wwPDB EM Validation Summary Report (i)

Sep 20, 2026 – 07:44 am BST

PDB ID	:	7PIN / pdb_00007pin
EMDB ID	:	EMD-13444
Title	:	Stacked compact Dunaliella PSII
Authors	:	Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on	:	2021-08-22
Resolution	:	3.60 Å(reported)
Based on initial model	:	6KAC

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:

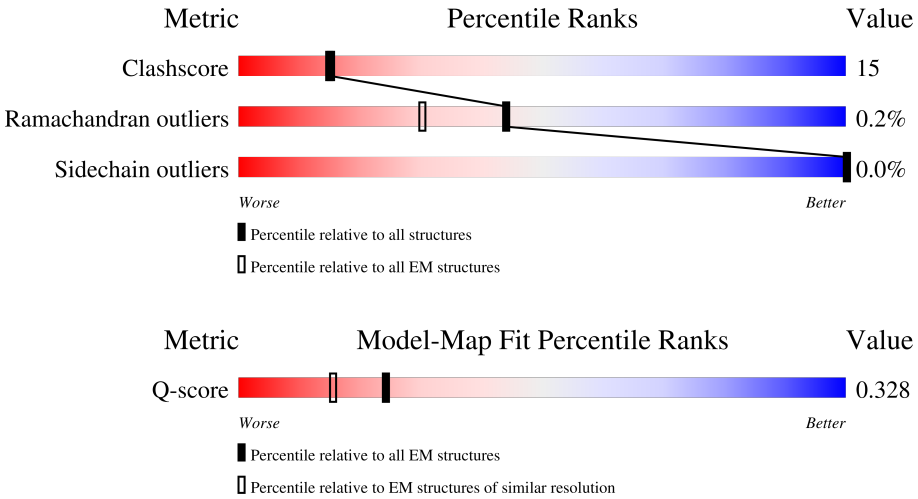
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	336	61% 70% 30%
1	A1	336	61% 63% 37%
1	a	336	54% 74% 26%
1	a1	336	70% 58% 42%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	484	74% 75% 25%
2	B1	484	66% 63% 37%
2	b	484	70% 69% 31%
2	b1	484	71% 68% 32%
3	V	32	94% 84% 16%
3	V1	32	69% 66% 34%
3	v	32	84% 84% 16%
3	v1	32	94% 59% 41%
4	C	449	55% 79% 21%
4	C1	449	42% 61% 38%
4	c	449	55% 81% 19%
4	c1	449	66% 63% 36%
5	D	348	63% 81% 19%
5	D1	348	63% 63% 37%
5	d	348	61% 73% 27%
5	d1	348	75% 61% 39%
6	E	76	92% 59% 41%
6	E1	76	50% 74% 26%
6	e	76	93% 75% 25%
6	e1	76	76% 67% 33%
7	F	31	74% 71% 29%
7	F1	31	58% 71% 29%
7	f	31	90% 52% 48%
7	f1	31	71% 58% 42%
8	H	67	84% 69% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H1	67	78% 63% 37%
8	h	67	88% 81% 19%
8	h1	67	84% 64% 36%
9	I	35	57% 80% 20%
9	I1	35	71% 54% 46%
9	i	35	60% 94% 6%
9	i1	35	74% 71% 29%
10	J	36	89% 83% 17%
10	J1	36	81% 75% 25%
10	j	36	86% 92% 8%
10	j1	36	81% 64% 36%
11	K	37	81% 78% 22%
11	K1	37	41% 68% 32%
11	k	37	76% 86% 14%
11	k1	37	73% 70% 30%
12	L	38	71% 84% 16%
12	L1	38	79% 74% 26%
12	l	38	74% 74% 26%
13	M	31	87% 84% 16%
13	M1	31	84% 74% 26%
13	m	31	84% 71% 29%
13	m1	31	77% 74% 26%
14	O	238	92% 77% 22%
14	O1	238	67% 65% 35%
14	o	238	94% 77% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	o1	238	72% 72% 28%
15	P	187	100% 77% 23%
15	P1	187	98% 75% 25%
15	p	187	100% 72% 28%
15	p1	187	99% 73% 27%
16	T	30	83% 90% 10%
16	T1	30	83% 67% 33%
16	t	30	90% 70% 30%
16	t1	30	80% 77% 23%
17	W	44	95% 84% 16%
17	W1	44	75% 64% 36%
17	w	44	86% 73% 27%
17	w1	44	82% 57% 43%
18	X	30	97% 97%
18	X1	30	57% 70% 30%
18	x	30	100% 67% 33%
18	x1	30	83% 77% 23%
19	Z	61	90% 90% 10%
19	Z1	61	52% 77% 23%
19	z	61	87% 87% 13%
19	z1	61	84% 80% 20%
20	N	222	94% 75% 25%
20	N1	222	37% 65% 34%
20	n	222	89% 77% 23%
20	n1	222	55% 65% 34%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
21	G	221	99% 75% 25%
21	G1	221	43% 71% 29%
21	g	221	97% 74% 26%
21	g1	221	62% 76% 24%
22	R	196	97% 82% 18%
22	R1	196	78% 82% 18%
22	r	196	98% 81% 19%
22	r1	196	78% 68% 32%
23	S	243	88% 82% 18%
23	S1	243	42% 72% 28%
23	s	243	90% 75% 25%
23	s1	243	75% 64% 36%
24	Y	222	83% 80% 20%
24	Y1	222	39% 68% 32%
24	y	222	83% 76% 23%
24	y1	222	66% 67% 33%
25	U	27	96% 63% 37%
25	U1	27	81% 59% 41%
25	u	27	100% 67% 33%
25	u1	27	96% 56% 44%

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
36	C7Z	B	620	X	-	-	-
36	C7Z	B1	620	X	-	-	-
36	C7Z	b	620	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	C7Z	b1	620	X	-	-	-
41	LMK	C	527	X	-	-	-
41	LMK	C1	527	X	-	-	-
41	LMK	c	527	X	-	-	-
41	LMK	c1	527	X	-	-	-
45	RRX	H	101	X	-	-	-
45	RRX	H1	101	X	-	-	-
45	RRX	h	101	X	-	-	-
45	RRX	h1	101	X	-	-	-
48	CHL	G	601	X	-	-	-
48	CHL	G	605	X	-	-	-
48	CHL	G	607	X	-	-	-
48	CHL	G	609	X	-	-	-
48	CHL	G1	601	X	-	-	-
48	CHL	G1	605	X	-	-	-
48	CHL	G1	607	X	-	-	-
48	CHL	G1	609	X	-	-	-
48	CHL	N	601	X	-	-	-
48	CHL	N	605	X	-	-	-
48	CHL	N	606	X	-	-	-
48	CHL	N	607	X	-	-	-
48	CHL	N	609	X	-	-	-
48	CHL	N1	601	X	-	-	-
48	CHL	N1	605	X	-	-	-
48	CHL	N1	606	X	-	-	-
48	CHL	N1	607	X	-	-	-
48	CHL	N1	609	X	-	-	-
48	CHL	S	608	X	-	-	-
48	CHL	S1	608	X	-	-	-
48	CHL	Y	601	X	-	-	-
48	CHL	Y	606	X	-	-	-
48	CHL	Y	607	X	-	-	-
48	CHL	Y	609	X	-	-	-
48	CHL	Y1	601	X	-	-	-
48	CHL	Y1	606	X	-	-	-
48	CHL	Y1	607	X	-	-	-
48	CHL	Y1	609	X	-	-	-
48	CHL	g	601	X	-	-	-
48	CHL	g	605	X	-	-	-
48	CHL	g	607	X	-	-	-
48	CHL	g	609	X	-	-	-
48	CHL	g1	601	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	g1	605	X	-	-	-
48	CHL	g1	607	X	-	-	-
48	CHL	g1	609	X	-	-	-
48	CHL	n	601	X	-	-	-
48	CHL	n	605	X	-	-	-
48	CHL	n	606	X	-	-	-
48	CHL	n	607	X	-	-	-
48	CHL	n	609	X	-	-	-
48	CHL	n1	601	X	-	-	-
48	CHL	n1	605	X	-	-	-
48	CHL	n1	606	X	-	-	-
48	CHL	n1	607	X	-	-	-
48	CHL	n1	609	X	-	-	-
48	CHL	s	608	X	-	-	-
48	CHL	s1	608	X	-	-	-
48	CHL	y	601	X	-	-	-
48	CHL	y	606	X	-	-	-
48	CHL	y	607	X	-	-	-
48	CHL	y	609	X	-	-	-
48	CHL	y1	601	X	-	-	-
48	CHL	y1	606	X	-	-	-
48	CHL	y1	607	X	-	-	-
48	CHL	y1	609	X	-	-	-
49	LUT	G	621	X	-	-	-
49	LUT	R	620	X	-	-	-
49	LUT	n1	621	X	-	-	-
50	XAT	G	622	X	-	-	-
50	XAT	G1	622	X	-	-	-
50	XAT	N	622	X	-	-	-
50	XAT	N1	622	X	-	-	-
50	XAT	Y1	622	X	-	-	-
50	XAT	g	622	X	-	-	-
50	XAT	g1	622	X	-	-	-
50	XAT	n	622	X	-	-	-
50	XAT	r	621	X	-	-	-
50	XAT	r1	621	X	-	-	-
51	NEX	g	623	X	-	-	-
51	NEX	g1	623	X	-	-	-
53	ERG	R	626	X	-	-	-
53	ERG	R1	626	X	-	-	-
53	ERG	r	626	X	-	-	-
53	ERG	r1	626	X	-	-	-

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 152240 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	A1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	B1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		
3	V1	32	Total	C	N	O	0	0
			227	152	37	38		
3	v1	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	C1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	D1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		
6	e	76	Total	C	N	O	0	0
			621	404	102	115		
6	E1	76	Total	C	N	O	0	0
			621	404	102	115		
6	e1	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	F1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	H1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	I1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

- Molecule 10 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		
10	j	36	Total	C	N	O	0	0
			266	183	40	43		
10	J1	36	Total	C	N	O	0	0
			266	183	40	43		
10	j1	36	Total	C	N	O	0	0
			266	183	40	43		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		
11	K1	37	Total	C	N	O	0	0
			297	207	43	47		
11	k1	37	Total	C	N	O	0	0
			297	207	43	47		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	L1	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

- Molecule 13 is a protein called PsbM.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		
13	M1	31	Total	C	N	O	0	0
			234	159	33	42		
13	m1	31	Total	C	N	O	0	0
			234	159	33	42		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	O1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	P1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	T1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	W1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		
18	X1	30	Total	C	N	O	0	0
			201	132	32	37		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
18	x1	30	Total 201	C 132	N 32	O 37	0	0

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total 457	C 312	N 68	O 76	S 1	0	0
19	z	61	Total 457	C 312	N 68	O 76	S 1	0	0
19	Z1	61	Total 457	C 312	N 68	O 76	S 1	0	0
19	z1	61	Total 457	C 312	N 68	O 76	S 1	0	0

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total 1703	C 1100	N 277	O 321	S 5	0	0
20	n	222	Total 1703	C 1100	N 277	O 321	S 5	0	0
20	N1	222	Total 1703	C 1100	N 277	O 321	S 5	0	0
20	n1	222	Total 1703	C 1100	N 277	O 321	S 5	0	0

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total 1680	C 1085	N 271	O 321	S 3	0	0
21	g	221	Total 1680	C 1085	N 271	O 321	S 3	0	0
21	G1	221	Total 1680	C 1085	N 271	O 321	S 3	0	0
21	g1	221	Total 1680	C 1085	N 271	O 321	S 3	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7
g	180	ALA	PRO	conflict	UNP A1XKU7
G1	180	ALA	PRO	conflict	UNP A1XKU7
g1	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	R	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	R1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
22	r1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

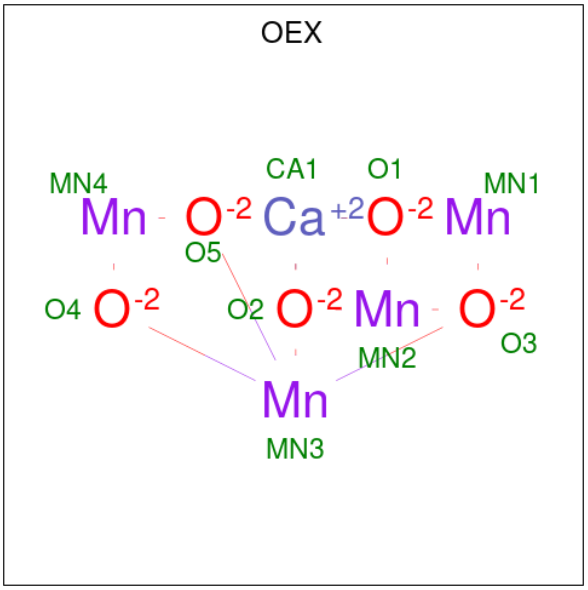
- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total 224	C 134	N 42	O 47	S 1	0	0
25	u	27	Total 224	C 134	N 42	O 47	S 1	0	0
25	U1	27	Total 224	C 134	N 42	O 47	S 1	0	0
25	u1	27	Total 224	C 134	N 42	O 47	S 1	0	0

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total 10	Ca 1	Mn 4	O 5	0
26	a	1	Total 10	Ca 1	Mn 4	O 5	0
26	A1	1	Total 10	Ca 1	Mn 4	O 5	0
26	a1	1	Total 10	Ca 1	Mn 4	O 5	0

- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total 1	Fe 1	0
27	a	1	Total 1	Fe 1	0

Continued on next page...

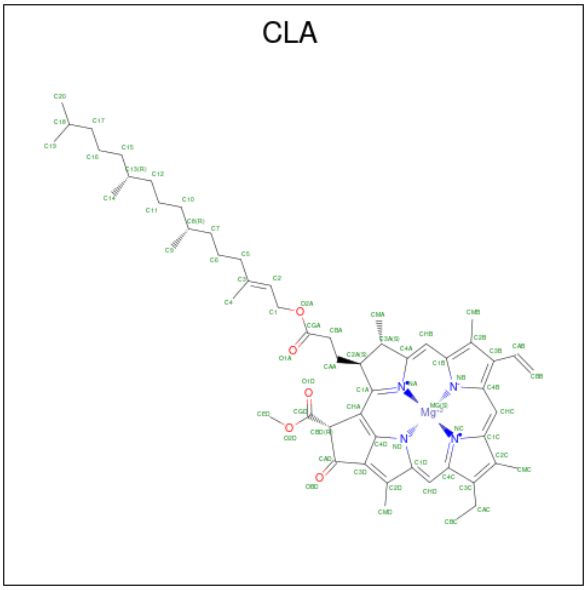
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
27	A1	1	Total Fe 1 1	0
27	a1	1	Total Fe 1 1	0

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
28	A	2	Total Cl 2 2	0
28	a	2	Total Cl 2 2	0
28	A1	2	Total Cl 2 2	0
28	a1	2	Total Cl 2 2	0

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C Mg N O 65 55 1 4 5	0
29	A	1	Total C Mg N O 65 55 1 4 5	0
29	A	1	Total C Mg N O 50 40 1 4 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	D1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	D1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	N1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G1	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
29	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	a1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	n1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

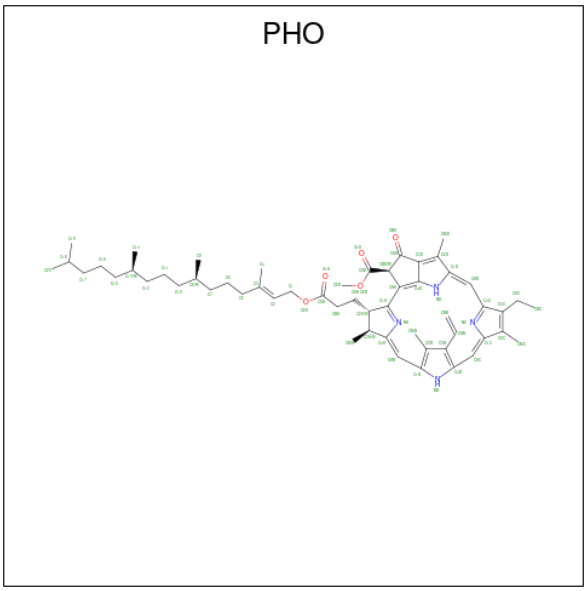
Mol	Chain	Residues	Atoms					AltConf
29	n1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g1	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
29	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	s1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

Continued on next page...

Continued from previous page...

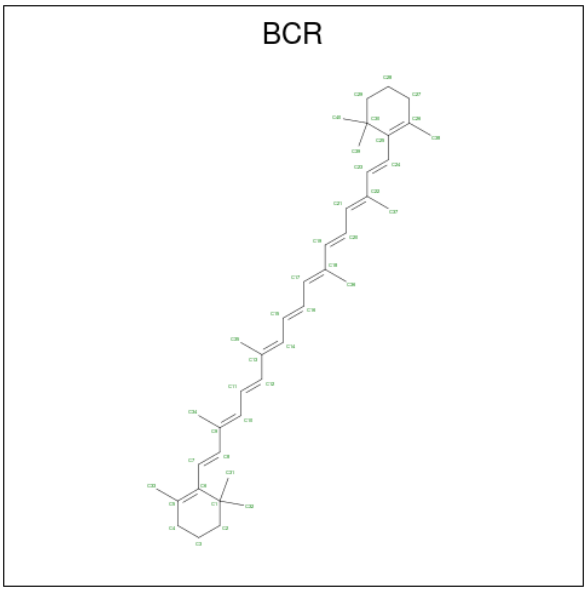
Mol	Chain	Residues	Atoms					AltConf
29	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s1	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s1	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s1	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y1	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y1	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	A1	1	Total	C	N	O	0
			64	55	4	5	
30	A1	1	Total	C	N	O	0
			64	55	4	5	
30	a1	1	Total	C	N	O	0
			64	55	4	5	
30	a1	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



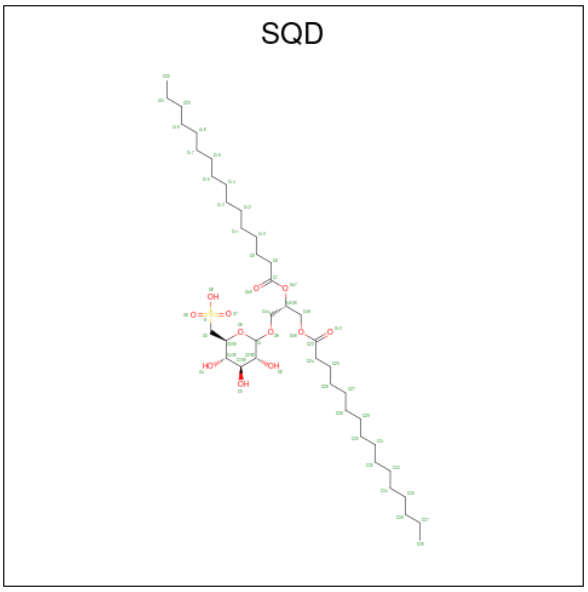
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	A1	1	Total C 40 40	0
31	B1	1	Total C 40 40	0
31	B1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	C1	1	Total C 40 40	0
31	D1	1	Total C 40 40	0
31	a1	1	Total C 40 40	0
31	b1	1	Total C 40 40	0
31	b1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	c1	1	Total C 40 40	0
31	d1	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



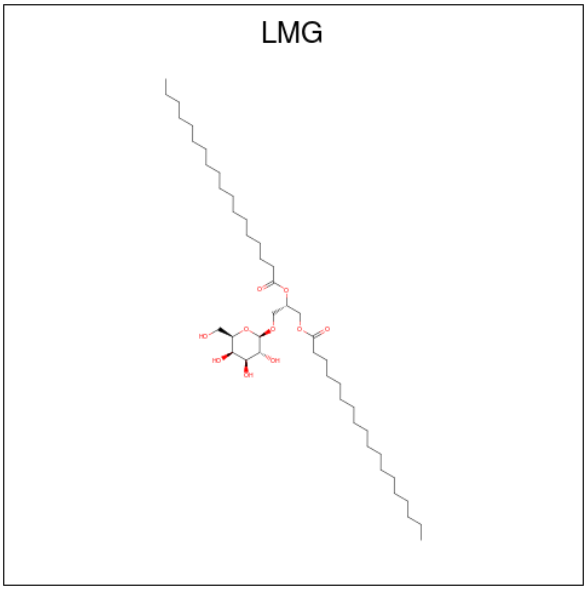
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			51	38	12	1	
32	B	1	Total	C	O	S	0
			42	29	12	1	
32	B	1	Total	C	O	S	0
			54	41	12	1	
32	C	1	Total	C	O	S	0
			54	41	12	1	
32	M	1	Total	C	O	S	0
			42	29	12	1	
32	a	1	Total	C	O	S	0
			51	38	12	1	
32	b	1	Total	C	O	S	0
			42	29	12	1	
32	b	1	Total	C	O	S	0
			54	41	12	1	
32	c	1	Total	C	O	S	0
			54	41	12	1	
32	m	1	Total	C	O	S	0
			42	29	12	1	
32	A1	1	Total	C	O	S	0
			51	38	12	1	
32	B1	1	Total	C	O	S	0
			42	29	12	1	
32	B1	1	Total	C	O	S	0
			54	41	12	1	
32	C1	1	Total	C	O	S	0
			54	41	12	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
32	M1	1	Total	C	O	S	0
			42	29	12	1	
32	a1	1	Total	C	O	S	0
			51	38	12	1	
32	b1	1	Total	C	O	S	0
			42	29	12	1	
32	b1	1	Total	C	O	S	0
			54	41	12	1	
32	c1	1	Total	C	O	S	0
			54	41	12	1	
32	m1	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			48	38	10	
33	B	1	Total	C	O	0
			44	34	10	
33	C	1	Total	C	O	0
			51	41	10	
33	C	1	Total	C	O	0
			55	45	10	
33	D	1	Total	C	O	0
			46	36	10	

Continued on next page...

Continued from previous page...

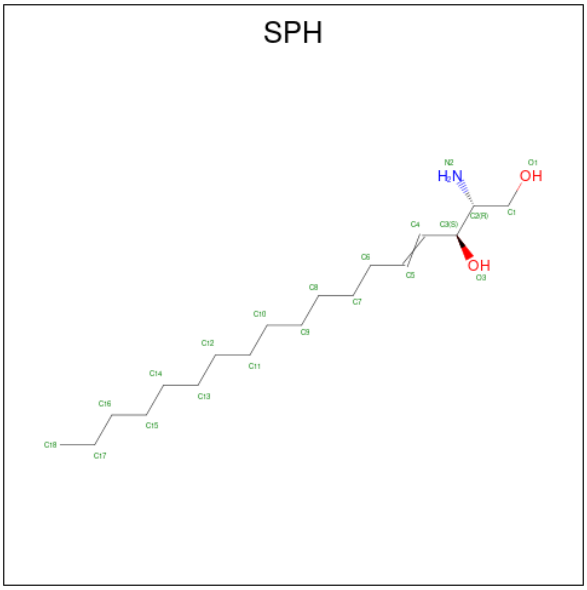
Mol	Chain	Residues	Atoms	AltConf
33	H	1	Total C O 48 38 10	0
33	W	1	Total C O 39 29 10	0
33	a	1	Total C O 48 38 10	0
33	b	1	Total C O 44 34 10	0
33	c	1	Total C O 51 41 10	0
33	c	1	Total C O 55 45 10	0
33	d	1	Total C O 46 36 10	0
33	h	1	Total C O 48 38 10	0
33	w	1	Total C O 39 29 10	0
33	A1	1	Total C O 48 38 10	0
33	B1	1	Total C O 44 34 10	0
33	C1	1	Total C O 51 41 10	0
33	C1	1	Total C O 55 45 10	0
33	D1	1	Total C O 46 36 10	0
33	H1	1	Total C O 48 38 10	0
33	W1	1	Total C O 39 29 10	0
33	a1	1	Total C O 48 38 10	0
33	b1	1	Total C O 44 34 10	0
33	c1	1	Total C O 51 41 10	0
33	c1	1	Total C O 55 45 10	0
33	d1	1	Total C O 46 36 10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
33	h1	1	Total C O 48 38 10	0
33	w1	1	Total C O 39 29 10	0

- Molecule 34 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).

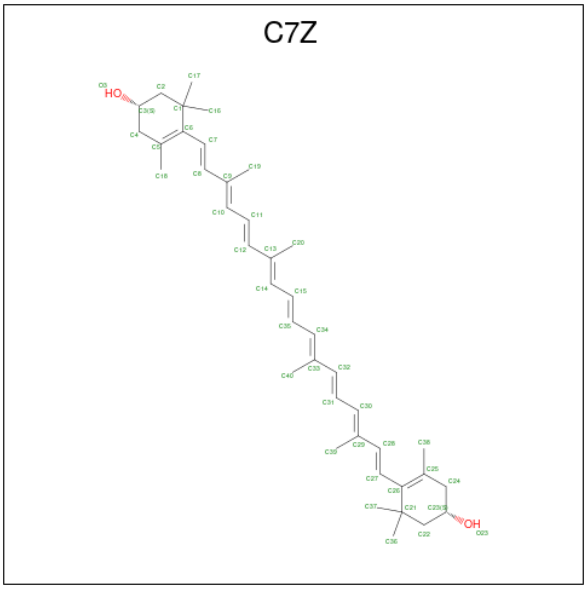


Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C N O 21 18 1 2	0
34	Y	1	Total C N O 21 18 1 2	0
34	a	1	Total C N O 21 18 1 2	0
34	y	1	Total C N O 21 18 1 2	0
34	A1	1	Total C N O 21 18 1 2	0
34	Y1	1	Total C N O 21 18 1 2	0
34	a1	1	Total C N O 21 18 1 2	0
34	y1	1	Total C N O 21 18 1 2	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

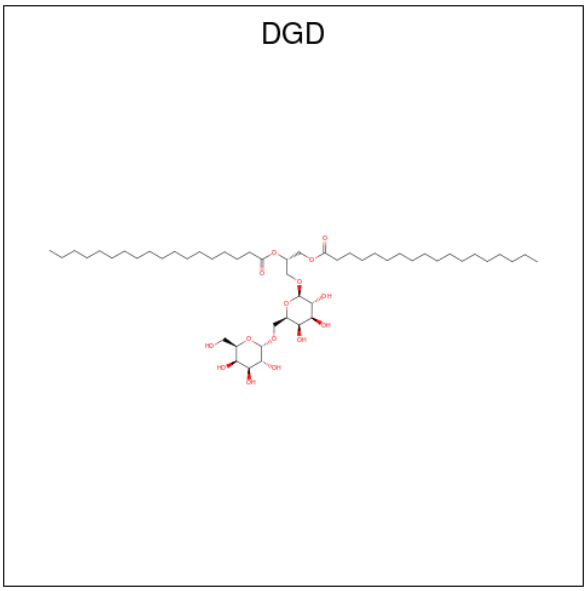
Mol	Chain	Residues	Atoms	AltConf
35	A	1	Total Na 1 1	0
35	a	1	Total Na 1 1	0
35	A1	1	Total Na 1 1	0
35	a1	1	Total Na 1 1	0

- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
36	B	1	Total C O 42 40 2	0
36	b	1	Total C O 42 40 2	0
36	B1	1	Total C O 42 40 2	0
36	b1	1	Total C O 42 40 2	0

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



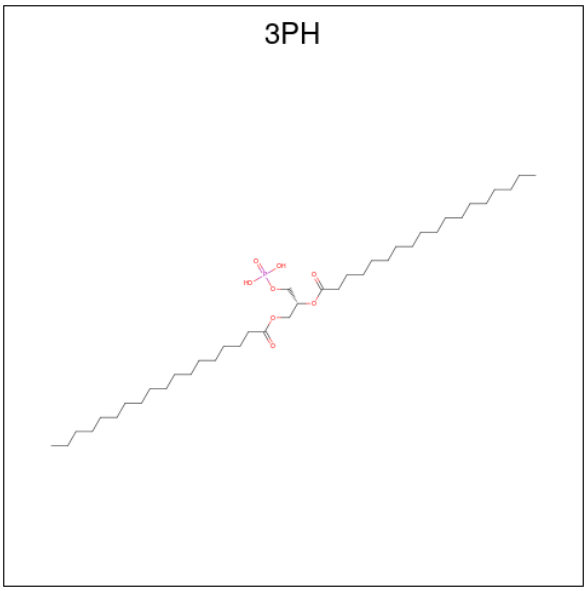
Mol	Chain	Residues	Atoms	AltConf
37	B	1	Total C O 43 28 15	0
37	C	1	Total C O 55 40 15	0
37	C	1	Total C O 62 47 15	0
37	C	1	Total C O 59 44 15	0
37	b	1	Total C O 43 28 15	0
37	c	1	Total C O 55 40 15	0
37	c	1	Total C O 62 47 15	0
37	c	1	Total C O 59 44 15	0
37	B1	1	Total C O 43 28 15	0
37	C1	1	Total C O 55 40 15	0
37	C1	1	Total C O 62 47 15	0
37	C1	1	Total C O 59 44 15	0
37	b1	1	Total C O 43 28 15	0
37	c1	1	Total C O 55 40 15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
37	c1	1	Total C O 62 47 15	0
37	c1	1	Total C O 59 44 15	0

- Molecule 38 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



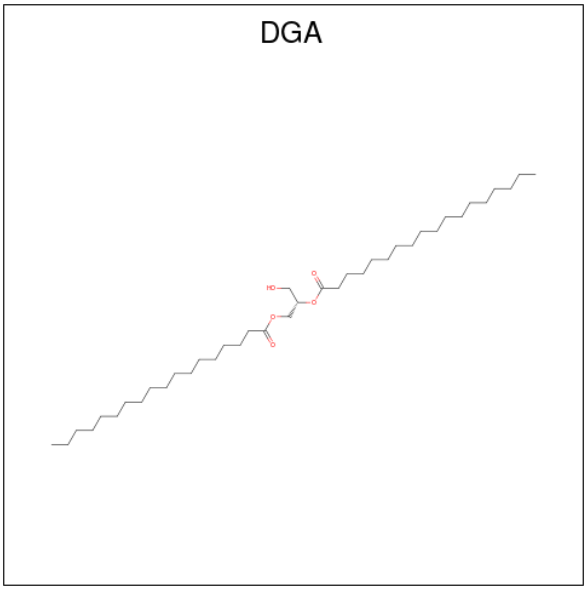
Mol	Chain	Residues	Atoms	AltConf
38	B	1	Total C O P 48 39 8 1	0
38	T	1	Total C O P 48 39 8 1	0
38	S	1	Total C O P 48 39 8 1	0
38	b	1	Total C O P 48 39 8 1	0
38	t	1	Total C O P 48 39 8 1	0
38	s	1	Total C O P 48 39 8 1	0
38	B1	1	Total C O P 48 39 8 1	0
38	T1	1	Total C O P 48 39 8 1	0
38	S1	1	Total C O P 48 39 8 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
38	b1	1	Total	C	O	P	0
			48	39	8	1	
38	t1	1	Total	C	O	P	0
			48	39	8	1	
38	s1	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 39 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



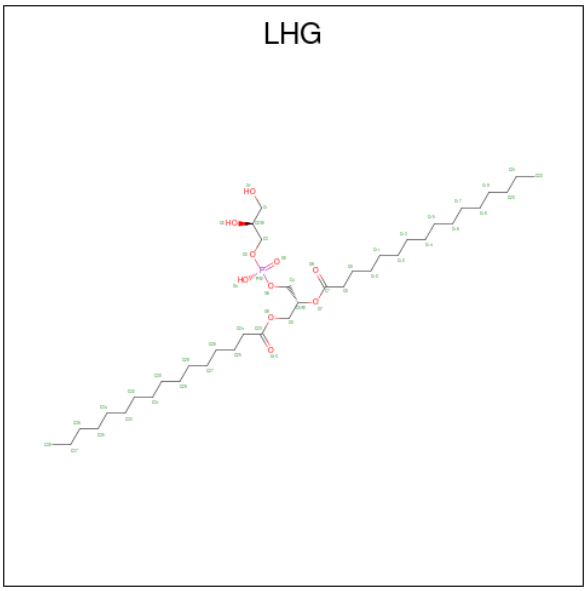
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			44	39	5	
39	C	1	Total	C	O	0
			44	39	5	
39	J	1	Total	C	O	0
			29	24	5	
39	b	1	Total	C	O	0
			44	39	5	
39	c	1	Total	C	O	0
			44	39	5	
39	j	1	Total	C	O	0
			29	24	5	
39	B1	1	Total	C	O	0
			44	39	5	
39	C1	1	Total	C	O	0
			44	39	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
39	J1	1	Total C O 29 24 5	0
39	b1	1	Total C O 44 39 5	0
39	c1	1	Total C O 44 39 5	0
39	j1	1	Total C O 29 24 5	0

- Molecule 40 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
40	C	1	Total C O P 47 36 10 1	0
40	D	1	Total C O P 44 33 10 1	0
40	D	1	Total C O P 49 38 10 1	0
40	D	1	Total C O P 39 28 10 1	0
40	L	1	Total C O P 49 38 10 1	0
40	N	1	Total C O P 49 38 10 1	0
40	G	1	Total C O P 49 38 10 1	0

Continued on next page...

Continued from previous page...

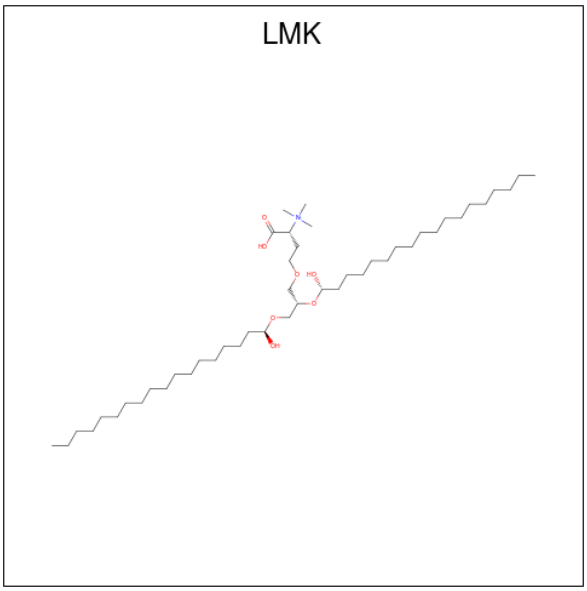
Mol	Chain	Residues	Atoms				AltConf
40	S	1	Total	C	O	P	0
			45	34	10	1	
40	Y	1	Total	C	O	P	0
			49	38	10	1	
40	c	1	Total	C	O	P	0
			47	36	10	1	
40	d	1	Total	C	O	P	0
			44	33	10	1	
40	d	1	Total	C	O	P	0
			49	38	10	1	
40	d	1	Total	C	O	P	0
			39	28	10	1	
40	l	1	Total	C	O	P	0
			49	38	10	1	
40	n	1	Total	C	O	P	0
			49	38	10	1	
40	g	1	Total	C	O	P	0
			49	38	10	1	
40	s	1	Total	C	O	P	0
			45	34	10	1	
40	y	1	Total	C	O	P	0
			49	38	10	1	
40	C1	1	Total	C	O	P	0
			47	36	10	1	
40	D1	1	Total	C	O	P	0
			44	33	10	1	
40	D1	1	Total	C	O	P	0
			49	38	10	1	
40	D1	1	Total	C	O	P	0
			39	28	10	1	
40	L1	1	Total	C	O	P	0
			49	38	10	1	
40	N1	1	Total	C	O	P	0
			49	38	10	1	
40	G1	1	Total	C	O	P	0
			49	38	10	1	
40	S1	1	Total	C	O	P	0
			45	34	10	1	
40	Y1	1	Total	C	O	P	0
			49	38	10	1	
40	c1	1	Total	C	O	P	0
			47	36	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
40	d1	1	Total	C	O	P	0
			44	33	10	1	
40	d1	1	Total	C	O	P	0
			49	38	10	1	
40	d1	1	Total	C	O	P	0
			39	28	10	1	
40	n1	1	Total	C	O	P	0
			49	38	10	1	
40	g1	1	Total	C	O	P	0
			49	38	10	1	
40	s1	1	Total	C	O	P	0
			45	34	10	1	
40	y1	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 41 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$).



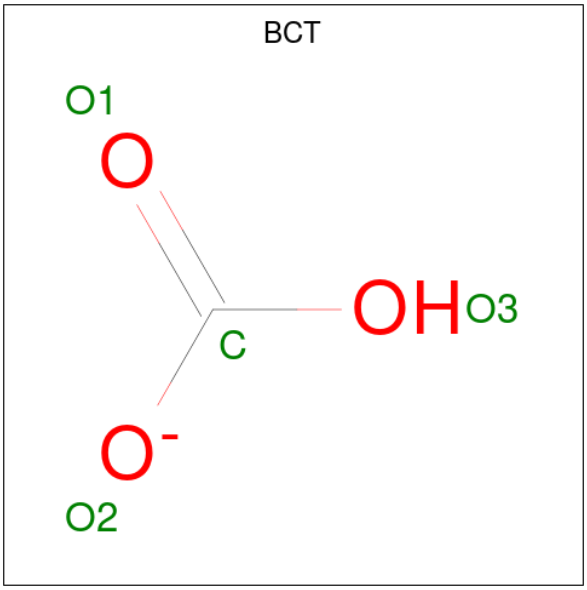
Mol	Chain	Residues	Atoms				AltConf
41	C	1	Total	C	N	O	0
			40	32	1	7	
41	c	1	Total	C	N	O	0
			40	32	1	7	
41	C1	1	Total	C	N	O	0
			40	32	1	7	

Continued on next page...

Continued from previous page...

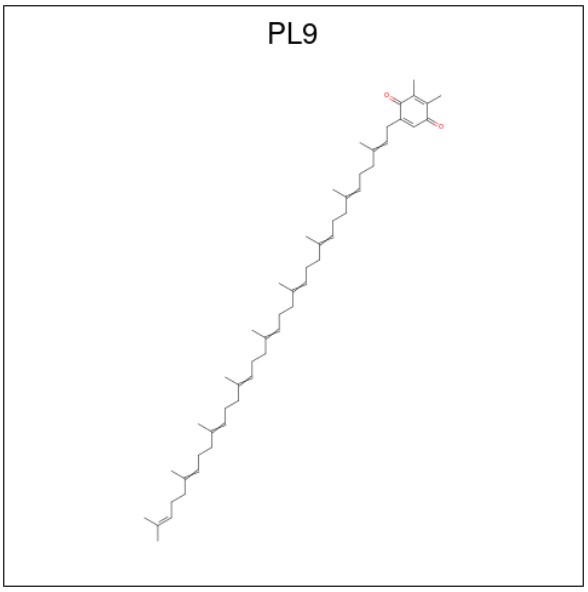
Mol	Chain	Residues	Atoms				AltConf
41	c1	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 42 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



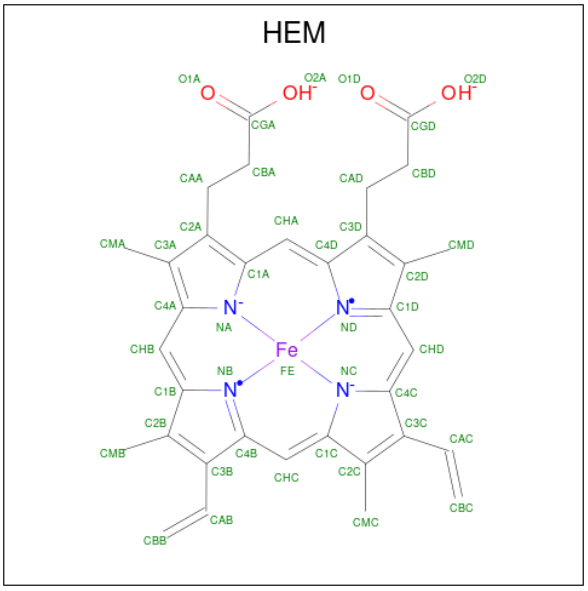
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			4	1	3	
42	d	1	Total	C	O	0
			4	1	3	
42	D1	1	Total	C	O	0
			4	1	3	
42	d1	1	Total	C	O	0
			4	1	3	

- Molecule 43 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



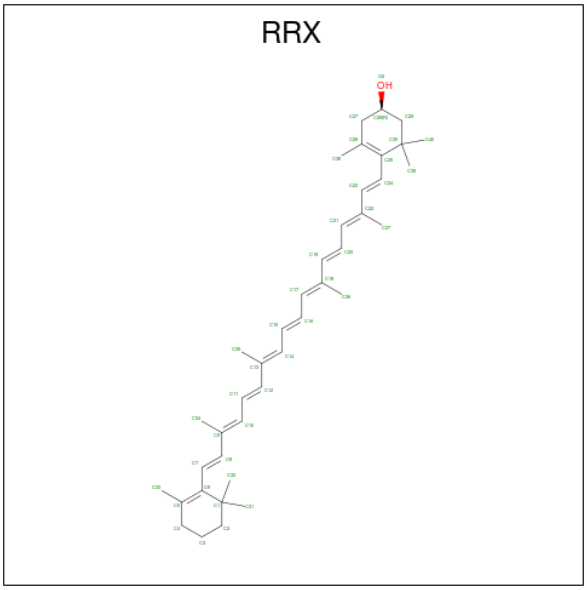
Mol	Chain	Residues	Atoms	AltConf
43	D	1	Total C O 55 53 2	0
43	d	1	Total C O 55 53 2	0
43	D1	1	Total C O 55 53 2	0
43	d1	1	Total C O 55 53 2	0

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



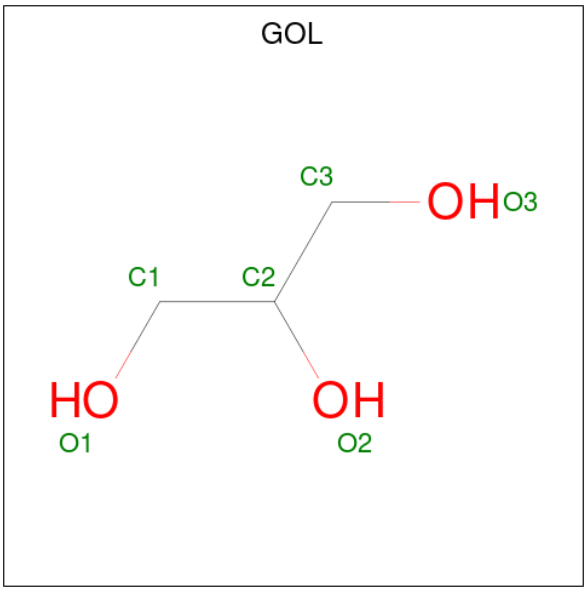
Mol	Chain	Residues	Atoms					AltConf
44	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	F1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
44	f1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



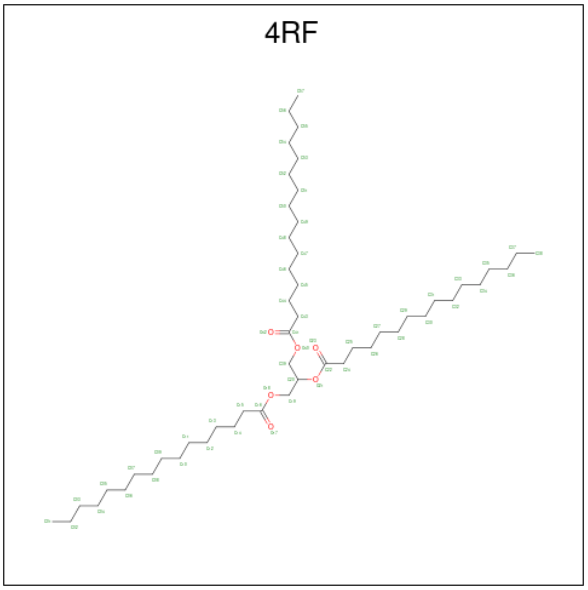
Mol	Chain	Residues	Atoms			AltConf
45	H	1	Total	C	O	0
			41	40	1	
45	h	1	Total	C	O	0
			41	40	1	
45	H1	1	Total	C	O	0
			41	40	1	
45	h1	1	Total	C	O	0
			41	40	1	

- Molecule 46 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	C	O	0
			6	3	3	
46	I1	1	Total	C	O	0
			6	3	3	

- Molecule 47 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



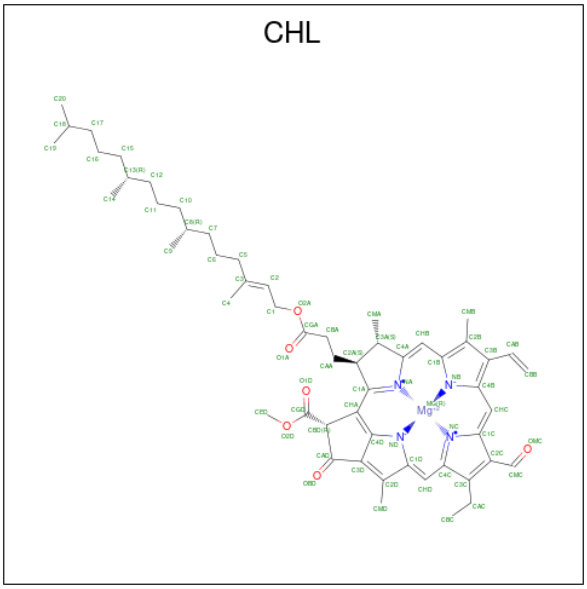
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	C	O	0
			57	51	6	
47	K	1	Total	C	O	0
			57	51	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
47	i	1	Total C O 57 51 6	0
47	k	1	Total C O 57 51 6	0
47	I1	1	Total C O 57 51 6	0
47	K1	1	Total C O 57 51 6	0
47	i1	1	Total C O 57 51 6	0
47	k1	1	Total C O 57 51 6	0

- Molecule 48 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms	AltConf
48	N	1	Total C Mg N O 66 55 1 4 6	0
48	N	1	Total C Mg N O 66 55 1 4 6	0
48	N	1	Total C Mg N O 66 55 1 4 6	0
48	N	1	Total C Mg N O 66 55 1 4 6	0
48	N	1	Total C Mg N O 50 39 1 4 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
48	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
48	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	G	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	R	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
48	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
48	S	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
48	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
48	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
48	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
48	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	g	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	r	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
48	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
48	s	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
48	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
48	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
48	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	N1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	G1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	G1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
48	G1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	G1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	G1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	G1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	R1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	R1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	S1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
48	S1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	S1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
48	S1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
48	Y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	Y1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
48	Y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	Y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

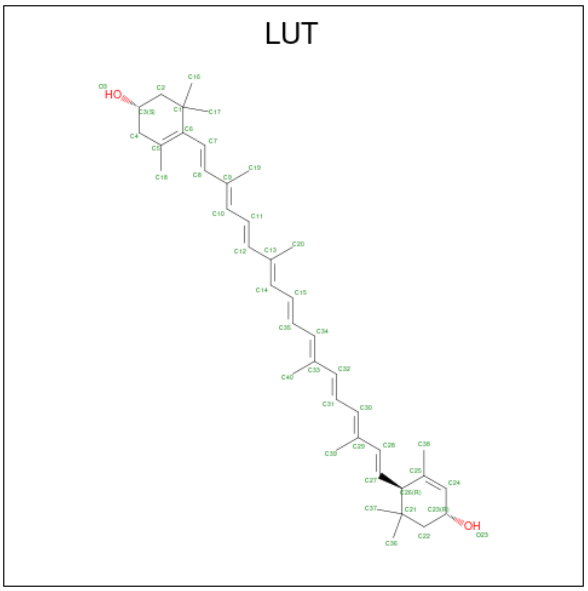
Mol	Chain	Residues	Atoms					AltConf
48	Y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	n1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	g1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	g1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
48	g1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	g1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	g1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	g1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	r1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	r1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
48	s1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
48	s1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
48	s1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
48	s1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
48	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 49 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			42	40	2	
49	N	1	Total	C	O	0
			42	40	2	
49	G	1	Total	C	O	0
			42	40	2	
49	G	1	Total	C	O	0
			42	40	2	
49	R	1	Total	C	O	0
			42	40	2	
49	S	1	Total	C	O	0
			42	40	2	
49	S	1	Total	C	O	0
			42	40	2	
49	Y	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

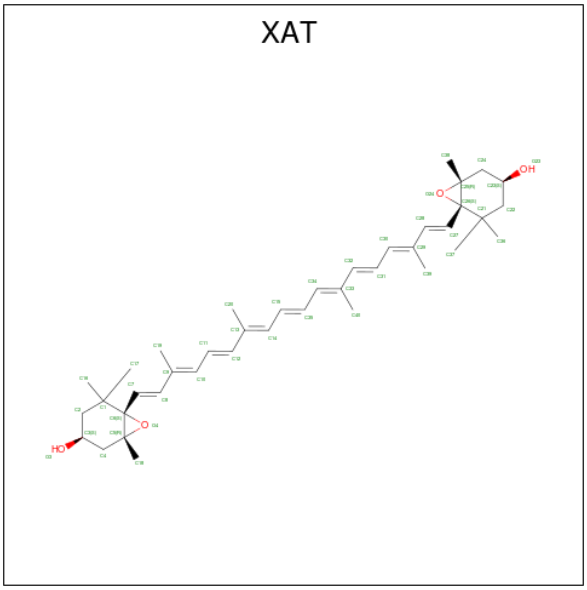
Mol	Chain	Residues	Atoms			AltConf
49	Y	1	Total	C	O	0
			42	40	2	
49	n	1	Total	C	O	0
			42	40	2	
49	n	1	Total	C	O	0
			42	40	2	
49	g	1	Total	C	O	0
			42	40	2	
49	g	1	Total	C	O	0
			42	40	2	
49	r	1	Total	C	O	0
			42	40	2	
49	s	1	Total	C	O	0
			42	40	2	
49	s	1	Total	C	O	0
			42	40	2	
49	y	1	Total	C	O	0
			42	40	2	
49	y	1	Total	C	O	0
			42	40	2	
49	N1	1	Total	C	O	0
			42	40	2	
49	N1	1	Total	C	O	0
			42	40	2	
49	G1	1	Total	C	O	0
			42	40	2	
49	G1	1	Total	C	O	0
			42	40	2	
49	R1	1	Total	C	O	0
			42	40	2	
49	S1	1	Total	C	O	0
			42	40	2	
49	S1	1	Total	C	O	0
			42	40	2	
49	Y1	1	Total	C	O	0
			42	40	2	
49	Y1	1	Total	C	O	0
			42	40	2	
49	n1	1	Total	C	O	0
			42	40	2	
49	n1	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
49	g1	1	Total C O 42 40 2	0
49	g1	1	Total C O 42 40 2	0
49	r1	1	Total C O 42 40 2	0
49	s1	1	Total C O 42 40 2	0
49	s1	1	Total C O 42 40 2	0
49	y1	1	Total C O 42 40 2	0
49	y1	1	Total C O 42 40 2	0

- Molecule 50 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



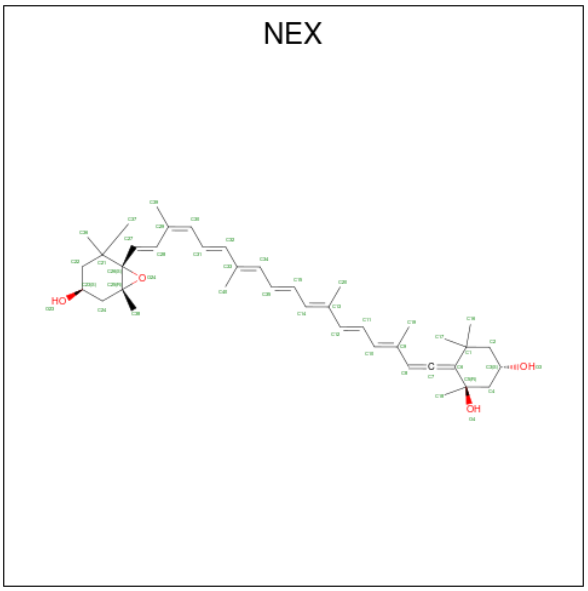
Mol	Chain	Residues	Atoms	AltConf
50	N	1	Total C O 44 40 4	0
50	G	1	Total C O 44 40 4	0
50	R	1	Total C O 44 40 4	0
50	Y	1	Total C O 44 40 4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
50	n	1	Total C O 44 40 4	0
50	g	1	Total C O 44 40 4	0
50	r	1	Total C O 44 40 4	0
50	y	1	Total C O 44 40 4	0
50	N1	1	Total C O 44 40 4	0
50	G1	1	Total C O 44 40 4	0
50	R1	1	Total C O 44 40 4	0
50	Y1	1	Total C O 44 40 4	0
50	n1	1	Total C O 44 40 4	0
50	g1	1	Total C O 44 40 4	0
50	r1	1	Total C O 44 40 4	0
50	y1	1	Total C O 44 40 4	0

- Molecule 51 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



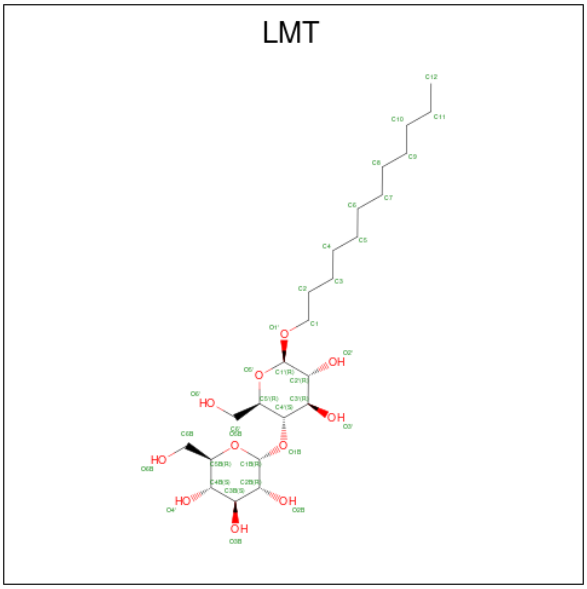
Mol	Chain	Residues	Atoms	AltConf
51	N	1	Total C O 44 40 4	0
51	G	1	Total C O 44 40 4	0
51	R	1	Total C O 44 40 4	0
51	S	1	Total C O 44 40 4	0
51	Y	1	Total C O 44 40 4	0
51	n	1	Total C O 44 40 4	0
51	g	1	Total C O 44 40 4	0
51	r	1	Total C O 44 40 4	0
51	s	1	Total C O 44 40 4	0
51	y	1	Total C O 44 40 4	0
51	N1	1	Total C O 44 40 4	0
51	G1	1	Total C O 44 40 4	0
51	R1	1	Total C O 44 40 4	0
51	S1	1	Total C O 44 40 4	0

Continued on next page...

Continued from previous page...

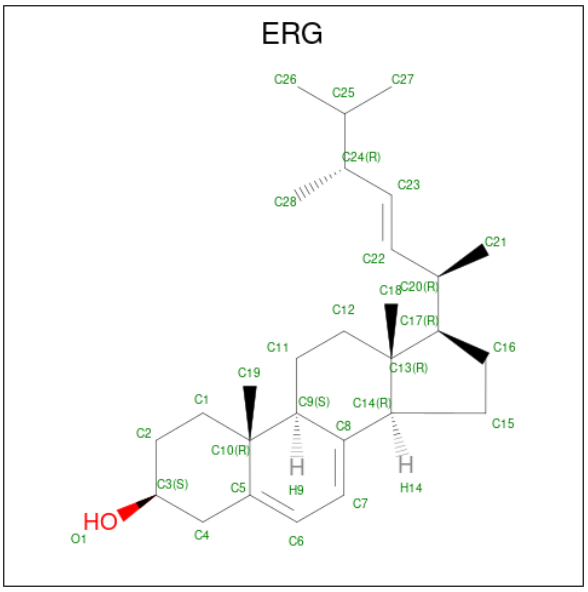
Mol	Chain	Residues	Atoms	AltConf
51	Y1	1	Total C O 44 40 4	0
51	n1	1	Total C O 44 40 4	0
51	g1	1	Total C O 44 40 4	0
51	r1	1	Total C O 44 40 4	0
51	s1	1	Total C O 44 40 4	0
51	y1	1	Total C O 44 40 4	0

- Molecule 52 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



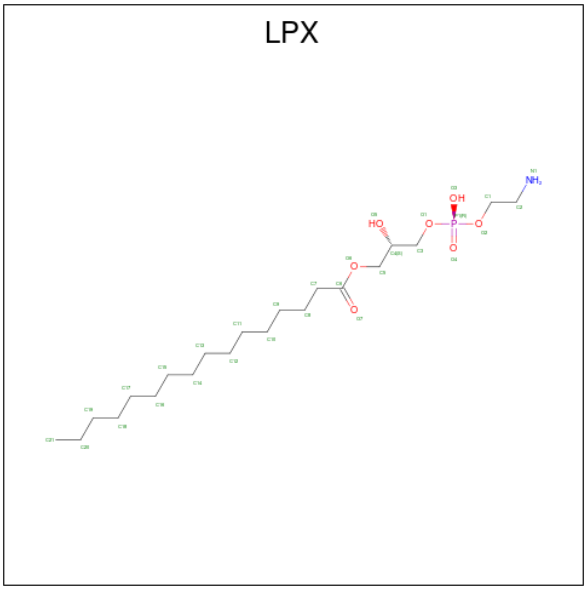
Mol	Chain	Residues	Atoms	AltConf
52	R	1	Total C O 35 24 11	0
52	r	1	Total C O 35 24 11	0
52	R1	1	Total C O 35 24 11	0
52	r1	1	Total C O 35 24 11	0

- Molecule 53 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



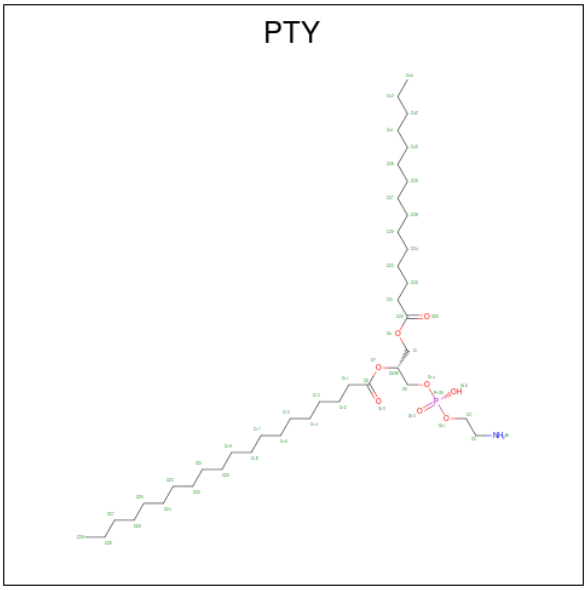
Mol	Chain	Residues	Atoms	AltConf
53	R	1	Total C O 29 28 1	0
53	r	1	Total C O 29 28 1	0
53	R1	1	Total C O 29 28 1	0
53	r1	1	Total C O 29 28 1	0

- Molecule 54 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
54	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	s	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	S1	1	Total	C	N	O	P	0
			30	21	1	7	1	
54	s1	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 55 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
55	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	Y	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	y	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	y	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	Y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	Y1	1	Total	C	N	O	P	0
			19	9	1	8	1	
55	y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
55	y1	1	Total	C	N	O	P	0
			19	9	1	8	1	

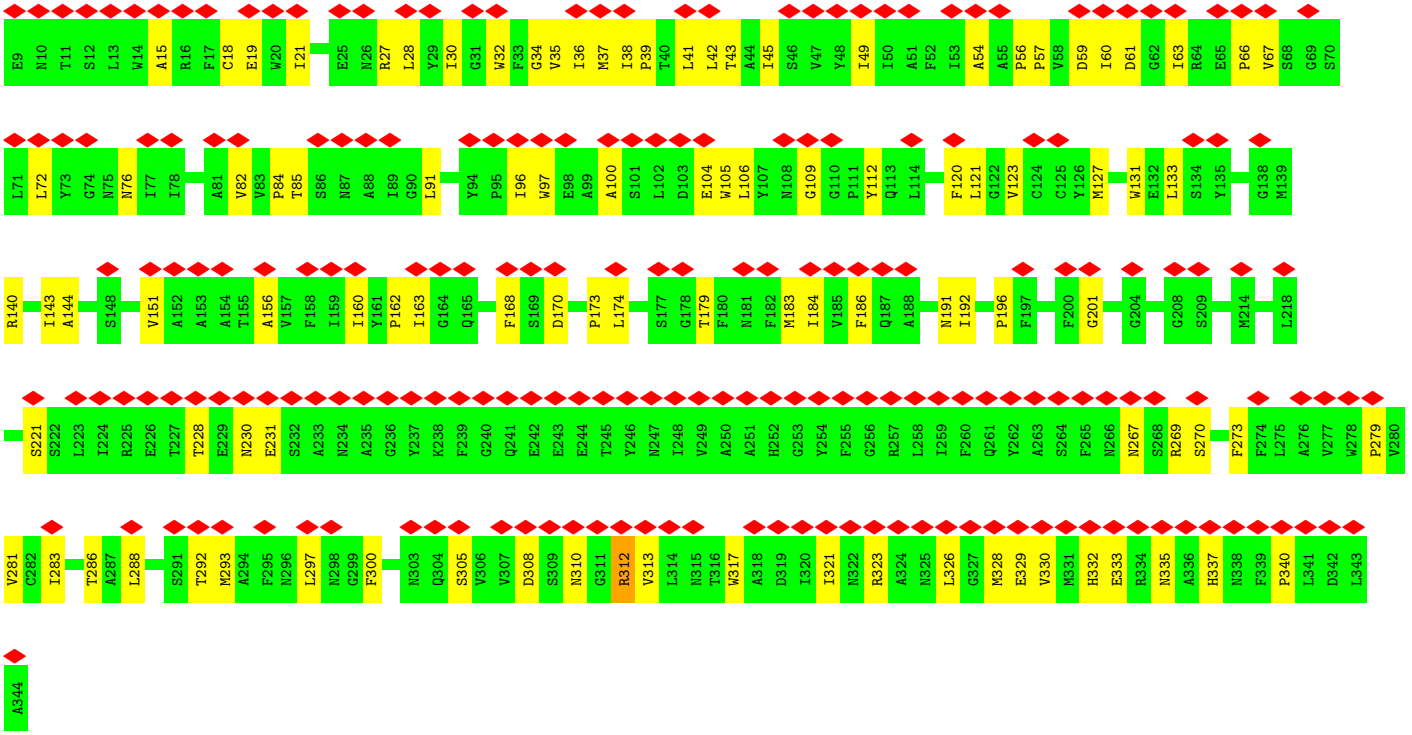
3 Residue-property plots (i)

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 II protein D1

Chain A:

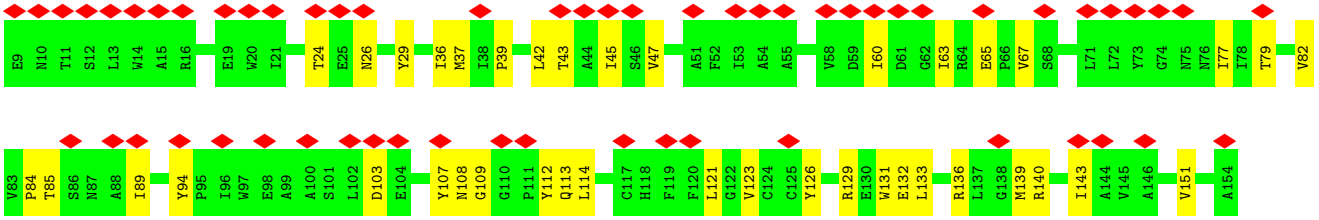


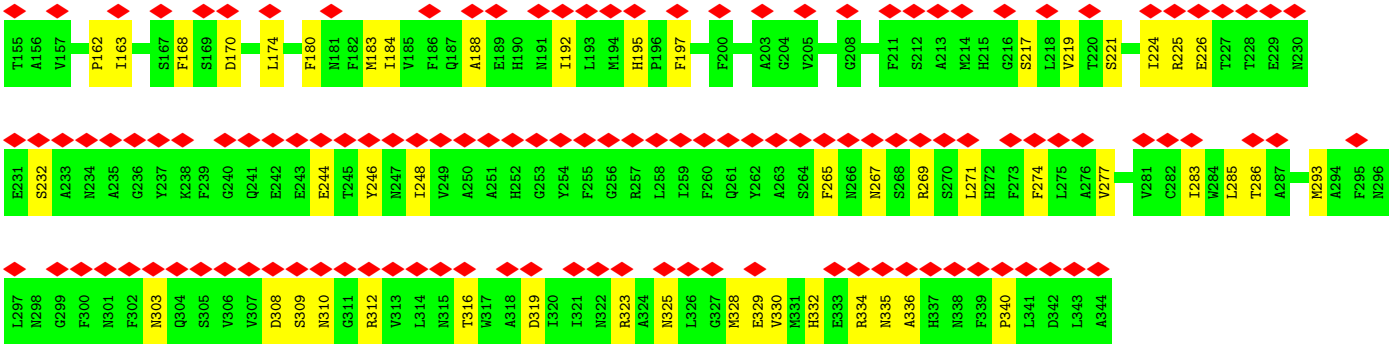


• Molecule 1: Photosystem II protein D1

Chain a:



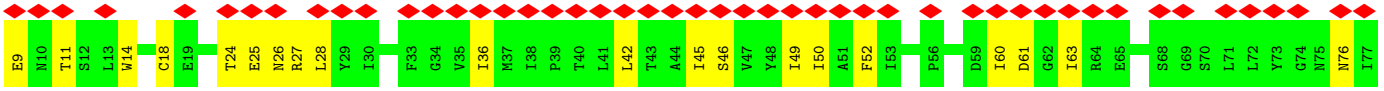




• Molecule 1: Photosystem II protein D1

Chain A1:

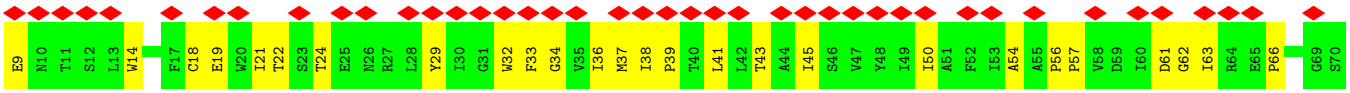


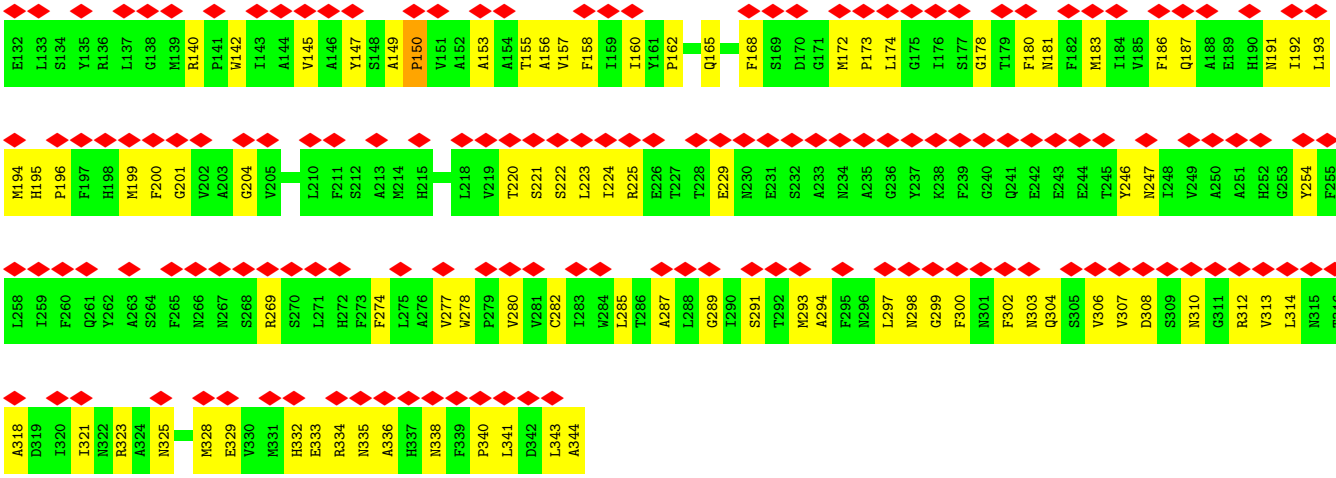


• Molecule 1: Photosystem II protein D1

Chain a1:



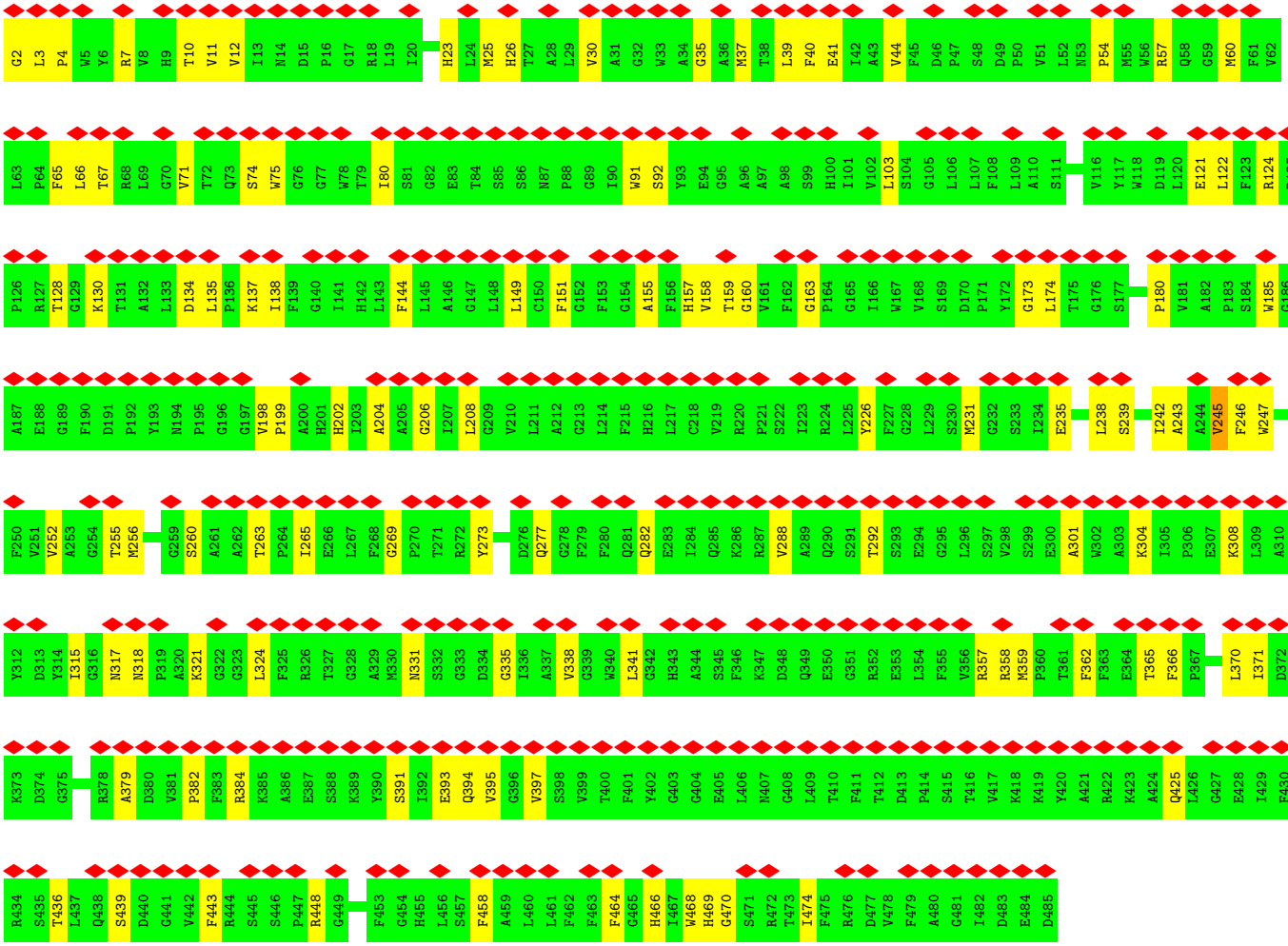




• Molecule 2: Photosystem II CP47 reaction center protein

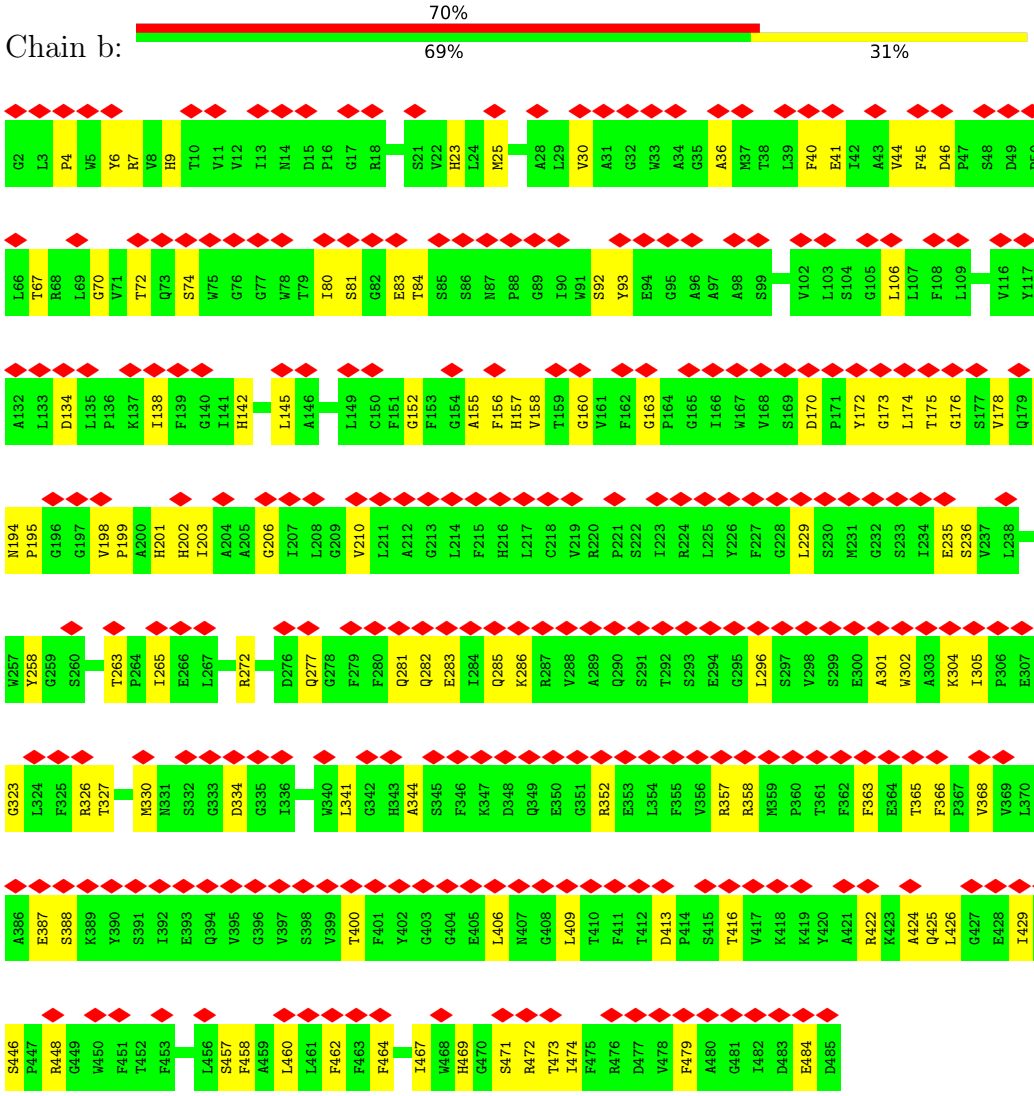
Chain B:





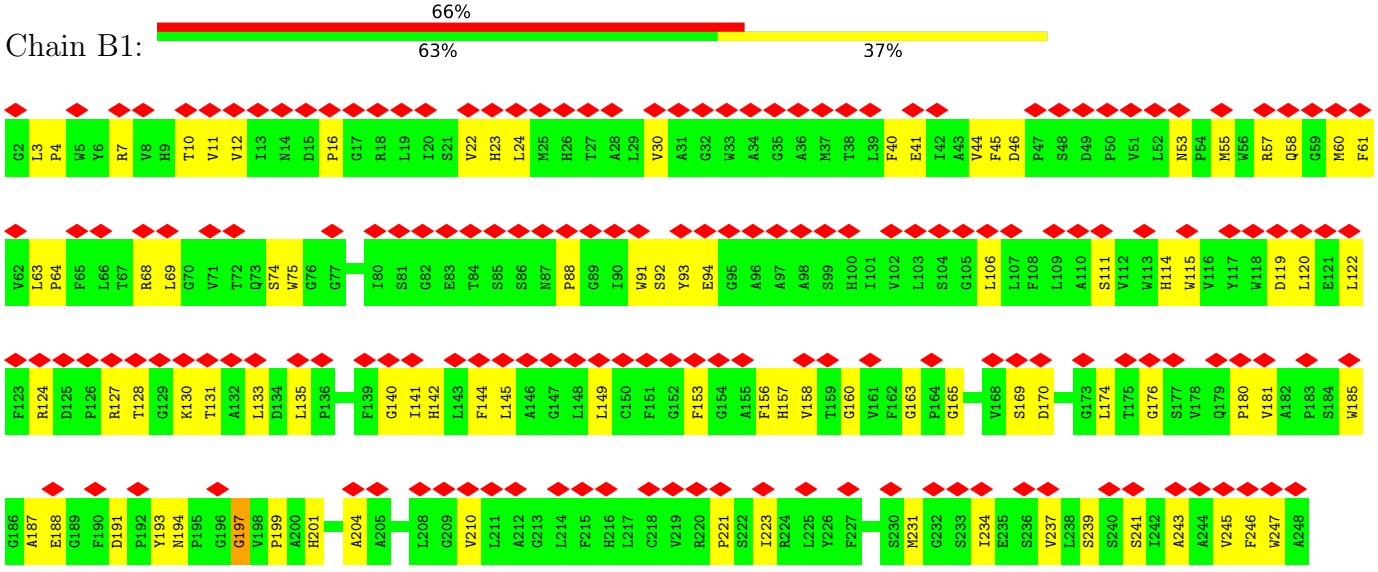
• Molecule 2: Photosystem II CP47 reaction center protein

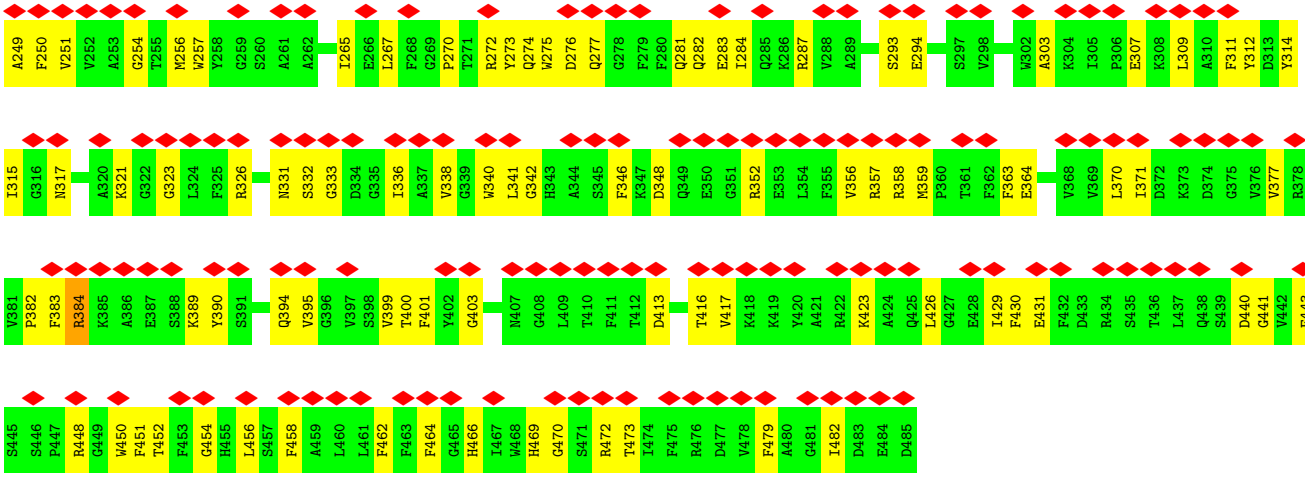
Chain b:



• Molecule 2: Photosystem II CP47 reaction center protein

Chain B1:

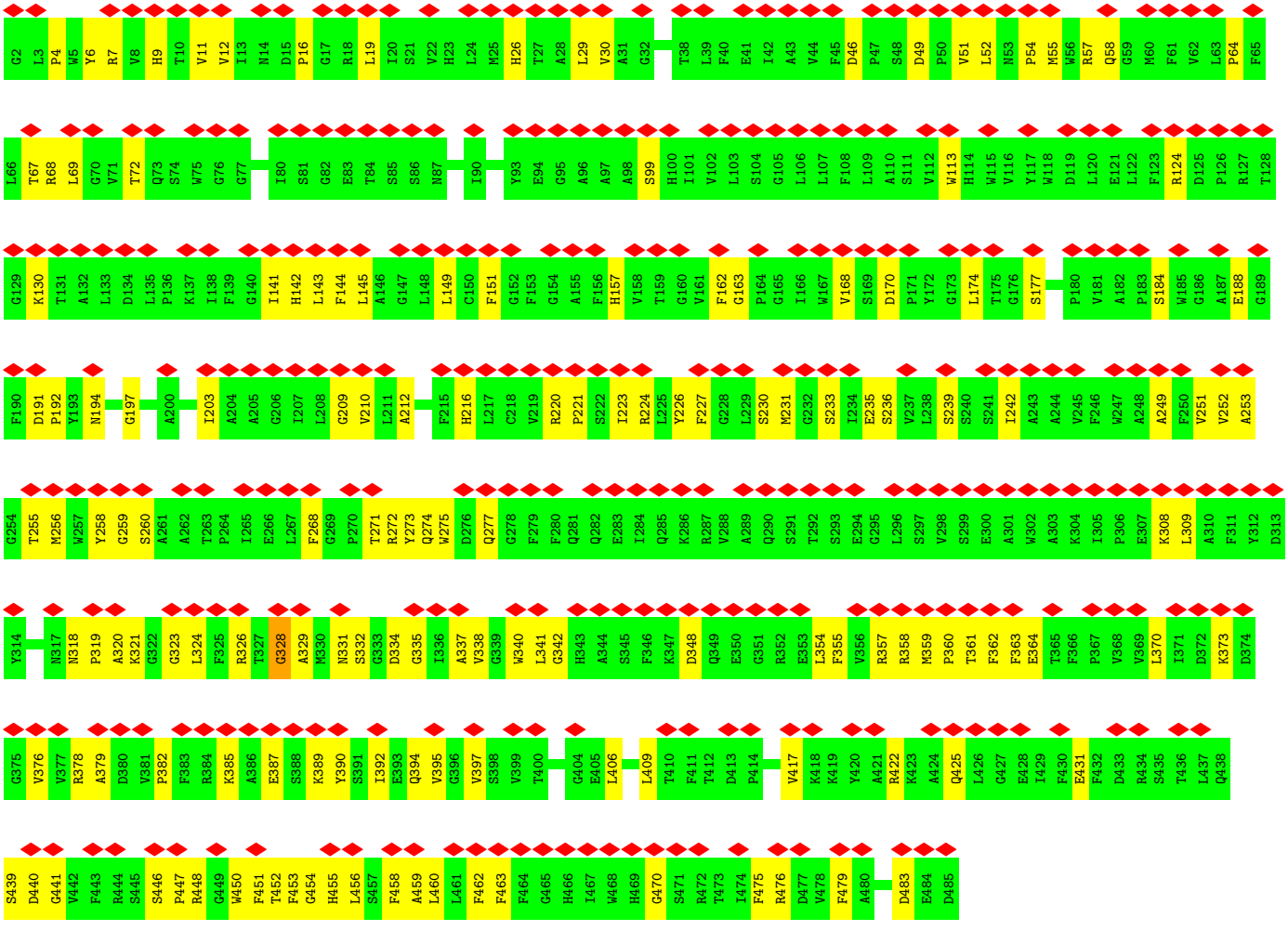




• Molecule 2: Photosystem II CP47 reaction center protein

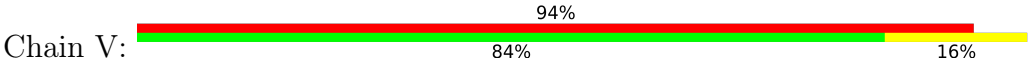
Chain b1:

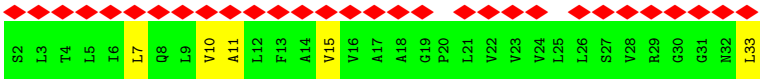




• Molecule 3: Photosystem II reaction center protein Ycf12

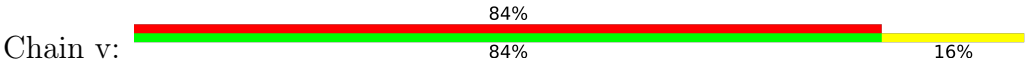
Chain V:

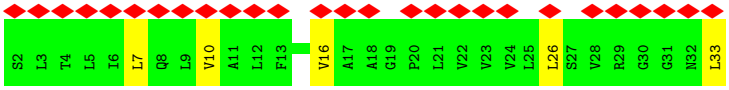




• Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:

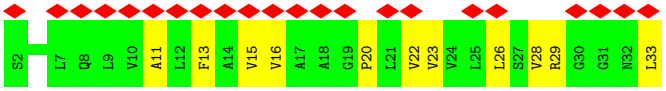




• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V1:





• Molecule 3: Photosystem II reaction center protein Ycf12

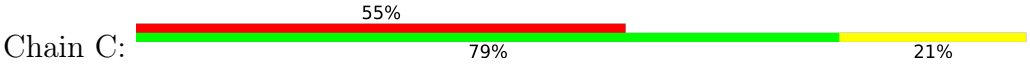
Chain v1:

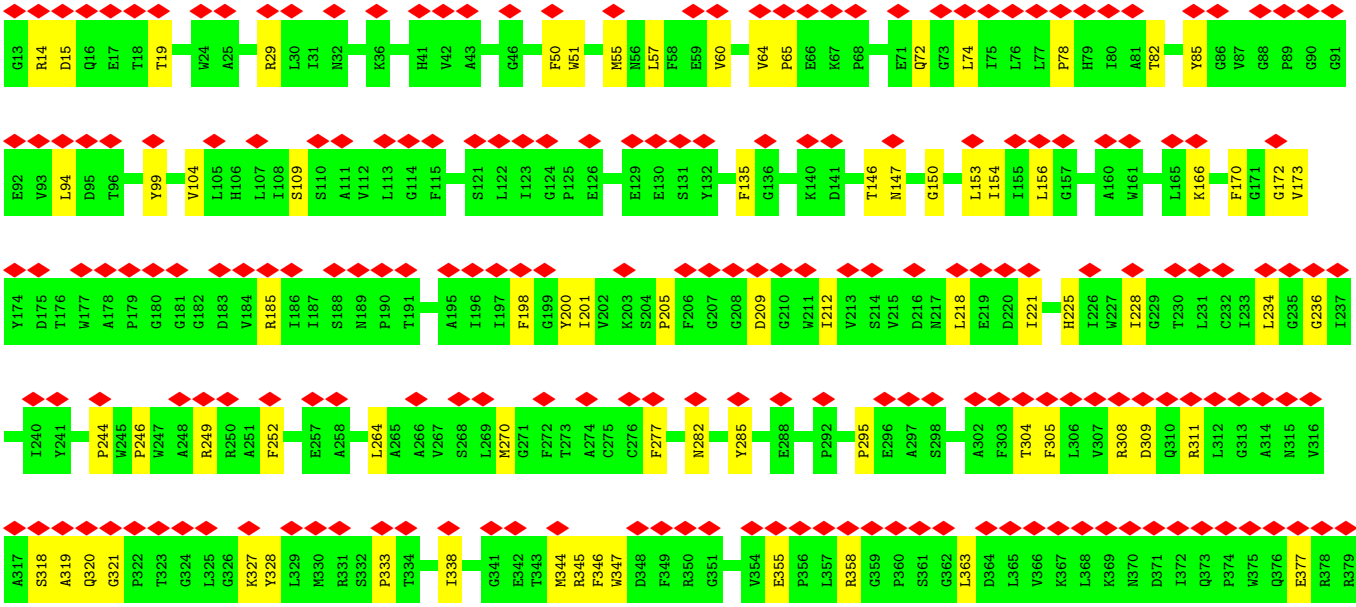


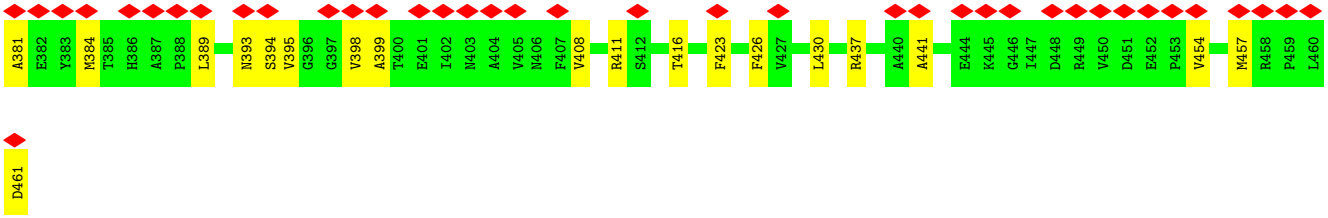


• Molecule 4: Photosystem II CP43 reaction center protein

Chain C:



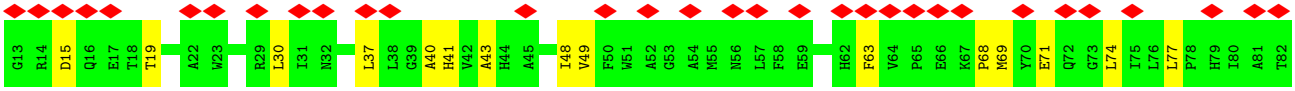




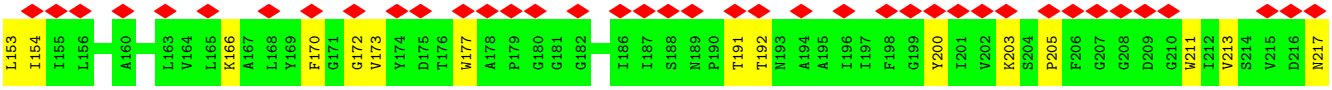
• Molecule 4: Photosystem II CP43 reaction center protein

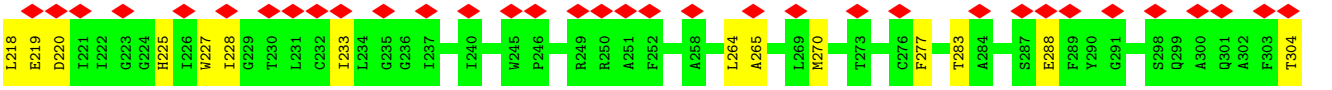
Chain c:

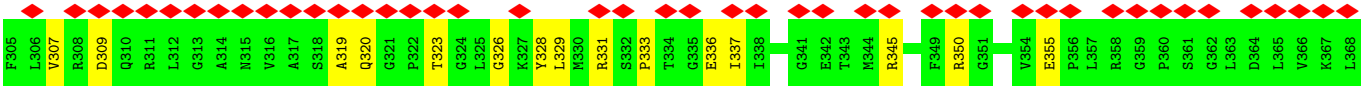


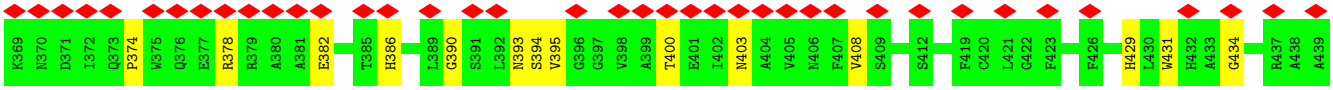


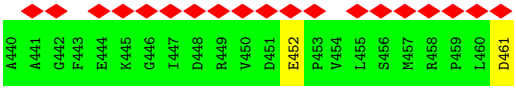








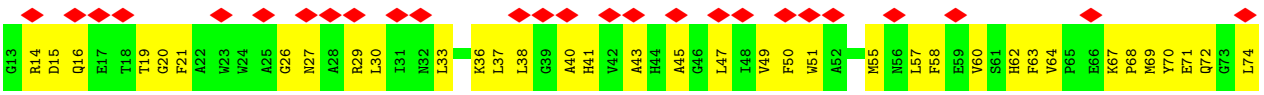




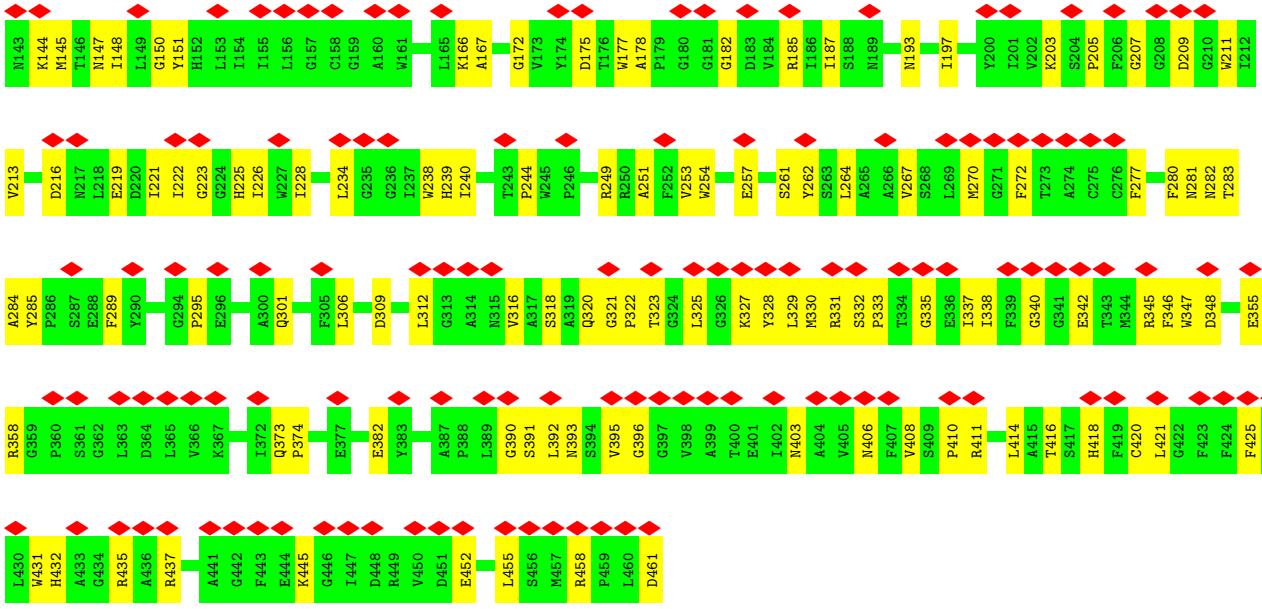
• Molecule 4: Photosystem II CP43 reaction center protein

Chain C1:





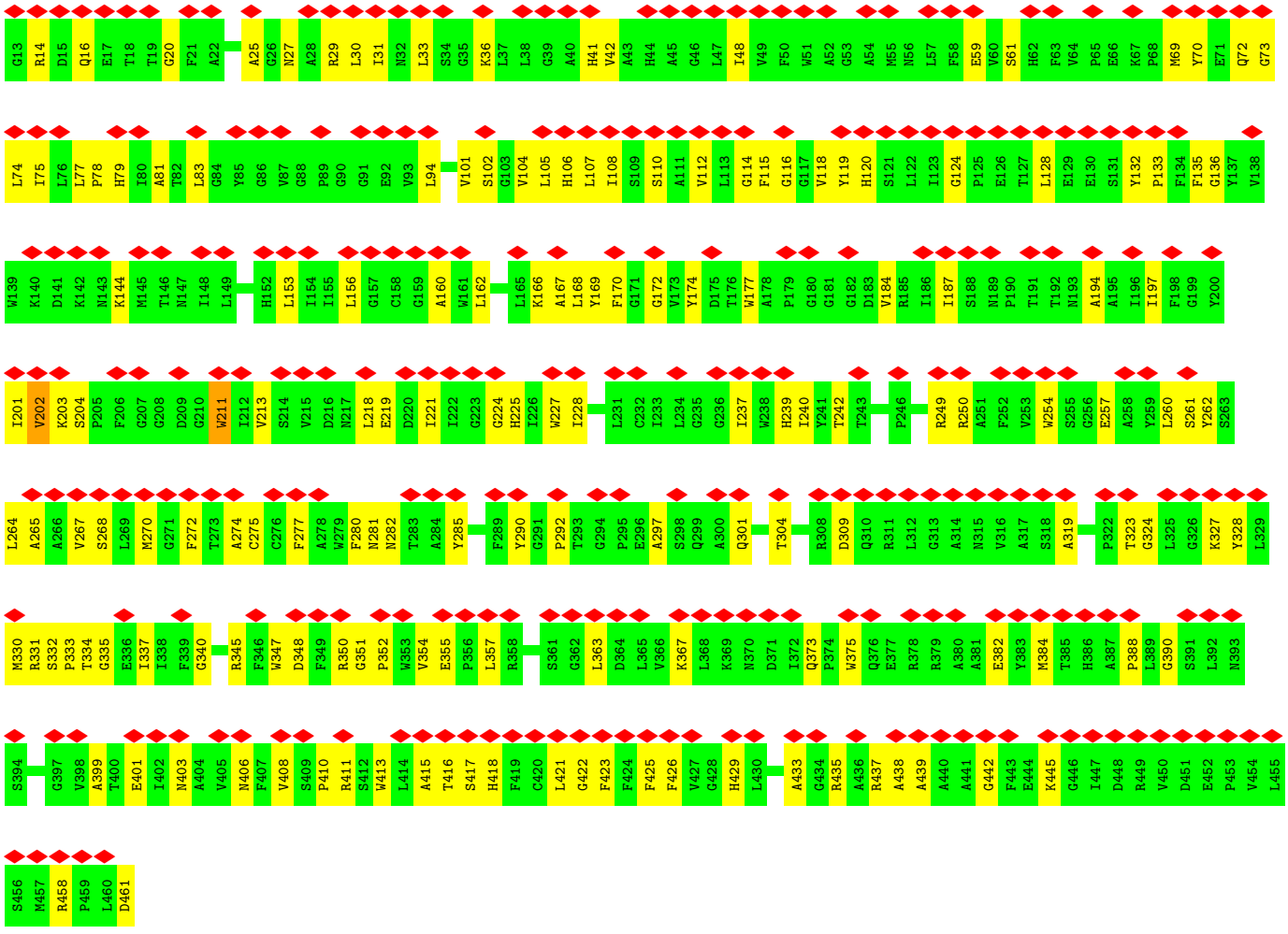




• Molecule 4: Photosystem II CP43 reaction center protein

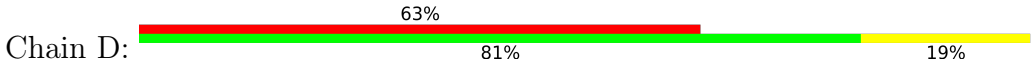
Chain c1:

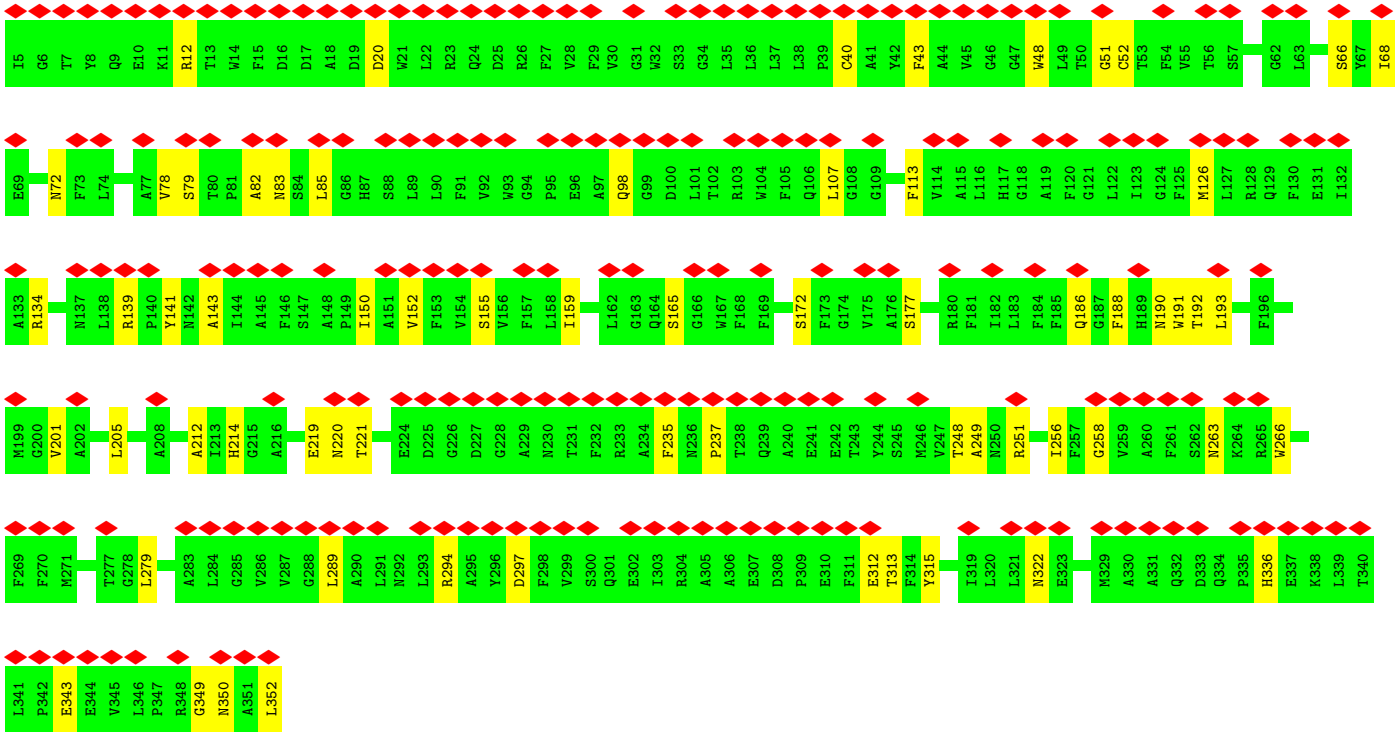




• Molecule 5: Photosystem II D2 protein

Chain D:

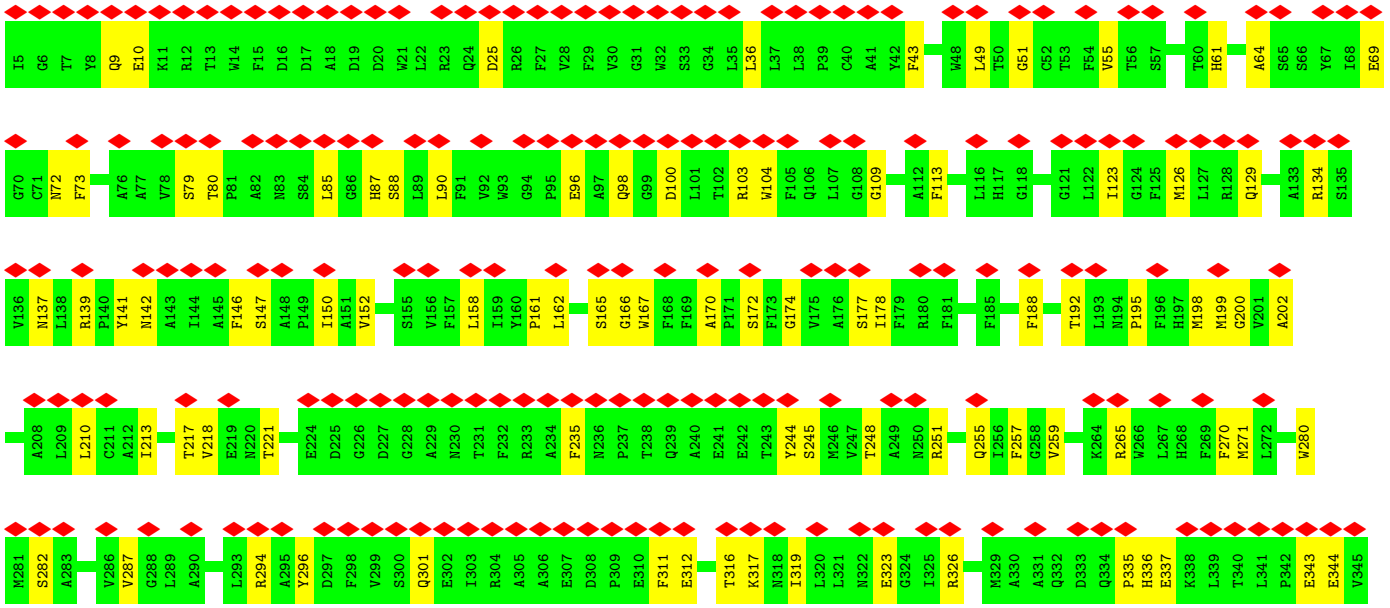


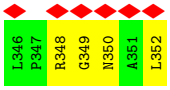


• Molecule 5: Photosystem II D2 protein

Chain d:



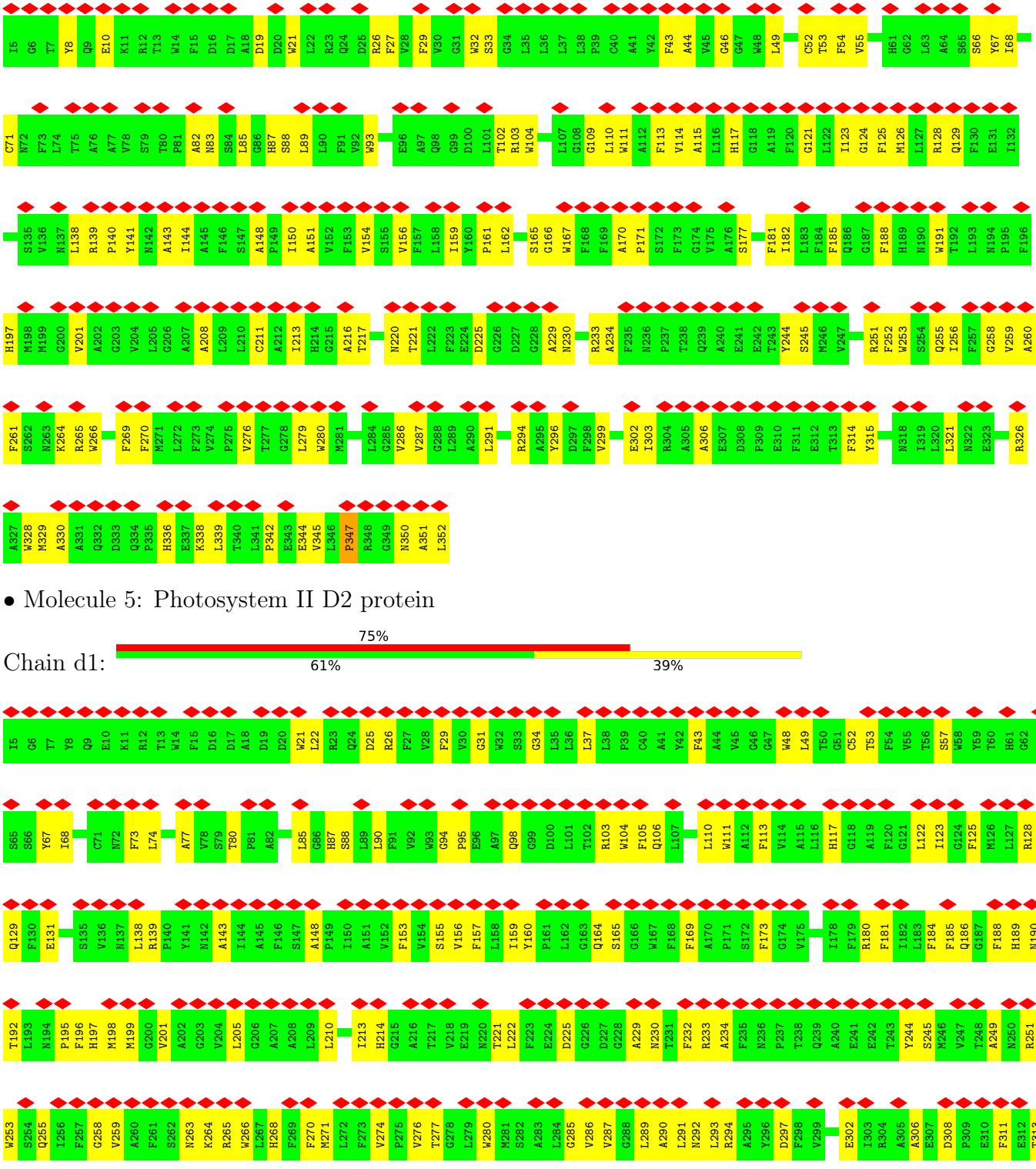




• Molecule 5: Photosystem II D2 protein

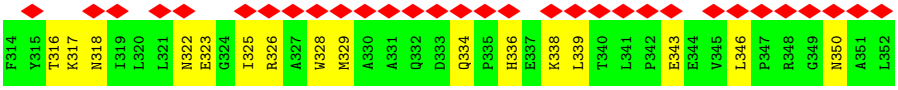
Chain D1:





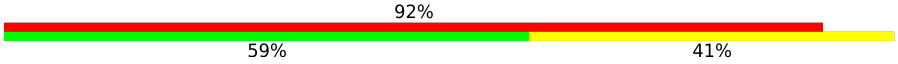
• Molecule 5: Photosystem II D2 protein

Chain d1:

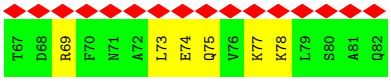


• Molecule 6: Cytochrome b559 subunit alpha

Chain E:

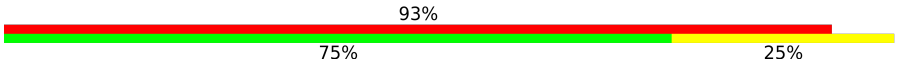


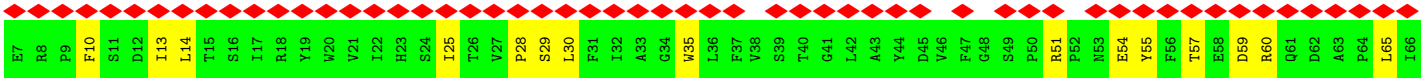


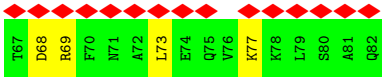


• Molecule 6: Cytochrome b559 subunit alpha

Chain e:

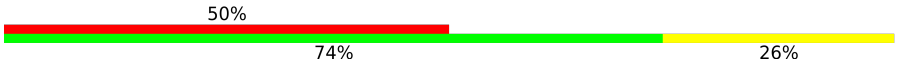


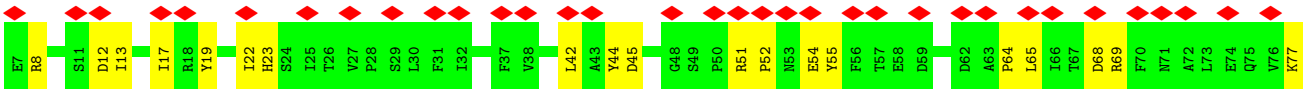


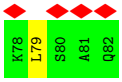


• Molecule 6: Cytochrome b559 subunit alpha

Chain E1:



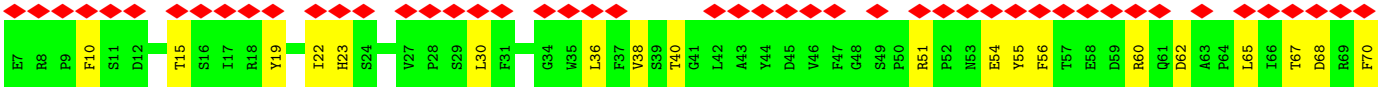


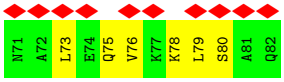


• Molecule 6: Cytochrome b559 subunit alpha

Chain e1:



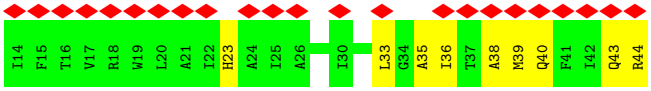




• Molecule 7: Cytochrome b559 subunit beta

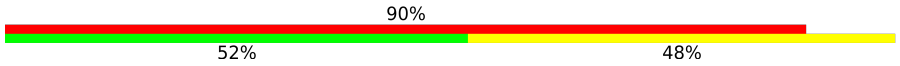
Chain F:

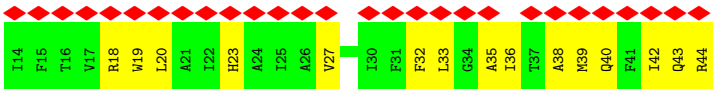




• Molecule 7: Cytochrome b559 subunit beta

Chain f:

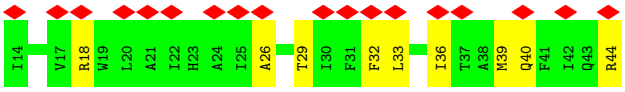




• Molecule 7: Cytochrome b559 subunit beta

Chain F1:

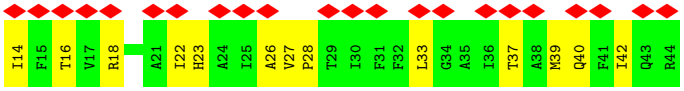




• Molecule 7: Cytochrome b559 subunit beta

Chain f1:

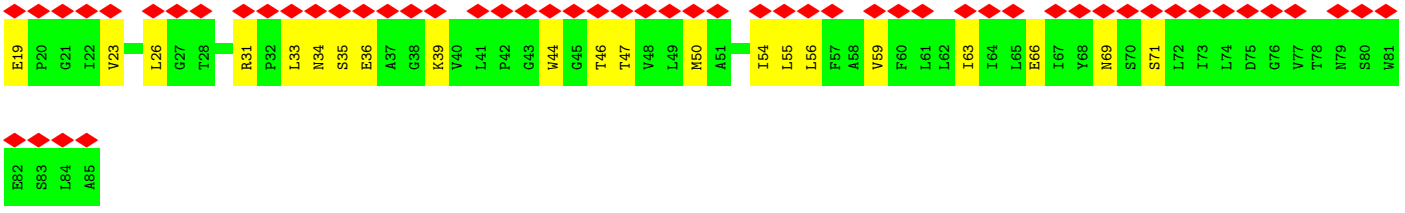




• Molecule 8: Photosystem II reaction center protein H

Chain H:

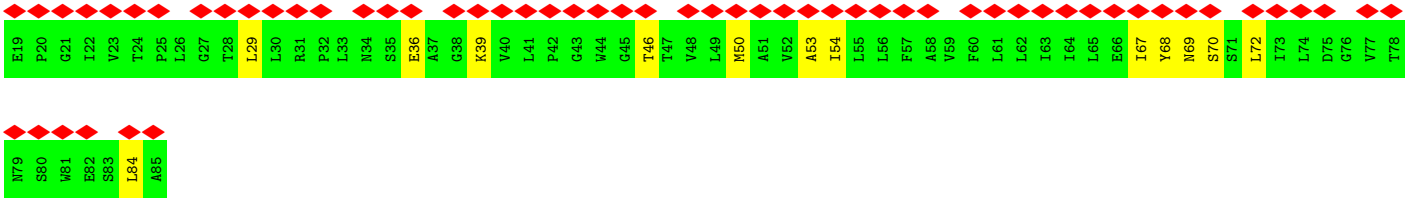




• Molecule 8: Photosystem II reaction center protein H

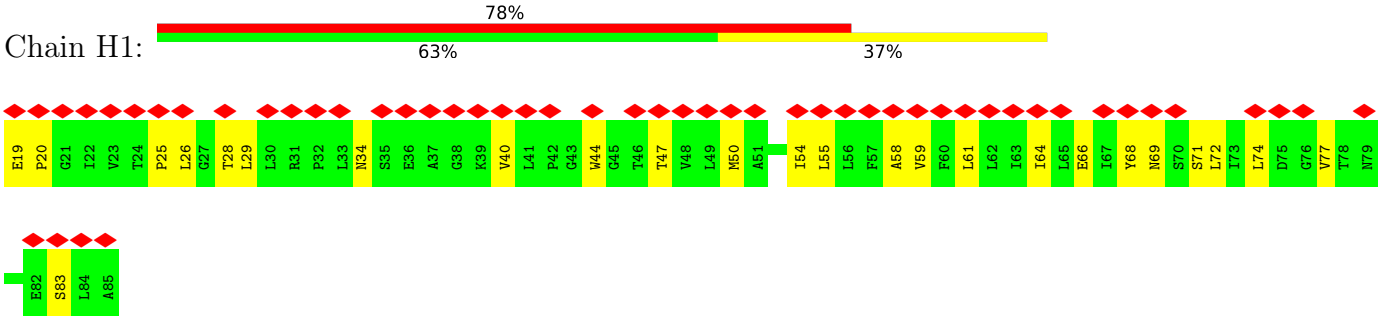
Chain h:





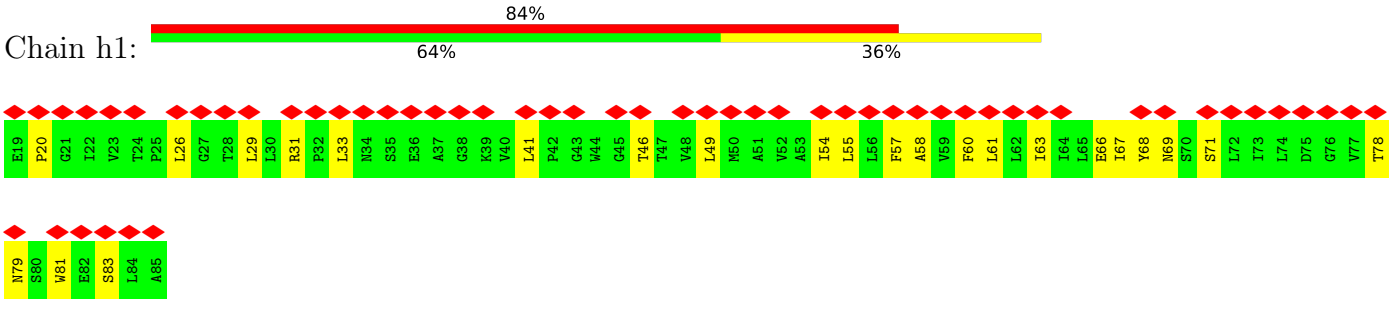
• Molecule 8: Photosystem II reaction center protein H

Chain H1:



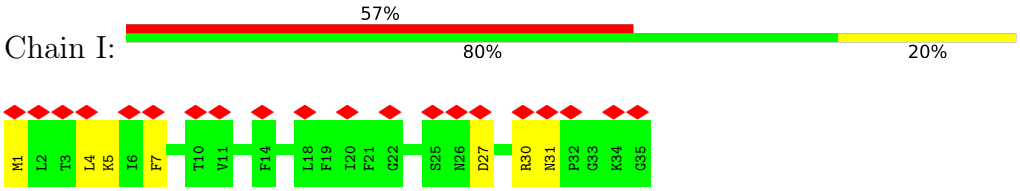
• Molecule 8: Photosystem II reaction center protein H

Chain h1:



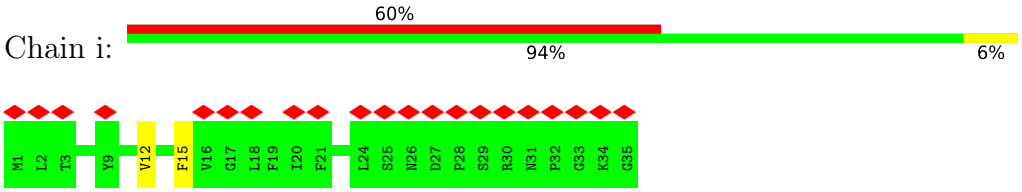
• Molecule 9: Photosystem II reaction center protein I

Chain I:



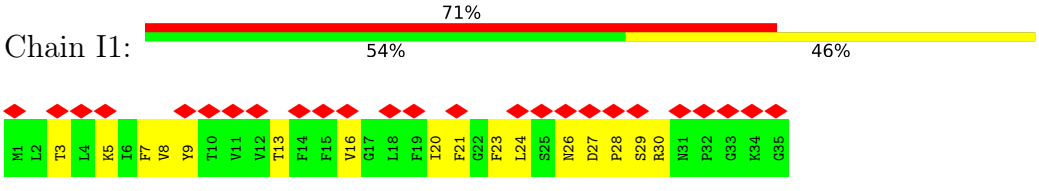
• Molecule 9: Photosystem II reaction center protein I

Chain i:



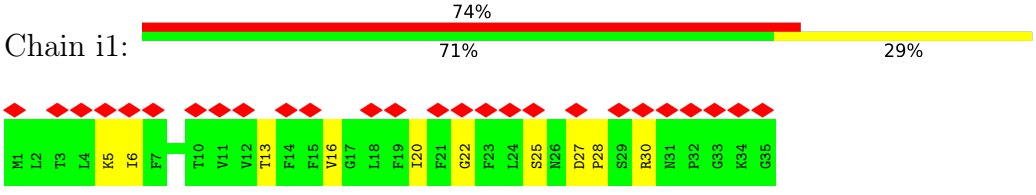
• Molecule 9: Photosystem II reaction center protein I

Chain I1:



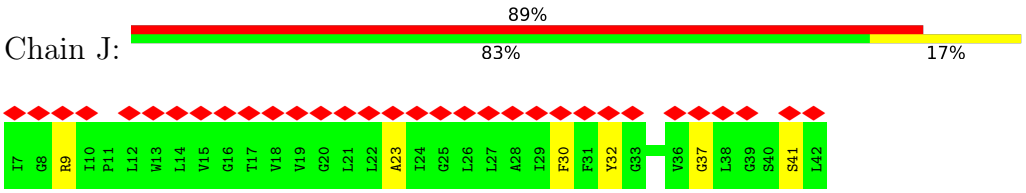
• Molecule 9: Photosystem II reaction center protein I

Chain i1:



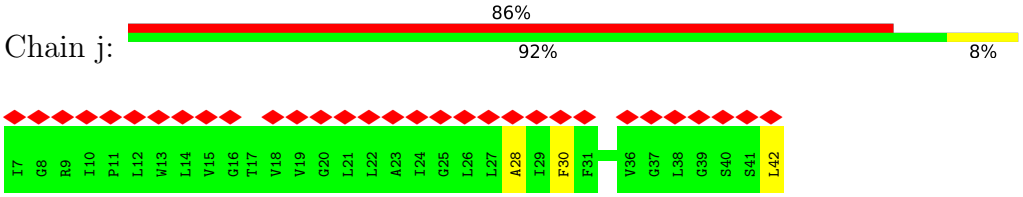
• Molecule 10: PsbJ

Chain J:



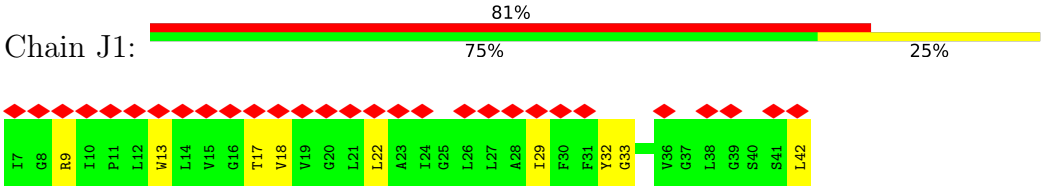
• Molecule 10: PsbJ

Chain j:



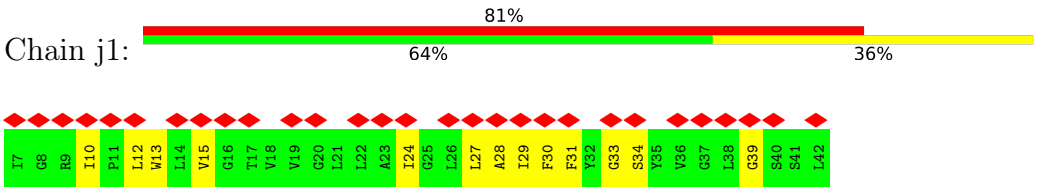
• Molecule 10: PsbJ

Chain J1:



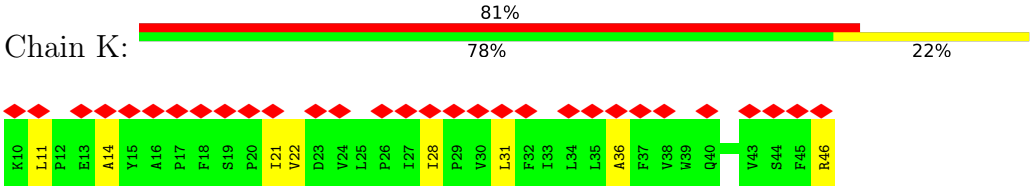
• Molecule 10: PsbJ

Chain j1:



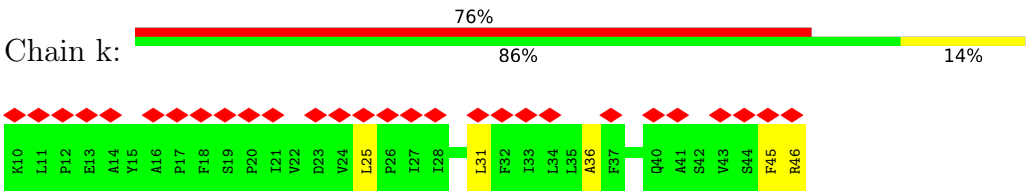
• Molecule 11: Photosystem II reaction center protein K

Chain K:



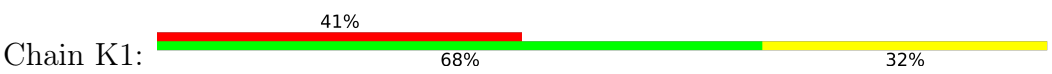
• Molecule 11: Photosystem II reaction center protein K

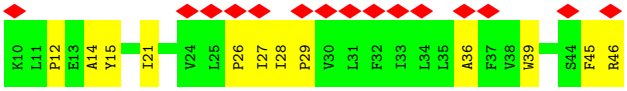
Chain k:



• Molecule 11: Photosystem II reaction center protein K

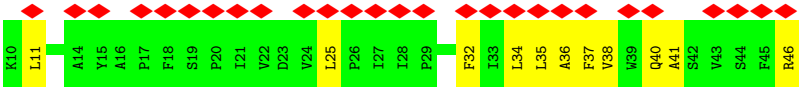
Chain K1:



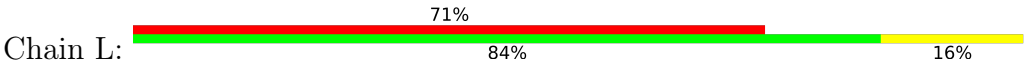


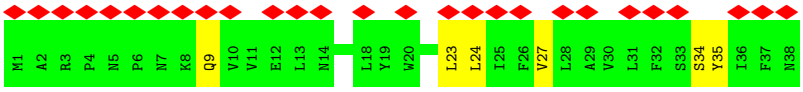
• Molecule 11: Photosystem II reaction center protein K





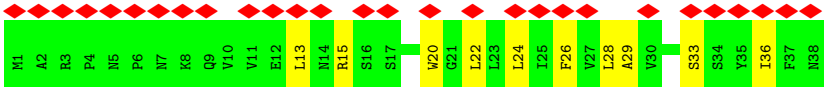
• Molecule 12: Photosystem II reaction center protein L



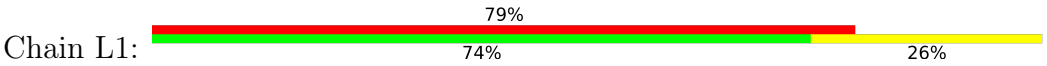


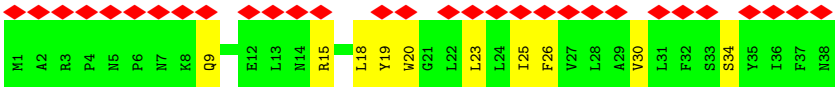
• Molecule 12: Photosystem II reaction center protein L



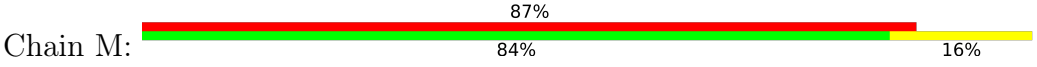


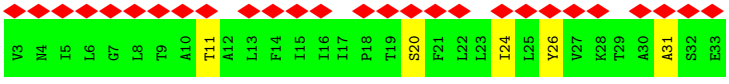
• Molecule 12: Photosystem II reaction center protein L



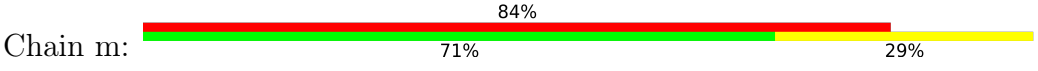


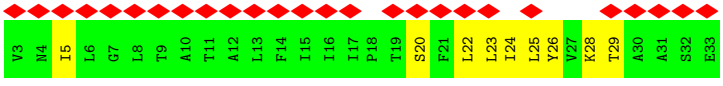
• Molecule 13: PsbM





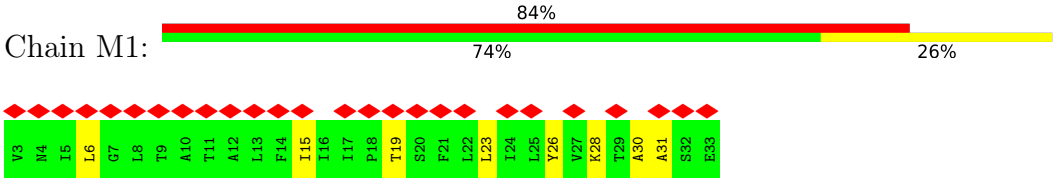
• Molecule 13: PsbM





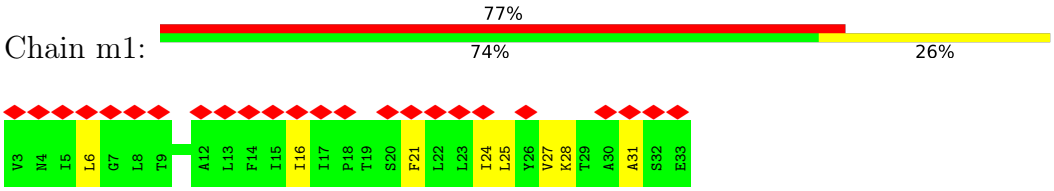
• Molecule 13: PsbM

Chain M1:



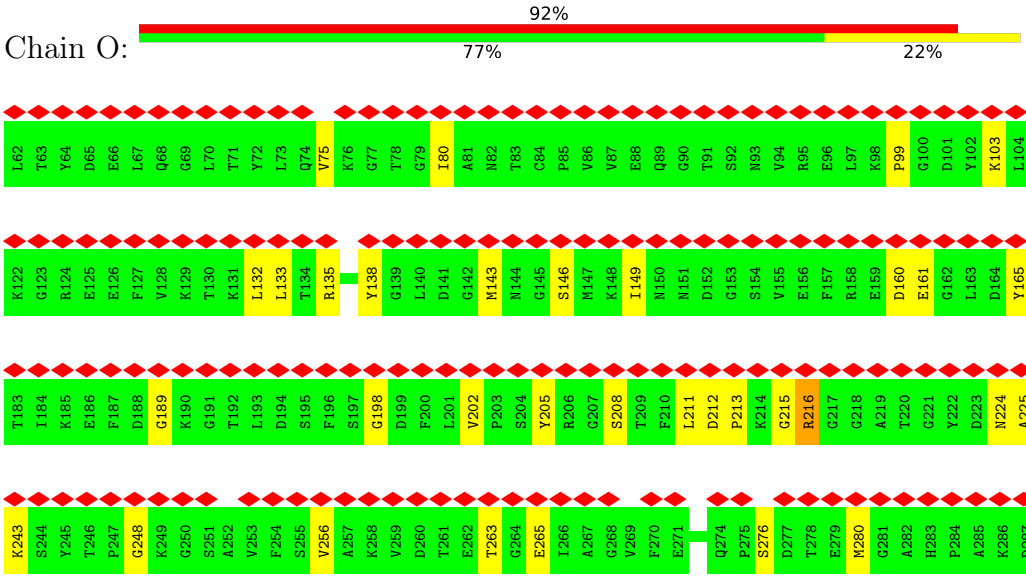
• Molecule 13: PsbM

Chain m1:



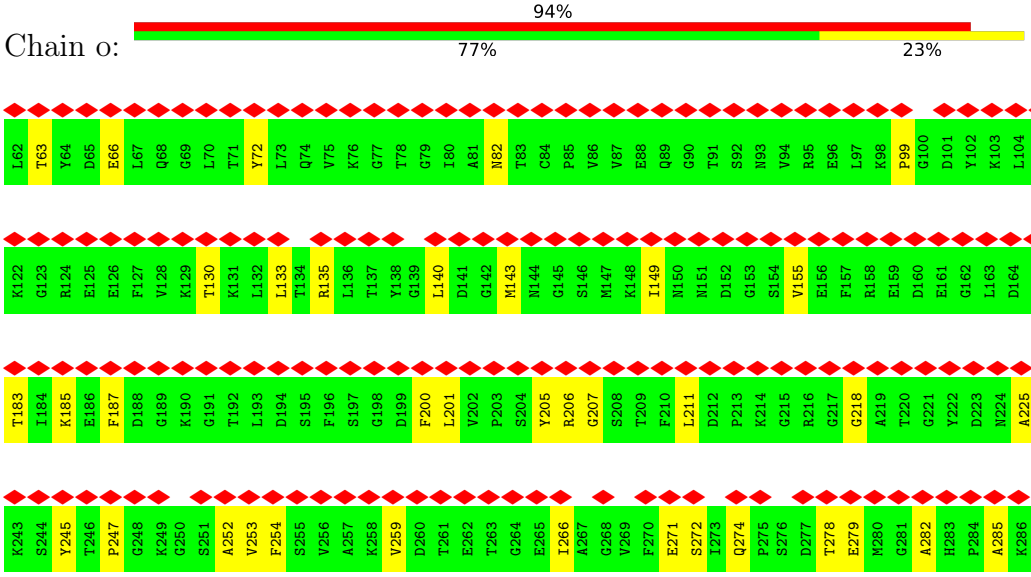
• Molecule 14: PsbO

Chain O:



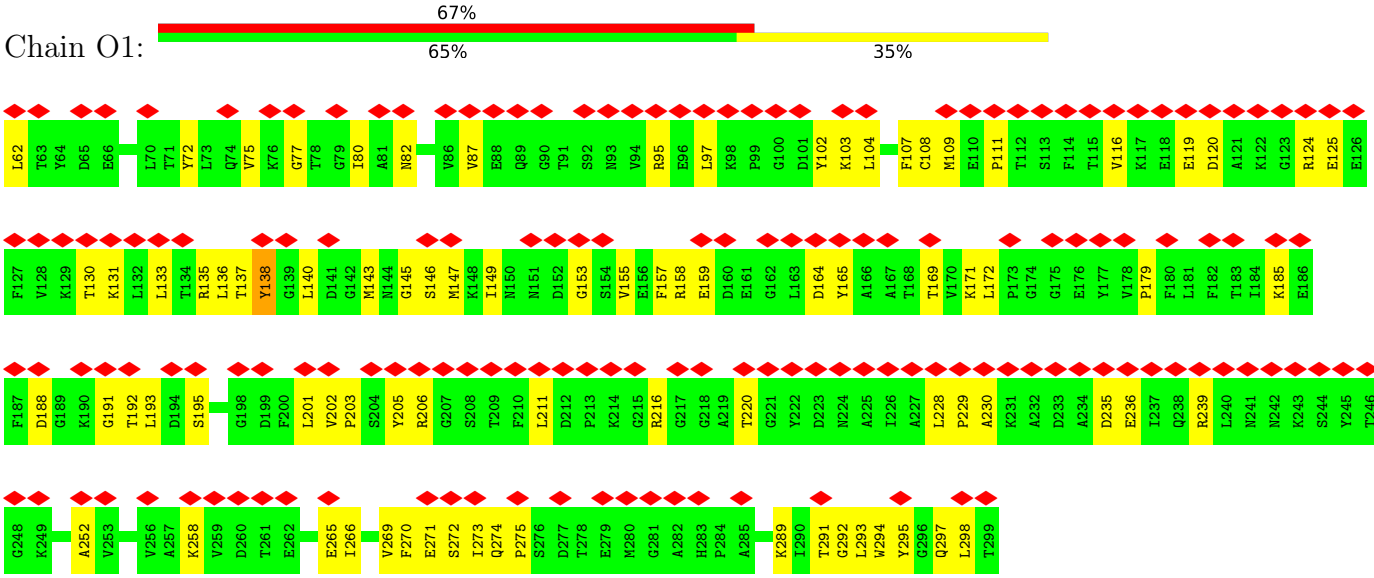
• Molecule 14: PsbO

Chain o:



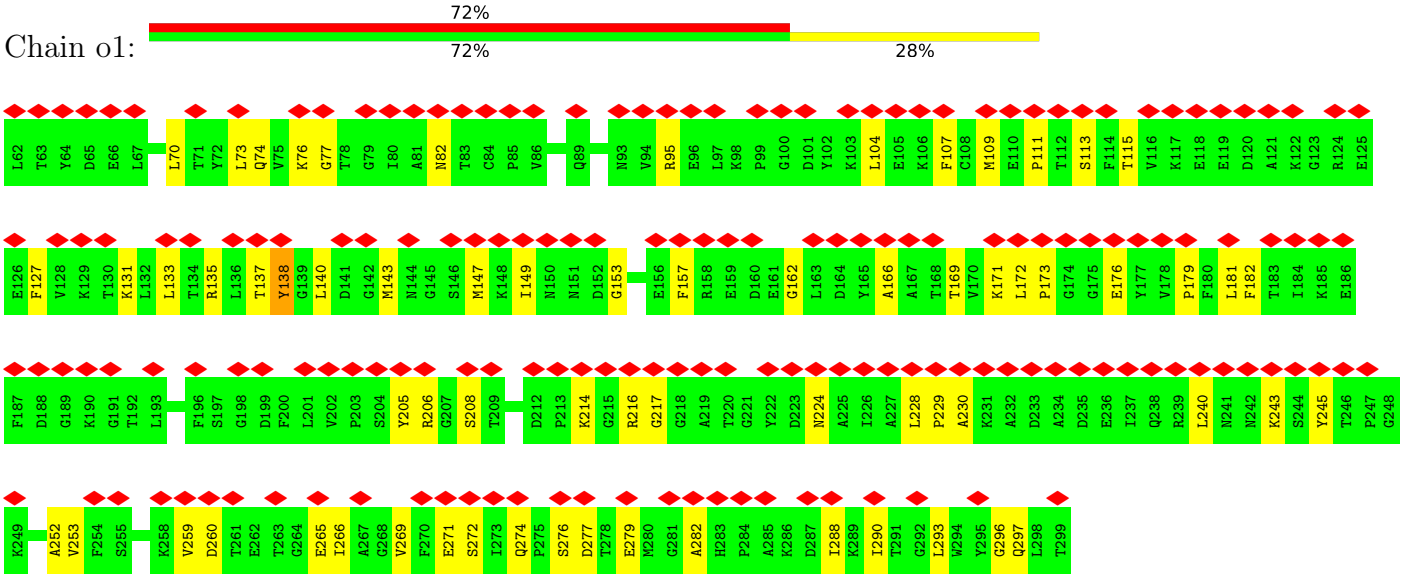
• Molecule 14: PsbO

Chain O1:



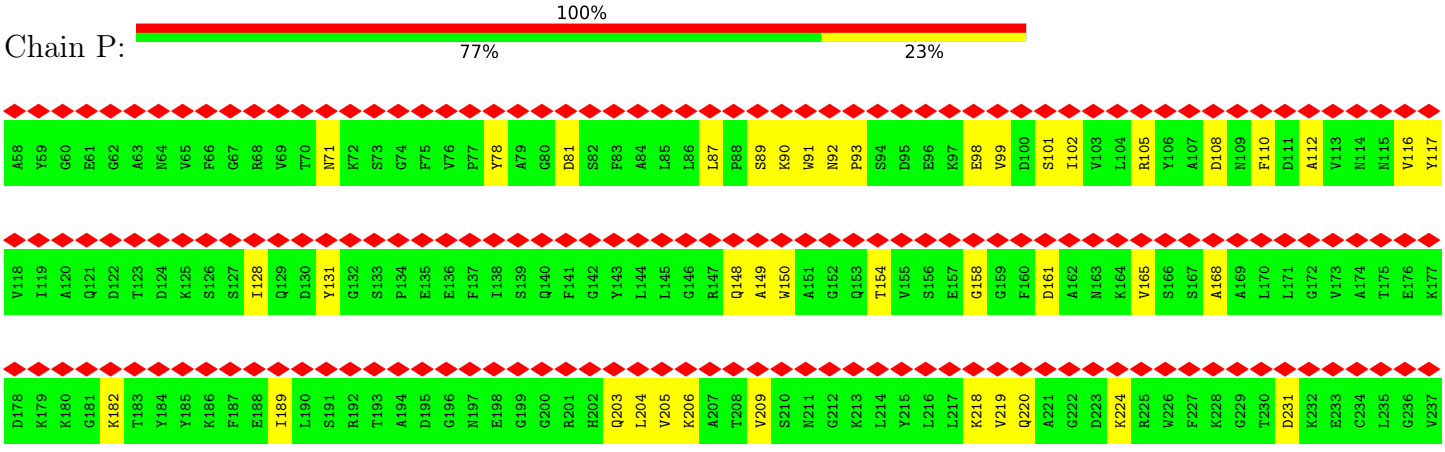
• Molecule 14: PsbO

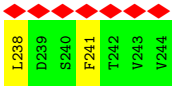
Chain o1:



• Molecule 15: PsbP

Chain P:



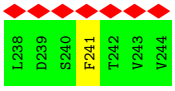


• Molecule 15: PsbP

Chain p:

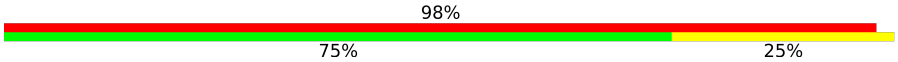




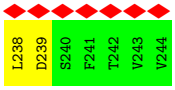


• Molecule 15: PsbP

Chain P1:

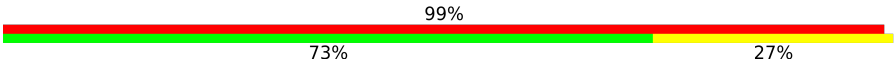


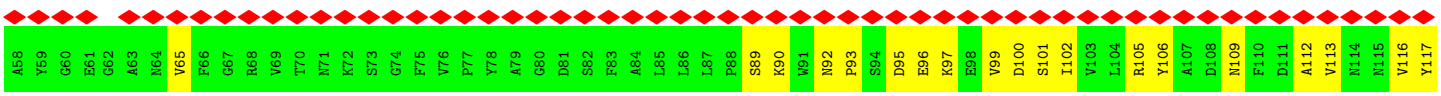


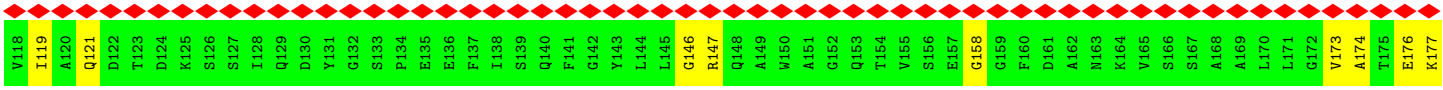


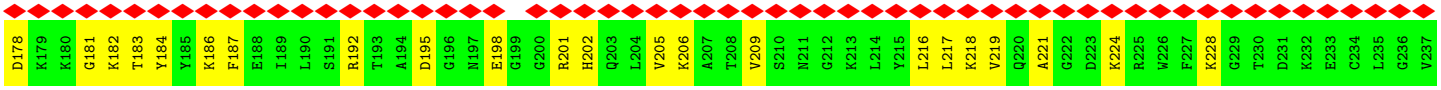
• Molecule 15: PsbP

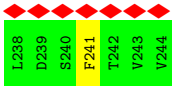
Chain p1:





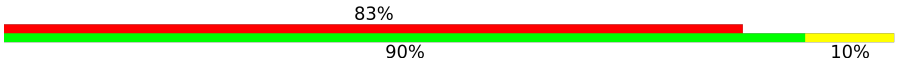


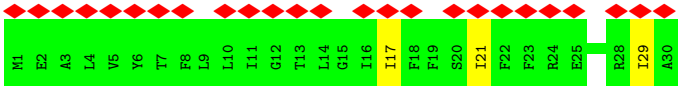




• Molecule 16: Photosystem II reaction center protein T

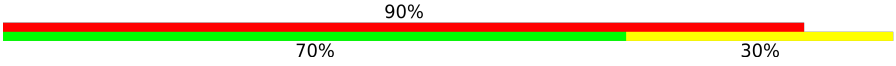
Chain T:

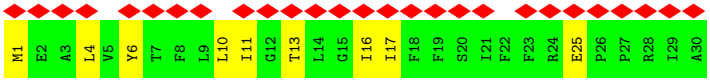




• Molecule 16: Photosystem II reaction center protein T

Chain t:

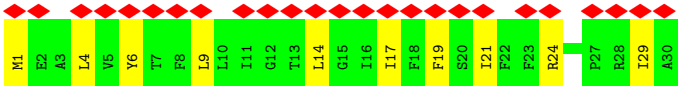




• Molecule 16: Photosystem II reaction center protein T

Chain T1:





• Molecule 16: Photosystem II reaction center protein T

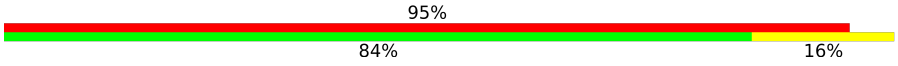
Chain t1:

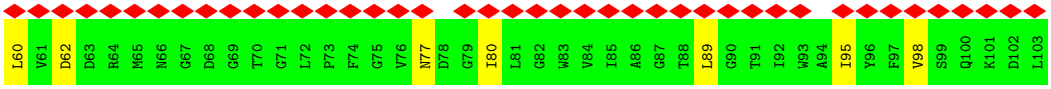




• Molecule 17: PsbW

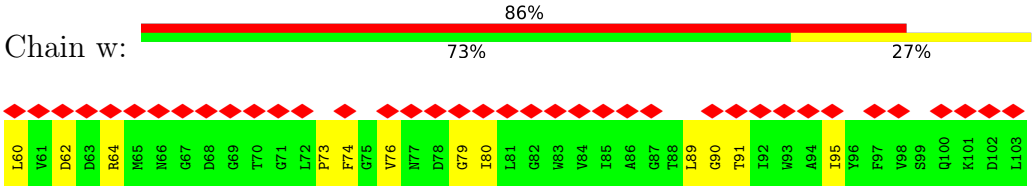
Chain W:





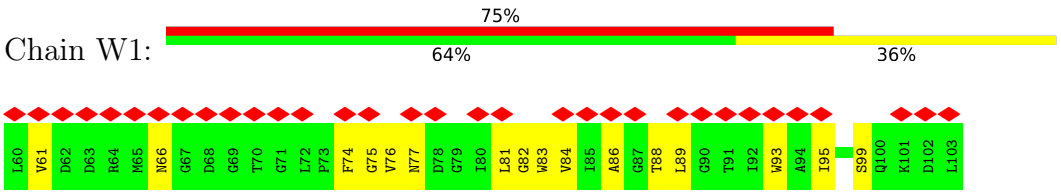
• Molecule 17: PsbW

Chain w:



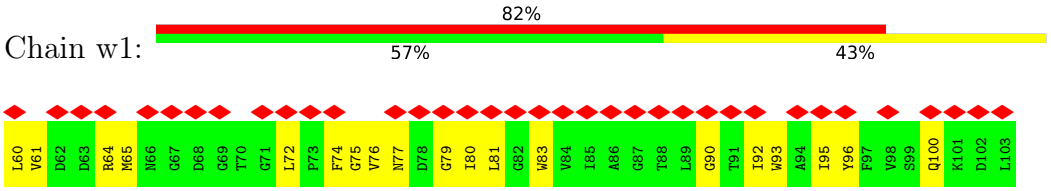
• Molecule 17: PsbW

Chain W1:



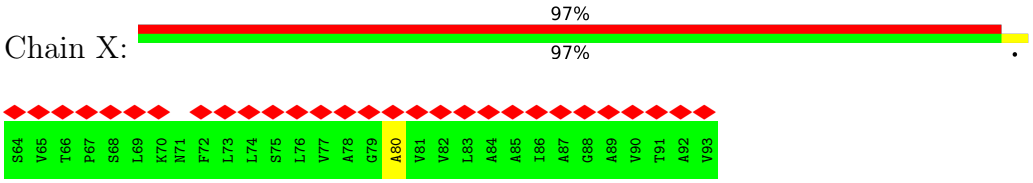
• Molecule 17: PsbW

Chain w1:



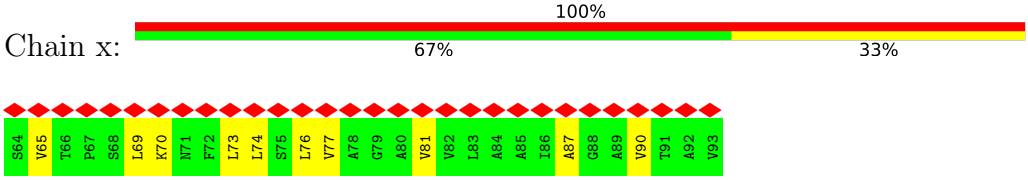
• Molecule 18: PsbX

Chain X:



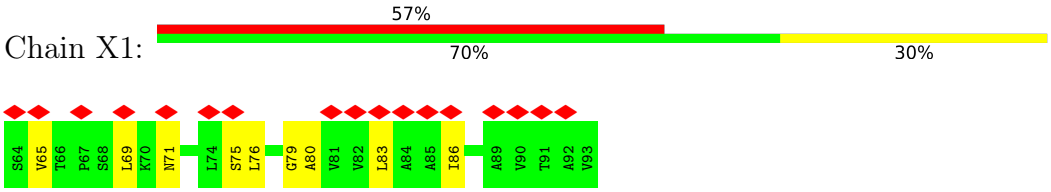
• Molecule 18: PsbX

Chain x:



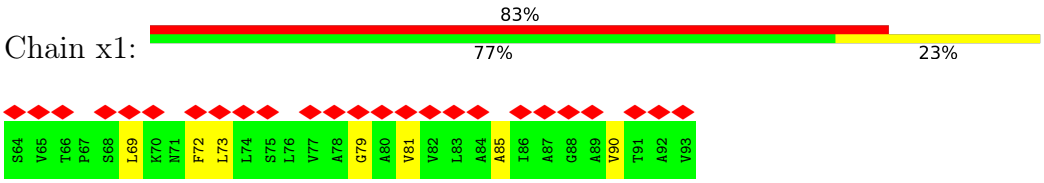
• Molecule 18: PsbX

Chain X1:



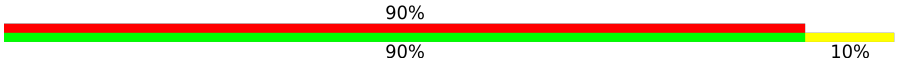
• Molecule 18: PsbX

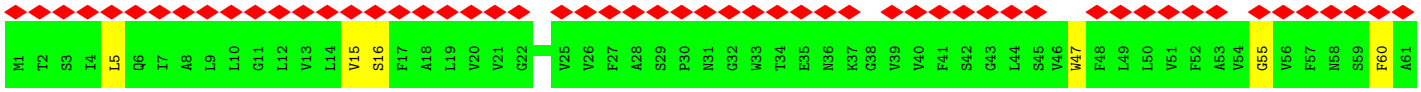
Chain x1:



• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

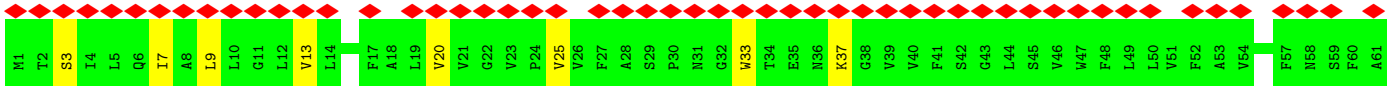




• Molecule 19: Photosystem II reaction center protein Z

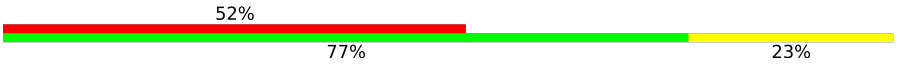
Chain z:

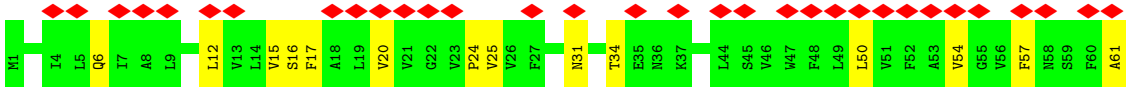




• Molecule 19: Photosystem II reaction center protein Z

Chain Z1:

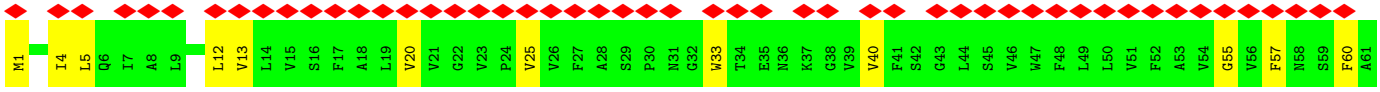




• Molecule 19: Photosystem II reaction center protein Z

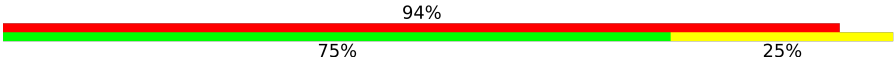
Chain z1:

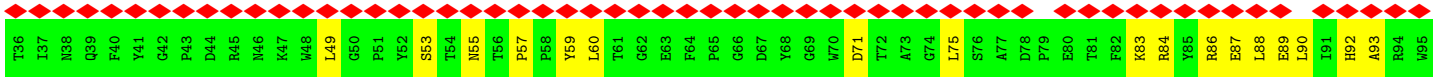


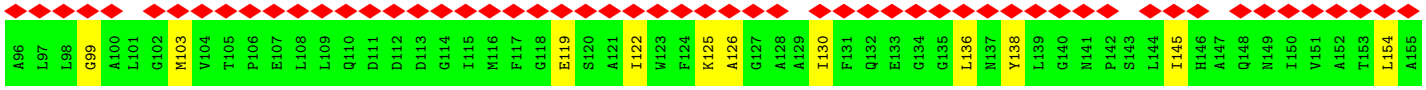


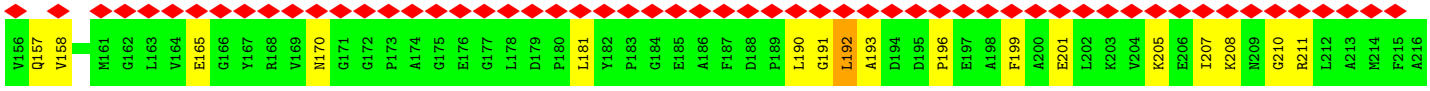
• Molecule 20: LHCII M3

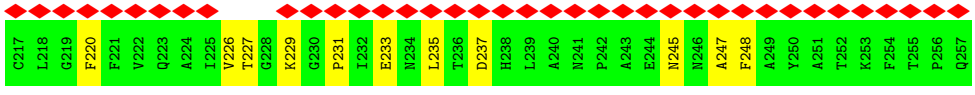
Chain N:







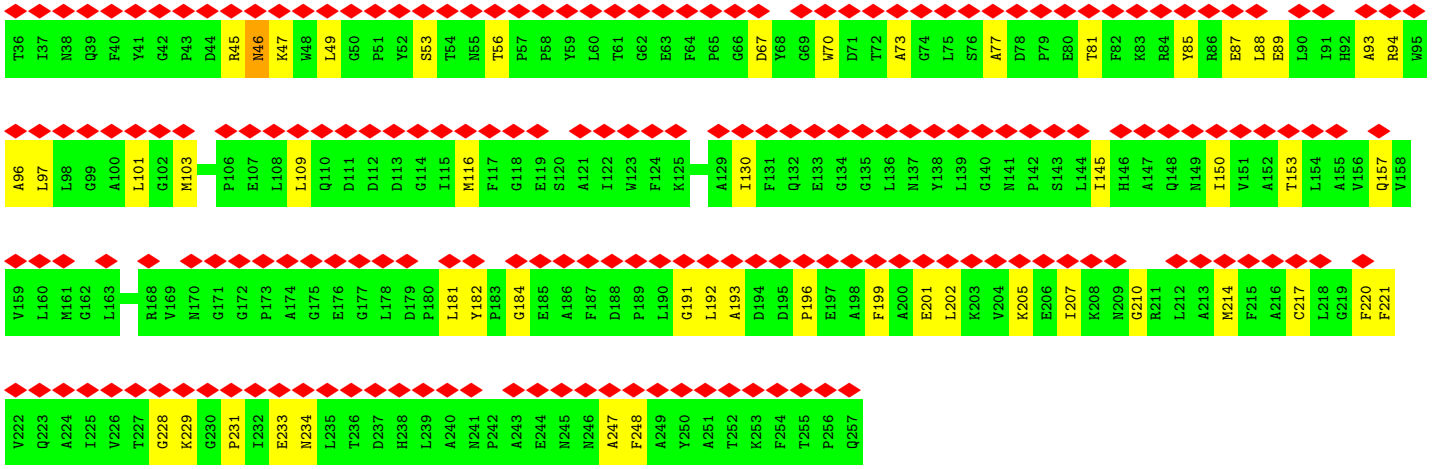




• Molecule 20: LHCII M3

Chain n:

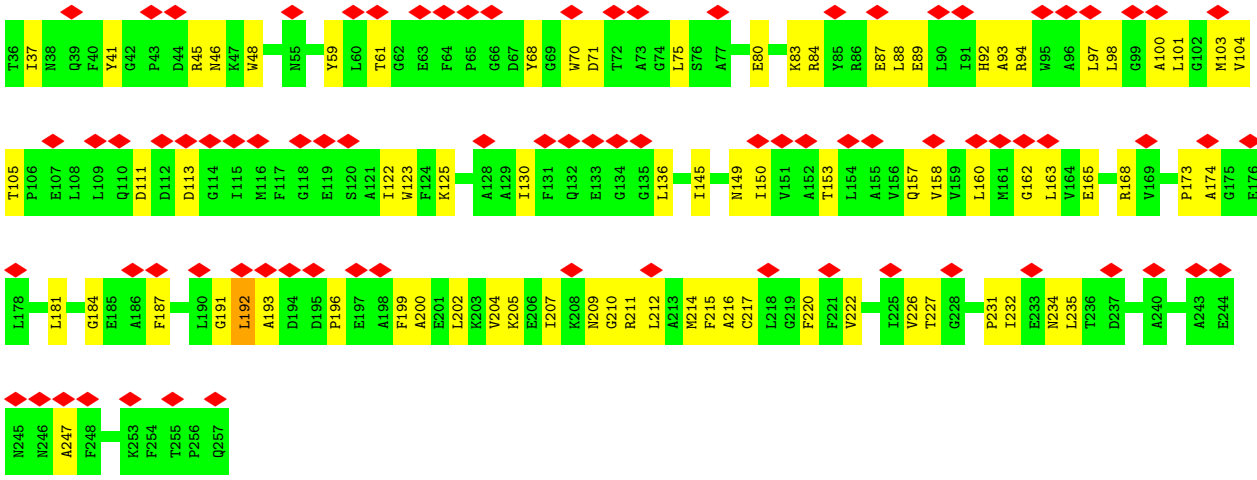




• Molecule 20: LHCII M3

Chain N1:

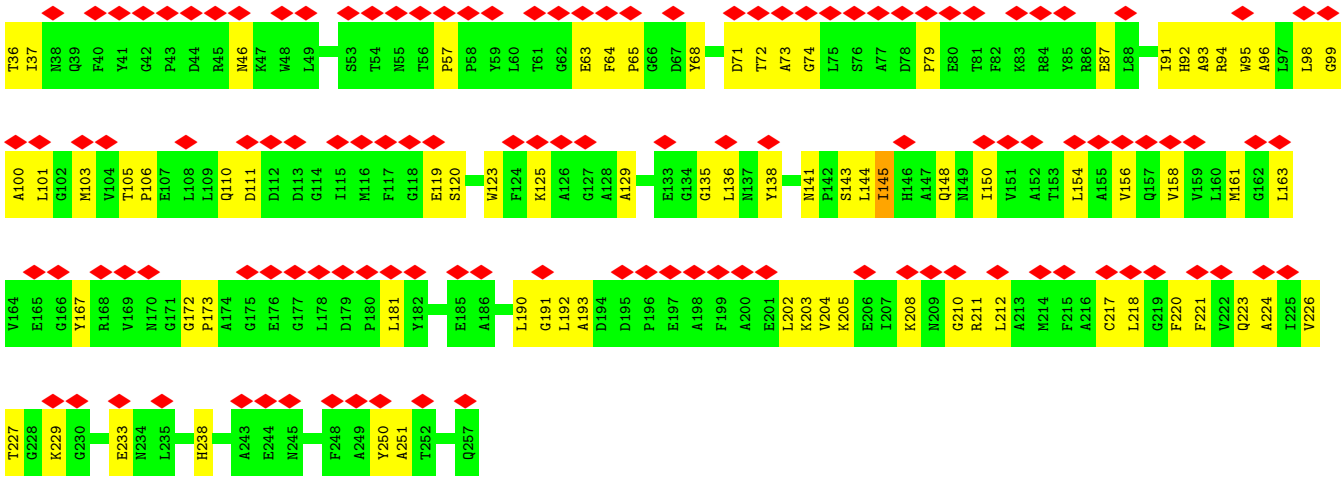




• Molecule 20: LHCII M3

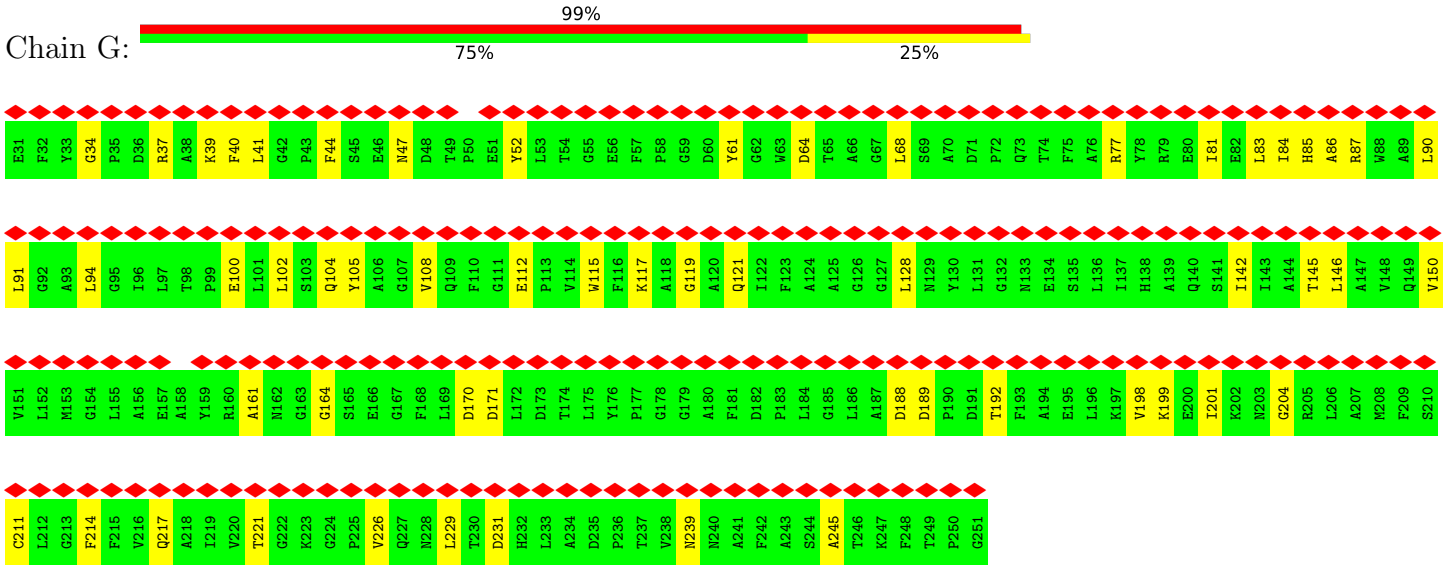
Chain n1:





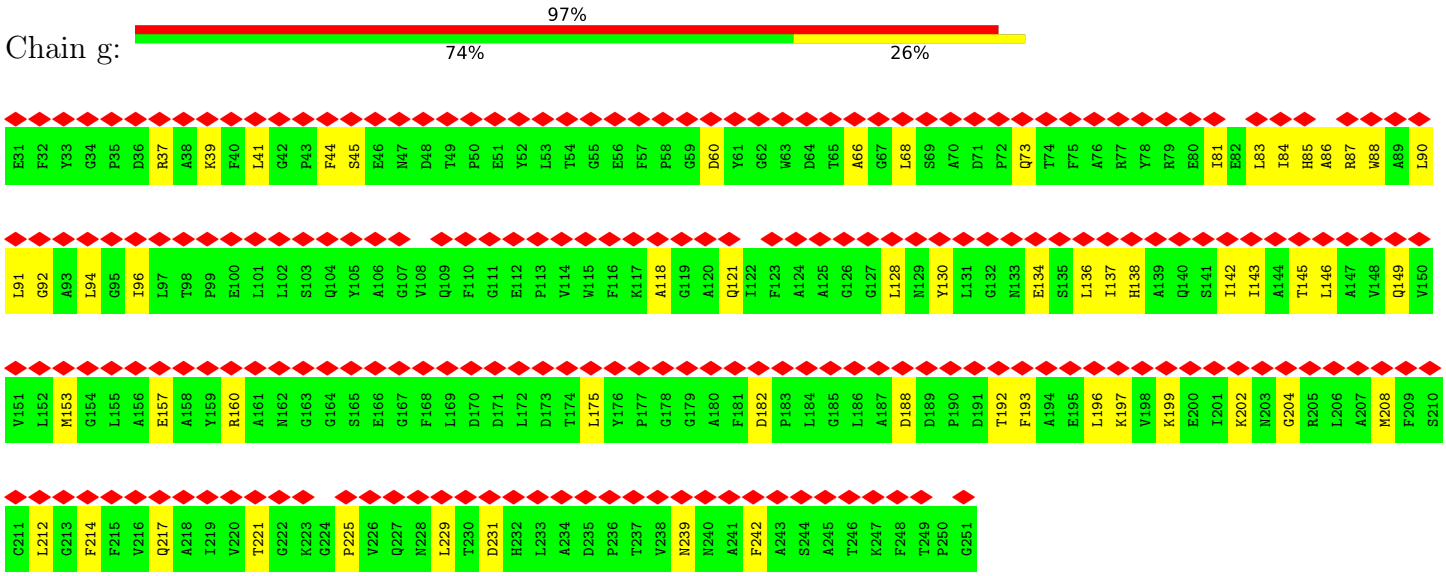
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G:



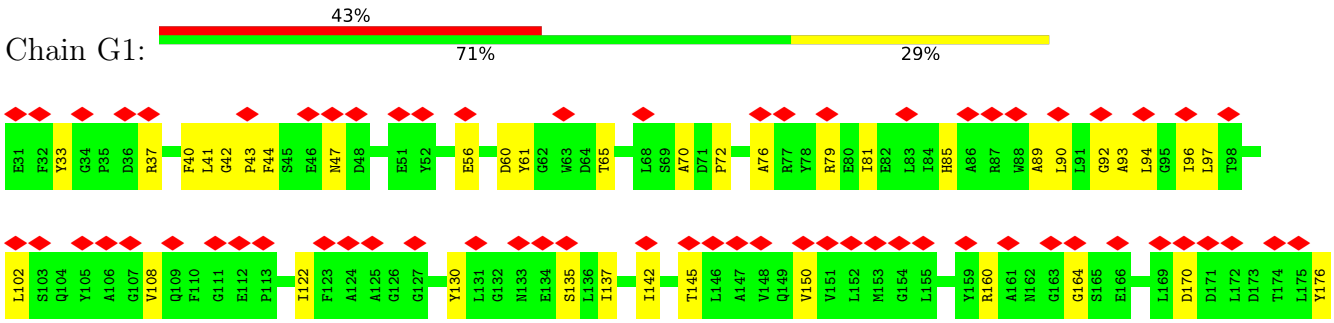
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

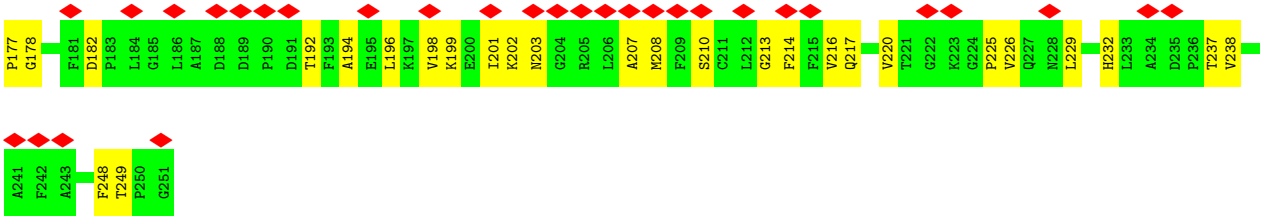
Chain g:



• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G1:

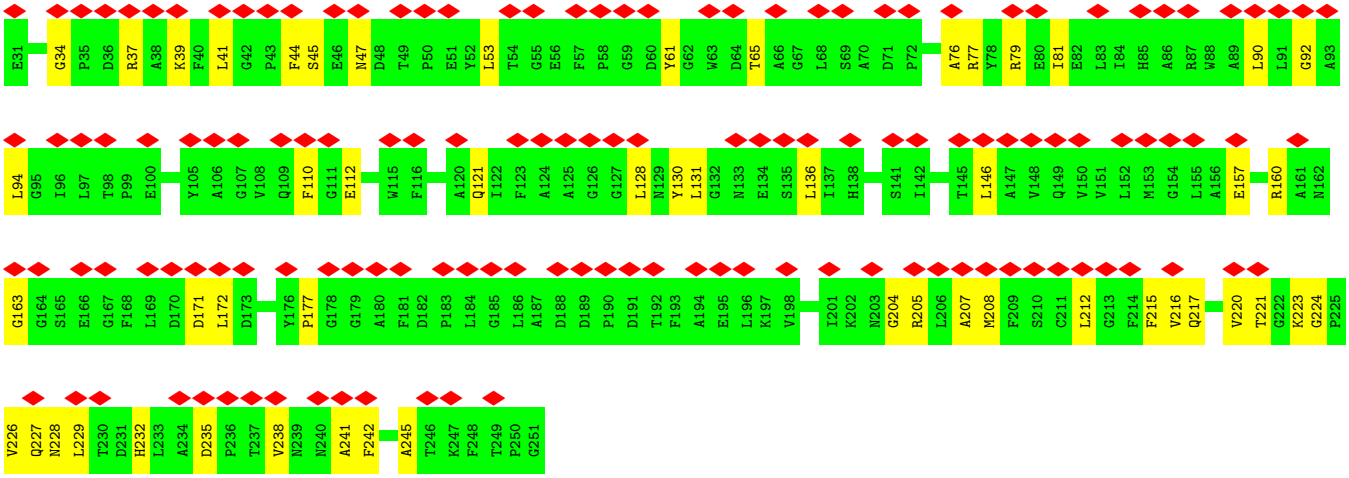




• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

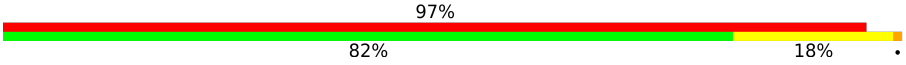
Chain g1:

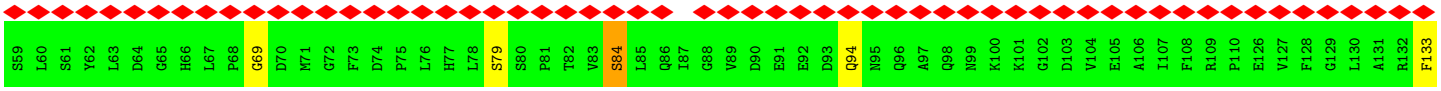


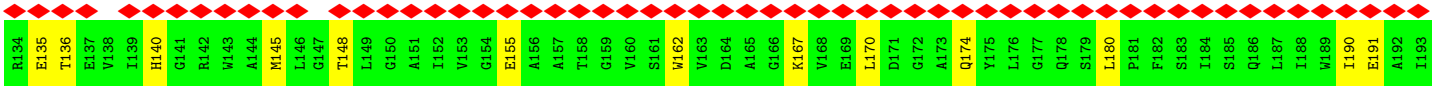


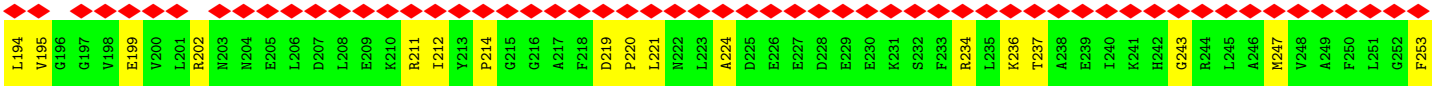
• Molecule 22: CP29

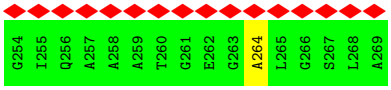
Chain R:





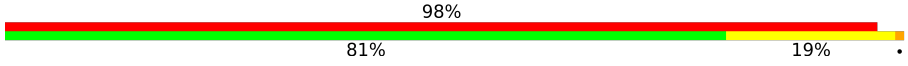






• Molecule 22: CP29

Chain r:

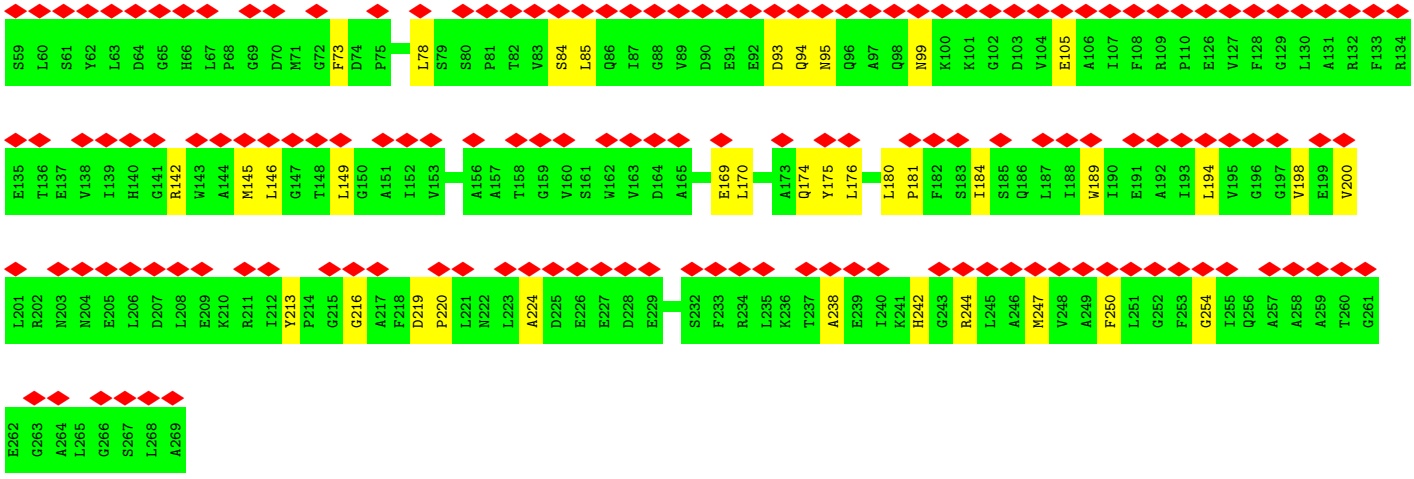




• Molecule 22: CP29

Chain R1:

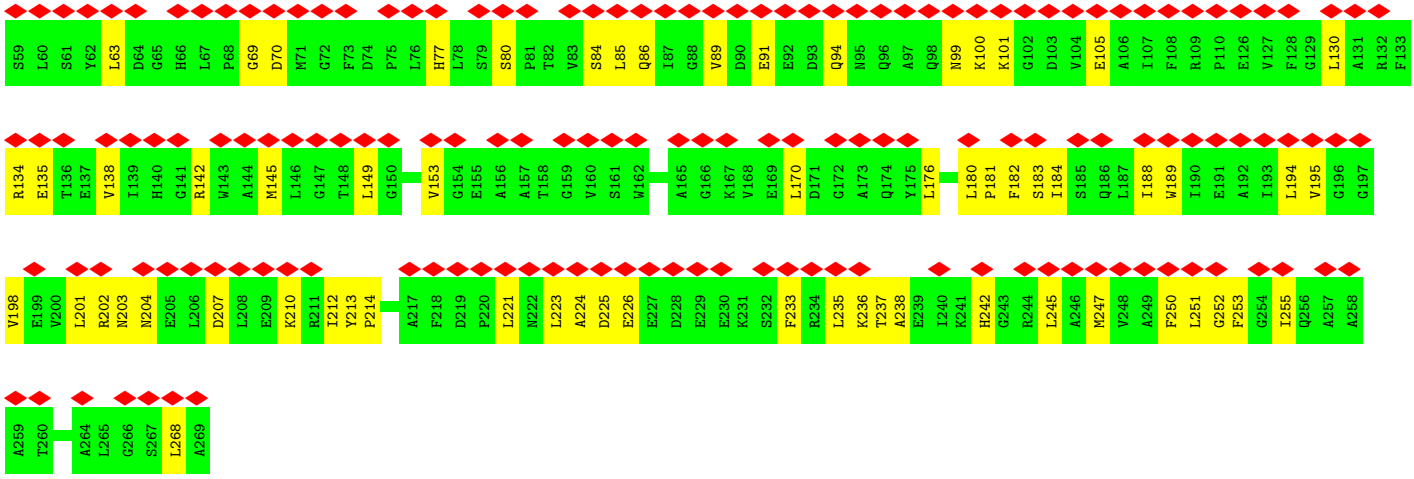




• Molecule 22: CP29

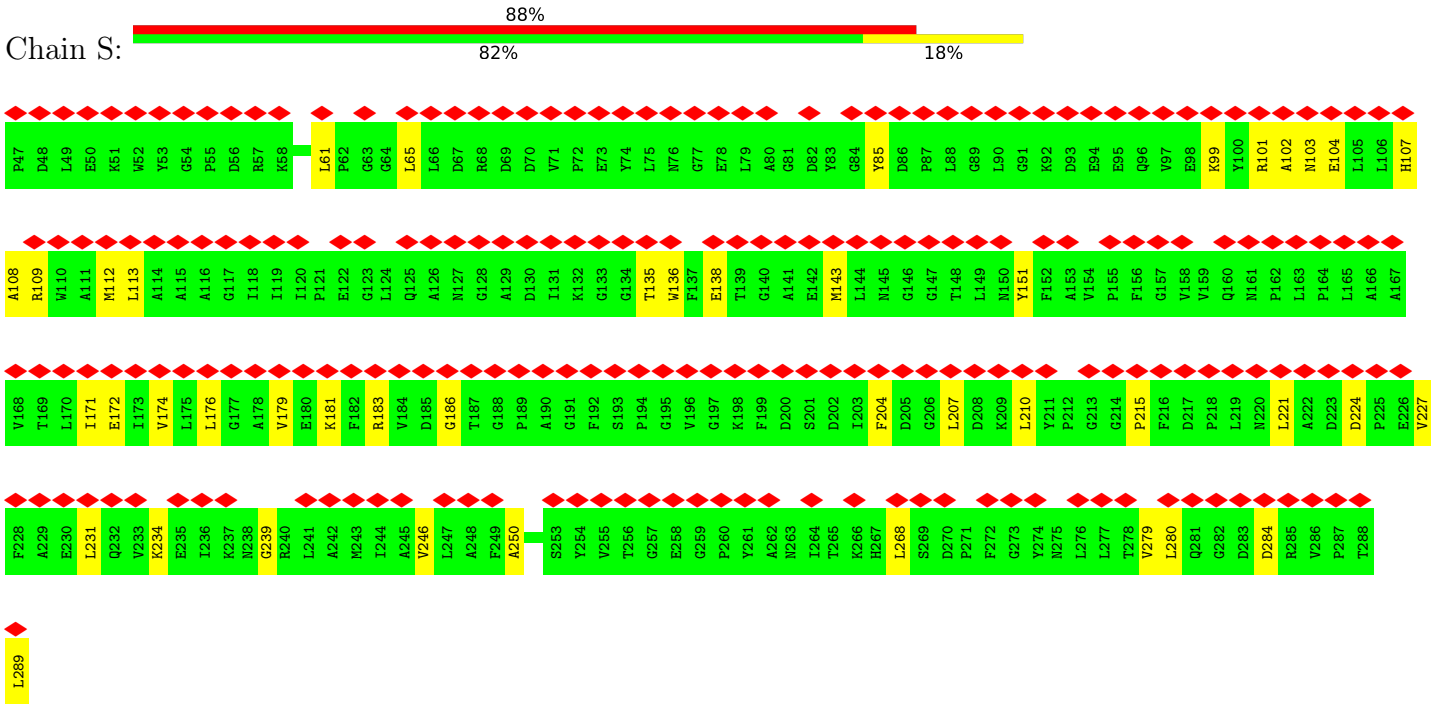
Chain r1:





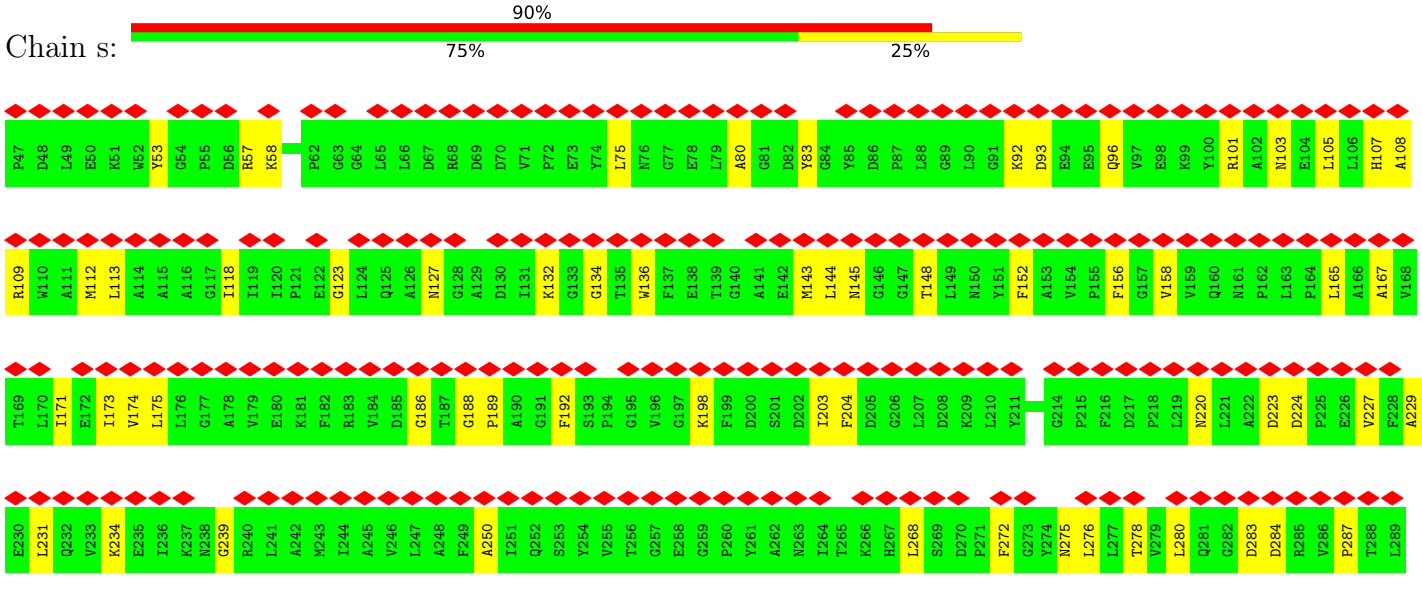
• Molecule 23: CP26

Chain S:



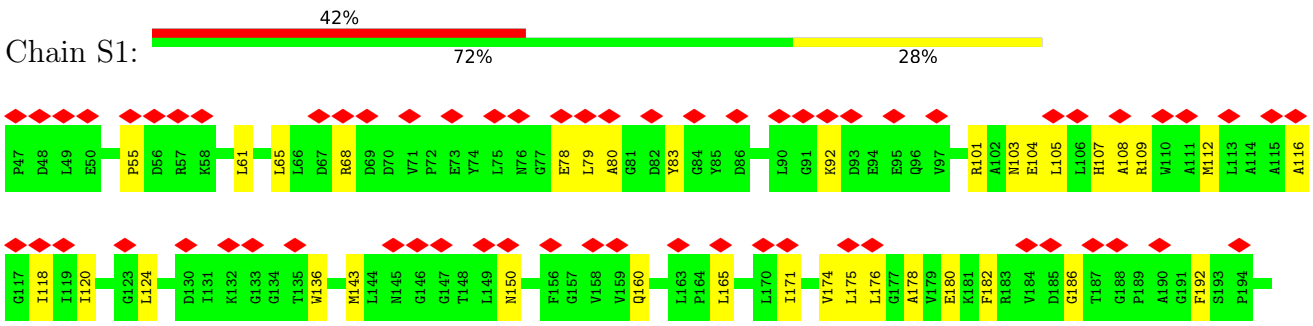
• Molecule 23: CP26

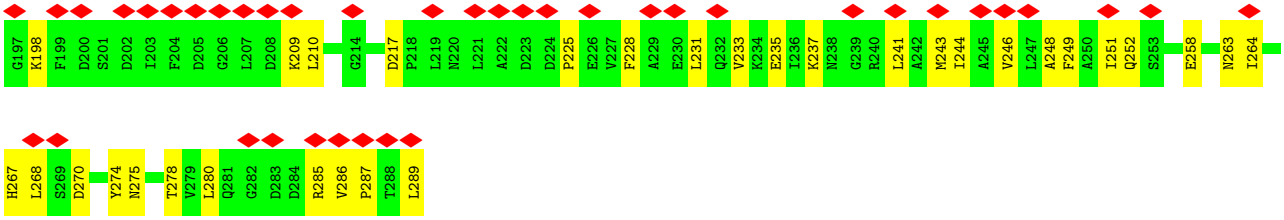
Chain s:



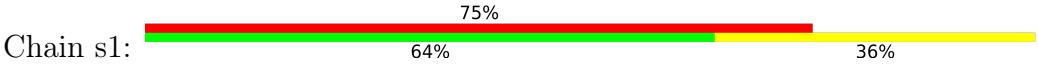
• Molecule 23: CP26

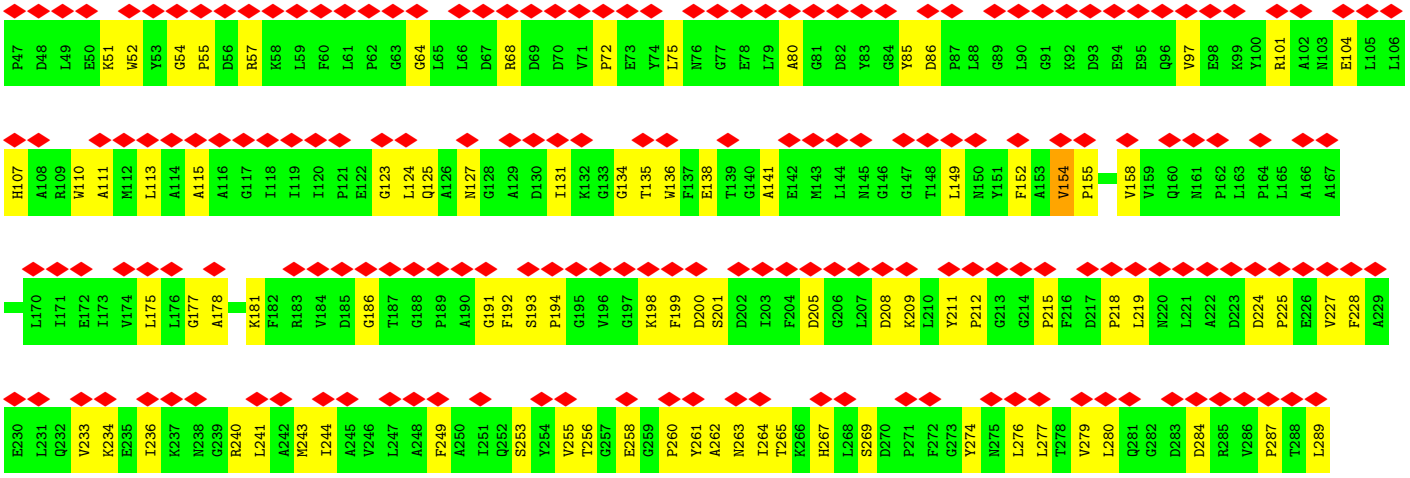
Chain S1:



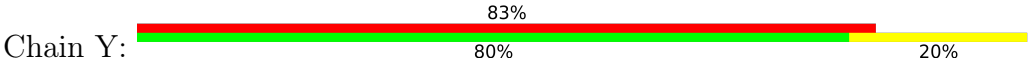


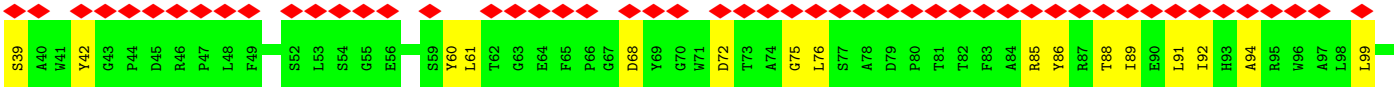
• Molecule 23: CP26

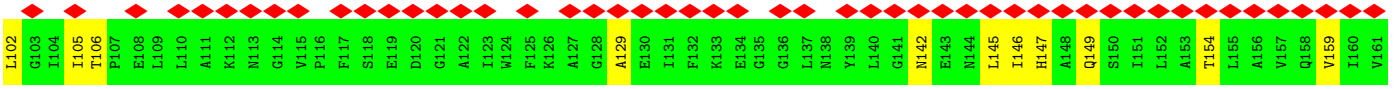


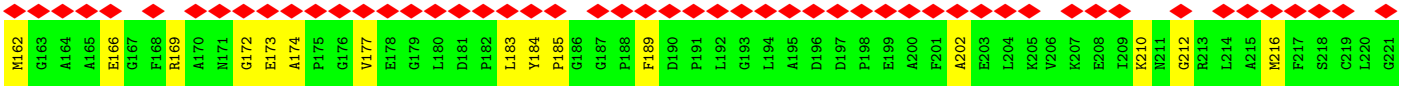


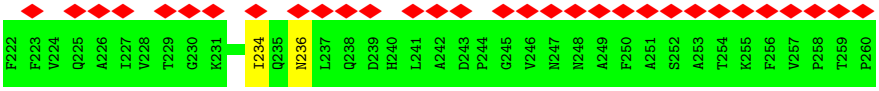
• Molecule 24: LHCII M1



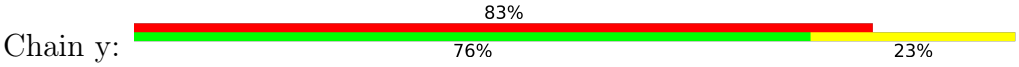


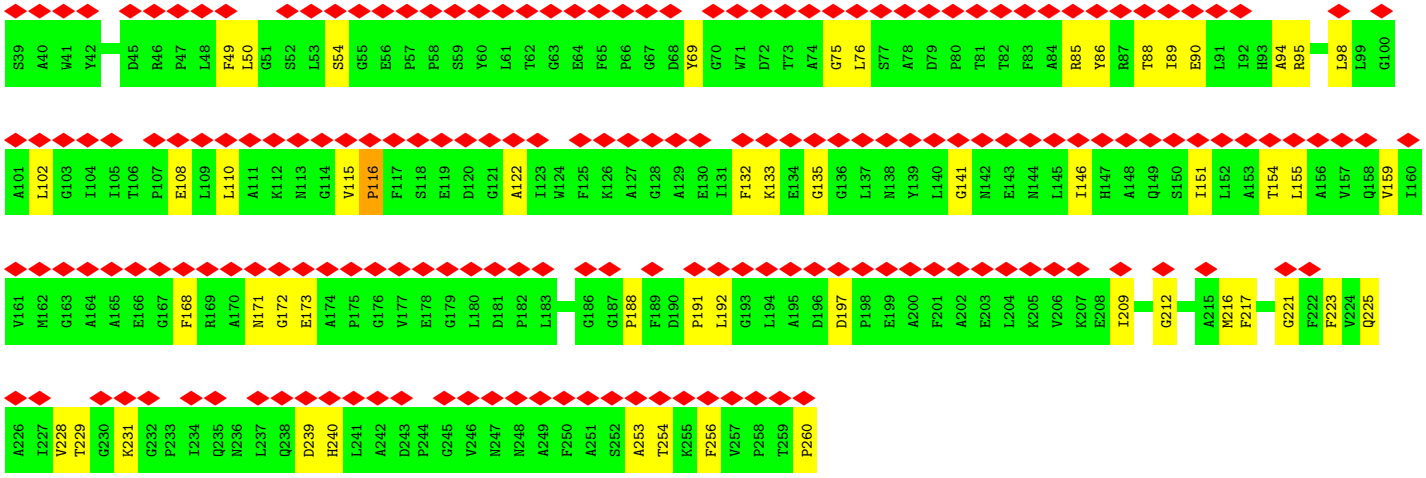






• Molecule 24: LHCII M1

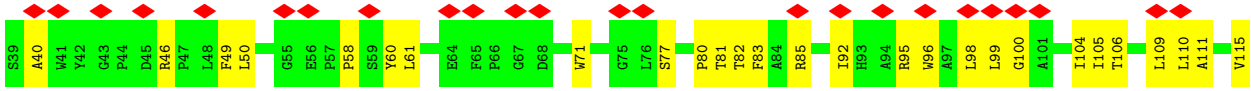


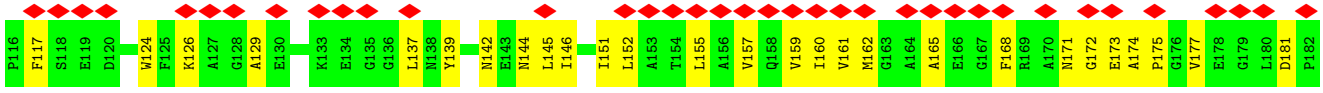


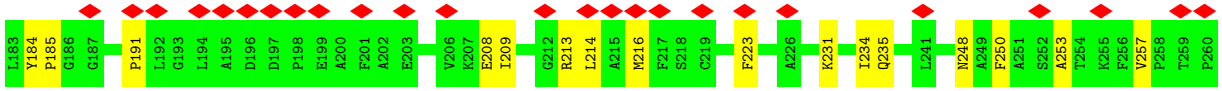
- Molecule 24: LHCII M1

Chain Y1:





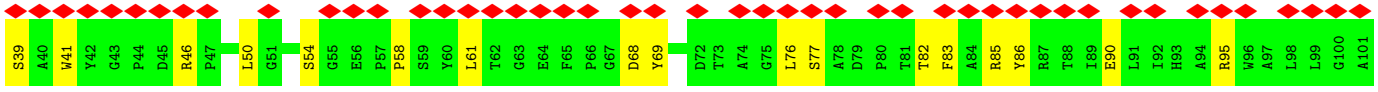


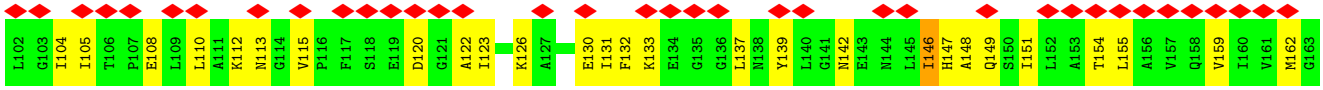


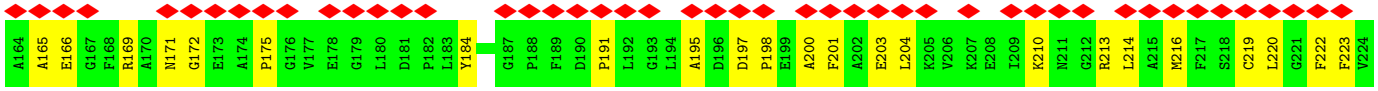
- Molecule 24: LHCII M1

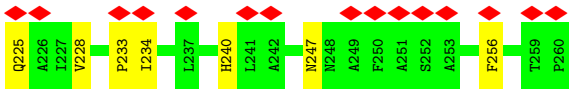
Chain y1:





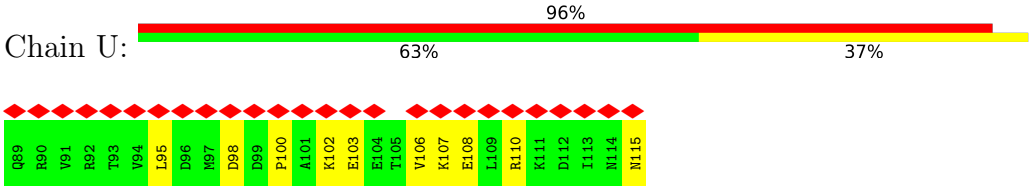






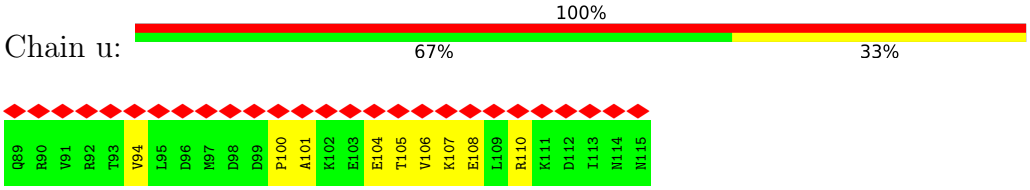
- Molecule 25: PsbU

Chain U:



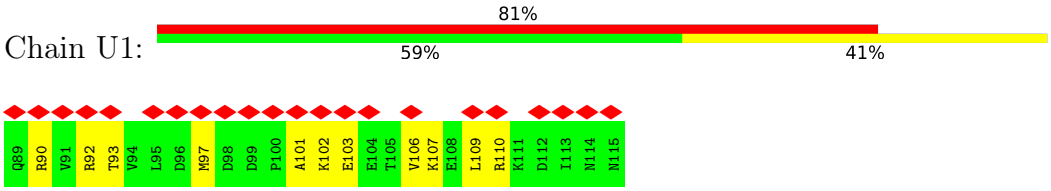
• Molecule 25: PsbU

Chain u:



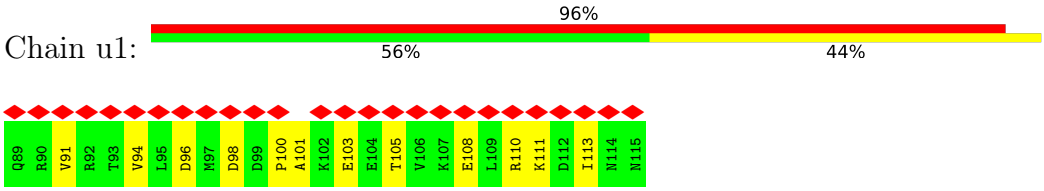
• Molecule 25: PsbU

Chain U1:



• Molecule 25: PsbU

Chain u1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	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: HEM, PL9, LUT, 3PH, LMK, RRX, XAT, SPH, ERG, LHG, BCT, CLA, LMT, SEP, CHL, DGD, OEX, PTY, FE2, 4RF, SQD, PHO, CL, GOL, LMG, NEX, BCR, LPX, C7Z, NA, DGA

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	0.34	0/2723	0.57	0/3715
1	A1	0.27	0/2723	0.61	2/3715 (0.1%)
1	a	0.34	0/2723	0.57	0/3715
1	a1	0.28	0/2723	0.65	2/3715 (0.1%)
2	B	0.31	0/3912	0.59	2/5327 (0.0%)
2	B1	0.27	0/3912	0.60	2/5327 (0.0%)
2	b	0.31	0/3912	0.54	1/5327 (0.0%)
2	b1	0.25	0/3912	0.56	3/5327 (0.1%)
3	V	0.25	0/228	0.57	0/311
3	V1	0.19	0/228	0.47	0/311
3	v	0.24	0/228	0.55	0/311
3	v1	0.25	0/228	0.67	0/311
4	C	0.39	2/3602 (0.1%)	0.65	4/4913 (0.1%)
4	C1	0.26	0/3602	0.54	1/4913 (0.0%)
4	c	0.31	0/3602	0.51	0/4913
4	c1	0.32	2/3602 (0.1%)	0.66	4/4913 (0.1%)
5	D	0.36	0/2860	0.60	2/3899 (0.1%)
5	D1	0.28	0/2860	0.63	2/3899 (0.1%)
5	d	0.32	0/2860	0.57	0/3899
5	d1	0.29	0/2860	0.64	0/3899
6	E	0.26	0/639	0.60	0/870
6	E1	0.26	0/639	0.63	0/870
6	e	0.50	1/639 (0.2%)	0.84	3/870 (0.3%)
6	e1	0.23	0/639	0.62	0/870
7	F	0.29	0/259	0.56	0/351
7	F1	0.26	0/259	0.58	0/351
7	f	0.37	0/259	0.71	0/351
7	f1	0.26	0/259	0.71	0/351
8	H	0.34	0/513	0.68	0/703
8	H1	0.25	0/513	0.57	0/703
8	h	0.30	0/513	0.58	0/703

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
8	h1	0.24	0/513	0.57	0/703
9	I	0.35	0/287	0.52	0/386
9	I1	0.24	0/287	0.57	0/386
9	i	0.30	0/287	0.55	0/386
9	i1	0.26	0/287	0.63	0/386
10	J	0.24	0/272	0.46	0/369
10	J1	0.21	0/272	0.55	0/369
10	j	0.27	0/272	0.56	0/369
10	j1	0.21	0/272	0.59	0/369
11	K	0.36	0/308	0.73	0/423
11	K1	0.28	0/308	0.64	0/423
11	k	0.33	0/308	0.58	0/423
11	k1	0.32	0/308	0.70	0/423
12	L	0.27	0/321	0.46	0/435
12	L1	0.35	0/321	0.68	0/435
12	l	0.33	0/321	0.59	0/435
13	M	0.30	0/237	0.53	0/323
13	M1	0.23	0/237	0.57	0/323
13	m	0.35	0/237	0.78	1/323 (0.3%)
13	m1	0.26	0/237	0.60	0/323
14	O	0.28	0/1855	0.63	0/2505
14	O1	0.27	0/1855	0.62	0/2505
14	o	0.28	0/1855	0.58	0/2505
14	o1	0.43	1/1855 (0.1%)	0.78	4/2505 (0.2%)
15	P	0.21	0/1473	0.56	2/1988 (0.1%)
15	P1	0.21	0/1473	0.53	0/1988
15	p	0.23	0/1473	0.53	0/1988
15	p1	0.27	0/1473	0.58	0/1988
16	T	0.29	0/254	0.60	0/342
16	T1	0.32	0/254	0.65	0/342
16	t	0.26	0/254	0.42	0/342
16	t1	0.24	0/254	0.57	0/342
17	W	0.28	0/339	0.63	0/460
17	W1	0.26	0/339	0.54	0/460
17	w	0.27	0/339	0.53	0/460
17	w1	0.24	0/339	0.60	0/460
18	X	0.26	0/202	0.55	0/276
18	X1	0.24	0/202	0.52	0/276
18	x	0.28	0/202	0.62	0/276
18	x1	0.22	0/202	0.55	0/276
19	Z	0.23	0/469	0.45	0/641
19	Z1	0.22	0/469	0.59	1/641 (0.2%)
19	z	0.24	0/469	0.45	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	z1	0.19	0/469	0.49	0/641
20	N	0.28	0/1751	0.56	0/2386
20	N1	0.25	0/1751	0.54	0/2386
20	n	0.29	0/1750	0.55	0/2382
20	n1	0.39	2/1750 (0.1%)	0.71	5/2382 (0.2%)
21	G	0.26	0/1725	0.58	0/2348
21	G1	0.28	0/1725	0.61	2/2348 (0.1%)
21	g	0.27	0/1725	0.60	0/2348
21	g1	0.25	0/1725	0.58	0/2348
22	R	0.26	0/1506	0.56	0/2035
22	R1	0.21	0/1506	0.50	0/2035
22	r	0.24	0/1506	0.56	0/2035
22	r1	0.24	0/1506	0.59	0/2035
23	S	0.28	0/1903	0.60	0/2590
23	S1	0.25	0/1903	0.59	0/2590
23	s	0.28	0/1903	0.63	0/2590
23	s1	0.34	1/1903 (0.1%)	0.71	3/2590 (0.1%)
24	Y	0.30	0/1715	0.51	0/2338
24	Y1	0.26	0/1715	0.58	0/2338
24	y	0.29	0/1715	0.53	1/2338 (0.0%)
24	y1	0.23	0/1715	0.53	0/2338
25	U	0.32	0/224	0.63	0/298
25	U1	0.33	0/224	0.62	0/298
25	u	0.33	0/224	0.67	0/298
25	u1	0.30	0/224	0.67	0/298
All	All	0.29	9/117985 (0.0%)	0.59	47/160485 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	A1	0	1
2	B1	0	1
All	All	0	3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	o1	111	PRO	CG-CD	-13.88	1.03	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	65	PRO	CG-CD	-12.67	1.07	1.50
6	e	28	PRO	CG-CD	-10.34	1.15	1.50
4	c1	352	PRO	CG-CD	-8.86	1.20	1.50
20	n1	57	PRO	CG-CD	-8.42	1.22	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	65	PRO	N-CD-CG	-18.59	75.32	103.20
14	o1	111	PRO	N-CD-CG	-18.29	75.77	103.20
23	s1	155	PRO	N-CD-CG	-12.66	88.60	103.80
6	e	28	PRO	N-CD-CG	-12.50	84.44	103.20
20	n1	57	PRO	N-CD-CG	-12.30	84.74	103.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ARG	Sidechain
1	A1	131	TRP	Peptide
2	B1	384	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2638	0	2541	95	0
1	A1	2638	0	2541	120	0
1	a	2638	0	2541	73	0
1	a1	2638	0	2541	128	0
2	B	3783	0	3663	99	0
2	B1	3783	0	3663	150	0
2	b	3783	0	3663	114	0
2	b1	3783	0	3663	137	0
3	V	227	0	261	4	0
3	V1	227	0	261	12	0
3	v	227	0	261	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	v1	227	0	261	10	0
4	C	3483	0	3376	76	0
4	C1	3483	0	3376	151	0
4	c	3483	0	3376	68	0
4	c1	3483	0	3376	154	0
5	D	2766	0	2654	61	0
5	D1	2766	0	2654	123	0
5	d	2766	0	2655	80	0
5	d1	2766	0	2655	149	0
6	E	621	0	605	25	0
6	E1	621	0	605	20	0
6	e	621	0	605	17	0
6	e1	621	0	605	23	0
7	F	252	0	265	9	0
7	F1	252	0	265	11	0
7	f	252	0	265	16	0
7	f1	252	0	265	13	0
8	H	503	0	532	18	0
8	H1	503	0	532	25	0
8	h	503	0	532	13	0
8	h1	503	0	532	23	0
9	I	279	0	288	7	0
9	I1	279	0	288	18	0
9	i	279	0	288	3	0
9	i1	279	0	288	12	0
10	J	266	0	286	6	0
10	J1	266	0	286	8	0
10	j	266	0	286	3	0
10	j1	266	0	286	15	0
11	K	297	0	312	7	0
11	K1	297	0	312	14	0
11	k	297	0	312	5	0
11	k1	297	0	312	16	0
12	L	313	0	325	8	0
12	L1	313	0	325	12	0
12	l	313	0	325	10	0
13	M	234	0	258	6	0
13	M1	234	0	258	9	0
13	m	234	0	258	8	0
13	m1	234	0	258	7	0
14	O	1820	0	1776	42	0
14	O1	1820	0	1776	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	o	1820	0	1776	34	0
14	o1	1820	0	1776	50	0
15	P	1444	0	1403	32	0
15	P1	1444	0	1403	33	0
15	p	1444	0	1403	40	0
15	p1	1444	0	1403	40	0
16	T	247	0	260	2	0
16	T1	247	0	260	15	0
16	t	247	0	260	12	0
16	t1	247	0	260	7	0
17	W	332	0	323	7	0
17	W1	332	0	323	21	0
17	w	332	0	323	11	0
17	w1	332	0	323	18	0
18	X	201	0	224	2	0
18	X1	201	0	224	7	0
18	x	201	0	224	6	0
18	x1	201	0	224	5	0
19	Z	457	0	478	5	0
19	Z1	457	0	478	10	0
19	z	457	0	478	6	0
19	z1	457	0	478	11	0
20	N	1703	0	1641	46	0
20	N1	1703	0	1641	72	0
20	n	1703	0	1641	43	0
20	n1	1703	0	1641	69	0
21	G	1680	0	1614	45	0
21	G1	1680	0	1613	52	0
21	g	1680	0	1614	53	0
21	g1	1680	0	1614	43	0
22	R	1490	0	1454	32	0
22	R1	1490	0	1454	31	0
22	r	1490	0	1454	31	0
22	r1	1490	0	1454	54	0
23	S	1856	0	1816	31	0
23	S1	1856	0	1816	61	0
23	s	1856	0	1816	45	0
23	s1	1856	0	1816	65	0
24	Y	1667	0	1624	44	0
24	Y1	1667	0	1624	62	0
24	y	1667	0	1624	45	0
24	y1	1667	0	1624	70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	U	224	0	226	11	0
25	U1	224	0	226	11	0
25	u	224	0	226	7	0
25	u1	224	0	226	13	0
26	A	10	0	0	1	0
26	A1	10	0	0	0	0
26	a	10	0	0	0	0
26	a1	10	0	0	1	0
27	A	1	0	0	0	0
27	A1	1	0	0	0	0
27	a	1	0	0	0	0
27	a1	1	0	0	0	0
28	A	2	0	0	1	0
28	A1	2	0	0	1	0
28	a	2	0	0	1	0
28	a1	2	0	0	1	0
29	A	240	0	242	17	0
29	A1	240	0	240	18	0
29	B	1040	0	1149	71	0
29	B1	1040	0	1147	93	0
29	C	845	0	933	55	0
29	C1	845	0	930	67	0
29	D	130	0	144	10	0
29	D1	130	0	143	10	0
29	G	466	0	467	24	0
29	G1	466	0	467	35	0
29	N	468	0	469	27	0
29	N1	468	0	468	43	0
29	R	409	0	391	19	0
29	R1	409	0	391	26	0
29	S	625	0	588	21	0
29	S1	625	0	586	25	0
29	Y	570	0	613	51	0
29	Y1	570	0	612	48	0
29	a	239	0	242	14	0
29	a1	239	0	241	29	0
29	b	1040	0	1151	62	0
29	b1	1040	0	1146	80	0
29	c	845	0	934	43	0
29	c1	845	0	931	69	0
29	d	130	0	143	8	0
29	d1	130	0	143	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	g	466	0	468	20	0
29	g1	466	0	465	36	0
29	n	468	0	468	21	0
29	n1	468	0	469	38	0
29	r	409	0	392	18	0
29	r1	409	0	390	23	0
29	s	625	0	588	22	0
29	s1	625	0	586	34	0
29	y	570	0	614	38	0
29	y1	570	0	612	51	0
30	A	128	0	148	11	0
30	A1	128	0	148	13	0
30	a	128	0	148	7	0
30	a1	128	0	148	20	0
31	A	40	0	53	2	0
31	A1	40	0	53	4	0
31	B	80	0	106	3	0
31	B1	80	0	105	2	0
31	C	160	0	210	16	0
31	C1	160	0	209	22	0
31	D	40	0	53	3	0
31	D1	40	0	53	4	0
31	a	40	0	53	3	0
31	a1	40	0	53	4	0
31	b	80	0	106	6	0
31	b1	80	0	106	6	0
31	c	160	0	211	12	0
31	c1	160	0	211	30	0
31	d	40	0	53	3	0
31	d1	40	0	53	3	0
32	A	51	0	68	5	0
32	A1	51	0	68	6	0
32	B	96	0	124	6	0
32	B1	96	0	124	6	0
32	C	54	0	77	4	0
32	C1	54	0	77	3	0
32	M	42	0	47	4	0
32	M1	42	0	47	4	0
32	a	51	0	68	2	0
32	a1	51	0	68	3	0
32	b	96	0	124	7	0
32	b1	96	0	124	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	c	54	0	77	0	0
32	c1	54	0	77	4	0
32	m	42	0	47	6	0
32	m1	42	0	47	3	0
33	A	48	0	66	3	0
33	A1	48	0	66	10	0
33	B	44	0	58	2	0
33	B1	44	0	58	5	0
33	C	106	0	158	7	0
33	C1	106	0	158	13	0
33	D	46	0	62	2	0
33	D1	46	0	62	2	0
33	H	48	0	66	2	0
33	H1	48	0	66	15	0
33	W	39	0	48	2	0
33	W1	39	0	48	8	0
33	a	48	0	66	5	0
33	a1	48	0	66	8	0
33	b	44	0	58	5	0
33	b1	44	0	58	5	0
33	c	106	0	158	12	0
33	c1	106	0	158	7	0
33	d	46	0	62	2	0
33	d1	46	0	62	2	0
33	h	48	0	66	5	0
33	h1	48	0	66	4	0
33	w	39	0	48	6	0
33	w1	39	0	48	4	0
34	A	21	0	37	1	0
34	A1	21	0	37	4	0
34	Y	21	0	37	4	0
34	Y1	21	0	37	7	0
34	a	21	0	37	3	0
34	a1	21	0	37	1	0
34	y	21	0	37	4	0
34	y1	21	0	37	2	0
35	A	1	0	0	0	0
35	A1	1	0	0	0	0
35	a	1	0	0	0	0
35	a1	1	0	0	0	0
36	B	42	0	0	0	0
36	B1	42	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	b	42	0	0	0	0
36	b1	42	0	0	0	0
37	B	43	0	44	3	0
37	B1	43	0	44	2	0
37	C	176	0	226	13	0
37	C1	176	0	226	31	0
37	b	43	0	44	3	0
37	b1	43	0	44	4	0
37	c	176	0	226	10	0
37	c1	176	0	226	26	0
38	B	48	0	75	7	0
38	B1	48	0	75	6	0
38	S	48	0	75	7	0
38	S1	48	0	75	4	0
38	T	48	0	75	2	0
38	T1	48	0	75	8	0
38	b	48	0	75	6	0
38	b1	48	0	75	8	0
38	s	48	0	75	6	0
38	s1	48	0	75	5	0
38	t	48	0	75	2	0
38	t1	48	0	75	5	0
39	B	44	0	76	1	0
39	B1	44	0	76	1	0
39	C	44	0	76	3	0
39	C1	44	0	76	6	0
39	J	29	0	40	2	0
39	J1	29	0	40	4	0
39	b	44	0	76	5	0
39	b1	44	0	76	4	0
39	c	44	0	76	9	0
39	c1	44	0	76	4	0
39	j	29	0	40	3	0
39	j1	29	0	40	4	0
40	C	47	0	67	7	0
40	C1	47	0	67	8	0
40	D	132	0	183	11	0
40	D1	132	0	183	12	0
40	G	49	0	74	4	0
40	G1	49	0	74	6	0
40	L	49	0	74	5	0
40	L1	49	0	74	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	N	49	0	74	4	0
40	N1	49	0	74	5	0
40	S	45	0	63	5	0
40	S1	45	0	63	5	0
40	Y	49	0	74	6	0
40	Y1	49	0	74	6	0
40	c	47	0	67	4	0
40	c1	47	0	67	11	0
40	d	132	0	183	12	0
40	d1	132	0	183	17	0
40	g	49	0	74	7	0
40	g1	49	0	74	7	0
40	l	49	0	74	4	0
40	n	49	0	74	3	0
40	n1	49	0	74	10	0
40	s	45	0	63	4	0
40	s1	45	0	63	7	0
40	y	49	0	74	5	0
40	y1	49	0	74	6	0
41	C	40	0	0	0	0
41	C1	40	0	0	0	0
41	c	40	0	0	0	0
41	c1	40	0	0	0	0
42	D	4	0	0	0	0
42	D1	4	0	0	1	0
42	d	4	0	0	0	0
42	d1	4	0	1	0	0
43	D	55	0	80	4	0
43	D1	55	0	80	11	0
43	d	55	0	80	7	0
43	d1	55	0	80	8	0
44	F	43	0	30	3	0
44	F1	43	0	30	3	0
44	f	43	0	30	1	0
44	f1	43	0	30	3	0
45	H	41	0	56	1	0
45	H1	41	0	56	3	0
45	h	41	0	56	3	0
45	h1	41	0	56	4	0
46	I	6	0	8	0	0
46	I1	6	0	8	0	0
47	I	57	0	98	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	I1	57	0	98	9	0
47	K	57	0	98	2	0
47	K1	57	0	98	5	0
47	i	57	0	98	6	0
47	i1	57	0	98	2	0
47	k	57	0	98	2	0
47	k1	57	0	98	2	0
48	G	340	0	306	18	0
48	G1	340	0	306	19	0
48	N	380	0	383	18	0
48	N1	380	0	383	37	0
48	R	94	0	67	4	0
48	R1	94	0	67	3	0
48	S	194	0	144	9	0
48	S1	194	0	144	12	0
48	Y	310	0	307	7	0
48	Y1	310	0	308	21	0
48	g	340	0	306	15	0
48	g1	340	0	306	19	0
48	n	380	0	385	18	0
48	n1	380	0	383	29	0
48	r	94	0	66	3	0
48	r1	94	0	67	6	0
48	s	194	0	146	9	0
48	s1	194	0	146	14	0
48	y	310	0	308	7	0
48	y1	310	0	308	15	0
49	G	84	0	110	13	0
49	G1	84	0	110	16	0
49	N	84	0	110	8	0
49	N1	84	0	110	12	0
49	R	42	0	55	6	0
49	R1	42	0	55	4	0
49	S	84	0	110	7	0
49	S1	84	0	110	13	0
49	Y	84	0	110	8	0
49	Y1	84	0	110	14	0
49	g	84	0	110	13	0
49	g1	84	0	110	22	0
49	n	84	0	110	5	0
49	n1	84	0	110	14	0
49	r	42	0	55	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	r1	42	0	55	7	0
49	s	84	0	110	4	0
49	s1	84	0	110	10	0
49	y	84	0	110	5	0
49	y1	84	0	110	13	0
50	G	44	0	56	6	0
50	G1	44	0	56	10	0
50	N	44	0	56	5	0
50	N1	44	0	56	9	0
50	R	44	0	56	4	0
50	R1	44	0	56	5	0
50	Y	44	0	56	6	0
50	Y1	44	0	56	4	0
50	g	44	0	56	9	0
50	g1	44	0	56	6	0
50	n	44	0	56	6	0
50	n1	44	0	56	5	0
50	r	44	0	56	2	0
50	r1	44	0	56	5	0
50	y	44	0	56	4	0
50	y1	44	0	56	9	0
51	G	44	0	54	0	0
51	G1	44	0	54	0	0
51	N	44	0	54	3	0
51	N1	44	0	55	6	0
51	R	44	0	54	2	0
51	R1	44	0	54	4	0
51	S	44	0	54	0	0
51	S1	44	0	55	4	0
51	Y	44	0	54	2	0
51	Y1	44	0	54	3	0
51	g	44	0	54	1	0
51	g1	44	0	54	0	0
51	n	44	0	54	3	0
51	n1	44	0	54	6	0
51	r	44	0	54	3	0
51	r1	44	0	54	5	0
51	s	44	0	54	3	0
51	s1	44	0	56	6	0
51	y	44	0	54	1	0
51	y1	44	0	55	2	0
52	R	35	0	44	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	R1	35	0	45	7	0
52	r	35	0	44	4	0
52	r1	35	0	45	2	0
53	R	29	0	38	7	0
53	R1	29	0	38	9	0
53	r	29	0	38	7	0
53	r1	29	0	38	5	0
54	S	30	0	43	4	0
54	S1	30	0	43	2	0
54	s	30	0	43	3	0
54	s1	30	0	43	3	0
55	Y	69	0	90	5	0
55	Y1	69	0	90	3	0
55	y	69	0	90	9	0
55	y1	69	0	90	9	0
All	All	152240	0	154365	4580	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 15.

The worst 5 of 4580 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:r:626:ERG:O1	53:r:626:ERG:C3	1.70	1.38
53:r1:626:ERG:O1	53:r1:626:ERG:C3	1.70	1.37
53:R:626:ERG:O1	53:R:626:ERG:C3	1.70	1.36
53:R1:626:ERG:O1	53:R1:626:ERG:C3	1.70	1.35
24:y1:76:LEU:CD1	29:y1:602:CLA:H42	1.79	1.10

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	335/336 (100%)	321 (96%)	14 (4%)	0	100	100
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a	335/336 (100%)	318 (95%)	17 (5%)	0	100	100
1	a1	335/336 (100%)	314 (94%)	21 (6%)	0	100	100
2	B	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	B1	482/484 (100%)	447 (93%)	35 (7%)	0	100	100
2	b	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	b1	482/484 (100%)	454 (94%)	28 (6%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	V1	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	30 (100%)	0	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	430 (96%)	17 (4%)	0	100	100
4	C1	447/449 (100%)	421 (94%)	26 (6%)	0	100	100
4	c	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
4	c1	447/449 (100%)	421 (94%)	25 (6%)	1 (0%)	43	72
5	D	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
5	D1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
5	d	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
5	d1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
6	E	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	E1	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	e	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	e1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	H1	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	29 (88%)	4 (12%)	0	100	100
9	i1	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
10	j1	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	K1	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k1	35/37 (95%)	35 (100%)	0	0	100	100
12	L	36/38 (95%)	36 (100%)	0	0	100	100
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	29 (100%)	0	0	100	100
13	M1	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	215 (91%)	19 (8%)	2 (1%)	16	49
14	O1	236/238 (99%)	212 (90%)	23 (10%)	1 (0%)	30	61
14	o	236/238 (99%)	218 (92%)	17 (7%)	1 (0%)	30	61
14	o1	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	30	61
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	170 (92%)	15 (8%)	0	100	100
15	p1	185/187 (99%)	169 (91%)	16 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	2	22
16	T1	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	2	22
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	t1	28/30 (93%)	27 (96%)	1 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	W	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
17	W1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	Z1	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
19	z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
20	N	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	14	46
20	N1	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	14	46
20	n	218/222 (98%)	199 (91%)	17 (8%)	2 (1%)	14	46
20	n1	218/222 (98%)	202 (93%)	14 (6%)	2 (1%)	14	46
21	G	219/221 (99%)	196 (90%)	23 (10%)	0	100	100
21	G1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
21	g	219/221 (99%)	197 (90%)	22 (10%)	0	100	100
21	g1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
22	R	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	R1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
22	r	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	r1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
23	S	241/243 (99%)	219 (91%)	21 (9%)	1 (0%)	30	61
23	S1	241/243 (99%)	208 (86%)	32 (13%)	1 (0%)	30	61
23	s	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	16	49
23	s1	241/243 (99%)	214 (89%)	26 (11%)	1 (0%)	30	61
24	Y	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	24	57
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	24	57
24	y	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
24	y1	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24 57
25	U	25/27 (93%)	23 (92%)	2 (8%)	0	100 100
25	U1	25/27 (93%)	24 (96%)	1 (4%)	0	100 100
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100 100
25	u1	25/27 (93%)	25 (100%)	0	0	100 100
All	All	14636/14846 (99%)	13696 (94%)	915 (6%)	25 (0%)	44 72

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
20	n	192	LEU
23	s	284	ASP

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	276/275 (100%)	276 (100%)	0	100 100
1	A1	276/275 (100%)	276 (100%)	0	100 100
1	a	276/275 (100%)	276 (100%)	0	100 100
1	a1	276/275 (100%)	276 (100%)	0	100 100
2	B	388/388 (100%)	388 (100%)	0	100 100
2	B1	388/388 (100%)	388 (100%)	0	100 100
2	b	388/388 (100%)	388 (100%)	0	100 100
2	b1	388/388 (100%)	387 (100%)	1 (0%)	86 83
3	V	25/25 (100%)	25 (100%)	0	100 100
3	V1	25/25 (100%)	25 (100%)	0	100 100
3	v	25/25 (100%)	25 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	v1	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	C1	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	279 (100%)	0	100	100
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
5	d1	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
9	i1	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	K1	33/33 (100%)	33 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k	33/33 (100%)	33 (100%)	0	100	100
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	M1	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
13	m1	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	O1	195/195 (100%)	194 (100%)	1 (0%)	81	80
14	o	195/195 (100%)	195 (100%)	0	100	100
14	o1	195/195 (100%)	194 (100%)	1 (0%)	81	80
15	P	151/151 (100%)	151 (100%)	0	100	100
15	P1	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
15	p1	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z	50/50 (100%)	50 (100%)	0	100	100
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	170 (99%)	1 (1%)	78	79
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	R1	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
22	r1	151/151 (100%)	151 (100%)	0	100	100
23	S	190/190 (100%)	190 (100%)	0	100	100
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
23	s1	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
25	u1	26/26 (100%)	26 (100%)	0	100	100
All	All	11841/11837 (100%)	11837 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	n	46	ASN
14	O1	138	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b1	425	GLN
14	o1	138	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
8	h1	79	ASN
18	x1	71	ASN
17	w	100	GLN
15	p	140	GLN
20	n1	245	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
22	SEP	R	84	22	8,9,10	1.58	1 (12%)	8,12,14	1.40	2 (25%)
22	SEP	R1	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.71	2 (25%)
22	SEP	r	84	22	8,9,10	1.51	1 (12%)	8,12,14	1.39	2 (25%)
22	SEP	r1	84	22	8,9,10	1.53	1 (12%)	8,12,14	1.69	2 (25%)

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
22	SEP	R	84	22	-	2/5/8/10	-
22	SEP	R1	84	22	-	4/5/8/10	-
22	SEP	r	84	22	-	2/5/8/10	-
22	SEP	r1	84	22	-	5/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.37	1.61	1.50
22	r1	84	SEP	P-O1P	3.30	1.61	1.50
22	R1	84	SEP	P-O1P	3.29	1.61	1.50
22	r	84	SEP	P-O1P	3.22	1.60	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r1	84	SEP	P-OG-CB	-3.36	109.03	118.30
22	R1	84	SEP	OG-CB-CA	3.23	111.29	108.14
22	R1	84	SEP	P-OG-CB	-3.07	109.85	118.30
22	r1	84	SEP	OG-CB-CA	2.79	110.86	108.14
22	r	84	SEP	P-OG-CB	-2.56	111.25	118.30

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	R1	84	SEP	N-CA-CB-OG
22	R1	84	SEP	CB-OG-P-O2P
22	R1	84	SEP	CB-OG-P-O3P
22	r1	84	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	84	SEP	1	0
22	r	84	SEP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 721 ligands modelled in this entry, 16 are monoatomic - leaving 705 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	y	612	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	19 (22%)
40	LHG	L1	101	-	48,48,48	0.37	0	51,54,54	1.11	3 (5%)
29	CLA	C1	505	4	69,73,73	1.37	7 (10%)	83,113,113	1.91	18 (21%)
29	CLA	S1	602	23	64,68,73	1.40	8 (12%)	77,107,113	2.06	18 (23%)
46	GOL	I1	101	-	5,5,5	0.56	0	5,5,5	0.31	0
49	LUT	y	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.98	14 (27%)
39	DGA	J1	101	-	28,28,43	1.27	2 (7%)	30,30,45	1.34	2 (6%)
49	LUT	y1	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.97	10 (19%)
29	CLA	B	617	2	69,73,73	1.37	7 (10%)	83,113,113	1.98	16 (19%)
29	CLA	s	617	-	54,58,73	1.55	7 (12%)	65,95,113	2.25	18 (27%)
29	CLA	c	507	-	69,73,73	1.39	7 (10%)	83,113,113	1.98	18 (21%)
32	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.92	2 (3%)
48	CHL	n1	608	-	54,58,74	0.92	2 (3%)	59,94,114	1.31	9 (15%)
29	CLA	c	501	4	69,73,73	1.35	7 (10%)	83,113,113	2.01	18 (21%)
29	CLA	y	610	24	69,73,73	1.35	7 (10%)	83,113,113	1.97	18 (21%)
34	SPH	y	625	-	19,20,20	0.61	0	18,21,21	1.21	2 (11%)
50	XAT	g1	622	-	39,47,47	0.75	1 (2%)	54,74,74	1.88	16 (29%)
55	PTY	y1	627	-	18,18,49	1.27	2 (11%)	21,23,54	1.45	2 (9%)
40	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.10	2 (4%)
55	PTY	y1	626	-	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)
29	CLA	B	603	2	69,73,73	1.37	8 (11%)	83,113,113	1.91	19 (22%)
29	CLA	b	602	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	g	614	-	53,57,73	1.57	8 (15%)	62,93,113	2.15	17 (27%)
29	CLA	a	406	-	69,73,73	1.36	7 (10%)	83,113,113	2.15	19 (22%)
29	CLA	d1	402	-	69,73,73	1.40	8 (11%)	83,113,113	1.91	19 (22%)
29	CLA	C1	508	4	69,73,73	1.40	8 (11%)	83,113,113	1.81	15 (18%)
26	OEX	A1	401	1,4	0,14,14	-	-	-		
33	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.19	4 (7%)
29	CLA	B1	609	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	16 (19%)
31	BCR	C	515	-	41,41,41	1.83	6 (14%)	56,56,56	4.20	16 (28%)
48	CHL	s	606	-	48,52,74	1.06	2 (4%)	53,87,114	1.39	7 (13%)
29	CLA	b1	613	-	69,73,73	1.38	7 (10%)	83,113,113	2.01	17 (20%)
49	LUT	R	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.03	17 (33%)
29	CLA	N	610	-	69,73,73	1.36	6 (8%)	83,113,113	2.03	20 (24%)
29	CLA	c	504	-	69,73,73	1.33	7 (10%)	83,113,113	1.99	18 (21%)
29	CLA	A1	406	-	69,73,73	1.40	7 (10%)	83,113,113	1.96	19 (22%)
29	CLA	Y1	611	-	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
29	CLA	r	603	-	64,68,73	1.45	7 (10%)	77,107,113	1.89	17 (22%)
38	3PH	s	626	-	47,47,47	0.87	3 (6%)	51,52,52	4.40	4 (7%)
50	XAT	G	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.11	15 (27%)
31	BCR	B1	619	-	41,41,41	1.82	4 (9%)	56,56,56	4.44	18 (32%)
32	SQD	b1	626	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
51	NEX	S	623	-	38,46,46	3.42	10 (26%)	50,70,70	1.71	12 (24%)
53	ERG	r	626	-	31,32,32	7.80	18 (58%)	47,50,50	3.01	16 (34%)
48	CHL	G1	601	21	70,74,74	0.84	2 (2%)	80,114,114	1.33	14 (17%)
40	LHG	g1	624	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
48	CHL	g1	609	-	70,74,74	0.85	2 (2%)	80,114,114	1.25	10 (12%)
29	CLA	r	608	-	64,68,73	1.42	9 (14%)	77,107,113	1.90	17 (22%)
29	CLA	B1	610	-	69,73,73	1.38	7 (10%)	83,113,113	1.84	14 (16%)
52	LMT	r	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.16	3 (6%)
29	CLA	g1	610	-	69,73,73	1.32	6 (8%)	83,113,113	2.19	20 (24%)
32	SQD	m	101	-	41,42,54	0.91	0	50,53,65	0.99	3 (6%)
29	CLA	C1	512	-	69,73,73	1.38	7 (10%)	83,113,113	1.97	22 (26%)
48	CHL	G1	605	21	52,56,74	0.91	2 (3%)	58,92,114	1.41	11 (18%)
33	LMG	b1	622	-	44,44,55	0.86	2 (4%)	52,52,63	1.17	3 (5%)
44	HEM	f1	101	7	50,50,50	1.59	7 (14%)	66,82,82	1.14	7 (10%)
48	CHL	Y1	609	-	70,74,74	0.79	2 (2%)	80,114,114	1.27	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	y1	604	-	69,73,73	1.34	6 (8%)	83,113,113	2.03	17 (20%)
29	CLA	s	604	-	59,63,73	1.48	6 (10%)	71,101,113	2.01	15 (21%)
47	4RF	K	101	-	56,56,56	1.08	3 (5%)	59,59,59	0.91	3 (5%)
40	LHG	d1	408	-	43,43,48	0.40	0	46,49,54	1.05	2 (4%)
29	CLA	b	616	2	69,73,73	1.35	7 (10%)	83,113,113	1.84	17 (20%)
31	BCR	d1	404	-	41,41,41	1.88	4 (9%)	56,56,56	4.27	22 (39%)
29	CLA	b1	614	-	69,73,73	1.38	9 (13%)	83,113,113	1.88	18 (21%)
29	CLA	C1	501	4	69,73,73	1.36	7 (10%)	83,113,113	2.08	21 (25%)
29	CLA	G	602	-	69,73,73	1.37	7 (10%)	83,113,113	2.01	20 (24%)
29	CLA	y	608	-	54,58,73	1.58	8 (14%)	65,95,113	2.16	17 (26%)
47	4RF	I1	102	-	56,56,56	1.06	4 (7%)	59,59,59	0.98	3 (5%)
29	CLA	a	410	1	64,68,73	1.41	8 (12%)	77,107,113	2.08	20 (25%)
29	CLA	g1	612	21	47,51,73	1.65	8 (17%)	56,86,113	2.21	15 (26%)
29	CLA	N	611	-	53,57,73	1.57	6 (11%)	62,93,113	2.15	17 (27%)
48	CHL	y1	607	-	70,74,74	0.78	2 (2%)	80,114,114	1.28	11 (13%)
29	CLA	n1	611	-	53,57,73	1.57	6 (11%)	62,93,113	2.20	17 (27%)
49	LUT	G1	620	-	42,43,43	2.26	1 (2%)	51,60,60	1.86	13 (25%)
37	DGD	C1	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.07	6 (8%)
51	NEX	S1	623	-	38,46,46	3.20	9 (23%)	50,70,70	1.79	10 (20%)
34	SPH	a1	414	-	19,20,20	0.73	1 (5%)	18,21,21	0.98	1 (5%)
29	CLA	N1	603	-	69,73,73	1.36	6 (8%)	83,113,113	2.06	23 (27%)
31	BCR	C	517	-	41,41,41	1.87	5 (12%)	56,56,56	4.32	18 (32%)
29	CLA	g1	602	-	69,73,73	1.38	8 (11%)	83,113,113	1.91	21 (25%)
50	XAT	Y1	622	-	39,47,47	0.69	1 (2%)	54,74,74	3.83	20 (37%)
29	CLA	A	407	-	54,58,73	1.55	8 (14%)	65,95,113	2.21	18 (27%)
31	BCR	c1	515	-	41,41,41	1.91	4 (9%)	56,56,56	4.38	13 (23%)
37	DGD	c	520	-	60,60,67	1.05	4 (6%)	74,74,81	1.03	3 (4%)
39	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
47	4RF	i1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.92	3 (5%)
49	LUT	S	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.10	19 (37%)
48	CHL	y	606	-	70,74,74	0.86	3 (4%)	80,114,114	1.24	11 (13%)
29	CLA	R	604	-	53,57,73	1.55	7 (13%)	62,93,113	2.22	16 (25%)
29	CLA	s	603	-	69,73,73	1.39	7 (10%)	83,113,113	1.98	19 (22%)
29	CLA	S	605	23	54,58,73	1.59	8 (14%)	65,95,113	2.32	17 (26%)
48	CHL	g	606	-	54,58,74	0.94	2 (3%)	59,94,114	1.53	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	XAT	n1	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.04	14 (25%)
44	HEM	F	101	6,7	50,50,50	1.34	7 (14%)	66,82,82	1.16	5 (7%)
48	CHL	G1	609	-	70,74,74	0.90	2 (2%)	80,114,114	1.22	11 (13%)
29	CLA	A1	410	-	64,68,73	1.40	7 (10%)	77,107,113	2.06	21 (27%)
50	XAT	r1	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.16	18 (33%)
37	DGD	C	520	-	60,60,67	1.06	6 (10%)	74,74,81	1.07	3 (4%)
41	LMK	c1	527	-	38,39,53	1.51	3 (7%)	41,46,60	1.24	2 (4%)
36	C7Z	b	620	-	43,43,43	5.32	27 (62%)	58,60,60	2.48	19 (32%)
55	PTY	y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.50	2 (9%)
29	CLA	s1	605	-	54,58,73	1.58	9 (16%)	65,95,113	2.20	20 (30%)
51	NEX	s	623	-	38,46,46	3.52	11 (28%)	50,70,70	2.12	14 (28%)
52	LMT	R1	625	-	36,36,36	1.27	8 (22%)	47,47,47	1.15	4 (8%)
49	LUT	S1	621	-	42,43,43	2.39	2 (4%)	51,60,60	1.99	19 (37%)
47	4RF	i	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.93	3 (5%)
48	CHL	N	608	-	54,58,74	0.99	3 (5%)	59,94,114	1.30	9 (15%)
31	BCR	b	619	-	41,41,41	1.83	5 (12%)	56,56,56	4.15	16 (28%)
29	CLA	c	513	-	69,73,73	1.41	8 (11%)	83,113,113	2.03	18 (21%)
29	CLA	B	604	-	69,73,73	1.39	6 (8%)	83,113,113	1.89	16 (19%)
29	CLA	R1	609	-	64,68,73	1.39	7 (10%)	77,107,113	4.35	21 (27%)
29	CLA	y1	614	-	69,73,73	1.38	8 (11%)	83,113,113	1.87	21 (25%)
33	LMG	B	622	-	44,44,55	0.86	3 (6%)	52,52,63	1.24	2 (3%)
29	CLA	Y1	610	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	18 (21%)
38	3PH	t	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.19	2 (3%)
54	LPX	s1	625	-	29,29,29	1.01	2 (6%)	31,33,33	1.05	2 (6%)
41	LMK	C	527	-	38,39,53	1.47	2 (5%)	41,46,60	1.56	4 (9%)
48	CHL	N	601	20	70,74,74	0.81	2 (2%)	80,114,114	1.36	11 (13%)
29	CLA	S1	609	-	64,68,73	1.40	7 (10%)	77,107,113	2.04	18 (23%)
29	CLA	C	506	-	69,73,73	1.41	7 (10%)	83,113,113	1.99	19 (22%)
29	CLA	C	512	-	69,73,73	1.38	6 (8%)	83,113,113	1.92	17 (20%)
40	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
29	CLA	y1	603	-	69,73,73	1.38	7 (10%)	83,113,113	1.90	18 (21%)
29	CLA	G1	602	-	69,73,73	1.42	6 (8%)	83,113,113	2.04	22 (26%)
30	PHO	a	408	-	58,69,69	2.01	12 (20%)	56,99,99	1.62	7 (12%)
37	DGD	c1	519	-	63,63,67	1.14	6 (9%)	77,77,81	1.04	3 (3%)
51	NEX	G	623	-	38,46,46	3.37	11 (28%)	50,70,70	1.92	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	CHL	N	605	20	70,74,74	0.87	3 (4%)	80,114,114	1.27	12 (15%)
48	CHL	g1	608	-	48,52,74	0.97	2 (4%)	53,87,114	1.39	8 (15%)
33	LMG	C1	523	-	55,55,55	1.12	6 (10%)	63,63,63	1.15	6 (9%)
43	PL9	d	405	-	55,55,55	1.75	10 (18%)	68,69,69	1.54	11 (16%)
29	CLA	s1	602	-	64,68,73	1.41	7 (10%)	77,107,113	2.19	21 (27%)
48	CHL	N	607	-	70,74,74	0.85	2 (2%)	80,114,114	1.18	12 (15%)
29	CLA	r	602	22	64,68,73	1.45	7 (10%)	77,107,113	1.92	19 (24%)
48	CHL	N1	601	-	70,74,74	0.88	2 (2%)	80,114,114	1.40	12 (15%)
29	CLA	R	608	-	64,68,73	1.47	9 (14%)	77,107,113	2.02	17 (22%)
30	PHO	a1	409	-	58,69,69	2.09	10 (17%)	56,99,99	1.82	9 (16%)
29	CLA	g1	604	-	53,57,73	1.54	7 (13%)	62,93,113	2.18	17 (27%)
51	NEX	N1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.68	10 (20%)
36	C7Z	B	620	-	43,43,43	5.27	26 (60%)	58,60,60	2.44	22 (37%)
49	LUT	Y	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.00	15 (29%)
37	DGD	C	519	-	63,63,67	1.13	7 (11%)	77,77,81	1.01	2 (2%)
29	CLA	y	603	-	69,73,73	1.36	8 (11%)	83,113,113	2.09	19 (22%)
47	4RF	k1	101	-	56,56,56	1.04	3 (5%)	59,59,59	0.88	3 (5%)
49	LUT	G	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	12 (23%)
39	DGA	c	524	-	43,43,43	1.10	3 (6%)	45,45,45	1.55	3 (6%)
29	CLA	c1	505	-	69,73,73	1.34	8 (11%)	83,113,113	2.02	18 (21%)
29	CLA	y	602	24	69,73,73	1.40	6 (8%)	83,113,113	1.86	16 (19%)
33	LMG	B1	622	-	44,44,55	0.88	3 (6%)	52,52,63	1.08	4 (7%)
48	CHL	r1	607	-	54,58,74	0.95	2 (3%)	59,94,114	1.59	12 (20%)
29	CLA	c	506	4	69,73,73	1.39	8 (11%)	83,113,113	1.96	17 (20%)
30	PHO	A	408	-	58,69,69	1.96	9 (15%)	56,99,99	1.56	7 (12%)
29	CLA	c1	506	-	69,73,73	1.34	6 (8%)	83,113,113	1.98	19 (22%)
49	LUT	n	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.09	17 (33%)
33	LMG	b	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.15	2 (3%)
37	DGD	C1	520	-	60,60,67	1.08	5 (8%)	74,74,81	0.95	2 (2%)
40	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.16	4 (9%)
29	CLA	B	612	2	69,73,73	1.39	6 (8%)	83,113,113	1.88	15 (18%)
51	NEX	r1	622	-	38,46,46	3.37	9 (23%)	50,70,70	1.83	12 (24%)
29	CLA	N	612	-	49,53,73	1.64	8 (16%)	59,89,113	2.00	14 (23%)
38	3PH	B1	624	-	47,47,47	0.86	3 (6%)	51,52,52	1.11	2 (3%)
29	CLA	C1	503	4	69,73,73	1.40	8 (11%)	83,113,113	1.94	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	B1	613	-	69,73,73	1.38	7 (10%)	83,113,113	1.92	16 (19%)
29	CLA	S1	614	-	59,63,73	1.49	6 (10%)	71,101,113	2.08	19 (26%)
48	CHL	Y	607	-	70,74,74	0.81	2 (2%)	80,114,114	1.22	9 (11%)
53	ERG	R	626	-	31,32,32	7.79	18 (58%)	47,50,50	3.10	19 (40%)
31	BCR	a1	411	-	41,41,41	1.92	5 (12%)	56,56,56	4.06	15 (26%)
29	CLA	b1	605	2	69,73,73	1.34	6 (8%)	83,113,113	2.05	21 (25%)
48	CHL	S	606	-	48,52,74	0.95	2 (4%)	53,87,114	1.46	11 (20%)
29	CLA	B	615	-	69,73,73	1.38	8 (11%)	83,113,113	1.94	18 (21%)
32	SQD	B	621	-	41,42,54	0.88	0	50,53,65	1.01	3 (6%)
31	BCR	c1	517	-	41,41,41	1.91	5 (12%)	56,56,56	4.37	19 (33%)
29	CLA	B	610	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	19 (22%)
31	BCR	C1	515	-	41,41,41	1.93	4 (9%)	56,56,56	3.77	16 (28%)
29	CLA	S1	605	-	54,58,73	1.58	8 (14%)	65,95,113	2.13	19 (29%)
29	CLA	Y1	614	-	69,73,73	1.36	6 (8%)	83,113,113	1.98	19 (22%)
33	LMG	c	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.16	4 (6%)
39	DGA	C1	524	-	43,43,43	1.17	3 (6%)	45,45,45	1.54	4 (8%)
37	DGD	c1	518	-	56,56,67	1.02	5 (8%)	70,70,81	1.11	4 (5%)
29	CLA	y1	611	40	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
29	CLA	c1	513	-	69,73,73	1.40	8 (11%)	83,113,113	2.01	20 (24%)
29	CLA	n	611	-	53,57,73	1.56	6 (11%)	62,93,113	2.21	19 (30%)
29	CLA	C	502	-	69,73,73	1.38	7 (10%)	83,113,113	1.95	17 (20%)
40	LHG	c1	525	-	46,46,48	0.39	0	49,52,54	1.01	2 (4%)
48	CHL	g	607	-	70,74,74	0.85	2 (2%)	80,114,114	1.22	11 (13%)
48	CHL	y1	606	-	70,74,74	0.82	2 (2%)	80,114,114	1.20	12 (15%)
29	CLA	R	610	-	64,68,73	1.49	9 (14%)	77,107,113	2.14	23 (29%)
40	LHG	d1	409	-	48,48,48	0.40	0	51,54,54	1.03	2 (3%)
32	SQD	B	626	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
49	LUT	N	620	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	15 (29%)
40	LHG	s	624	29	44,44,48	0.43	0	47,50,54	1.13	3 (6%)
49	LUT	n1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.77	10 (19%)
48	CHL	g1	605	-	52,56,74	0.89	1 (1%)	58,92,114	1.49	11 (18%)
42	BCT	D	401	27	2,3,3	1.26	0	2,3,3	2.71	2 (100%)
29	CLA	c	509	4	69,73,73	1.37	6 (8%)	83,113,113	1.84	15 (18%)
29	CLA	g	612	-	47,51,73	1.69	6 (12%)	56,86,113	2.10	15 (26%)
40	LHG	y	624	29	48,48,48	0.40	0	51,54,54	1.06	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	c1	509	4	69,73,73	1.38	8 (11%)	83,113,113	1.76	16 (19%)
40	LHG	C	525	-	46,46,48	0.42	0	49,52,54	1.04	2 (4%)
29	CLA	Y	602	-	69,73,73	1.41	7 (10%)	83,113,113	1.98	19 (22%)
29	CLA	s1	614	-	59,63,73	1.48	8 (13%)	71,101,113	2.11	18 (25%)
26	OEX	a1	401	1	0,14,14	-	-	-		
29	CLA	B1	607	-	69,73,73	1.35	7 (10%)	83,113,113	2.05	21 (25%)
29	CLA	b	617	2	69,73,73	1.36	7 (10%)	83,113,113	1.95	17 (20%)
48	CHL	n1	601	-	70,74,74	0.79	2 (2%)	80,114,114	1.29	10 (12%)
29	CLA	b	614	-	69,73,73	1.36	7 (10%)	83,113,113	2.06	16 (19%)
29	CLA	G	614	-	53,57,73	1.58	7 (13%)	62,93,113	2.20	19 (30%)
54	LPX	S	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
29	CLA	b1	608	-	69,73,73	1.40	7 (10%)	83,113,113	1.93	20 (24%)
50	XAT	r	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	13 (24%)
31	BCR	b1	618	-	41,41,41	2.03	4 (9%)	56,56,56	4.25	19 (33%)
29	CLA	N	614	-	53,57,73	1.57	6 (11%)	62,93,113	2.27	17 (27%)
48	CHL	r	607	-	54,58,74	0.95	2 (3%)	59,94,114	1.44	10 (16%)
29	CLA	C	508	4	69,73,73	1.45	6 (8%)	83,113,113	1.93	22 (26%)
29	CLA	n1	614	-	53,57,73	1.54	7 (13%)	62,93,113	2.30	17 (27%)
48	CHL	s	607	-	47,51,74	0.98	2 (4%)	52,86,114	1.51	11 (21%)
29	CLA	A1	405	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	17 (20%)
29	CLA	c1	503	4	69,73,73	1.36	8 (11%)	83,113,113	2.02	21 (25%)
48	CHL	r1	606	-	48,52,74	1.07	3 (6%)	53,87,114	1.21	6 (11%)
29	CLA	C	509	4	69,73,73	1.38	7 (10%)	83,113,113	1.99	19 (22%)
29	CLA	b	615	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
29	CLA	C1	510	-	69,73,73	1.36	8 (11%)	83,113,113	1.89	17 (20%)
29	CLA	N1	612	-	49,53,73	1.62	7 (14%)	59,89,113	2.09	14 (23%)
40	LHG	d	409	-	48,48,48	0.41	0	51,54,54	1.06	3 (5%)
33	LMG	A	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.20	4 (7%)
48	CHL	n	605	20	70,74,74	0.89	3 (4%)	80,114,114	1.27	10 (12%)
54	LPX	S1	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.93	1 (3%)
29	CLA	R1	610	-	64,68,73	1.45	8 (12%)	77,107,113	2.21	19 (24%)
48	CHL	Y	606	-	70,74,74	0.85	2 (2%)	80,114,114	1.20	9 (11%)
49	LUT	s1	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.02	16 (31%)
39	DGA	B1	625	-	43,43,43	1.14	3 (6%)	45,45,45	1.46	3 (6%)
29	CLA	g	611	-	69,73,73	1.35	6 (8%)	83,113,113	2.04	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	PHO	a	409	-	58,69,69	1.98	9 (15%)	56,99,99	1.63	11 (19%)
49	LUT	G1	621	-	42,43,43	2.23	1 (2%)	51,60,60	2.08	10 (19%)
48	CHL	S	607	-	47,51,74	1.01	2 (4%)	52,86,114	1.45	9 (17%)
29	CLA	S1	613	-	59,63,73	1.43	6 (10%)	71,101,113	2.10	18 (25%)
49	LUT	y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.41	16 (31%)
29	CLA	N1	610	-	69,73,73	1.34	6 (8%)	83,113,113	1.92	19 (22%)
33	LMG	c1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	3 (4%)
29	CLA	a1	407	-	53,57,73	1.57	7 (13%)	62,93,113	2.31	17 (27%)
43	PL9	d1	405	-	55,55,55	1.13	3 (5%)	68,69,69	1.57	14 (20%)
50	XAT	n	622	-	39,47,47	0.78	1 (2%)	54,74,74	2.09	13 (24%)
29	CLA	G1	603	-	69,73,73	1.35	6 (8%)	83,113,113	2.00	19 (22%)
52	LMT	R	625	-	36,36,36	1.22	6 (16%)	47,47,47	1.14	3 (6%)
31	BCR	c	517	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	17 (30%)
52	LMT	r1	625	-	36,36,36	1.18	4 (11%)	47,47,47	1.08	4 (8%)
29	CLA	C1	504	-	69,73,73	1.38	6 (8%)	83,113,113	1.97	19 (22%)
29	CLA	a1	405	-	69,73,73	1.35	6 (8%)	83,113,113	2.02	17 (20%)
44	HEM	f	101	6,7	50,50,50	1.43	5 (10%)	66,82,82	1.15	7 (10%)
48	CHL	N1	606	-	70,74,74	0.88	2 (2%)	80,114,114	1.19	10 (12%)
29	CLA	B1	616	-	69,73,73	1.34	7 (10%)	83,113,113	1.97	18 (21%)
29	CLA	C1	507	-	69,73,73	1.39	7 (10%)	83,113,113	1.89	19 (22%)
48	CHL	g1	601	-	70,74,74	0.77	1 (1%)	80,114,114	1.30	11 (13%)
53	ERG	R1	626	-	31,32,32	7.67	19 (61%)	47,50,50	2.83	19 (40%)
29	CLA	Y1	608	-	54,58,73	1.58	7 (12%)	65,95,113	2.19	18 (27%)
29	CLA	s	602	-	64,68,73	1.41	7 (10%)	77,107,113	2.04	22 (28%)
29	CLA	R1	612	-	64,68,73	1.44	6 (9%)	77,107,113	2.02	19 (24%)
29	CLA	g1	611	-	69,73,73	1.39	8 (11%)	83,113,113	1.84	17 (20%)
29	CLA	s1	611	40	69,73,73	1.38	6 (8%)	83,113,113	1.97	20 (24%)
26	OEX	A	401	1,4	0,14,14	-	-	-		
32	SQD	M	101	-	41,42,54	0.90	0	50,53,65	0.98	3 (6%)
29	CLA	N	602	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	21 (25%)
33	LMG	w	201	-	39,39,55	0.89	2 (5%)	47,47,63	1.29	4 (8%)
48	CHL	g	609	-	70,74,74	0.87	2 (2%)	80,114,114	1.29	10 (12%)
29	CLA	n1	602	20	69,73,73	1.33	7 (10%)	83,113,113	1.98	20 (24%)
54	LPX	s	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
29	CLA	C	501	4	69,73,73	1.36	7 (10%)	83,113,113	1.98	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	G1	610	-	69,73,73	1.38	8 (11%)	83,113,113	2.00	20 (24%)
31	BCR	c1	514	-	41,41,41	1.85	4 (9%)	56,56,56	4.49	17 (30%)
48	CHL	n1	607	-	70,74,74	0.78	2 (2%)	80,114,114	1.24	9 (11%)
29	CLA	s	613	-	59,63,73	1.44	6 (10%)	71,101,113	2.18	19 (26%)
49	LUT	r1	620	-	42,43,43	2.36	2 (4%)	51,60,60	2.32	15 (29%)
50	XAT	R1	621	-	39,47,47	0.68	1 (2%)	54,74,74	1.91	18 (33%)
29	CLA	Y	604	-	69,73,73	1.34	5 (7%)	83,113,113	1.93	17 (20%)
48	CHL	y1	609	-	70,74,74	0.85	2 (2%)	80,114,114	1.35	11 (13%)
48	CHL	R1	607	-	54,58,74	0.89	2 (3%)	59,94,114	1.43	11 (18%)
31	BCR	C1	517	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	16 (28%)
41	LMK	C1	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.47	2 (4%)
47	4RF	I	102	-	56,56,56	1.05	4 (7%)	59,59,59	0.97	3 (5%)
45	RRX	h	101	-	42,42,42	4.74	24 (57%)	57,58,58	3.10	25 (43%)
29	CLA	y1	610	24	69,73,73	1.41	8 (11%)	83,113,113	1.96	22 (26%)
48	CHL	y	607	-	70,74,74	0.83	2 (2%)	80,114,114	1.26	12 (15%)
32	SQD	b	621	-	41,42,54	0.87	0	50,53,65	1.02	3 (6%)
29	CLA	b1	606	-	69,73,73	1.38	7 (10%)	83,113,113	1.98	18 (21%)
29	CLA	S	617	23	54,58,73	1.52	7 (12%)	65,95,113	2.21	19 (29%)
40	LHG	C1	525	-	46,46,48	0.39	0	49,52,54	1.04	3 (6%)
51	NEX	g1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.91	15 (30%)
34	SPH	A1	414	-	19,20,20	0.67	1 (5%)	18,21,21	1.17	1 (5%)
29	CLA	C	511	-	69,73,73	1.36	7 (10%)	83,113,113	1.90	17 (20%)
29	CLA	S1	611	40	69,73,73	1.41	8 (11%)	83,113,113	1.93	17 (20%)
48	CHL	R	607	-	54,58,74	0.93	2 (3%)	59,94,114	1.45	11 (18%)
29	CLA	b	611	-	69,73,73	1.38	6 (8%)	83,113,113	1.94	20 (24%)
40	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.03	2 (4%)
48	CHL	g	605	21	52,56,74	0.91	2 (3%)	58,92,114	1.59	13 (22%)
29	CLA	B	613	2	69,73,73	1.41	7 (10%)	83,113,113	1.94	15 (18%)
40	LHG	S	624	29	44,44,48	0.43	0	47,50,54	1.05	3 (6%)
29	CLA	N	613	-	69,73,73	1.38	6 (8%)	83,113,113	1.96	15 (18%)
36	C7Z	B1	620	-	43,43,43	5.38	26 (60%)	58,60,60	2.39	22 (37%)
51	NEX	G1	623	-	38,46,46	3.38	10 (26%)	50,70,70	1.77	11 (22%)
29	CLA	n1	612	-	49,53,73	1.64	8 (16%)	59,89,113	1.98	15 (25%)
29	CLA	b	605	-	69,73,73	1.39	7 (10%)	83,113,113	2.14	23 (27%)
32	SQD	a1	412	-	50,51,54	0.82	0	59,62,65	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	PTY	y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.12	3 (5%)
49	LUT	Y	620	-	42,43,43	2.31	1 (2%)	51,60,60	1.81	13 (25%)
49	LUT	G	620	-	42,43,43	2.25	1 (2%)	51,60,60	1.99	17 (33%)
29	CLA	Y	603	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	21 (25%)
29	CLA	c1	501	-	69,73,73	1.40	7 (10%)	83,113,113	2.00	20 (24%)
29	CLA	y1	612	-	69,73,73	1.35	7 (10%)	83,113,113	1.97	21 (25%)
40	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.45	4 (7%)
49	LUT	n1	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.13	18 (35%)
49	LUT	g	620	-	42,43,43	2.32	1 (2%)	51,60,60	2.16	16 (31%)
34	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.00	0
29	CLA	G1	611	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	17 (20%)
40	LHG	S1	624	29	44,44,48	0.44	0	47,50,54	1.12	4 (8%)
48	CHL	y1	601	24	70,74,74	0.79	2 (2%)	80,114,114	1.22	9 (11%)
45	RRX	H	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.85	22 (38%)
29	CLA	c	508	4	69,73,73	1.39	7 (10%)	83,113,113	1.88	16 (19%)
48	CHL	S1	601	23	50,54,74	0.95	3 (6%)	56,90,114	1.42	10 (17%)
29	CLA	c	503	4	69,73,73	1.38	7 (10%)	83,113,113	1.90	20 (24%)
29	CLA	b1	615	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	14 (16%)
48	CHL	G	601	21	70,74,74	0.82	2 (2%)	80,114,114	1.27	12 (15%)
48	CHL	y	605	24	50,54,74	0.96	2 (4%)	56,90,114	1.49	11 (19%)
49	LUT	g1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.33	14 (27%)
29	CLA	C	505	4	69,73,73	1.39	7 (10%)	83,113,113	1.97	18 (21%)
31	BCR	C	514	-	41,41,41	1.87	5 (12%)	56,56,56	4.28	14 (25%)
39	DGA	c1	524	-	43,43,43	1.14	3 (6%)	45,45,45	1.51	3 (6%)
31	BCR	b	618	-	41,41,41	1.89	5 (12%)	56,56,56	4.48	20 (35%)
29	CLA	b	604	-	69,73,73	1.40	7 (10%)	83,113,113	1.82	16 (19%)
29	CLA	B	602	-	69,73,73	1.35	6 (8%)	83,113,113	1.92	17 (20%)
48	CHL	Y1	601	-	70,74,74	0.91	3 (4%)	80,114,114	1.15	9 (11%)
29	CLA	C1	509	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	17 (20%)
29	CLA	b1	609	-	69,73,73	1.36	7 (10%)	83,113,113	2.01	17 (20%)
32	SQD	B1	626	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
49	LUT	g1	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.93	11 (21%)
29	CLA	N	604	-	69,73,73	1.38	6 (8%)	83,113,113	2.01	20 (24%)
29	CLA	R	612	-	64,68,73	1.43	8 (12%)	77,107,113	2.10	20 (25%)
29	CLA	n1	604	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	B1	606	-	69,73,73	1.37	8 (11%)	83,113,113	1.97	19 (22%)
29	CLA	s	612	-	49,53,73	1.63	8 (16%)	59,89,113	2.05	15 (25%)
29	CLA	B	608	-	69,73,73	1.36	6 (8%)	83,113,113	1.95	16 (19%)
29	CLA	A	410	1	64,68,73	1.45	8 (12%)	77,107,113	2.06	20 (25%)
29	CLA	Y	613	24	69,73,73	1.38	7 (10%)	83,113,113	2.10	23 (27%)
29	CLA	G	613	-	69,73,73	1.35	7 (10%)	83,113,113	2.00	22 (26%)
29	CLA	n	610	-	69,73,73	1.40	8 (11%)	83,113,113	2.06	20 (24%)
29	CLA	C1	502	-	69,73,73	1.39	6 (8%)	83,113,113	1.94	19 (22%)
31	BCR	D1	404	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	16 (28%)
29	CLA	N1	611	-	53,57,73	1.56	7 (13%)	62,93,113	2.22	18 (29%)
29	CLA	N1	602	-	69,73,73	1.38	7 (10%)	83,113,113	1.92	18 (21%)
29	CLA	B1	614	-	69,73,73	1.38	8 (11%)	83,113,113	1.94	14 (16%)
48	CHL	G1	608	-	48,52,74	1.03	2 (4%)	53,87,114	1.46	9 (16%)
55	PTY	Y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.02	2 (3%)
33	LMG	w1	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.17	3 (6%)
29	CLA	N1	613	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	17 (20%)
48	CHL	Y	609	-	70,74,74	0.87	3 (4%)	80,114,114	1.43	15 (18%)
40	LHG	G	624	29	48,48,48	0.37	0	51,54,54	1.06	3 (5%)
30	PHO	A1	409	-	58,69,69	2.04	9 (15%)	56,99,99	1.75	8 (14%)
43	PL9	D	405	-	55,55,55	1.56	5 (9%)	68,69,69	1.47	12 (17%)
48	CHL	Y	601	24	70,74,74	0.94	3 (4%)	80,114,114	1.17	9 (11%)
47	4RF	k	101	-	56,56,56	1.06	5 (8%)	59,59,59	0.83	3 (5%)
29	CLA	S1	612	-	49,53,73	1.61	6 (12%)	59,89,113	2.03	14 (23%)
29	CLA	g	603	-	69,73,73	1.38	8 (11%)	83,113,113	1.98	19 (22%)
42	BCT	d	401	-	2,3,3	1.27	0	2,3,3	2.80	2 (100%)
29	CLA	g	604	-	53,57,73	1.56	8 (15%)	62,93,113	2.13	18 (29%)
29	CLA	Y1	612	-	69,73,73	1.39	7 (10%)	83,113,113	1.93	20 (24%)
48	CHL	Y	605	24	50,54,74	0.98	2 (4%)	56,90,114	1.50	11 (19%)
48	CHL	G	605	21	52,56,74	0.93	2 (3%)	58,92,114	1.31	9 (15%)
29	CLA	d	402	-	69,73,73	1.37	7 (10%)	83,113,113	1.91	18 (21%)
31	BCR	D	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	16 (28%)
50	XAT	G1	622	-	39,47,47	0.76	1 (2%)	54,74,74	1.88	17 (31%)
29	CLA	R1	608	-	64,68,73	1.43	7 (10%)	77,107,113	2.03	18 (23%)
51	NEX	Y	623	-	38,46,46	3.34	9 (23%)	50,70,70	1.85	12 (24%)
29	CLA	G1	613	-	69,73,73	1.35	7 (10%)	83,113,113	2.10	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	SPH	a	414	-	19,20,20	0.70	1 (5%)	18,21,21	1.10	1 (5%)
40	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.12	3 (6%)
29	CLA	b	612	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	16 (19%)
29	CLA	S1	617	23	54,58,73	1.54	8 (14%)	65,95,113	2.21	18 (27%)
48	CHL	G1	607	-	70,74,74	0.86	2 (2%)	80,114,114	1.12	8 (10%)
33	LMG	W1	201	-	39,39,55	0.87	2 (5%)	47,47,63	1.37	6 (12%)
48	CHL	n	607	-	70,74,74	0.83	2 (2%)	80,114,114	1.21	11 (13%)
29	CLA	b	606	-	69,73,73	1.37	7 (10%)	83,113,113	2.02	16 (19%)
29	CLA	S	609	-	64,68,73	1.42	7 (10%)	77,107,113	1.93	18 (23%)
33	LMG	h	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.22	4 (7%)
34	SPH	A	414	-	19,20,20	0.66	0	18,21,21	1.13	2 (11%)
38	3PH	b1	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.15	2 (3%)
29	CLA	c1	511	-	69,73,73	1.36	6 (8%)	83,113,113	2.03	19 (22%)
29	CLA	s1	603	-	69,73,73	1.36	7 (10%)	83,113,113	2.02	19 (22%)
29	CLA	S	614	-	59,63,73	1.49	6 (10%)	71,101,113	2.05	17 (23%)
48	CHL	n1	606	-	70,74,74	0.81	2 (2%)	80,114,114	1.24	11 (13%)
29	CLA	B1	602	-	69,73,73	1.40	7 (10%)	83,113,113	1.98	18 (21%)
43	PL9	D1	405	-	55,55,55	1.18	5 (9%)	68,69,69	1.72	15 (22%)
48	CHL	n	609	-	70,74,74	0.79	2 (2%)	80,114,114	1.40	13 (16%)
48	CHL	R1	606	-	48,52,74	1.00	2 (4%)	53,87,114	1.35	11 (20%)
29	CLA	S	604	-	59,63,73	1.45	7 (11%)	71,101,113	2.13	19 (26%)
29	CLA	b1	617	2	69,73,73	1.38	5 (7%)	83,113,113	1.92	20 (24%)
29	CLA	y1	602	-	69,73,73	1.36	9 (13%)	83,113,113	1.97	21 (25%)
38	3PH	T1	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.09	2 (3%)
48	CHL	g1	607	-	70,74,74	0.82	2 (2%)	80,114,114	1.19	9 (11%)
29	CLA	n1	603	-	69,73,73	1.35	6 (8%)	83,113,113	1.98	18 (21%)
29	CLA	Y	612	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	19 (22%)
29	CLA	G	612	-	47,51,73	1.65	5 (10%)	56,86,113	2.12	16 (28%)
29	CLA	B1	617	-	69,73,73	1.39	7 (10%)	83,113,113	1.93	18 (21%)
32	SQD	b	626	-	53,54,54	0.82	0	62,65,65	0.91	3 (4%)
40	LHG	d1	410	-	38,38,48	0.44	0	41,44,54	1.04	2 (4%)
29	CLA	S	613	-	59,63,73	1.49	7 (11%)	71,101,113	2.08	16 (22%)
29	CLA	D1	402	-	69,73,73	1.38	7 (10%)	83,113,113	1.99	20 (24%)
40	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
55	PTY	Y1	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	SPH	y1	625	-	19,20,20	0.62	0	18,21,21	1.27	2 (11%)
49	LUT	N	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	12 (23%)
48	CHL	Y1	605	-	50,54,74	0.96	2 (4%)	56,90,114	1.39	9 (16%)
49	LUT	n	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.78	12 (23%)
29	CLA	R1	602	-	64,68,73	1.45	8 (12%)	77,107,113	2.00	19 (24%)
31	BCR	A1	411	-	41,41,41	1.88	4 (9%)	56,56,56	4.17	15 (26%)
51	NEX	Y1	623	-	38,46,46	3.15	10 (26%)	50,70,70	1.99	13 (26%)
29	CLA	c	510	4	69,73,73	1.37	6 (8%)	83,113,113	2.01	19 (22%)
29	CLA	R	603	-	64,68,73	1.47	8 (12%)	77,107,113	1.94	17 (22%)
29	CLA	y1	608	-	54,58,73	1.55	8 (14%)	65,95,113	2.13	19 (29%)
48	CHL	G1	606	-	54,58,74	1.02	2 (3%)	59,94,114	1.36	11 (18%)
32	SQD	B1	621	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
29	CLA	B	605	2	69,73,73	1.40	7 (10%)	83,113,113	2.03	20 (24%)
29	CLA	b	608	-	69,73,73	1.34	6 (8%)	83,113,113	1.93	15 (18%)
29	CLA	b1	611	-	69,73,73	1.44	6 (8%)	83,113,113	1.98	20 (24%)
40	LHG	y1	624	29	48,48,48	0.41	0	51,54,54	0.98	2 (3%)
48	CHL	G	609	21	70,74,74	0.84	2 (2%)	80,114,114	1.20	13 (16%)
29	CLA	s1	610	-	69,73,73	1.37	6 (8%)	83,113,113	1.94	19 (22%)
29	CLA	C	504	-	69,73,73	1.34	7 (10%)	83,113,113	1.89	14 (16%)
33	LMG	D1	411	-	46,46,55	0.91	4 (8%)	54,54,63	1.12	3 (5%)
29	CLA	S	603	-	69,73,73	1.37	8 (11%)	83,113,113	1.83	19 (22%)
32	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.94	3 (5%)
29	CLA	R	602	-	64,68,73	1.46	8 (12%)	77,107,113	1.94	20 (25%)
48	CHL	Y1	607	-	70,74,74	0.87	3 (4%)	80,114,114	1.15	9 (11%)
29	CLA	y1	613	-	69,73,73	1.34	6 (8%)	83,113,113	2.01	19 (22%)
29	CLA	b1	607	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	20 (24%)
29	CLA	C	507	-	69,73,73	1.39	7 (10%)	83,113,113	1.99	17 (20%)
29	CLA	b	610	-	69,73,73	1.35	7 (10%)	83,113,113	1.95	17 (20%)
29	CLA	r1	602	-	64,68,73	1.42	6 (9%)	77,107,113	2.03	20 (25%)
32	SQD	C	526	-	53,54,54	0.81	1 (1%)	62,65,65	0.94	3 (4%)
33	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.12	3 (4%)
40	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.46	5 (9%)
42	BCT	d1	401	-	2,3,3	1.18	0	2,3,3	4.36	2 (100%)
32	SQD	b1	621	-	41,42,54	0.89	0	50,53,65	0.98	3 (6%)
33	LMG	A1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.20	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	LHG	d	410	-	38,38,48	0.43	0	41,44,54	1.11	3 (7%)
29	CLA	C	513	-	69,73,73	1.38	6 (8%)	83,113,113	1.94	19 (22%)
37	DGD	B	623	-	44,44,67	0.89	1 (2%)	58,58,81	1.36	6 (10%)
29	CLA	C1	511	-	69,73,73	1.36	7 (10%)	83,113,113	2.09	21 (25%)
29	CLA	s1	617	-	54,58,73	1.53	8 (14%)	65,95,113	2.14	19 (29%)
37	DGD	b	623	-	44,44,67	0.89	2 (4%)	58,58,81	1.26	6 (10%)
49	LUT	g	621	-	42,43,43	2.37	2 (4%)	51,60,60	1.91	12 (23%)
29	CLA	c1	502	-	69,73,73	1.41	7 (10%)	83,113,113	1.82	15 (18%)
29	CLA	B	611	-	69,73,73	1.39	7 (10%)	83,113,113	1.95	19 (22%)
29	CLA	g1	613	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	18 (21%)
31	BCR	C1	516	-	41,41,41	1.89	4 (9%)	56,56,56	4.66	17 (30%)
48	CHL	s1	601	23	50,54,74	1.01	3 (6%)	56,90,114	1.44	12 (21%)
29	CLA	Y	614	-	69,73,73	1.36	8 (11%)	83,113,113	1.99	21 (25%)
48	CHL	s1	607	-	47,51,74	0.94	2 (4%)	52,86,114	1.47	11 (21%)
51	NEX	s1	623	-	38,46,46	3.40	12 (31%)	50,70,70	2.71	15 (30%)
31	BCR	B1	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.43	19 (33%)
29	CLA	B1	604	-	69,73,73	1.39	6 (8%)	83,113,113	1.78	16 (19%)
39	DGA	B	625	-	43,43,43	1.09	2 (4%)	45,45,45	1.52	3 (6%)
29	CLA	A	405	-	69,73,73	1.38	6 (8%)	83,113,113	1.98	16 (19%)
29	CLA	R1	603	-	64,68,73	1.46	7 (10%)	77,107,113	1.84	16 (20%)
51	NEX	y1	623	-	38,46,46	3.26	10 (26%)	50,70,70	2.03	18 (36%)
29	CLA	c1	507	-	69,73,73	1.38	7 (10%)	83,113,113	1.98	19 (22%)
29	CLA	Y1	602	-	69,73,73	1.39	8 (11%)	83,113,113	2.03	19 (22%)
29	CLA	b1	602	-	69,73,73	1.38	9 (13%)	83,113,113	1.90	20 (24%)
40	LHG	n1	624	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
48	CHL	y	609	-	70,74,74	0.84	3 (4%)	80,114,114	1.24	10 (12%)
29	CLA	B1	608	-	69,73,73	1.38	7 (10%)	83,113,113	1.93	18 (21%)
33	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.19	4 (7%)
49	LUT	N1	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.99	14 (27%)
32	SQD	C1	526	-	53,54,54	0.81	0	62,65,65	0.88	2 (3%)
51	NEX	n1	623	-	38,46,46	3.26	9 (23%)	50,70,70	1.71	11 (22%)
48	CHL	g	601	21	70,74,74	0.83	3 (4%)	80,114,114	1.28	11 (13%)
29	CLA	B1	605	-	69,73,73	1.35	7 (10%)	83,113,113	2.00	18 (21%)
49	LUT	s1	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.37	13 (25%)
31	BCR	C1	514	-	41,41,41	1.84	5 (12%)	56,56,56	4.05	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	XAT	y1	622	-	39,47,47	0.74	1 (2%)	54,74,74	3.88	20 (37%)
29	CLA	n	604	-	69,73,73	1.35	7 (10%)	83,113,113	1.95	18 (21%)
29	CLA	S1	610	-	69,73,73	1.37	6 (8%)	83,113,113	1.97	18 (21%)
29	CLA	A	406	-	69,73,73	1.36	7 (10%)	83,113,113	2.01	16 (19%)
29	CLA	b1	616	2	69,73,73	1.40	6 (8%)	83,113,113	1.90	15 (18%)
29	CLA	a1	406	-	69,73,73	1.39	8 (11%)	83,113,113	1.99	20 (24%)
29	CLA	r1	609	-	64,68,73	1.40	7 (10%)	77,107,113	2.02	20 (25%)
32	SQD	M1	101	-	41,42,54	0.90	0	50,53,65	0.97	2 (4%)
29	CLA	d1	403	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	19 (22%)
33	LMG	W	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.21	4 (8%)
29	CLA	G	604	-	53,57,73	1.58	7 (13%)	62,93,113	2.15	17 (27%)
29	CLA	a	405	-	69,73,73	1.38	6 (8%)	83,113,113	1.97	19 (22%)
29	CLA	N1	614	-	53,57,73	1.55	7 (13%)	62,93,113	2.21	17 (27%)
29	CLA	G1	612	-	47,51,73	1.69	7 (14%)	56,86,113	2.10	14 (25%)
29	CLA	Y1	613	-	69,73,73	1.35	7 (10%)	83,113,113	2.05	18 (21%)
37	DGD	C1	519	-	63,63,67	1.10	7 (11%)	77,77,81	1.05	3 (3%)
29	CLA	G	611	40	69,73,73	1.37	6 (8%)	83,113,113	1.96	18 (21%)
40	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
47	4RF	K1	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.84	3 (5%)
29	CLA	r1	604	-	53,57,73	1.57	7 (13%)	62,93,113	2.14	16 (25%)
29	CLA	s1	612	-	49,53,73	1.67	9 (18%)	59,89,113	1.93	13 (22%)
48	CHL	N	606	-	70,74,74	0.86	2 (2%)	80,114,114	1.25	14 (17%)
46	GOL	I	101	-	5,5,5	0.54	0	5,5,5	0.39	0
38	3PH	T	101	-	47,47,47	0.85	3 (6%)	51,52,52	1.19	2 (3%)
33	LMG	d1	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.11	3 (5%)
29	CLA	s	614	-	59,63,73	1.48	6 (10%)	71,101,113	2.03	16 (22%)
29	CLA	S	610	-	69,73,73	1.39	8 (11%)	83,113,113	1.87	21 (25%)
29	CLA	b	603	2	69,73,73	1.39	7 (10%)	83,113,113	1.98	18 (21%)
31	BCR	a	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	14 (25%)
29	CLA	S	611	40	69,73,73	1.36	6 (8%)	83,113,113	1.91	18 (21%)
34	SPH	Y1	625	-	19,20,20	0.64	0	18,21,21	1.03	1 (5%)
29	CLA	s	605	-	54,58,73	1.55	7 (12%)	65,95,113	2.21	18 (27%)
29	CLA	S1	603	-	69,73,73	1.39	7 (10%)	83,113,113	1.96	18 (21%)
29	CLA	n	602	-	69,73,73	1.42	7 (10%)	83,113,113	1.90	21 (25%)
48	CHL	g	608	-	48,52,74	0.97	2 (4%)	53,87,114	1.46	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	c	502	4	69,73,73	1.37	6 (8%)	83,113,113	1.99	16 (19%)
29	CLA	C1	506	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)
48	CHL	g1	606	-	54,58,74	1.01	4 (7%)	59,94,114	1.37	10 (16%)
29	CLA	b1	610	-	69,73,73	1.37	8 (11%)	83,113,113	1.87	18 (21%)
29	CLA	S1	604	-	59,63,73	1.49	7 (11%)	71,101,113	2.14	20 (28%)
29	CLA	d	403	-	69,73,73	1.38	7 (10%)	83,113,113	1.94	17 (20%)
51	NEX	y	623	-	38,46,46	3.41	9 (23%)	50,70,70	1.96	15 (30%)
33	LMG	H1	102	-	48,48,55	1.02	5 (10%)	56,56,63	1.16	3 (5%)
29	CLA	B	607	2	69,73,73	1.38	8 (11%)	83,113,113	1.89	16 (19%)
37	DGD	c	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.14	4 (5%)
53	ERG	r1	626	-	31,32,32	7.77	19 (61%)	47,50,50	2.72	18 (38%)
45	RRX	h1	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.65	25 (43%)
29	CLA	Y1	604	-	69,73,73	1.38	5 (7%)	83,113,113	1.92	17 (20%)
48	CHL	S	601	23	50,54,74	1.04	3 (6%)	56,90,114	1.43	9 (16%)
48	CHL	N1	605	20	70,74,74	0.89	2 (2%)	80,114,114	1.31	13 (16%)
33	LMG	a1	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.31	4 (7%)
50	XAT	g	622	-	39,47,47	0.80	1 (2%)	54,74,74	2.22	16 (29%)
48	CHL	N1	607	-	70,74,74	0.83	2 (2%)	80,114,114	1.22	11 (13%)
29	CLA	g	613	-	69,73,73	1.34	6 (8%)	83,113,113	1.99	20 (24%)
49	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.92	15 (29%)
29	CLA	B	609	2	69,73,73	1.38	7 (10%)	83,113,113	2.13	17 (20%)
29	CLA	C1	513	4	69,73,73	1.37	7 (10%)	83,113,113	1.89	20 (24%)
48	CHL	S	608	-	65,69,74	0.84	2 (3%)	74,108,114	1.29	12 (16%)
33	LMG	c1	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.10	3 (5%)
29	CLA	n	613	-	69,73,73	1.38	6 (8%)	83,113,113	2.04	18 (21%)
40	LHG	d	408	-	43,43,48	0.40	0	46,49,54	1.04	3 (6%)
29	CLA	s	609	-	64,68,73	1.43	8 (12%)	77,107,113	1.97	16 (20%)
41	LMK	c	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.25	2 (4%)
26	OEX	a	401	1,4	0,14,14	-	-	-		
40	LHG	D1	410	-	38,38,48	0.43	0	41,44,54	1.09	3 (7%)
30	PHO	A	409	-	58,69,69	1.98	9 (15%)	56,99,99	1.70	8 (14%)
29	CLA	B	606	2	69,73,73	1.36	7 (10%)	83,113,113	2.04	16 (19%)
29	CLA	s1	604	-	59,63,73	1.48	5 (8%)	71,101,113	2.10	17 (23%)
29	CLA	G	603	21	69,73,73	1.35	7 (10%)	83,113,113	1.99	22 (26%)
30	PHO	a1	408	-	58,69,69	2.04	10 (17%)	56,99,99	1.48	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	c	512	-	69,73,73	1.43	9 (13%)	83,113,113	1.89	20 (24%)
48	CHL	s1	608	-	65,69,74	0.95	4 (6%)	74,108,114	1.39	12 (16%)
31	BCR	A	411	-	41,41,41	1.86	4 (9%)	56,56,56	4.22	14 (25%)
48	CHL	s1	606	-	48,52,74	0.96	2 (4%)	53,87,114	1.31	8 (15%)
29	CLA	s1	609	-	64,68,73	1.39	7 (10%)	77,107,113	2.12	17 (22%)
31	BCR	b1	619	-	41,41,41	1.91	4 (9%)	56,56,56	4.36	15 (26%)
29	CLA	N	603	-	69,73,73	1.33	7 (10%)	83,113,113	2.02	20 (24%)
55	PTY	Y	627	-	18,18,49	1.31	3 (16%)	21,23,54	1.40	2 (9%)
29	CLA	n	603	-	69,73,73	1.36	7 (10%)	83,113,113	2.01	22 (26%)
33	LMG	C	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.19	3 (5%)
38	3PH	t1	101	-	47,47,47	0.87	3 (6%)	51,52,52	1.05	2 (3%)
29	CLA	y	614	-	69,73,73	1.34	6 (8%)	83,113,113	1.97	20 (24%)
51	NEX	R	622	-	38,46,46	3.42	11 (28%)	50,70,70	1.98	12 (24%)
48	CHL	S1	608	-	65,69,74	0.83	2 (3%)	74,108,114	1.33	12 (16%)
39	DGA	b	625	-	43,43,43	1.11	2 (4%)	45,45,45	1.45	3 (6%)
29	CLA	s1	613	-	59,63,73	1.51	8 (13%)	71,101,113	2.05	19 (26%)
29	CLA	Y	611	-	69,73,73	1.35	8 (11%)	83,113,113	1.84	13 (15%)
29	CLA	c1	510	-	69,73,73	1.40	7 (10%)	83,113,113	1.89	17 (20%)
29	CLA	B1	611	-	69,73,73	1.40	6 (8%)	83,113,113	2.03	17 (20%)
29	CLA	r1	612	-	64,68,73	1.43	7 (10%)	77,107,113	1.96	19 (24%)
29	CLA	a	407	-	53,57,73	1.55	6 (11%)	62,93,113	2.39	18 (29%)
48	CHL	n	601	20	70,74,74	0.87	3 (4%)	80,114,114	1.28	11 (13%)
29	CLA	b	607	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	20 (24%)
32	SQD	c1	526	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
48	CHL	y1	605	24	50,54,74	0.97	2 (4%)	56,90,114	1.35	10 (17%)
29	CLA	S	612	-	49,53,73	1.64	7 (14%)	59,89,113	2.09	13 (22%)
49	LUT	S	620	-	42,43,43	2.29	1 (2%)	51,60,60	2.12	18 (35%)
29	CLA	Y	610	-	69,73,73	1.38	7 (10%)	83,113,113	2.06	18 (21%)
29	CLA	G	610	21	69,73,73	1.38	7 (10%)	83,113,113	1.96	18 (21%)
51	NEX	n	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.66	11 (22%)
37	DGD	b1	623	-	44,44,67	0.92	2 (4%)	58,58,81	1.32	5 (8%)
49	LUT	Y1	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.87	14 (27%)
29	CLA	g1	603	-	69,73,73	1.40	8 (11%)	83,113,113	1.84	17 (20%)
29	CLA	B	616	-	69,73,73	1.36	9 (13%)	83,113,113	1.93	21 (25%)
29	CLA	C	510	4	69,73,73	1.39	6 (8%)	83,113,113	1.90	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	CHL	Y1	606	-	70,74,74	0.85	3 (4%)	80,114,114	1.29	11 (13%)
29	CLA	b	609	2	69,73,73	1.42	9 (13%)	83,113,113	1.93	20 (24%)
29	CLA	R	609	-	64,68,73	1.43	7 (10%)	77,107,113	4.30	20 (25%)
29	CLA	B1	612	-	69,73,73	1.37	6 (8%)	83,113,113	2.02	20 (24%)
48	CHL	S1	607	-	47,51,74	0.97	2 (4%)	52,86,114	1.49	10 (19%)
33	LMG	h1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.23	4 (7%)
29	CLA	A1	407	-	54,58,73	1.57	7 (12%)	65,95,113	2.10	17 (26%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	14 (25%)
29	CLA	Y1	603	-	69,73,73	1.38	8 (11%)	83,113,113	1.91	18 (21%)
50	XAT	R	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	18 (33%)
37	DGD	c1	520	-	60,60,67	1.09	6 (10%)	74,74,81	1.00	3 (4%)
29	CLA	B1	615	-	69,73,73	1.38	7 (10%)	83,113,113	1.91	18 (21%)
29	CLA	N1	604	-	69,73,73	1.36	7 (10%)	83,113,113	2.11	18 (21%)
32	SQD	A1	412	-	50,51,54	0.81	0	59,62,65	0.98	4 (6%)
33	LMG	H	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.10	2 (3%)
50	XAT	N1	622	-	39,47,47	0.72	1 (2%)	54,74,74	2.10	15 (27%)
55	PTY	Y1	627	-	18,18,49	1.28	2 (11%)	21,23,54	1.41	2 (9%)
29	CLA	r1	610	-	64,68,73	1.45	7 (10%)	77,107,113	1.92	17 (22%)
40	LHG	g	624	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
49	LUT	S1	620	-	42,43,43	2.32	1 (2%)	51,60,60	1.76	9 (17%)
49	LUT	Y1	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.33	13 (25%)
29	CLA	g	602	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	22 (26%)
29	CLA	D	403	-	69,73,73	1.35	7 (10%)	83,113,113	2.02	20 (24%)
33	LMG	D	411	-	46,46,55	0.91	4 (8%)	54,54,63	0.99	2 (3%)
40	LHG	N	624	-	48,48,48	0.40	0	51,54,54	1.08	3 (5%)
40	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.08	2 (3%)
48	CHL	N	609	-	70,74,74	0.82	3 (4%)	80,114,114	1.17	10 (12%)
48	CHL	n1	609	-	70,74,74	0.80	2 (2%)	80,114,114	1.30	12 (15%)
48	CHL	r	606	-	48,52,74	0.96	2 (4%)	53,87,114	1.38	9 (16%)
48	CHL	R	606	-	48,52,74	1.08	2 (4%)	53,87,114	1.34	8 (15%)
29	CLA	c1	512	-	69,73,73	1.40	7 (10%)	83,113,113	1.93	18 (21%)
37	DGD	B1	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.21	6 (10%)
38	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
32	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
32	SQD	m1	101	-	41,42,54	0.88	0	50,53,65	0.99	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.77	16 (29%)
31	BCR	c	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.24	12 (21%)
31	BCR	B	618	-	41,41,41	1.88	5 (12%)	56,56,56	4.32	18 (32%)
51	NEX	N	623	-	38,46,46	3.40	9 (23%)	50,70,70	1.64	11 (22%)
29	CLA	n1	613	-	69,73,73	1.36	7 (10%)	83,113,113	2.10	19 (22%)
37	DGD	c	519	-	63,63,67	1.12	5 (7%)	77,77,81	1.01	2 (2%)
50	XAT	N	622	-	39,47,47	0.70	1 (2%)	54,74,74	2.21	13 (24%)
29	CLA	D1	403	-	69,73,73	1.37	9 (13%)	83,113,113	1.96	22 (26%)
36	C7Z	b1	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.51	22 (37%)
40	LHG	s1	624	29	44,44,48	0.43	0	47,50,54	1.08	4 (8%)
29	CLA	g1	614	-	53,57,73	1.60	9 (16%)	62,93,113	2.21	18 (29%)
38	3PH	s1	626	-	47,47,47	0.86	3 (6%)	51,52,52	4.37	4 (7%)
49	LUT	r	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.12	14 (27%)
49	LUT	s	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.91	15 (29%)
33	LMG	C1	521	-	51,51,55	1.07	5 (9%)	59,59,63	1.14	2 (3%)
48	CHL	s	601	-	50,54,74	0.99	2 (4%)	56,90,114	1.52	12 (21%)
31	BCR	d	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
51	NEX	r	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.78	11 (22%)
29	CLA	c	505	4	69,73,73	1.40	7 (10%)	83,113,113	1.94	17 (20%)
31	BCR	C	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
29	CLA	G1	604	-	53,57,73	1.57	6 (11%)	62,93,113	2.26	20 (32%)
29	CLA	G1	614	-	53,57,73	1.54	6 (11%)	62,93,113	2.24	17 (27%)
29	CLA	b1	612	-	69,73,73	1.38	7 (10%)	83,113,113	2.06	18 (21%)
31	BCR	B	619	-	41,41,41	1.85	4 (9%)	56,56,56	3.81	21 (37%)
48	CHL	G	608	-	48,52,74	1.00	2 (4%)	53,87,114	1.46	9 (16%)
40	LHG	Y1	624	-	48,48,48	0.40	0	51,54,54	1.11	4 (7%)
29	CLA	r	610	-	64,68,73	1.42	8 (12%)	77,107,113	2.13	21 (27%)
29	CLA	s	610	-	69,73,73	1.38	8 (11%)	83,113,113	1.94	19 (22%)
29	CLA	R1	604	-	53,57,73	1.57	7 (13%)	62,93,113	2.22	14 (22%)
44	HEM	F1	101	7	50,50,50	1.40	5 (10%)	66,82,82	1.32	9 (13%)
29	CLA	s	611	40	69,73,73	1.36	7 (10%)	83,113,113	1.89	15 (18%)
30	PHO	A1	408	-	58,69,69	2.07	10 (17%)	56,99,99	1.65	8 (14%)
29	CLA	y	604	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
39	DGA	j1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.26	2 (6%)
37	DGD	C	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.95	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	n1	610	-	69,73,73	1.35	5 (7%)	83,113,113	1.95	18 (21%)
48	CHL	N1	608	-	54,58,74	1.01	2 (3%)	59,94,114	1.43	9 (15%)
38	3PH	S	626	-	47,47,47	0.87	2 (4%)	51,52,52	4.41	4 (7%)
45	RRX	H1	101	-	42,42,42	4.95	24 (57%)	57,58,58	2.34	19 (33%)
29	CLA	y	611	40	69,73,73	1.37	7 (10%)	83,113,113	1.80	15 (18%)
29	CLA	c	511	4	69,73,73	1.38	7 (10%)	83,113,113	1.92	19 (22%)
49	LUT	N1	621	-	42,43,43	2.33	2 (4%)	51,60,60	2.10	13 (25%)
40	LHG	D1	409	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
29	CLA	a1	410	1	64,68,73	1.45	8 (12%)	77,107,113	2.08	20 (25%)
31	BCR	c1	516	-	41,41,41	1.91	4 (9%)	56,56,56	4.43	13 (23%)
39	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.50	3 (6%)
29	CLA	y	613	-	69,73,73	1.39	7 (10%)	83,113,113	1.95	17 (20%)
48	CHL	G	607	-	70,74,74	0.90	2 (2%)	80,114,114	1.19	10 (12%)
48	CHL	S1	606	-	48,52,74	1.01	2 (4%)	53,87,114	1.49	9 (16%)
29	CLA	r	612	-	64,68,73	1.43	7 (10%)	77,107,113	1.98	18 (23%)
51	NEX	g	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.86	15 (30%)
29	CLA	B1	603	2	69,73,73	1.40	8 (11%)	83,113,113	2.06	20 (24%)
49	LUT	s	621	-	42,43,43	2.30	1 (2%)	51,60,60	1.98	16 (31%)
48	CHL	N1	609	-	70,74,74	0.82	2 (2%)	80,114,114	1.46	13 (16%)
49	LUT	R1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	10 (19%)
29	CLA	D	402	-	69,73,73	1.39	8 (11%)	83,113,113	1.88	15 (18%)
38	3PH	S1	626	-	47,47,47	0.87	4 (8%)	51,52,52	4.40	4 (7%)
51	NEX	R1	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.93	14 (28%)
39	DGA	b1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.50	3 (6%)
48	CHL	y	601	24	70,74,74	0.90	3 (4%)	80,114,114	1.31	12 (15%)
40	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
39	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.27	2 (6%)
29	CLA	g	610	-	69,73,73	1.35	7 (10%)	83,113,113	2.04	20 (24%)
48	CHL	s	608	-	65,69,74	0.85	2 (3%)	74,108,114	1.34	13 (17%)
29	CLA	r	609	-	64,68,73	1.43	6 (9%)	77,107,113	1.98	18 (23%)
29	CLA	n	612	-	49,53,73	1.62	6 (12%)	59,89,113	2.01	15 (25%)
29	CLA	Y	608	-	54,58,73	1.55	8 (14%)	65,95,113	2.20	18 (27%)
29	CLA	n	614	-	53,57,73	1.55	7 (13%)	62,93,113	2.27	22 (35%)
29	CLA	C	503	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	19 (22%)
42	BCT	D1	401	27	2,3,3	1.29	0	2,3,3	3.02	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	b1	604	-	69,73,73	1.38	7 (10%)	83,113,113	1.99	19 (22%)
29	CLA	c1	508	4	69,73,73	1.38	8 (11%)	83,113,113	1.89	19 (22%)
31	BCR	c	515	-	41,41,41	1.88	5 (12%)	56,56,56	4.18	16 (28%)
29	CLA	c1	504	-	69,73,73	1.38	7 (10%)	83,113,113	2.04	15 (18%)
29	CLA	r	604	-	53,57,73	1.54	7 (13%)	62,93,113	2.28	15 (24%)
50	XAT	y	622	-	39,47,47	0.73	1 (2%)	54,74,74	3.68	19 (35%)
29	CLA	r1	603	22	64,68,73	1.40	7 (10%)	77,107,113	2.04	19 (24%)
48	CHL	n1	605	-	70,74,74	0.88	3 (4%)	80,114,114	1.28	11 (13%)
48	CHL	G	606	-	54,58,74	0.94	2 (3%)	59,94,114	1.48	12 (20%)
38	3PH	b	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.18	3 (5%)
29	CLA	B	614	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	18 (21%)
29	CLA	S	602	-	64,68,73	1.47	7 (10%)	77,107,113	2.07	17 (22%)
33	LMG	C	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	2 (3%)
29	CLA	b	613	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	13 (15%)
48	CHL	n	608	-	54,58,74	1.02	3 (5%)	59,94,114	1.21	10 (16%)
48	CHL	n	606	-	70,74,74	0.88	3 (4%)	80,114,114	1.27	13 (16%)
29	CLA	r1	608	-	64,68,73	1.44	7 (10%)	77,107,113	1.99	18 (23%)
29	CLA	b1	603	-	69,73,73	1.37	6 (8%)	83,113,113	1.97	21 (25%)

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
29	CLA	y	612	-	-	19/39/115/115	-
40	LHG	L1	101	-	-	36/53/53/53	-
29	CLA	C1	505	4	-	19/39/115/115	-
29	CLA	S1	602	23	-	19/33/109/115	-
46	GOL	I1	101	-	-	2/4/4/4	-
49	LUT	y	621	-	-	2/29/67/67	0/2/2/2
39	DGA	J1	101	-	-	15/30/30/45	-
49	LUT	y1	620	-	-	3/29/67/67	0/2/2/2
29	CLA	B	617	2	-	19/39/115/115	-
29	CLA	s	617	-	-	8/21/97/115	-
29	CLA	c	507	-	-	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	c	526	-	-	20/49/69/69	0/1/1/1
48	CHL	n1	608	-	-	8/22/98/117	-
29	CLA	c	501	4	-	21/39/115/115	-
29	CLA	y	610	24	-	15/39/115/115	-
34	SPH	y	625	-	-	8/21/21/21	-
50	XAT	g1	622	-	1/1/12/26	7/31/93/93	0/4/4/4
55	PTY	y1	627	-	-	11/20/20/53	-
40	LHG	D	408	-	-	23/48/48/53	-
55	PTY	y1	626	-	-	33/53/53/53	-
29	CLA	B	603	2	-	23/39/115/115	-
29	CLA	b	602	-	-	23/39/115/115	-
29	CLA	g	614	-	-	13/20/96/115	-
29	CLA	a	406	-	-	17/39/115/115	-
29	CLA	d1	402	-	-	12/39/115/115	-
29	CLA	C1	508	4	-	13/39/115/115	-
33	LMG	d	411	-	-	19/41/61/70	0/1/1/1
29	CLA	B1	609	-	-	17/39/115/115	-
31	BCR	C	515	-	-	9/29/63/63	0/2/2/2
48	CHL	s	606	-	-	3/15/91/117	-
29	CLA	b1	613	-	-	17/39/115/115	-
49	LUT	R	620	-	1/1/12/27	2/29/67/67	0/2/2/2
29	CLA	N	610	-	-	21/39/115/115	-
29	CLA	c	504	-	-	20/39/115/115	-
29	CLA	A1	406	-	-	21/39/115/115	-
29	CLA	Y1	611	-	-	18/39/115/115	-
29	CLA	r	603	-	-	19/33/109/115	-
50	XAT	G	622	-	1/1/12/26	2/31/93/93	0/4/4/4
38	3PH	s	626	-	-	22/49/49/49	-
31	BCR	B1	619	-	-	6/29/63/63	0/2/2/2
32	SQD	b1	626	-	-	26/49/69/69	0/1/1/1
51	NEX	S	623	-	-	8/27/83/83	0/3/3/3
53	ERG	r	626	-	5/5/11/15	8/13/71/71	0/4/4/4
48	CHL	G1	601	21	1/1/15/21	13/41/117/117	-
48	CHL	g1	609	-	1/1/15/21	7/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LHG	g1	624	-	-	35/53/53/53	-
29	CLA	r	608	-	-	17/33/109/115	-
29	CLA	B1	610	-	-	23/39/115/115	-
52	LMT	r	625	-	-	13/21/61/61	0/2/2/2
29	CLA	g1	610	-	-	18/39/115/115	-
32	SQD	m	101	-	-	20/37/57/69	0/1/1/1
29	CLA	C1	512	-	-	16/39/115/115	-
48	CHL	G1	605	21	1/1/11/21	5/20/96/117	-
33	LMG	b1	622	-	-	19/39/59/70	0/1/1/1
48	CHL	Y1	609	-	1/1/15/21	8/41/117/117	-
44	HEM	f1	101	7	-	2/14/54/54	-
29	CLA	y1	604	-	-	15/39/115/115	-
29	CLA	s	604	-	-	11/27/103/115	-
47	4RF	K	101	-	-	32/59/59/59	-
40	LHG	d1	408	-	-	30/48/48/53	-
29	CLA	b	616	2	-	17/39/115/115	-
31	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
29	CLA	b1	614	-	-	12/39/115/115	-
29	CLA	C1	501	4	-	15/39/115/115	-
29	CLA	G	602	-	-	17/39/115/115	-
29	CLA	y	608	-	-	10/21/97/115	-
47	4RF	I1	102	-	-	24/59/59/59	-
29	CLA	a	410	1	-	15/33/109/115	-
29	CLA	g1	612	21	-	5/13/89/115	-
29	CLA	N	611	-	-	9/20/96/115	-
48	CHL	y1	607	-	1/1/15/21	4/41/117/117	-
29	CLA	n1	611	-	-	11/20/96/115	-
49	LUT	G1	620	-	-	5/29/67/67	0/2/2/2
37	DGD	C1	518	-	-	12/44/84/95	0/2/2/2
51	NEX	S1	623	-	-	4/27/83/83	0/3/3/3
34	SPH	a1	414	-	-	10/21/21/21	-
29	CLA	N1	603	-	-	17/39/115/115	-
31	BCR	C	517	-	-	13/29/63/63	0/2/2/2
50	XAT	Y1	622	-	1/1/12/26	4/31/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	g1	602	-	-	19/39/115/115	-
29	CLA	A	407	-	-	9/21/97/115	-
31	BCR	c1	515	-	-	11/29/63/63	0/2/2/2
37	DGD	c	520	-	-	9/48/88/95	0/2/2/2
39	DGA	j	101	-	-	20/30/30/45	-
47	4RF	i1	101	-	-	30/59/59/59	-
49	LUT	S	621	-	-	4/29/67/67	0/2/2/2
48	CHL	y	606	-	1/1/15/21	12/41/117/117	-
29	CLA	R	604	-	-	10/20/96/115	-
29	CLA	s	603	-	-	17/39/115/115	-
29	CLA	S	605	23	-	11/21/97/115	-
48	CHL	g	606	-	-	4/22/98/117	-
50	XAT	n1	622	-	-	4/31/93/93	0/4/4/4
44	HEM	F	101	6,7	-	1/14/54/54	-
48	CHL	G1	609	-	1/1/15/21	10/41/117/117	-
29	CLA	A1	410	-	-	12/33/109/115	-
50	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
41	LMK	c1	527	-	2/2/6/6	14/46/46/60	-
36	C7Z	b	620	-	1/1/12/26	13/29/67/67	0/2/2/2
55	PTY	y	627	-	-	15/20/20/53	-
29	CLA	s1	605	-	-	11/21/97/115	-
51	NEX	s	623	-	-	4/27/83/83	0/3/3/3
52	LMT	R1	625	-	-	10/21/61/61	0/2/2/2
49	LUT	S1	621	-	-	7/29/67/67	0/2/2/2
47	4RF	i	101	-	-	31/59/59/59	-
48	CHL	N	608	-	-	3/22/98/117	-
31	BCR	b	619	-	-	6/29/63/63	0/2/2/2
29	CLA	c	513	-	-	23/39/115/115	-
29	CLA	B	604	-	-	18/39/115/115	-
29	CLA	R1	609	-	-	16/33/109/115	-
29	CLA	y1	614	-	-	18/39/115/115	-
33	LMG	B	622	-	-	20/39/59/70	0/1/1/1
29	CLA	Y1	610	-	-	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	3PH	t	101	-	-	27/49/49/49	-
54	LPX	s1	625	-	-	18/31/31/31	-
41	LMK	C	527	-	2/2/6/6	21/46/46/60	-
48	CHL	N	601	20	1/1/15/21	5/41/117/117	-
29	CLA	S1	609	-	-	12/33/109/115	-
29	CLA	C	506	-	-	15/39/115/115	-
29	CLA	C	512	-	-	15/39/115/115	-
40	LHG	N1	624	-	-	34/53/53/53	-
29	CLA	y1	603	-	-	20/39/115/115	-
29	CLA	G1	602	-	-	23/39/115/115	-
30	PHO	a	408	-	-	11/37/103/103	0/5/6/6
37	DGD	c1	519	-	-	24/51/91/95	0/2/2/2
51	NEX	G	623	-	-	5/27/83/83	0/3/3/3
48	CHL	N	605	20	1/1/15/21	10/41/117/117	-
48	CHL	g1	608	-	-	1/15/91/117	-
33	LMG	C1	523	-	-	19/50/70/70	0/1/1/1
43	PL9	d	405	-	-	9/53/73/73	0/1/1/1
29	CLA	s1	602	-	-	13/33/109/115	-
48	CHL	N	607	-	1/1/15/21	8/41/117/117	-
29	CLA	r	602	22	-	14/33/109/115	-
48	CHL	N1	601	-	1/1/15/21	10/41/117/117	-
29	CLA	R	608	-	-	21/33/109/115	-
30	PHO	a1	409	-	-	12/37/103/103	0/5/6/6
29	CLA	g1	604	-	-	9/20/96/115	-
51	NEX	N1	623	-	-	6/27/83/83	0/3/3/3
36	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
49	LUT	Y	621	-	-	4/29/67/67	0/2/2/2
49	LUT	G	621	-	1/1/12/27	4/29/67/67	0/2/2/2
29	CLA	y	603	-	-	20/39/115/115	-
37	DGD	C	519	-	-	26/51/91/95	0/2/2/2
47	4RF	k1	101	-	-	37/59/59/59	-
39	DGA	c	524	-	-	31/45/45/45	-
29	CLA	c1	505	-	-	18/39/115/115	-
29	CLA	y	602	24	-	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	B1	622	-	-	19/39/59/70	0/1/1/1
48	CHL	r1	607	-	-	5/22/98/117	-
29	CLA	c	506	4	-	17/39/115/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
29	CLA	c1	506	-	-	16/39/115/115	-
49	LUT	n	620	-	-	3/29/67/67	0/2/2/2
33	LMG	b	622	-	-	17/39/59/70	0/1/1/1
37	DGD	C1	520	-	-	16/48/88/95	0/2/2/2
40	LHG	D	410	-	-	26/43/43/53	-
29	CLA	B	612	2	-	16/39/115/115	-
51	NEX	r1	622	-	-	8/27/83/83	0/3/3/3
29	CLA	N	612	-	-	6/15/91/115	-
38	3PH	B1	624	-	-	27/49/49/49	-
29	CLA	C1	503	4	-	19/39/115/115	-
29	CLA	B1	613	-	-	21/39/115/115	-
48	CHL	Y	607	-	1/1/15/21	7/41/117/117	-
53	ERG	R	626	-	5/5/11/15	6/13/71/71	0/4/4/4
29	CLA	S1	614	-	-	10/27/103/115	-
31	BCR	a1	411	-	-	6/29/63/63	0/2/2/2
29	CLA	b1	605	2	-	20/39/115/115	-
48	CHL	S	606	-	-	2/15/91/117	-
29	CLA	B	615	-	-	15/39/115/115	-
32	SQD	B	621	-	-	20/37/57/69	0/1/1/1
31	BCR	c1	517	-	-	9/29/63/63	0/2/2/2
29	CLA	B	610	-	-	23/39/115/115	-
31	BCR	C1	515	-	-	12/29/63/63	0/2/2/2
29	CLA	S1	605	-	-	10/21/97/115	-
29	CLA	Y1	614	-	-	14/39/115/115	-
33	LMG	c	521	-	-	14/46/66/70	0/1/1/1
39	DGA	C1	524	-	-	23/45/45/45	-
37	DGD	c1	518	-	-	14/44/84/95	0/2/2/2
29	CLA	y1	611	40	-	20/39/115/115	-
29	CLA	c1	513	-	-	25/39/115/115	-
29	CLA	n	611	-	-	10/20/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C	502	-	-	15/39/115/115	-
40	LHG	c1	525	-	-	33/51/51/53	-
48	CHL	g	607	-	1/1/15/21	11/41/117/117	-
48	CHL	y1	606	-	1/1/15/21	6/41/117/117	-
29	CLA	R	610	-	-	16/33/109/115	-
40	LHG	d1	409	-	-	30/53/53/53	-
32	SQD	B	626	-	-	23/49/69/69	0/1/1/1
49	LUT	N	620	-	-	2/29/67/67	0/2/2/2
40	LHG	s	624	29	-	26/49/49/53	-
49	LUT	n1	620	-	-	5/29/67/67	0/2/2/2
48	CHL	g1	605	-	1/1/11/21	7/20/96/117	-
29	CLA	c	509	4	-	16/39/115/115	-
29	CLA	g	612	-	-	8/13/89/115	-
40	LHG	y	624	29	-	30/53/53/53	-
29	CLA	c1	509	4	-	20/39/115/115	-
40	LHG	C	525	-	-	32/51/51/53	-
29	CLA	Y	602	-	-	18/39/115/115	-
29	CLA	s1	614	-	-	17/27/103/115	-
29	CLA	B1	607	-	-	16/39/115/115	-
48	CHL	n1	601	-	1/1/15/21	11/41/117/117	-
29	CLA	b	617	2	-	15/39/115/115	-
29	CLA	b	614	-	-	13/39/115/115	-
29	CLA	G	614	-	-	10/20/96/115	-
54	LPX	S	625	-	-	14/31/31/31	-
29	CLA	b1	608	-	-	25/39/115/115	-
50	XAT	r	621	-	2/2/12/26	2/31/93/93	0/4/4/4
31	BCR	b1	618	-	-	11/29/63/63	0/2/2/2
29	CLA	N	614	-	-	7/20/96/115	-
48	CHL	r	607	-	-	4/22/98/117	-
29	CLA	C	508	4	-	12/39/115/115	-
29	CLA	n1	614	-	-	11/20/96/115	-
48	CHL	s	607	-	-	1/14/90/117	-
29	CLA	A1	405	-	-	12/39/115/115	-
29	CLA	c1	503	4	-	20/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	r1	606	-	-	4/15/91/117	-
29	CLA	C	509	4	-	20/39/115/115	-
29	CLA	b	615	-	-	19/39/115/115	-
29	CLA	C1	510	-	-	19/39/115/115	-
29	CLA	N1	612	-	-	6/15/91/115	-
40	LHG	d	409	-	-	26/53/53/53	-
33	LMG	A	413	-	-	15/43/63/70	0/1/1/1
48	CHL	n	605	20	1/1/15/21	8/41/117/117	-
54	LPX	S1	625	-	-	15/31/31/31	-
29	CLA	R1	610	-	-	19/33/109/115	-
48	CHL	Y	606	-	1/1/15/21	7/41/117/117	-
49	LUT	s1	620	-	-	6/29/67/67	0/2/2/2
39	DGA	B1	625	-	-	26/45/45/45	-
29	CLA	g	611	-	-	17/39/115/115	-
30	PHO	a	409	-	-	11/37/103/103	0/5/6/6
49	LUT	G1	621	-	-	3/29/67/67	0/2/2/2
48	CHL	S	607	-	-	1/14/90/117	-
29	CLA	S1	613	-	-	11/27/103/115	-
49	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
29	CLA	N1	610	-	-	21/39/115/115	-
33	LMG	c1	523	-	-	18/50/70/70	0/1/1/1
29	CLA	a1	407	-	-	7/20/96/115	-
43	PL9	d1	405	-	-	20/53/73/73	0/1/1/1
50	XAT	n	622	-	1/1/12/26	4/31/93/93	0/4/4/4
29	CLA	G1	603	-	-	25/39/115/115	-
52	LMT	R	625	-	-	9/21/61/61	0/2/2/2
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
52	LMT	r1	625	-	-	10/21/61/61	0/2/2/2
29	CLA	C1	504	-	-	20/39/115/115	-
29	CLA	a1	405	-	-	17/39/115/115	-
44	HEM	f	101	6,7	-	1/14/54/54	-
48	CHL	N1	606	-	1/1/15/21	12/41/117/117	-
48	CHL	g1	601	-	1/1/15/21	12/41/117/117	-
53	ERG	R1	626	-	5/5/11/15	9/13/71/71	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B1	616	-	-	18/39/115/115	-
29	CLA	C1	507	-	-	16/39/115/115	-
29	CLA	Y1	608	-	-	9/21/97/115	-
29	CLA	s	602	-	-	18/33/109/115	-
29	CLA	R1	612	-	-	21/33/109/115	-
29	CLA	g1	611	-	-	20/39/115/115	-
29	CLA	s1	611	40	-	22/39/115/115	-
32	SQD	M	101	-	-	24/37/57/69	0/1/1/1
48	CHL	g	609	-	1/1/15/21	10/41/117/117	-
29	CLA	N	602	-	-	15/39/115/115	-
33	LMG	w	201	-	-	17/34/54/70	0/1/1/1
29	CLA	n1	602	20	-	19/39/115/115	-
54	LPX	s	625	-	-	15/31/31/31	-
29	CLA	C	501	4	-	20/39/115/115	-
29	CLA	G1	610	-	-	17/39/115/115	-
31	BCR	c1	514	-	-	12/29/63/63	0/2/2/2
48	CHL	n1	607	-	1/1/15/21	7/41/117/117	-
29	CLA	s	613	-	-	11/27/103/115	-
49	LUT	r1	620	-	-	4/29/67/67	0/2/2/2
50	XAT	R1	621	-	-	4/31/93/93	0/4/4/4
29	CLA	Y	604	-	-	17/39/115/115	-
48	CHL	y1	609	-	1/1/15/21	8/41/117/117	-
48	CHL	R1	607	-	-	4/22/98/117	-
31	BCR	C1	517	-	-	11/29/63/63	0/2/2/2
41	LMK	C1	527	-	2/2/6/6	19/46/46/60	-
47	4RF	I	102	-	-	30/59/59/59	-
45	RRX	h	101	-	1/1/11/25	4/29/65/65	0/2/2/2
48	CHL	y	607	-	1/1/15/21	9/41/117/117	-
29	CLA	y1	610	24	-	13/39/115/115	-
32	SQD	b	621	-	-	19/37/57/69	0/1/1/1
29	CLA	b1	606	-	-	13/39/115/115	-
29	CLA	S	617	23	-	9/21/97/115	-
51	NEX	g1	623	-	1/1/12/25	7/27/83/83	0/3/3/3
40	LHG	C1	525	-	-	30/51/51/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SPH	A1	414	-	-	16/21/21/21	-
29	CLA	C	511	-	-	14/39/115/115	-
29	CLA	S1	611	40	-	18/39/115/115	-
48	CHL	R	607	-	-	7/22/98/117	-
48	CHL	g	605	21	1/1/11/21	5/20/96/117	-
29	CLA	b	611	-	-	7/39/115/115	-
40	LHG	D1	408	-	-	26/48/48/53	-
29	CLA	B	613	2	-	18/39/115/115	-
40	LHG	S	624	29	-	27/49/49/53	-
29	CLA	N	613	-	-	19/39/115/115	-
36	C7Z	B1	620	-	1/1/12/26	7/29/67/67	0/2/2/2
51	NEX	G1	623	-	-	12/27/83/83	0/3/3/3
29	CLA	n1	612	-	-	7/15/91/115	-
29	CLA	b	605	-	-	21/39/115/115	-
32	SQD	a1	412	-	-	19/46/66/69	0/1/1/1
55	PTY	y	626	-	-	27/53/53/53	-
49	LUT	Y	620	-	-	5/29/67/67	0/2/2/2
49	LUT	G	620	-	-	3/29/67/67	0/2/2/2
29	CLA	Y	603	-	-	19/39/115/115	-
29	CLA	c1	501	-	-	19/39/115/115	-
49	LUT	n1	621	-	1/1/12/27	5/29/67/67	0/2/2/2
29	CLA	y1	612	-	-	18/39/115/115	-
40	LHG	l	101	-	-	38/53/53/53	-
49	LUT	g	620	-	-	4/29/67/67	0/2/2/2
34	SPH	Y	625	-	-	10/21/21/21	-
29	CLA	G1	611	-	-	21/39/115/115	-
40	LHG	S1	624	29	-	32/49/49/53	-
48	CHL	y1	601	24	1/1/15/21	5/41/117/117	-
45	RRX	H	101	-	1/1/11/25	7/29/65/65	0/2/2/2
29	CLA	c	508	4	-	12/39/115/115	-
48	CHL	S1	601	23	-	3/17/93/117	-
29	CLA	c	503	4	-	20/39/115/115	-
29	CLA	b1	615	-	-	17/39/115/115	-
48	CHL	G	601	21	1/1/15/21	11/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	y	605	24	-	3/17/93/117	-
49	LUT	g1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	C	505	4	-	18/39/115/115	-
31	BCR	C	514	-	-	17/29/63/63	0/2/2/2
48	CHL	Y1	601	-	1/1/15/21	7/41/117/117	-
31	BCR	b	618	-	-	9/29/63/63	0/2/2/2
29	CLA	b	604	-	-	16/39/115/115	-
29	CLA	B	602	-	-	20/39/115/115	-
39	DGA	c1	524	-	-	28/45/45/45	-
29	CLA	C1	509	-	-	10/39/115/115	-
29	CLA	b1	609	-	-	18/39/115/115	-
32	SQD	B1	626	-	-	17/49/69/69	0/1/1/1
49	LUT	g1	620	-	-	6/29/67/67	0/2/2/2
29	CLA	N	604	-	-	21/39/115/115	-
29	CLA	R	612	-	-	12/33/109/115	-
29	CLA	n1	604	-	-	15/39/115/115	-
29	CLA	B1	606	-	-	20/39/115/115	-
29	CLA	s	612	-	-	5/15/91/115	-
29	CLA	B	608	-	-	27/39/115/115	-
29	CLA	A	410	1	-	14/33/109/115	-
29	CLA	Y	613	24	-	24/39/115/115	-
29	CLA	G	613	-	-	21/39/115/115	-
29	CLA	n	610	-	-	20/39/115/115	-
29	CLA	C1	502	-	-	14/39/115/115	-
31	BCR	D1	404	-	-	14/29/63/63	0/2/2/2
29	CLA	N1	611	-	-	12/20/96/115	-
29	CLA	N1	602	-	-	17/39/115/115	-
29	CLA	B1	614	-	-	16/39/115/115	-
48	CHL	G1	608	-	-	1/15/91/117	-
55	PTY	Y	626	-	-	31/53/53/53	-
33	LMG	w1	201	-	-	17/34/54/70	0/1/1/1
29	CLA	N1	613	-	-	14/39/115/115	-
48	CHL	Y	609	-	1/1/15/21	6/41/117/117	-
40	LHG	G	624	29	-	33/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PHO	A1	409	-	-	11/37/103/103	0/5/6/6
43	PL9	D	405	-	-	9/53/73/73	0/1/1/1
48	CHL	Y	601	24	1/1/15/21	7/41/117/117	-
47	4RF	k	101	-	-	31/59/59/59	-
29	CLA	S1	612	-	-	6/15/91/115	-
29	CLA	g	603	-	-	23/39/115/115	-
29	CLA	g	604	-	-	9/20/96/115	-
29	CLA	Y1	612	-	-	20/39/115/115	-
48	CHL	Y	605	24	-	3/17/93/117	-
48	CHL	G	605	21	1/1/11/21	6/20/96/117	-
50	XAT	G1	622	-	1/1/12/26	2/31/93/93	0/4/4/4
29	CLA	d	402	-	-	13/39/115/115	-
31	BCR	D	404	-	-	13/29/63/63	0/2/2/2
29	CLA	R1	608	-	-	11/33/109/115	-
51	NEX	Y	623	-	-	7/27/83/83	0/3/3/3
29	CLA	G1	613	-	-	15/39/115/115	-
34	SPH	a	414	-	-	11/21/21/21	-
40	LHG	c	525	-	-	30/51/51/53	-
29	CLA	b	612	-	-	16/39/115/115	-
29	CLA	S1	617	23	-	7/21/97/115	-
48	CHL	G1	607	-	1/1/15/21	11/41/117/117	-
48	CHL	n	607	-	1/1/15/21	8/41/117/117	-
33	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
29	CLA	b	606	-	-	15/39/115/115	-
29	CLA	S	609	-	-	12/33/109/115	-
33	LMG	h	102	-	-	11/43/63/70	0/1/1/1
34	SPH	A	414	-	-	12/21/21/21	-
38	3PH	b1	624	-	-	24/49/49/49	-
29	CLA	c1	511	-	-	20/39/115/115	-
29	CLA	s1	603	-	-	17/39/115/115	-
29	CLA	S	614	-	-	8/27/103/115	-
48	CHL	n1	606	-	1/1/15/21	8/41/117/117	-
29	CLA	B1	602	-	-	25/39/115/115	-
48	CHL	n	609	-	1/1/15/21	5/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	PL9	D1	405	-	-	18/53/73/73	0/1/1/1
48	CHL	R1	606	-	-	4/15/91/117	-
29	CLA	S	604	-	-	11/27/103/115	-
29	CLA	b1	617	2	-	16/39/115/115	-
29	CLA	y1	602	-	-	17/39/115/115	-
38	3PH	T1	101	-	-	29/49/49/49	-
48	CHL	g1	607	-	1/1/15/21	8/41/117/117	-
29	CLA	n1	603	-	-	14/39/115/115	-
29	CLA	Y	612	-	-	15/39/115/115	-
29	CLA	G	612	-	-	7/13/89/115	-
29	CLA	B1	617	-	-	18/39/115/115	-
32	SQD	b	626	-	-	17/49/69/69	0/1/1/1
40	LHG	d1	410	-	-	33/43/43/53	-
29	CLA	S	613	-	-	12/27/103/115	-
29	CLA	D1	402	-	-	13/39/115/115	-
40	LHG	Y	624	-	-	29/53/53/53	-
55	PTY	Y1	626	-	-	26/53/53/53	-
34	SPH	y1	625	-	-	12/21/21/21	-
49	LUT	N	621	-	-	4/29/67/67	0/2/2/2
48	CHL	Y1	605	-	-	3/17/93/117	-
49	LUT	n	621	-	-	2/29/67/67	0/2/2/2
29	CLA	R1	602	-	-	14/33/109/115	-
31	BCR	A1	411	-	-	9/29/63/63	0/2/2/2
51	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
29	CLA	c	510	4	-	16/39/115/115	-
29	CLA	R	603	-	-	18/33/109/115	-
29	CLA	y1	608	-	-	11/21/97/115	-
48	CHL	G1	606	-	-	4/22/98/117	-
32	SQD	B1	621	-	-	11/37/57/69	0/1/1/1
29	CLA	B	605	2	-	21/39/115/115	-
29	CLA	b	608	-	-	28/39/115/115	-
29	CLA	b1	611	-	-	10/39/115/115	-
48	CHL	G	609	21	1/1/15/21	10/41/117/117	-
40	LHG	y1	624	29	-	25/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s1	610	-	-	20/39/115/115	-
29	CLA	C	504	-	-	18/39/115/115	-
33	LMG	D1	411	-	-	10/41/61/70	0/1/1/1
29	CLA	S	603	-	-	19/39/115/115	-
32	SQD	A	412	-	-	24/46/66/69	0/1/1/1
29	CLA	R	602	-	-	12/33/109/115	-
48	CHL	Y1	607	-	1/1/15/21	12/41/117/117	-
29	CLA	y1	613	-	-	20/39/115/115	-
29	CLA	b1	607	-	-	14/39/115/115	-
29	CLA	C	507	-	-	14/39/115/115	-
29	CLA	b	610	-	-	15/39/115/115	-
29	CLA	r1	602	-	-	13/33/109/115	-
32	SQD	C	526	-	-	23/49/69/69	0/1/1/1
33	LMG	c	523	-	-	21/50/70/70	0/1/1/1
40	LHG	L	101	-	-	38/53/53/53	-
32	SQD	b1	621	-	-	17/37/57/69	0/1/1/1
33	LMG	A1	413	-	-	18/43/63/70	0/1/1/1
40	LHG	d	410	-	-	20/43/43/53	-
29	CLA	C	513	-	-	22/39/115/115	-
37	DGD	B	623	-	-	15/32/72/95	0/2/2/2
29	CLA	C1	511	-	-	12/39/115/115	-
29	CLA	s1	617	-	-	11/21/97/115	-
37	DGD	b	623	-	-	13/32/72/95	0/2/2/2
49	LUT	g	621	-	-	4/29/67/67	0/2/2/2
29	CLA	c1	502	-	-	16/39/115/115	-
29	CLA	B	611	-	-	13/39/115/115	-
29	CLA	g1	613	-	-	24/39/115/115	-
31	BCR	C1	516	-	-	15/29/63/63	0/2/2/2
48	CHL	s1	601	23	-	4/17/93/117	-
29	CLA	Y	614	-	-	19/39/115/115	-
48	CHL	s1	607	-	-	0/14/90/117	-
51	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
31	BCR	B1	618	-	-	15/29/63/63	0/2/2/2
29	CLA	B1	604	-	-	14/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGA	B	625	-	-	23/45/45/45	-
29	CLA	A	405	-	-	14/39/115/115	-
29	CLA	R1	603	-	-	19/33/109/115	-
51	NEX	y1	623	-	-	10/27/83/83	0/3/3/3
29	CLA	c1	507	-	-	16/39/115/115	-
29	CLA	Y1	602	-	-	20/39/115/115	-
29	CLA	b1	602	-	-	22/39/115/115	-
40	LHG	n1	624	-	-	29/53/53/53	-
48	CHL	y	609	-	1/1/15/21	6/41/117/117	-
29	CLA	B1	608	-	-	28/39/115/115	-
33	LMG	a	413	-	-	20/43/63/70	0/1/1/1
49	LUT	N1	620	-	-	8/29/67/67	0/2/2/2
32	SQD	C1	526	-	-	25/49/69/69	0/1/1/1
51	NEX	n1	623	-	-	5/27/83/83	0/3/3/3
48	CHL	g	601	21	1/1/15/21	16/41/117/117	-
29	CLA	B1	605	-	-	17/39/115/115	-
49	LUT	s1	621	-	-	5/29/67/67	0/2/2/2
31	BCR	C1	514	-	-	12/29/63/63	0/2/2/2
50	XAT	y1	622	-	-	7/31/93/93	0/4/4/4
29	CLA	n	604	-	-	15/39/115/115	-
29	CLA	S1	610	-	-	22/39/115/115	-
29	CLA	A	406	-	-	14/39/115/115	-
29	CLA	b1	616	2	-	9/39/115/115	-
29	CLA	a1	406	-	-	16/39/115/115	-
29	CLA	r1	609	-	-	19/33/109/115	-
32	SQD	M1	101	-	-	17/37/57/69	0/1/1/1
29	CLA	d1	403	-	-	12/39/115/115	-
33	LMG	W	201	-	-	14/34/54/70	0/1/1/1
29	CLA	G	604	-	-	8/20/96/115	-
29	CLA	a	405	-	-	15/39/115/115	-
29	CLA	N1	614	-	-	7/20/96/115	-
29	CLA	G1	612	-	-	8/13/89/115	-
29	CLA	Y1	613	-	-	21/39/115/115	-
37	DGD	C1	519	-	-	22/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	611	40	-	19/39/115/115	-
40	LHG	G1	624	-	-	29/53/53/53	-
47	4RF	K1	101	-	-	32/59/59/59	-
29	CLA	r1	604	-	-	10/20/96/115	-
29	CLA	s1	612	-	-	8/15/91/115	-
48	CHL	N	606	-	1/1/15/21	10/41/117/117	-
46	GOL	I	101	-	-	2/4/4/4	-
38	3PH	T	101	-	-	26/49/49/49	-
33	LMG	d1	411	-	-	19/41/61/70	0/1/1/1
29	CLA	s	614	-	-	4/27/103/115	-
29	CLA	S	610	-	-	22/39/115/115	-
29	CLA	b	603	2	-	22/39/115/115	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
29	CLA	S	611	40	-	18/39/115/115	-
34	SPH	Y1	625	-	-	9/21/21/21	-
29	CLA	s	605	-	-	13/21/97/115	-
29	CLA	S1	603	-	-	14/39/115/115	-
29	CLA	n	602	-	-	16/39/115/115	-
48	CHL	g	608	-	-	3/15/91/117	-
29	CLA	c	502	4	-	14/39/115/115	-
29	CLA	C1	506	-	-	21/39/115/115	-
48	CHL	g1	606	-	-	3/22/98/117	-
29	CLA	b1	610	-	-	19/39/115/115	-
29	CLA	S1	604	-	-	12/27/103/115	-
29	CLA	d	403	-	-	16/39/115/115	-
51	NEX	y	623	-	-	6/27/83/83	0/3/3/3
33	LMG	H1	102	-	-	17/43/63/70	0/1/1/1
29	CLA	B	607	2	-	18/39/115/115	-
37	DGD	c	518	-	-	9/44/84/95	0/2/2/2
53	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
45	RRX	h1	101	-	1/1/11/25	10/29/65/65	0/2/2/2
29	CLA	Y1	604	-	-	15/39/115/115	-
48	CHL	S	601	23	-	3/17/93/117	-
48	CHL	N1	605	20	1/1/15/21	9/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	XAT	g	622	-	2/2/12/26	3/31/93/93	0/4/4/4
33	LMG	a1	413	-	-	20/43/63/70	0/1/1/1
48	CHL	N1	607	-	1/1/15/21	11/41/117/117	-
29	CLA	g	613	-	-	21/39/115/115	-
49	LUT	y	620	-	-	4/29/67/67	0/2/2/2
29	CLA	B	609	2	-	12/39/115/115	-
29	CLA	C1	513	4	-	16/39/115/115	-
48	CHL	S	608	-	1/1/14/21	7/35/111/117	-
33	LMG	c1	521	-	-	14/46/66/70	0/1/1/1
29	CLA	n	613	-	-	18/39/115/115	-
40	LHG	d	408	-	-	26/48/48/53	-
29	CLA	s	609	-	-	18/33/109/115	-
41	LMK	c	527	-	2/2/6/6	13/46/46/60	-
40	LHG	D1	410	-	-	25/43/43/53	-
30	PHO	A	409	-	-	14/37/103/103	0/5/6/6
29	CLA	B	606	2	-	20/39/115/115	-
29	CLA	s1	604	-	-	8/27/103/115	-
29	CLA	G	603	21	-	16/39/115/115	-
30	PHO	a1	408	-	-	17/37/103/103	0/5/6/6
29	CLA	c	512	-	-	18/39/115/115	-
48	CHL	s1	608	-	1/1/14/21	5/35/111/117	-
31	BCR	A	411	-	-	12/29/63/63	0/2/2/2
48	CHL	s1	606	-	-	0/15/91/117	-
29	CLA	s1	609	-	-	19/33/109/115	-
31	BCR	b1	619	-	-	9/29/63/63	0/2/2/2
29	CLA	N	603	-	-	19/39/115/115	-
55	PTY	Y	627	-	-	15/20/20/53	-
29	CLA	n	603	-	-	25/39/115/115	-
33	LMG	C	521	-	-	16/46/66/70	0/1/1/1
38	3PH	t1	101	-	-	30/49/49/49	-
29	CLA	y	614	-	-	17/39/115/115	-
51	NEX	R	622	-	-	8/27/83/83	0/3/3/3
48	CHL	S1	608	-	1/1/14/21	10/35/111/117	-
39	DGA	b	625	-	-	26/45/45/45	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s1	613	-	-	13/27/103/115	-
29	CLA	Y	611	-	-	12/39/115/115	-
29	CLA	c1	510	-	-	14/39/115/115	-
29	CLA	B1	611	-	-	13/39/115/115	-
29	CLA	r1	612	-	-	16/33/109/115	-
29	CLA	a	407	-	-	9/20/96/115	-
48	CHL	n	601	20	1/1/15/21	4/41/117/117	-
29	CLA	b	607	-	-	18/39/115/115	-
32	SQD	c1	526	-	-	22/49/69/69	0/1/1/1
48	CHL	y1	605	24	-	4/17/93/117	-
29	CLA	S	612	-	-	6/15/91/115	-
49	LUT	S	620	-	-	3/29/67/67	0/2/2/2
29	CLA	Y	610	-	-	12/39/115/115	-
29	CLA	G	610	21	-	16/39/115/115	-
51	NEX	n	623	-	-	5/27/83/83	1/3/3/3
37	DGD	b1	623	-	-	14/32/72/95	0/2/2/2
49	LUT	Y1	620	-	-	8/29/67/67	0/2/2/2
29	CLA	g1	603	-	-	18/39/115/115	-
29	CLA	B	616	-	-	7/39/115/115	-
29	CLA	C	510	4	-	13/39/115/115	-
48	CHL	Y1	606	-	1/1/15/21	7/41/117/117	-
29	CLA	b	609	2	-	13/39/115/115	-
29	CLA	R	609	-	-	15/33/109/115	-
29	CLA	B1	612	-	-	15/39/115/115	-
48	CHL	S1	607	-	-	2/14/90/117	-
33	LMG	h1	102	-	-	22/43/63/70	0/1/1/1
29	CLA	A1	407	-	-	9/21/97/115	-
31	BCR	c	514	-	-	14/29/63/63	0/2/2/2
29	CLA	Y1	603	-	-	16/39/115/115	-
50	XAT	R	621	-	-	2/31/93/93	0/4/4/4
37	DGD	c1	520	-	-	11/48/88/95	0/2/2/2
29	CLA	B1	615	-	-	14/39/115/115	-
29	CLA	N1	604	-	-	20/39/115/115	-
32	SQD	A1	412	-	-	15/46/66/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
33	LMG	H	102	-	-	14/43/63/70	0/1/1/1
55	PTY	Y1	627	-	-	12/20/20/53	-
29	CLA	r1	610	-	-	15/33/109/115	-
40	LHG	g	624	-	-	27/53/53/53	-
49	LUT	S1	620	-	-	4/29/67/67	0/2/2/2
49	LUT	Y1	621	-	-	6/29/67/67	0/2/2/2
48	CHL	N	609	-	1/1/15/21	11/41/117/117	-
29	CLA	D	403	-	-	18/39/115/115	-
29	CLA	g	602	-	-	22/39/115/115	-
33	LMG	D	411	-	-	11/41/61/70	0/1/1/1
40	LHG	N	624	-	-	31/53/53/53	-
48	CHL	n1	609	-	1/1/15/21	5/41/117/117	-
40	LHG	n	624	-	-	35/53/53/53	-
48	CHL	r	606	-	-	3/15/91/117	-
48	CHL	R	606	-	-	1/15/91/117	-
29	CLA	c1	512	-	-	17/39/115/115	-
37	DGD	B1	623	-	-	11/32/72/95	0/2/2/2
38	3PH	B	624	-	-	34/49/49/49	-
32	SQD	a	412	-	-	14/46/66/69	0/1/1/1
32	SQD	m1	101	-	-	22/37/57/69	0/1/1/1
50	XAT	Y	622	-	-	7/31/93/93	0/4/4/4
31	BCR	c	516	-	-	15/29/63/63	0/2/2/2
31	BCR	B	618	-	-	11/29/63/63	0/2/2/2
51	NEX	N	623	-	-	4/27/83/83	1/3/3/3
29	CLA	n1	613	-	-	22/39/115/115	-
37	DGD	c	519	-	-	23/51/91/95	0/2/2/2
50	XAT	N	622	-	1/1/12/26	2/31/93/93	0/4/4/4
36	C7Z	b1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
29	CLA	D1	403	-	-	17/39/115/115	-
40	LHG	s1	624	29	-	27/49/49/53	-
29	CLA	g1	614	-	-	13/20/96/115	-
38	3PH	s1	626	-	-	27/49/49/49	-
49	LUT	r	620	-	-	6/29/67/67	0/2/2/2
49	LUT	s	620	-	-	1/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
48	CHL	s	601	-	-	4/17/93/117	-
31	BCR	d	404	-	-	13/29/63/63	0/2/2/2
51	NEX	r	622	-	-	9/27/83/83	0/3/3/3
29	CLA	c	505	4	-	21/39/115/115	-
31	BCR	C	516	-	-	13/29/63/63	0/2/2/2
29	CLA	G1	604	-	-	10/20/96/115	-
29	CLA	G1	614	-	-	8/20/96/115	-
29	CLA	b1	612	-	-	18/39/115/115	-
31	BCR	B	619	-	-	8/29/63/63	0/2/2/2
48	CHL	G	608	-	-	1/15/91/117	-
40	LHG	Y1	624	-	-	18/53/53/53	-
29	CLA	r	610	-	-	13/33/109/115	-
29	CLA	s	610	-	-	20/39/115/115	-
29	CLA	R1	604	-	-	12/20/96/115	-
44	HEM	F1	101	7	-	1/14/54/54	-
29	CLA	s	611	40	-	17/39/115/115	-
30	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
29	CLA	y	604	-	-	15/39/115/115	-
39	DGA	j1	101	-	-	20/30/30/45	-
37	DGD	C	518	-	-	18/44/84/95	0/2/2/2
29	CLA	n1	610	-	-	22/39/115/115	-
48	CHL	N1	608	-	-	6/22/98/117	-
45	RRX	H1	101	-	1/1/11/25	9/29/65/65	0/2/2/2
38	3PH	S	626	-	-	24/49/49/49	-
29	CLA	y	611	40	-	16/39/115/115	-
29	CLA	c	511	4	-	9/39/115/115	-
49	LUT	N1	621	-	-	4/29/67/67	0/2/2/2
40	LHG	D1	409	-	-	31/53/53/53	-
29	CLA	a1	410	1	-	13/33/109/115	-
31	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
39	DGA	C	524	-	-	18/45/45/45	-
29	CLA	y	613	-	-	24/39/115/115	-
48	CHL	G	607	-	1/1/15/21	11/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	S1	606	-	-	2/15/91/117	-
29	CLA	r	612	-	-	16/33/109/115	-
51	NEX	g	623	-	1/1/12/25	9/27/83/83	0/3/3/3
29	CLA	B1	603	2	-	21/39/115/115	-
49	LUT	s	621	-	-	3/29/67/67	0/2/2/2
48	CHL	N1	609	-	1/1/15/21	10/41/117/117	-
49	LUT	R1	620	-	-	9/29/67/67	0/2/2/2
29	CLA	D	402	-	-	19/39/115/115	-
38	3PH	S1	626	-	-	30/49/49/49	-
51	NEX	R1	622	-	-	14/27/83/83	0/3/3/3
39	DGA	b1	625	-	-	22/45/45/45	-
48	CHL	y	601	24	1/1/15/21	9/41/117/117	-
40	LHG	D	409	-	-	25/53/53/53	-
39	DGA	J	101	-	-	12/30/30/45	-
48	CHL	s	608	-	1/1/14/21	5/35/111/117	-
29	CLA	g	610	-	-	21/39/115/115	-
29	CLA	r	609	-	-	12/33/109/115	-
29	CLA	n	612	-	-	7/15/91/115	-
29	CLA	Y	608	-	-	9/21/97/115	-
29	CLA	n	614	-	-	6/20/96/115	-
29	CLA	C	503	-	-	20/39/115/115	-
29	CLA	b1	604	-	-	20/39/115/115	-
29	CLA	c1	508	4	-	12/39/115/115	-
31	BCR	c	515	-	-	10/29/63/63	0/2/2/2
29	CLA	c1	504	-	-	21/39/115/115	-
29	CLA	r	604	-	-	11/20/96/115	-
50	XAT	y	622	-	-	8/31/93/93	0/4/4/4
48	CHL	n1	605	-	1/1/15/21	7/41/117/117	-
29	CLA	r1	603	22	-	20/33/109/115	-
48	CHL	G	606	-	-	5/22/98/117	-
38	3PH	b	624	-	-	23/49/49/49	-
29	CLA	B	614	-	-	14/39/115/115	-
29	CLA	S	602	-	-	16/33/109/115	-
33	LMG	C	523	-	-	21/50/70/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	613	-	-	21/39/115/115	-
48	CHL	n	608	-	-	6/22/98/117	-
48	CHL	n	606	-	1/1/15/21	7/41/117/117	-
29	CLA	r1	608	-	-	16/33/109/115	-
29	CLA	b1	603	-	-	21/39/115/115	-

The worst 5 of 3547 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	R	626	ERG	C1-C10	-23.16	1.10	1.54
53	r	626	ERG	C1-C10	-22.96	1.10	1.54
53	R1	626	ERG	C1-C10	-22.89	1.10	1.54
53	r1	626	ERG	C1-C10	-22.73	1.11	1.54
53	r	626	ERG	C10-C9	-20.15	1.28	1.55

The worst 5 of 9056 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	L	101	LHG	O7-C7-C8	22.97	161.00	111.50
40	l	101	LHG	O7-C7-C8	22.96	160.99	111.50
29	R	609	CLA	C4-C3-C5	-22.39	77.60	115.27
38	S	626	3PH	O21-C21-C22	22.18	159.31	111.50
38	S1	626	3PH	O21-C21-C22	22.13	159.19	111.50

5 of 109 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	B	620	C7Z	C3
36	b	620	C7Z	C3
36	B1	620	C7Z	C3
36	b1	620	C7Z	C3
41	C	527	LMK	C8

5 of 9888 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	O2A-C1-C2-C3
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA
29	A	407	CLA	C2-C1-O2A-CGA

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
51	N	623	NEX	C1-C2-C3-C4-C5-C6
51	n	623	NEX	C1-C2-C3-C4-C5-C6

662 monomers are involved in 2295 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	612	CLA	5	0
40	L1	101	LHG	6	0
29	C1	505	CLA	4	0
29	S1	602	CLA	6	0
49	y	621	LUT	3	0
39	J1	101	DGA	4	0
49	y1	620	LUT	6	0
29	B	617	CLA	5	0
29	c	507	CLA	6	0
48	n1	608	CHL	5	0
29	c	501	CLA	5	0
29	y	610	CLA	1	0
34	y	625	SPH	4	0
50	g1	622	XAT	6	0
40	D	408	LHG	3	0
55	y1	626	PTY	9	0
29	B	603	CLA	8	0
29	b	602	CLA	1	0
29	g	614	CLA	2	0
29	a	406	CLA	5	0
29	d1	402	CLA	9	0
29	C1	508	CLA	7	0
33	d	411	LMG	2	0
29	B1	609	CLA	9	0
31	C	515	BCR	3	0
48	s	606	CHL	3	0
29	b1	613	CLA	6	0
49	R	620	LUT	6	0
29	N	610	CLA	4	0
29	c	504	CLA	4	0
29	A1	406	CLA	4	0
29	Y1	611	CLA	8	0
29	r	603	CLA	3	0
38	s	626	3PH	6	0
50	G	622	XAT	6	0
31	B1	619	BCR	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	b1	626	SQD	4	0
53	r	626	ERG	7	0
48	G1	601	CHL	3	0
40	g1	624	LHG	7	0
48	g1	609	CHL	4	0
29	r	608	CLA	4	0
29	B1	610	CLA	5	0
52	r	625	LMT	4	0
29	g1	610	CLA	4	0
32	m	101	SQD	6	0
29	C1	512	CLA	8	0
48	G1	605	CHL	1	0
33	b1	622	LMG	5	0
44	f1	101	HEM	3	0
48	Y1	609	CHL	7	0
29	y1	604	CLA	2	0
29	s	604	CLA	2	0
47	K	101	4RF	2	0
40	d1	408	LHG	4	0
29	b	616	CLA	8	0
31	d1	404	BCR	3	0
29	b1	614	CLA	7	0
29	C1	501	CLA	8	0
29	G	602	CLA	8	0
29	y	608	CLA	3	0
47	I1	102	4RF	9	0
29	a	410	CLA	6	0
29	g1	612	CLA	1	0
29	N	611	CLA	4	0
48	y1	607	CHL	8	0
29	n1	611	CLA	2	0
49	G1	620	LUT	6	0
37	C1	518	DGD	11	0
51	S1	623	NEX	4	0
34	a1	414	SPH	1	0
29	N1	603	CLA	7	0
31	C	517	BCR	1	0
29	g1	602	CLA	12	0
50	Y1	622	XAT	4	0
29	A	407	CLA	1	0
31	c1	515	BCR	7	0
37	c	520	DGD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	j	101	DGA	3	0
47	i1	101	4RF	2	0
49	S	621	LUT	5	0
48	y	606	CHL	2	0
29	s	603	CLA	2	0
48	g	606	CHL	3	0
50	n1	622	XAT	5	0
44	F	101	HEM	3	0
48	G1	609	CHL	6	0
29	A1	410	CLA	7	0
50	r1	621	XAT	5	0
37	C	520	DGD	2	0
51	s	623	NEX	3	0
52	R1	625	LMT	7	0
49	S1	621	LUT	6	0
47	i	101	4RF	6	0
48	N	608	CHL	1	0
31	b	619	BCR	1	0
29	c	513	CLA	3	0
29	B	604	CLA	4	0
29	R1	609	CLA	4	0
29	y1	614	CLA	6	0
33	B	622	LMG	2	0
29	Y1	610	CLA	4	0
38	t	101	3PH	2	0
54	s1	625	LPX	3	0
48	N	601	CHL	4	0
29	S1	609	CLA	2	0
29	C	506	CLA	7	0
29	C	512	CLA	3	0
40	N1	624	LHG	5	0
29	y1	603	CLA	6	0
29	G1	602	CLA	8	0
30	a	408	PHO	5	0
37	c1	519	DGD	9	0
48	N	605	CHL	3	0
48	g1	608	CHL	2	0
33	C1	523	LMG	4	0
43	d	405	PL9	7	0
29	s1	602	CLA	4	0
48	N	607	CHL	3	0
29	r	602	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	N1	601	CHL	8	0
29	R	608	CLA	4	0
30	a1	409	PHO	11	0
29	g1	604	CLA	3	0
51	N1	623	NEX	6	0
49	Y	621	LUT	6	0
37	C	519	DGD	9	0
29	y	603	CLA	3	0
47	k1	101	4RF	2	0
49	G	621	LUT	7	0
39	c	524	DGA	9	0
29	c1	505	CLA	9	0
29	y	602	CLA	9	0
33	B1	622	LMG	5	0
48	r1	607	CHL	2	0
29	c	506	CLA	6	0
30	A	408	PHO	5	0
29	c1	506	CLA	3	0
49	n	620	LUT	3	0
33	b	622	LMG	5	0
37	C1	520	DGD	12	0
40	D	410	LHG	2	0
29	B	612	CLA	8	0
51	r1	622	NEX	5	0
29	N	612	CLA	3	0
38	B1	624	3PH	6	0
29	C1	503	CLA	2	0
29	B1	613	CLA	3	0
29	S1	614	CLA	1	0
48	Y	607	CHL	1	0
53	R	626	ERG	7	0
31	a1	411	BCR	4	0
29	b1	605	CLA	9	0
48	S	606	CHL	3	0
29	B	615	CLA	2	0
32	B	621	SQD	2	0
31	c1	517	BCR	8	0
29	B	610	CLA	7	0
31	C1	515	BCR	5	0
29	Y1	614	CLA	3	0
33	c	521	LMG	4	0
39	C1	524	DGA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	c1	518	DGD	11	0
29	y1	611	CLA	4	0
29	c1	513	CLA	8	0
29	C	502	CLA	2	0
40	c1	525	LHG	11	0
48	g	607	CHL	2	0
48	y1	606	CHL	1	0
29	R	610	CLA	5	0
40	d1	409	LHG	6	0
32	B	626	SQD	4	0
49	N	620	LUT	6	0
40	s	624	LHG	4	0
49	n1	620	LUT	4	0
48	g1	605	CHL	2	0
29	c	509	CLA	4	0
29	g	612	CLA	1	0
40	y	624	LHG	5	0
29	c1	509	CLA	4	0
40	C	525	LHG	7	0
29	Y	602	CLA	15	0
29	s1	614	CLA	2	0
26	a1	401	OEX	1	0
29	B1	607	CLA	4	0
29	b	617	CLA	5	0
48	n1	601	CHL	6	0
29	b	614	CLA	4	0
29	G	614	CLA	1	0
54	S	625	LPX	4	0
29	b1	608	CLA	4	0
50	r	621	XAT	2	0
31	b1	618	BCR	2	0
29	N	614	CLA	1	0
48	r	607	CHL	1	0
29	C	508	CLA	3	0
29	n1	614	CLA	1	0
48	s	607	CHL	2	0
29	A1	405	CLA	6	0
29	c1	503	CLA	5	0
48	r1	606	CHL	4	0
29	C	509	CLA	3	0
29	b	615	CLA	6	0
29	C1	510	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	N1	612	CLA	3	0
40	d	409	LHG	7	0
33	A	413	LMG	3	0
48	n	605	CHL	4	0
54	S1	625	LPX	2	0
29	R1	610	CLA	7	0
49	s1	620	LUT	4	0
39	B1	625	DGA	1	0
29	g	611	CLA	3	0
30	a	409	PHO	2	0
49	G1	621	LUT	10	0
48	S	607	CHL	1	0
29	S1	613	CLA	2	0
49	y1	621	LUT	7	0
29	N1	610	CLA	8	0
33	c1	523	LMG	4	0
29	a1	407	CLA	3	0
43	d1	405	PL9	8	0
50	n	622	XAT	6	0
29	G1	603	CLA	9	0
52	R	625	LMT	4	0
31	c	517	BCR	1	0
52	r1	625	LMT	2	0
29	C1	504	CLA	6	0
29	a1	405	CLA	9	0
44	f	101	HEM	1	0
48	N1	606	CHL	7	0
29	B1	616	CLA	11	0
29	C1	507	CLA	8	0
48	g1	601	CHL	7	0
53	R1	626	ERG	9	0
29	Y1	608	CLA	5	0
29	s	602	CLA	1	0
29	R1	612	CLA	2	0
29	g1	611	CLA	3	0
29	s1	611	CLA	7	0
26	A	401	OEX	1	0
32	M	101	SQD	4	0
29	N	602	CLA	6	0
33	w	201	LMG	6	0
48	g	609	CHL	4	0
29	n1	602	CLA	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	s	625	LPX	3	0
29	C	501	CLA	8	0
29	G1	610	CLA	2	0
31	c1	514	BCR	9	0
48	n1	607	CHL	6	0
29	s	613	CLA	2	0
49	r1	620	LUT	7	0
50	R1	621	XAT	5	0
29	Y	604	CLA	4	0
48	y1	609	CHL	6	0
48	R1	607	CHL	2	0
31	C1	517	BCR	5	0
47	I	102	4RF	2	0
45	h	101	RRX	3	0
29	y1	610	CLA	7	0
48	y	607	CHL	3	0
32	b	621	SQD	5	0
29	b1	606	CLA	8	0
29	S	617	CLA	1	0
40	C1	525	LHG	8	0
34	A1	414	SPH	4	0
29	C	511	CLA	1	0
29	S1	611	CLA	4	0
48	R	607	CHL	2	0
29	b	611	CLA	5	0
40	D1	408	LHG	3	0
48	g	605	CHL	1	0
29	B	613	CLA	5	0
40	S	624	LHG	5	0
29	N	613	CLA	4	0
29	n1	612	CLA	1	0
29	b	605	CLA	4	0
32	a1	412	SQD	3	0
55	y	626	PTY	9	0
49	Y	620	LUT	2	0
49	G	620	LUT	6	0
29	Y	603	CLA	4	0
29	c1	501	CLA	8	0
29	y1	612	CLA	6	0
40	l	101	LHG	4	0
49	n1	621	LUT	10	0
49	g	620	LUT	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	Y	625	SPH	4	0
29	G1	611	CLA	6	0
40	S1	624	LHG	5	0
45	H	101	RRX	1	0
29	c	508	CLA	4	0
48	S1	601	CHL	2	0
29	c	503	CLA	4	0
29	b1	615	CLA	3	0
48	G	601	CHL	4	0
48	y	605	CHL	1	0
49	g1	621	LUT	13	0
29	C	505	CLA	6	0
31	C	514	BCR	10	0
39	c1	524	DGA	4	0
31	b	618	BCR	5	0
29	b	604	CLA	3	0
29	B	602	CLA	2	0
48	Y1	601	CHL	4	0
29	C1	509	CLA	3	0
29	b1	609	CLA	8	0
32	B1	626	SQD	3	0
49	g1	620	LUT	9	0
29	N	604	CLA	2	0
29	R	612	CLA	1	0
29	n1	604	CLA	6	0
29	B1	606	CLA	5	0
29	s	612	CLA	2	0
29	B	608	CLA	4	0
29	A	410	CLA	6	0
29	Y	613	CLA	9	0
29	G	613	CLA	2	0
29	n	610	CLA	3	0
29	C1	502	CLA	2	0
31	D1	404	BCR	4	0
29	N1	611	CLA	3	0
29	N1	602	CLA	8	0
29	B1	614	CLA	8	0
48	G1	608	CHL	2	0
55	Y	626	PTY	5	0
33	w1	201	LMG	4	0
29	N1	613	CLA	10	0
48	Y	609	CHL	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	G	624	LHG	4	0
30	A1	409	PHO	8	0
43	D	405	PL9	4	0
48	Y	601	CHL	1	0
47	k	101	4RF	2	0
29	g	603	CLA	4	0
29	g	604	CLA	1	0
29	Y1	612	CLA	6	0
48	Y	605	CHL	2	0
48	G	605	CHL	1	0
29	d	402	CLA	5	0
31	D	404	BCR	3	0
50	G1	622	XAT	10	0
29	R1	608	CLA	2	0
51	Y	623	NEX	2	0
29	G1	613	CLA	6	0
34	a	414	SPH	3	0
40	c	525	LHG	4	0
29	b	612	CLA	2	0
48	G1	607	CHL	6	0
33	W1	201	LMG	8	0
48	n	607	CHL	7	0
29	b	606	CLA	5	0
29	S	609	CLA	3	0
33	h	102	LMG	5	0
34	A	414	SPH	1	0
38	b1	624	3PH	8	0
29	c1	511	CLA	9	0
29	s1	603	CLA	3	0
48	n1	606	CHL	7	0
29	B1	602	CLA	5	0
43	D1	405	PL9	11	0
48	n	609	CHL	2	0
48	R1	606	CHL	2	0
29	S	604	CLA	3	0
29	b1	617	CLA	7	0
29	y1	602	CLA	17	0
38	T1	101	3PH	8	0
48	g1	607	CHL	3	0
29	n1	603	CLA	8	0
29	Y	612	CLA	2	0
29	G	612	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B1	617	CLA	7	0
32	b	626	SQD	2	0
40	d1	410	LHG	7	0
29	S	613	CLA	1	0
29	D1	402	CLA	8	0
40	Y	624	LHG	6	0
55	Y1	626	PTY	3	0
34	y1	625	SPH	2	0
49	N	621	LUT	2	0
48	Y1	605	CHL	2	0
49	n	621	LUT	2	0
29	R1	602	CLA	4	0
31	A1	411	BCR	4	0
51	Y1	623	NEX	3	0
29	c	510	CLA	2	0
29	R	603	CLA	2	0
29	y1	608	CLA	2	0
48	G1	606	CHL	1	0
32	B1	621	SQD	3	0
29	B	605	CLA	5	0
29	b	608	CLA	7	0
29	b1	611	CLA	7	0
40	y1	624	LHG	6	0
48	G	609	CHL	4	0
29	s1	610	CLA	6	0
29	C	504	CLA	7	0
33	D1	411	LMG	2	0
29	S	603	CLA	3	0
32	A	412	SQD	5	0
29	R	602	CLA	4	0
48	Y1	607	CHL	4	0
29	y1	613	CLA	5	0
29	b1	607	CLA	5	0
29	C	507	CLA	4	0
29	b	610	CLA	6	0
29	r1	602	CLA	4	0
32	C	526	SQD	4	0
33	c	523	LMG	8	0
40	L	101	LHG	5	0
32	b1	621	SQD	4	0
33	A1	413	LMG	10	0
40	d	410	LHG	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	C	513	CLA	10	0
37	B	623	DGD	3	0
29	C1	511	CLA	7	0
29	s1	617	CLA	1	0
37	b	623	DGD	3	0
49	g	621	LUT	9	0
29	c1	502	CLA	7	0
29	B	611	CLA	2	0
29	g1	613	CLA	7	0
31	C1	516	BCR	3	0
48	s1	601	CHL	4	0
29	Y	614	CLA	9	0
48	s1	607	CHL	3	0
51	s1	623	NEX	6	0
31	B1	618	BCR	2	0
29	B1	604	CLA	5	0
39	B	625	DGA	1	0
29	A	405	CLA	4	0
29	R1	603	CLA	6	0
51	y1	623	NEX	2	0
29	c1	507	CLA	8	0
29	Y1	602	CLA	10	0
29	b1	602	CLA	2	0
40	n1	624	LHG	10	0
48	y	609	CHL	2	0
29	B1	608	CLA	7	0
33	a	413	LMG	5	0
49	N1	620	LUT	5	0
32	C1	526	SQD	3	0
51	n1	623	NEX	6	0
48	g	601	CHL	4	0
29	B1	605	CLA	4	0
49	s1	621	LUT	6	0
31	C1	514	BCR	9	0
50	y1	622	XAT	9	0
29	n	604	CLA	1	0
29	S1	610	CLA	6	0
29	A	406	CLA	6	0
29	b1	616	CLA	3	0
29	a1	406	CLA	9	0
29	r1	609	CLA	4	0
32	M1	101	SQD	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d1	403	CLA	4	0
33	W	201	LMG	2	0
29	G	604	CLA	2	0
29	a	405	CLA	3	0
29	Y1	613	CLA	4	0
37	C1	519	DGD	8	0
29	G	611	CLA	3	0
40	G1	624	LHG	6	0
47	K1	101	4RF	5	0
29	r1	604	CLA	1	0
29	s1	612	CLA	1	0
48	N	606	CHL	3	0
38	T	101	3PH	2	0
33	d1	411	LMG	2	0
29	s	614	CLA	1	0
29	S	610	CLA	6	0
29	b	603	CLA	5	0
31	a	411	BCR	3	0
29	S	611	CLA	3	0
34	Y1	625	SPH	7	0
29	S1	603	CLA	1	0
29	n	602	CLA	4	0
48	g	608	CHL	1	0
29	c	502	CLA	3	0
29	C1	506	CLA	5	0
48	g1	606	CHL	2	0
29	b1	610	CLA	9	0
29	S1	604	CLA	3	0
29	d	403	CLA	3	0
51	y	623	NEX	1	0
33	H1	102	LMG	15	0
29	B	607	CLA	5	0
37	c	518	DGD	7	0
53	r1	626	ERG	5	0
45	h1	101	RRX	4	0
29	Y1	604	CLA	7	0
48	S	601	CHL	2	0
48	N1	605	CHL	4	0
33	a1	413	LMG	8	0
50	g	622	XAT	9	0
48	N1	607	CHL	8	0
29	g	613	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	y	620	LUT	2	0
29	B	609	CLA	8	0
29	C1	513	CLA	14	0
48	S	608	CHL	3	0
33	c1	521	LMG	3	0
29	n	613	CLA	8	0
40	d	408	LHG	2	0
29	s	609	CLA	2	0
40	D1	410	LHG	4	0
30	A	409	PHO	6	0
29	B	606	CLA	8	0
29	s1	604	CLA	3	0
29	G	603	CLA	3	0
30	a1	408	PHO	9	0
29	c	512	CLA	1	0
48	s1	608	CHL	5	0
31	A	411	BCR	2	0
48	s1	606	CHL	2	0
29	s1	609	CLA	6	0
31	b1	619	BCR	4	0
29	N	603	CLA	4	0
29	n	603	CLA	5	0
33	C	521	LMG	3	0
38	t1	101	3PH	5	0
29	y	614	CLA	7	0
51	R	622	NEX	2	0
48	S1	608	CHL	5	0
39	b	625	DGA	5	0
29	s1	613	CLA	4	0
29	Y	611	CLA	3	0
29	c1	510	CLA	5	0
29	B1	611	CLA	6	0
29	r1	612	CLA	3	0
29	a	407	CLA	1	0
48	n	601	CHL	2	0
29	b	607	CLA	4	0
32	c1	526	SQD	4	0
48	y1	605	CHL	1	0
49	S	620	LUT	2	0
29	Y	610	CLA	4	0
29	G	610	CLA	6	0
51	n	623	NEX	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	b1	623	DGD	4	0
49	Y1	620	LUT	6	0
29	g1	603	CLA	8	0
29	B	616	CLA	7	0
29	C	510	CLA	2	0
48	Y1	606	CHL	4	0
29	b	609	CLA	4	0
29	R	609	CLA	3	0
29	B1	612	CLA	9	0
48	S1	607	CHL	1	0
33	h1	102	LMG	4	0
29	A1	407	CLA	2	0
31	c	514	BCR	3	0
29	Y1	603	CLA	5	0
50	R	621	XAT	4	0
37	c1	520	DGD	6	0
29	B1	615	CLA	5	0
29	N1	604	CLA	5	0
32	A1	412	SQD	6	0
33	H	102	LMG	2	0
50	N1	622	XAT	9	0
29	r1	610	CLA	6	0
40	g	624	LHG	7	0
49	S1	620	LUT	7	0
49	Y1	621	LUT	8	0
29	g	602	CLA	6	0
29	D	403	CLA	4	0
33	D	411	LMG	2	0
40	N	624	LHG	4	0
40	n	624	LHG	3	0
48	N	609	CHL	5	0
48	n1	609	CHL	4	0
48	r	606	CHL	2	0
48	R	606	CHL	2	0
29	c1	512	CLA	5	0
37	B1	623	DGD	2	0
38	B	624	3PH	7	0
32	a	412	SQD	2	0
32	m1	101	SQD	3	0
50	Y	622	XAT	6	0
31	c	516	BCR	5	0
31	B	618	BCR	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	N	623	NEX	3	0
29	n1	613	CLA	10	0
37	c	519	DGD	1	0
50	N	622	XAT	5	0
29	D1	403	CLA	2	0
40	s1	624	LHG	7	0
29	g1	614	CLA	1	0
38	s1	626	3PH	5	0
49	r	620	LUT	4	0
49	s	620	LUT	3	0
33	C1	521	LMG	9	0
31	d	404	BCR	3	0
51	r	622	NEX	3	0
29	c	505	CLA	5	0
31	C	516	BCR	2	0
29	G1	604	CLA	3	0
29	G1	614	CLA	3	0
29	b1	612	CLA	6	0
48	G	608	CHL	2	0
40	Y1	624	LHG	6	0
29	r	610	CLA	5	0
29	s	610	CLA	5	0
29	R1	604	CLA	2	0
44	F1	101	HEM	3	0
29	s	611	CLA	6	0
30	A1	408	PHO	5	0
29	y	604	CLA	1	0
39	j1	101	DGA	4	0
37	C	518	DGD	4	0
29	n1	610	CLA	4	0
48	N1	608	CHL	4	0
38	S	626	3PH	7	0
45	H1	101	RRX	3	0
29	y	611	CLA	6	0
29	c	511	CLA	4	0
49	N1	621	LUT	7	0
40	D1	409	LHG	5	0
29	a1	410	CLA	11	0
31	c1	516	BCR	7	0
39	C	524	DGA	3	0
29	y	613	CLA	6	0
48	G	607	CHL	6	0

Continued on next page...

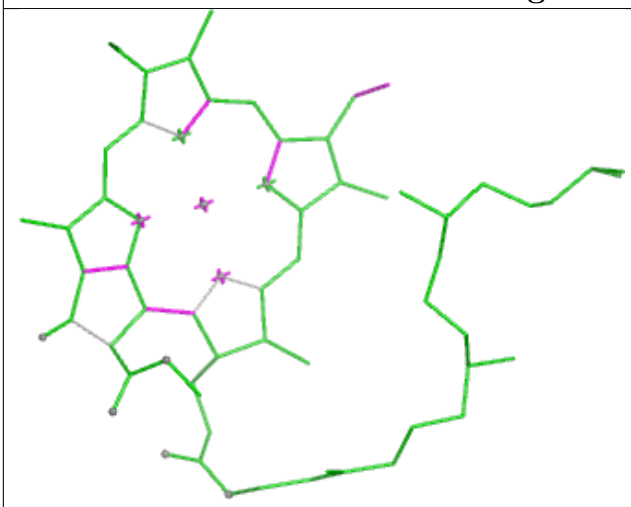
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	S1	606	CHL	4	0
29	r	612	CLA	1	0
51	g	623	NEX	1	0
29	B1	603	CLA	13	0
49	s	621	LUT	1	0
48	N1	609	CHL	9	0
49	R1	620	LUT	4	0
29	D	402	CLA	6	0
38	S1	626	3PH	4	0
51	R1	622	NEX	4	0
39	b1	625	DGA	4	0
48	y	601	CHL	1	0
40	D	409	LHG	6	0
39	J	101	DGA	2	0
29	g	610	CLA	3	0
48	s	608	CHL	5	0
29	r	609	CLA	2	0
29	n	612	CLA	1	0
29	Y	608	CLA	2	0
29	C	503	CLA	2	0
42	D1	401	BCT	1	0
29	b1	604	CLA	9	0
29	c1	508	CLA	8	0
31	c	515	BCR	3	0
29	c1	504	CLA	4	0
29	r	604	CLA	1	0
50	y	622	XAT	4	0
29	r1	603	CLA	2	0
48	n1	605	CHL	3	0
48	G	606	CHL	2	0
38	b	624	3PH	6	0
29	B	614	CLA	6	0
29	S	602	CLA	3	0
33	C	523	LMG	4	0
29	b	613	CLA	4	0
48	n	606	CHL	6	0
29	r1	608	CLA	3	0
29	b1	603	CLA	3	0

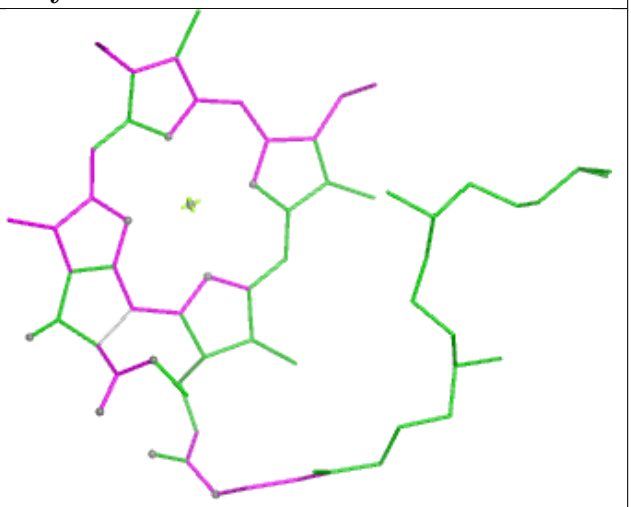
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

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

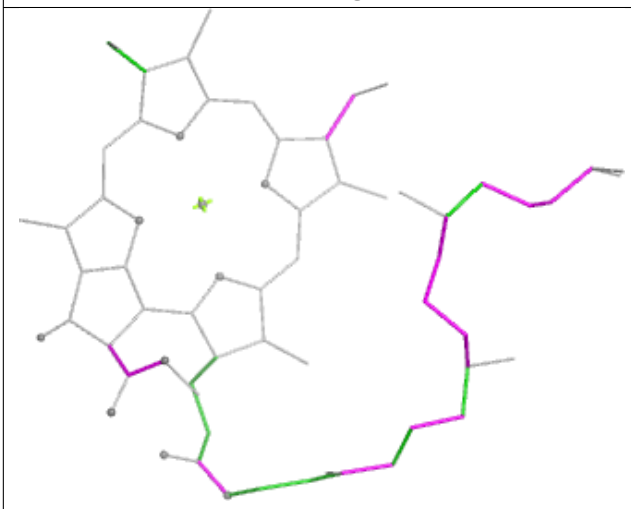
Ligand CLA y 612



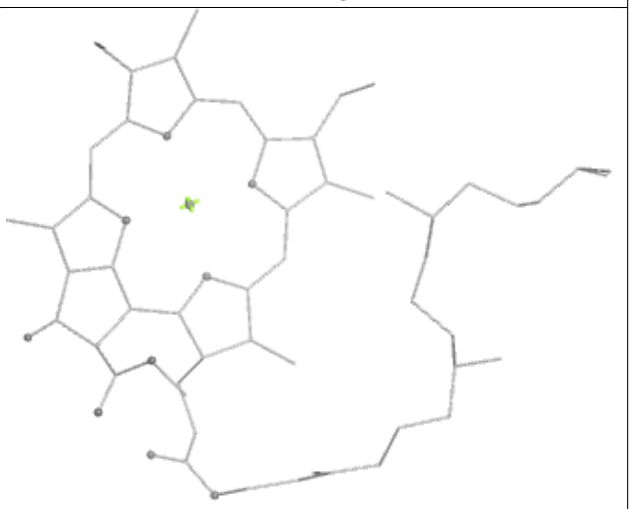
Bond lengths



Bond angles

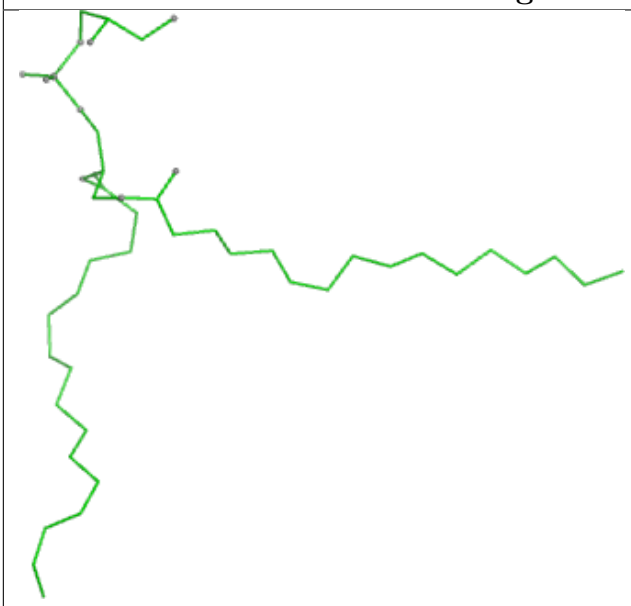


Torsions



Rings

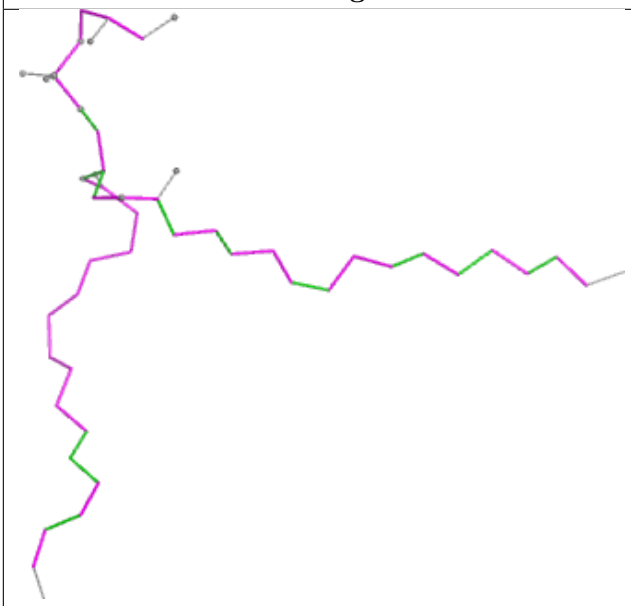
Ligand LHG L1 101



Bond lengths



Bond angles

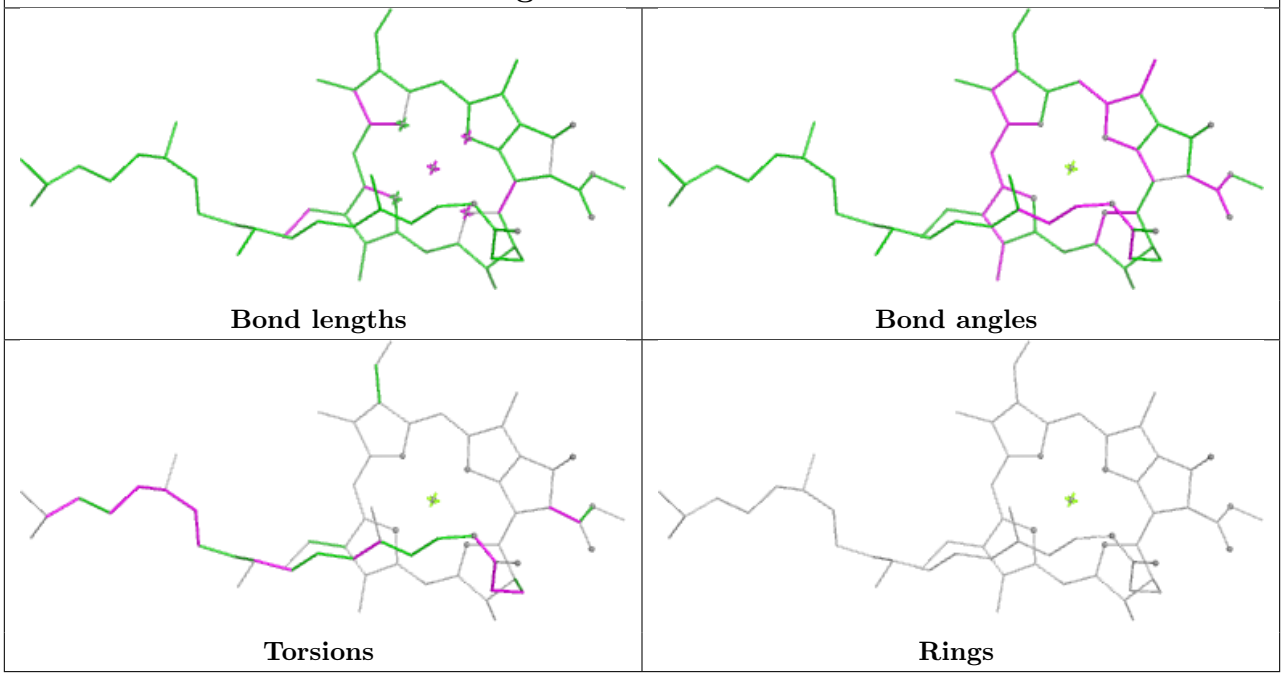


Torsions

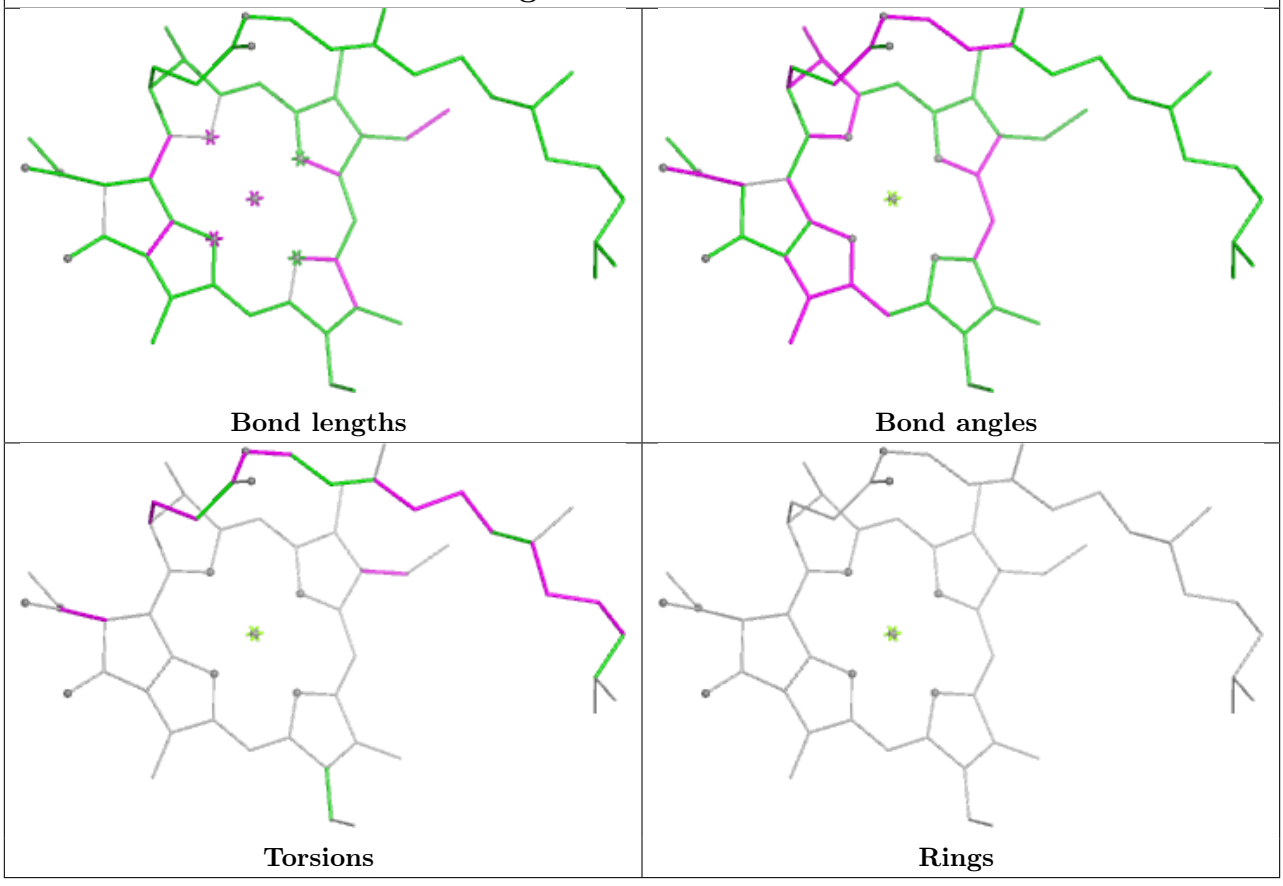


Rings

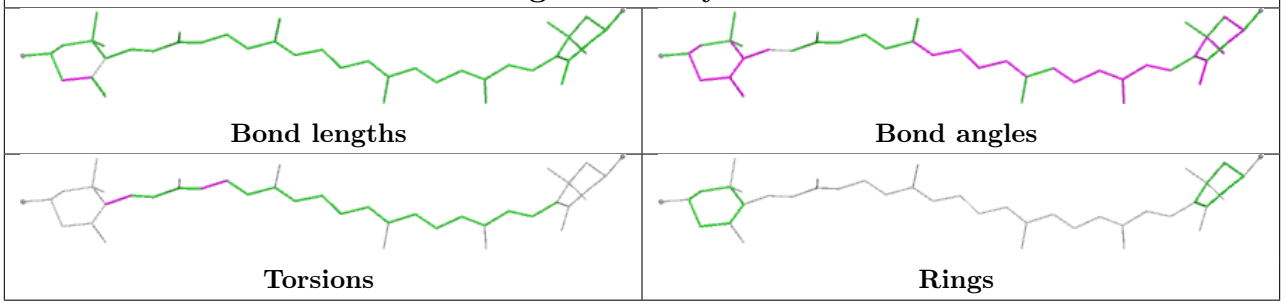
Ligand CLA C1 505



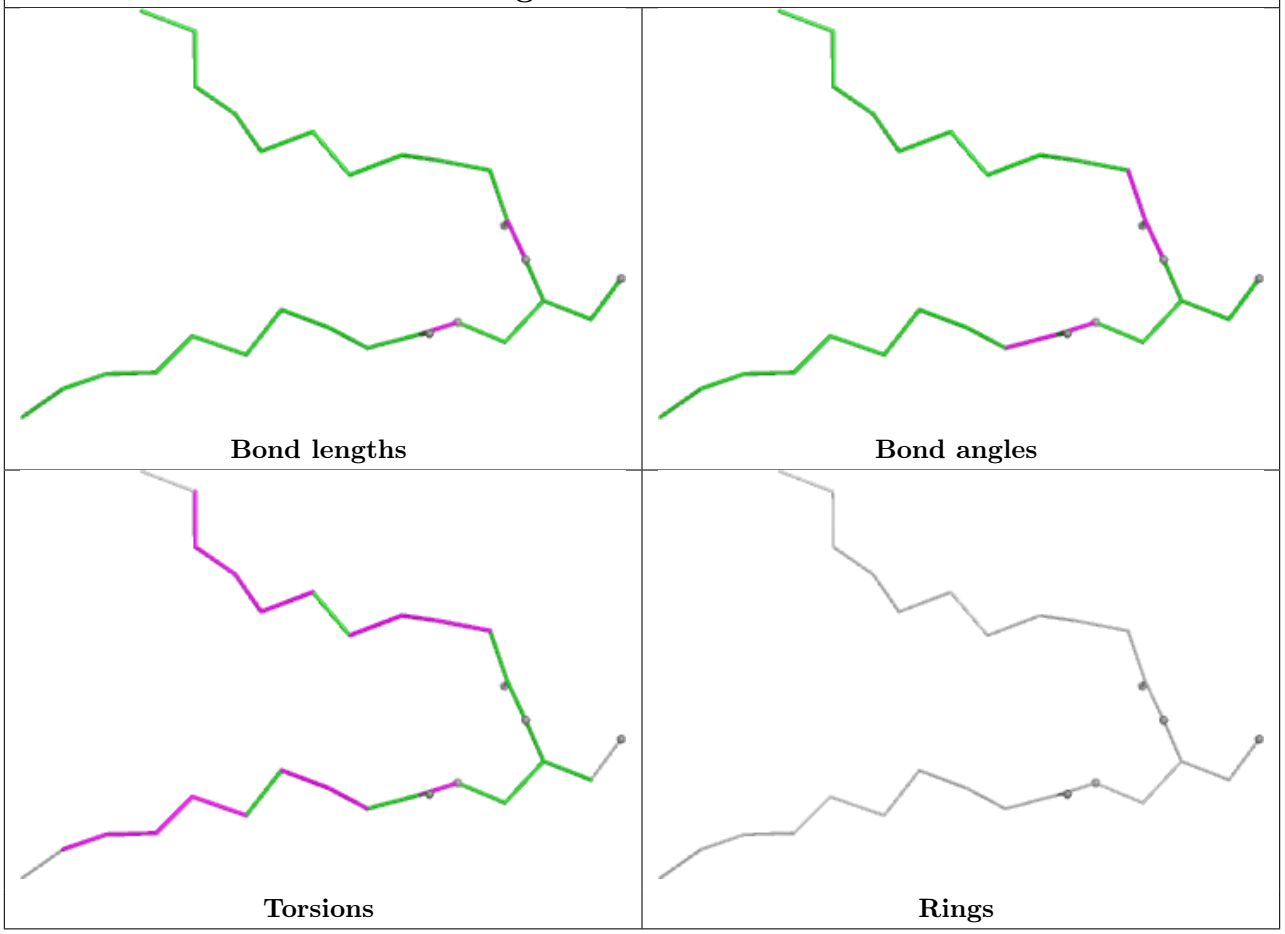
Ligand CLA S1 602



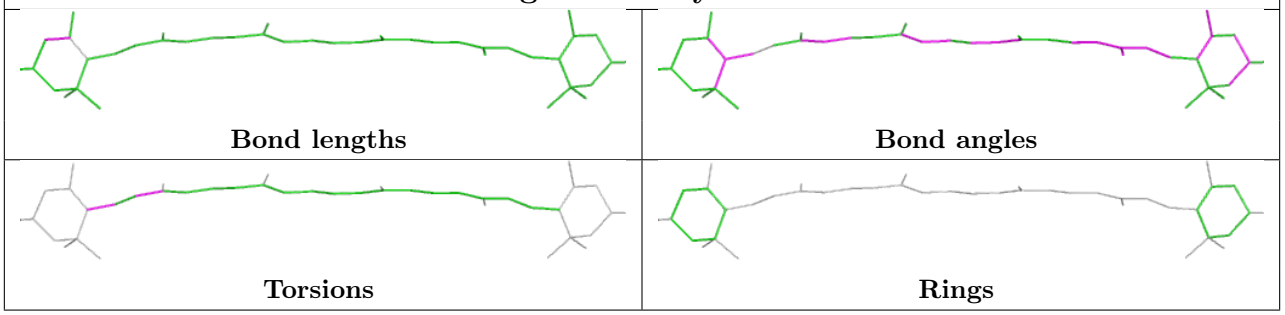
Ligand LUT y 621



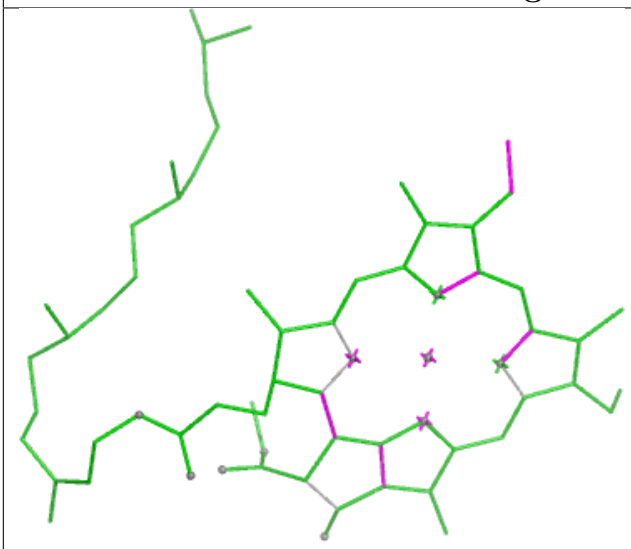
Ligand DGA J1 101



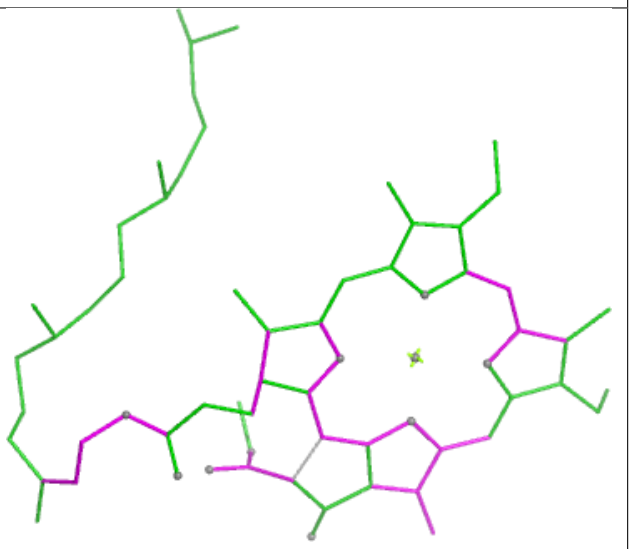
Ligand LUT y1 620



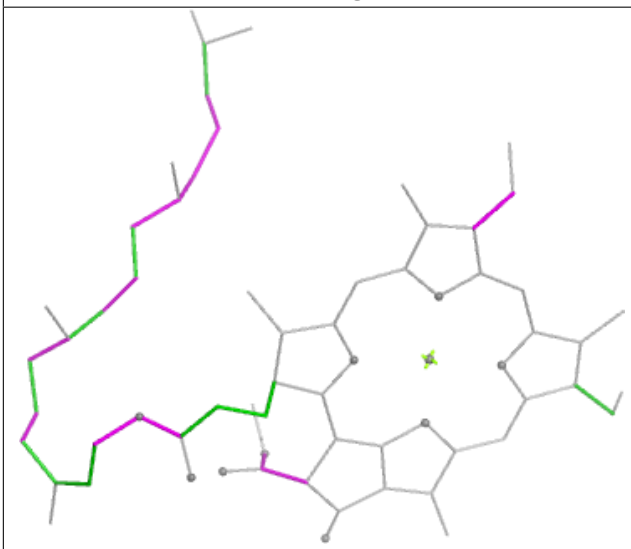
Ligand CLA B 617



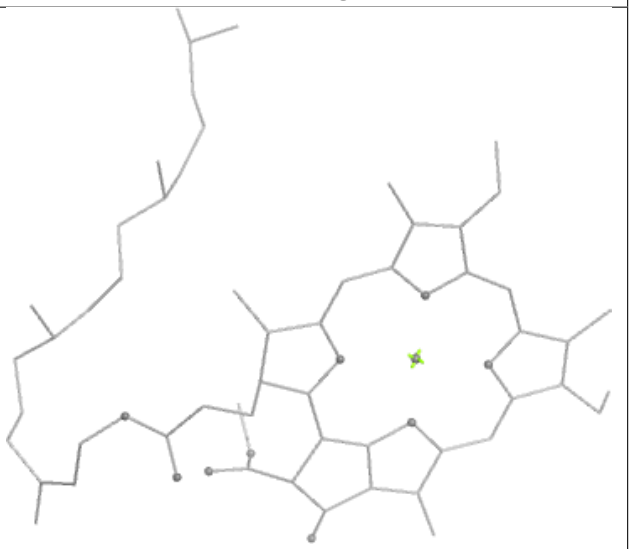
Bond lengths



Bond angles

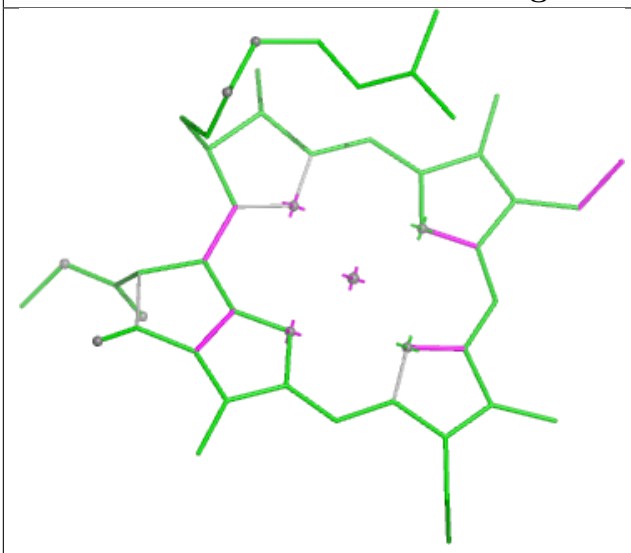


Torsions

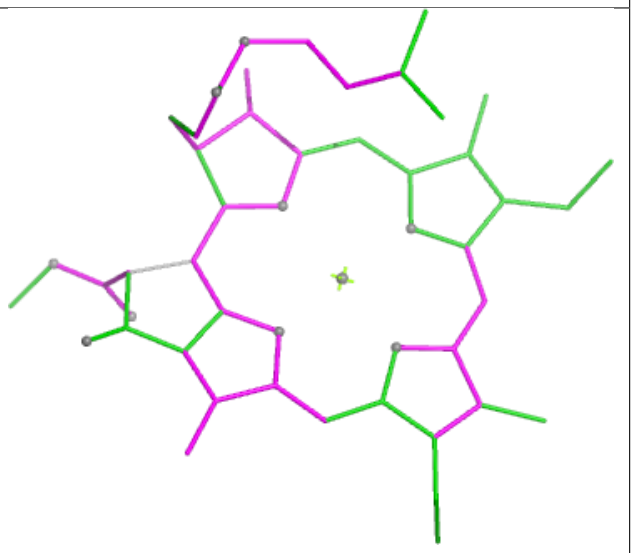


Rings

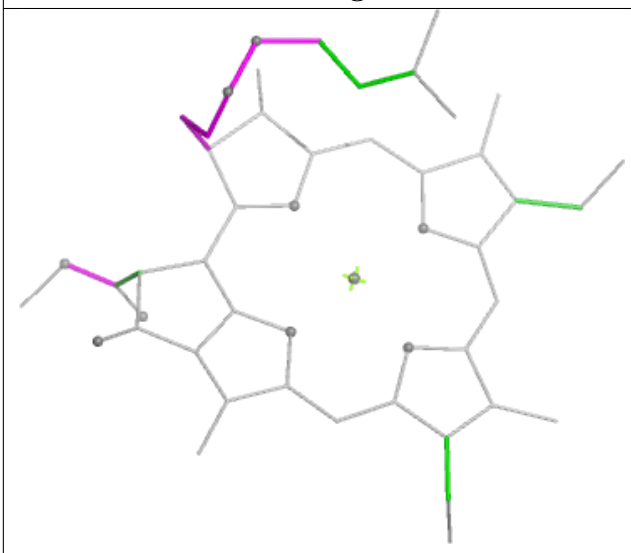
Ligand CLA s 617



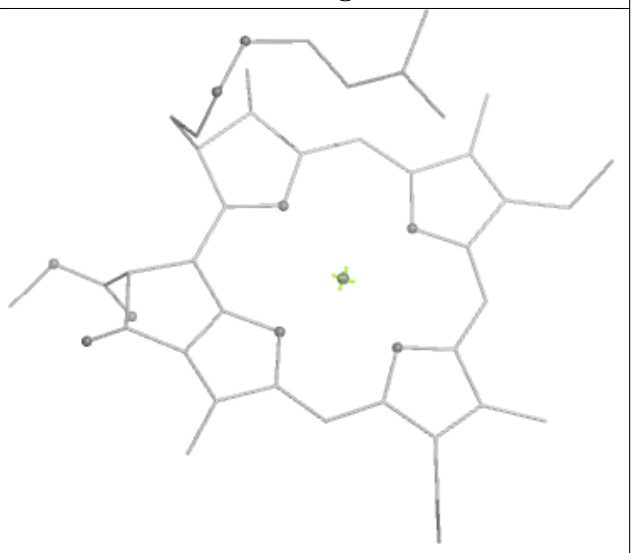
Bond lengths



Bond angles



Torsions

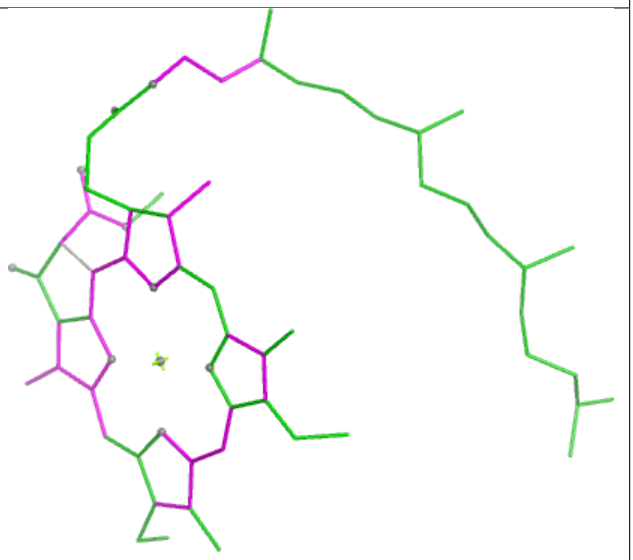


Rings

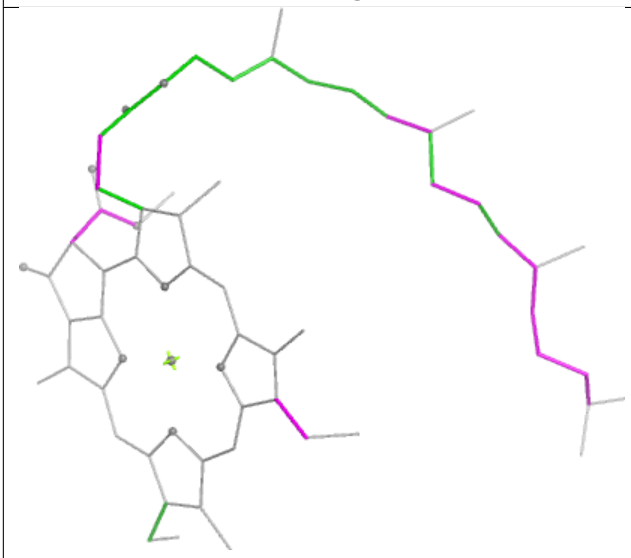
Ligand CLA c 507



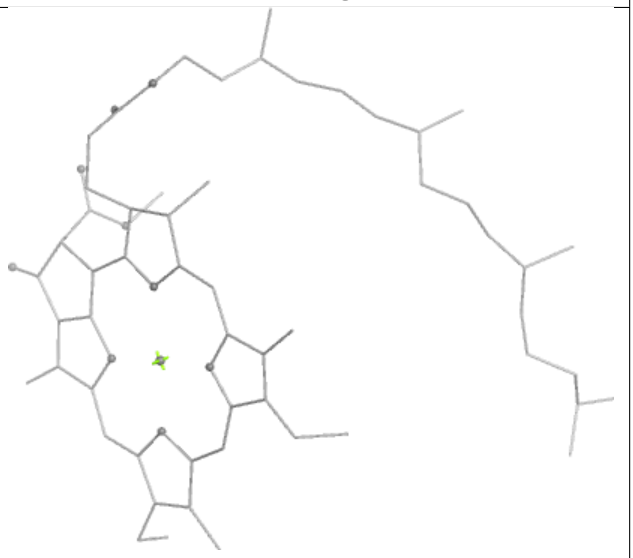
Bond lengths



Bond angles

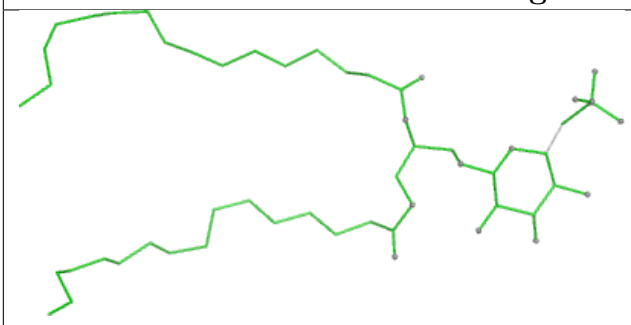


Torsions

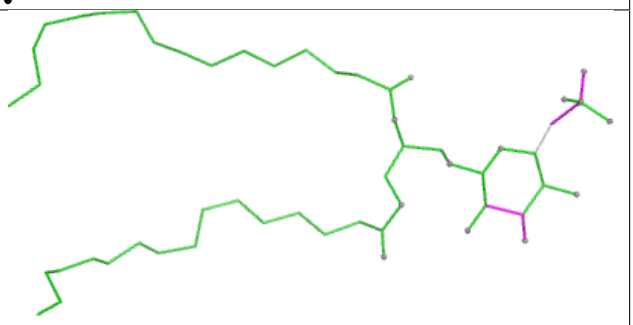


Rings

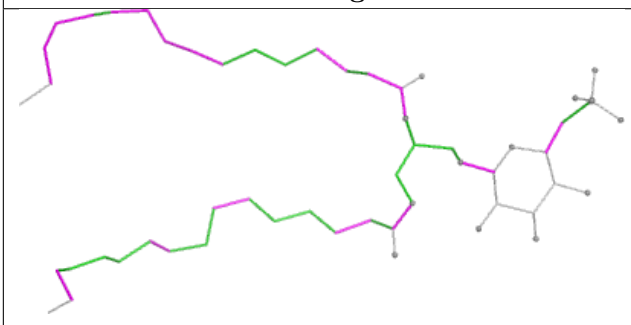
Ligand SQD c 526



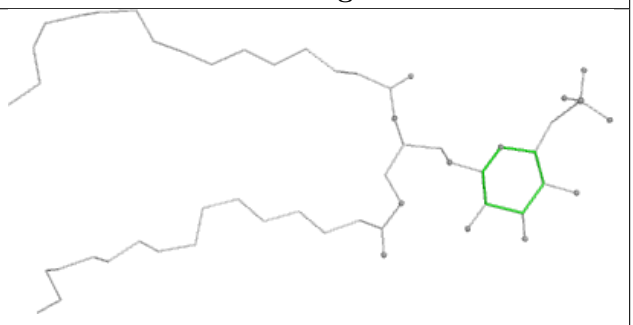
Bond lengths



Bond angles

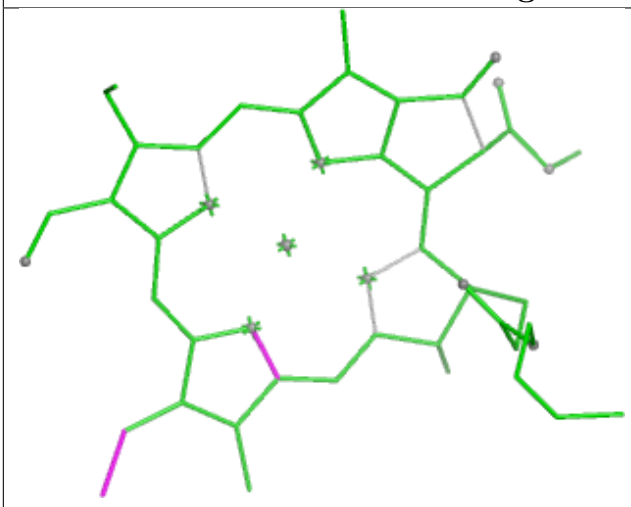


Torsions

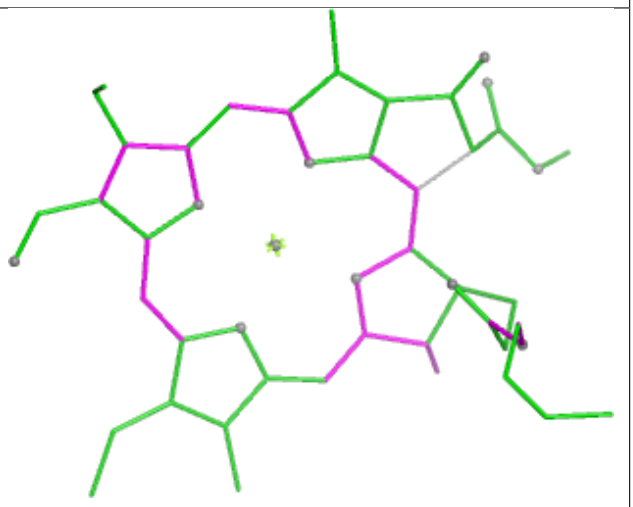


Rings

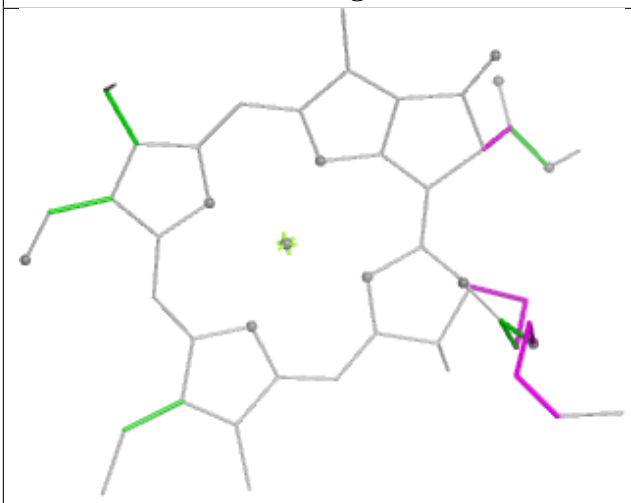
Ligand CHL n1 608



Bond lengths



Bond angles

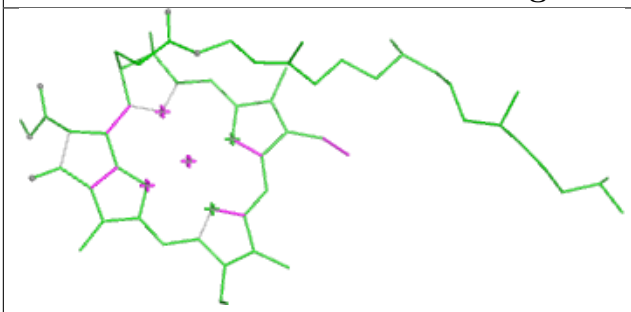


Torsions

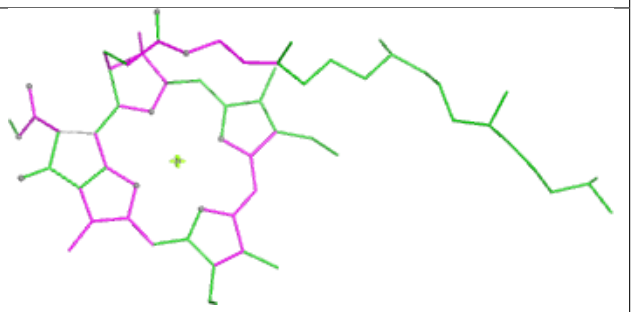


Rings

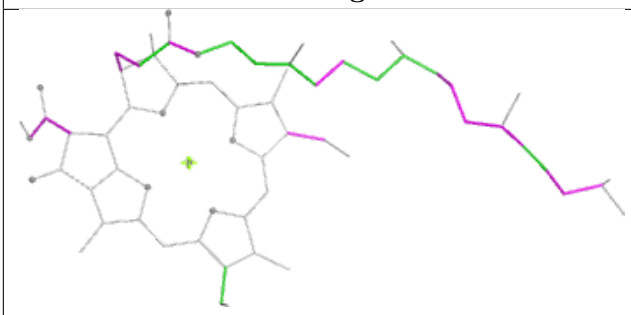
Ligand CLA c 501



Bond lengths



Bond angles

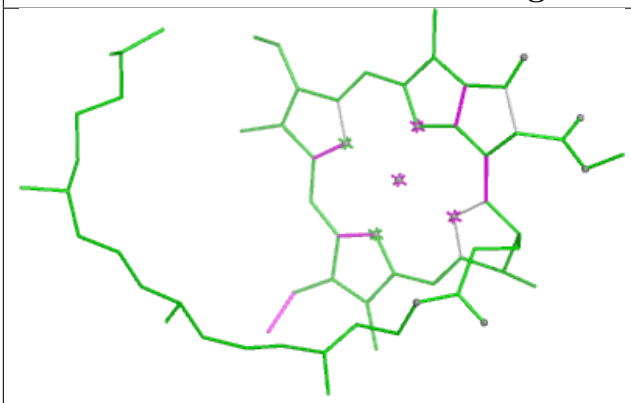


Torsions

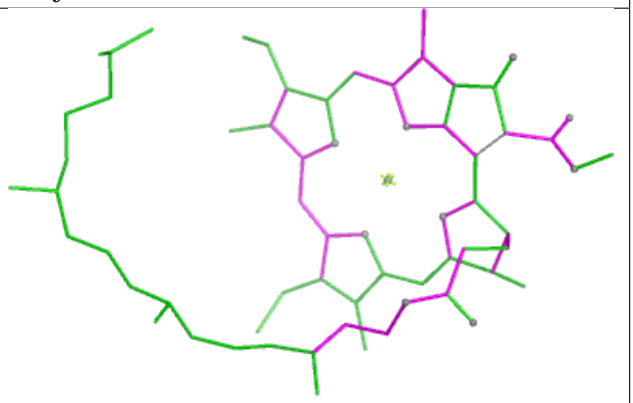


Rings

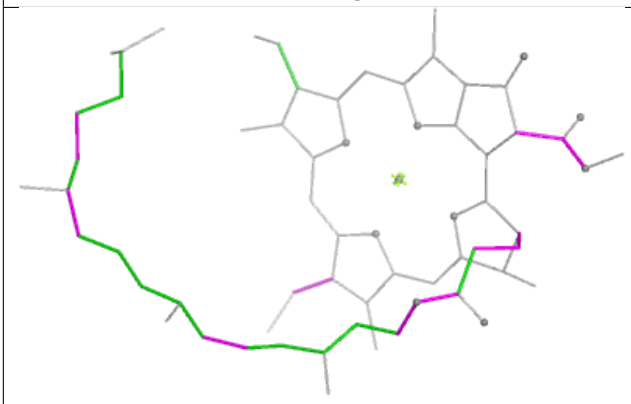
Ligand CLA y 610



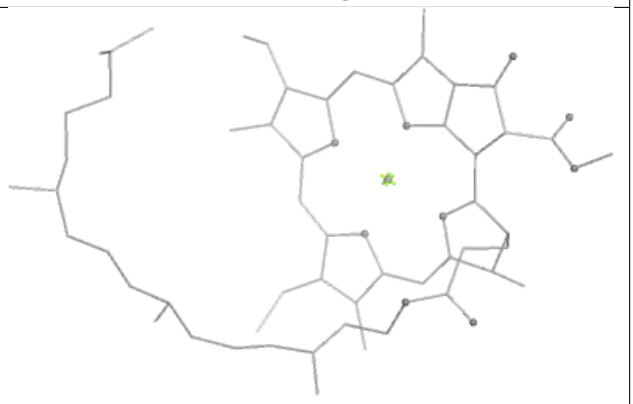
Bond lengths



Bond angles

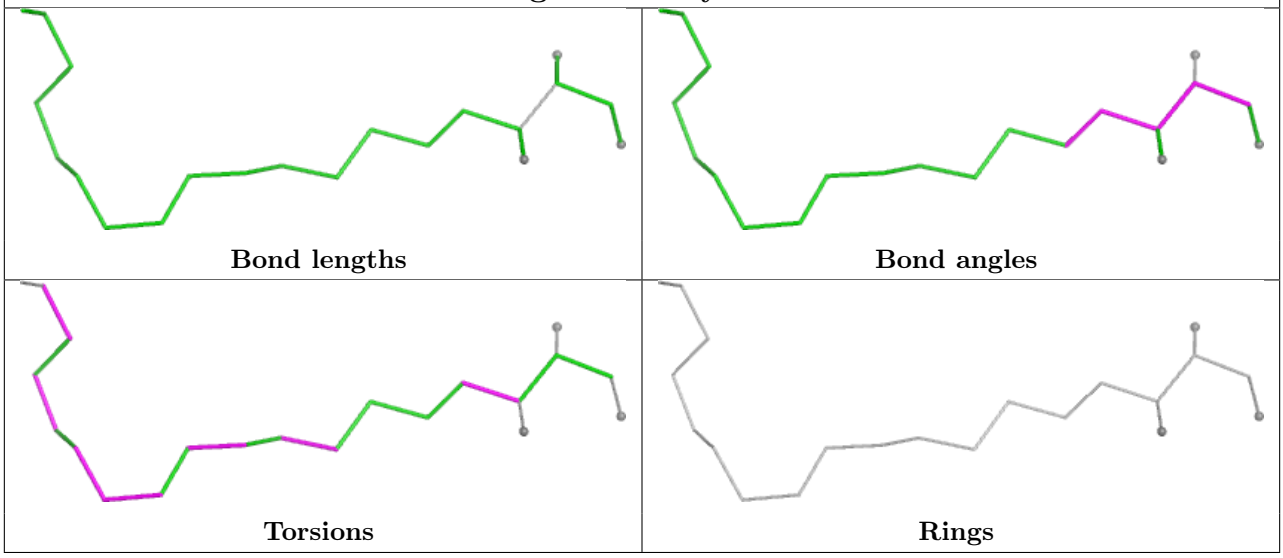


Torsions

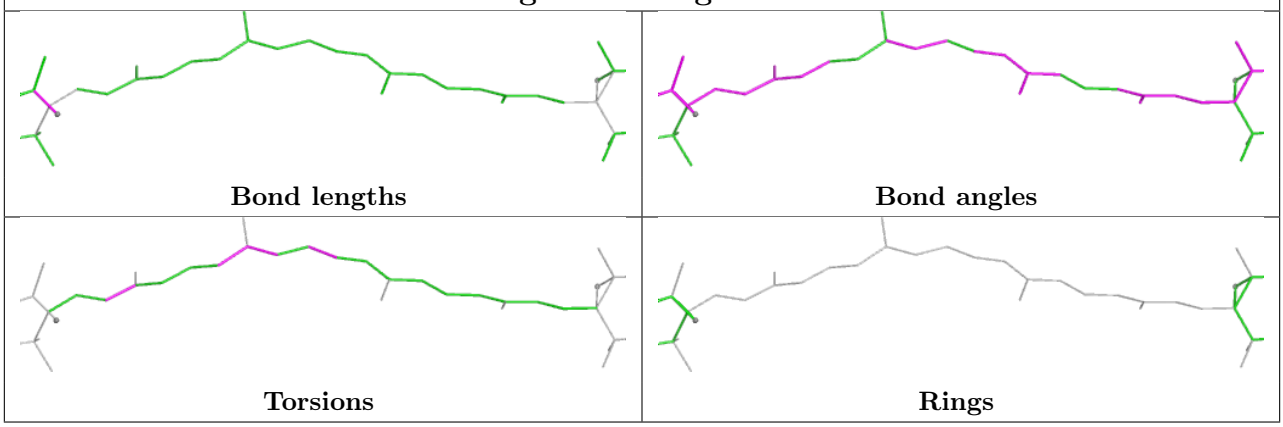


Rings

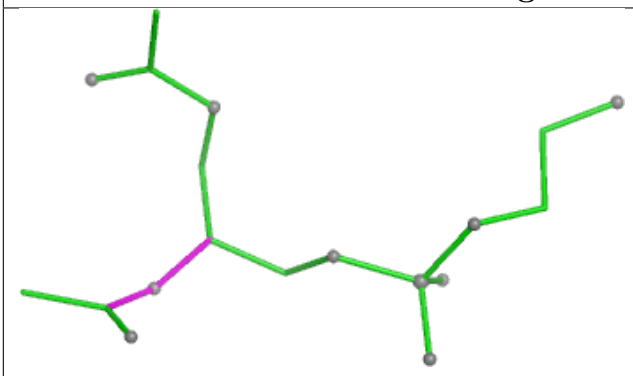
Ligand SPH y 625



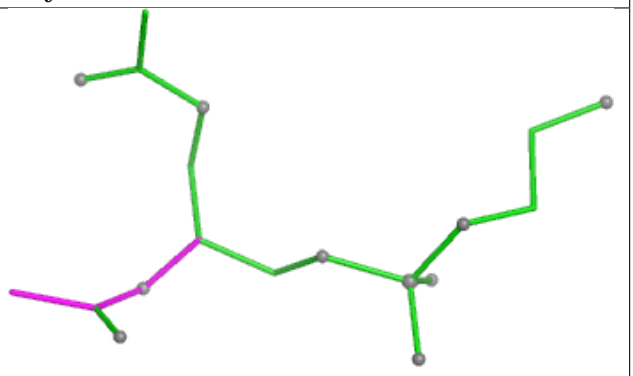
Ligand XAT g1 622



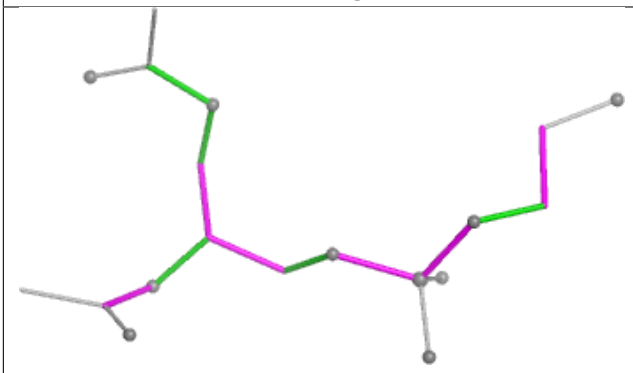
Ligand PTY y1 627



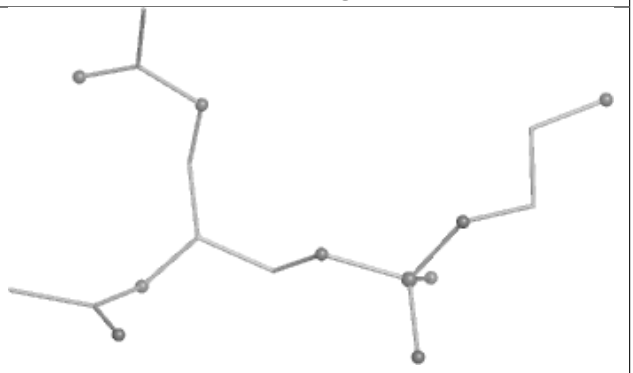
Bond lengths



Bond angles

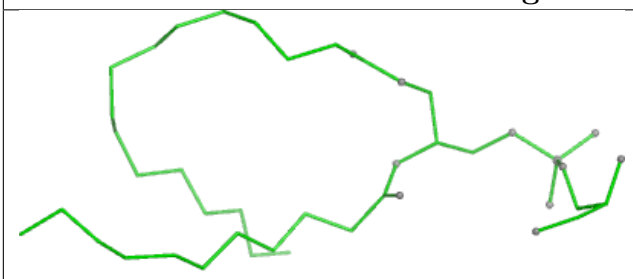


Torsions

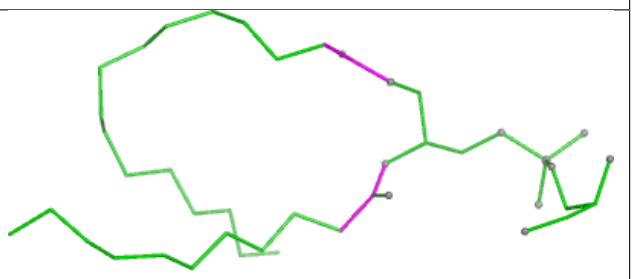


Rings

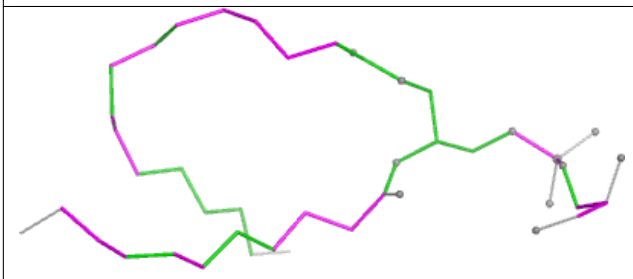
Ligand LHG D 408



Bond lengths



Bond angles

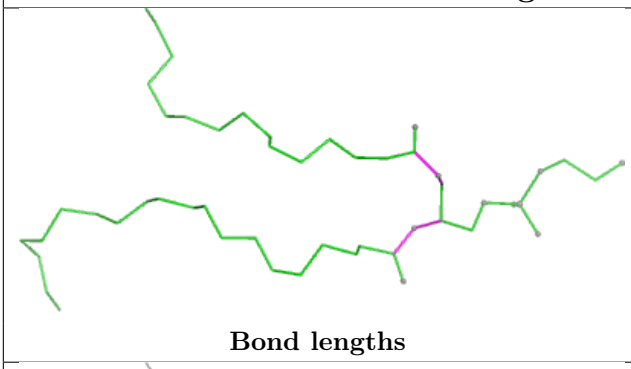


Torsions

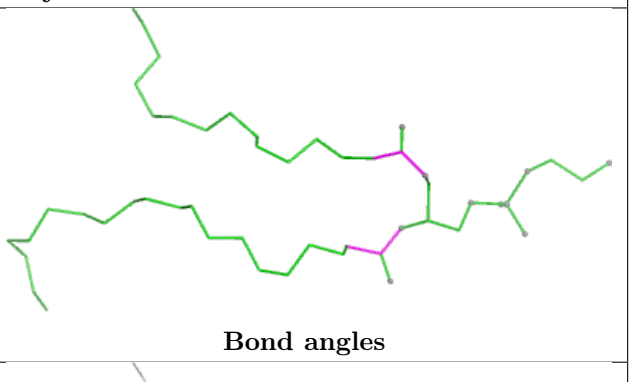


Rings

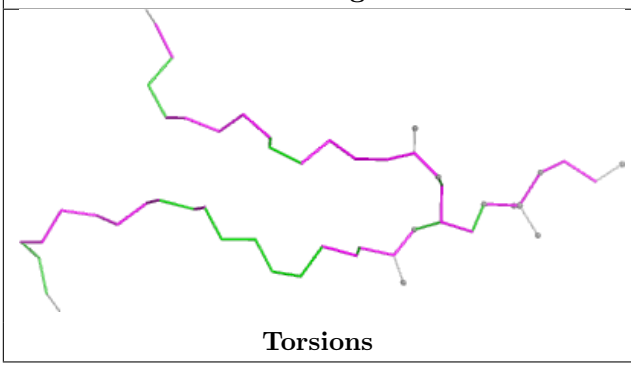
Ligand PTY y1 626



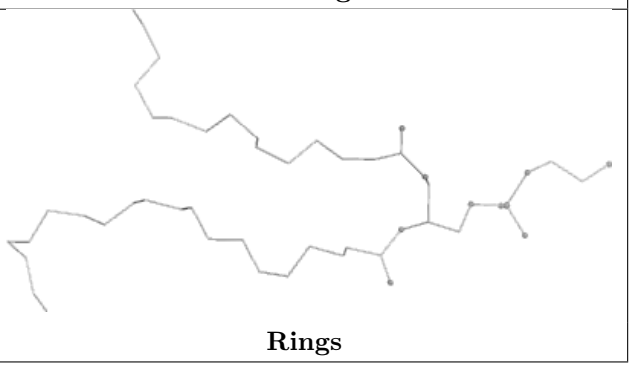
Bond lengths



Bond angles

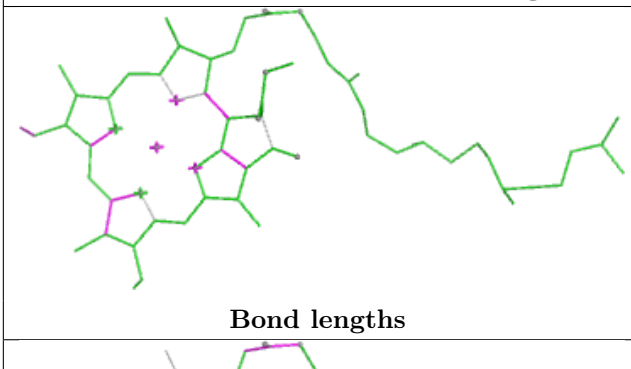


Torsions

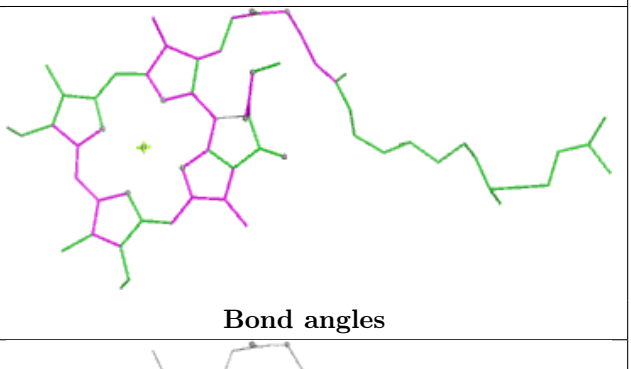


Rings

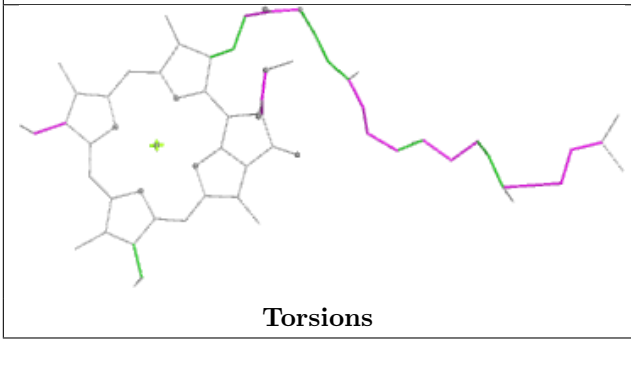
Ligand CLA B 603



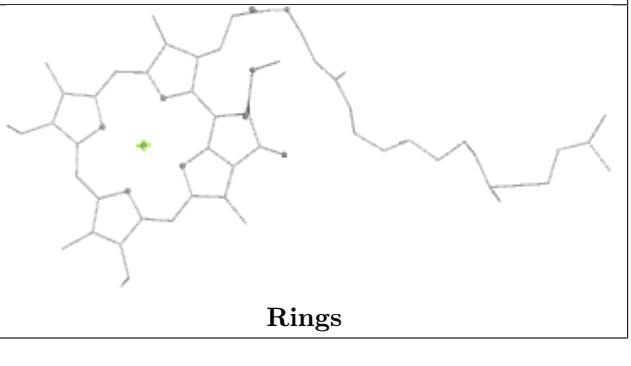
Bond lengths



Bond angles

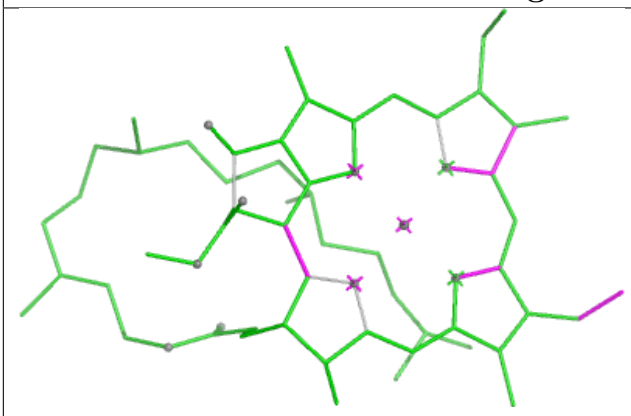


Torsions

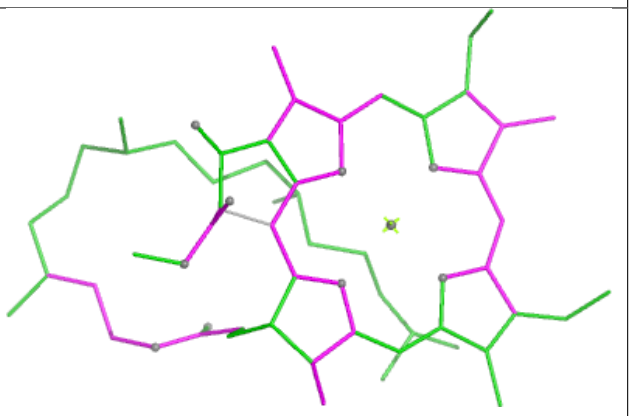


Rings

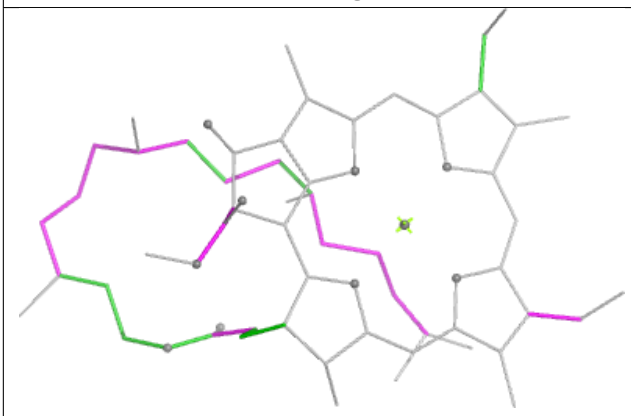
Ligand CLA b 602



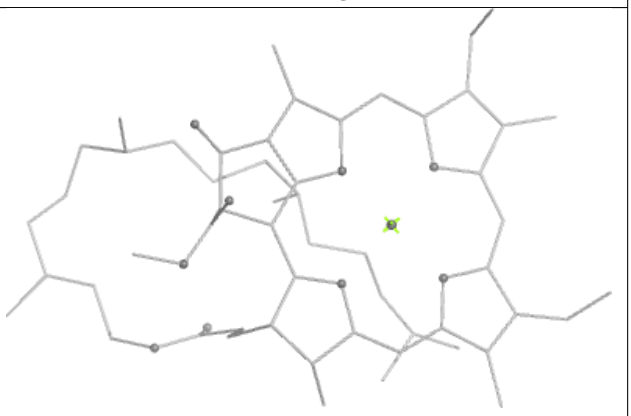
Bond lengths



Bond angles

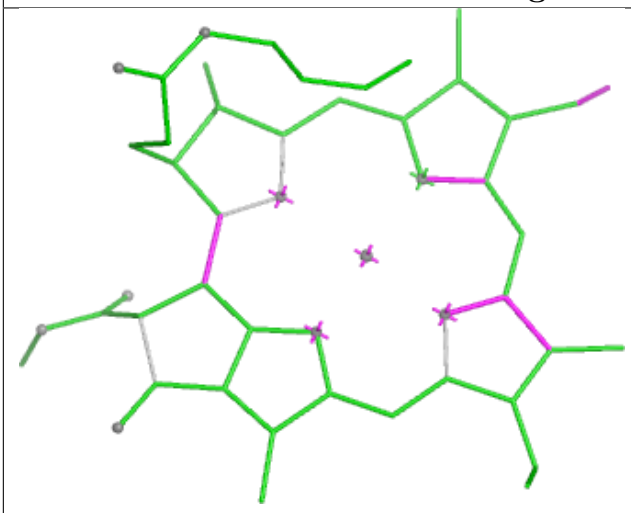


Torsions

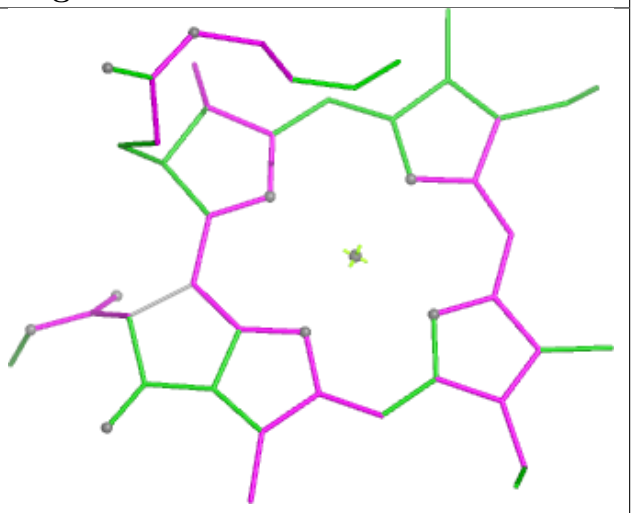


Rings

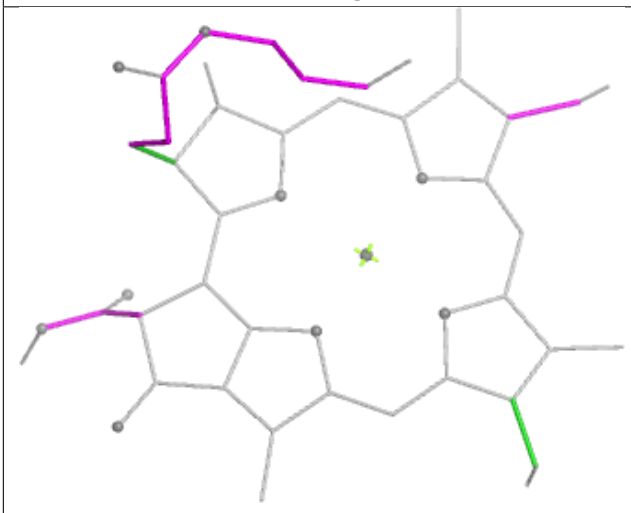
Ligand CLA g 614



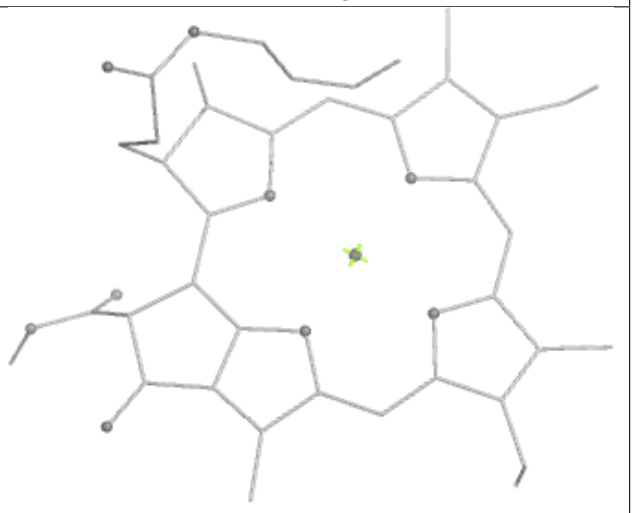
Bond lengths



Bond angles

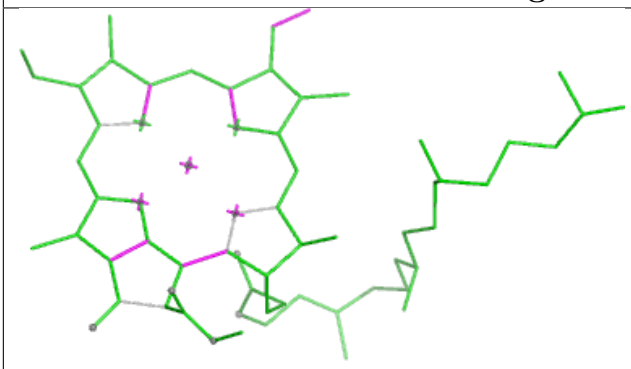


Torsions

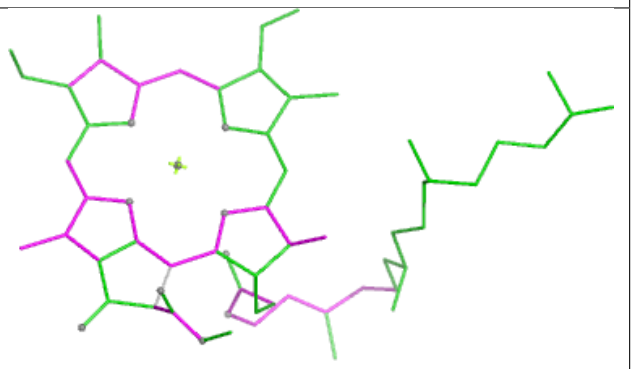


Rings

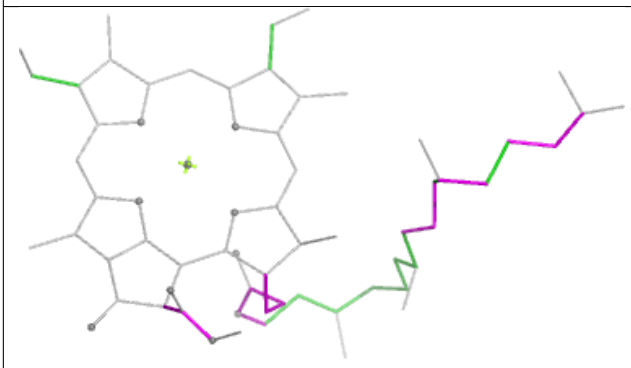
Ligand CLA a 406



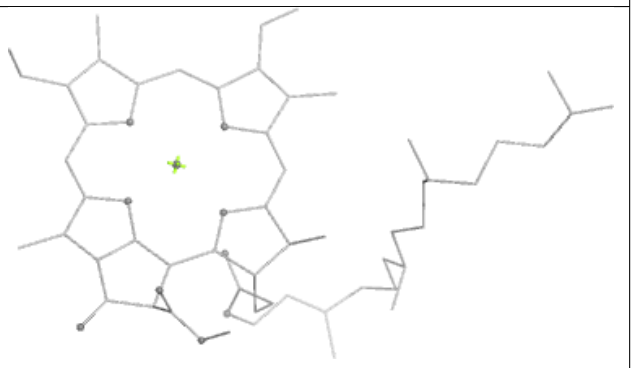
Bond lengths



Bond angles

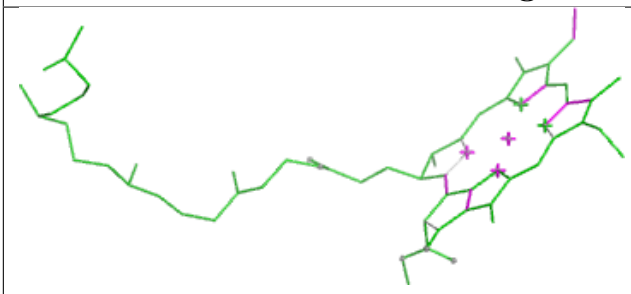


Torsions

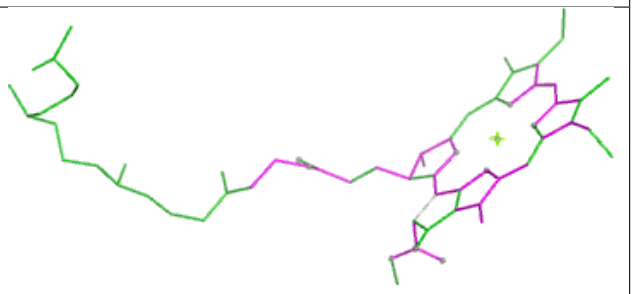


Rings

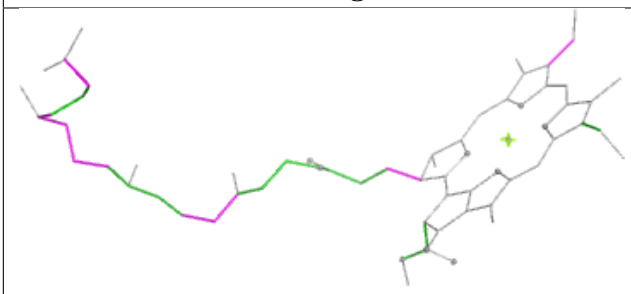
Ligand CLA d1 402



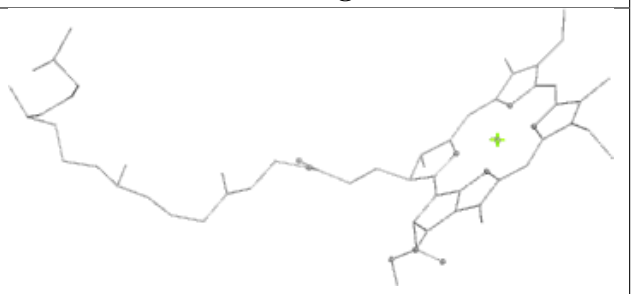
Bond lengths



Bond angles

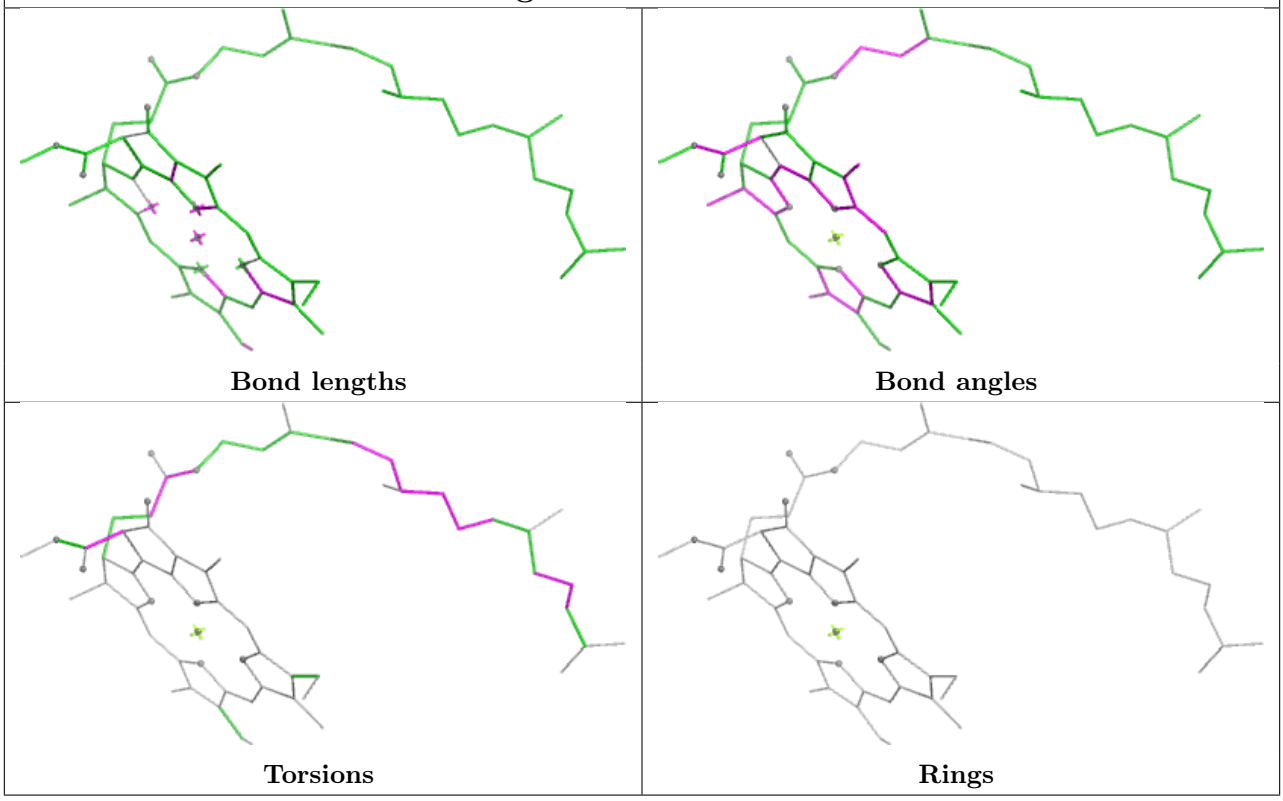


Torsions

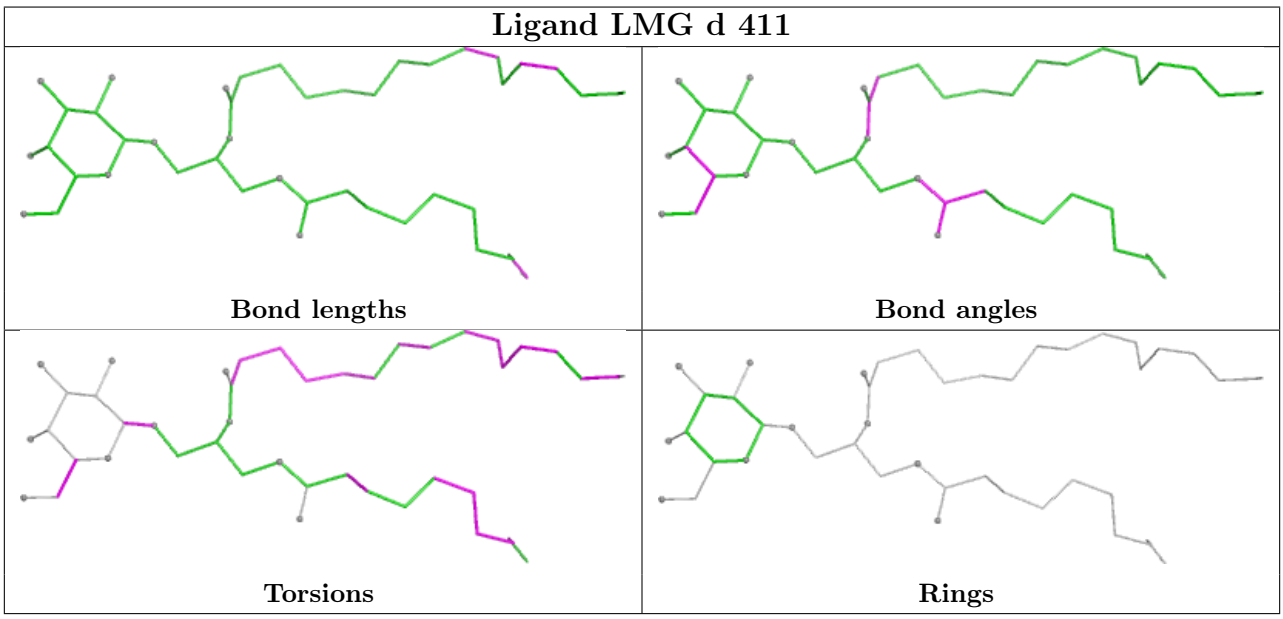


Rings

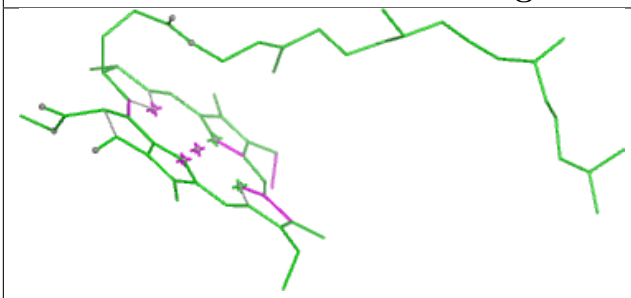
Ligand CLA C1 508



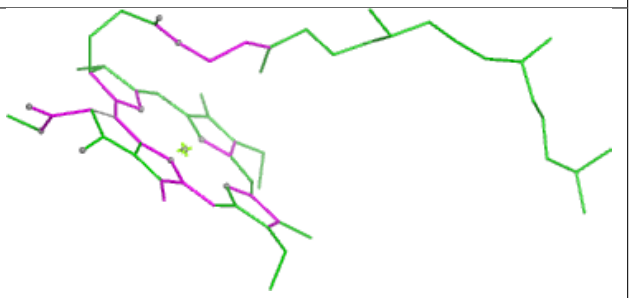
Ligand LMG d 411



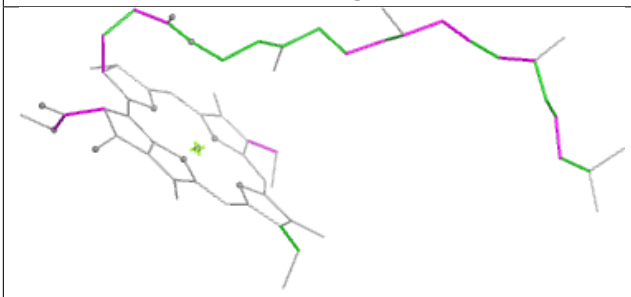
Ligand CLA B1 609



Bond lengths



Bond angles

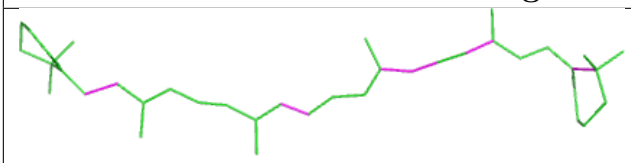


Torsions

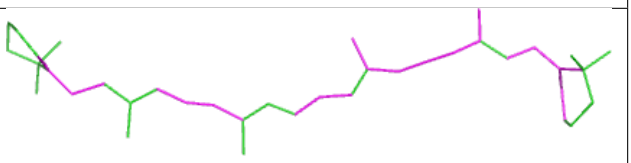


Rings

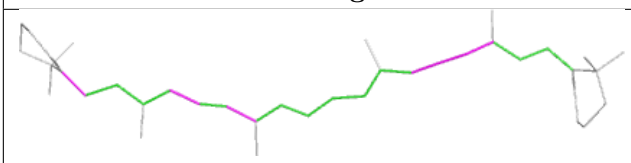
Ligand BCR C 515



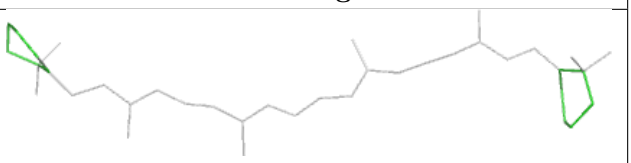
Bond lengths



Bond angles

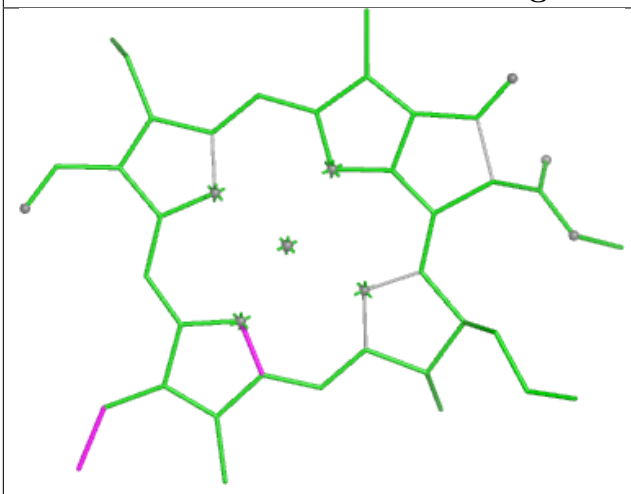


Torsions

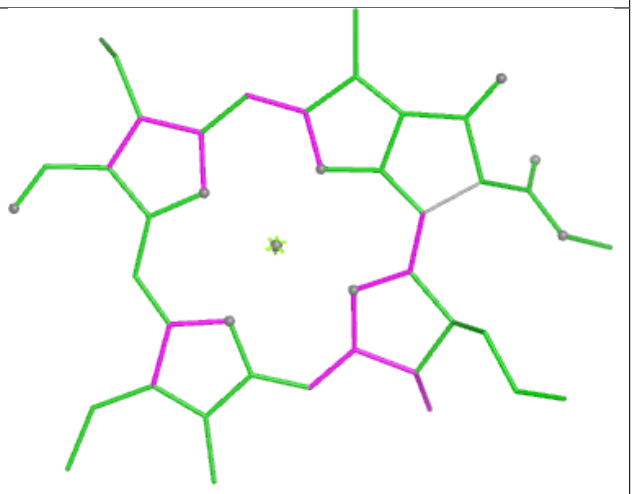


Rings

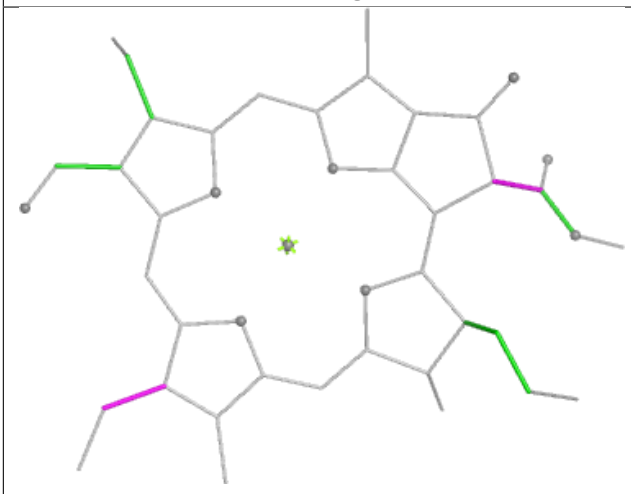
Ligand CHL s 606



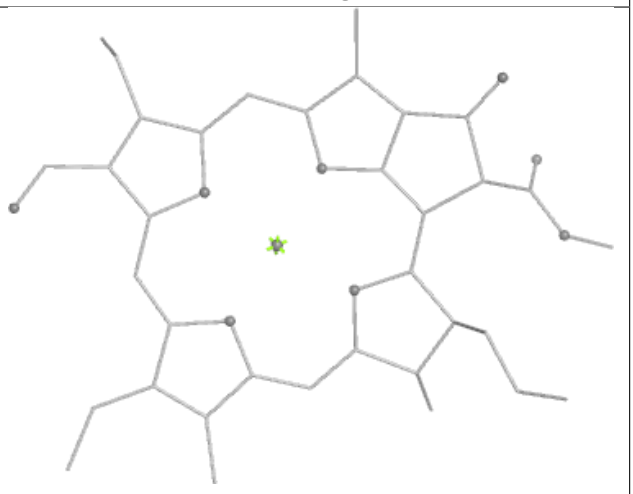
Bond lengths



Bond angles

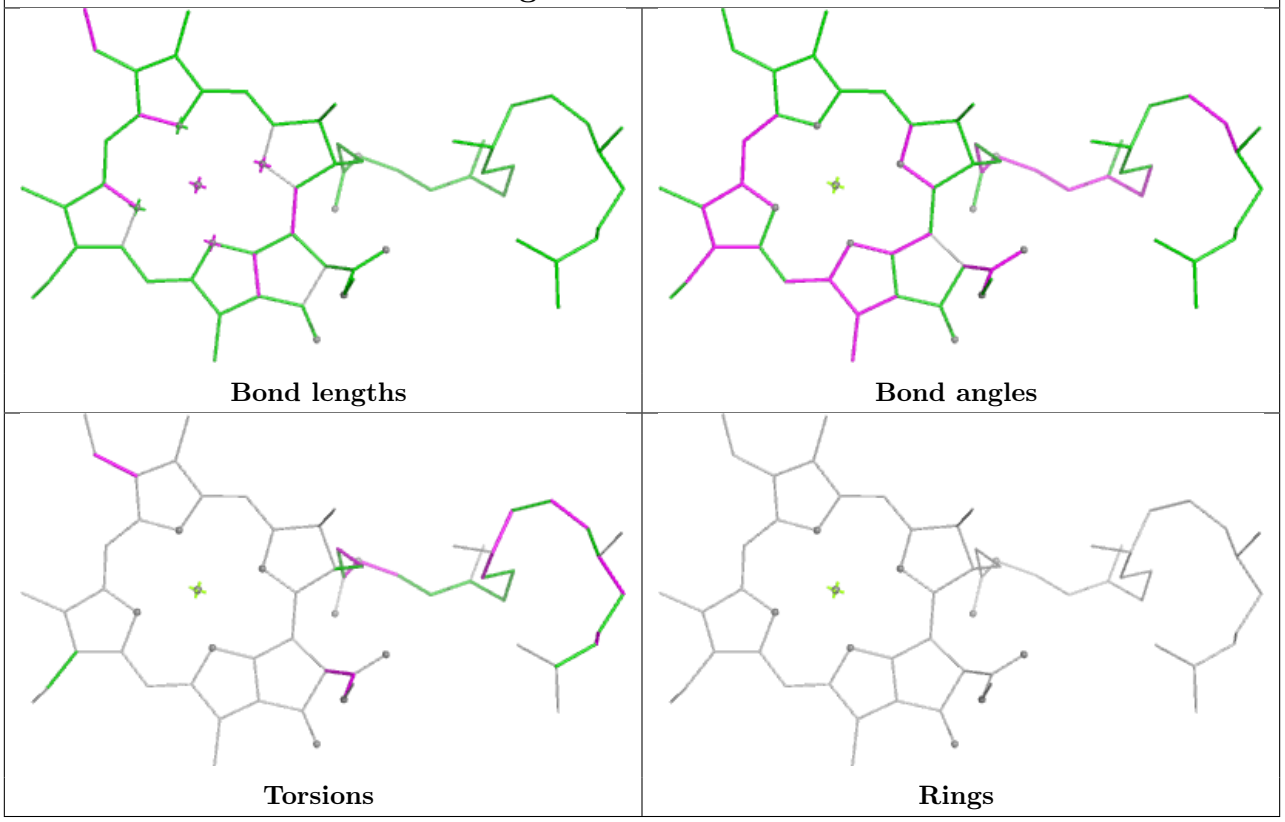


Torsions

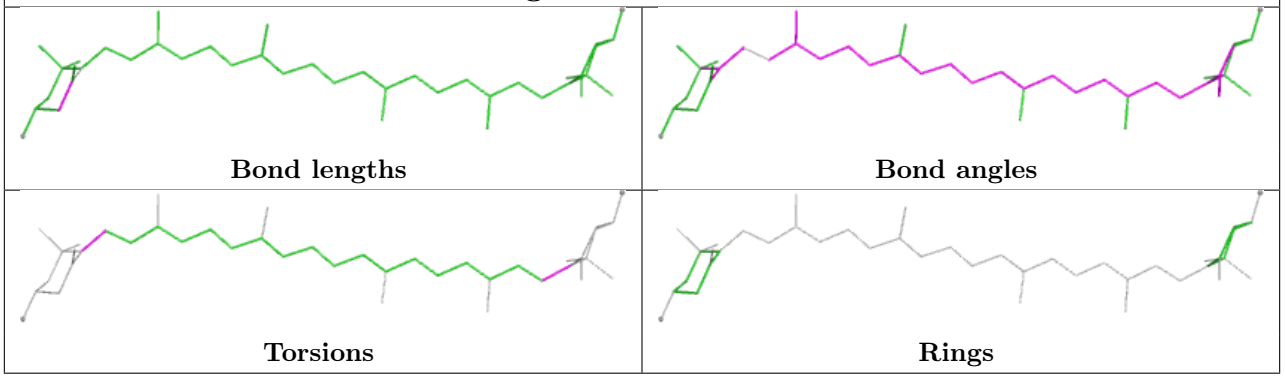


Rings

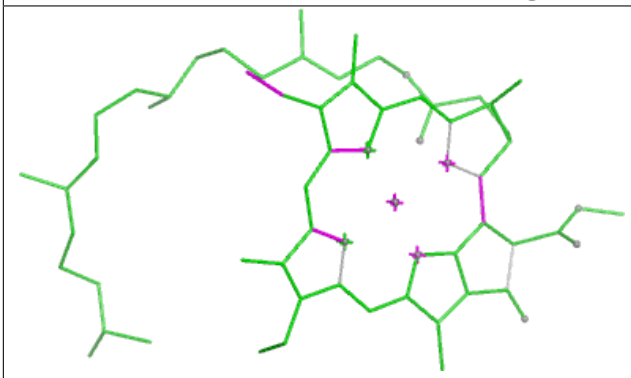
Ligand CLA b1 613



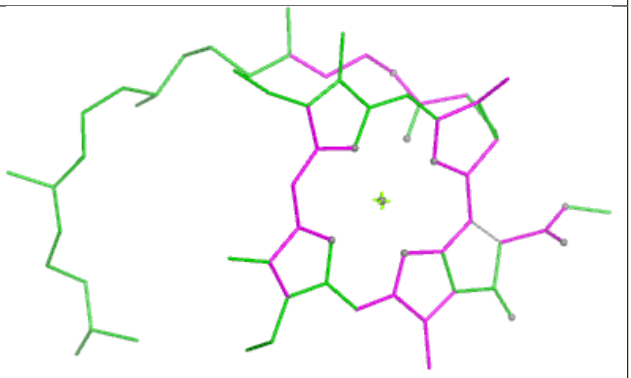
Ligand LUT R 620



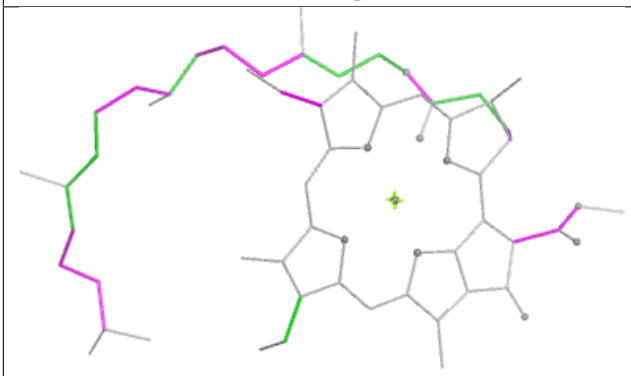
Ligand CLA N 610



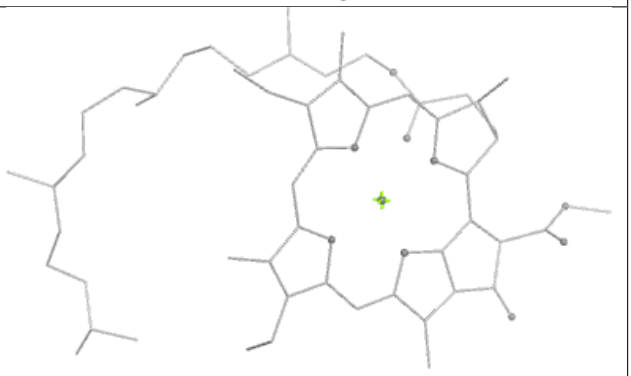
Bond lengths



Bond angles

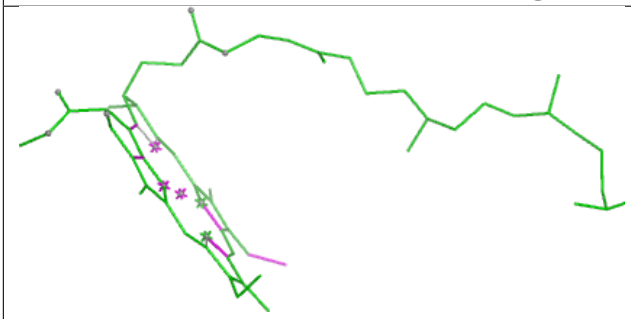


Torsions

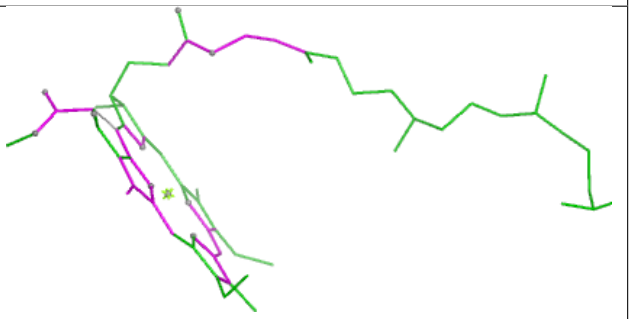


Rings

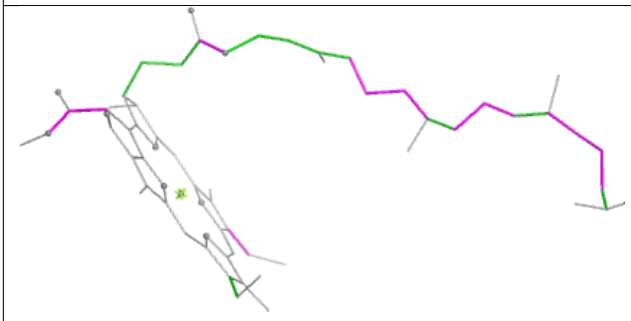
Ligand CLA c 504



Bond lengths



Bond angles

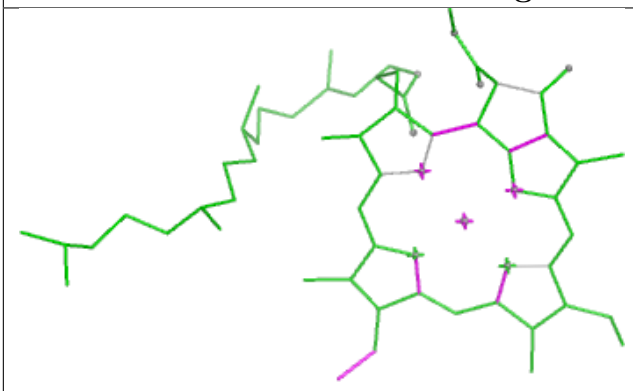


Torsions

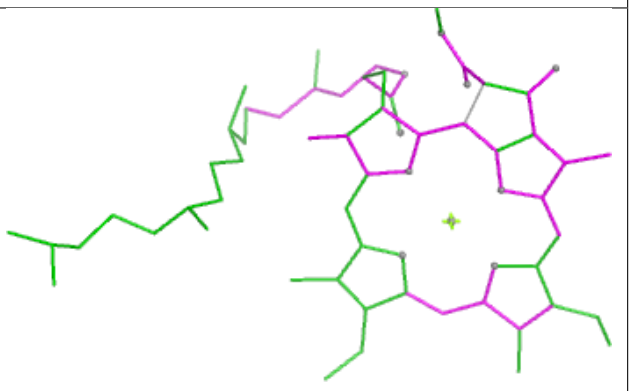


Rings

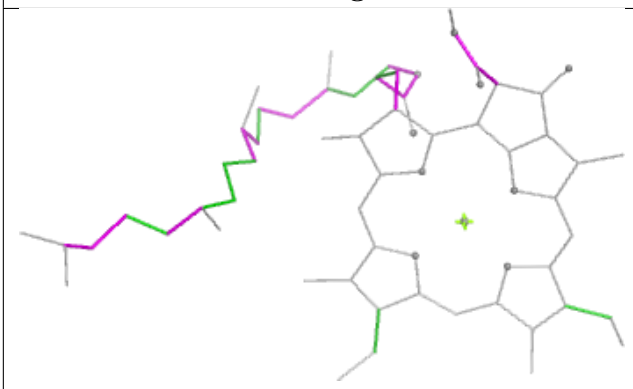
Ligand CLA A1 406



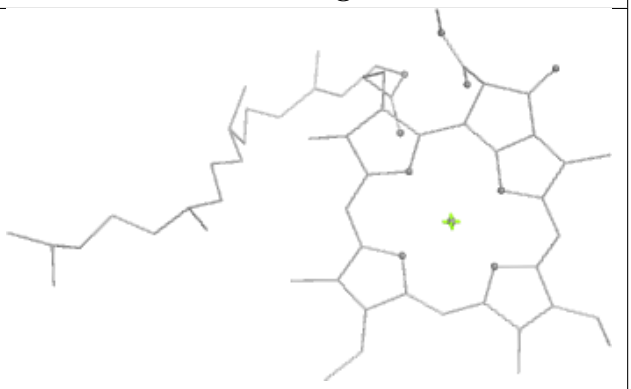
Bond lengths



Bond angles

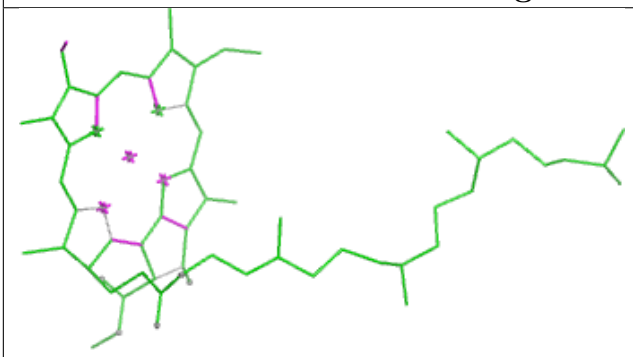


Torsions

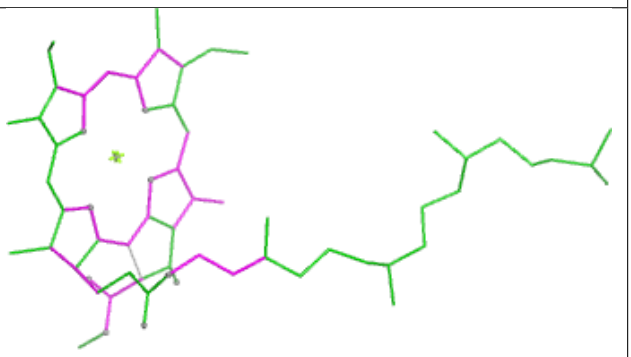


Rings

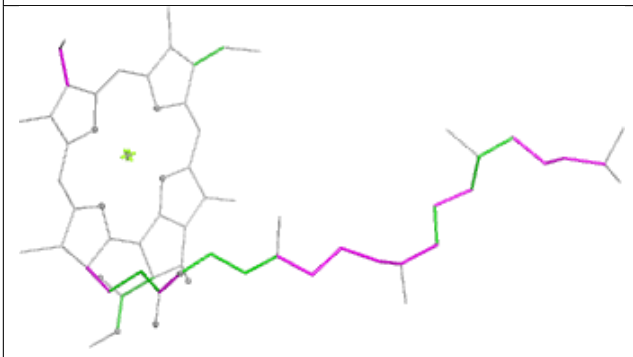
Ligand CLA Y1 611



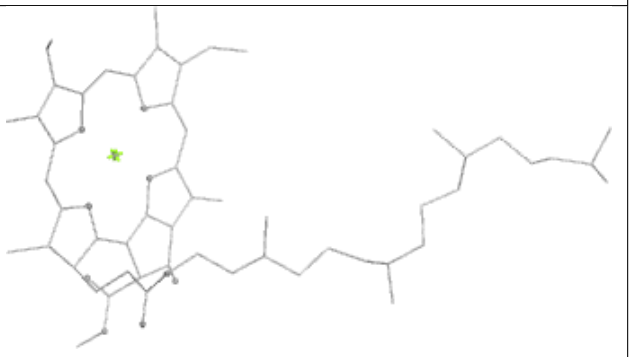
Bond lengths



Bond angles

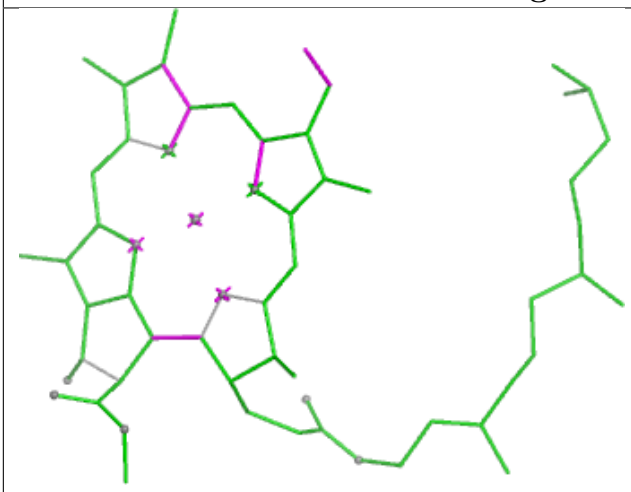


Torsions

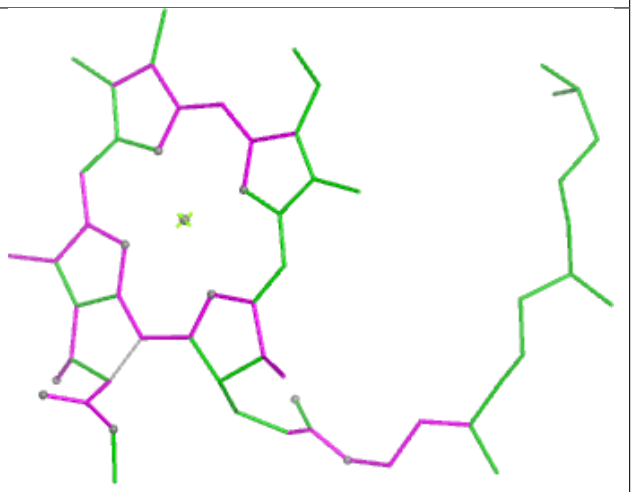


Rings

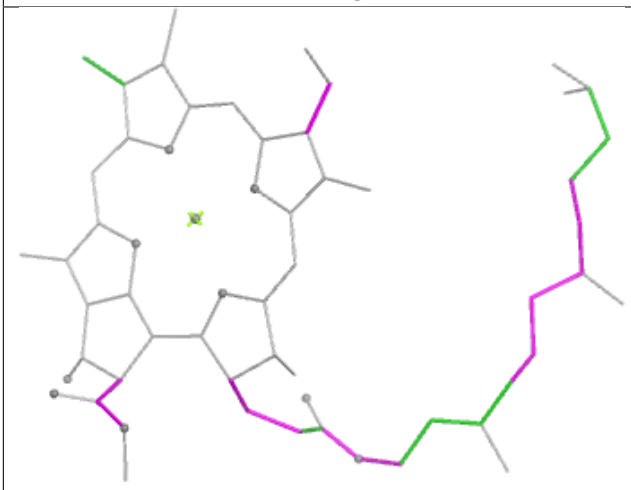
Ligand CLA r 603



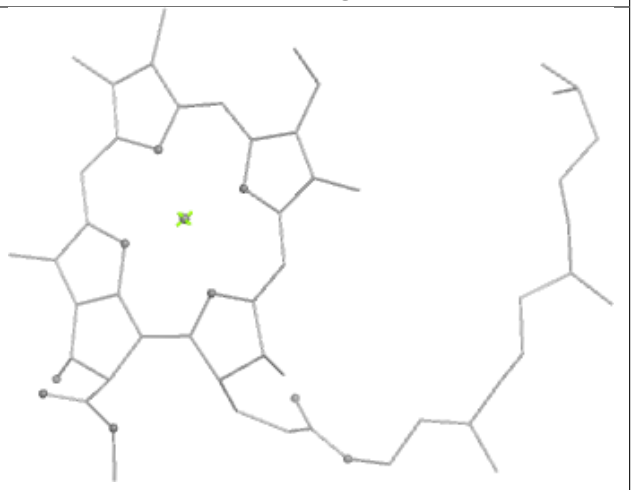
Bond lengths



Bond angles

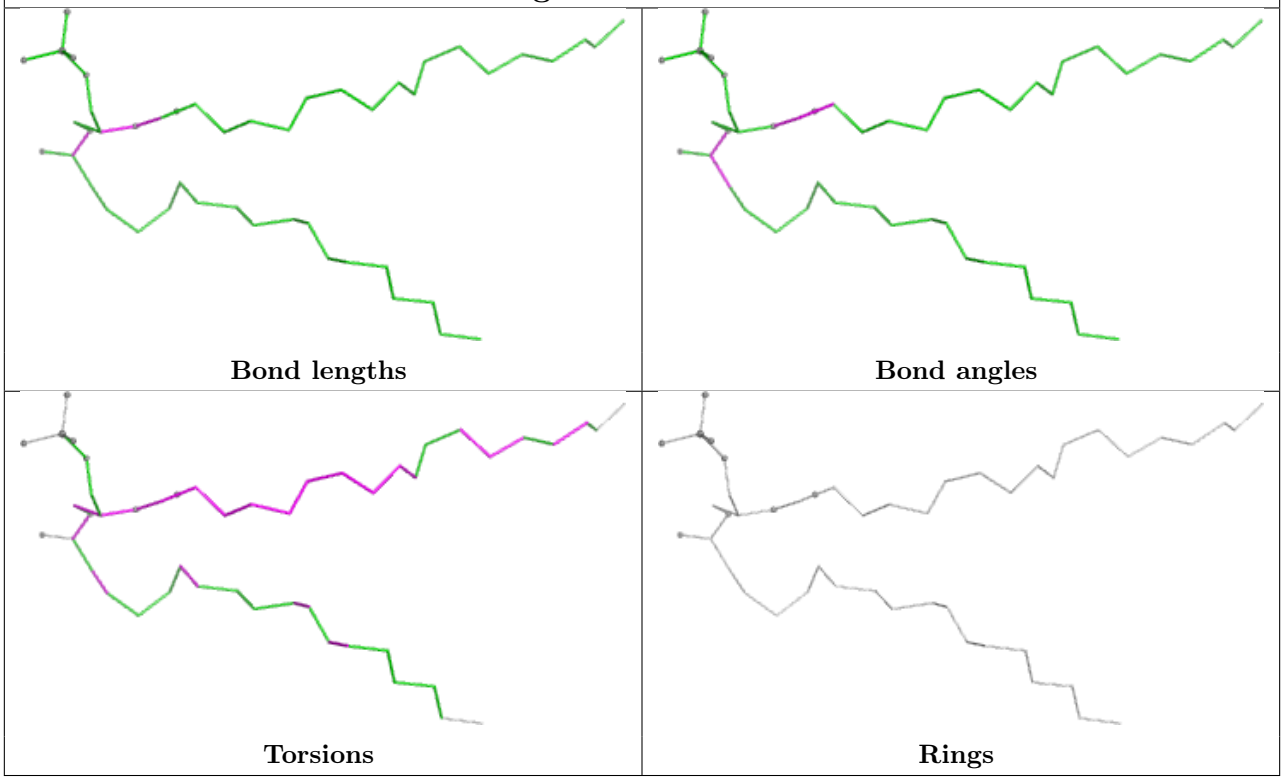


Torsions

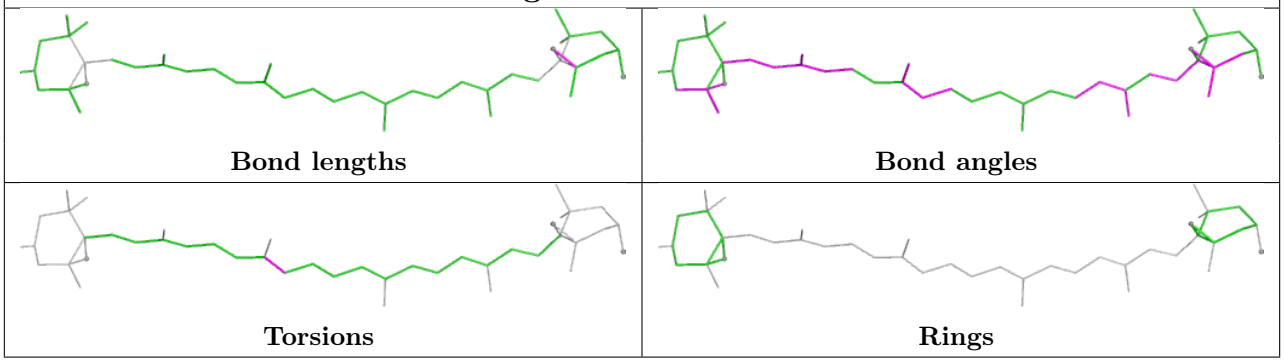


Rings

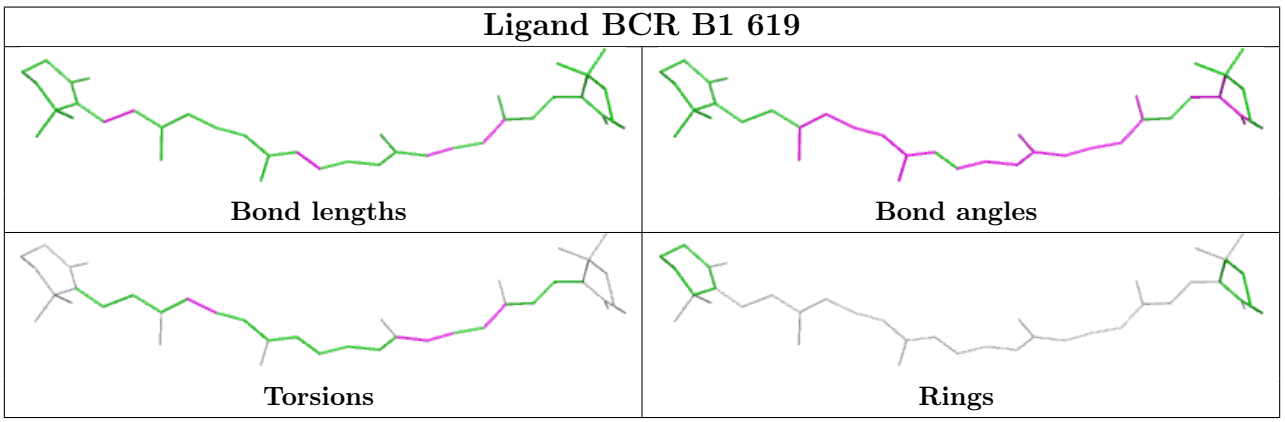
Ligand 3PH s 626



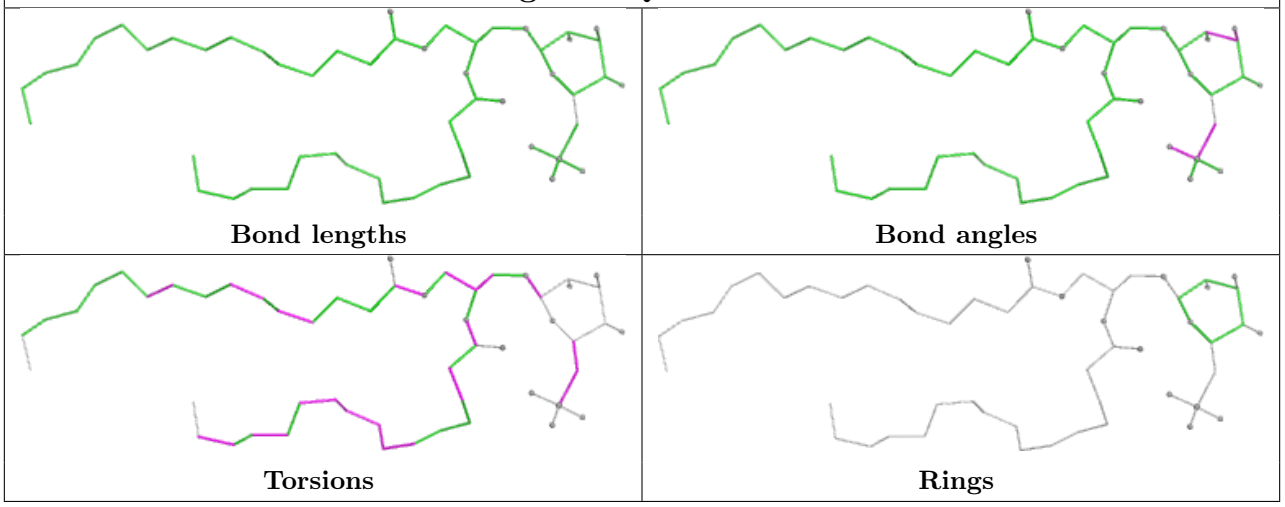
Ligand XAT G 622



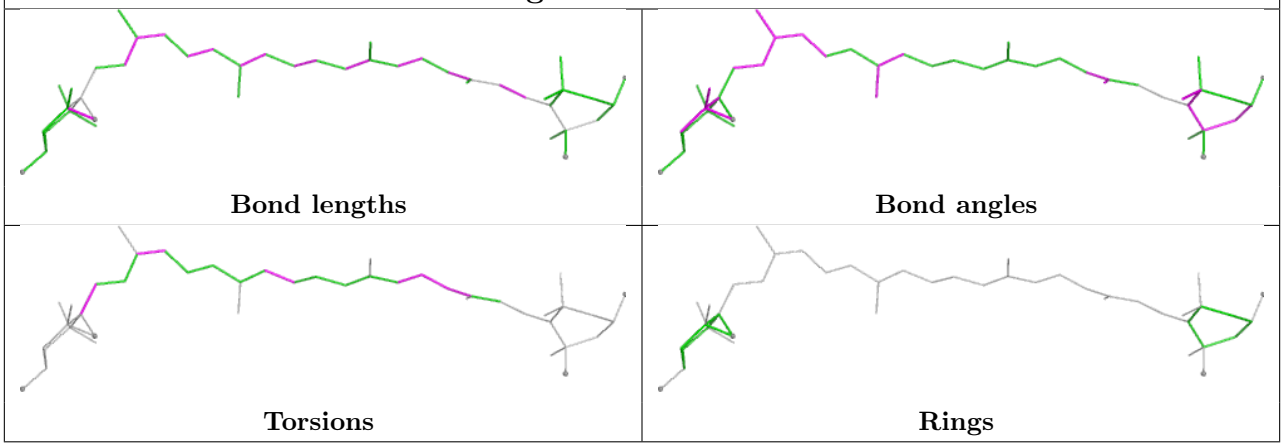
Ligand BCR B1 619



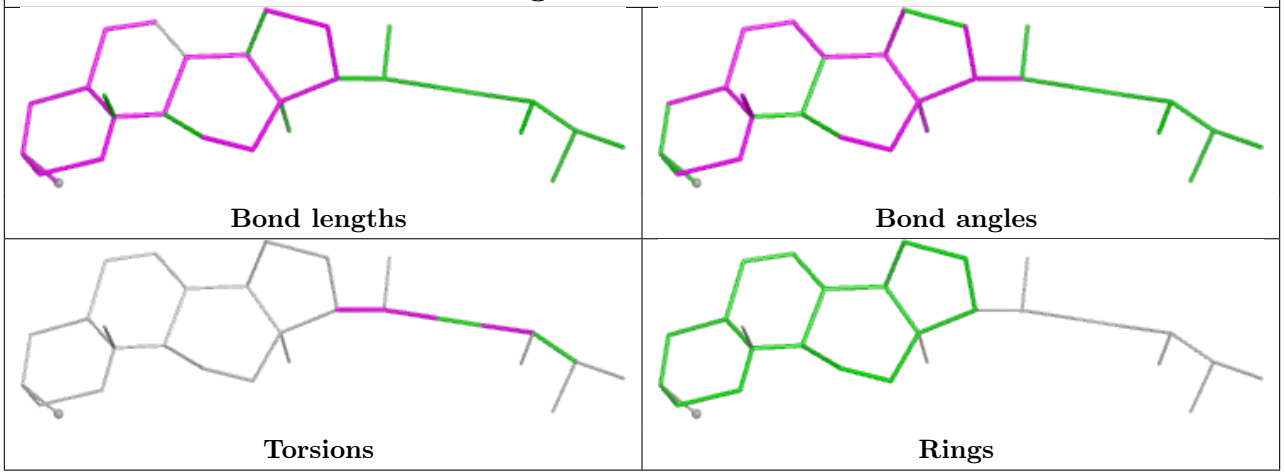
Ligand SQD b1 626



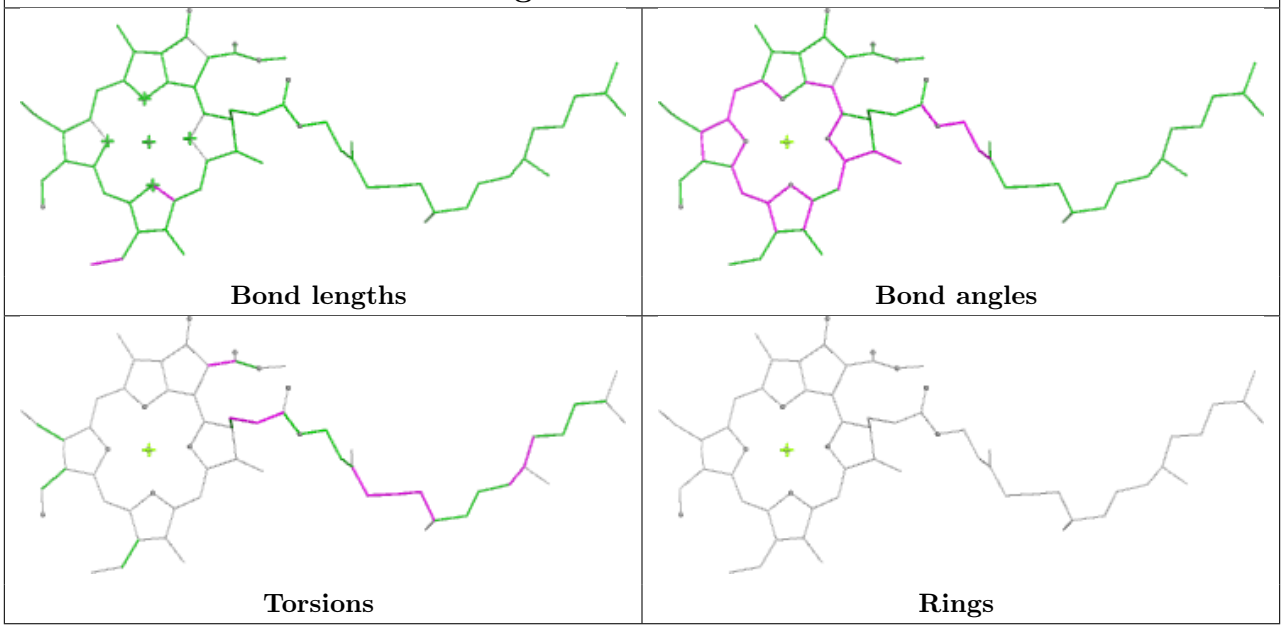
Ligand NEX S 623



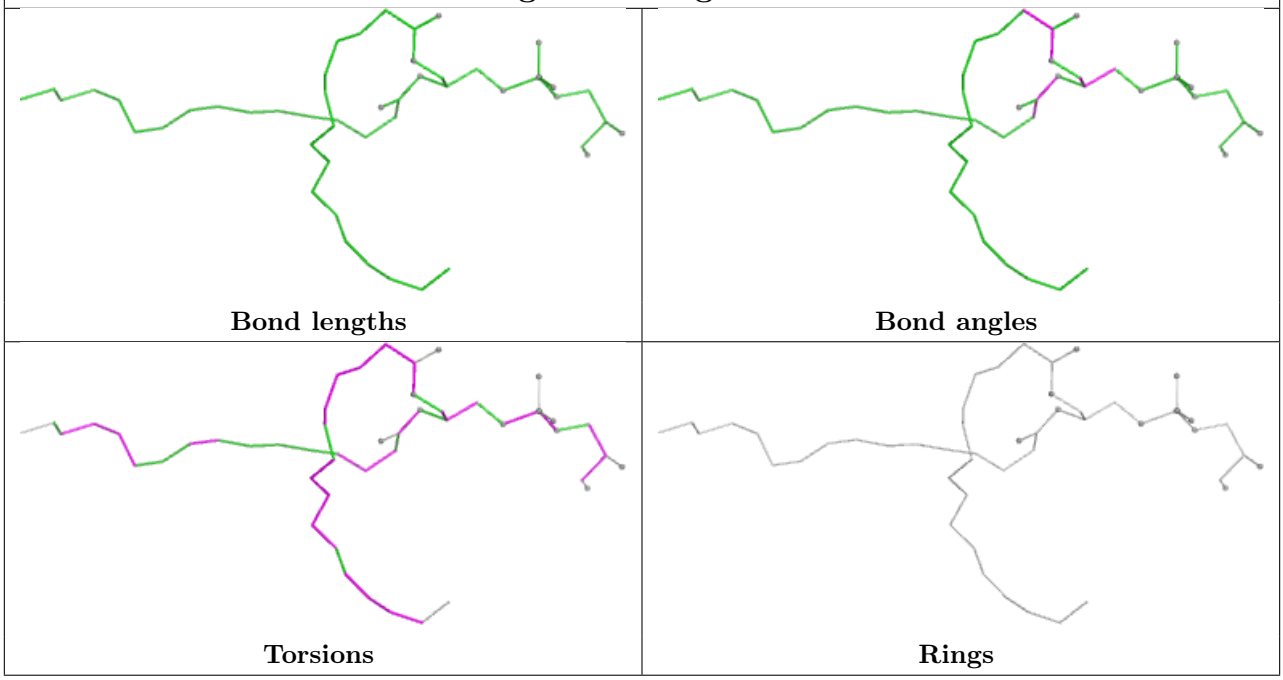
Ligand ERG r 626



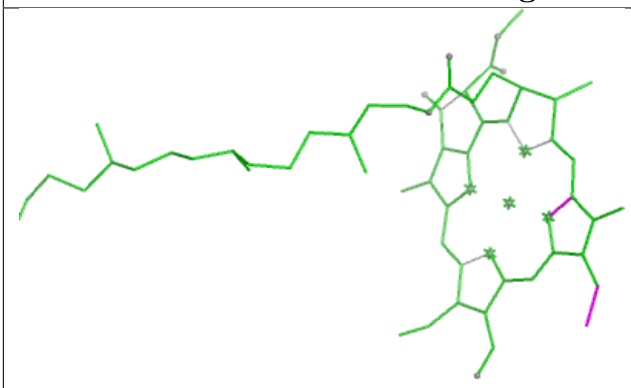
Ligand CHL G1 601



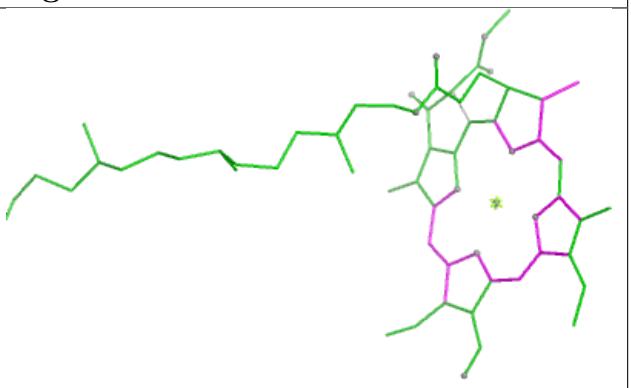
Ligand LHG g1 624



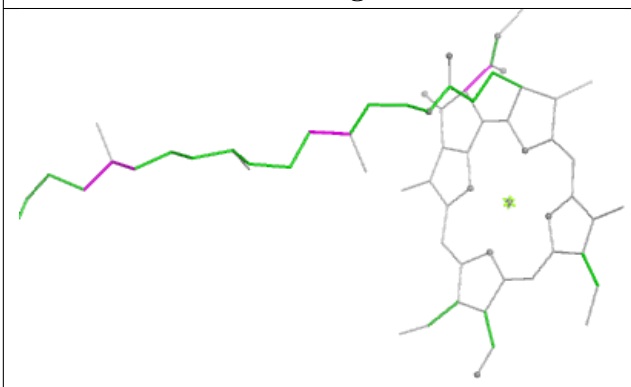
Ligand CHL g1 609



Bond lengths



Bond angles

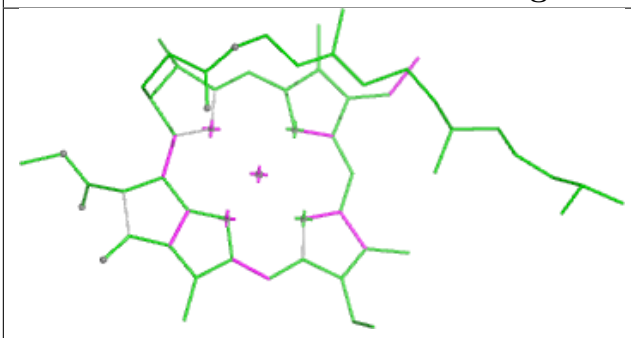


Torsions

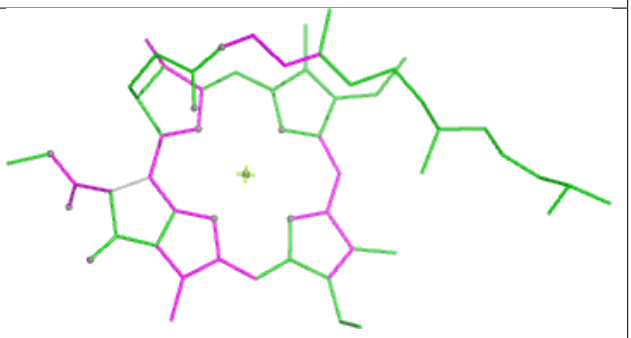


Rings

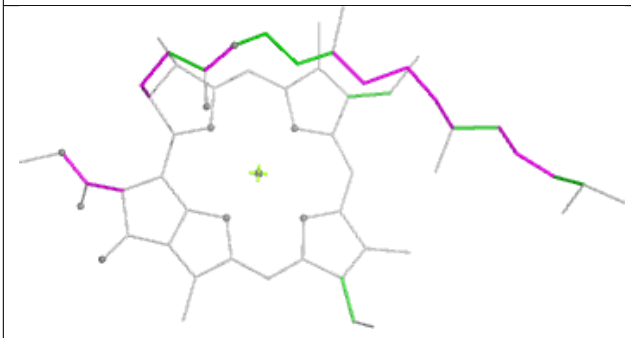
Ligand CLA r 608



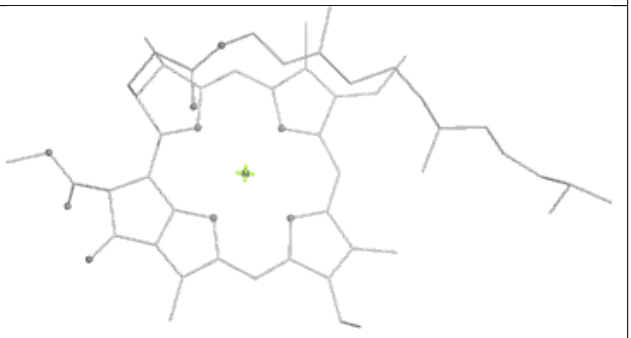
Bond lengths



Bond angles

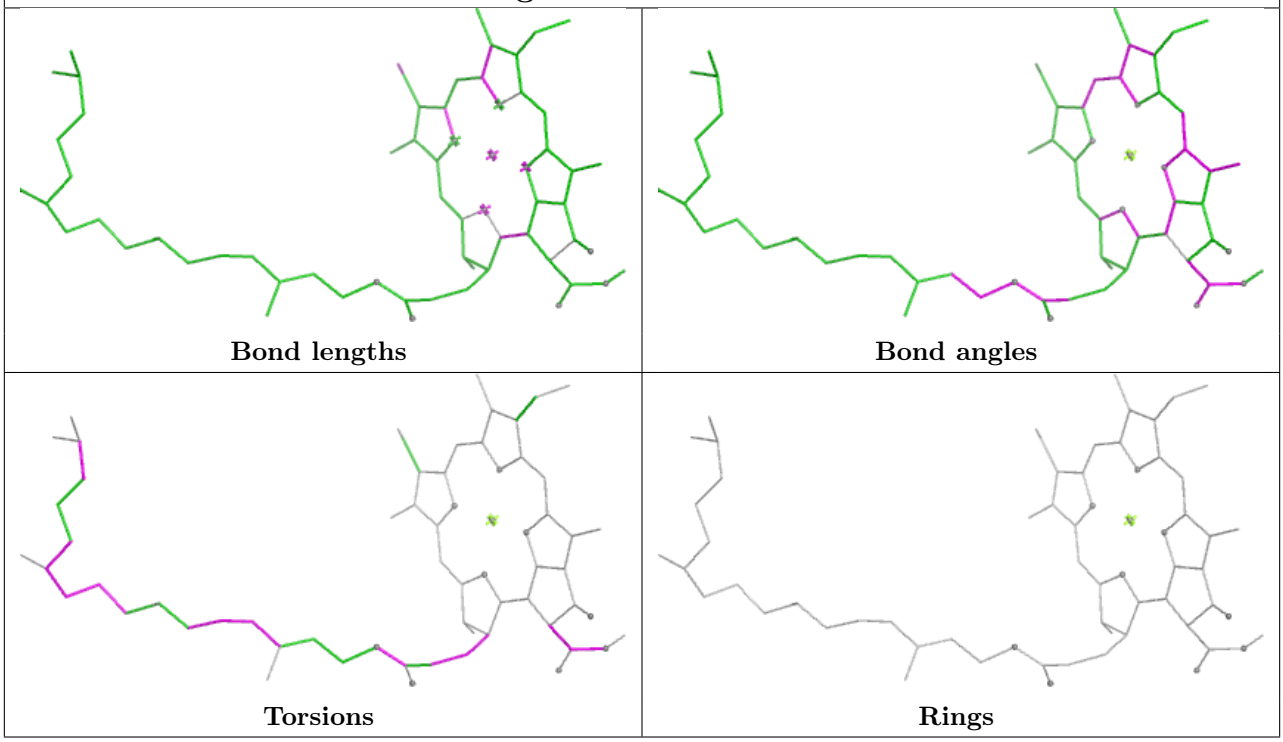


Torsions

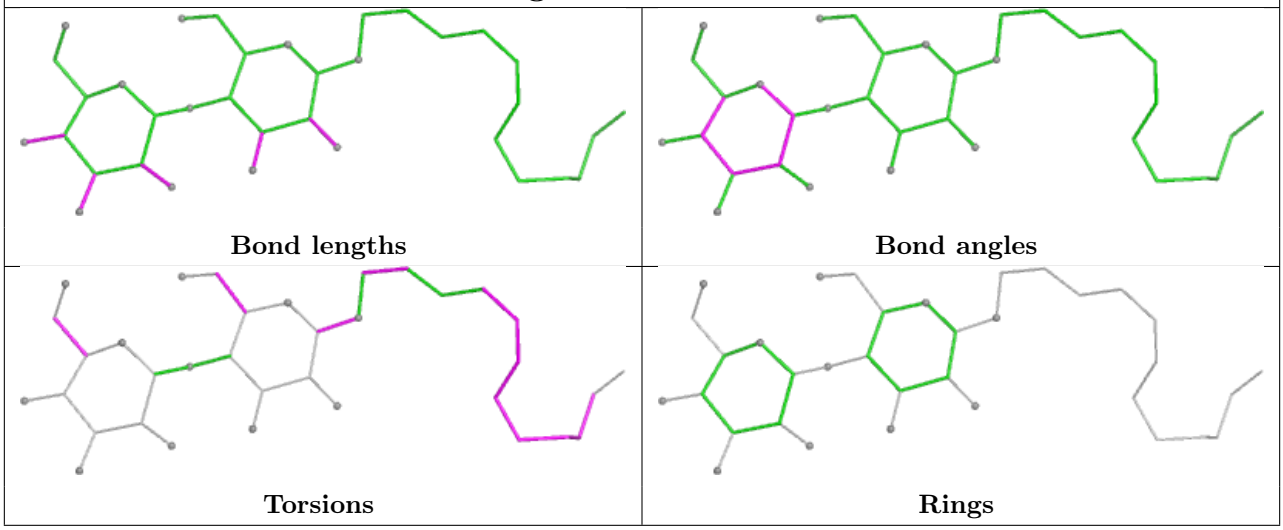


Rings

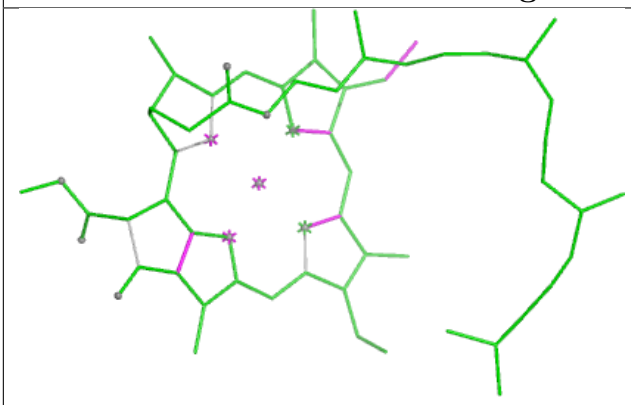
Ligand CLA B1 610



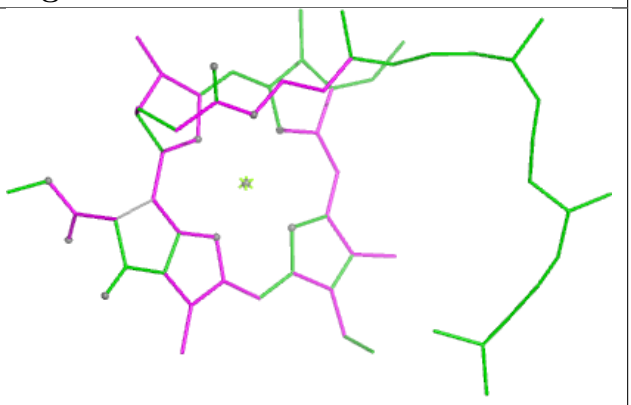
Ligand LMT r 625



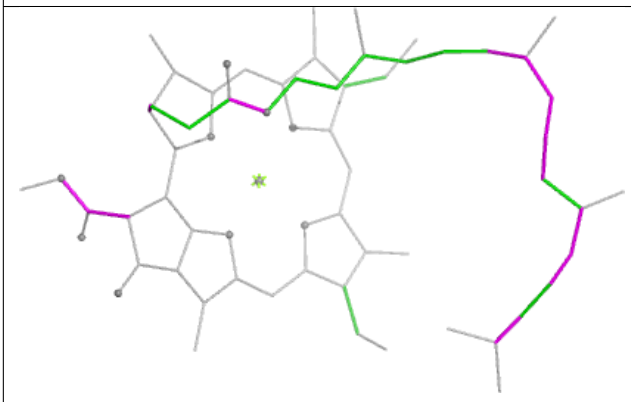
Ligand CLA g1 610



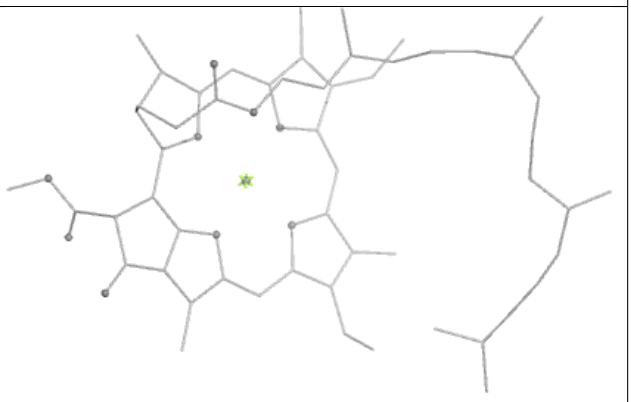
Bond lengths



Bond angles

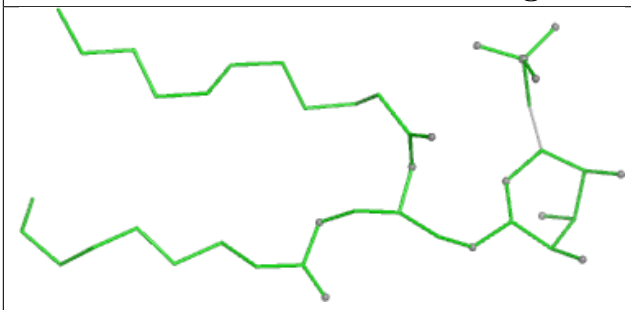


Torsions

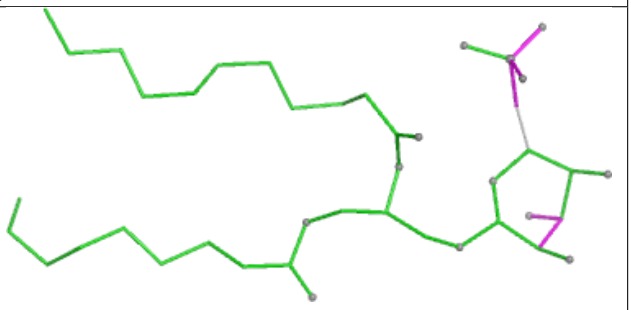


Rings

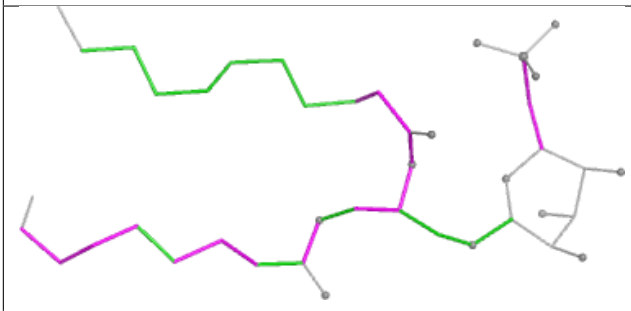
Ligand SQD m 101



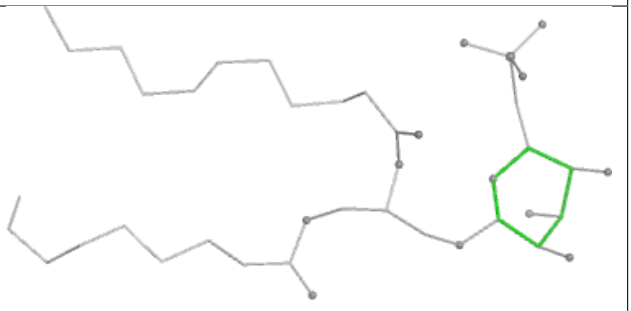
Bond lengths



Bond angles

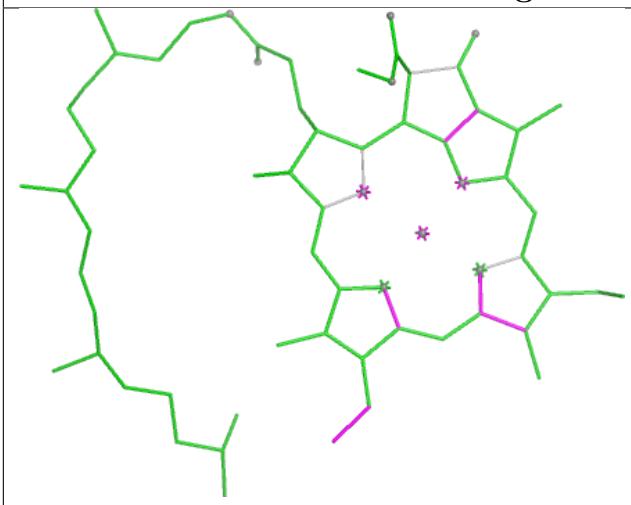


Torsions

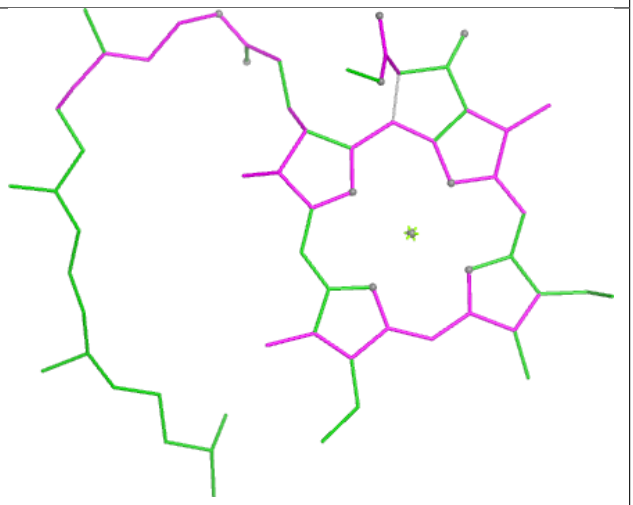


Rings

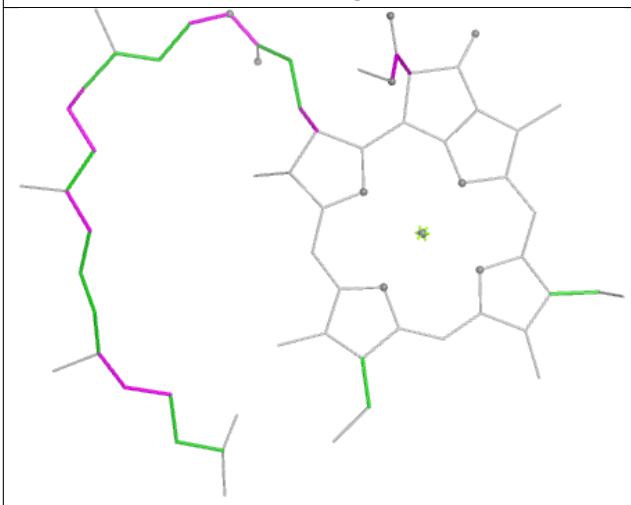
Ligand CLA C1 512



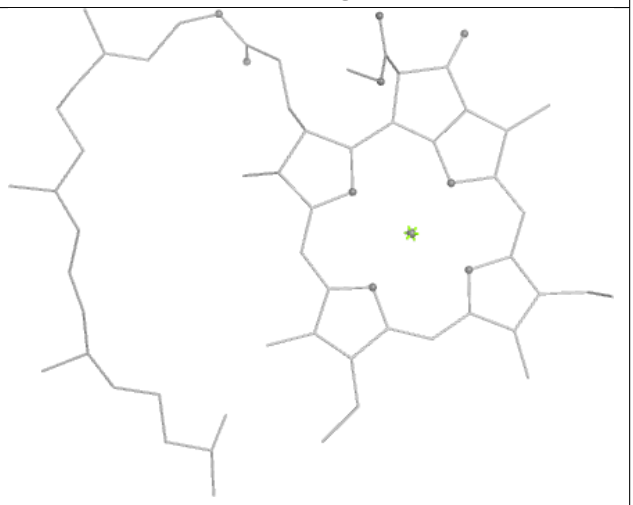
Bond lengths



Bond angles

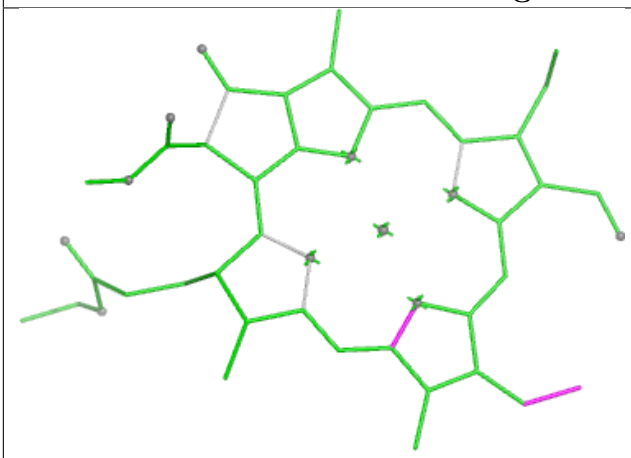


Torsions

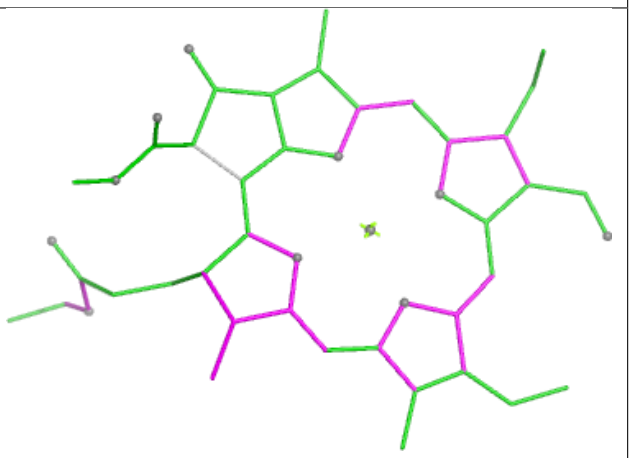


Rings

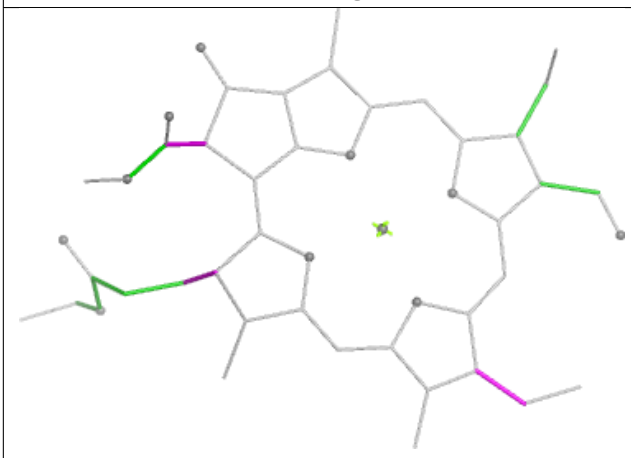
Ligand CHL G1 605



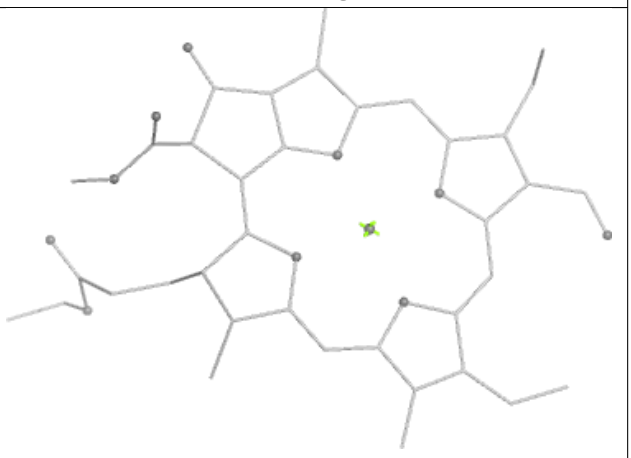
Bond lengths



Bond angles

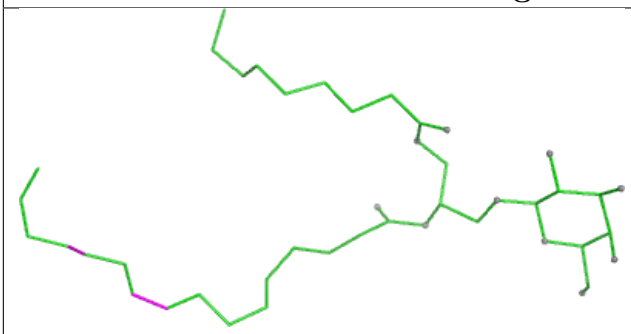


Torsions

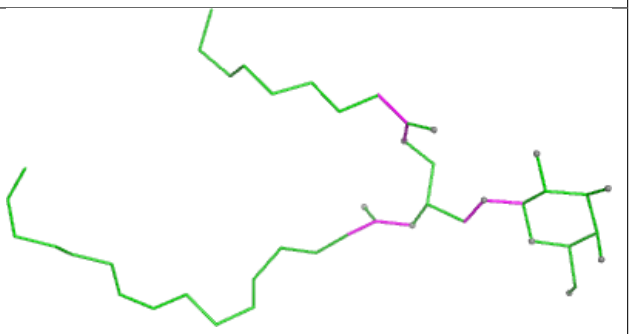


Rings

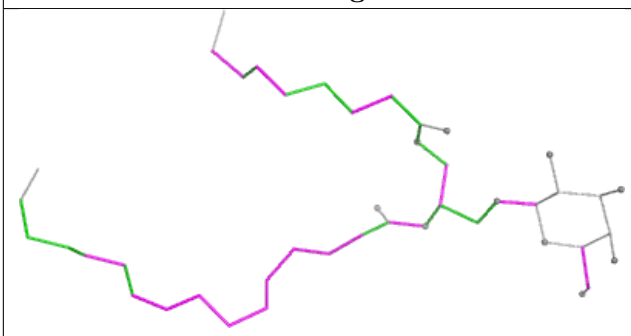
Ligand LMG b1 622



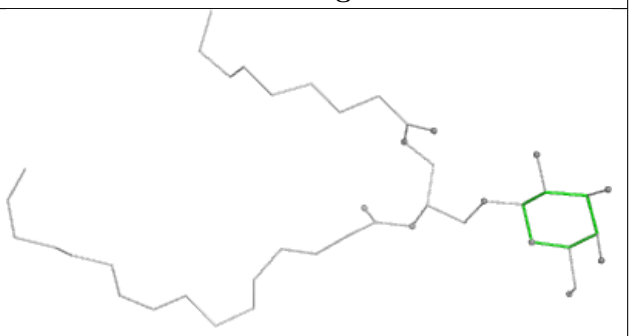
Bond lengths



Bond angles

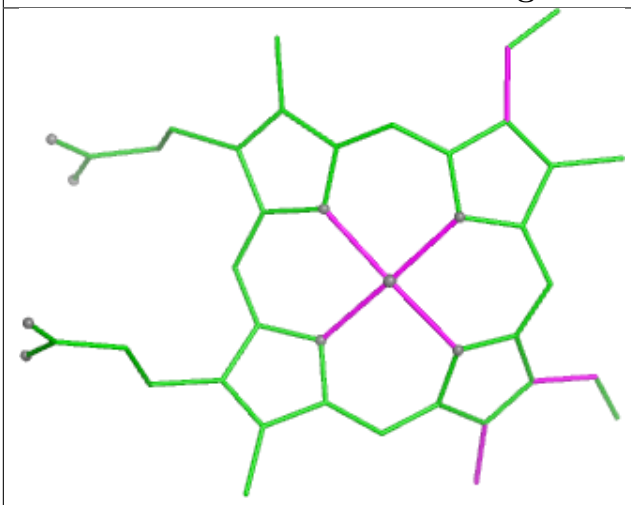


Torsions

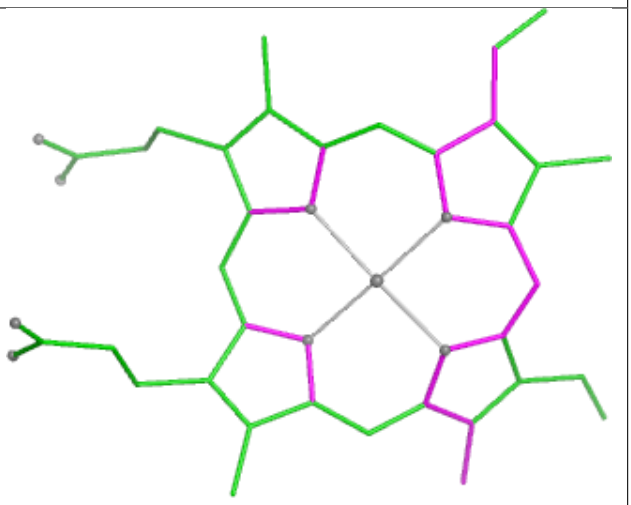


Rings

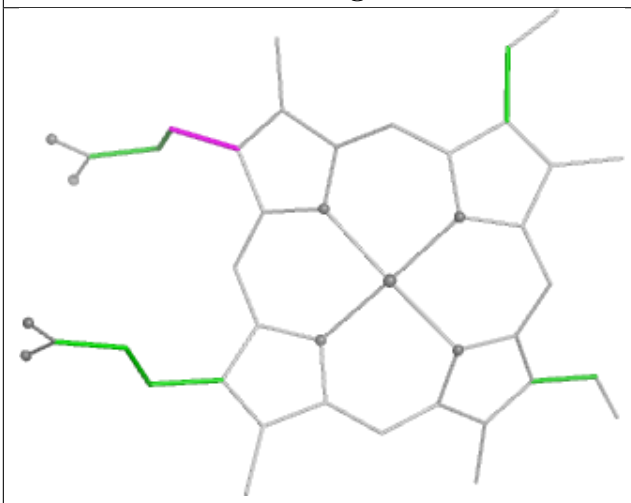
Ligand HEM f1 101



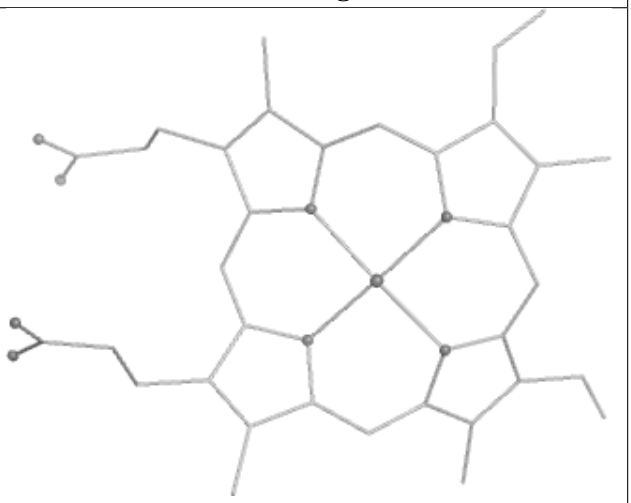
Bond lengths



Bond angles

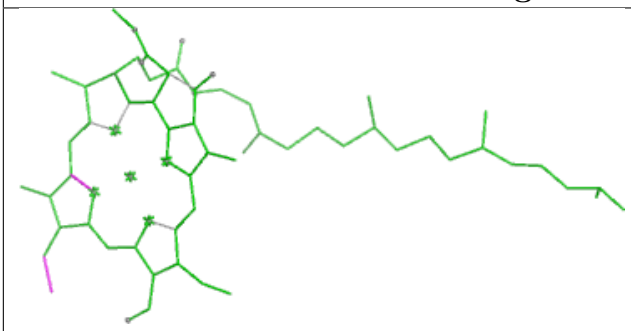


Torsions

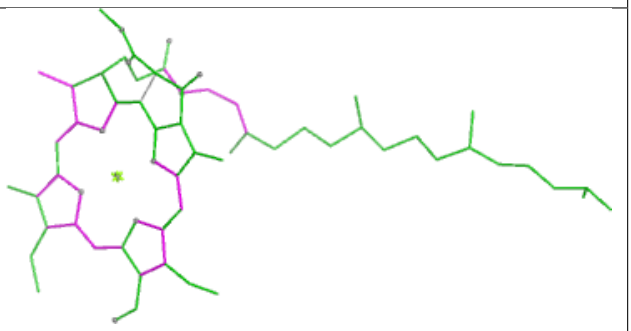


Rings

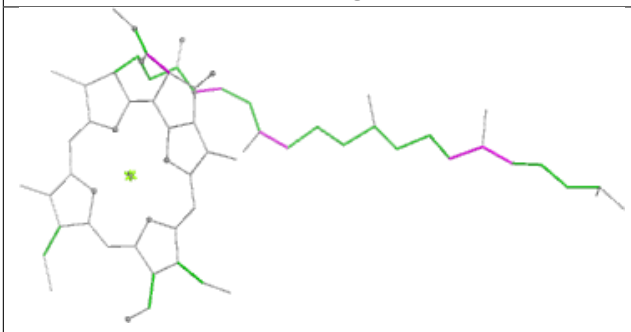
Ligand CHL Y1 609



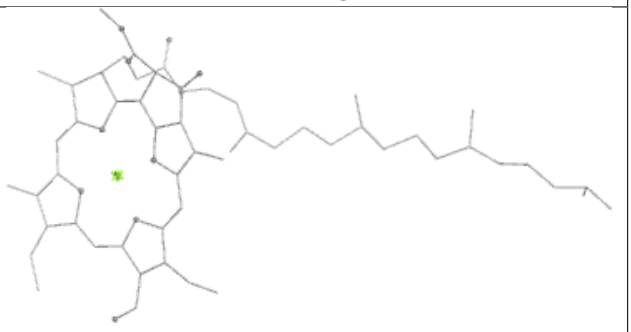
Bond lengths



Bond angles

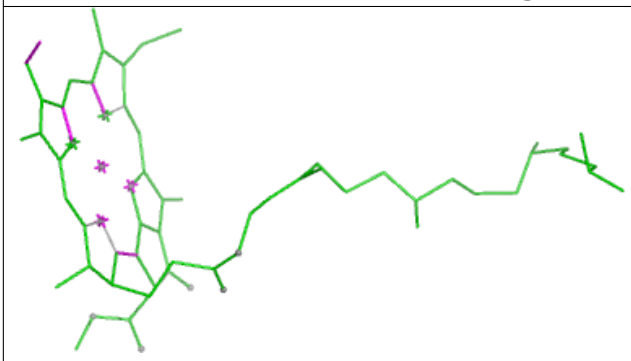


Torsions

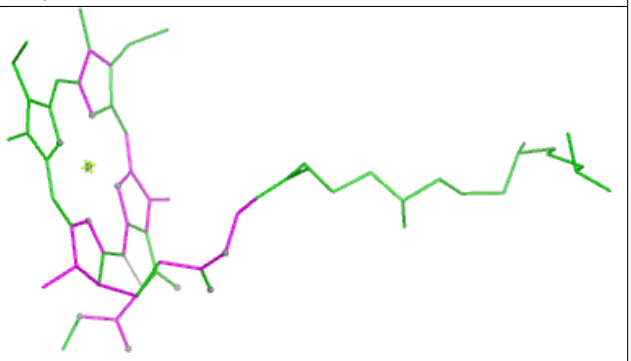


Rings

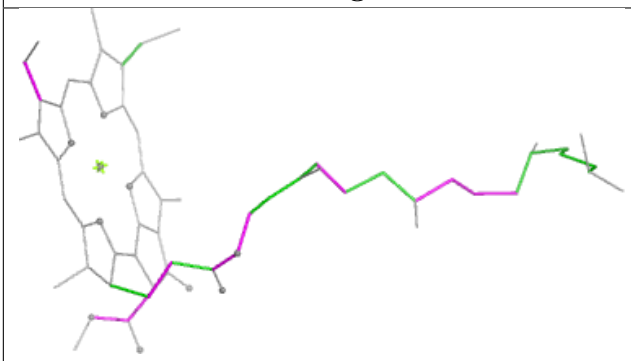
Ligand CLA y1 604



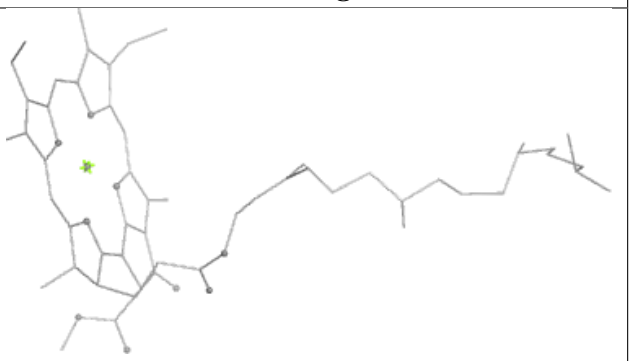
Bond lengths



Bond angles



Torsions

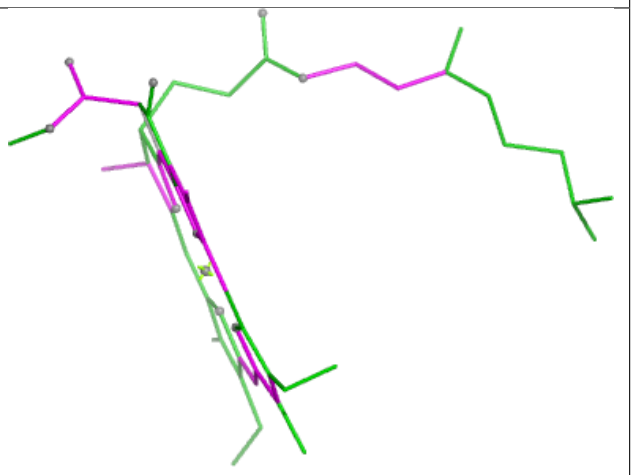


Rings

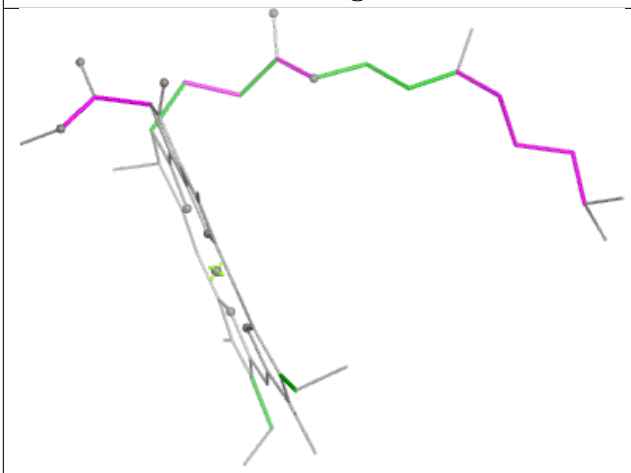
Ligand CLA s 604



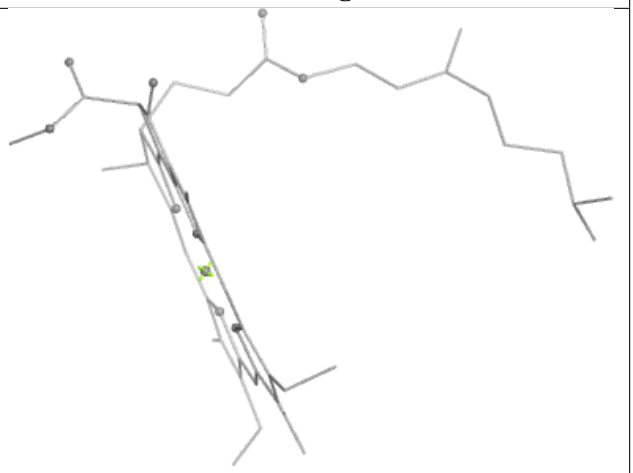
Bond lengths



Bond angles

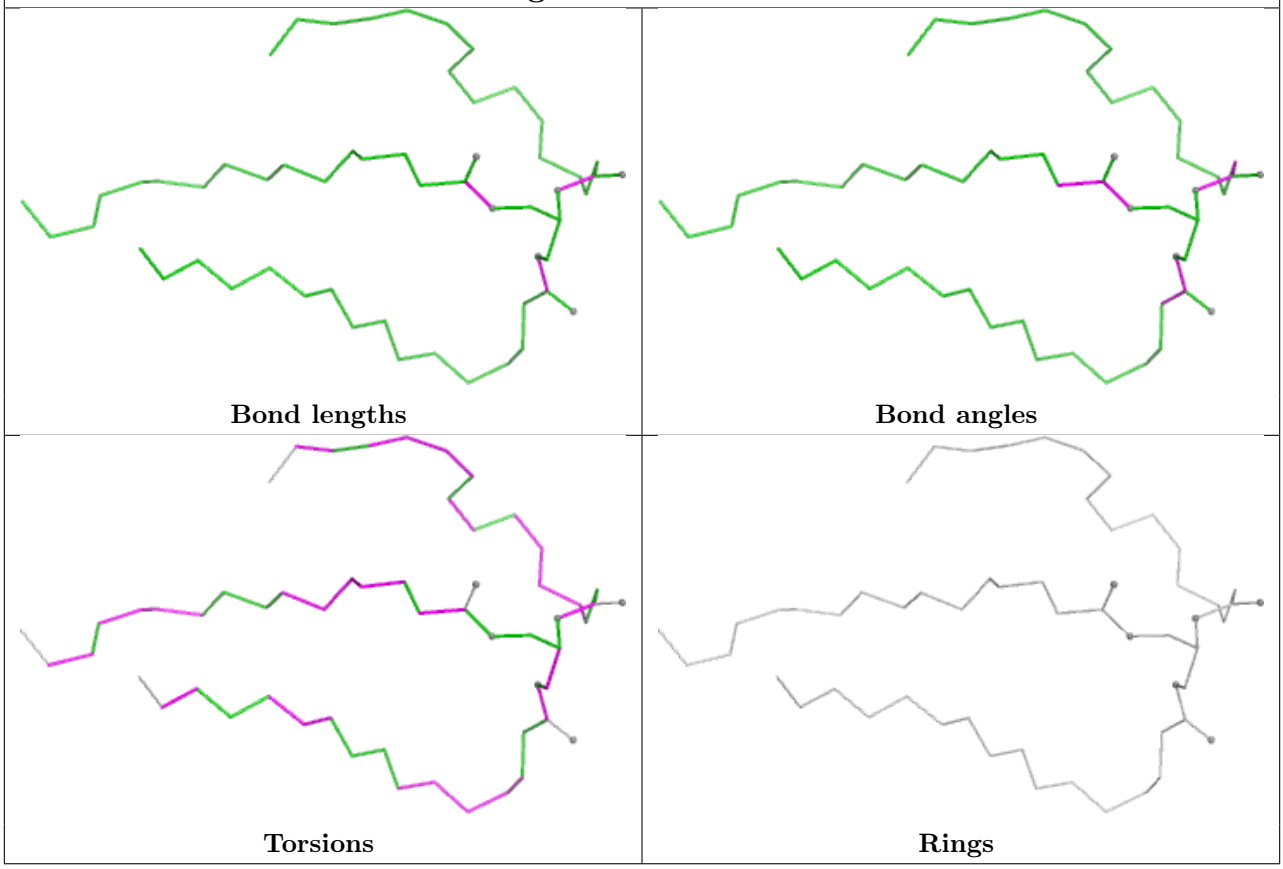


Torsions

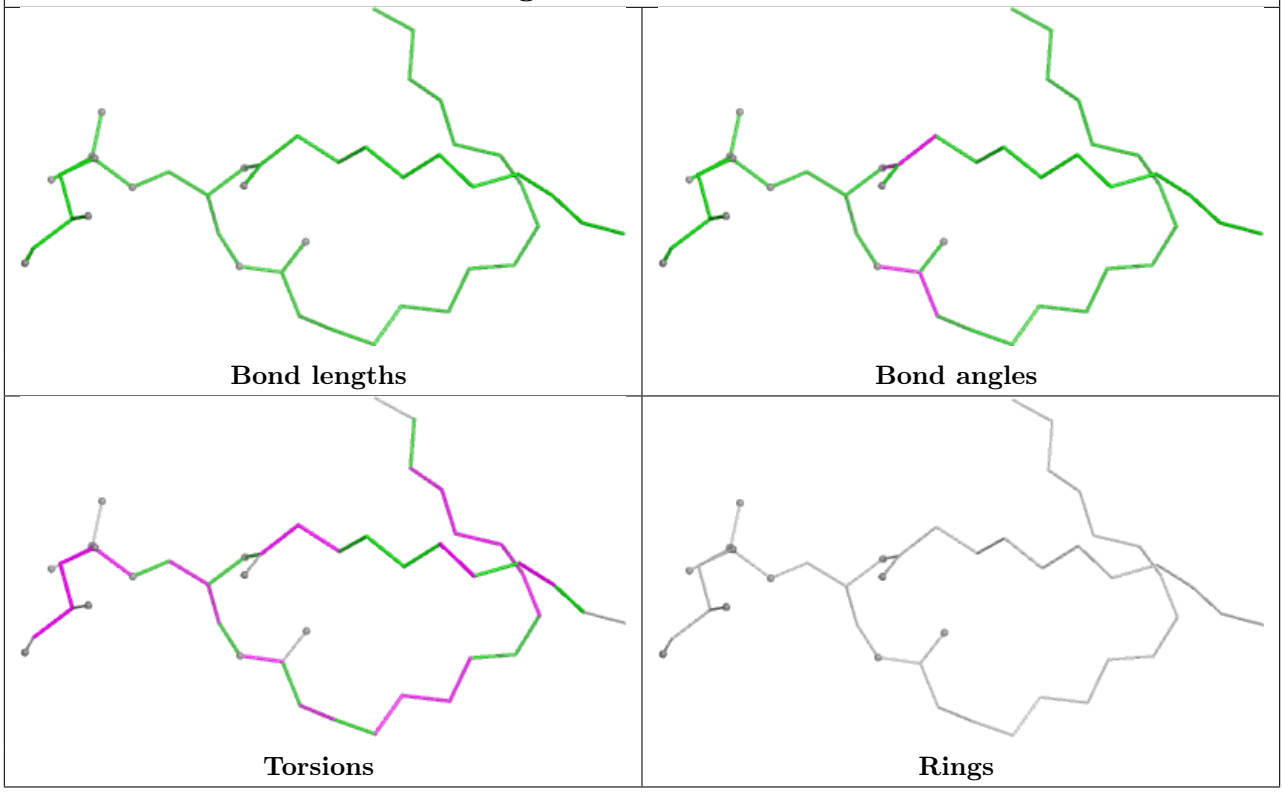


Rings

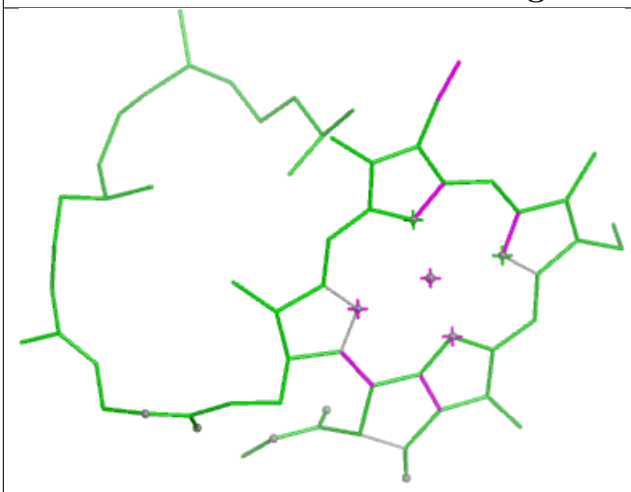
Ligand 4RF K 101



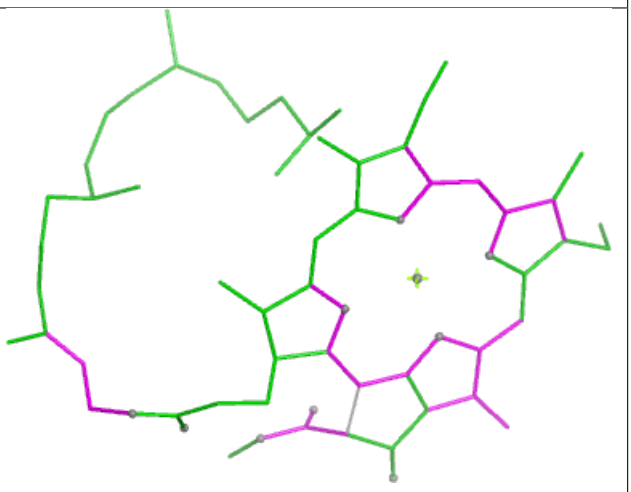
Ligand LHG d1 408



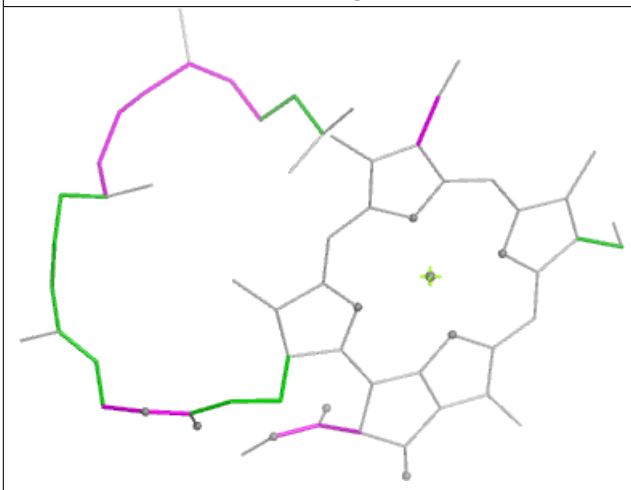
Ligand CLA b 616



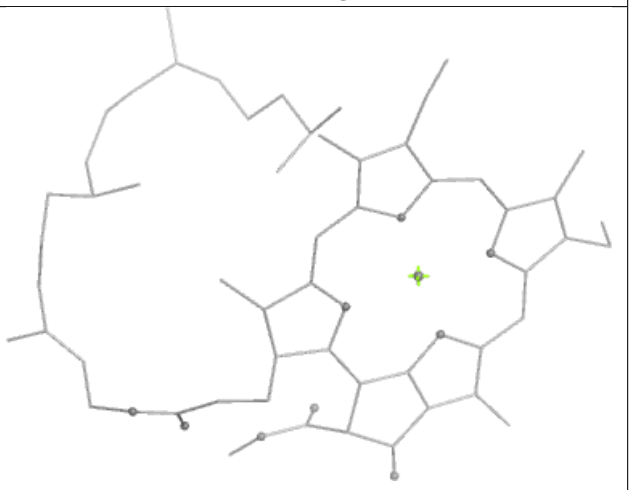
Bond lengths



Bond angles

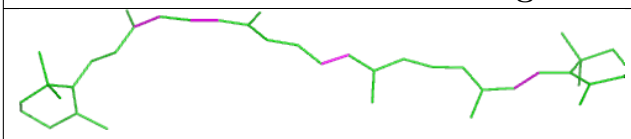


Torsions

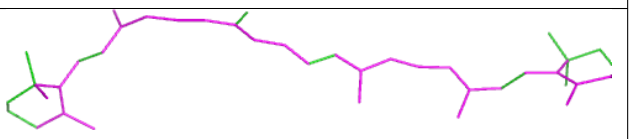


Rings

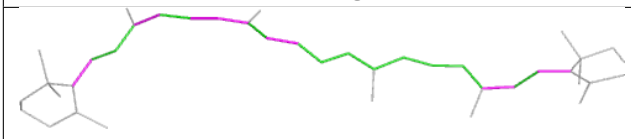
Ligand BCR d1 404



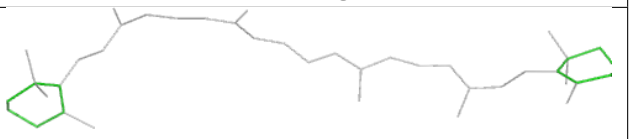
Bond lengths



Bond angles

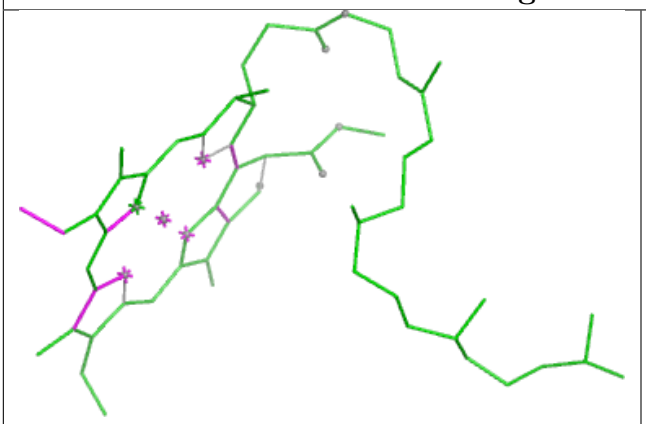


Torsions

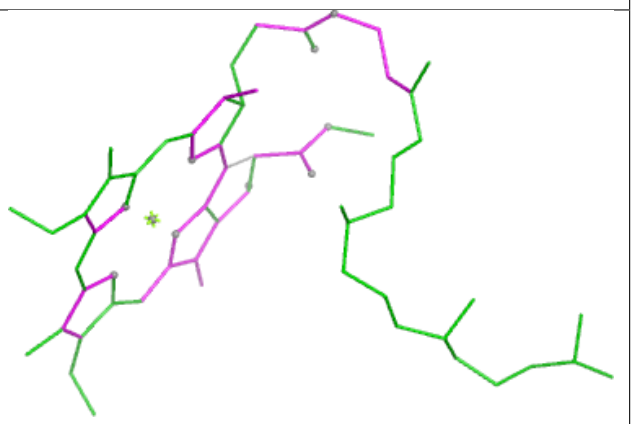


Rings

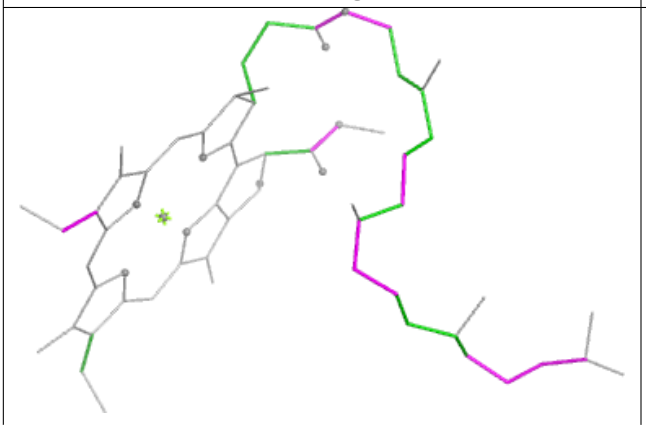
Ligand CLA b1 614



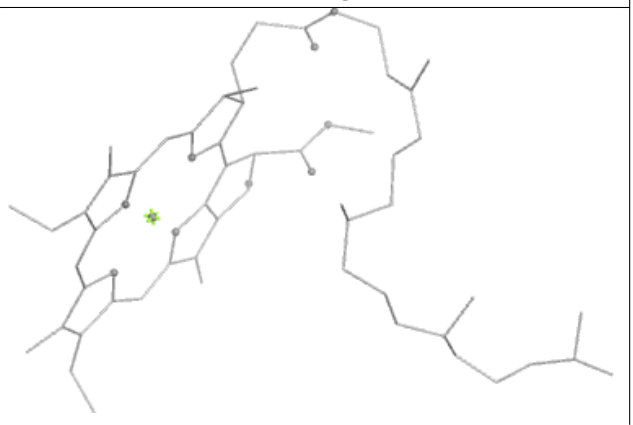
Bond lengths



Bond angles

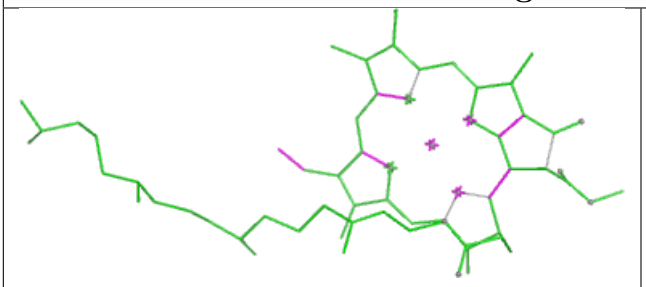


Torsions

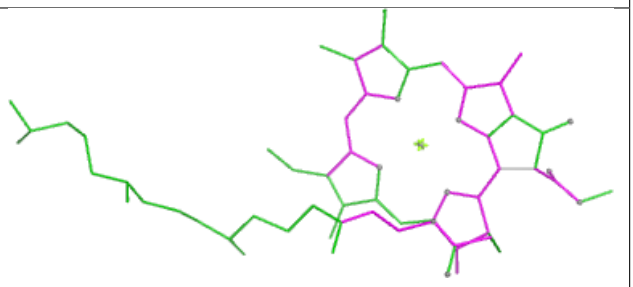


Rings

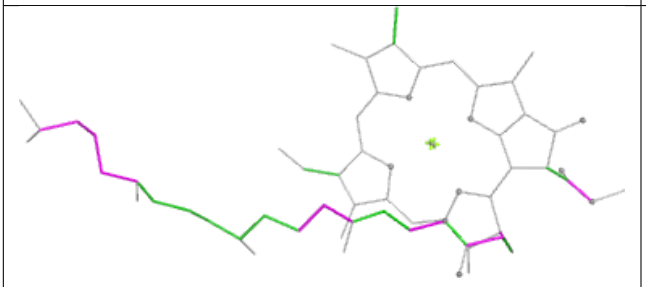
Ligand CLA C1 501



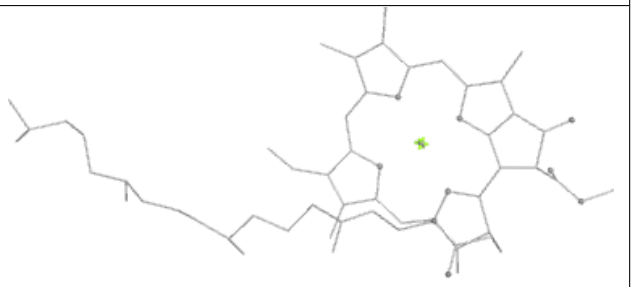
Bond lengths



Bond angles

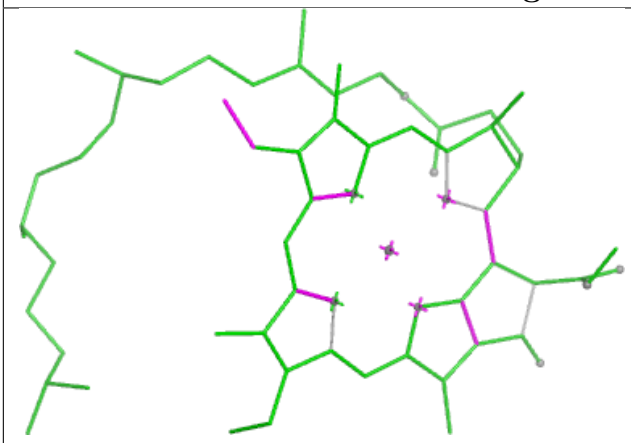


Torsions

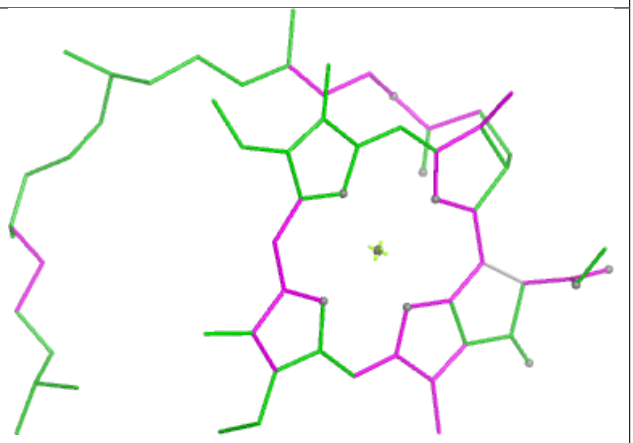


Rings

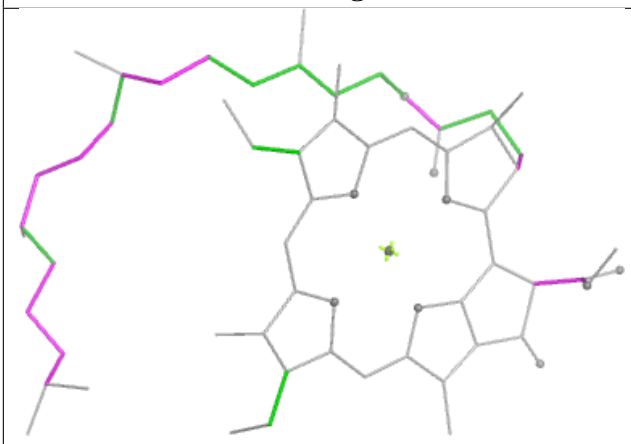
Ligand CLA G 602



Bond lengths



Bond angles

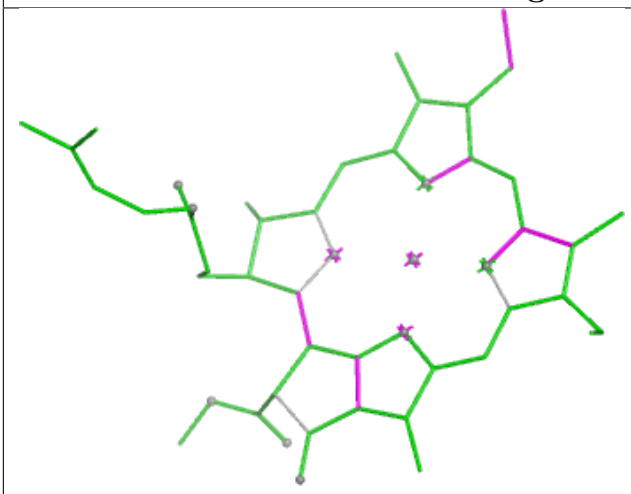


Torsions

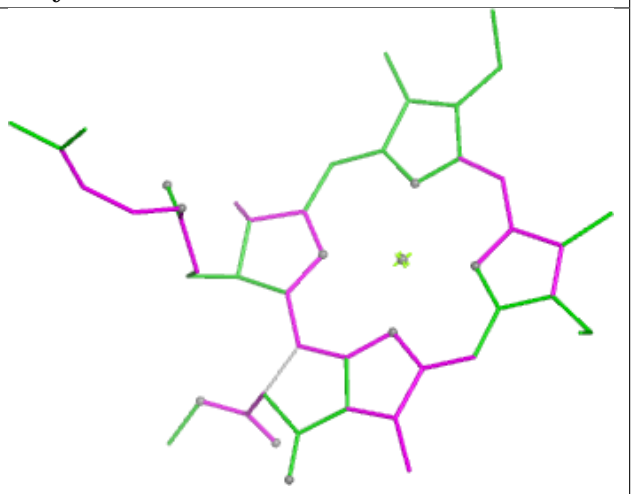


Rings

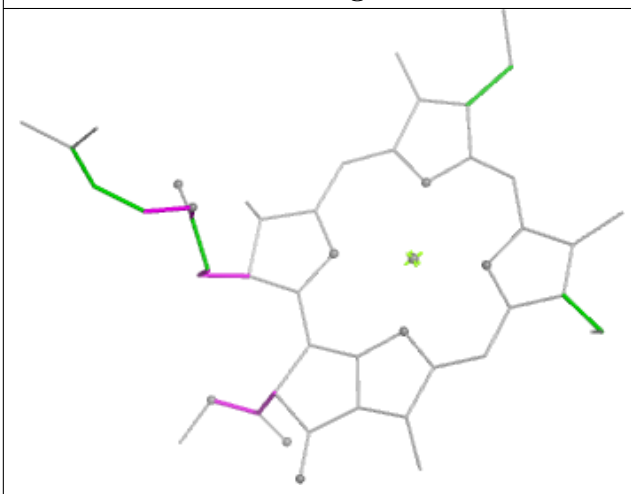
Ligand CLA y 608



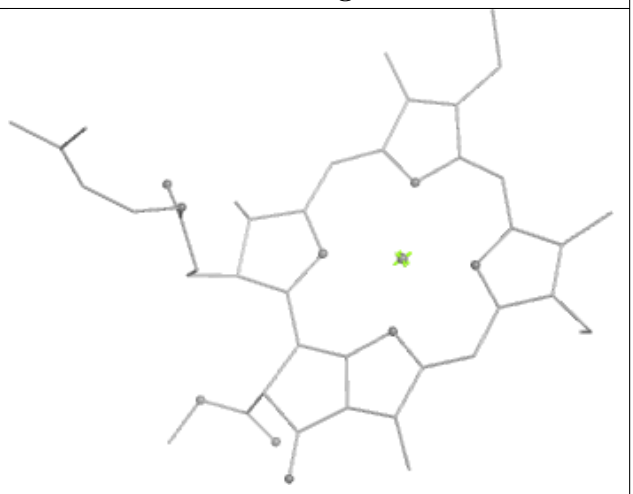
Bond lengths



Bond angles

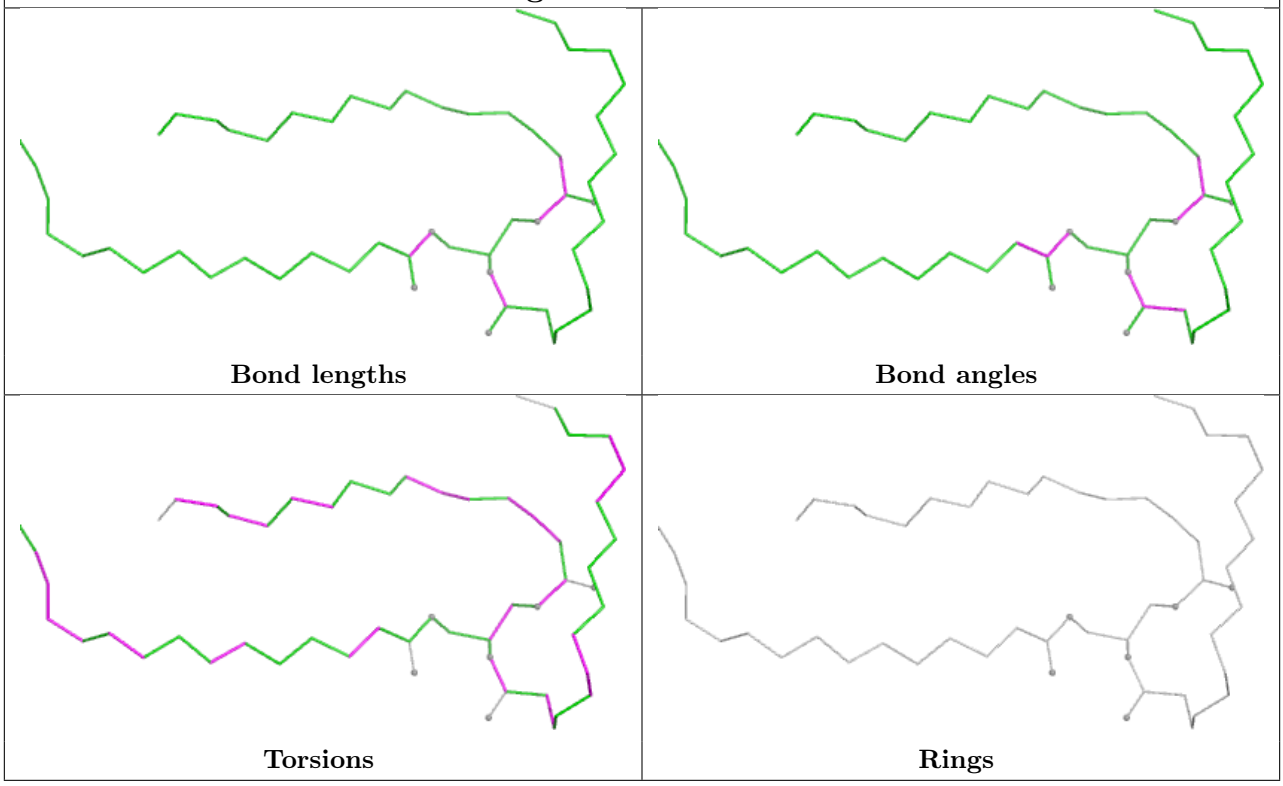


Torsions

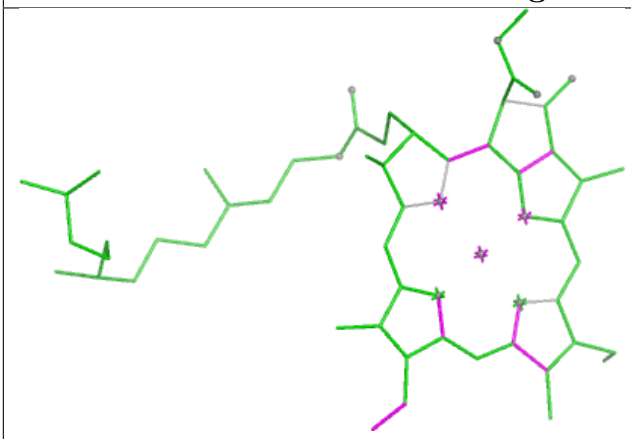


Rings

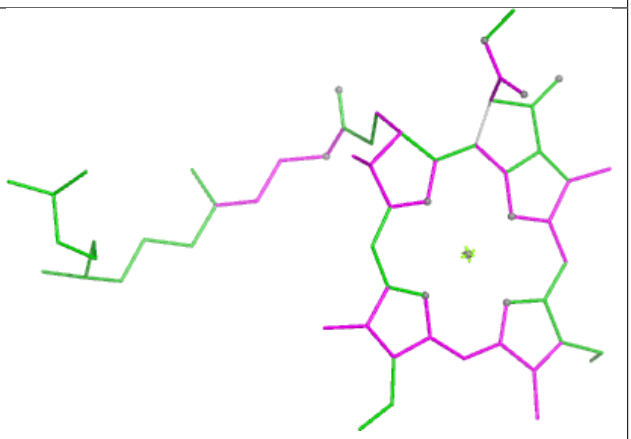
Ligand 4RF I1 102



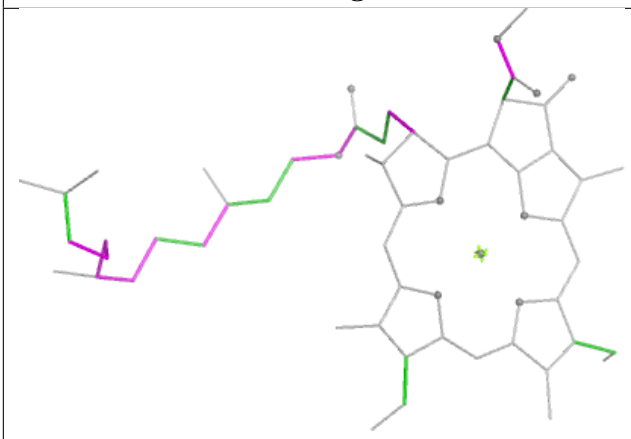
Ligand CLA a 410



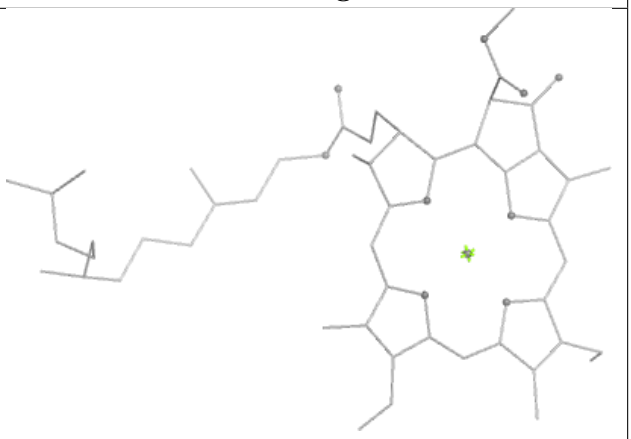
Bond lengths



Bond angles

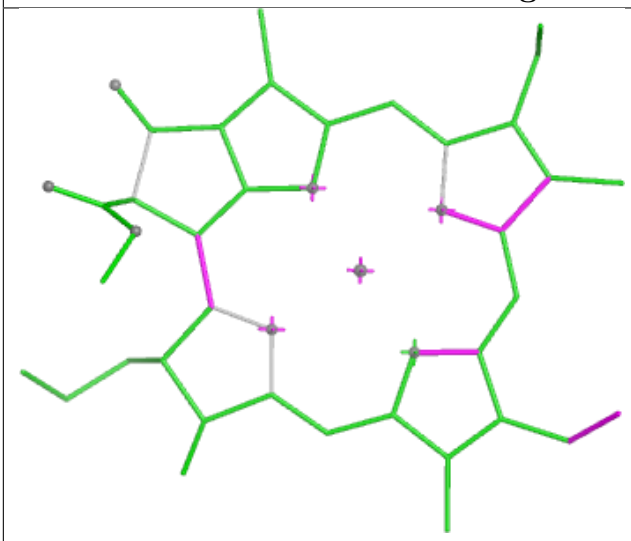


Torsions

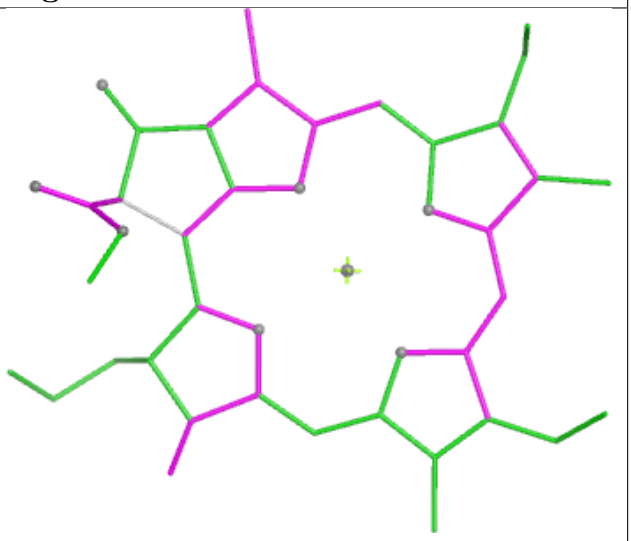


Rings

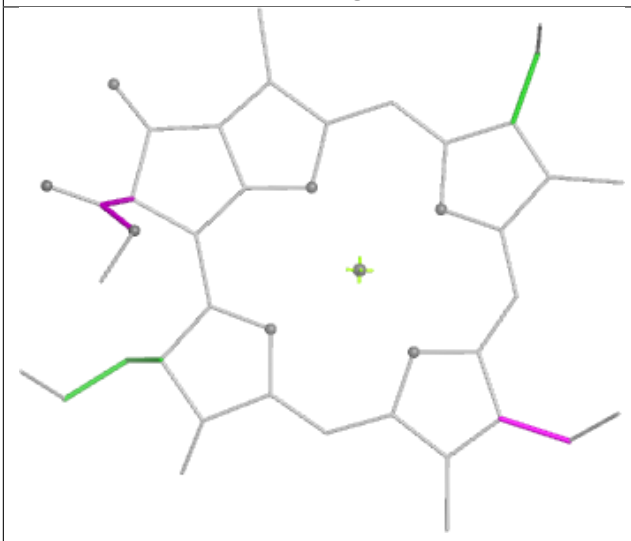
Ligand CLA g1 612



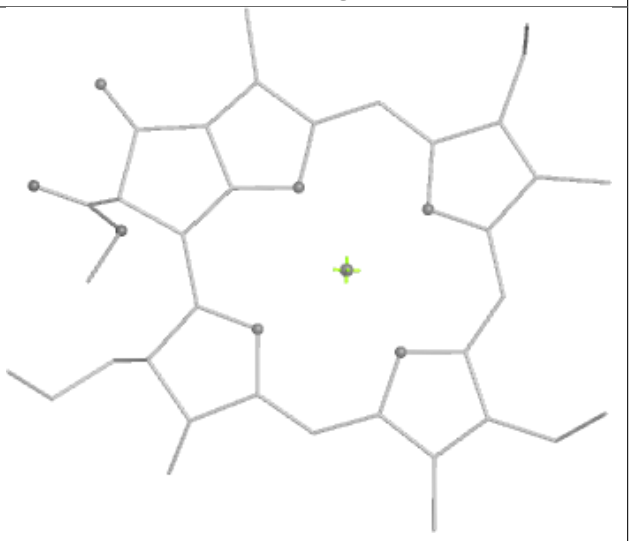
Bond lengths



Bond angles

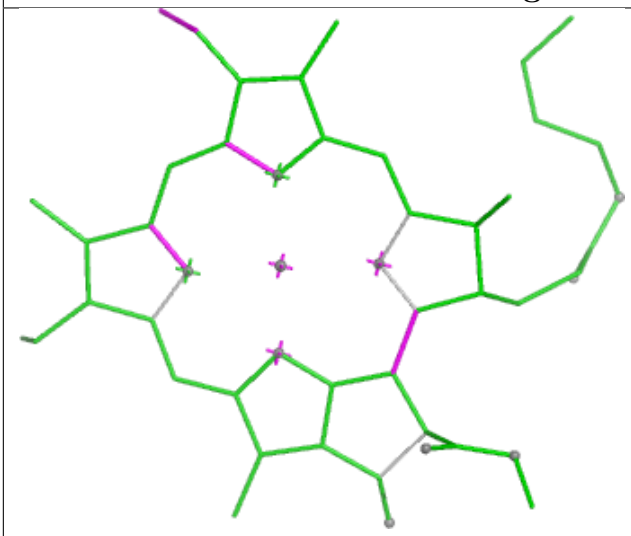


Torsions

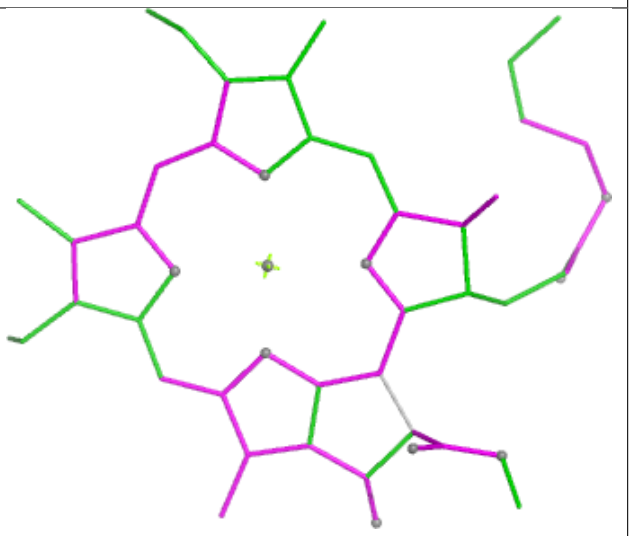


Rings

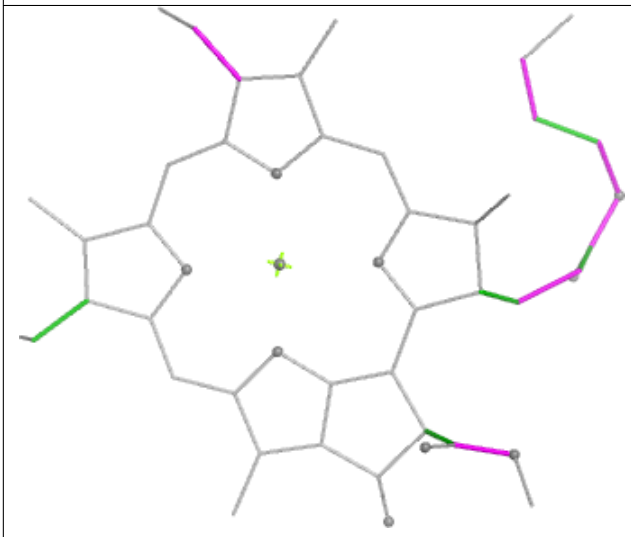
Ligand CLA N 611



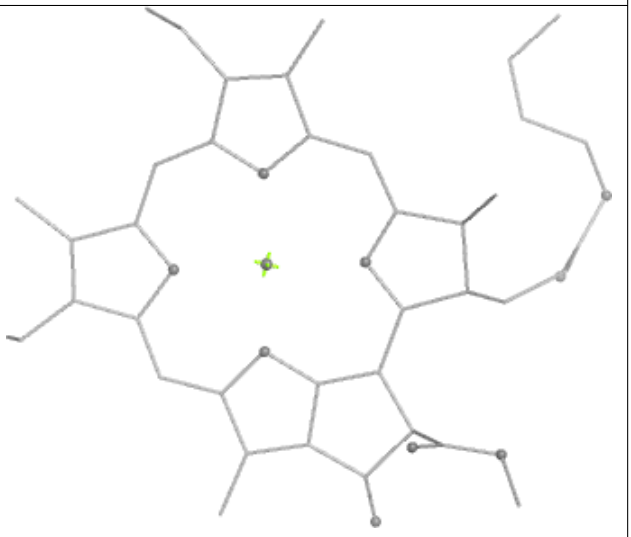
Bond lengths



Bond angles

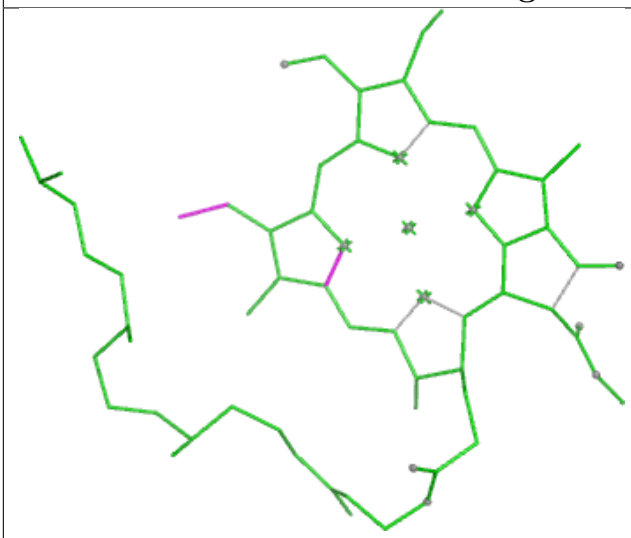


Torsions

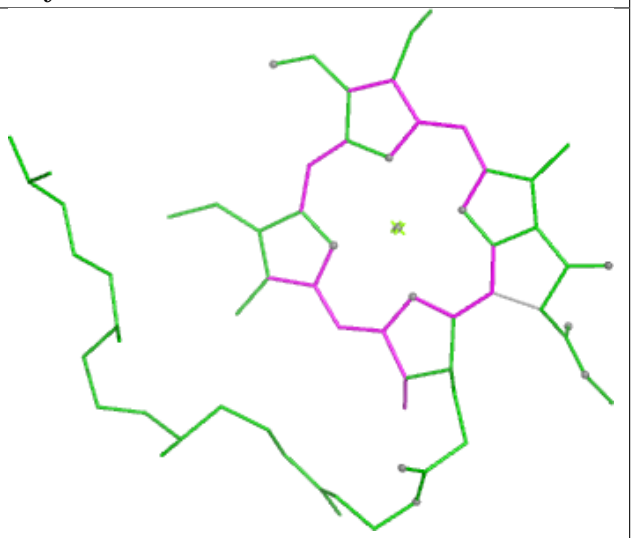


Rings

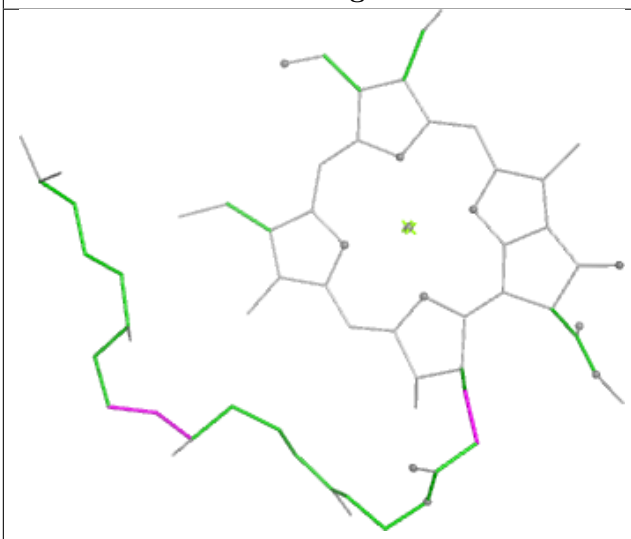
Ligand CHL y1 607



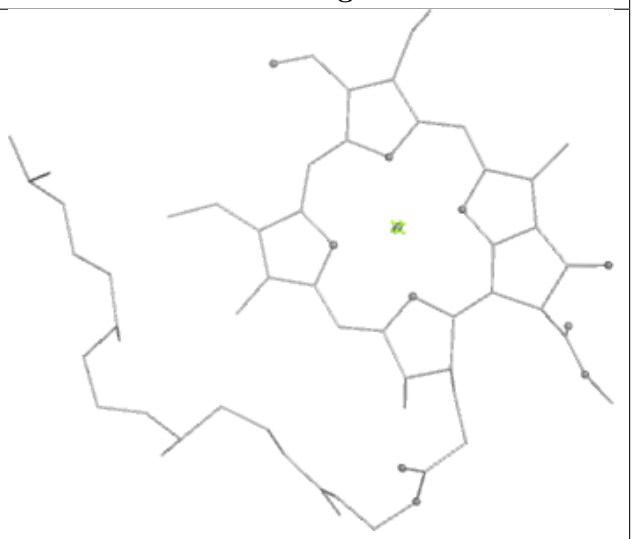
Bond lengths



Bond angles

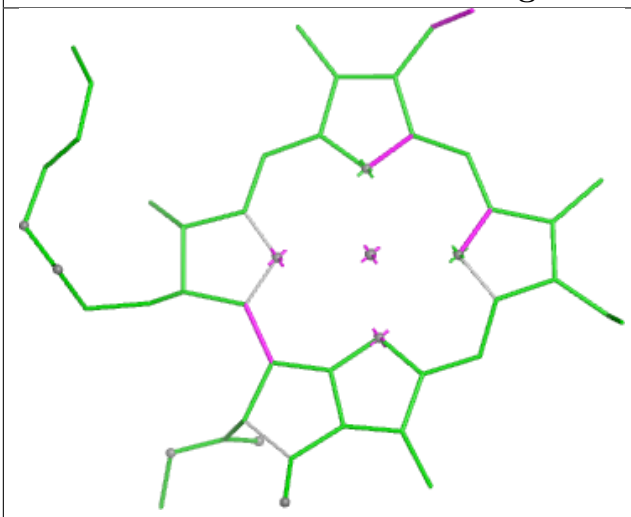


Torsions

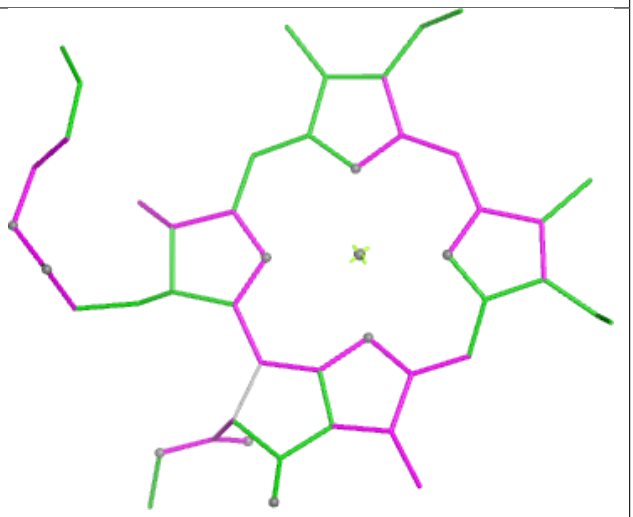


Rings

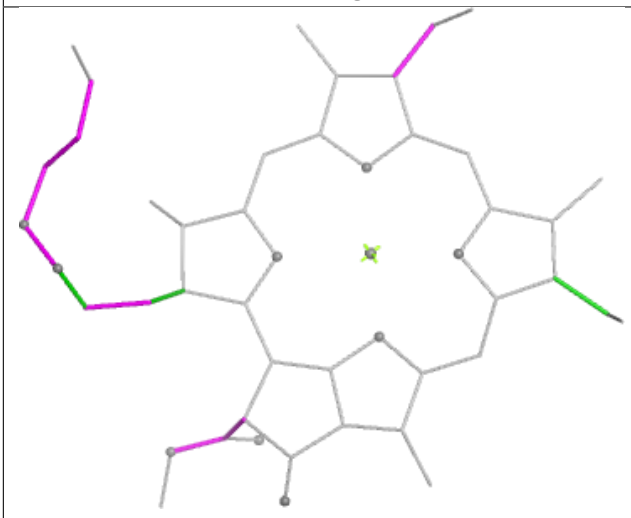
Ligand CLA n1 611



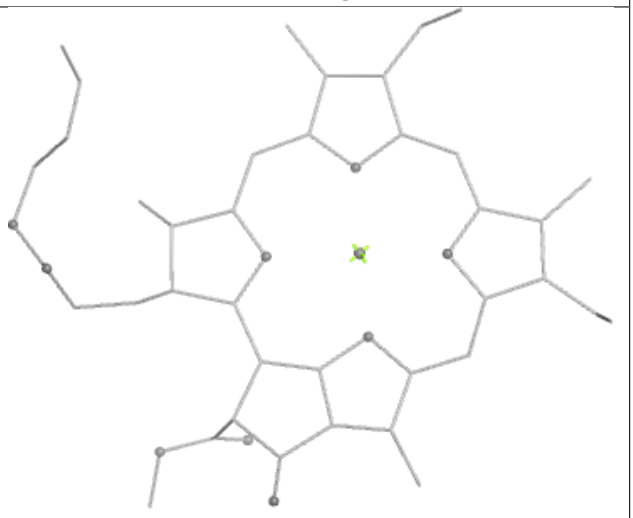
Bond lengths



Bond angles

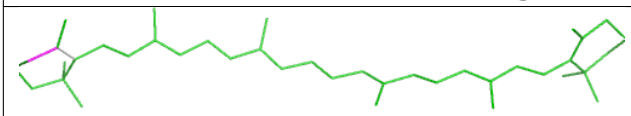


Torsions

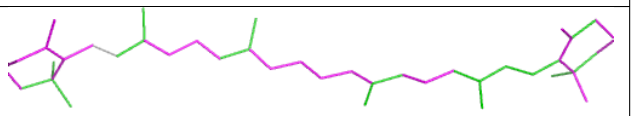


Rings

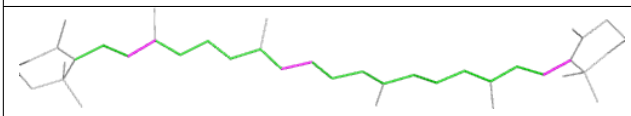
Ligand LUT G1 620



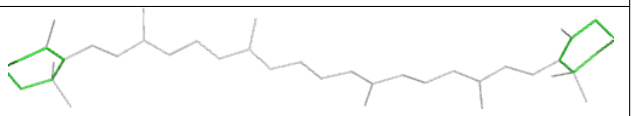
Bond lengths



Bond angles

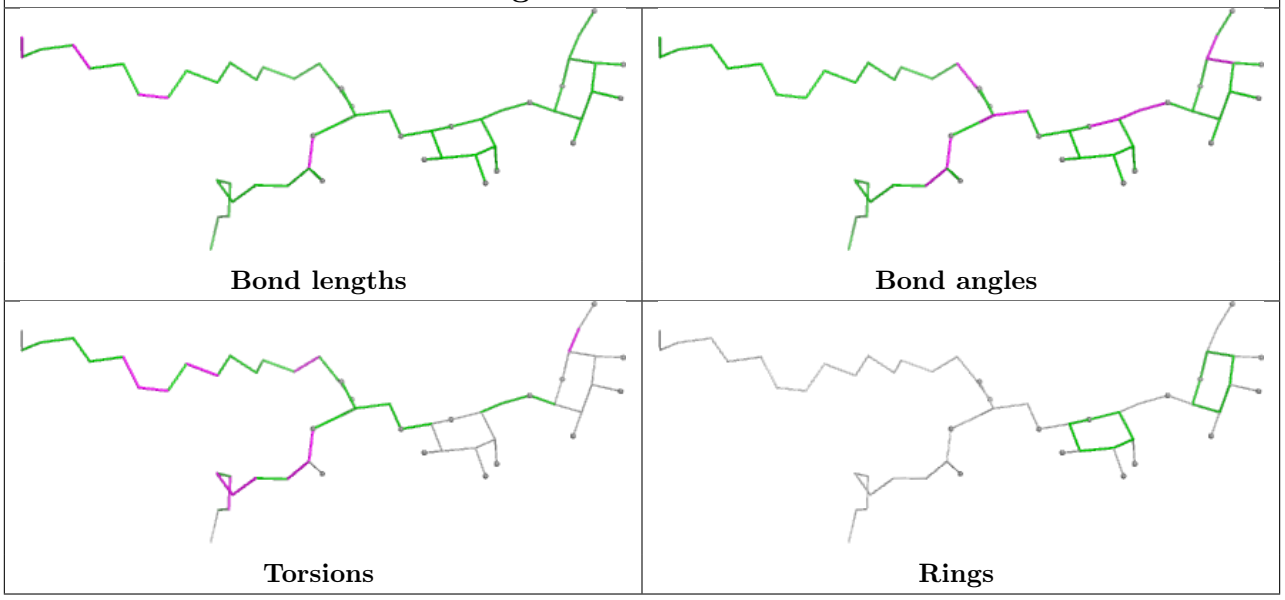


Torsions

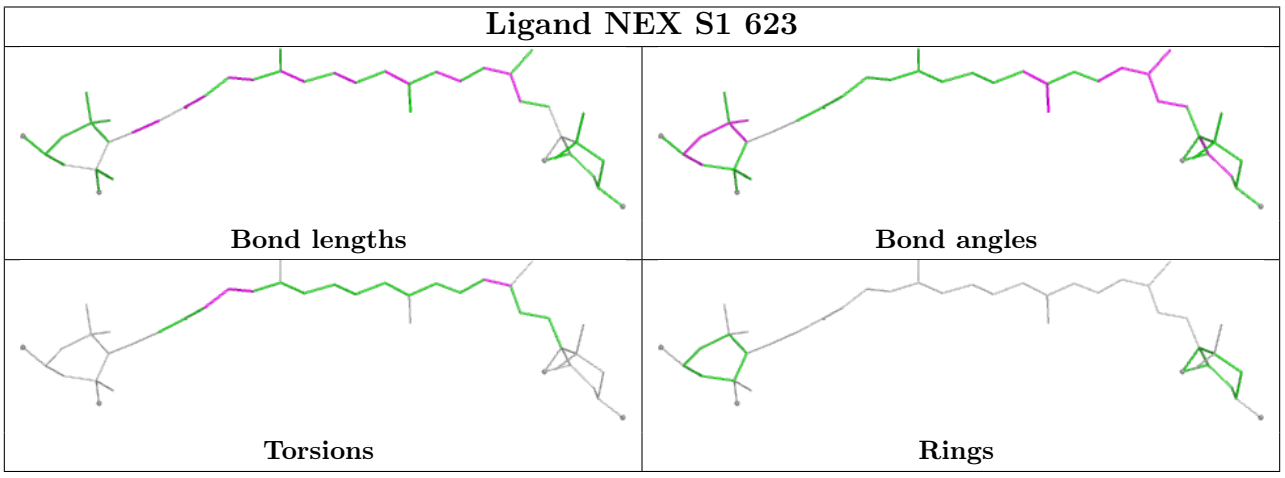


Rings

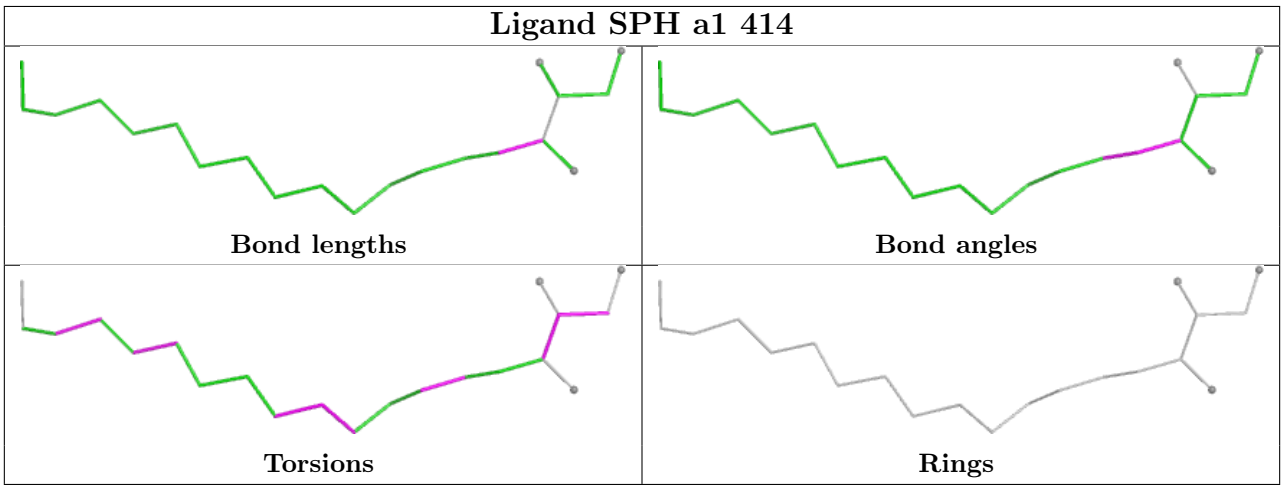
Ligand DGD C1 518



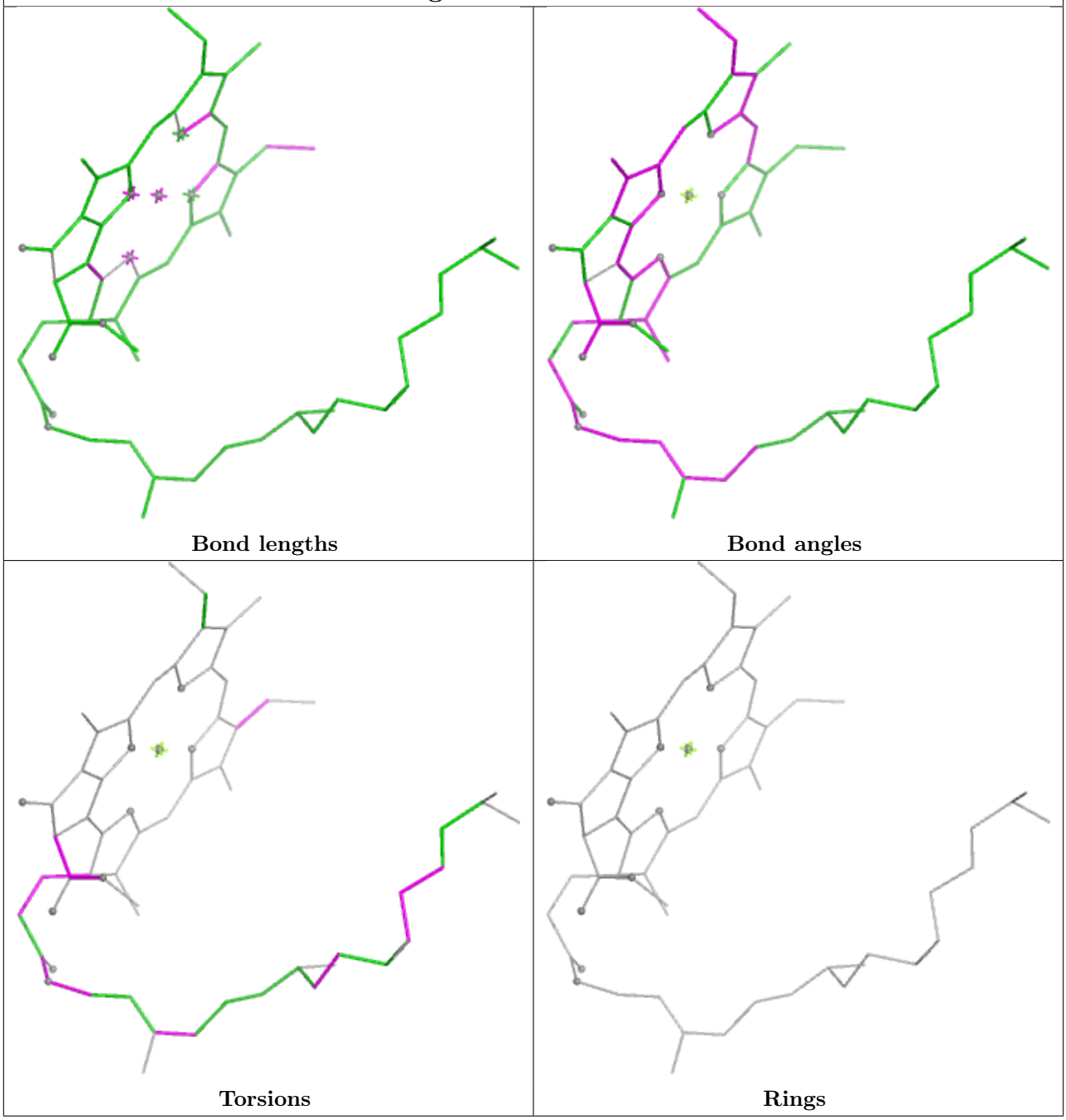
Ligand NEX S1 623



Ligand SPH a1 414



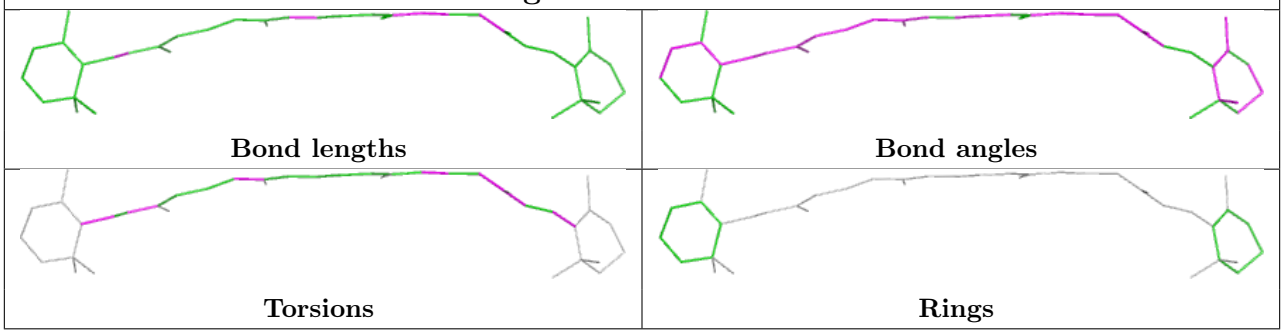
Ligand CLA N1 603



Bond lengths | Bond angles

Torsions | Rings

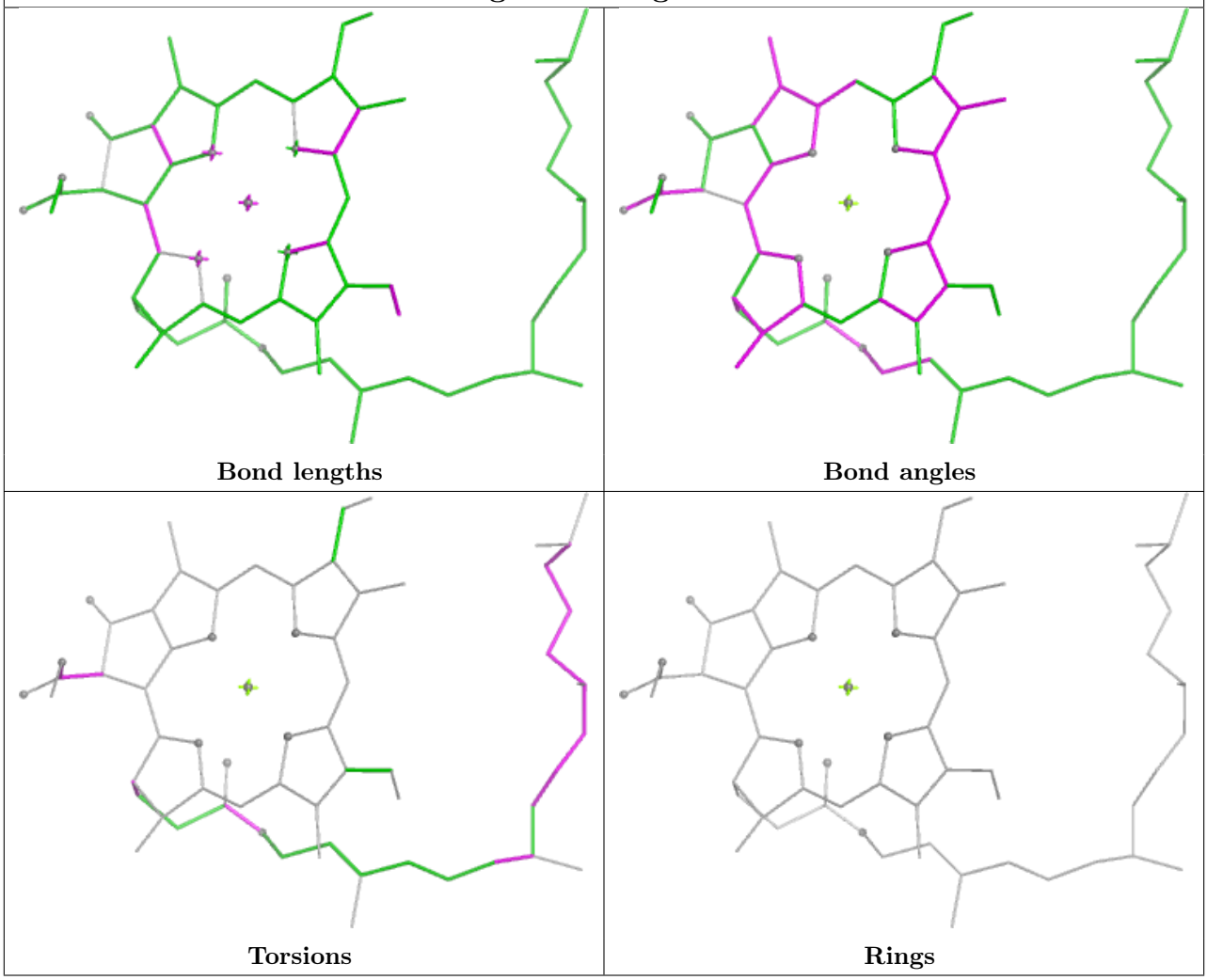
Ligand BCR C 517



Bond lengths | Bond angles

Torsions | Rings

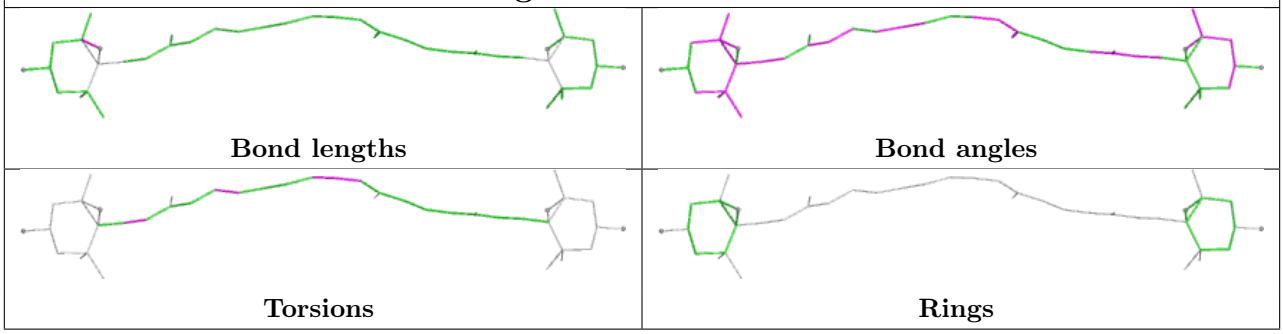
Ligand CLA g1 602



Bond lengths | Bond angles

Torsions | Rings

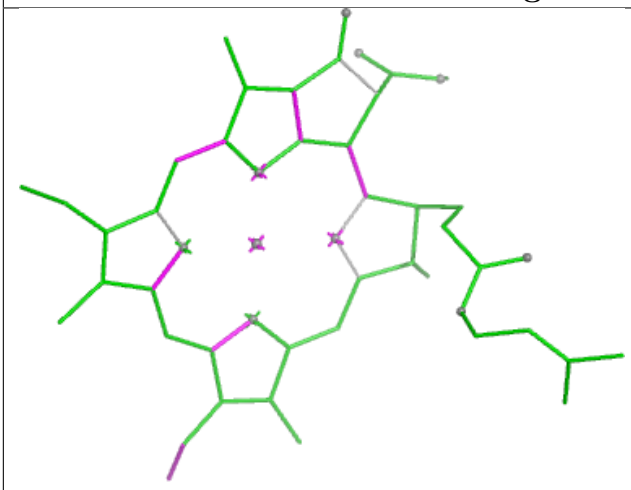
Ligand XAT Y1 622



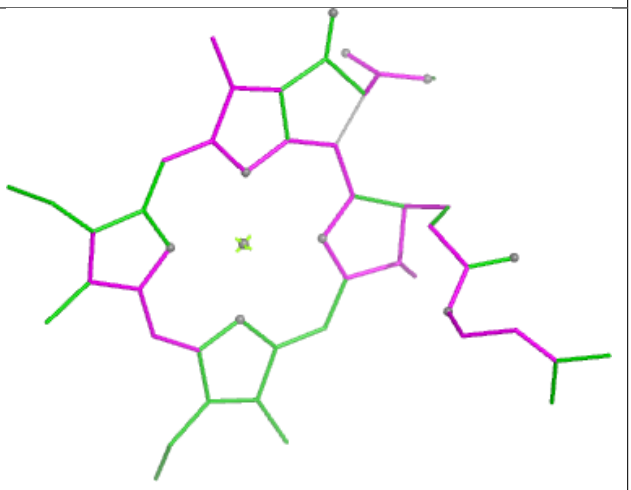
Bond lengths | Bond angles

Torsions | Rings

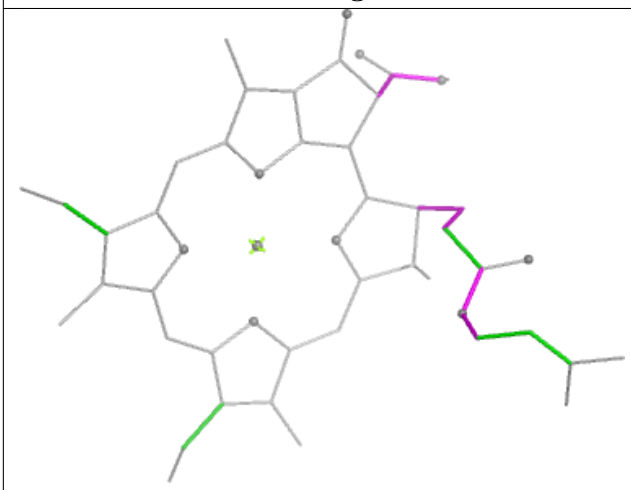
Ligand CLA A 407



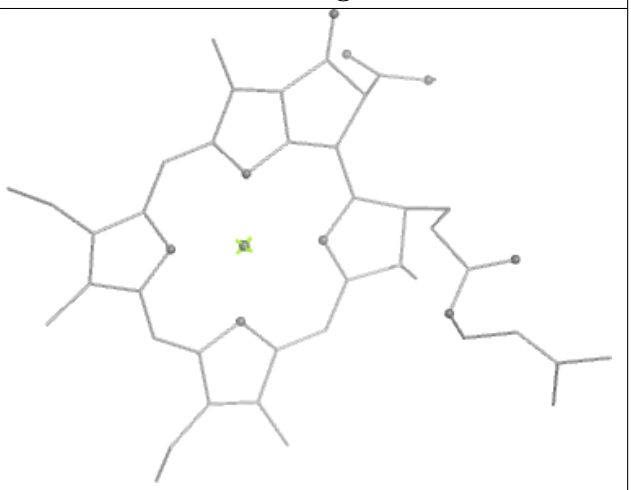
Bond lengths



Bond angles

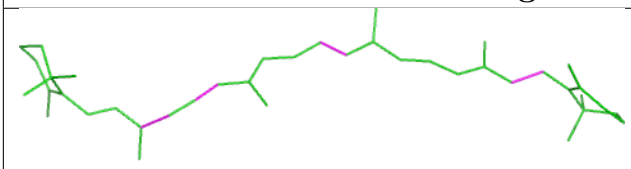


Torsions

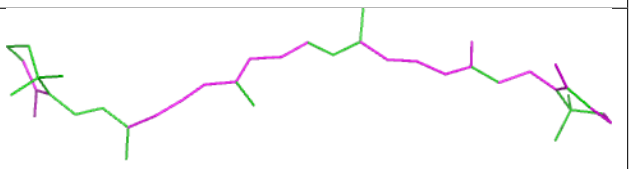


Rings

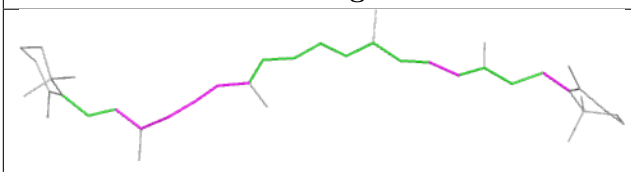
Ligand BCR c1 515



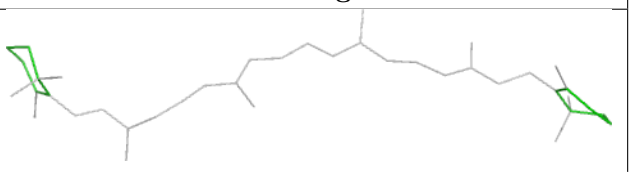
Bond lengths



Bond angles

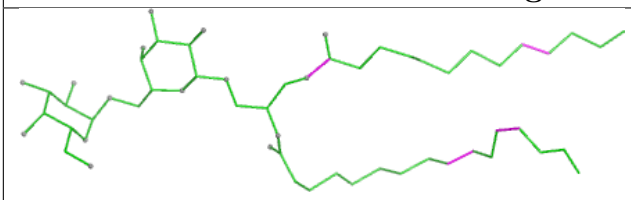


Torsions

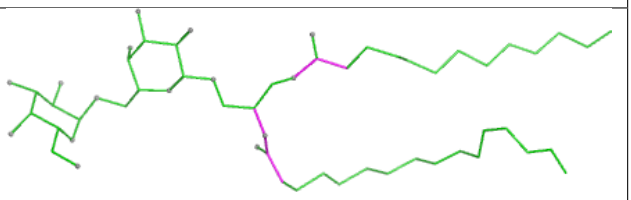


Rings

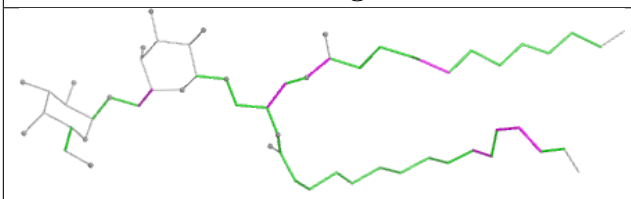
Ligand DGD c 520



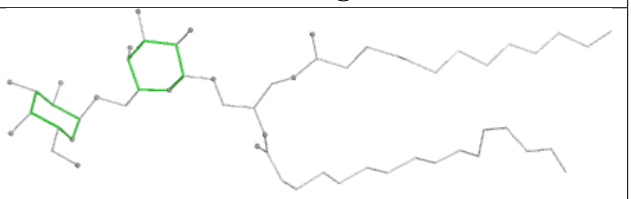
Bond lengths



Bond angles

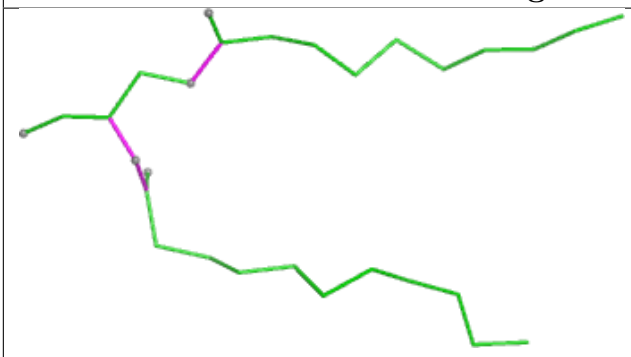


Torsions

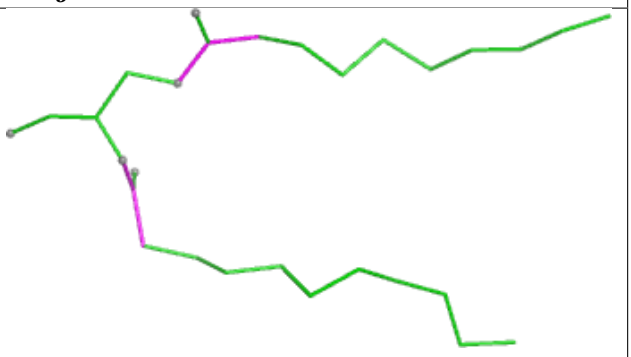


Rings

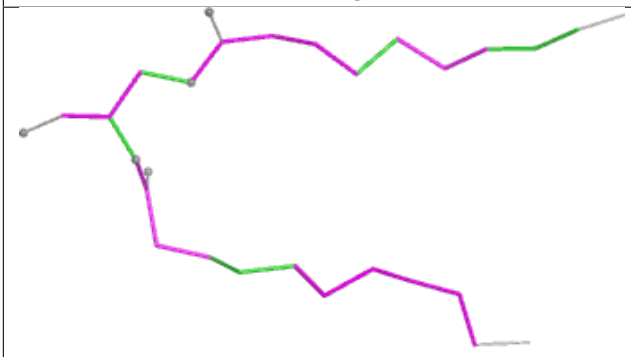
Ligand DGA j 101



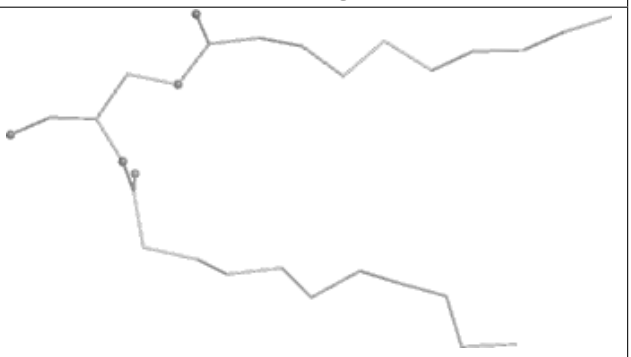
Bond lengths



Bond angles

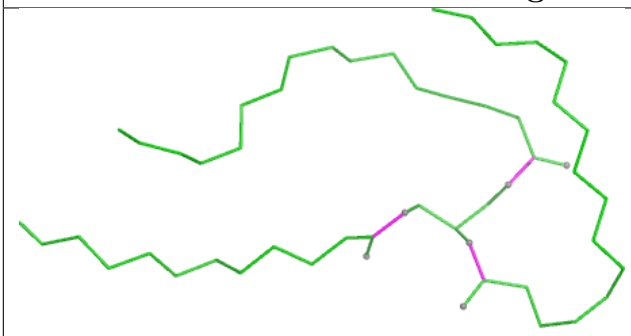


Torsions

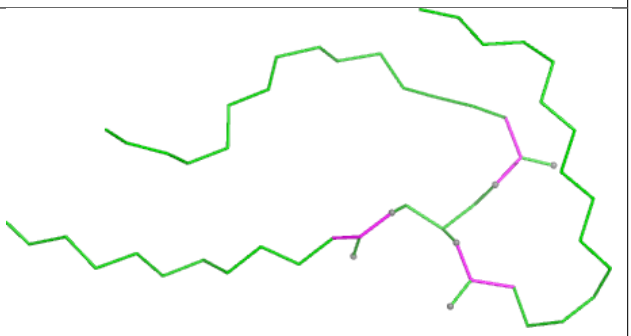


Rings

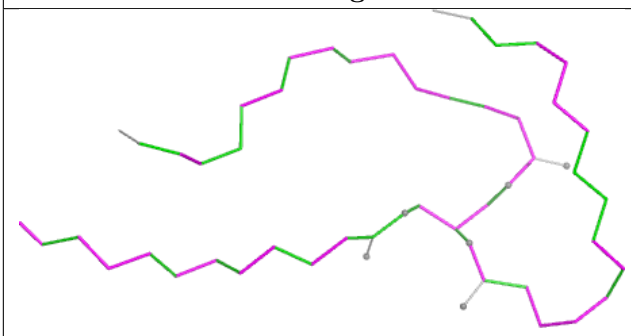
Ligand 4RF i1 101



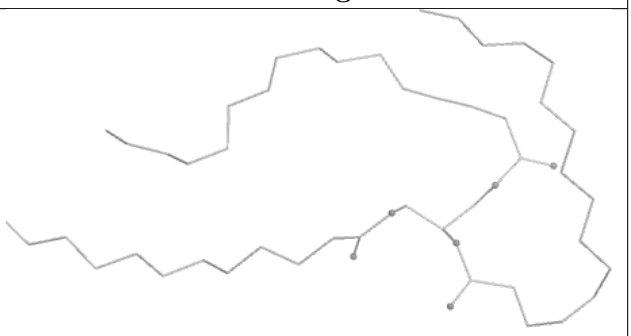
Bond lengths



Bond angles

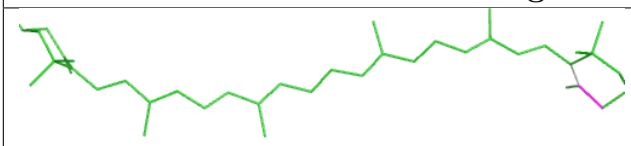


Torsions

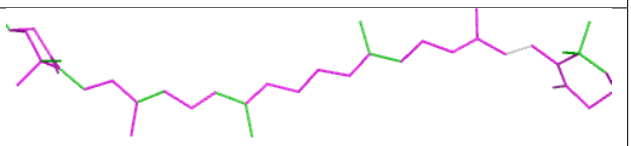


Rings

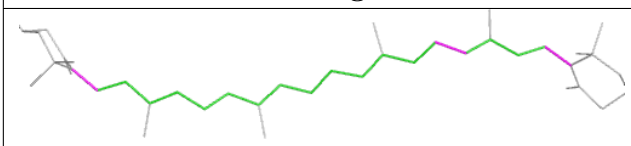
Ligand LUT S 621



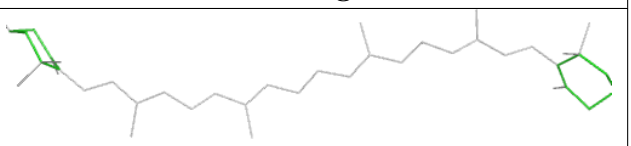
Bond lengths



Bond angles

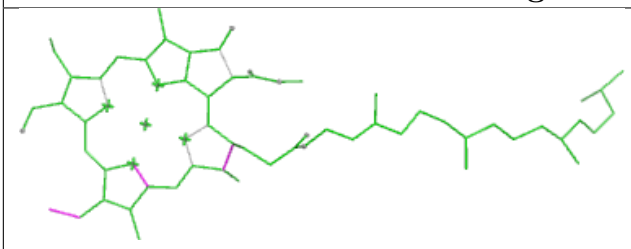


Torsions

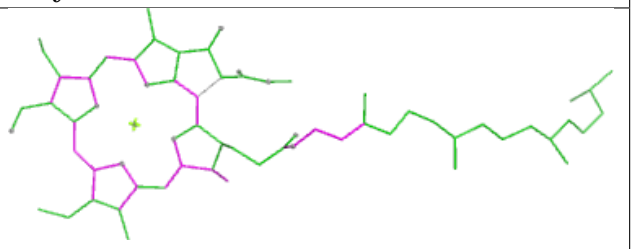


Rings

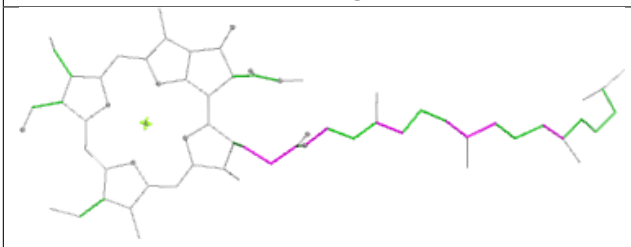
Ligand CHL y 606



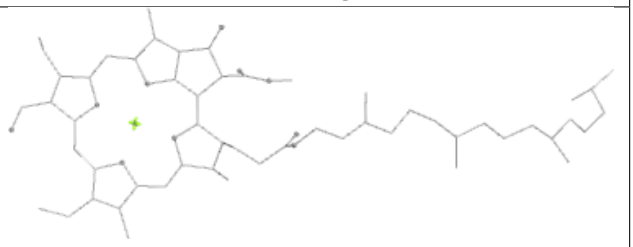
Bond lengths



Bond angles

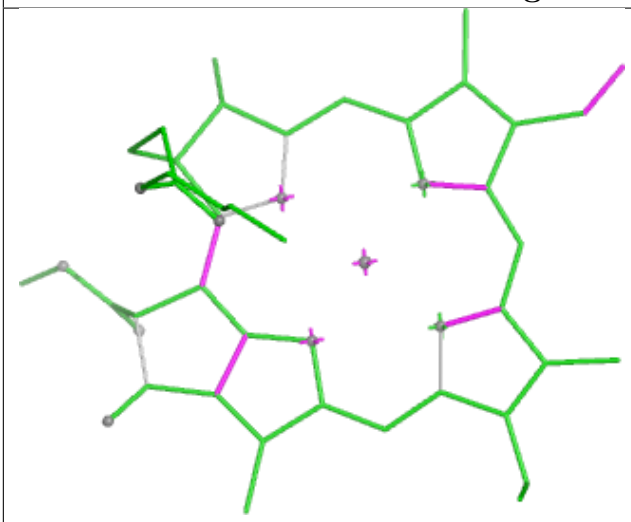


Torsions

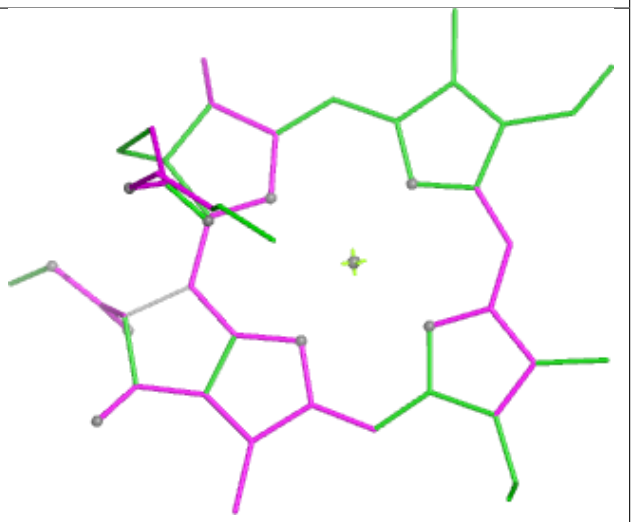


Rings

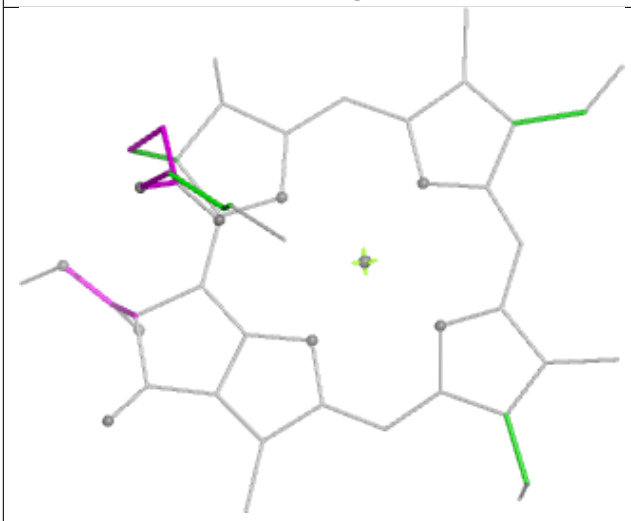
Ligand CLA R 604



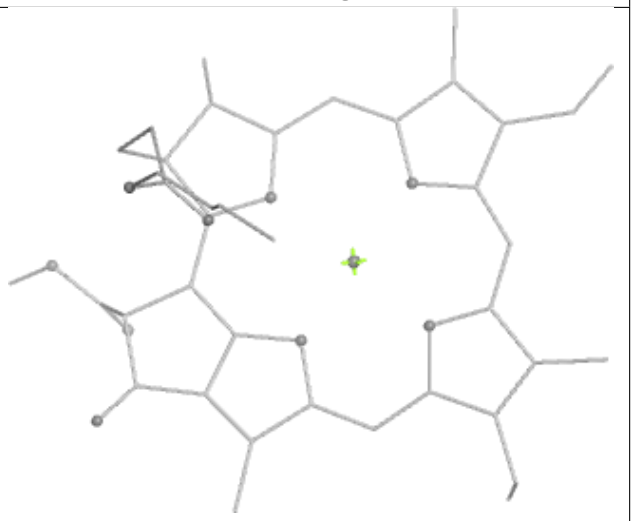
Bond lengths



Bond angles

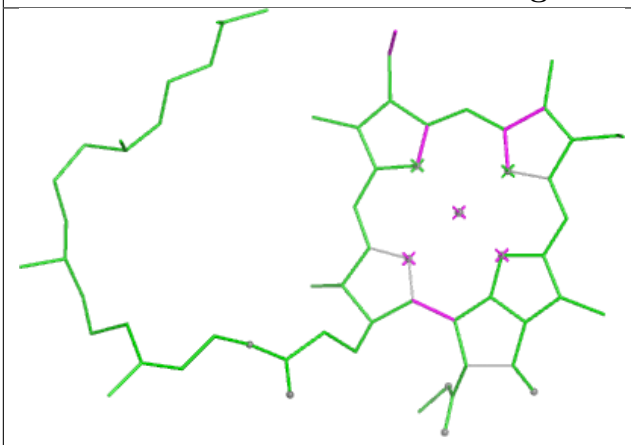


Torsions

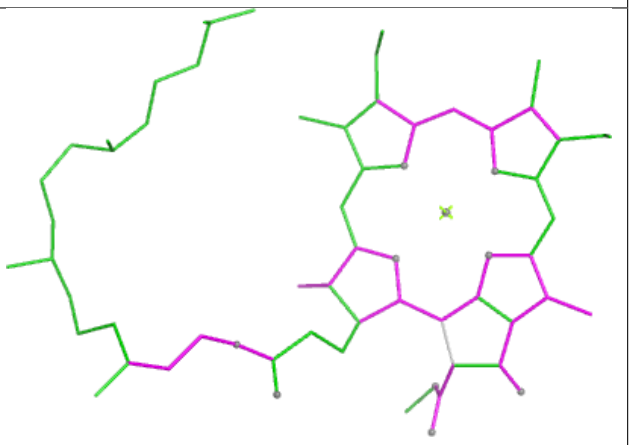


Rings

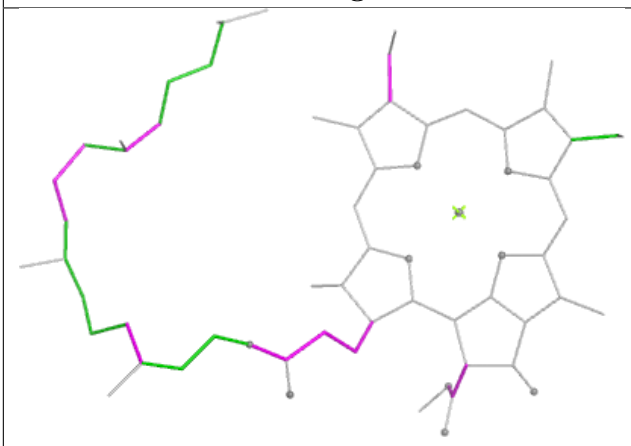
Ligand CLA s 603



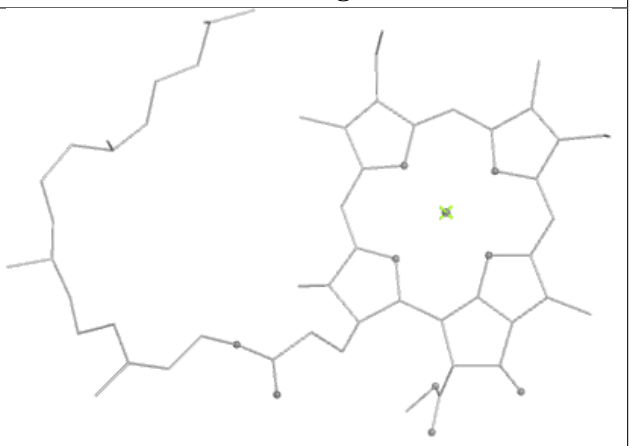
Bond lengths



Bond angles

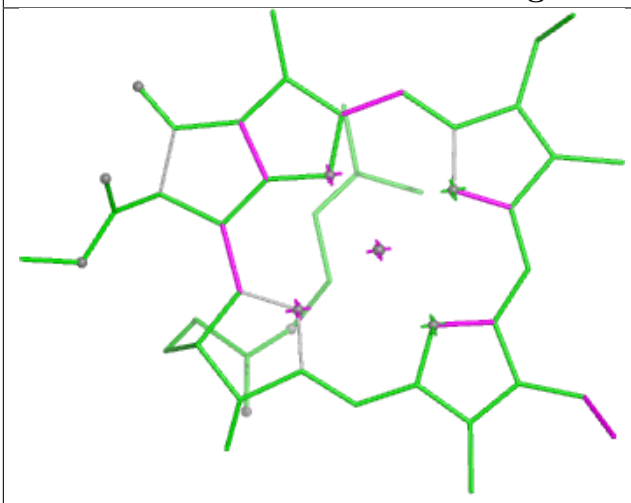


Torsions

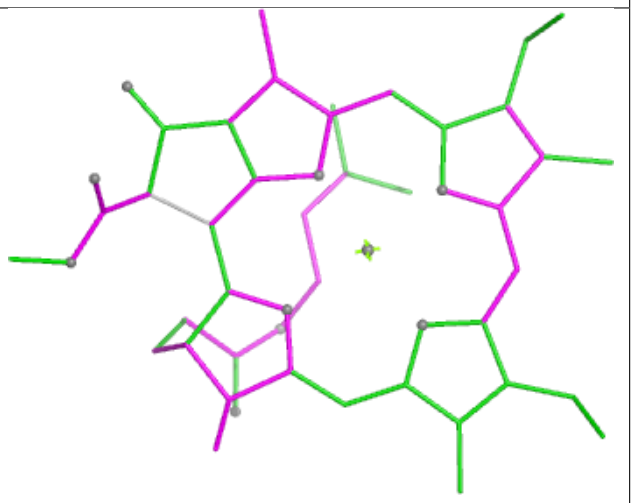


Rings

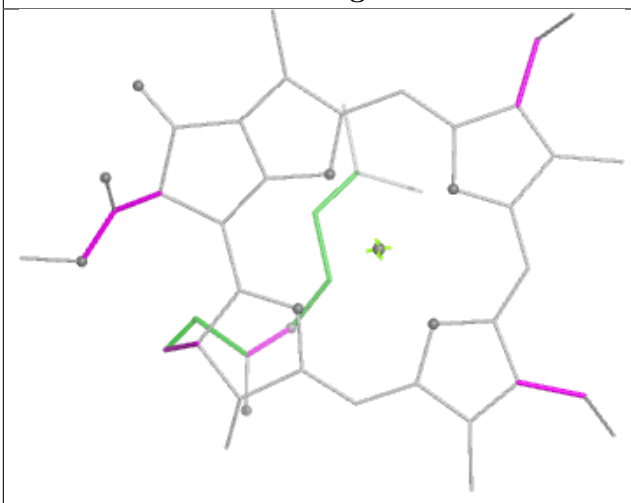
Ligand CLA S 605



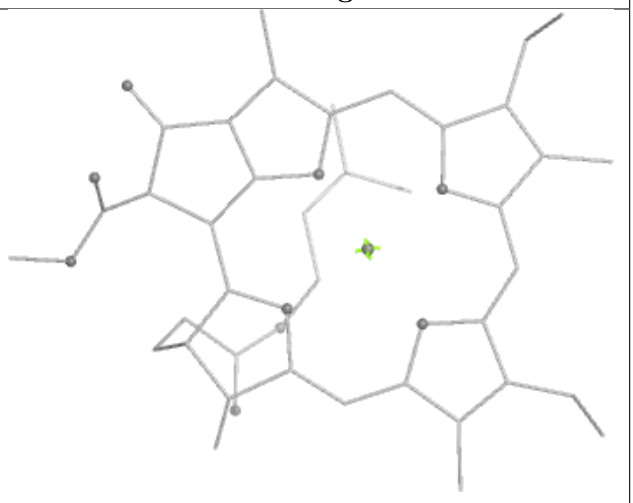
Bond lengths



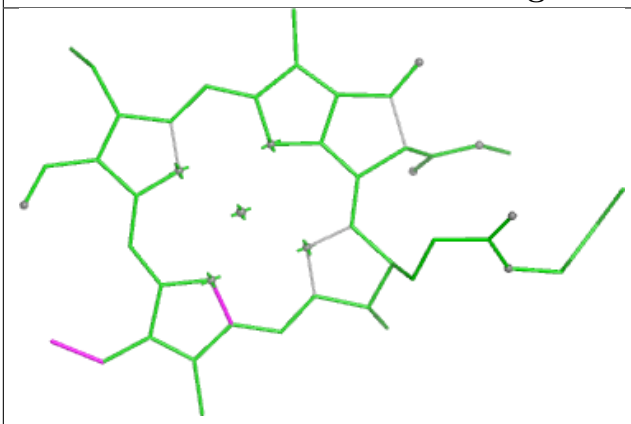
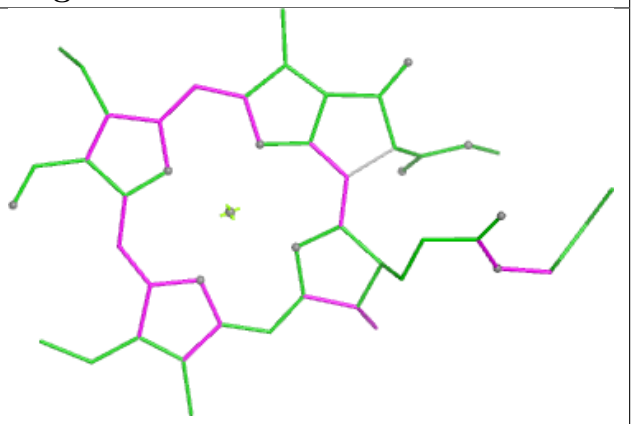
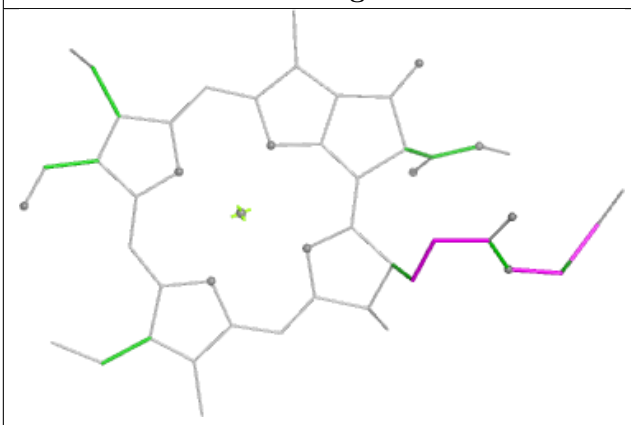
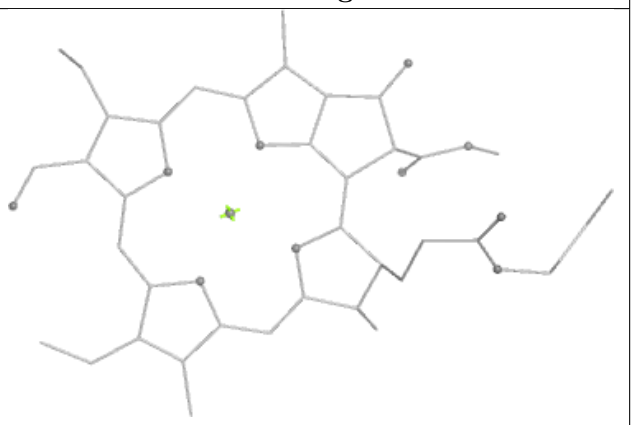
Bond angles

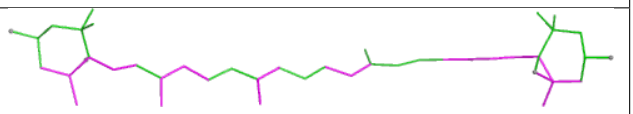
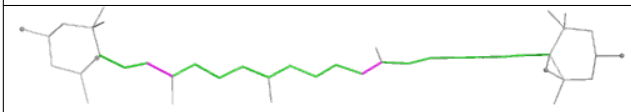
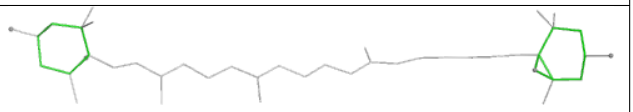


Torsions

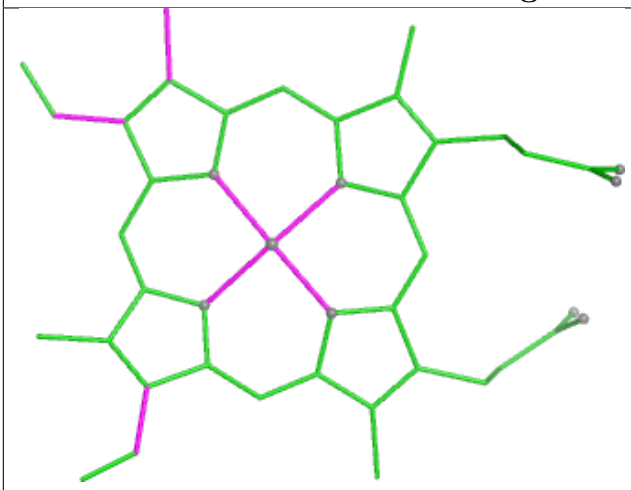


Rings

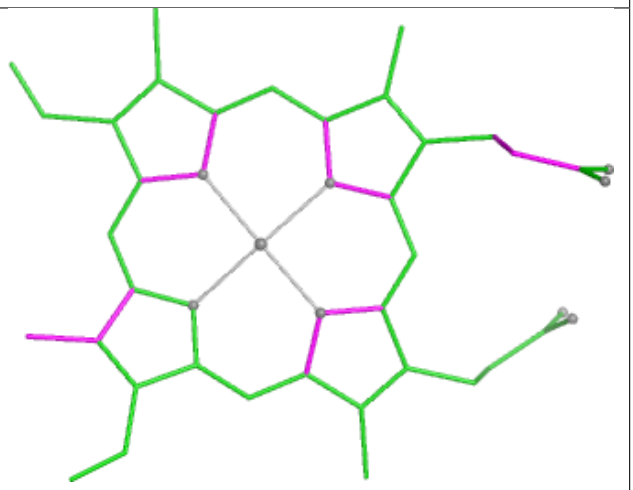
Ligand CHL g 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT n1 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

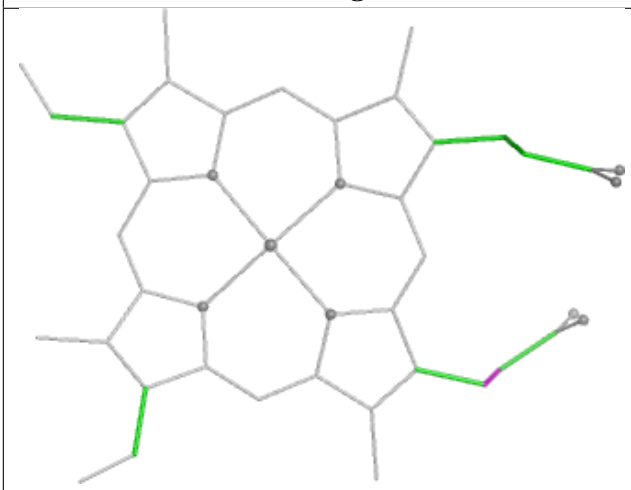
Ligand HEM F 101



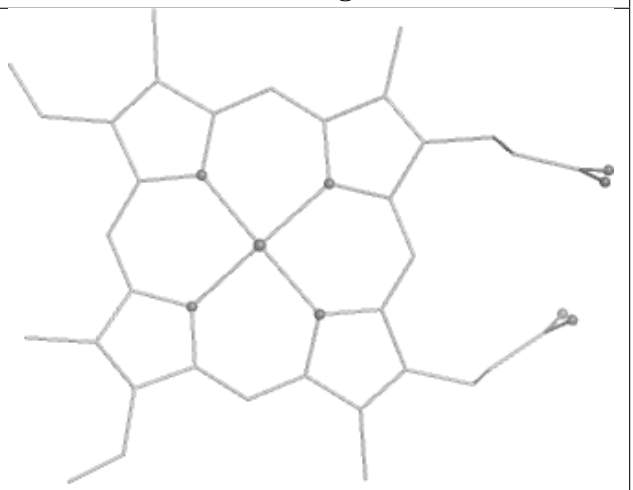
Bond lengths



Bond angles

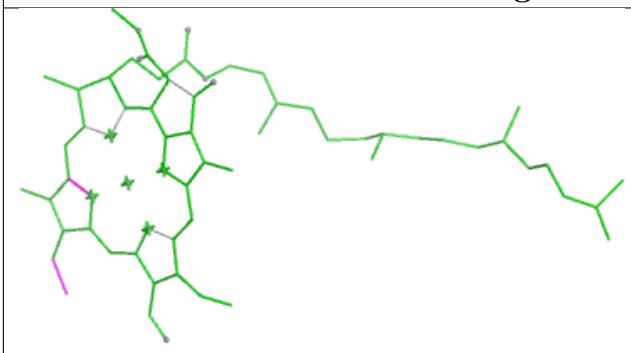


Torsions

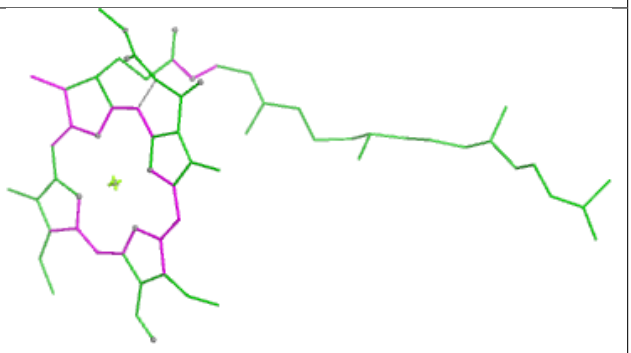


Rings

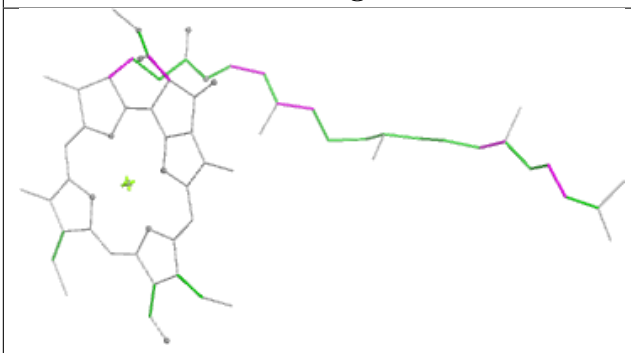
Ligand CHL G1 609



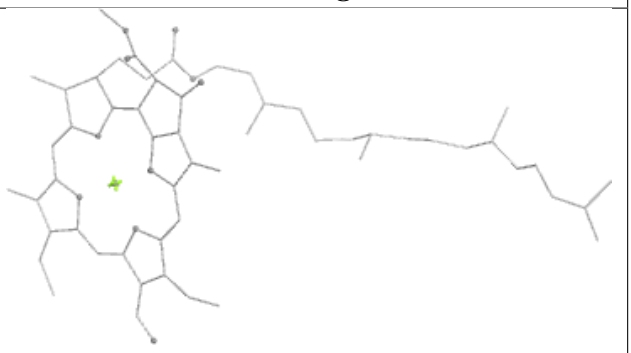
Bond lengths



Bond angles

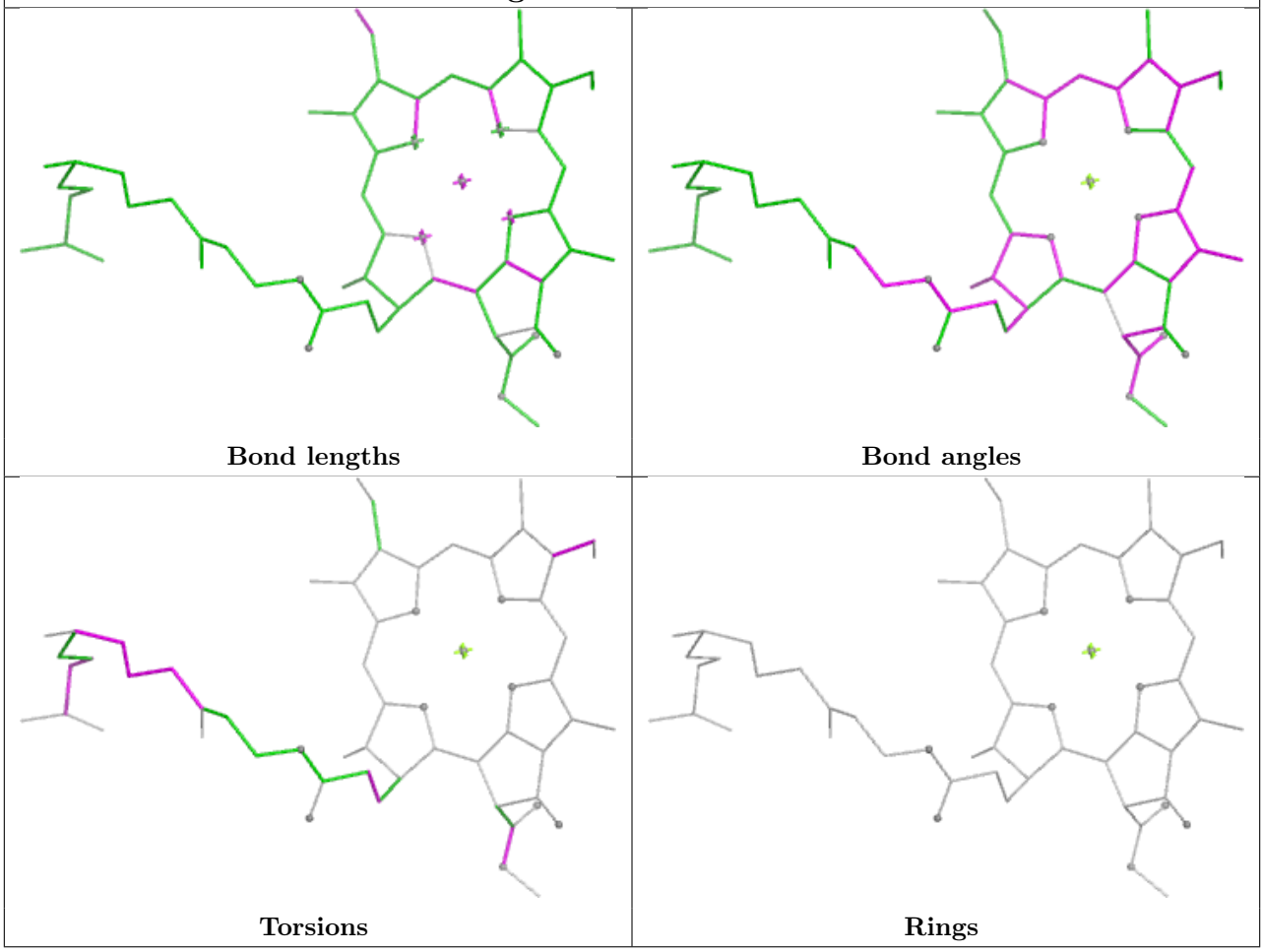


Torsions

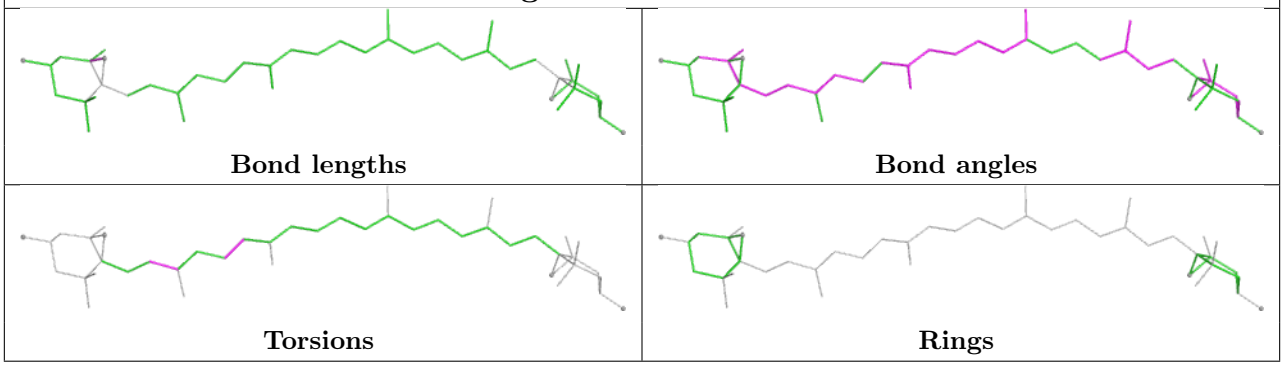


Rings

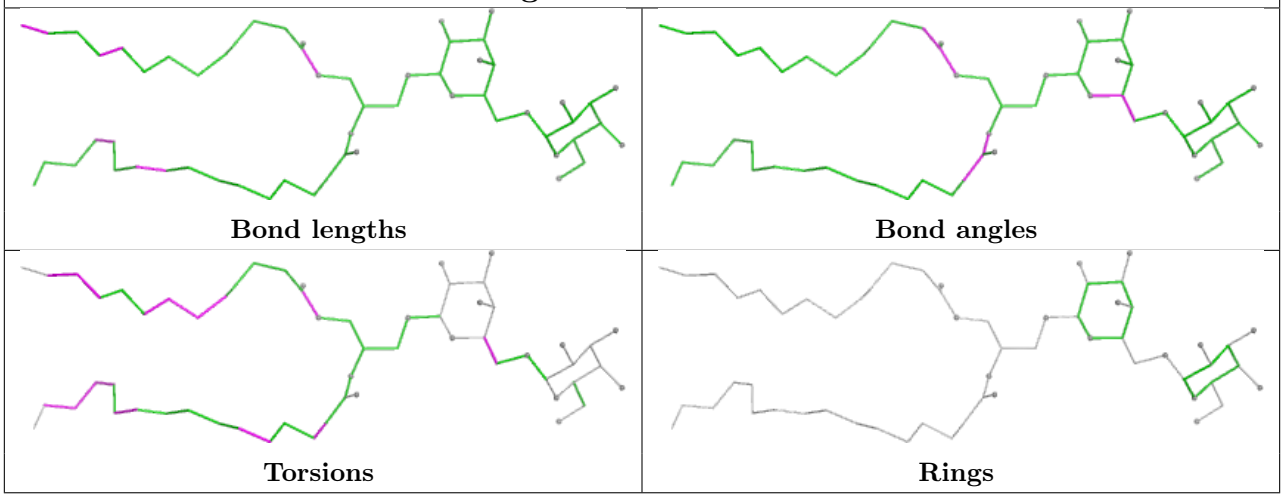
Ligand CLA A1 410



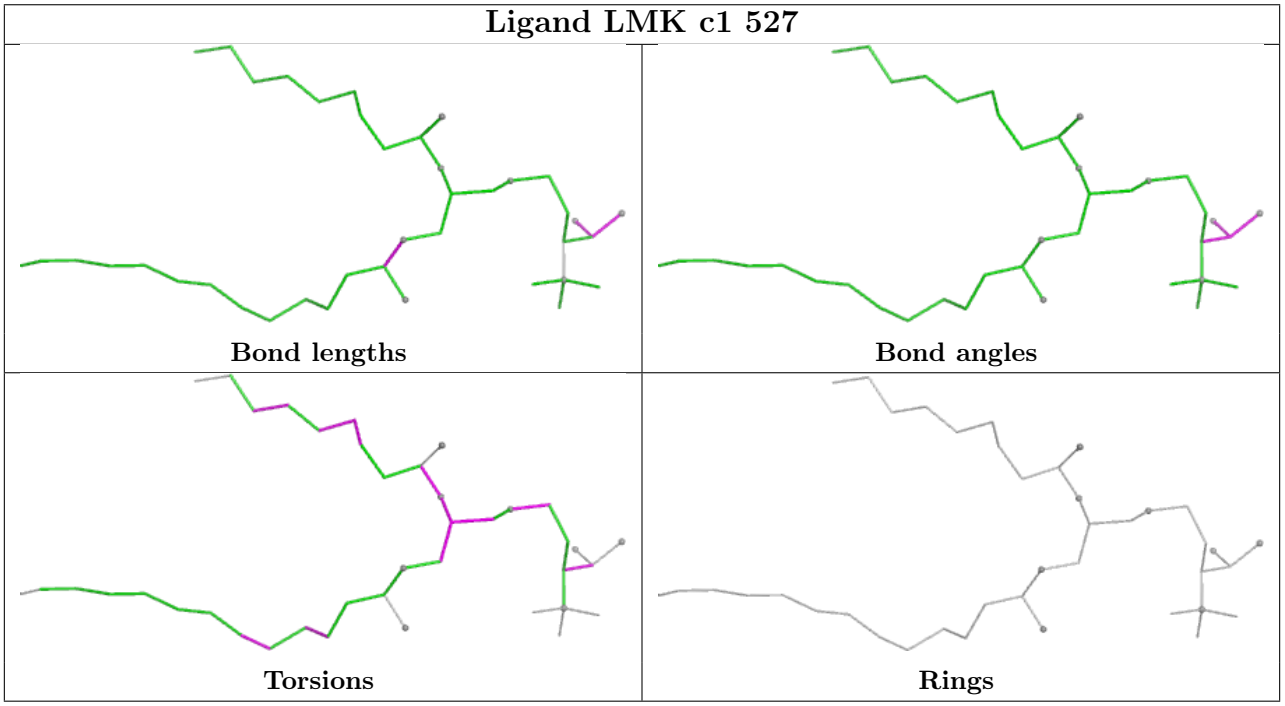
Ligand XAT r1 621



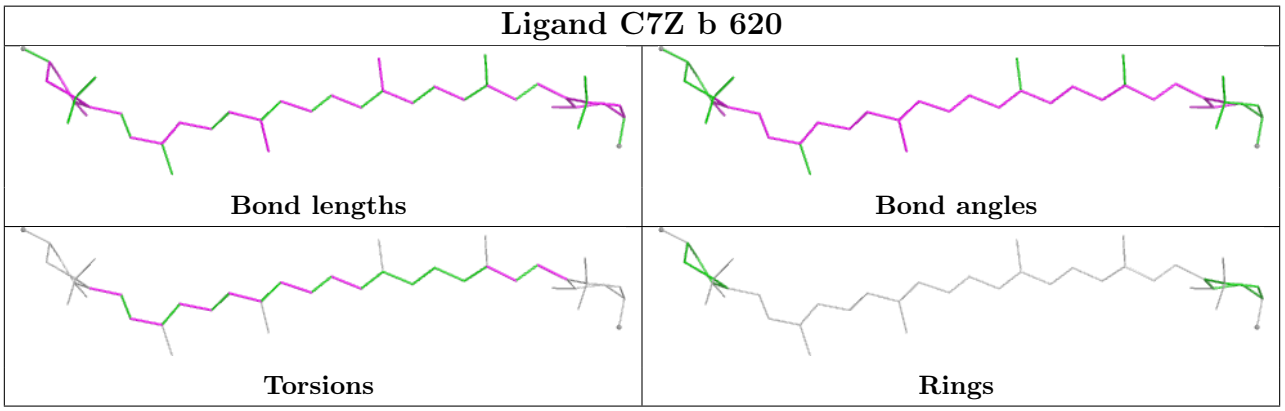
Ligand DGD C 520



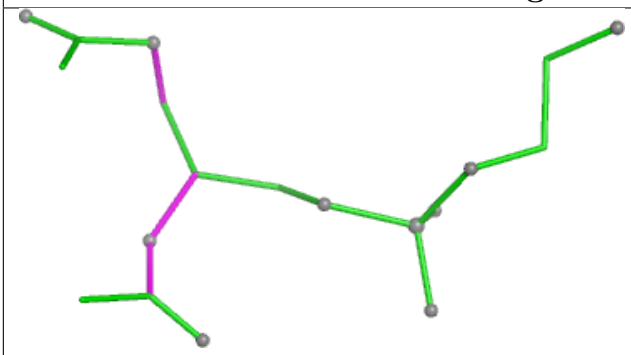
Ligand LMK c1 527



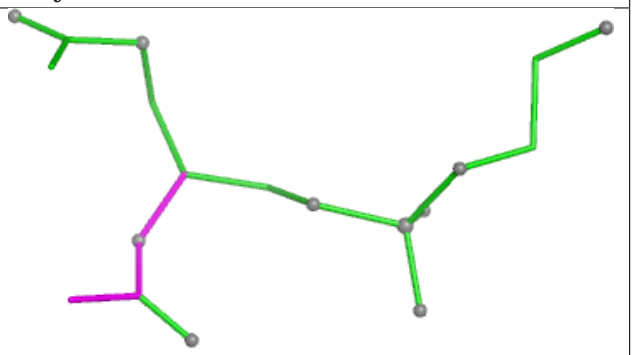
Ligand C7Z b 620



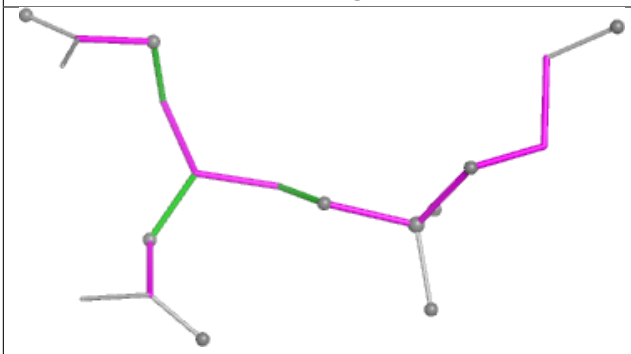
Ligand PTY y 627



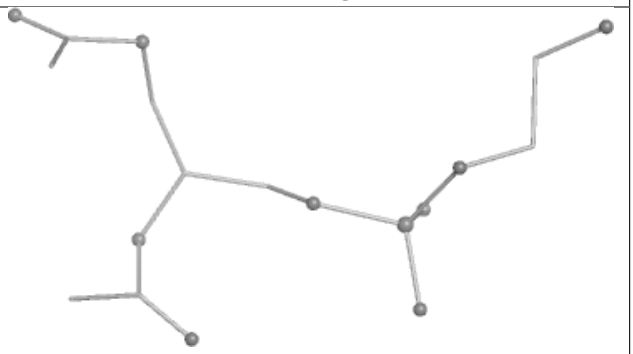
Bond lengths



Bond angles

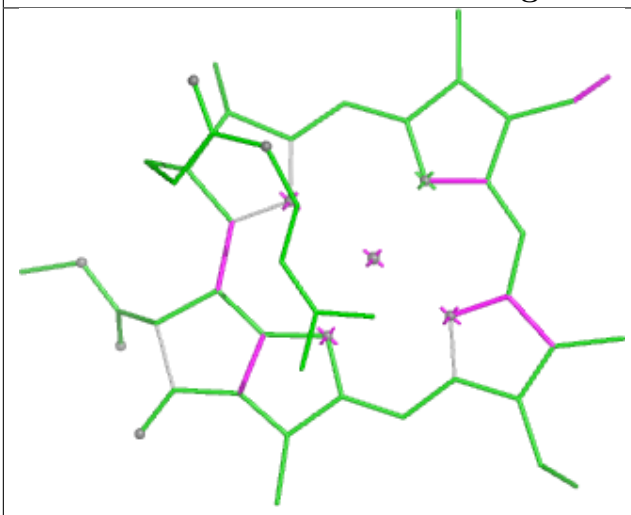


Torsions

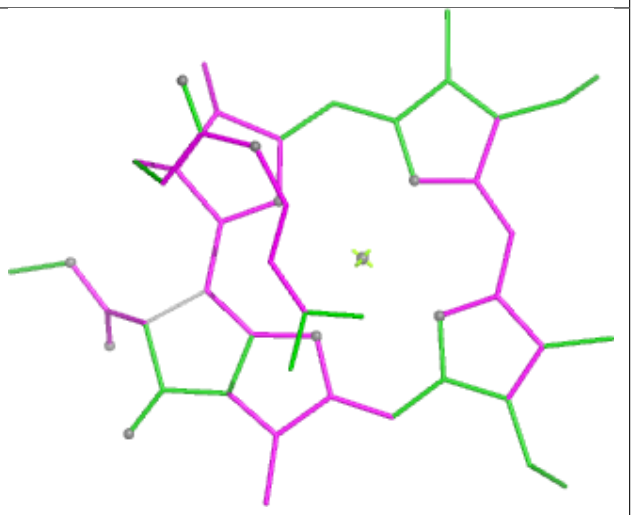


Rings

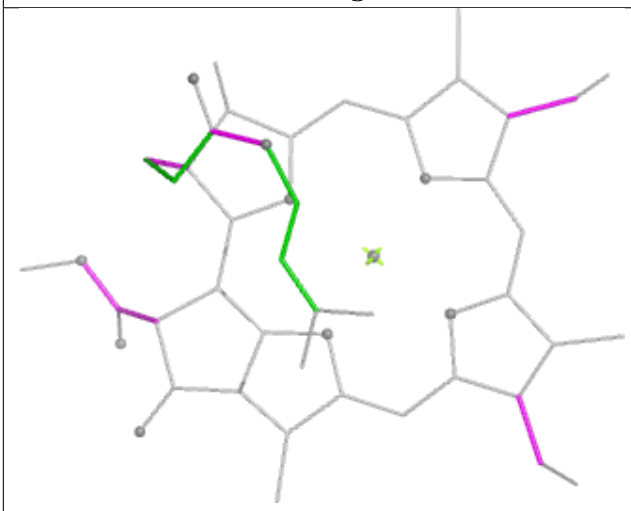
Ligand CLA s1 605



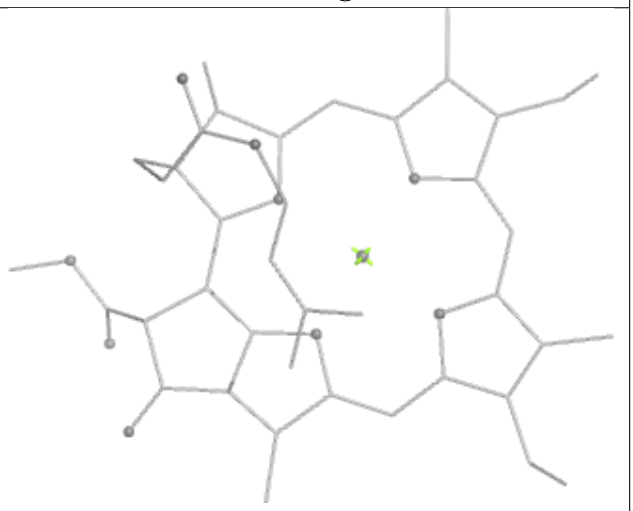
Bond lengths



Bond angles

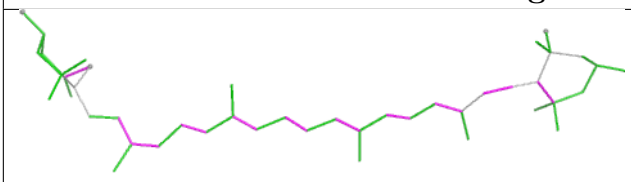


Torsions

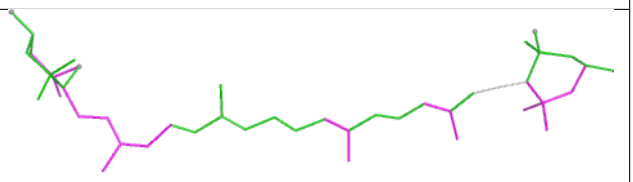


Rings

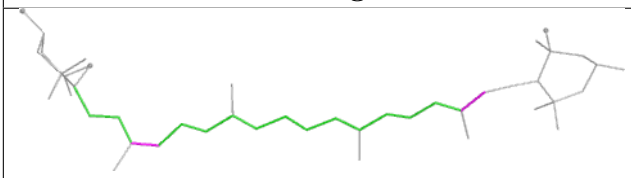
Ligand NEX s 623



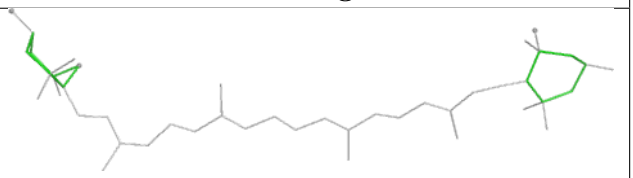
Bond lengths



Bond angles

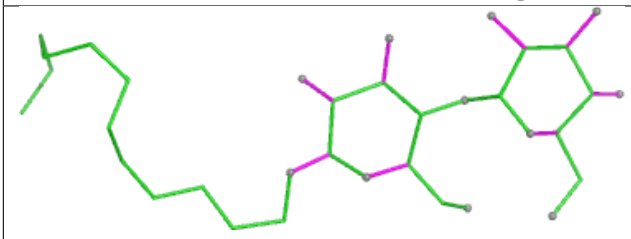


Torsions

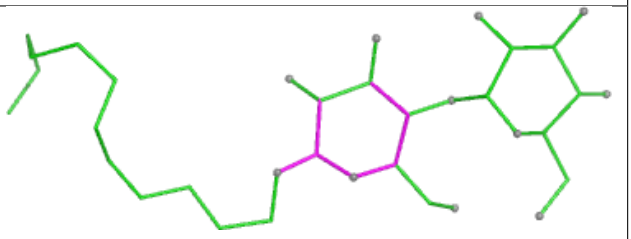


Rings

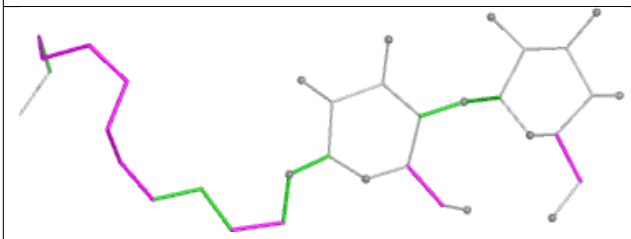
Ligand LMT R1 625



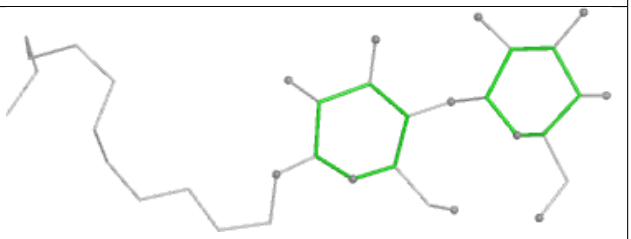
Bond lengths



Bond angles



Torsions



Rings

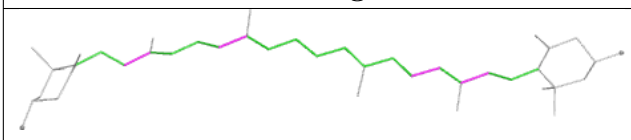
Ligand LUT S1 621



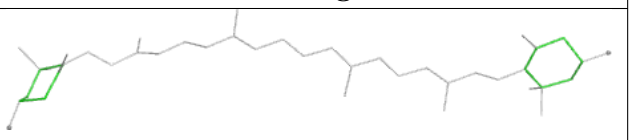
Bond lengths



Bond angles

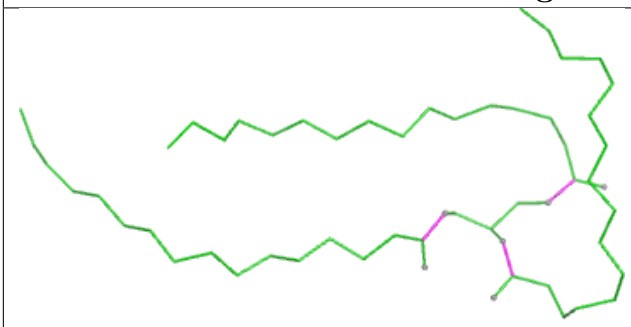


Torsions

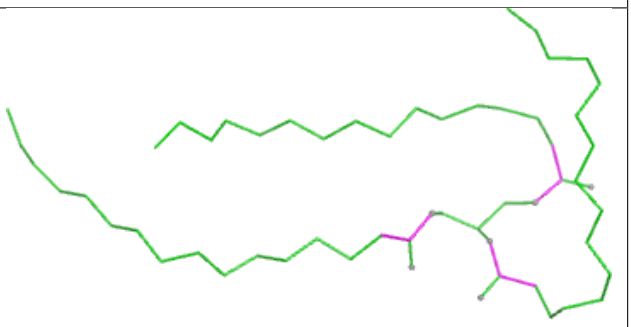


Rings

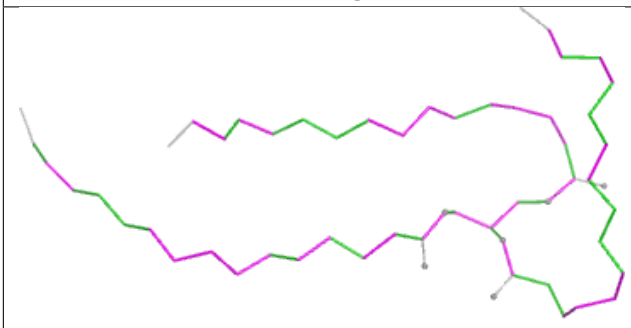
Ligand 4RF i 101



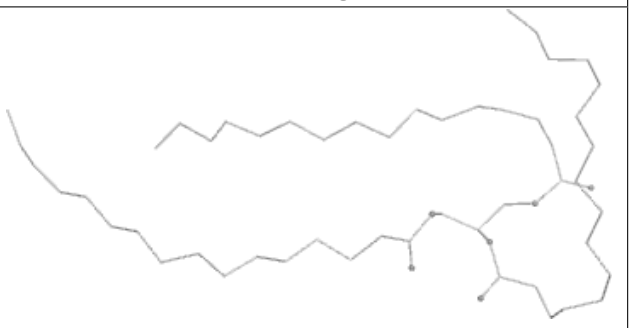
Bond lengths



Bond angles

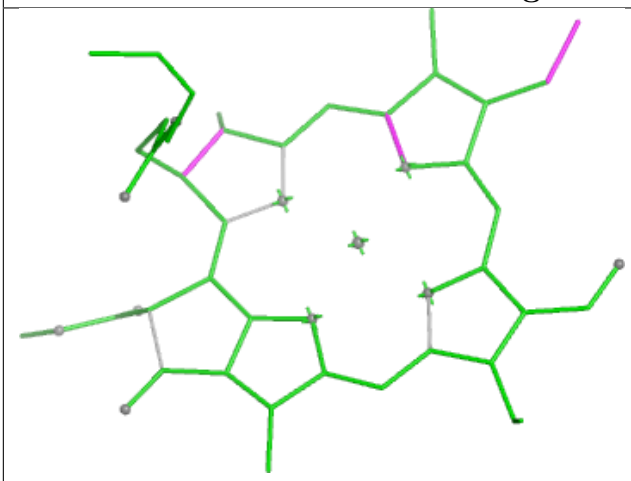


Torsions

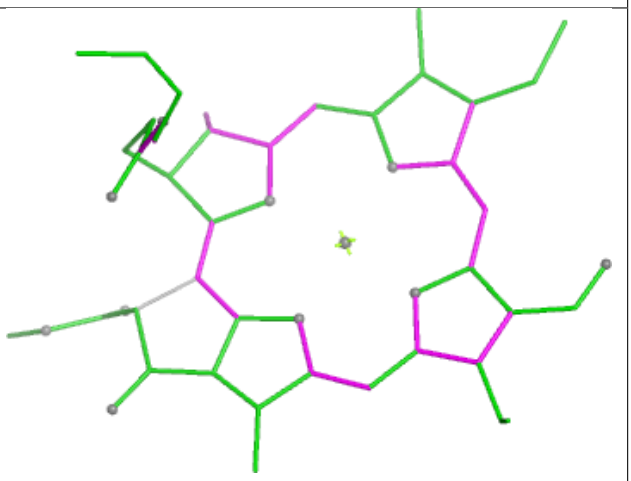


Rings

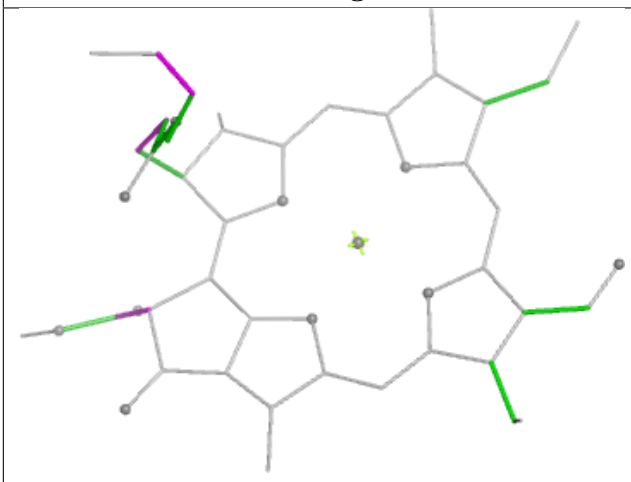
Ligand CHL N 608



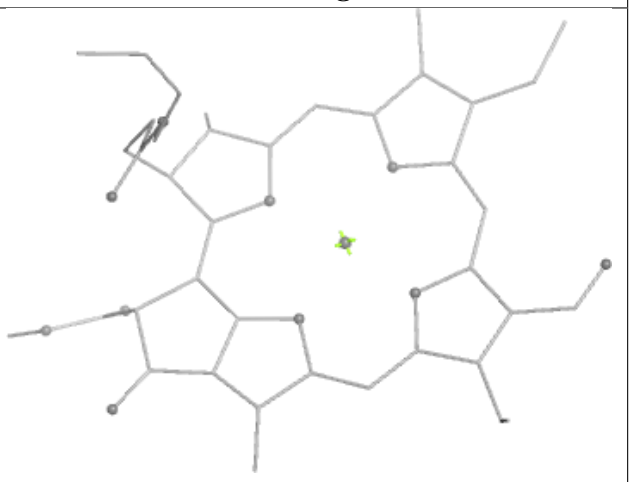
Bond lengths



Bond angles

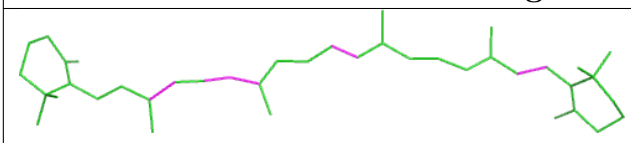


Torsions

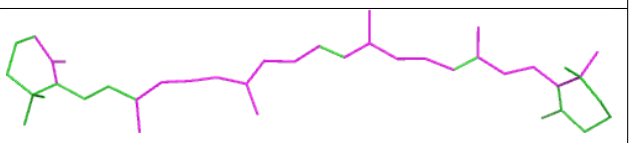


Rings

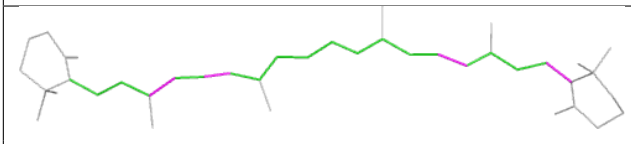
Ligand BCR b 619



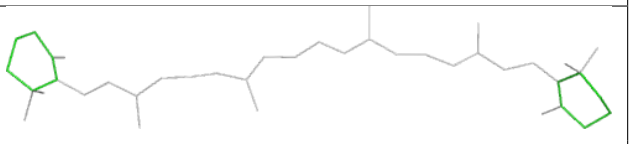
Bond lengths



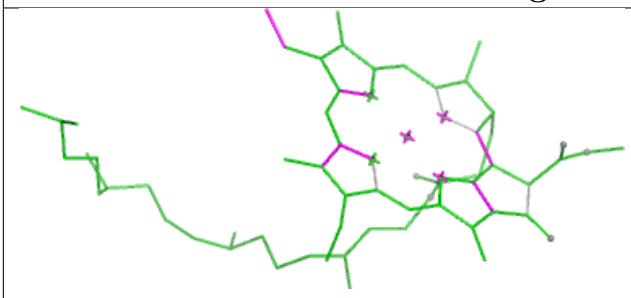
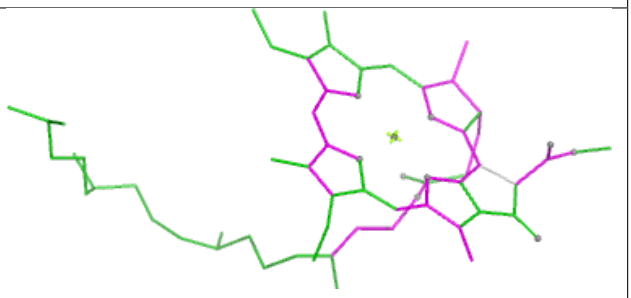
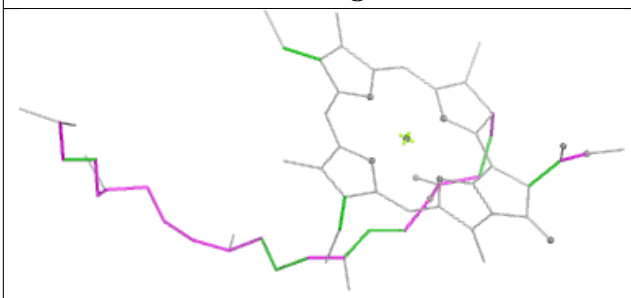
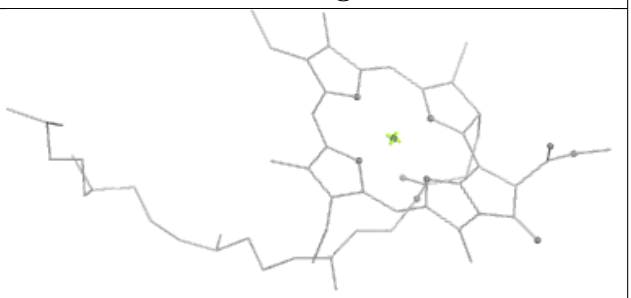
Bond angles

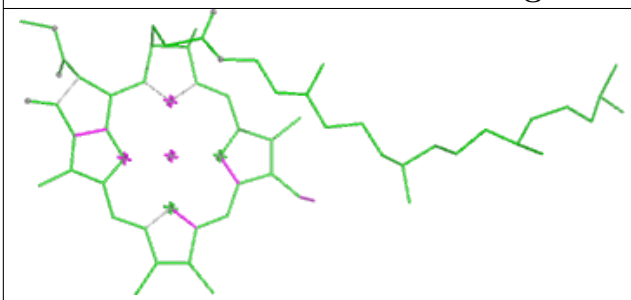
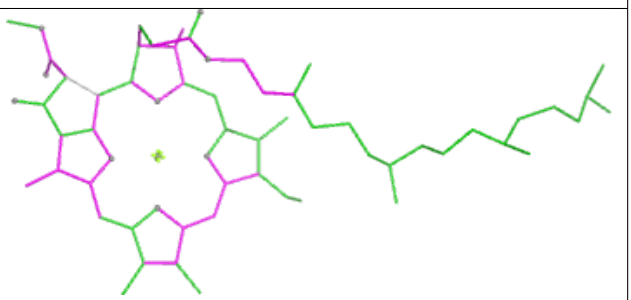
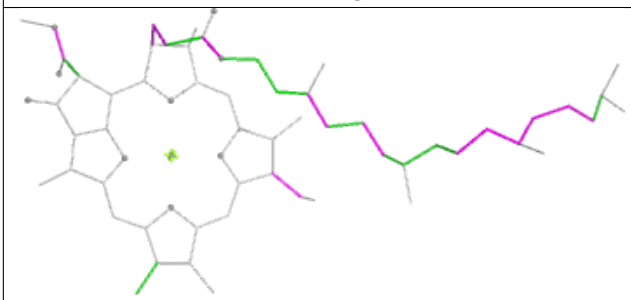
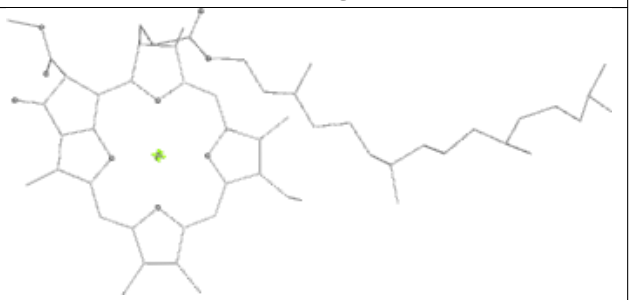


Torsions

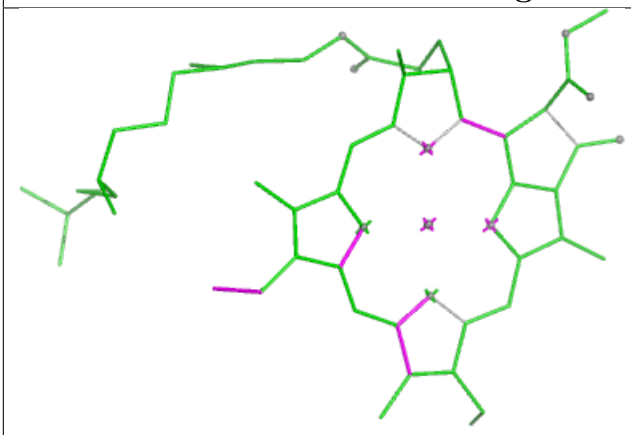


Rings

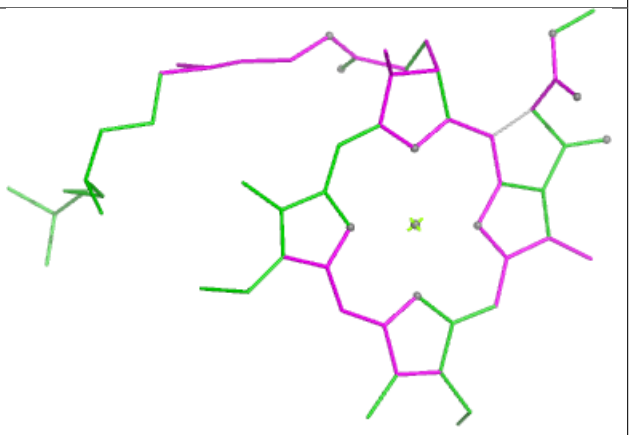
Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

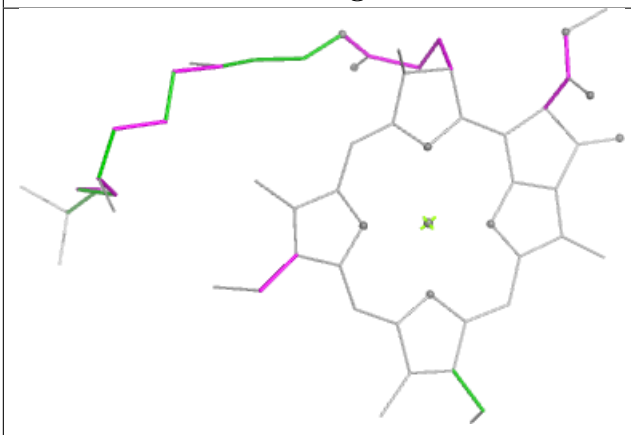
Ligand CLA R1 609



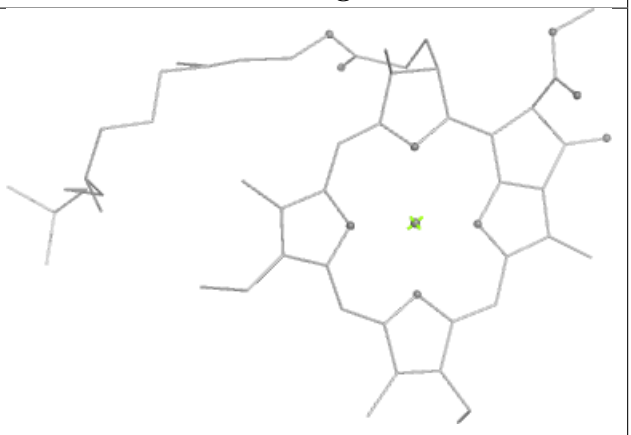
Bond lengths



Bond angles

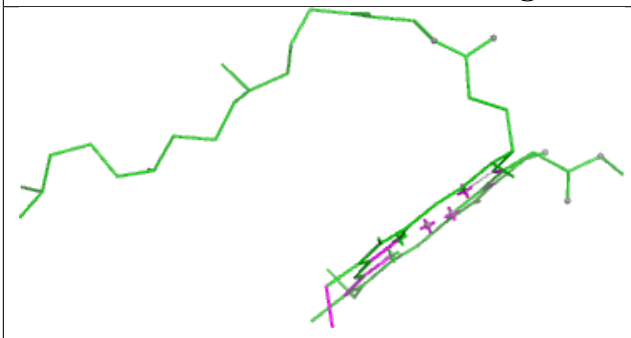


Torsions

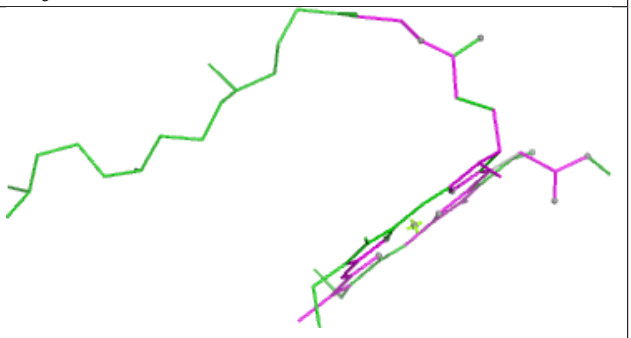


Rings

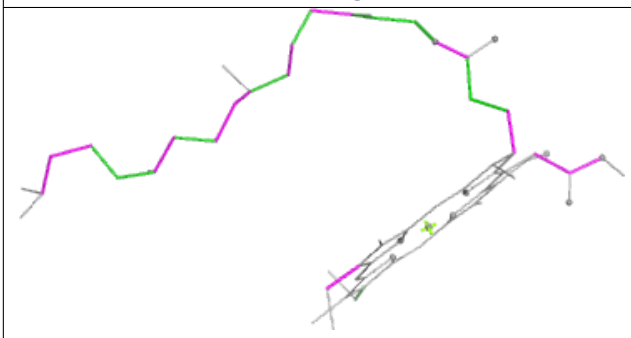
Ligand CLA y1 614



Bond lengths



Bond angles

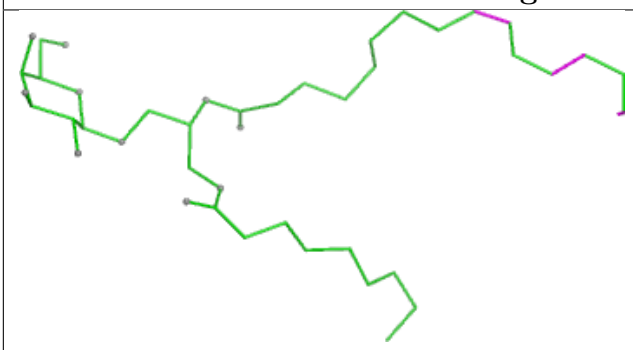


Torsions

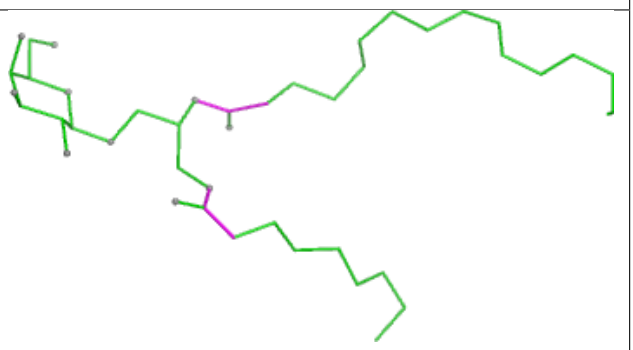


Rings

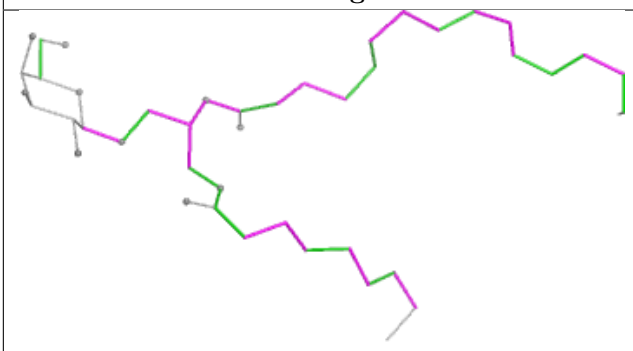
Ligand LMG B 622



Bond lengths



Bond angles

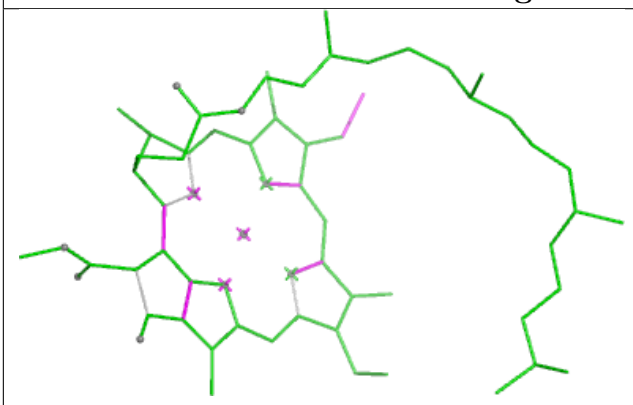


Torsions

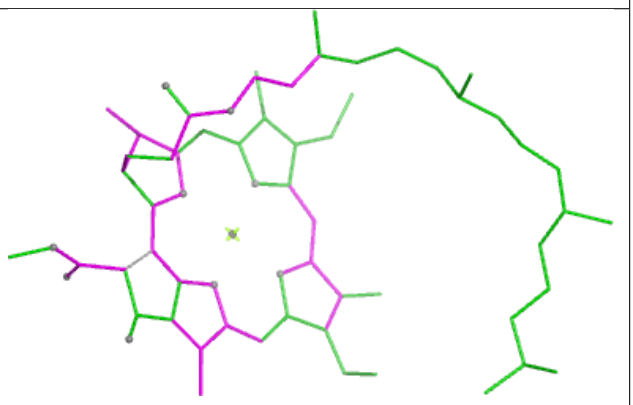


Rings

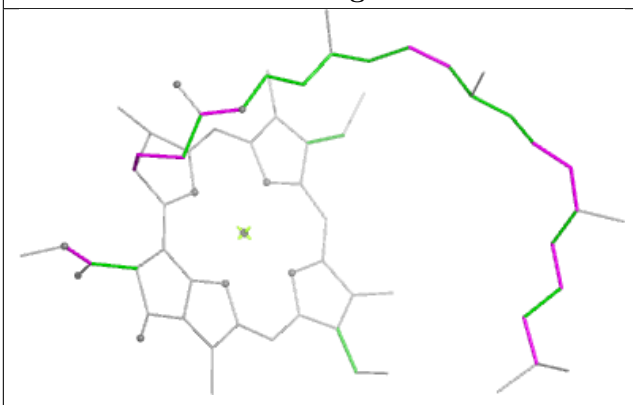
Ligand CLA Y1 610



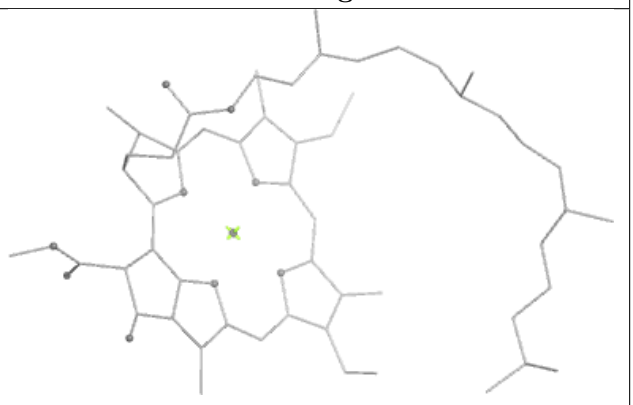
Bond lengths



Bond angles

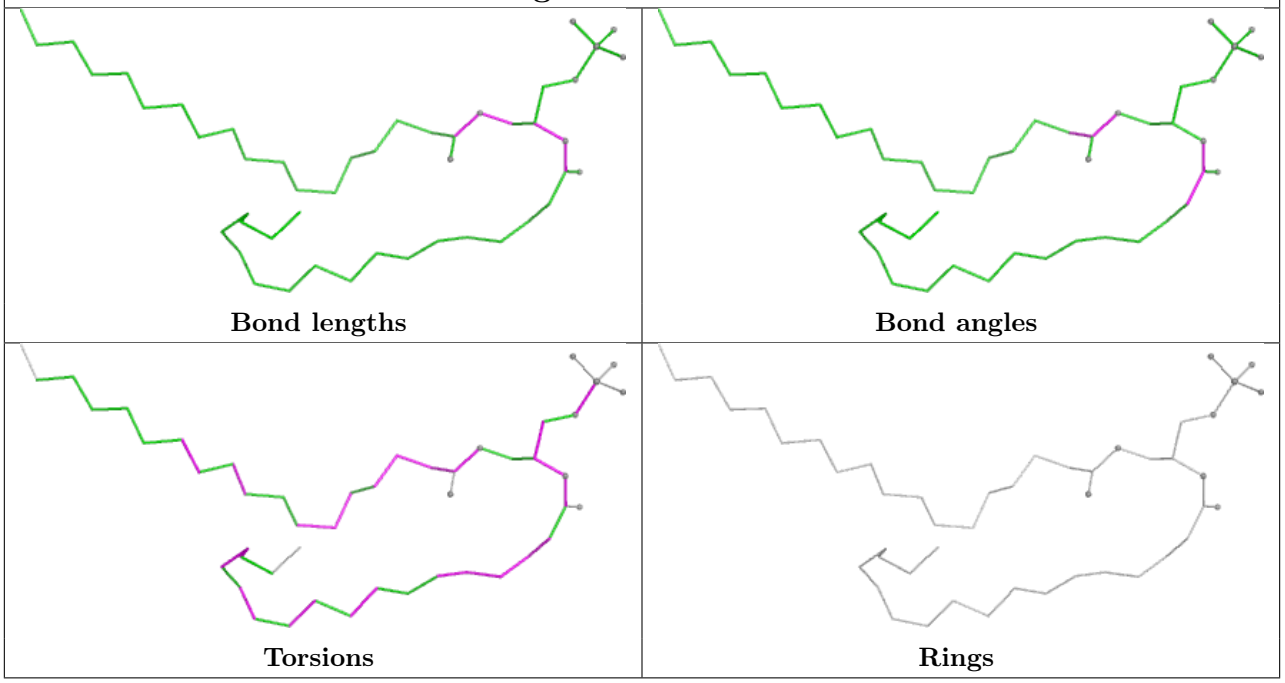


Torsions

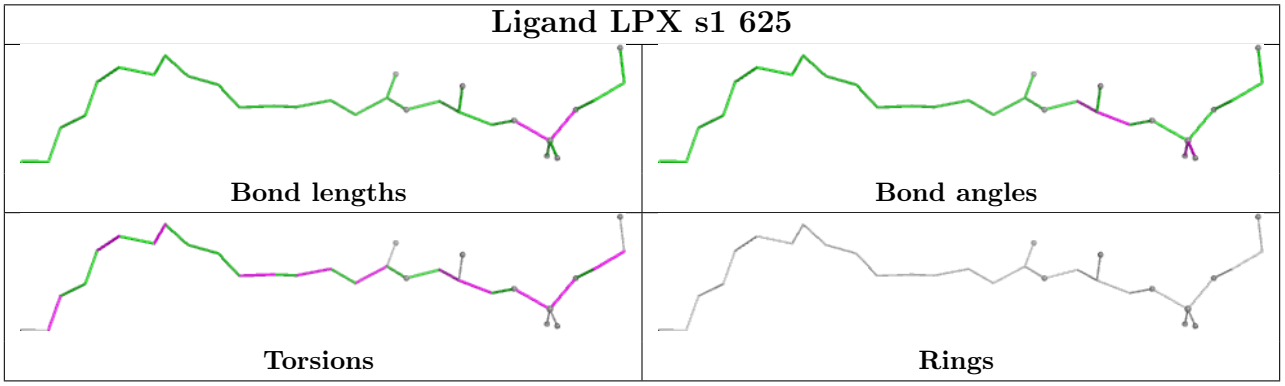


Rings

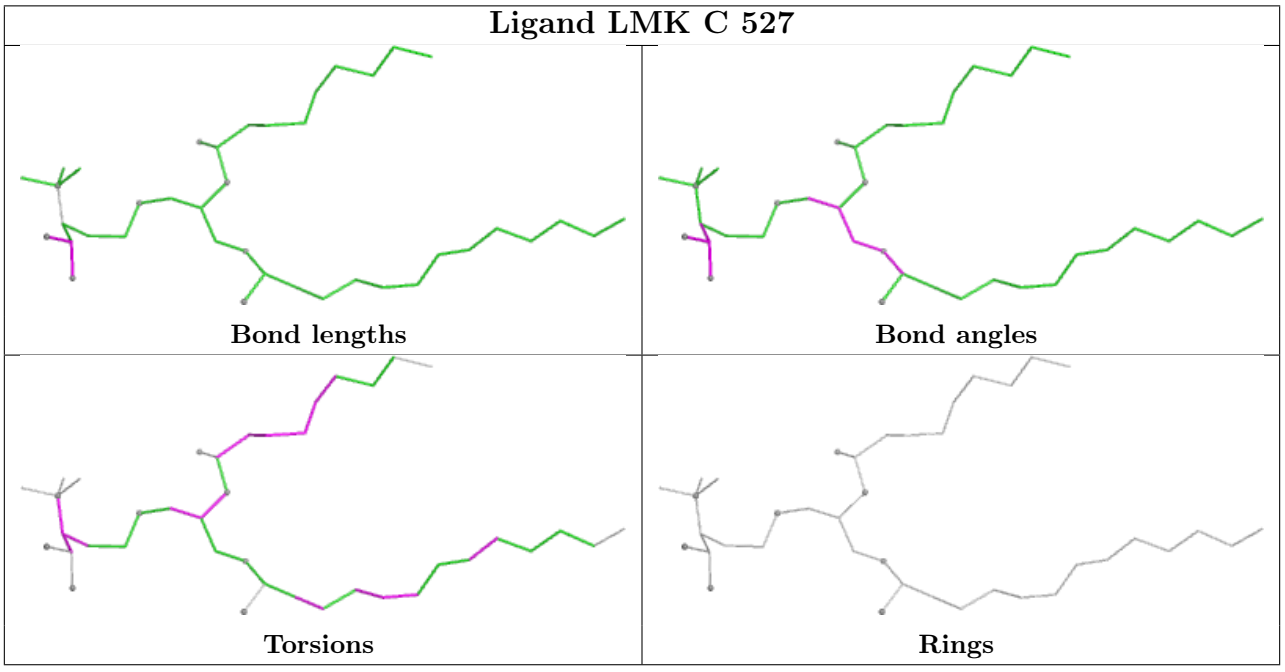
Ligand 3PH t 101



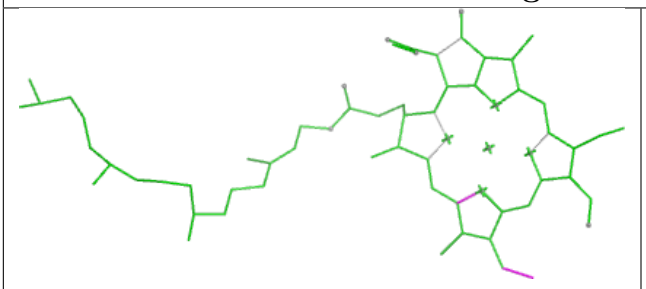
Ligand LPX s1 625



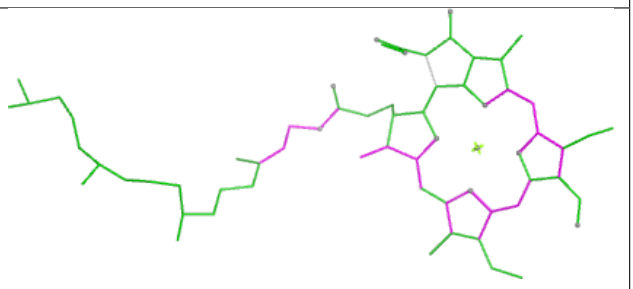
Ligand LMK C 527



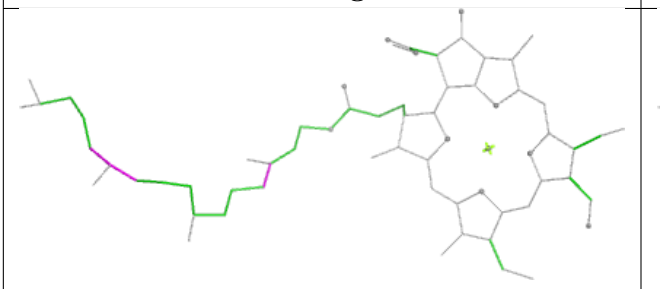
Ligand CHL N 601



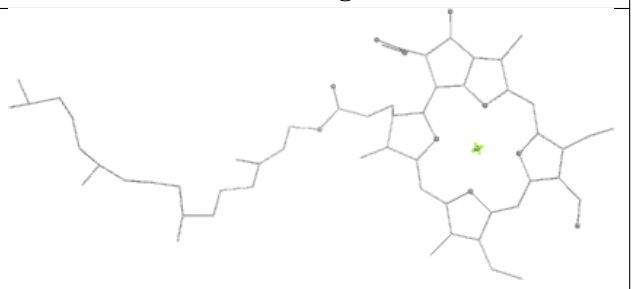
Bond lengths



Bond angles

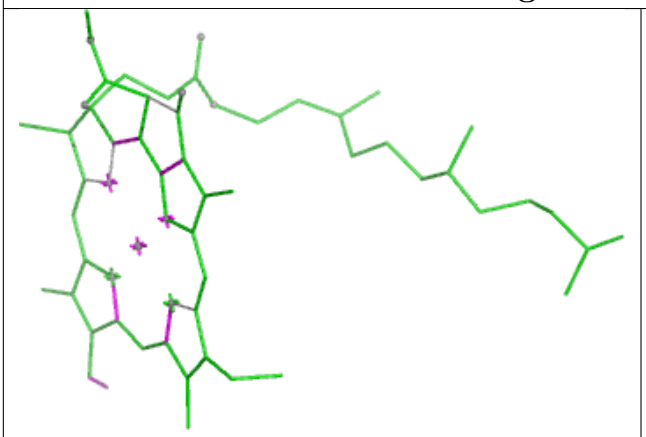


Torsions

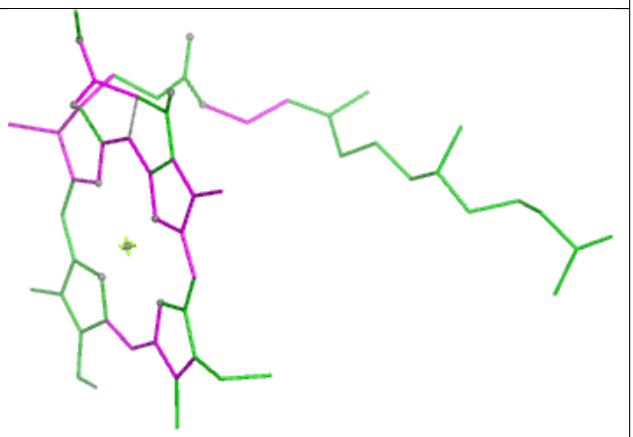


Rings

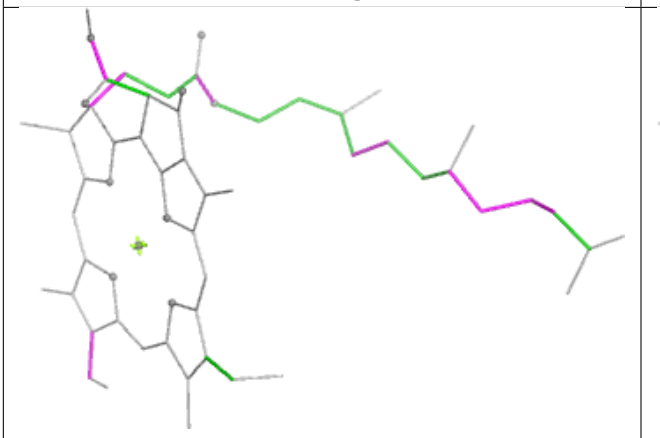
Ligand CLA S1 609



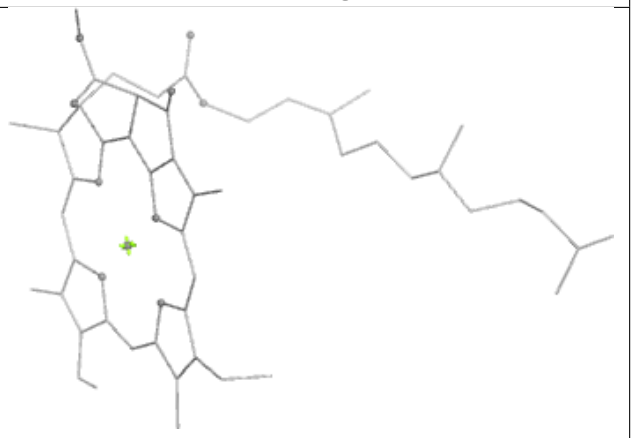
Bond lengths



Bond angles

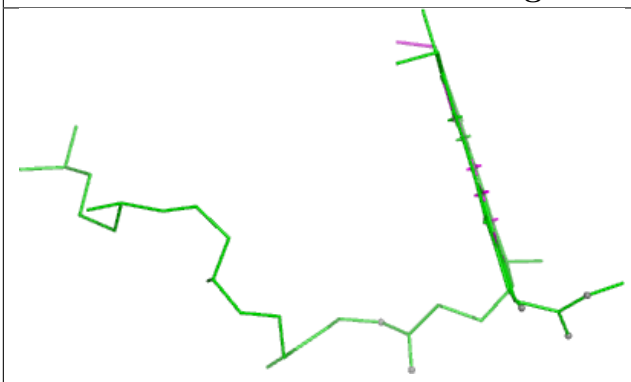


Torsions

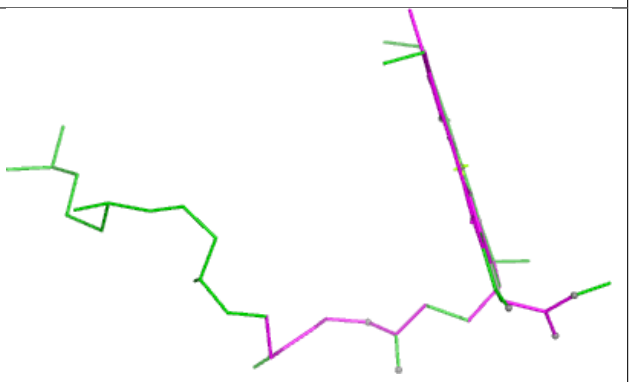


Rings

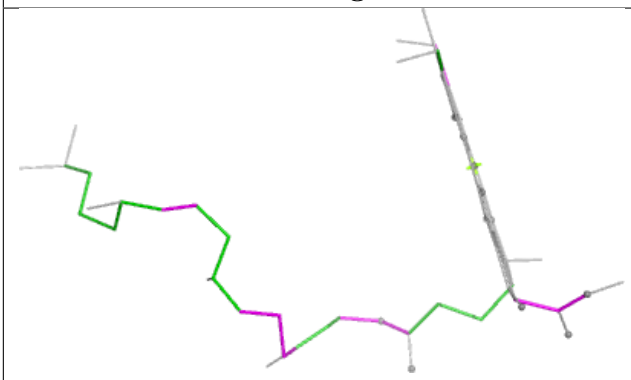
Ligand CLA C 506



Bond lengths



Bond angles

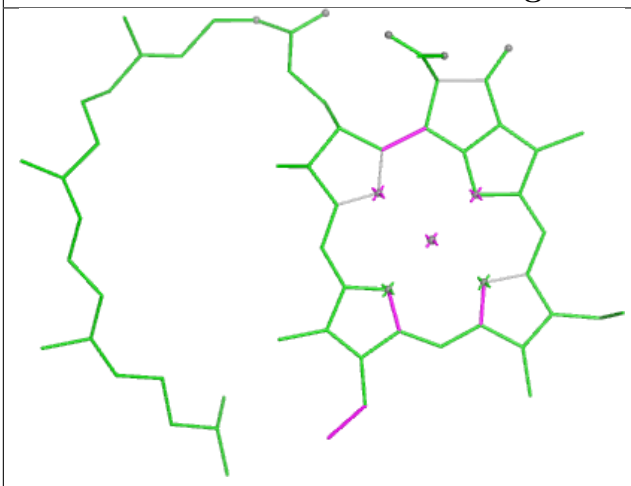


Torsions

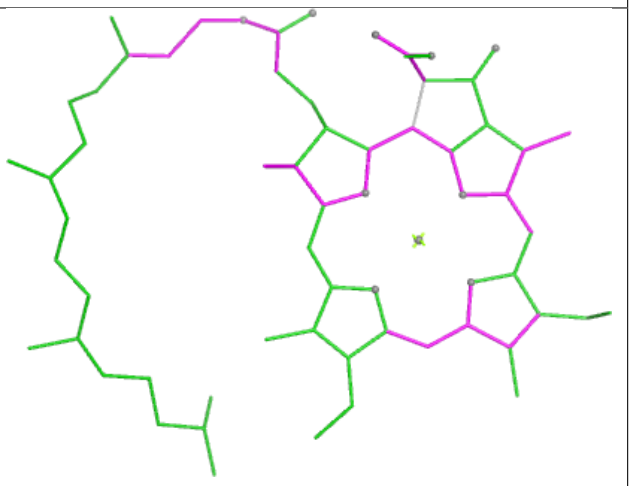


Rings

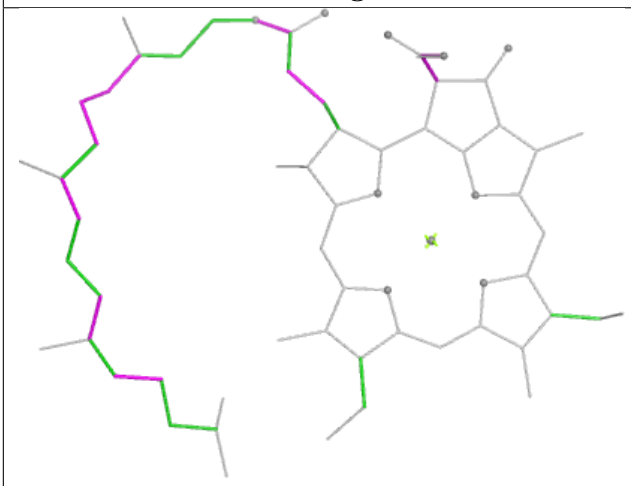
Ligand CLA C 512



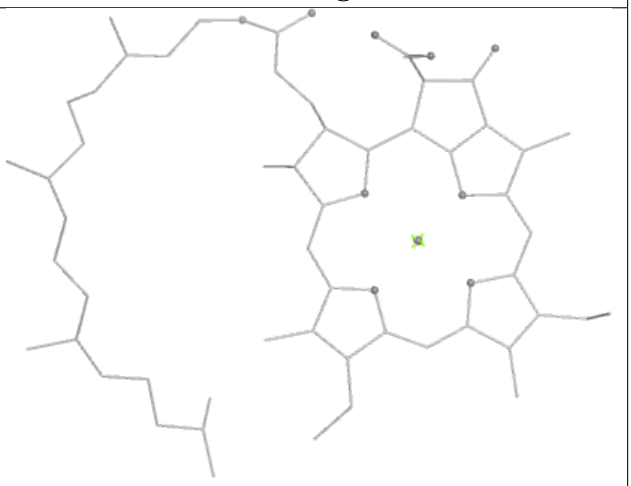
Bond lengths



Bond angles

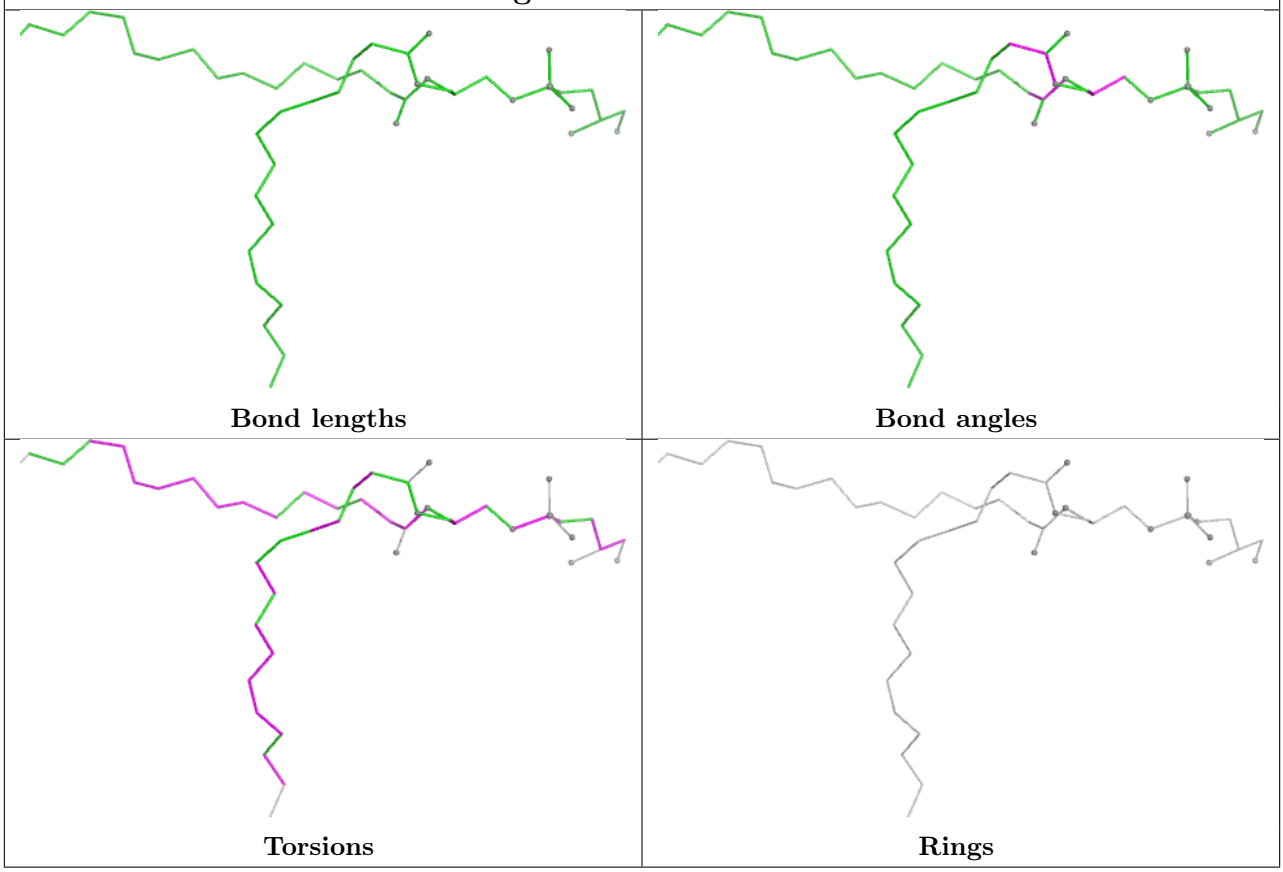


Torsions



Rings

Ligand LHG N1 624



Ligand CLA y1 603



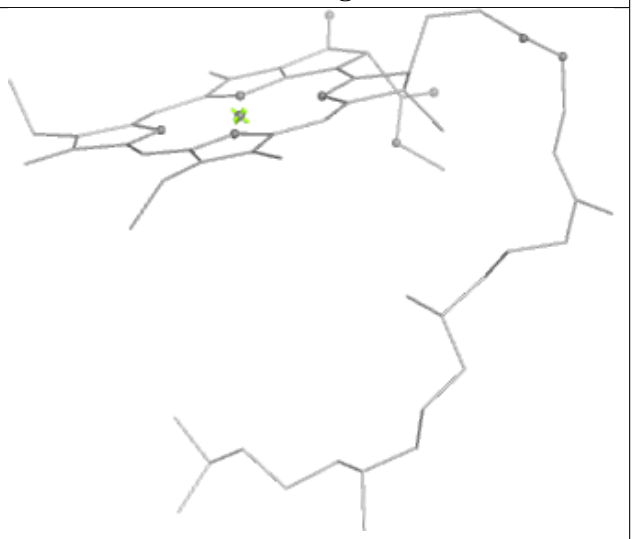
Bond lengths



Bond angles

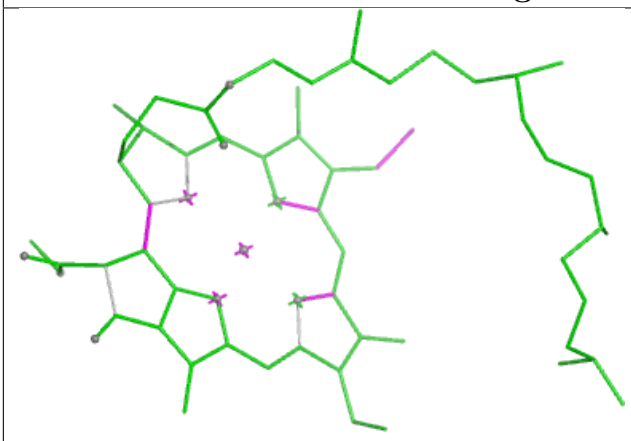


Torsions

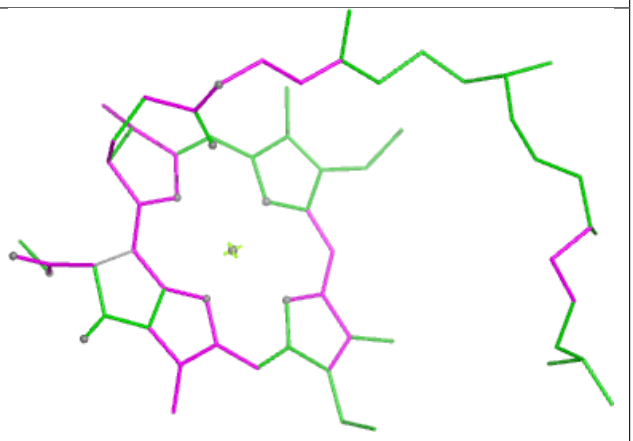


Rings

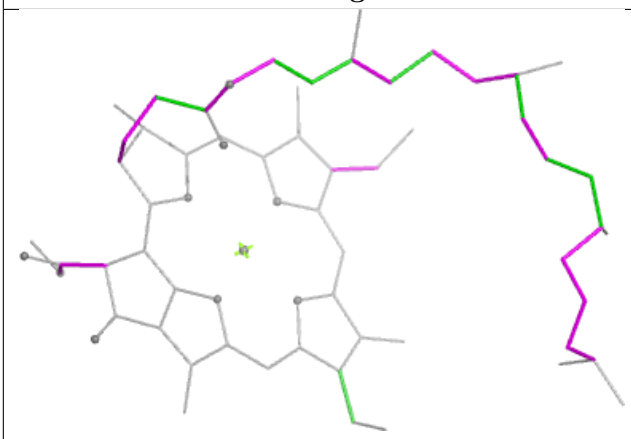
Ligand CLA G1 602



Bond lengths



Bond angles

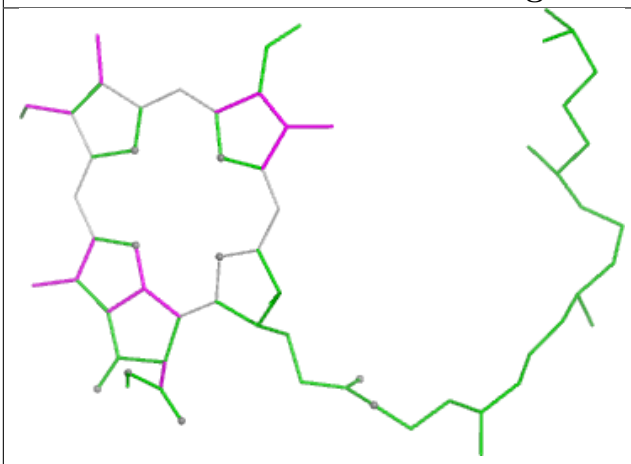


Torsions

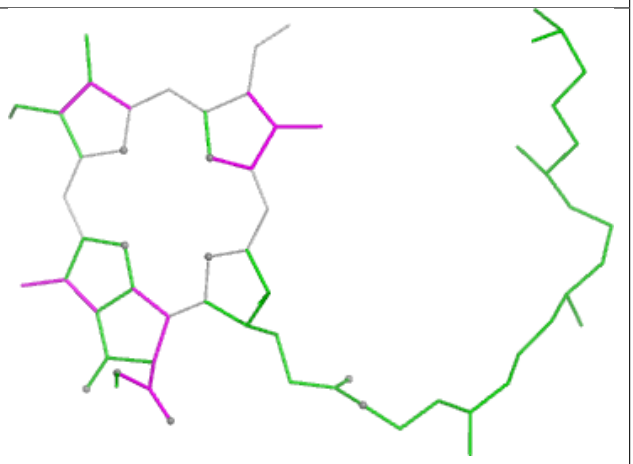


Rings

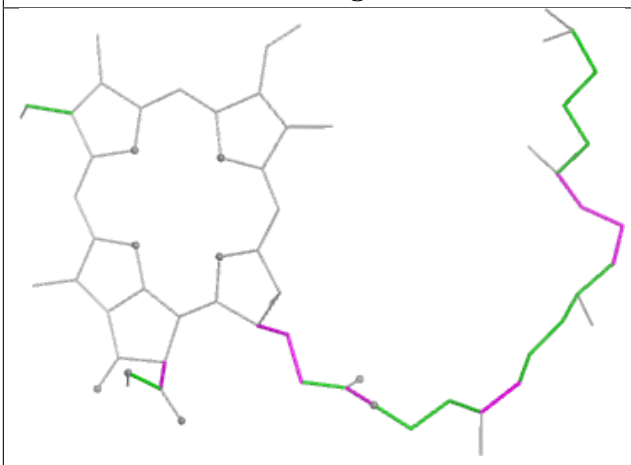
Ligand PHO a 408



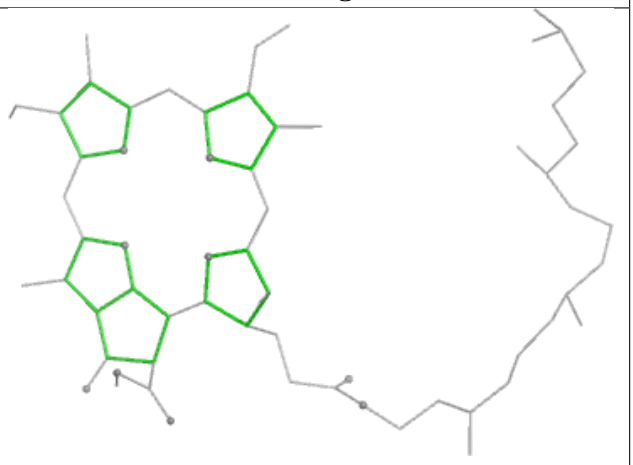
Bond lengths



Bond angles

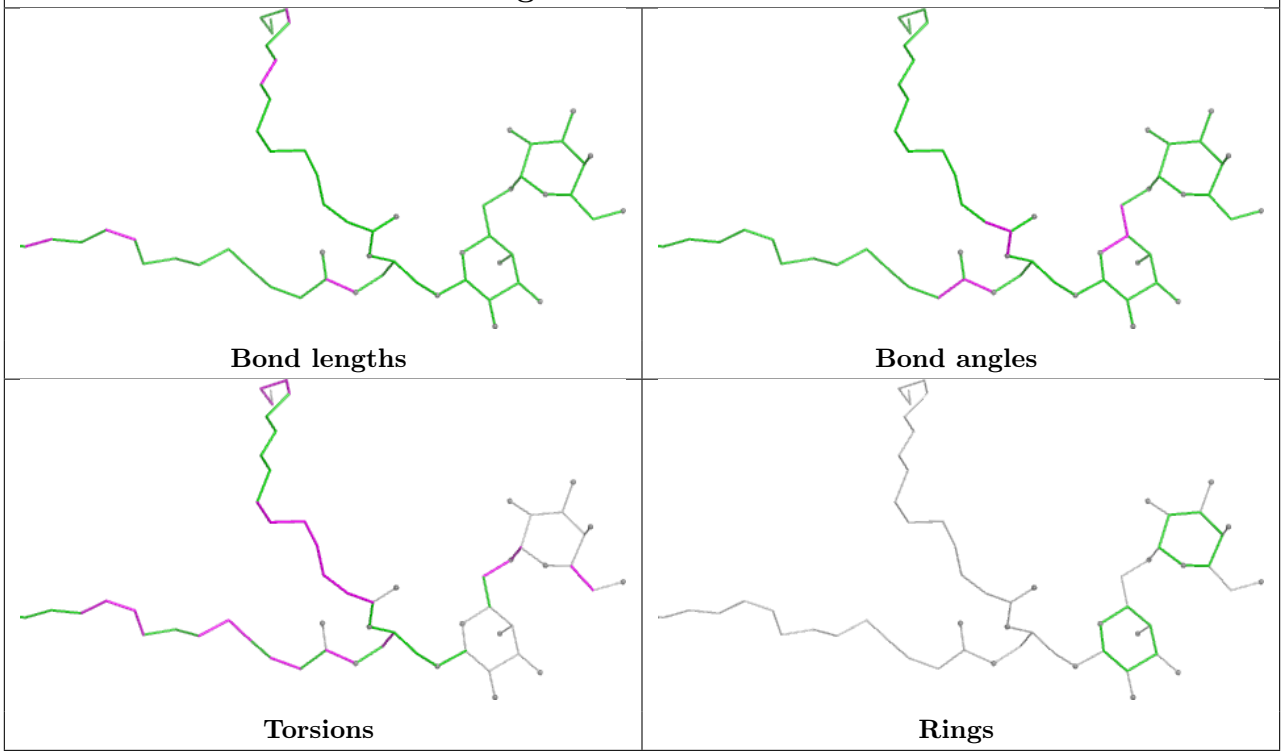


Torsions



Rings

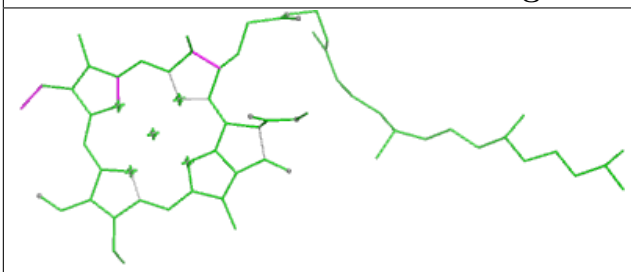
Ligand DGD c1 519



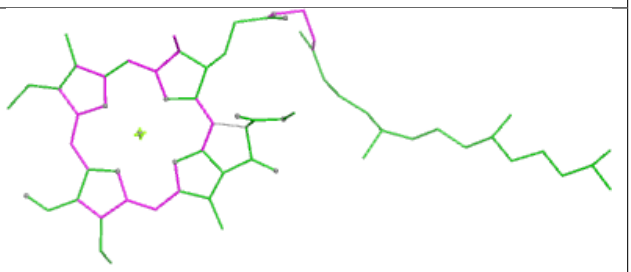
Ligand NEX G 623



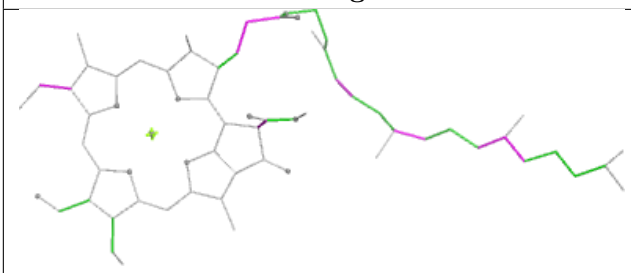
Ligand CHL N 605



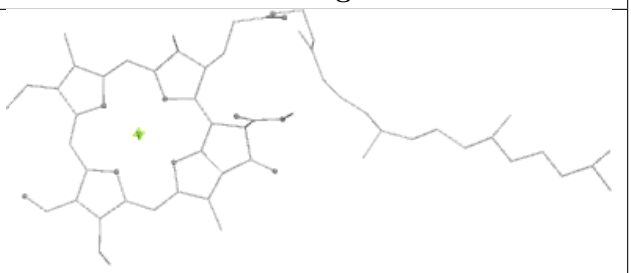
Bond lengths



Bond angles

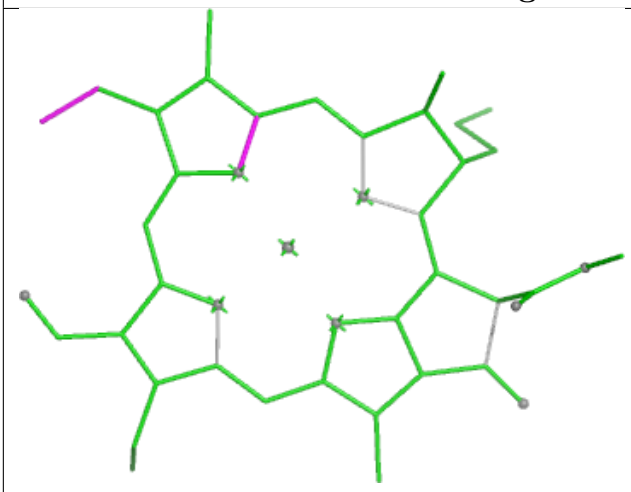


Torsions

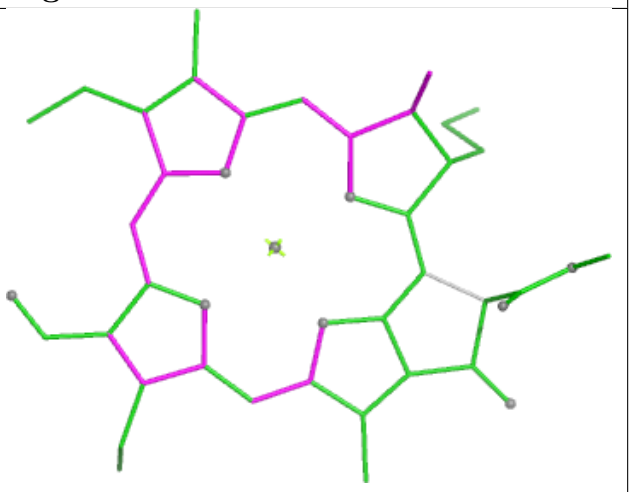


Rings

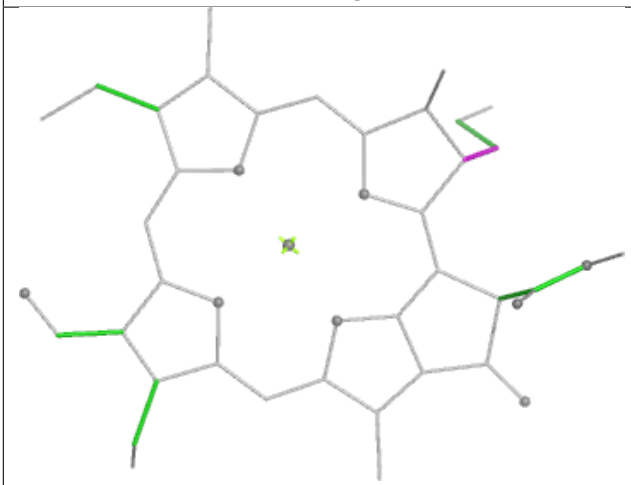
Ligand CHL g1 608



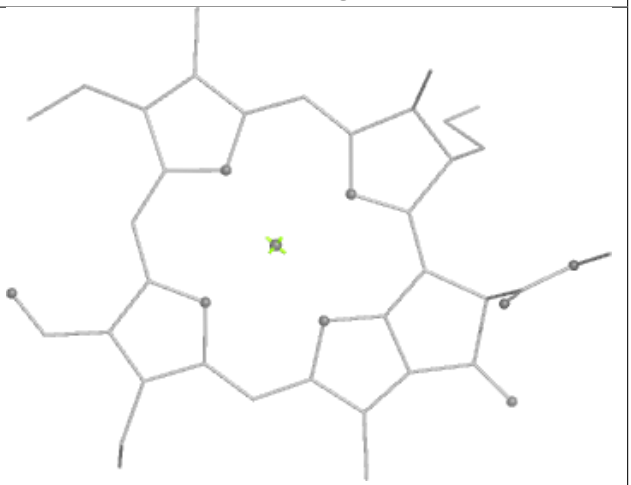
Bond lengths



Bond angles

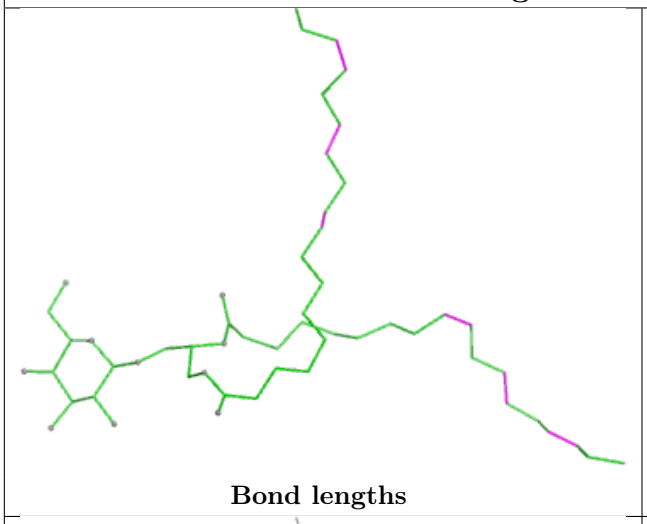


Torsions

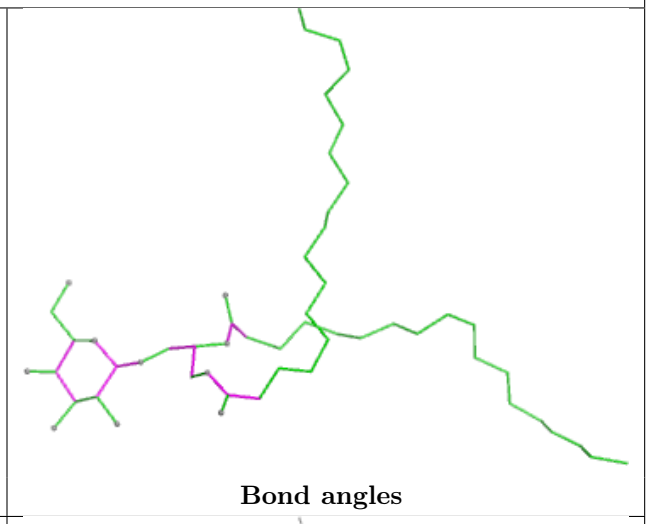


Rings

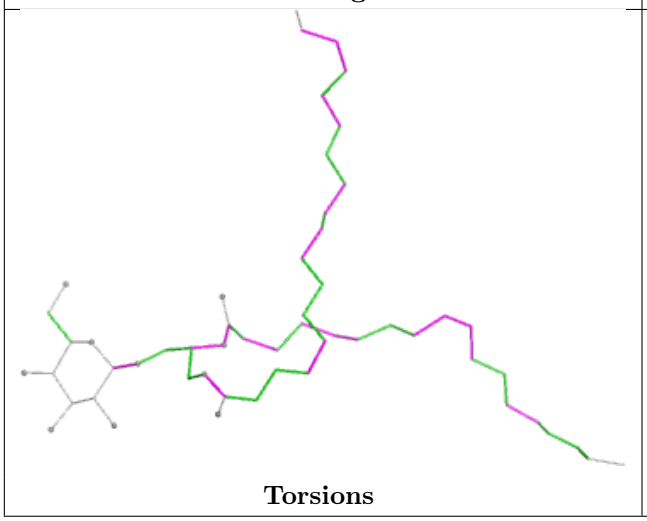
Ligand LMG C1 523



Bond lengths



Bond angles

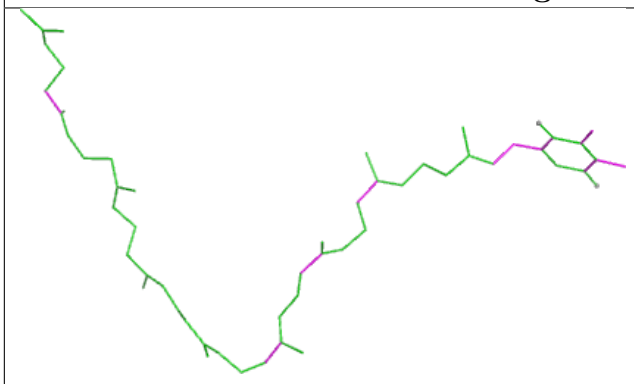


Torsions

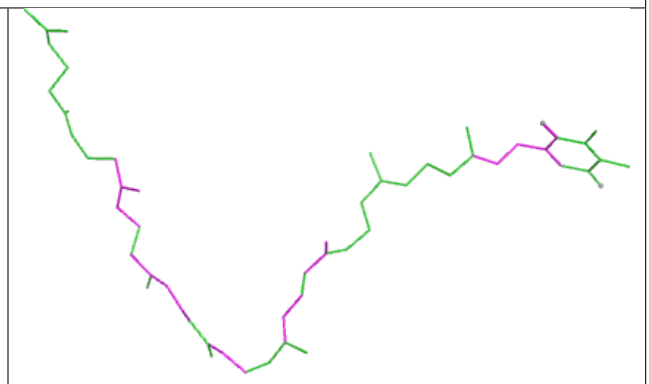


Rings

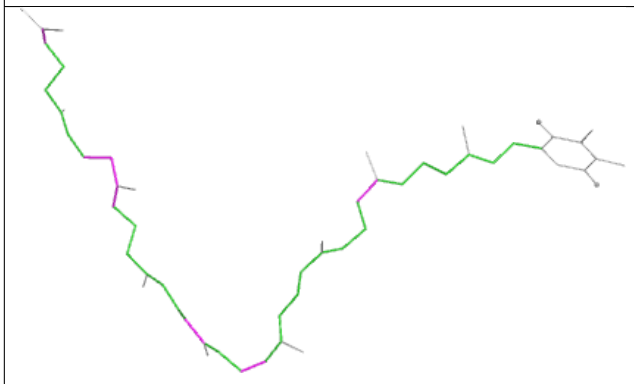
Ligand PL9 d 405



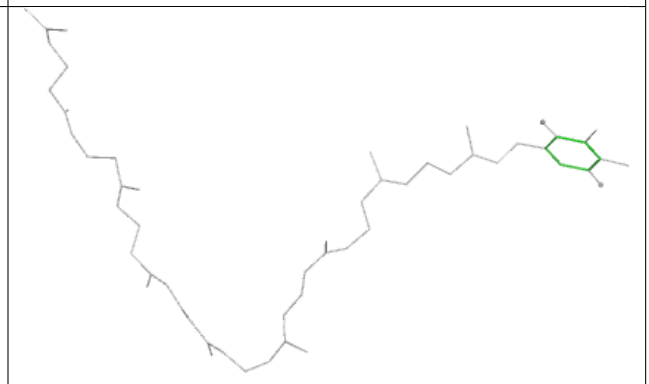
Bond lengths



Bond angles

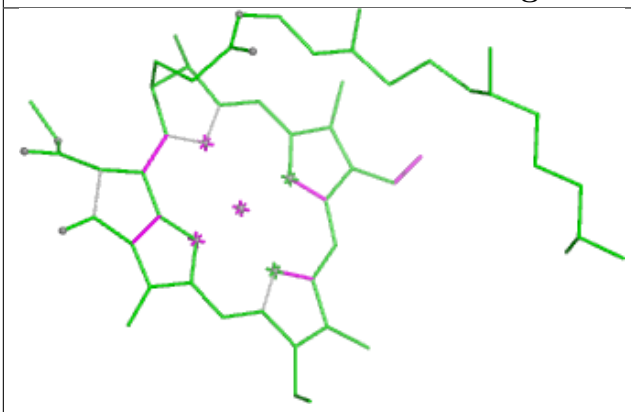


Torsions

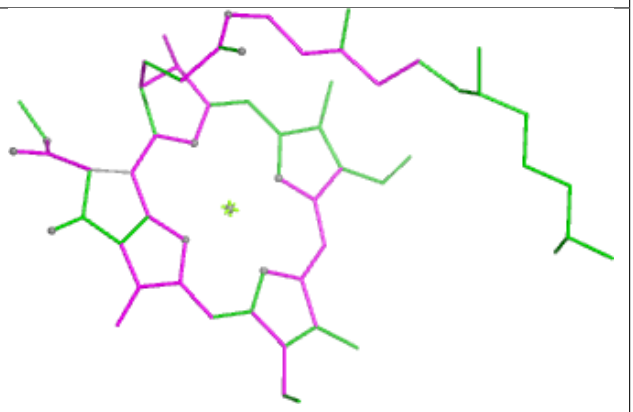


Rings

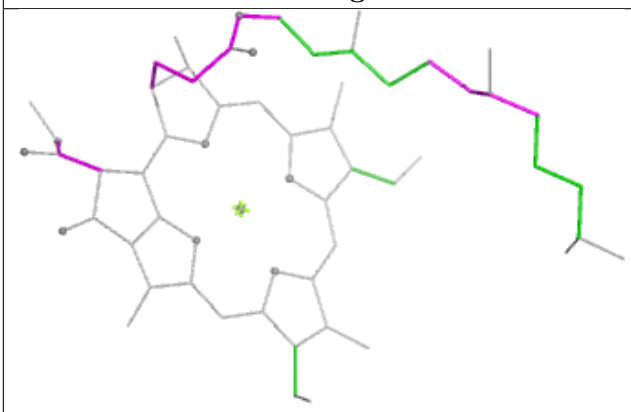
Ligand CLA s1 602



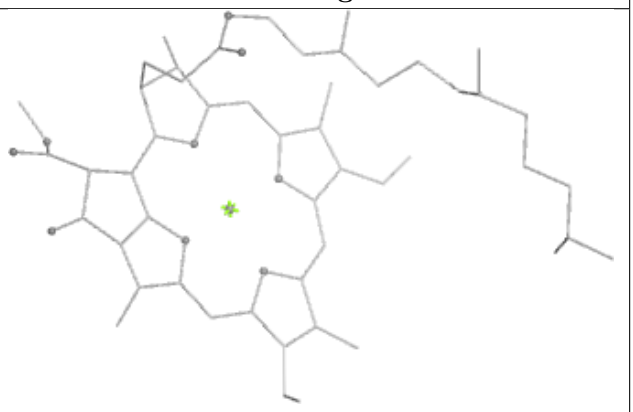
Bond lengths



Bond angles

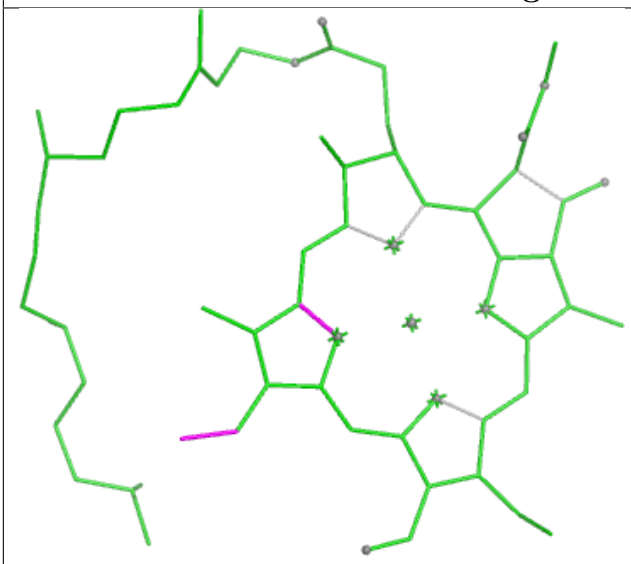


Torsions

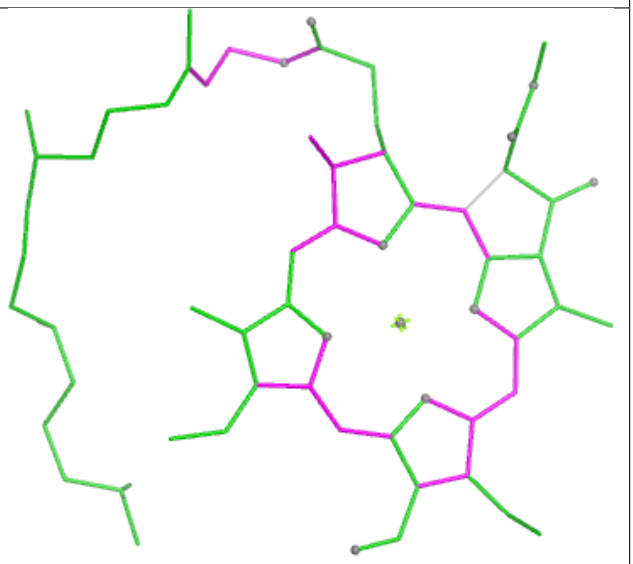


Rings

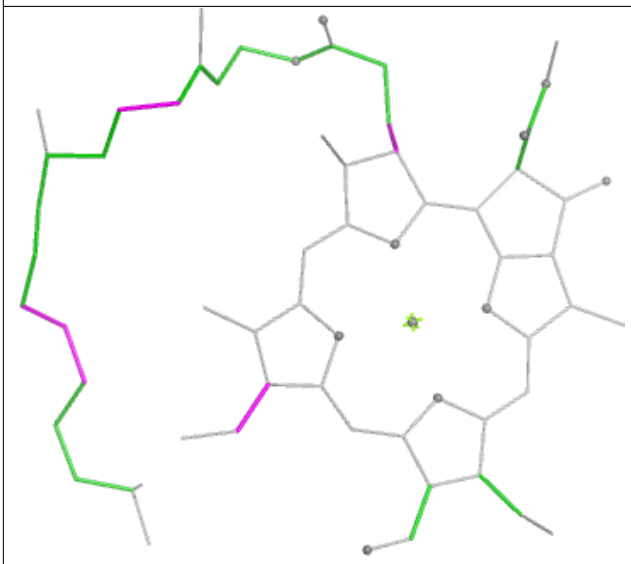
Ligand CHL N 607



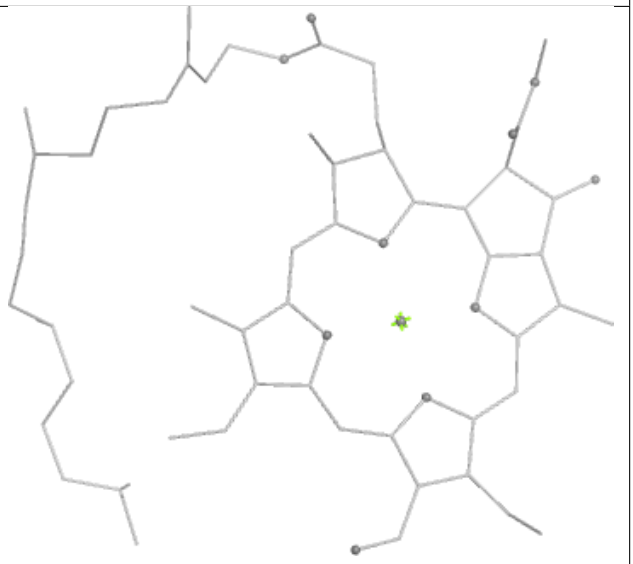
Bond lengths



Bond angles

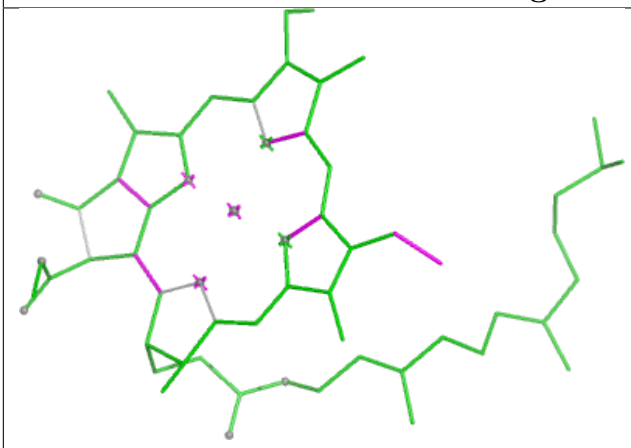


Torsions

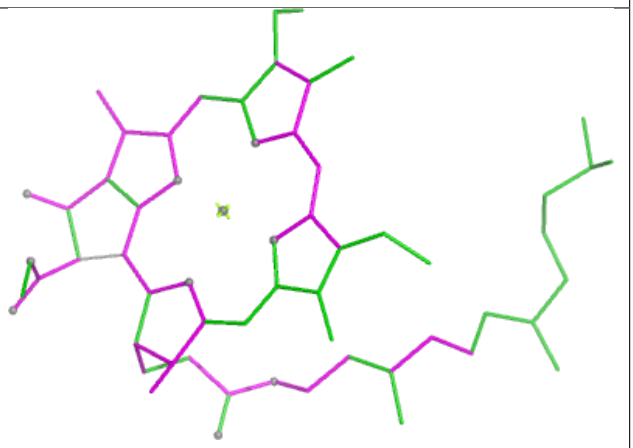


Rings

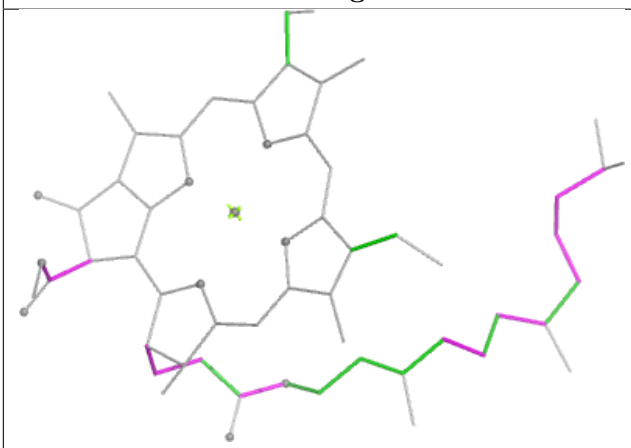
Ligand CLA r 602



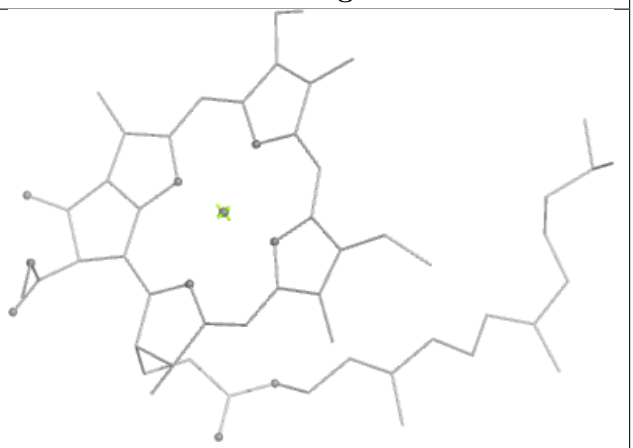
Bond lengths



Bond angles

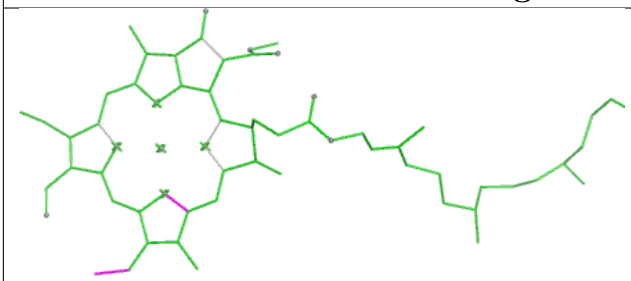


Torsions

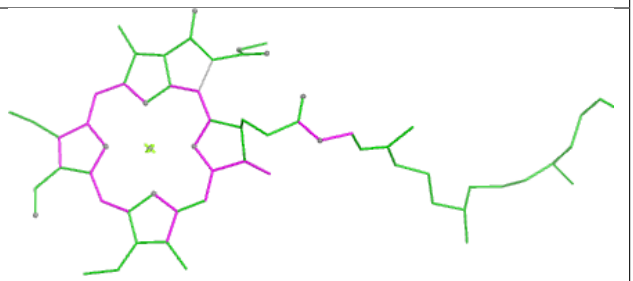


Rings

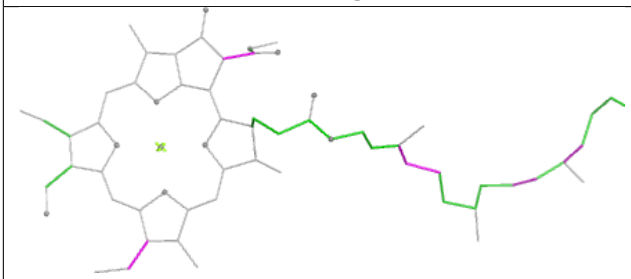
Ligand CHL N1 601



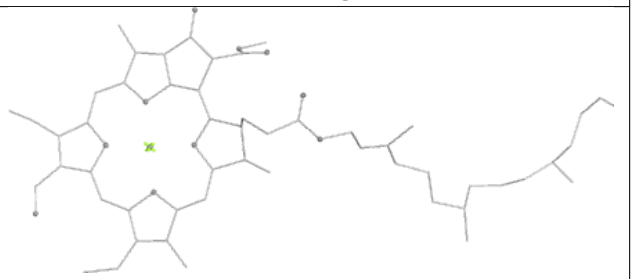
Bond lengths



Bond angles

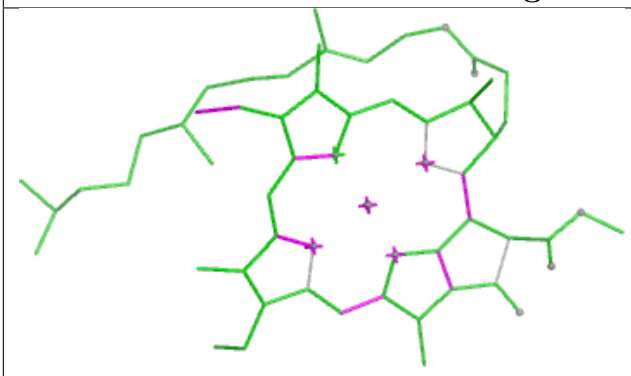


Torsions

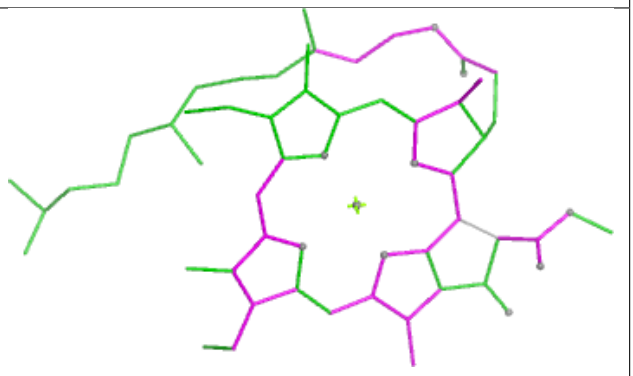


Rings

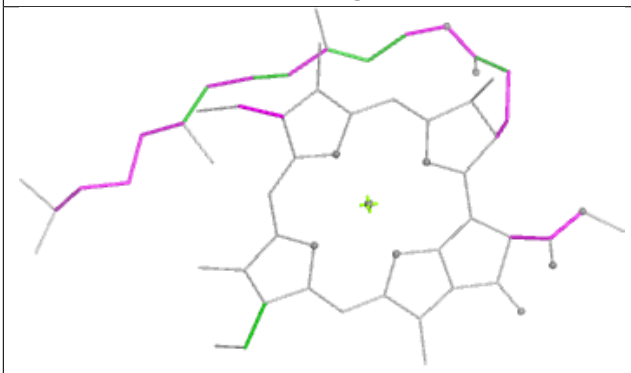
Ligand CLA R 608



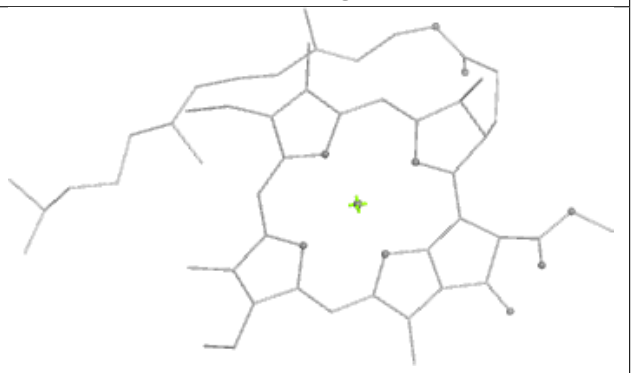
Bond lengths



Bond angles

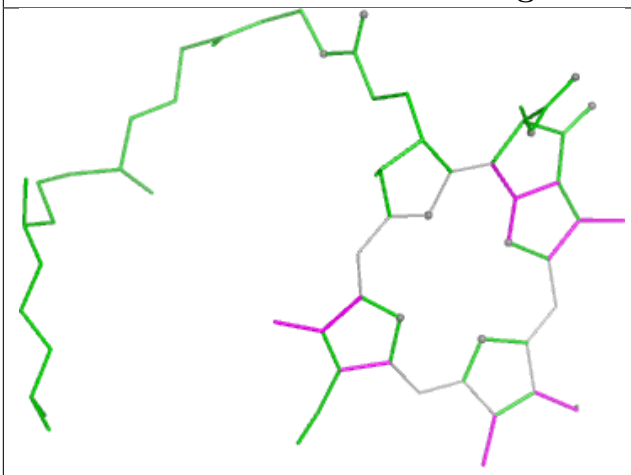


Torsions

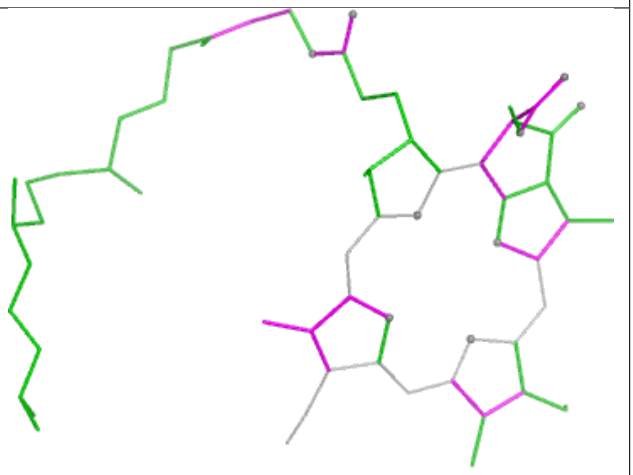


Rings

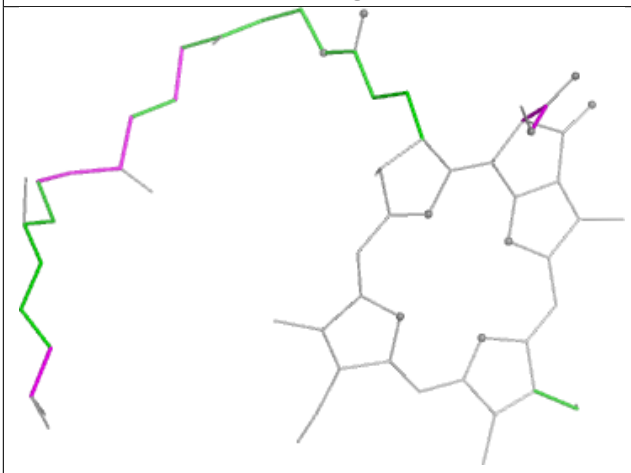
Ligand PHO a1 409



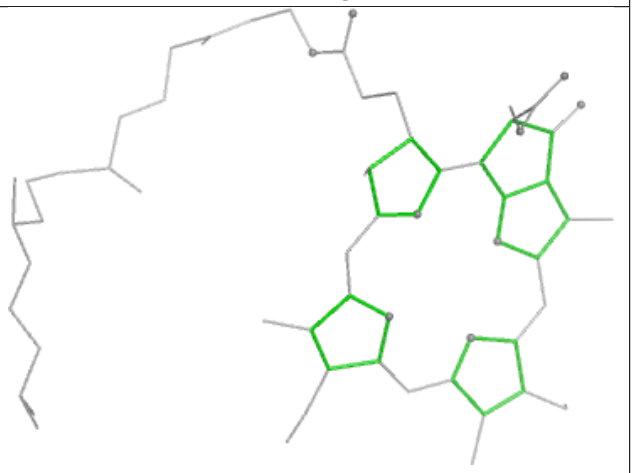
Bond lengths



Bond angles

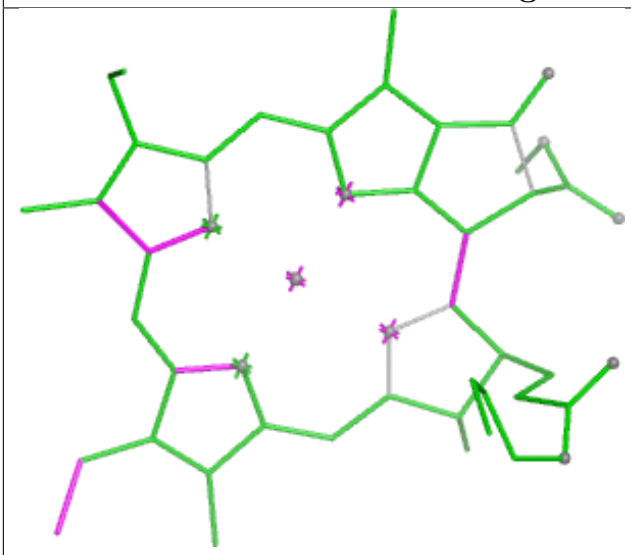


Torsions

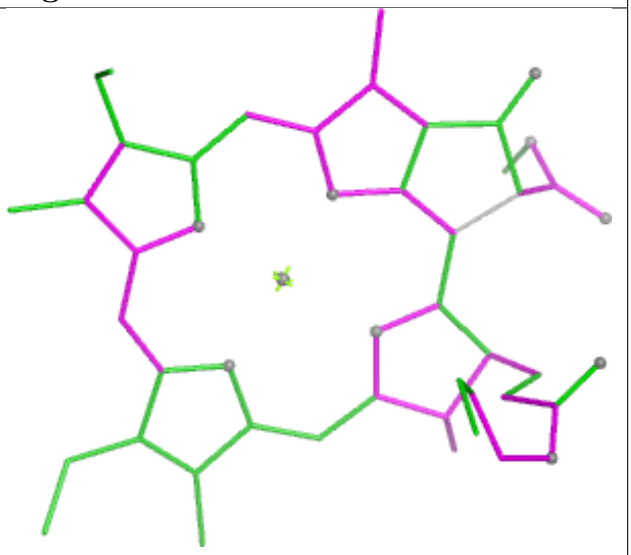


Rings

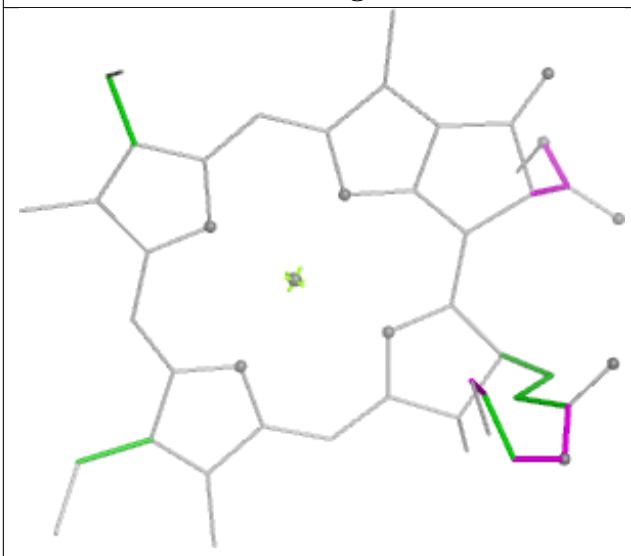
Ligand CLA g1 604



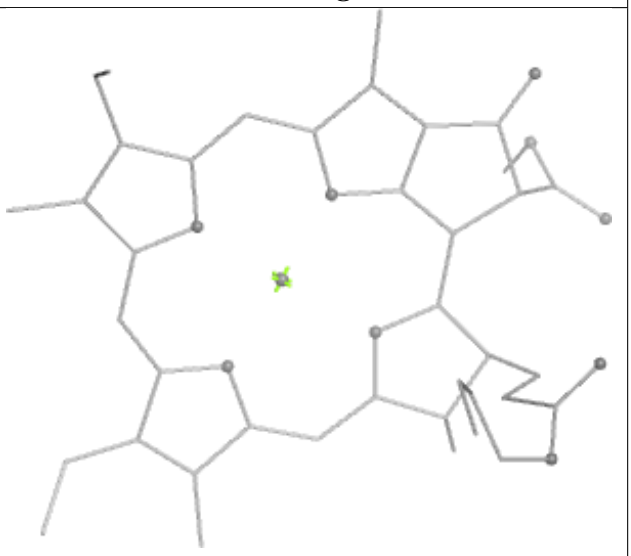
Bond lengths



Bond angles

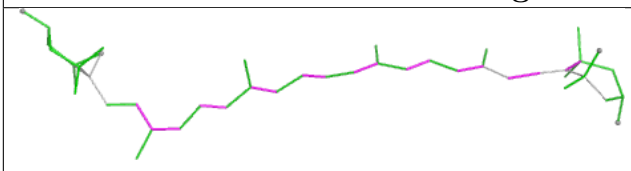


Torsions

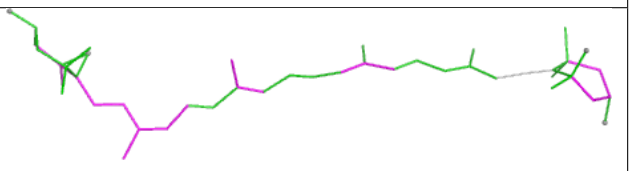


Rings

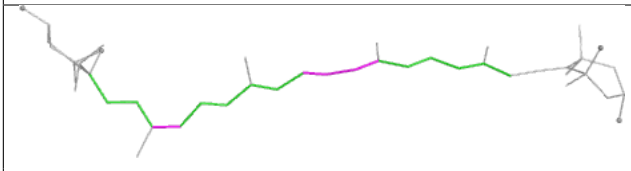
Ligand NEX N1 623



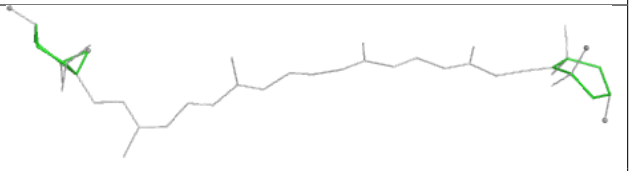
Bond lengths



Bond angles

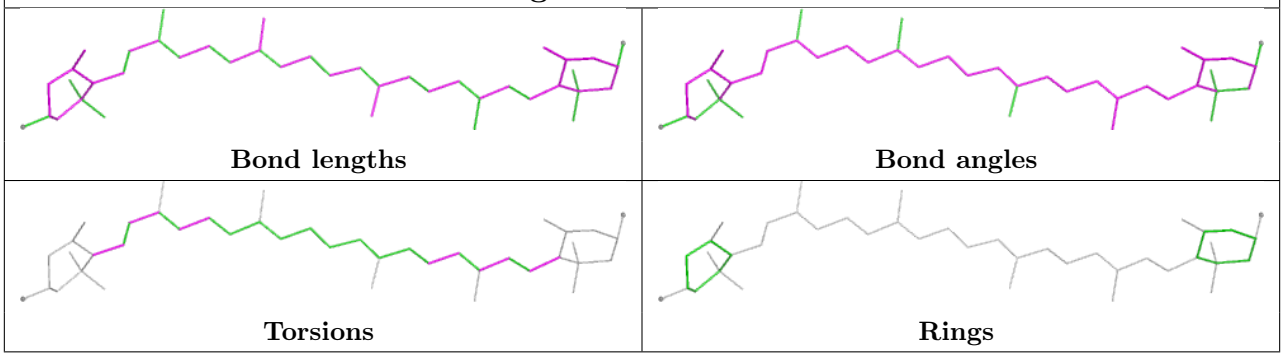


Torsions

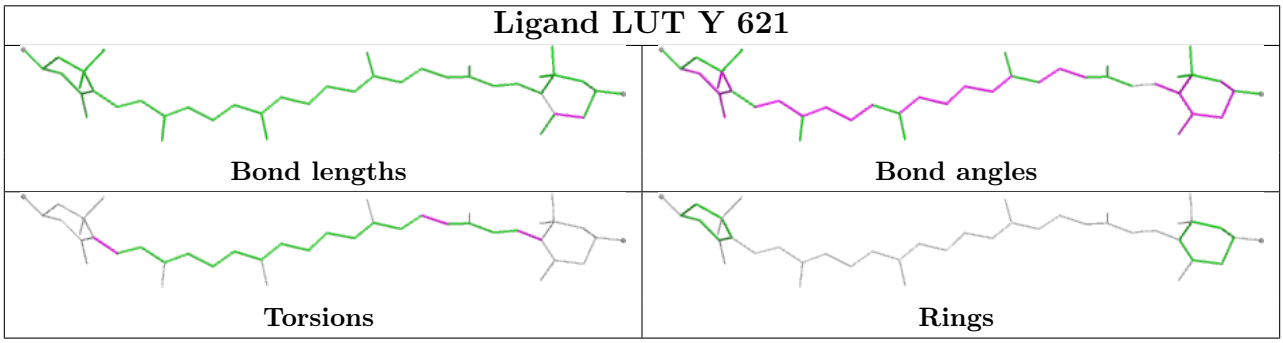


Rings

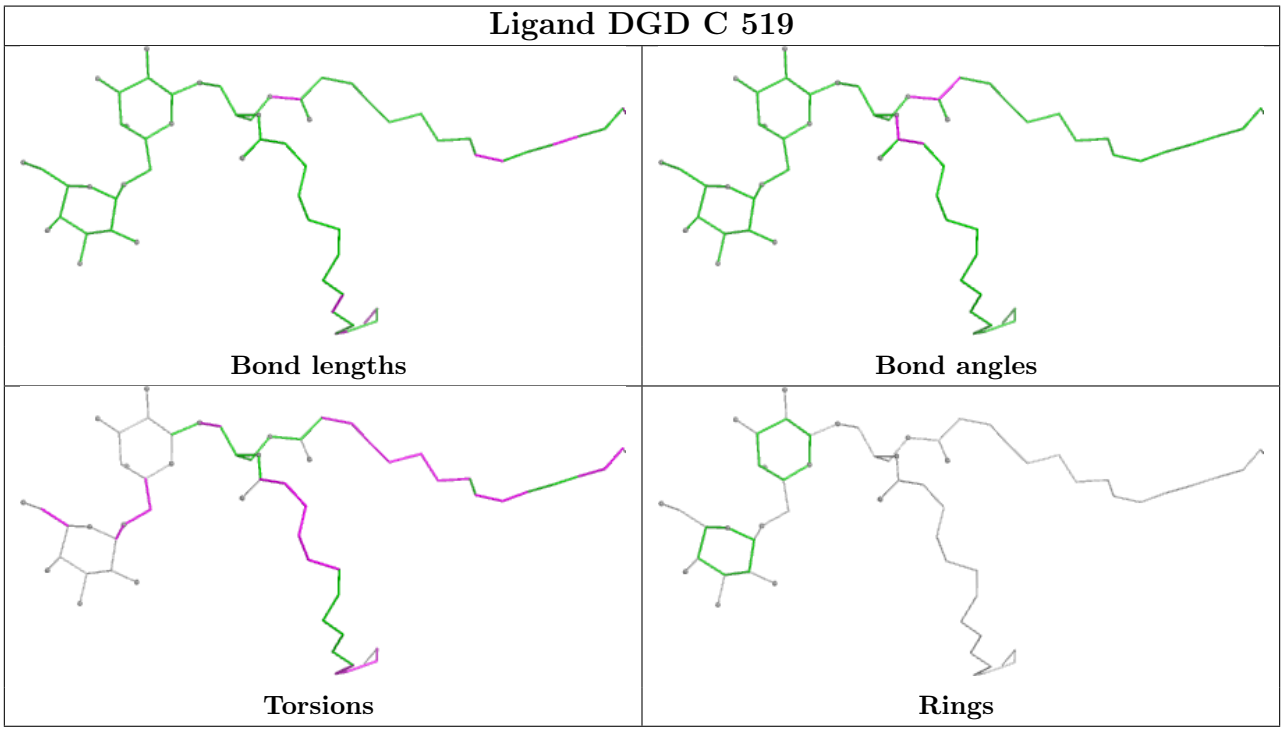
Ligand C7Z B 620



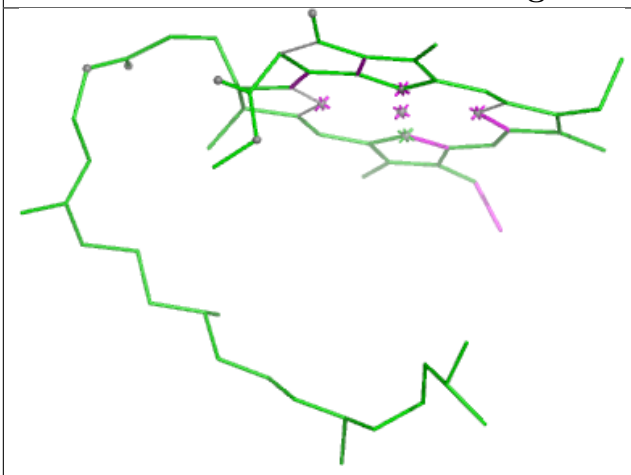
Ligand LUT Y 621



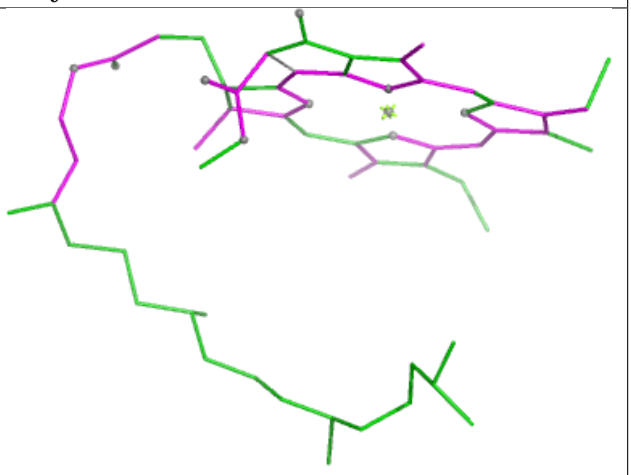
Ligand DGD C 519



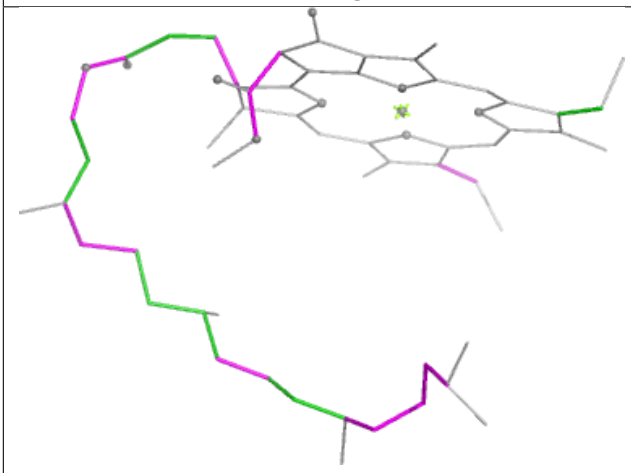
Ligand CLA y 603



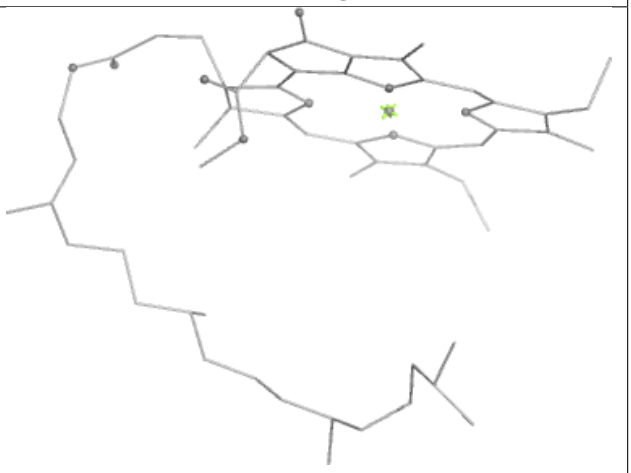
Bond lengths



Bond angles

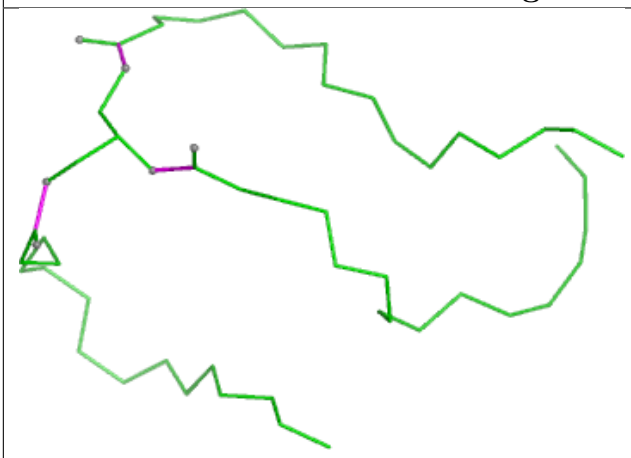


Torsions

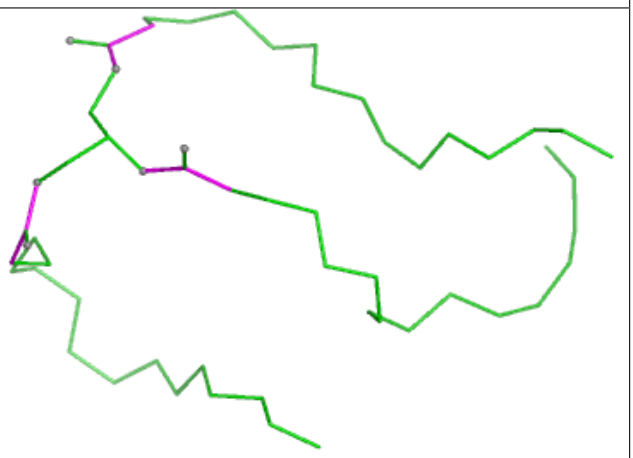


Rings

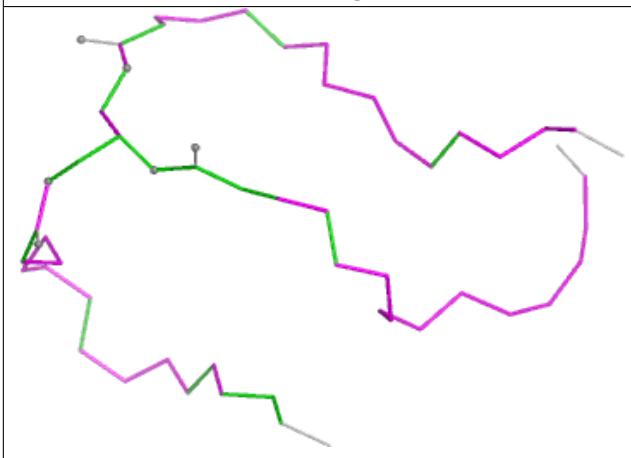
Ligand 4RF k1 101



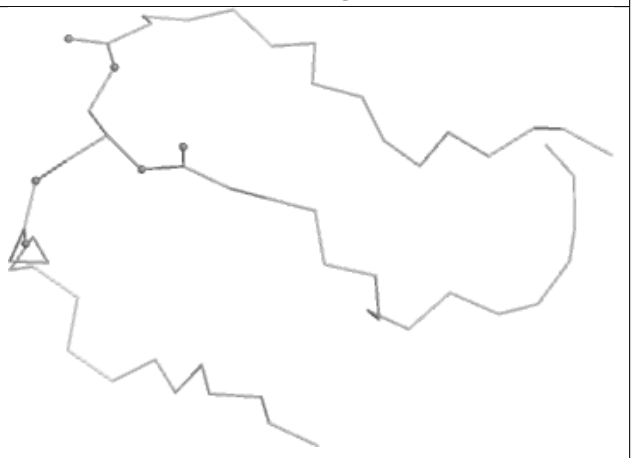
Bond lengths



Bond angles



Torsions

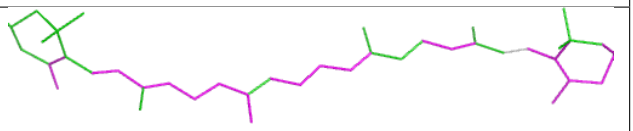


Rings

Ligand LUT G 621



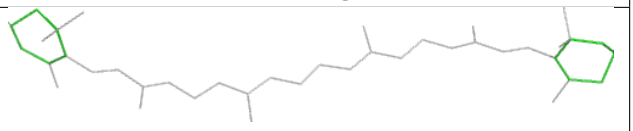
Bond lengths



Bond angles

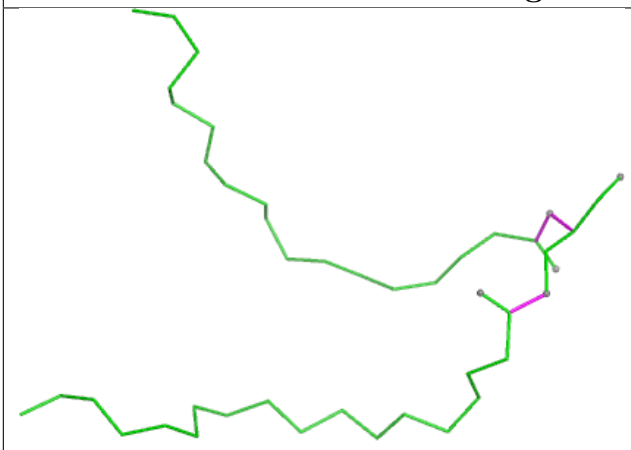


Torsions

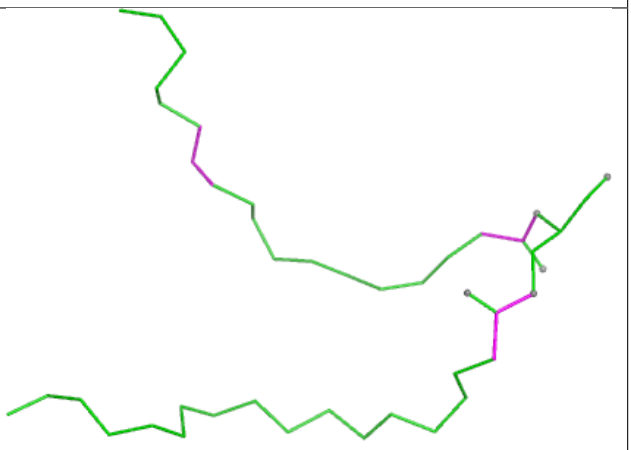


Rings

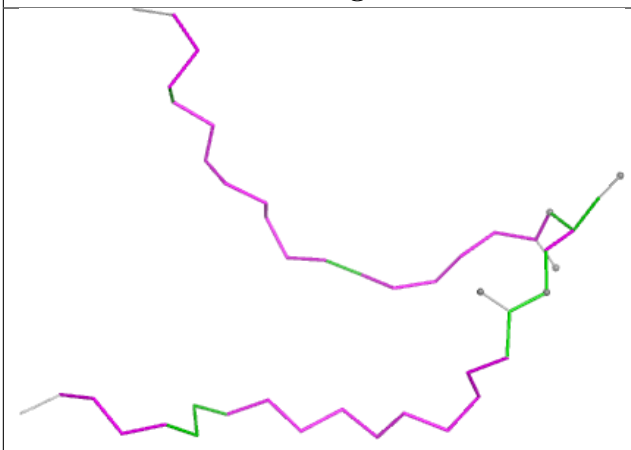
Ligand DGA c 524



Bond lengths



Bond angles

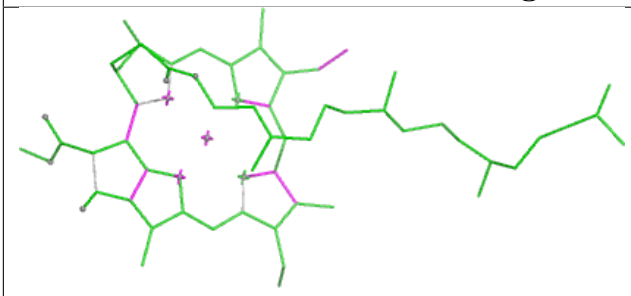


Torsions

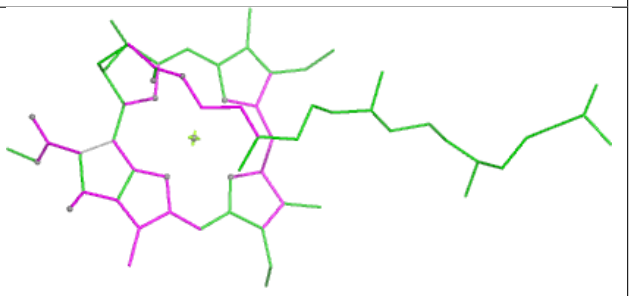


Rings

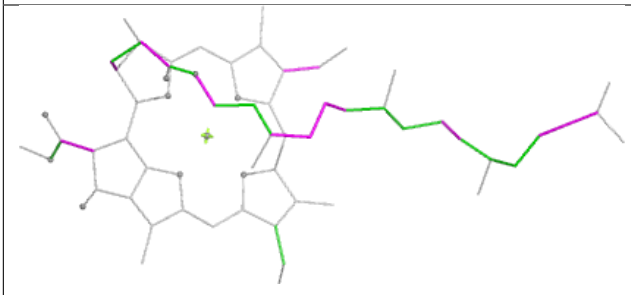
Ligand CLA c1 505



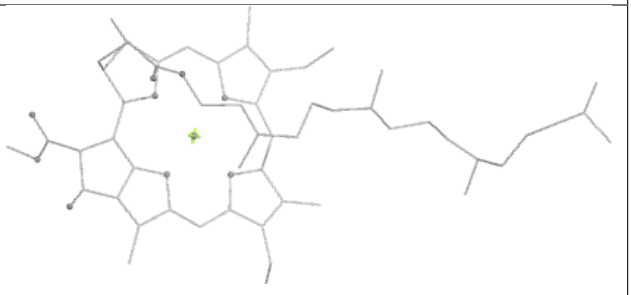
Bond lengths



Bond angles

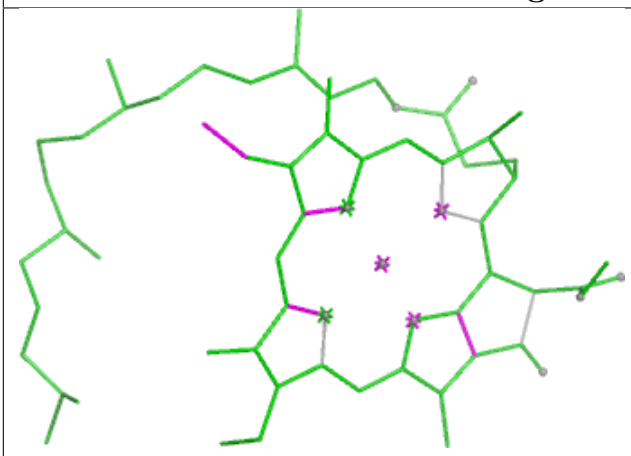


Torsions

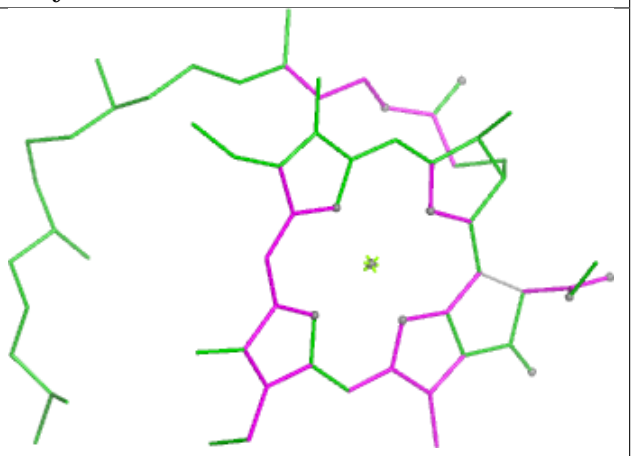


Rings

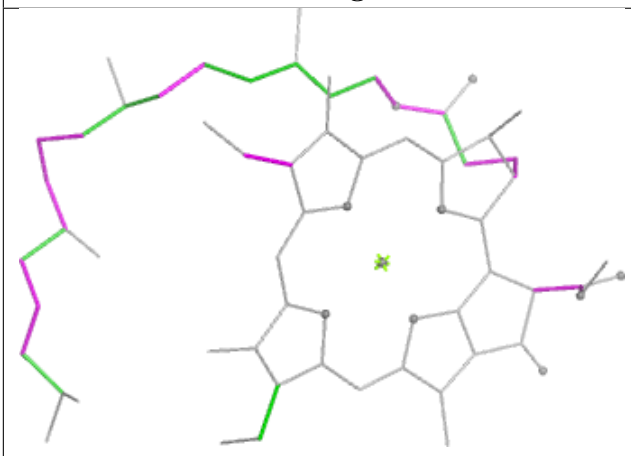
Ligand CLA y 602



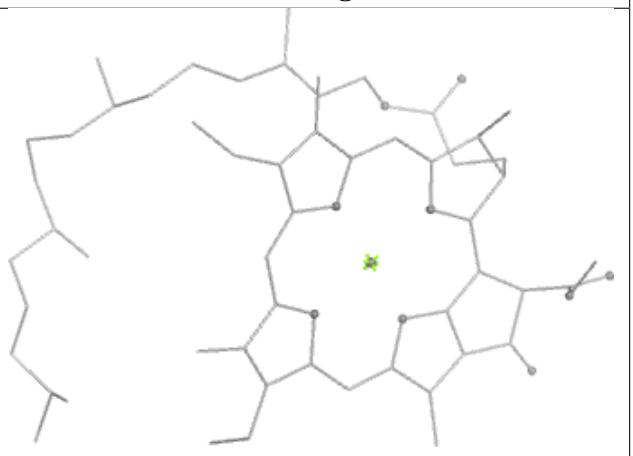
Bond lengths



Bond angles

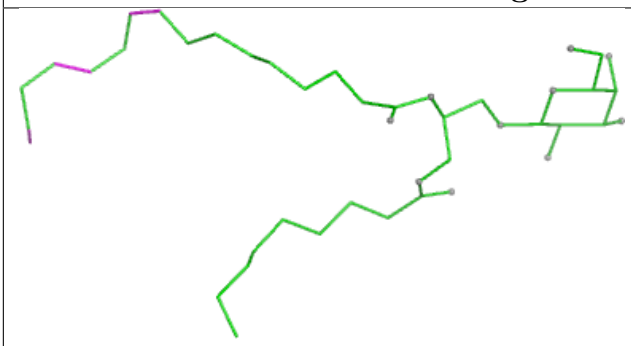


Torsions

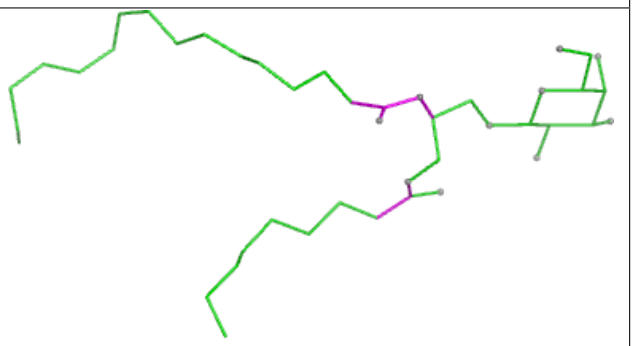


Rings

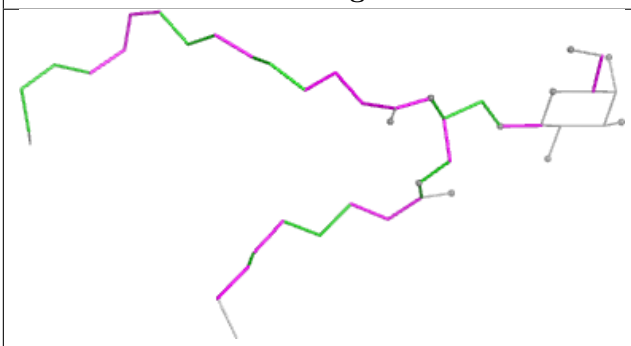
Ligand LMG B1 622



Bond lengths



Bond angles

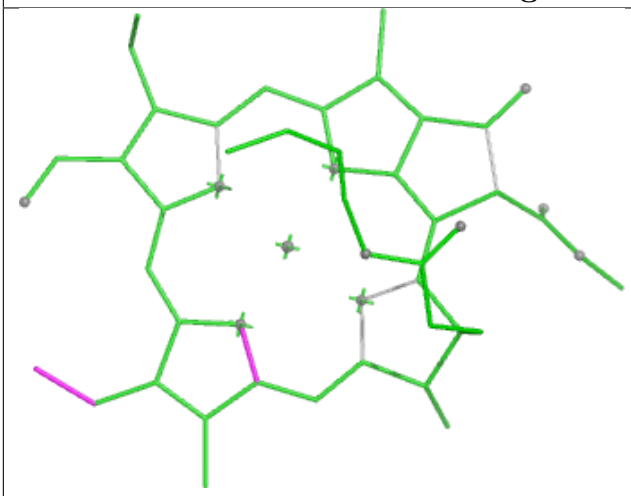


Torsions

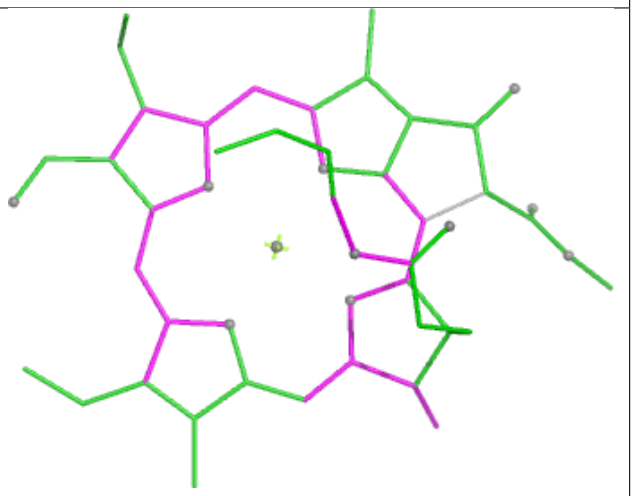


Rings

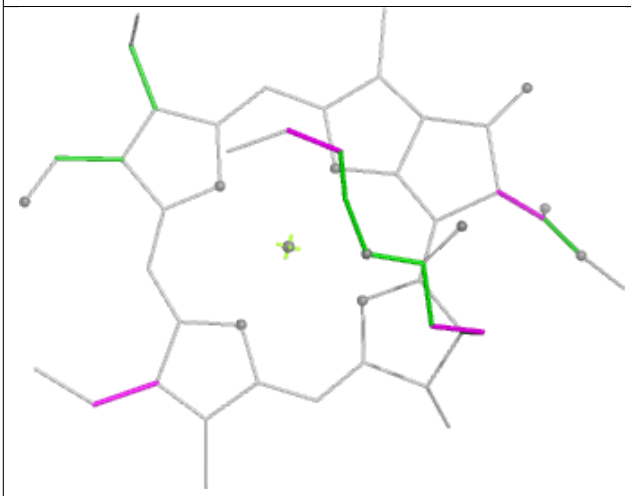
Ligand CHL r1 607



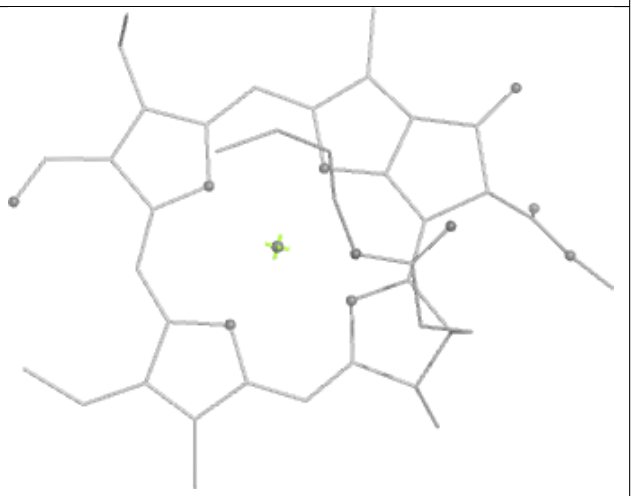
Bond lengths



Bond angles

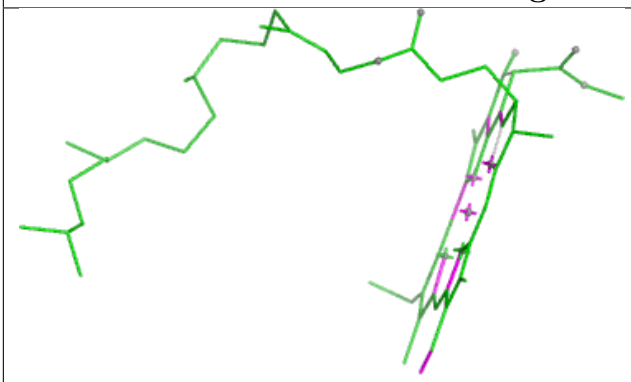


Torsions

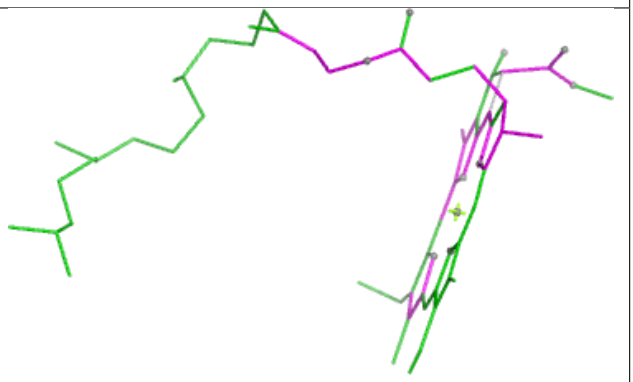


Rings

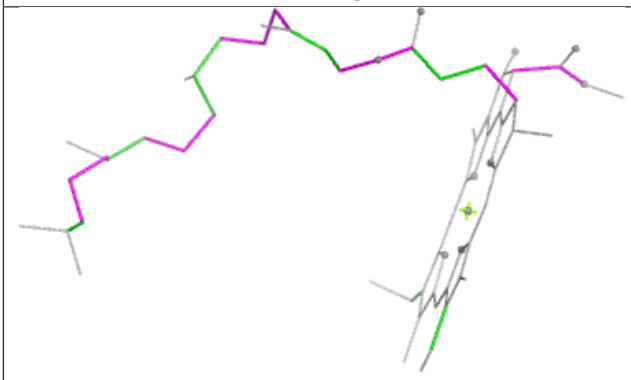
Ligand CLA c 506



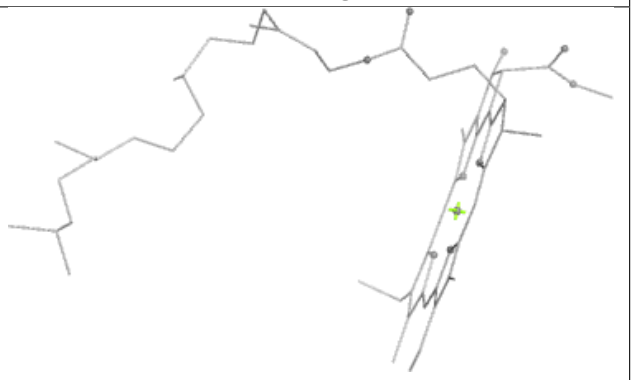
Bond lengths



Bond angles

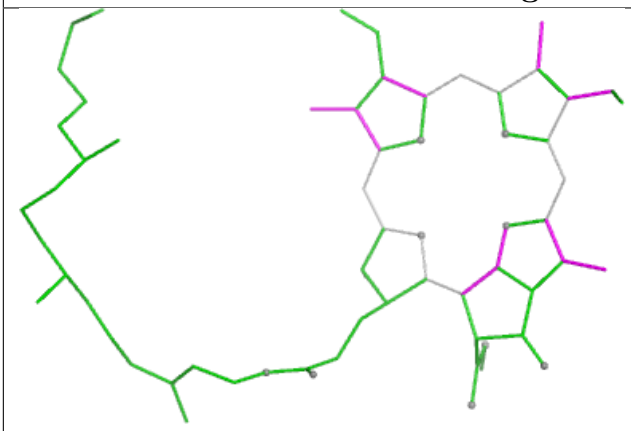


Torsions

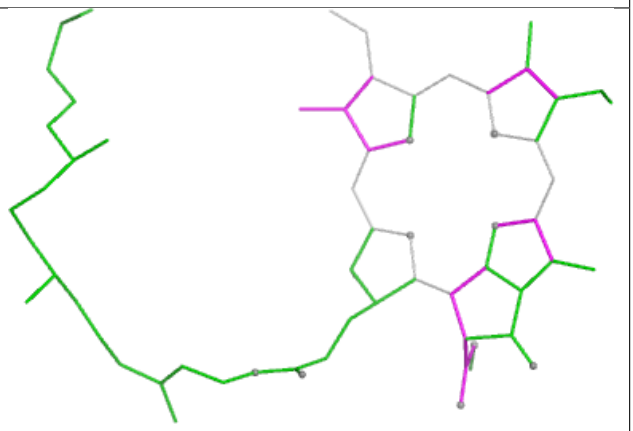


Rings

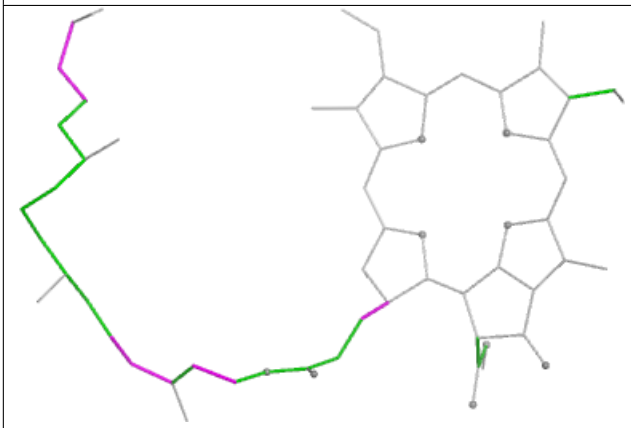
Ligand PHO A 408



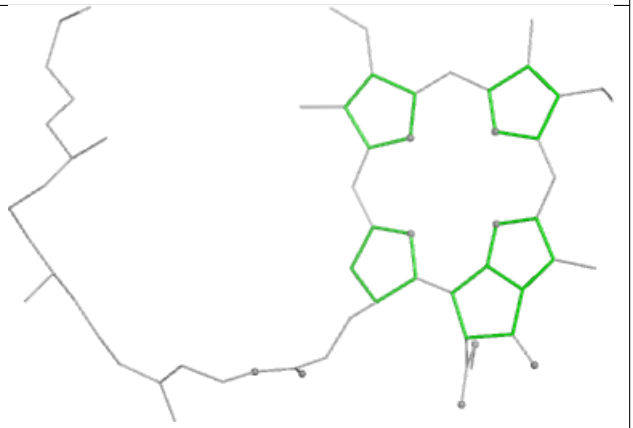
Bond lengths



Bond angles

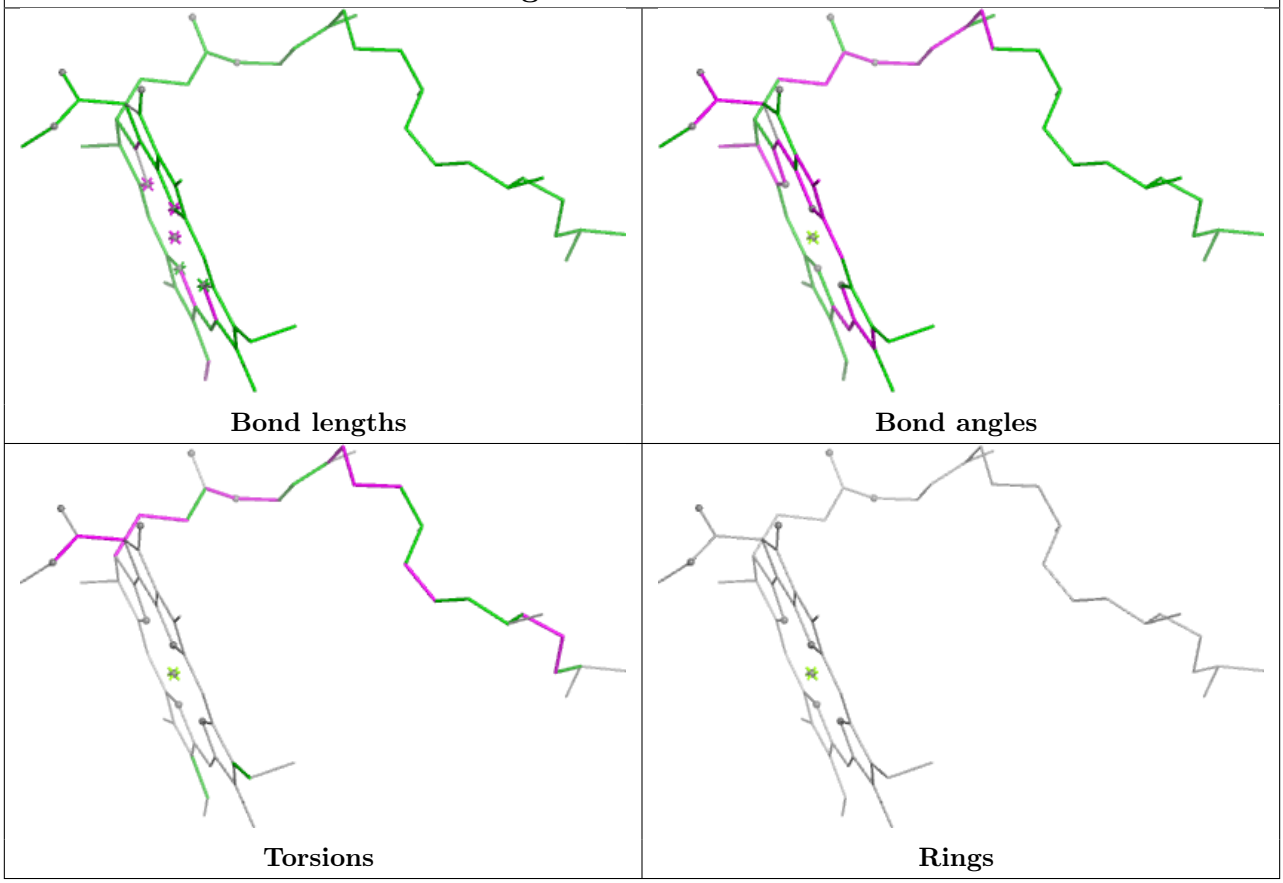


Torsions

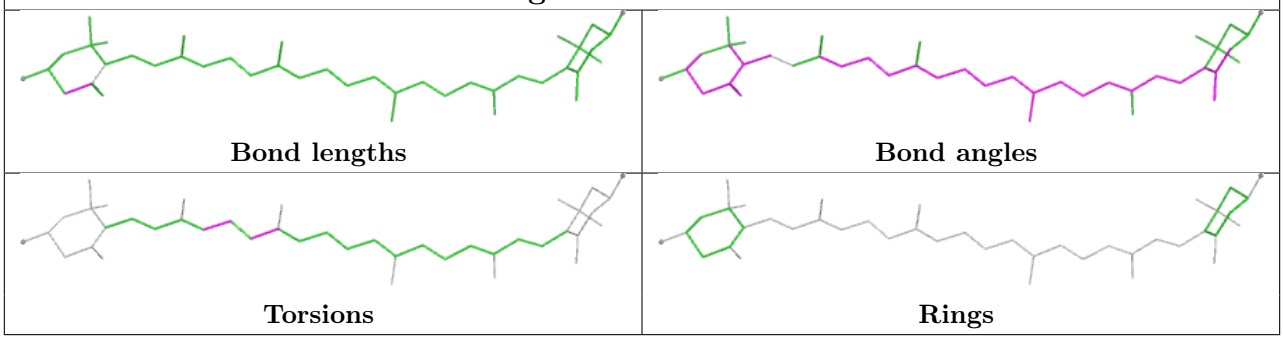


Rings

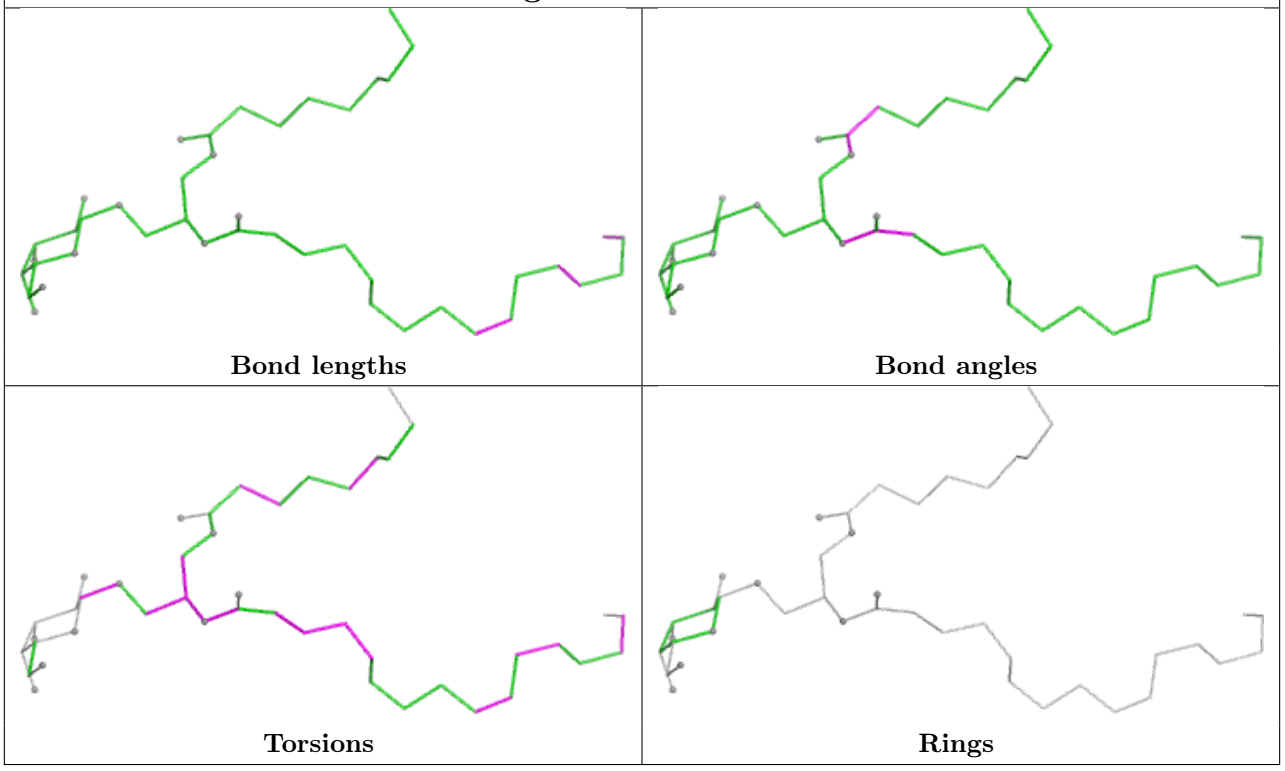
Ligand CLA c1 506



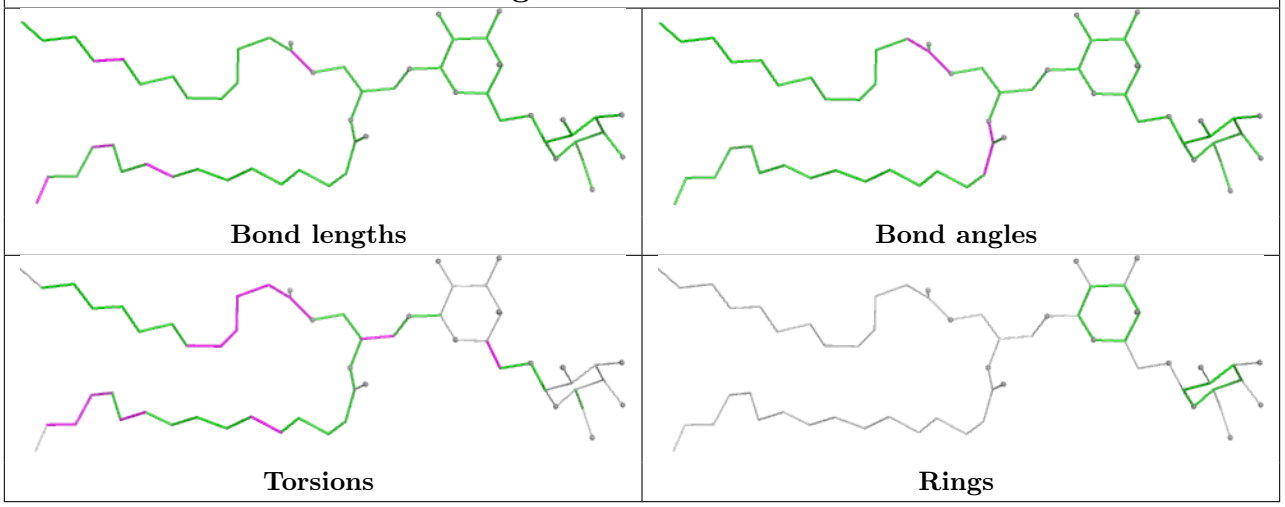
Ligand LUT n 620



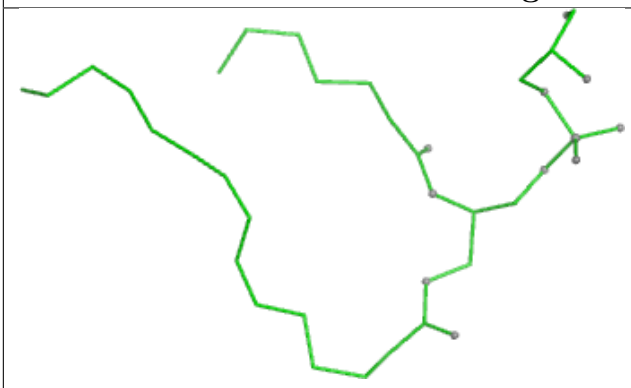
Ligand LMG b 622



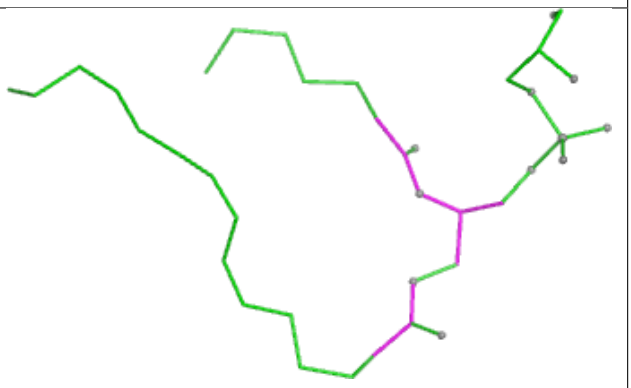
Ligand DGD C1 520



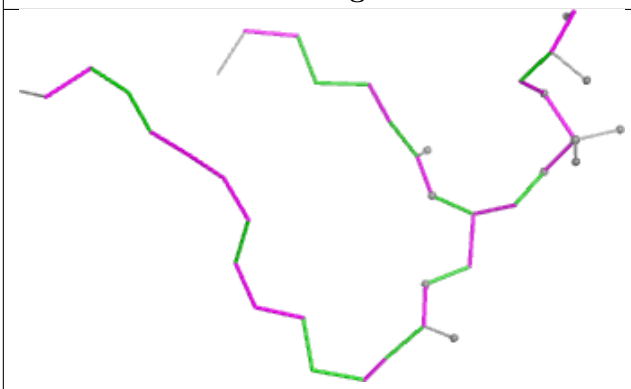
Ligand LHG D 410



Bond lengths



Bond angles

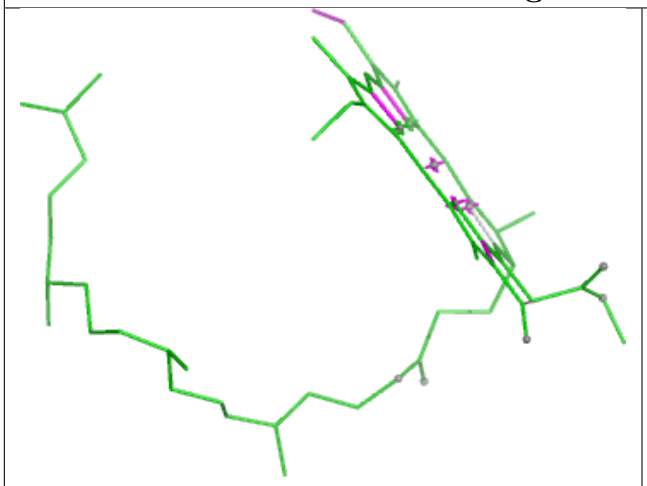


Torsions



Rings

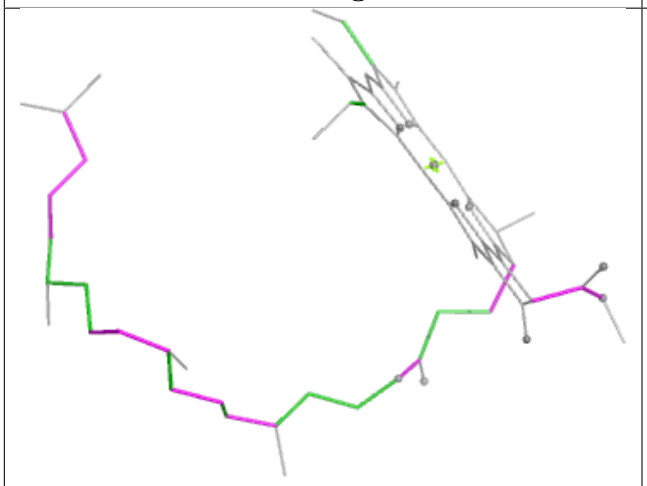
Ligand CLA B 612



Bond lengths



Bond angles

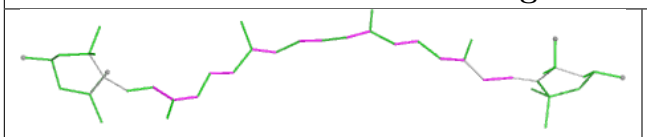


Torsions

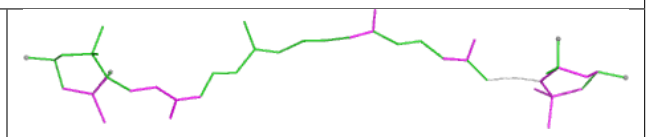


Rings

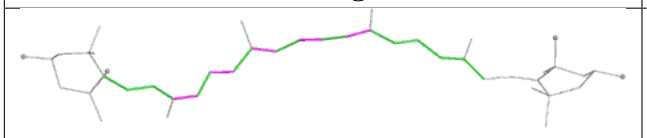
Ligand NEX r1 622



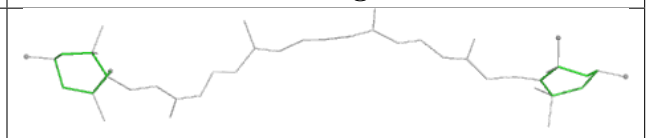
Bond lengths



Bond angles

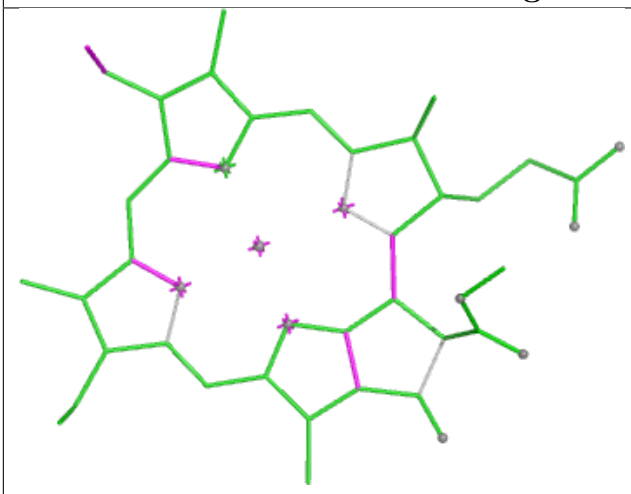


Torsions

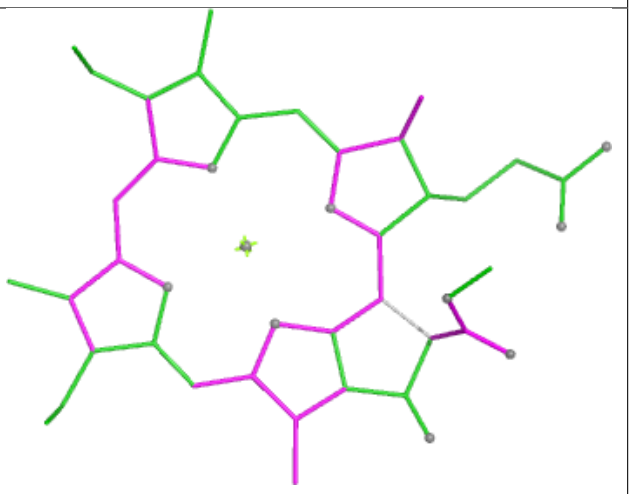


Rings

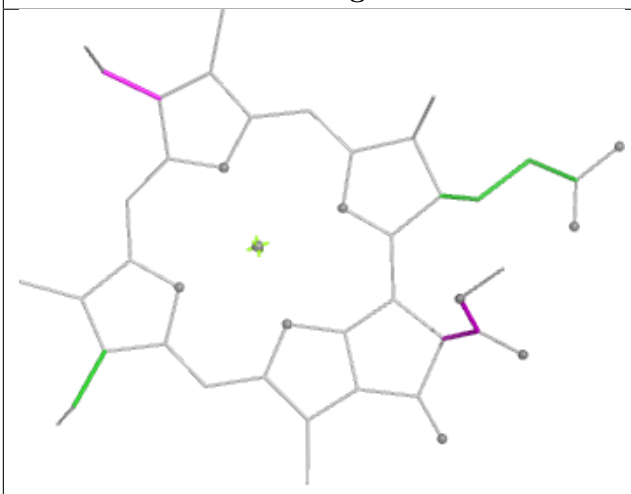
Ligand CLA N 612



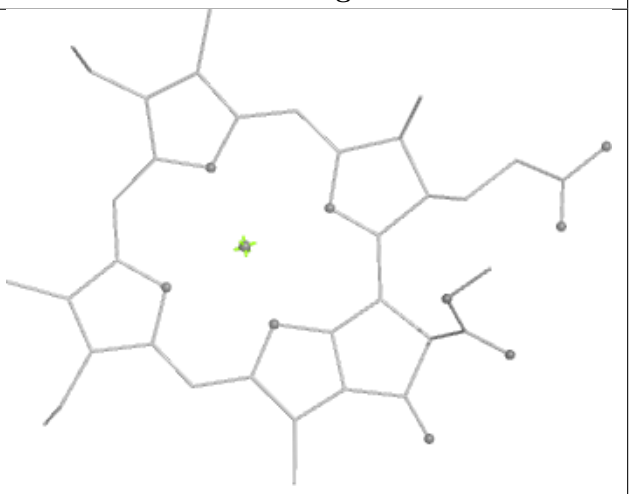
Bond lengths



Bond angles

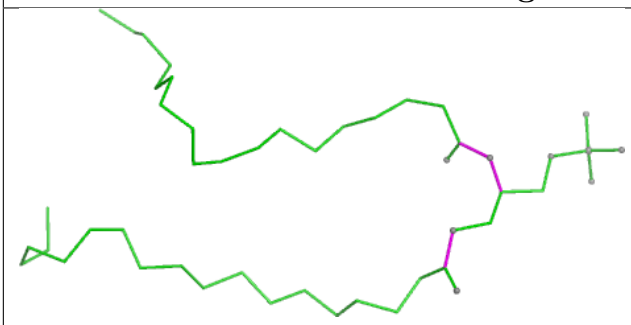


Torsions

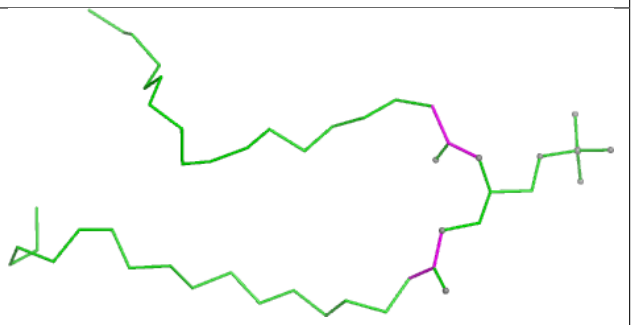


Rings

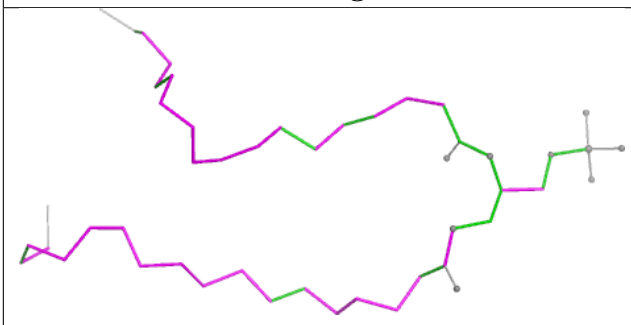
Ligand 3PH B1 624



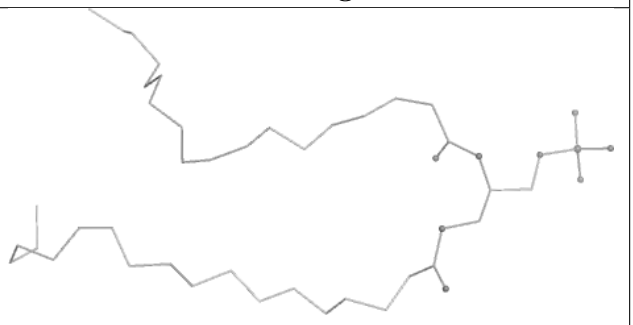
Bond lengths



Bond angles

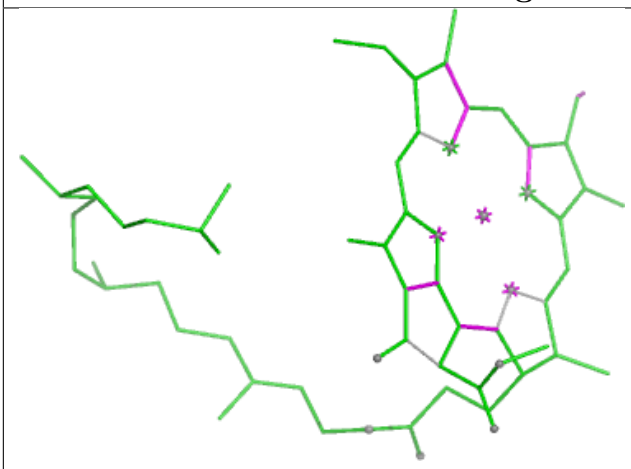


Torsions

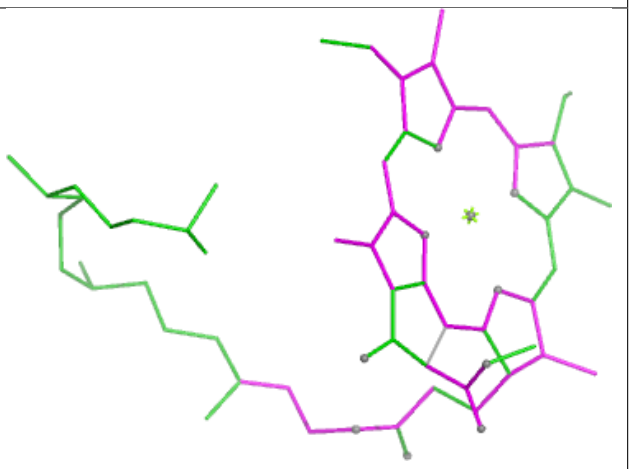


Rings

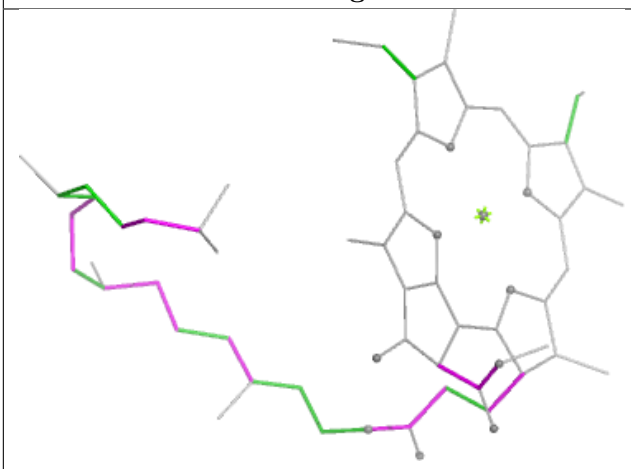
Ligand CLA C1 503



Bond lengths



Bond angles

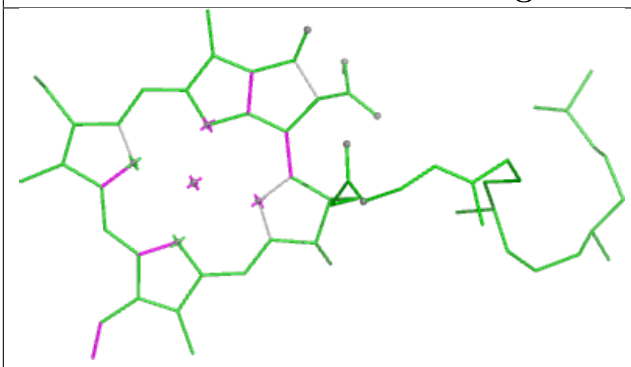


Torsions

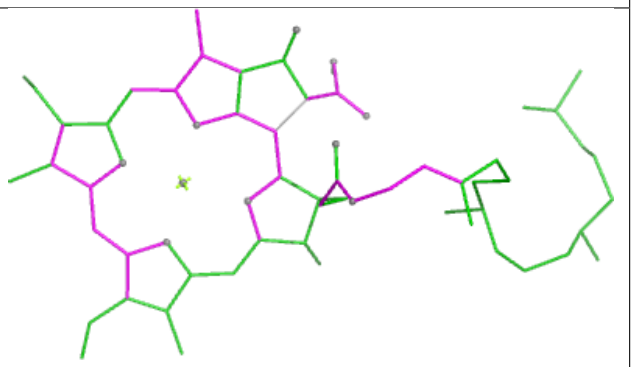


Rings

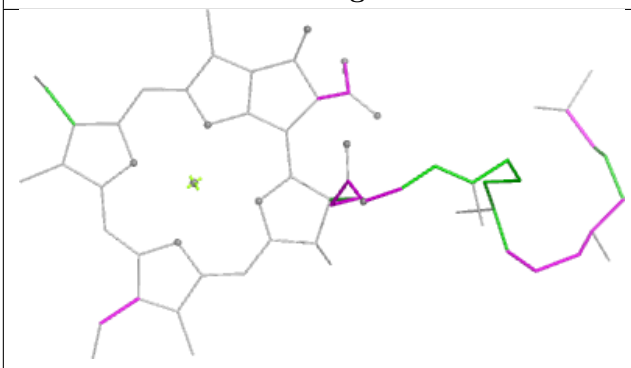
Ligand CLA B1 613



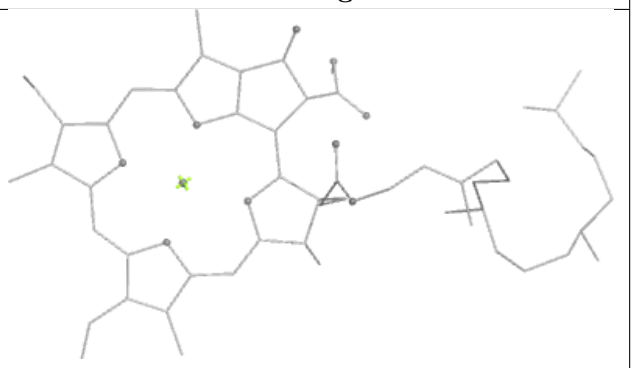
Bond lengths



Bond angles

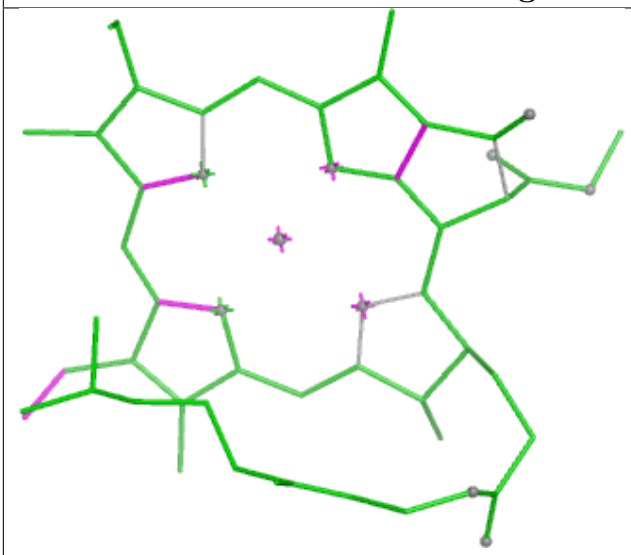


Torsions

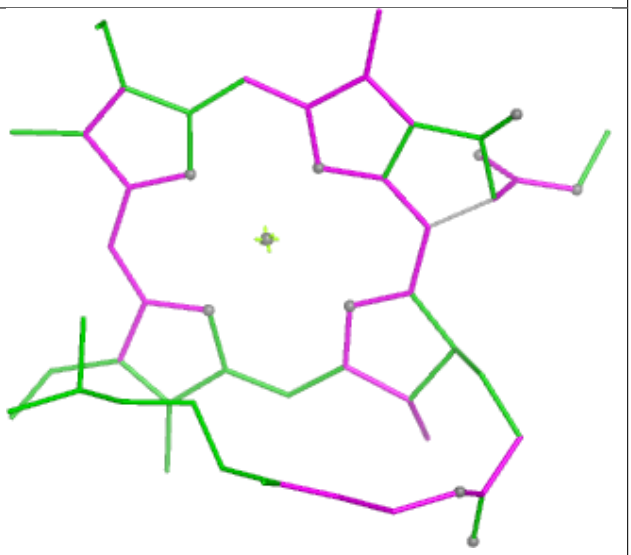


Rings

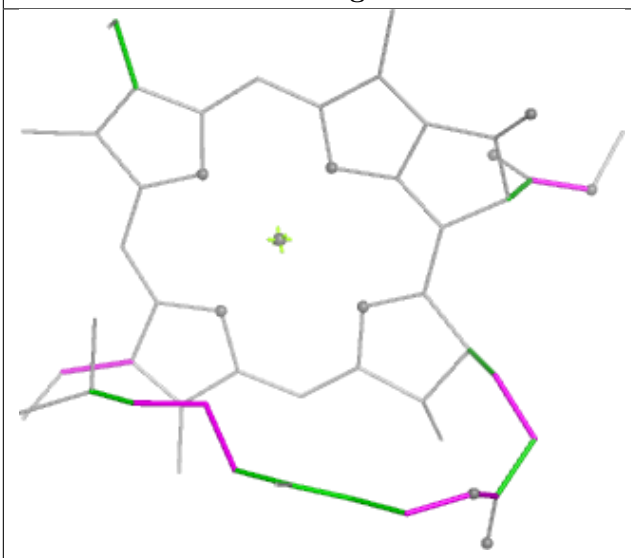
Ligand CLA S1 614



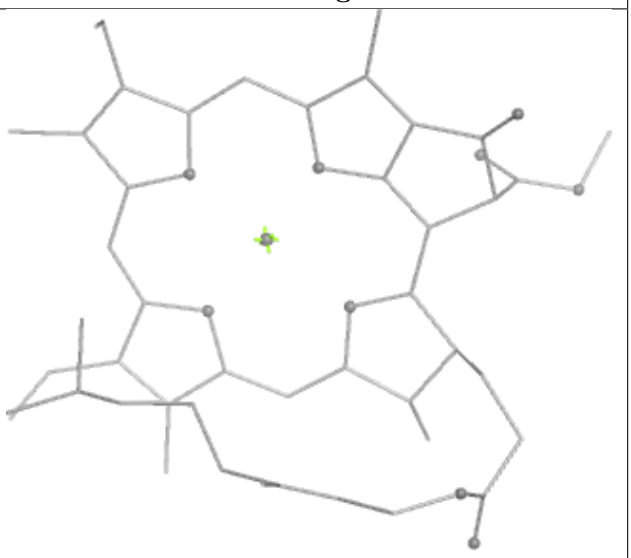
Bond lengths



Bond angles

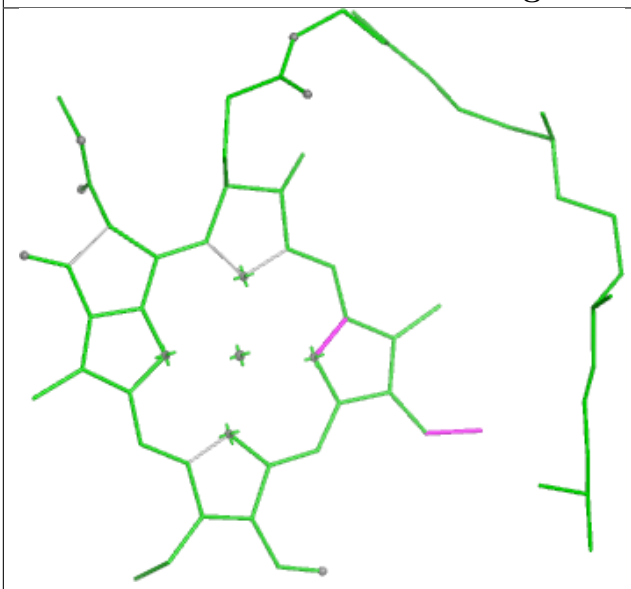


Torsions

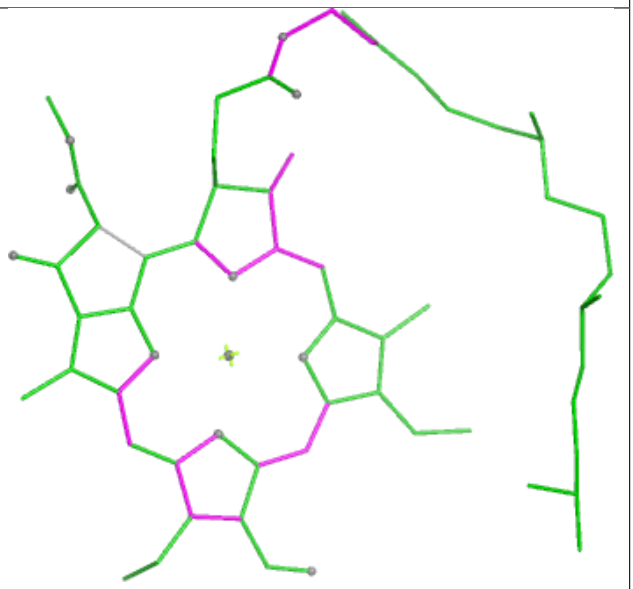


Rings

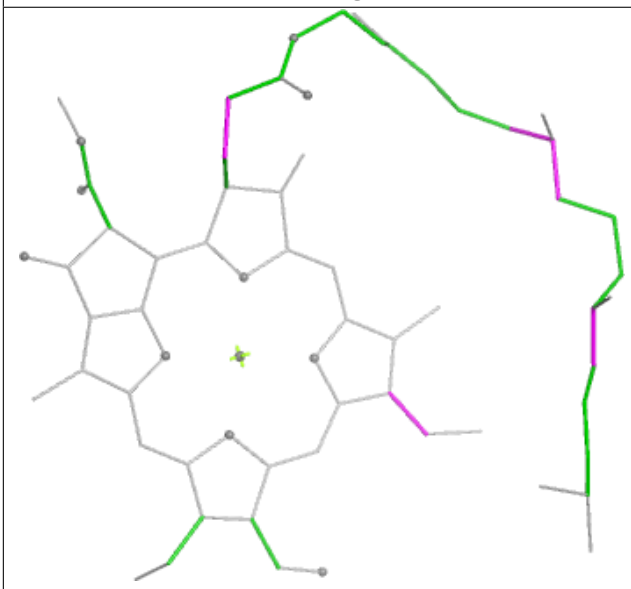
Ligand CHL Y 607



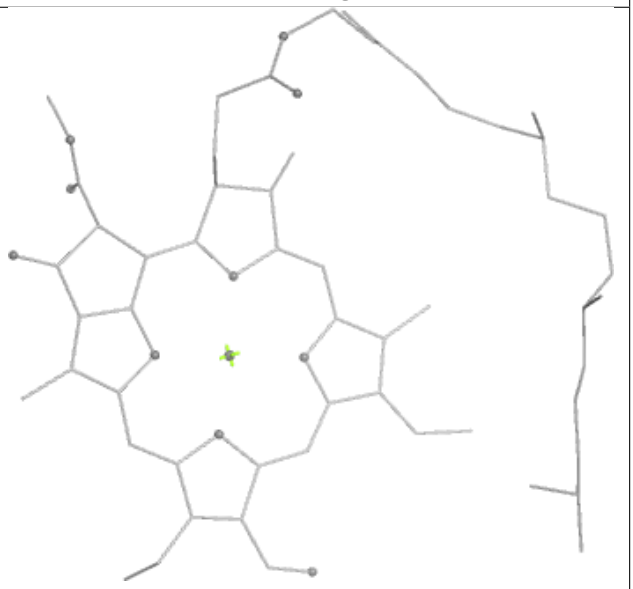
Bond lengths



Bond angles

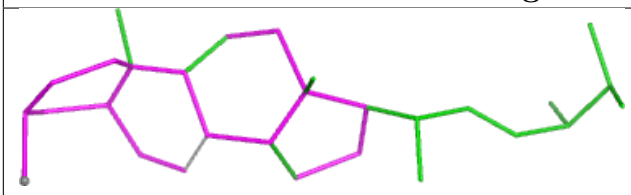


Torsions

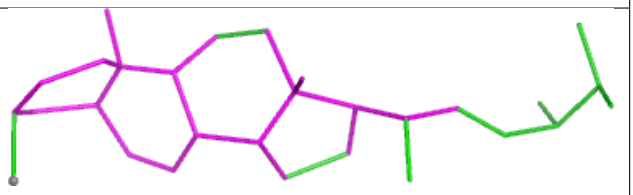


Rings

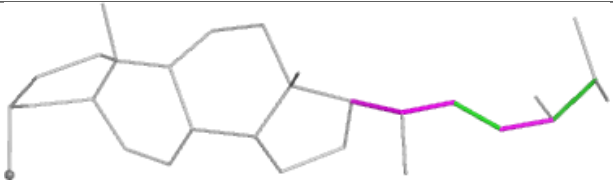
Ligand ERG R 626



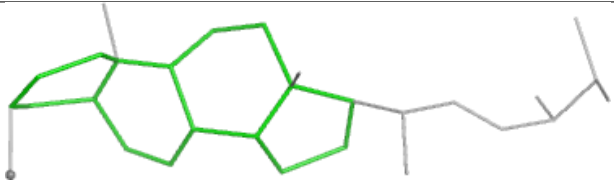
Bond lengths



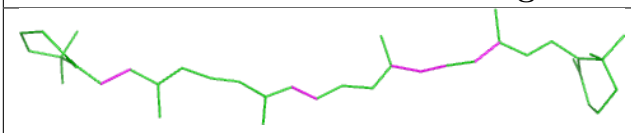
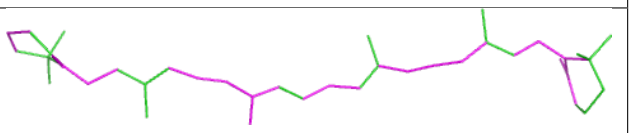
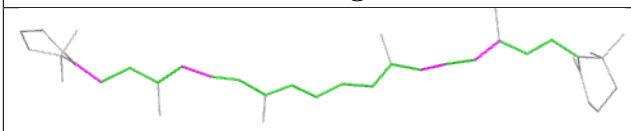
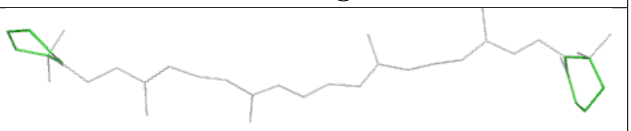
Bond angles

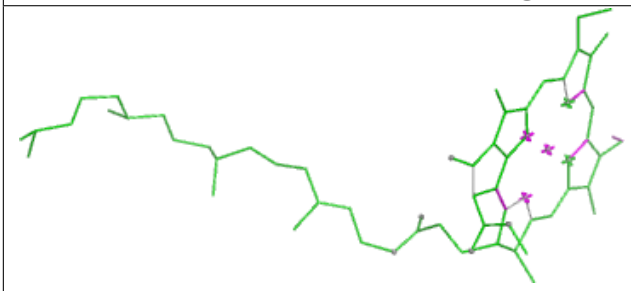
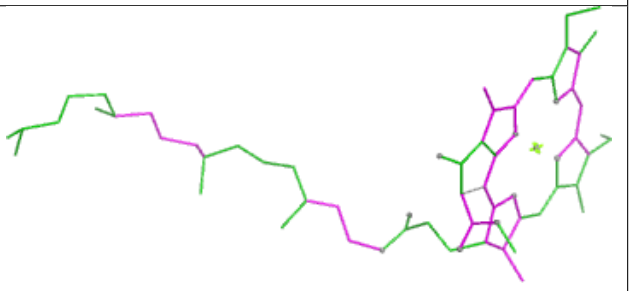
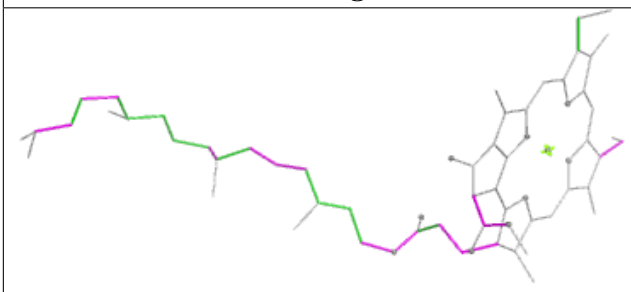
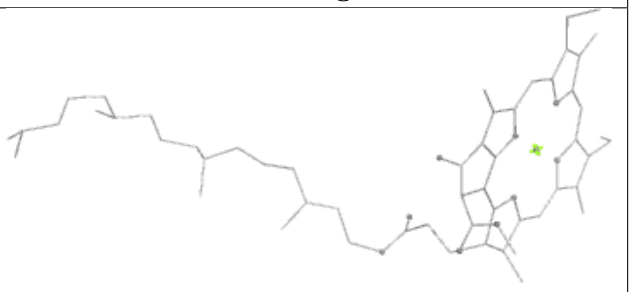


Torsions

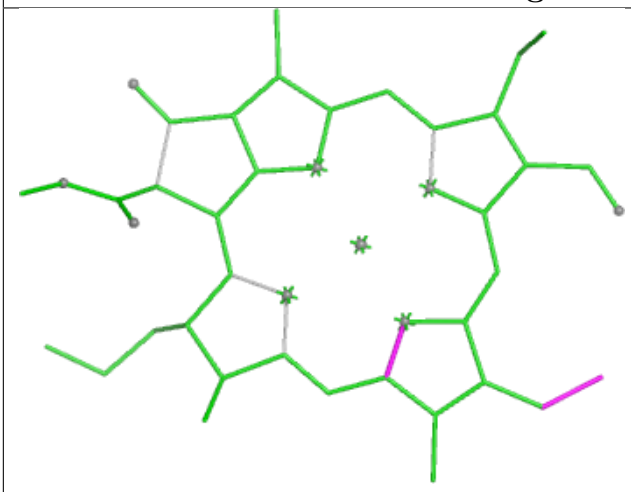


Rings

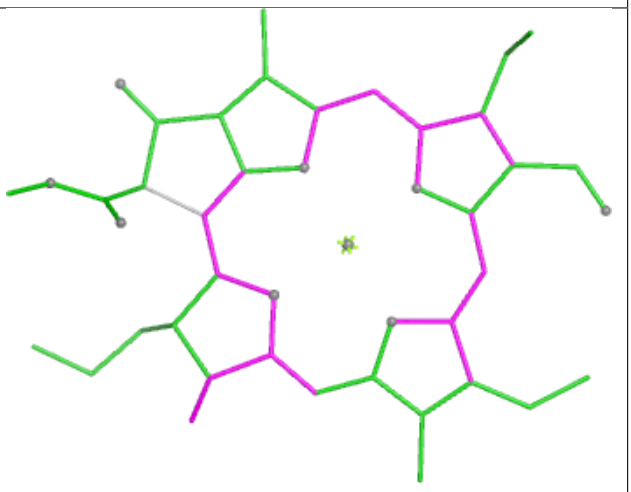
Ligand BCR a1 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b1 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

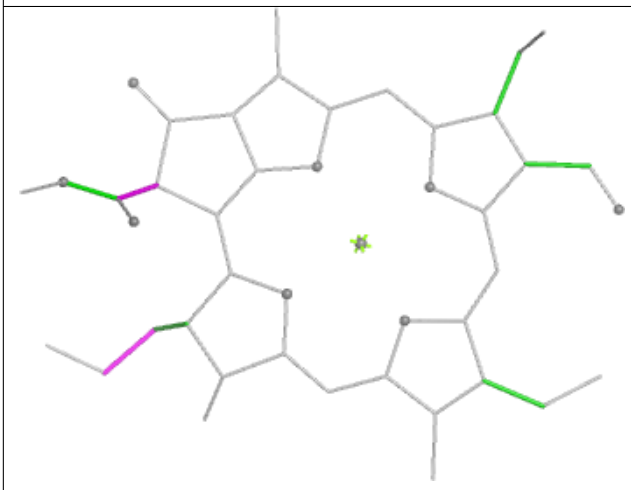
Ligand CHL S 606



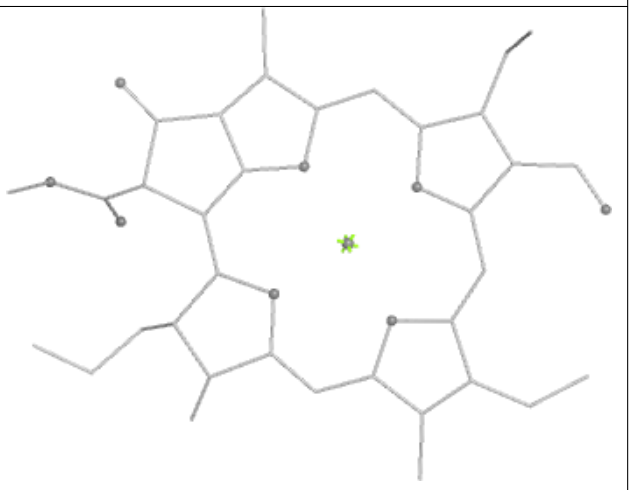
Bond lengths



Bond angles

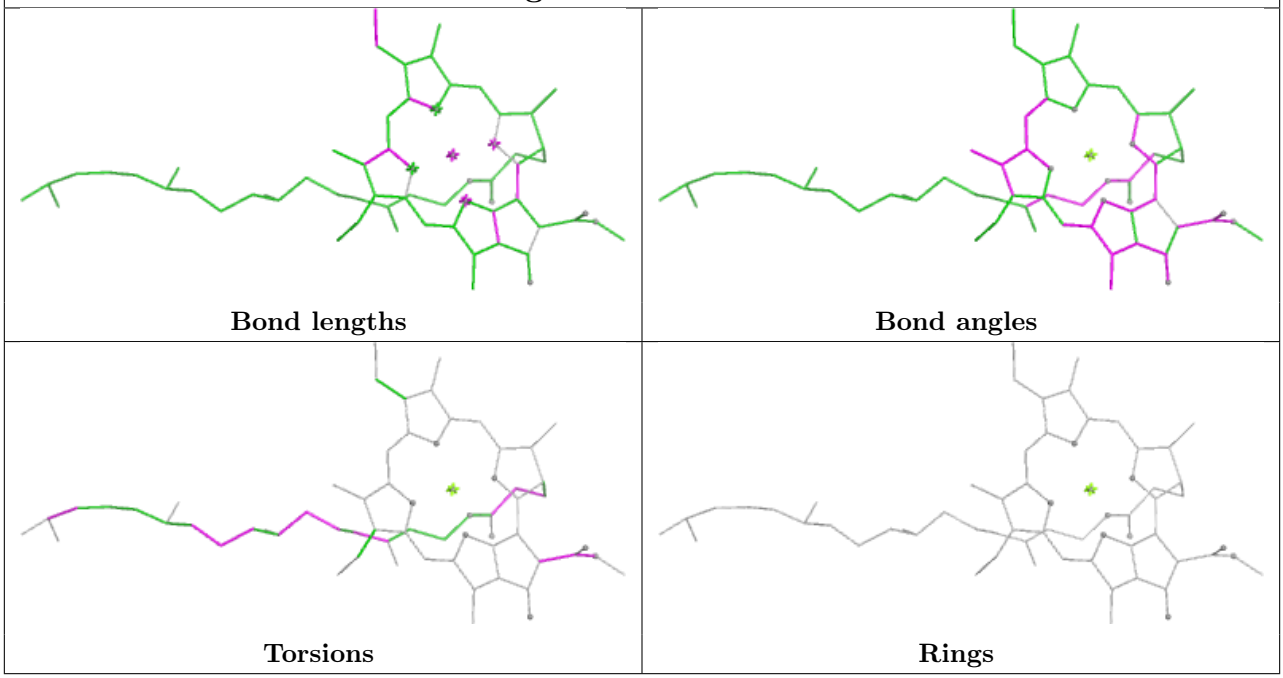


Torsions

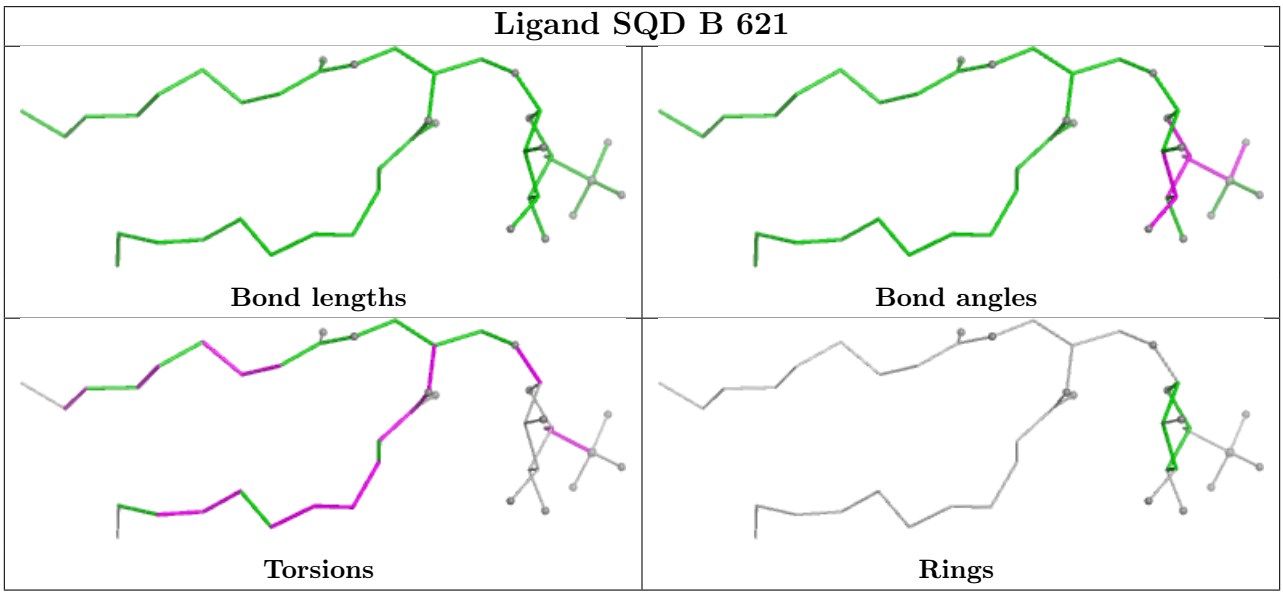


Rings

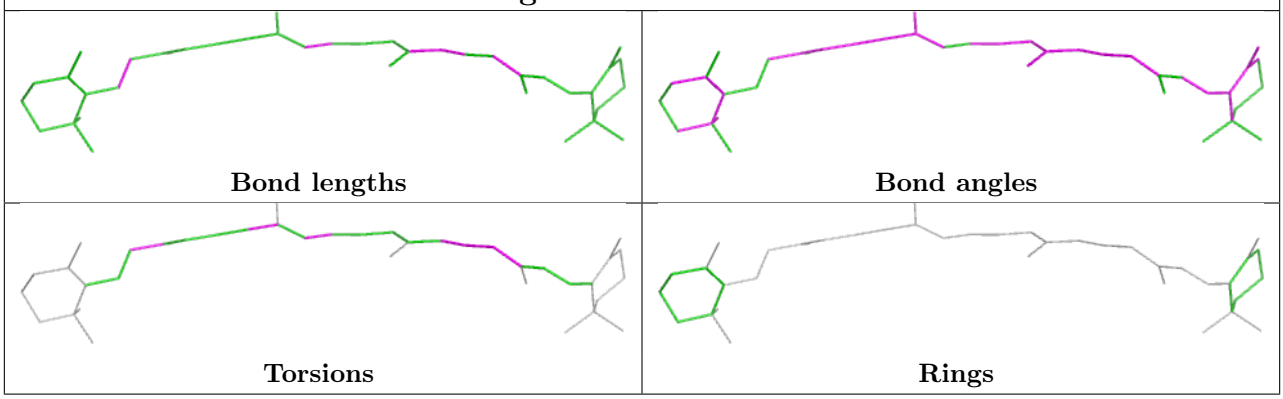
Ligand CLA B 615



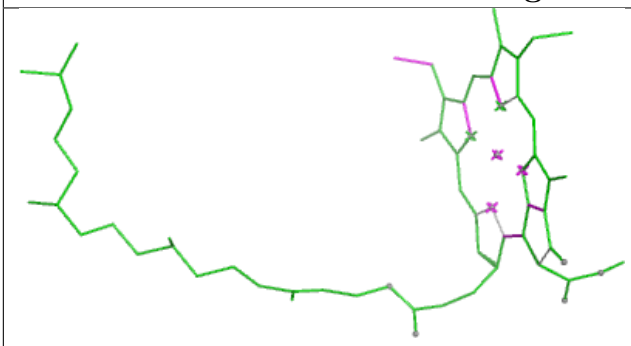
Ligand SQD B 621



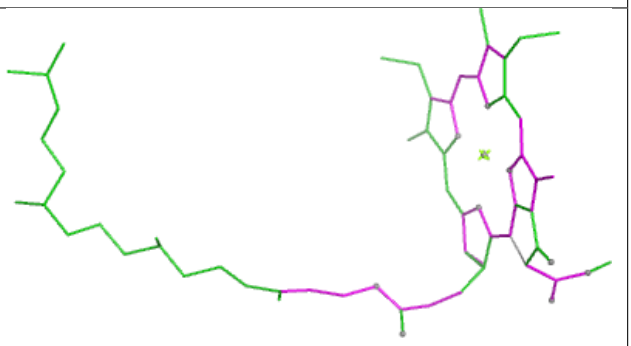
Ligand BCR c1 517



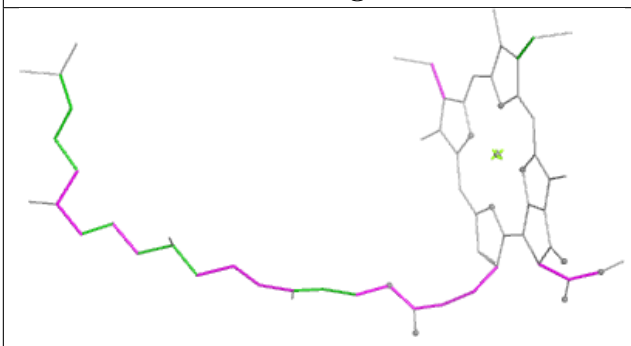
Ligand CLA B 610



Bond lengths



Bond angles

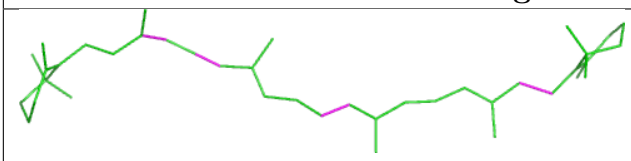


Torsions

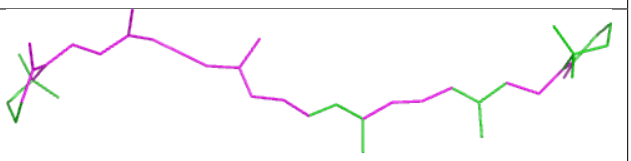


Rings

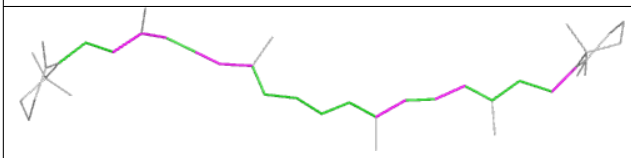
Ligand BCR C1 515



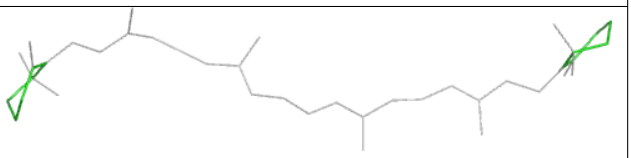
Bond lengths



Bond angles

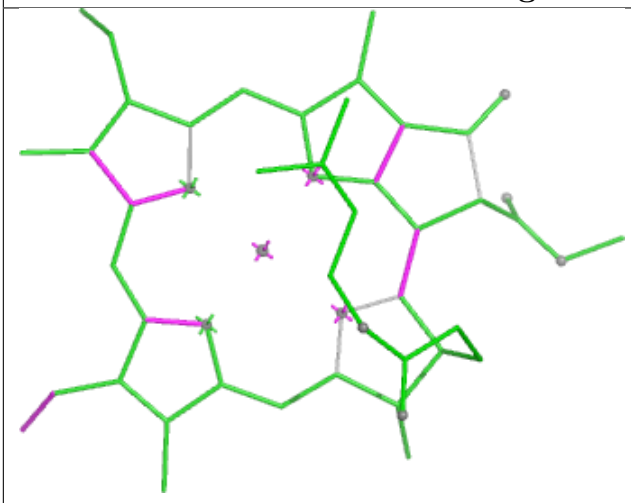


Torsions

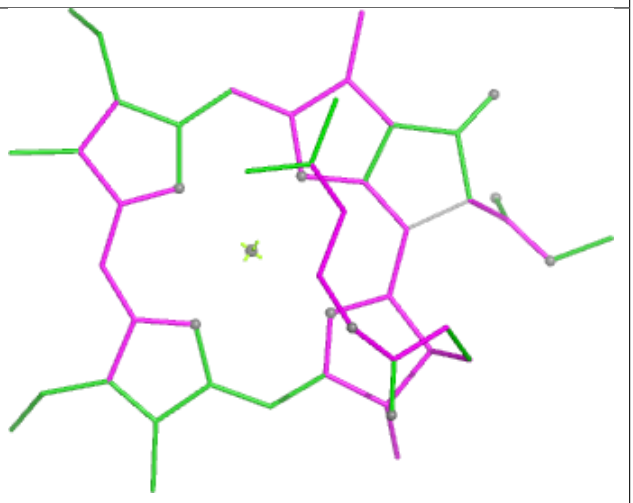


Rings

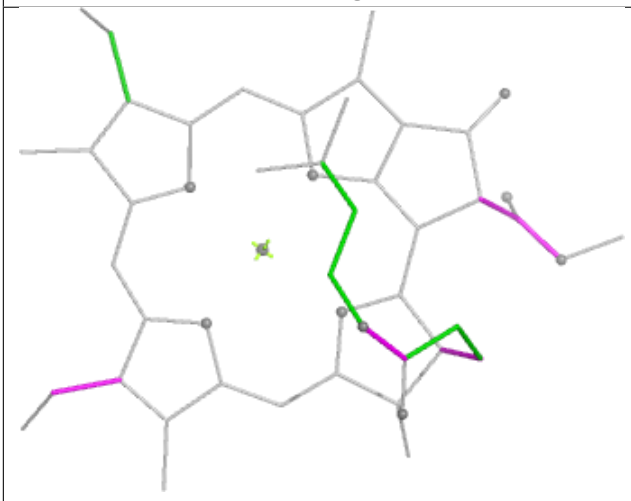
Ligand CLA S1 605



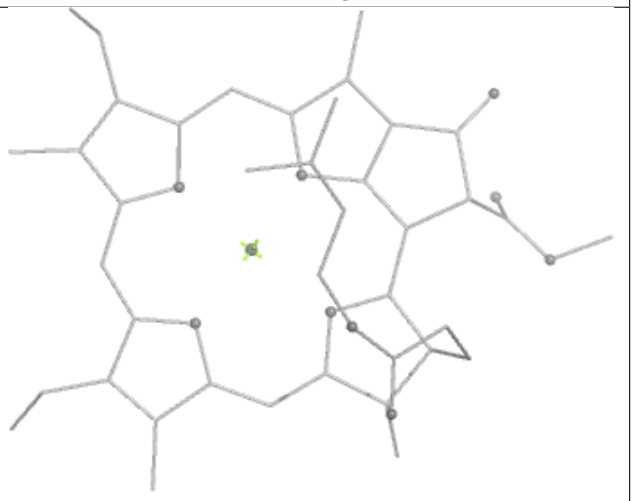
Bond lengths



Bond angles



Torsions



Rings

Ligand CLA Y1 614



Bond lengths



Bond angles

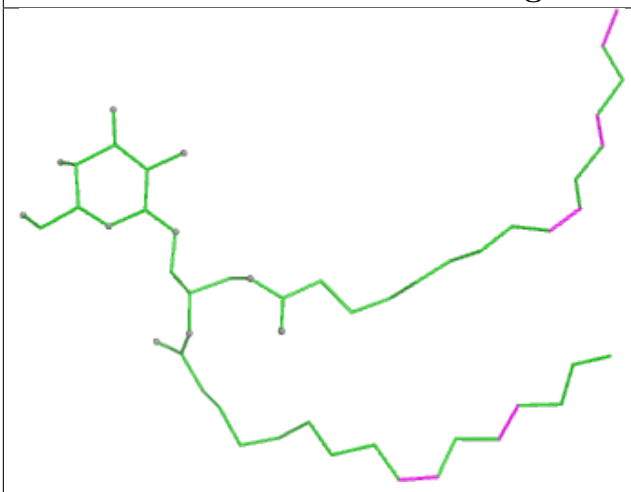


Torsions

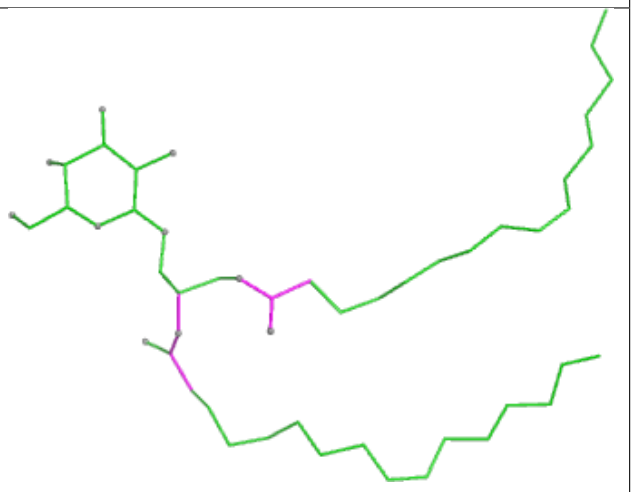


Rings

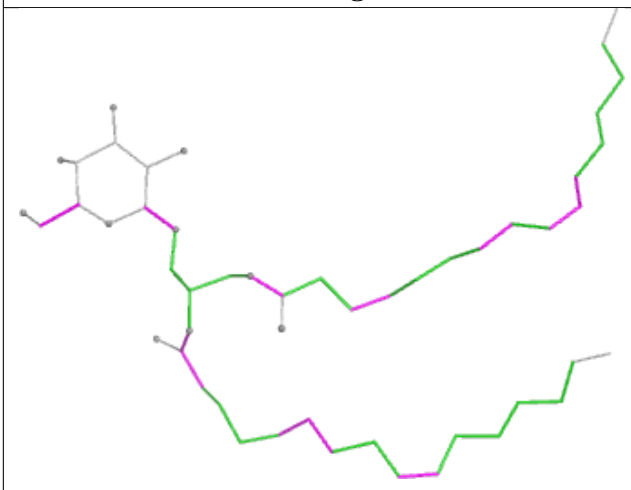
Ligand LMG c 521



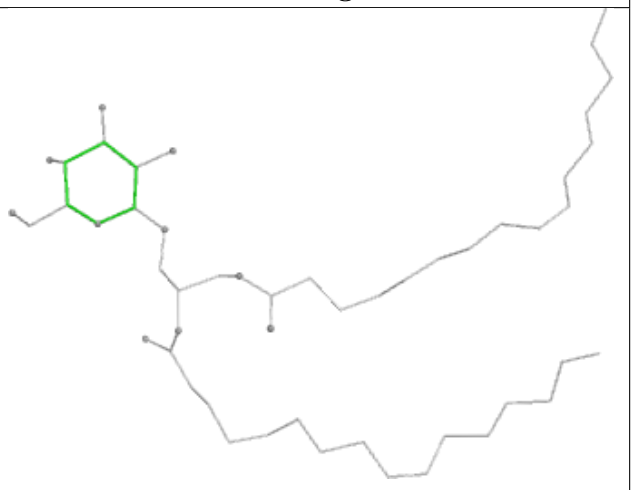
Bond lengths



Bond angles

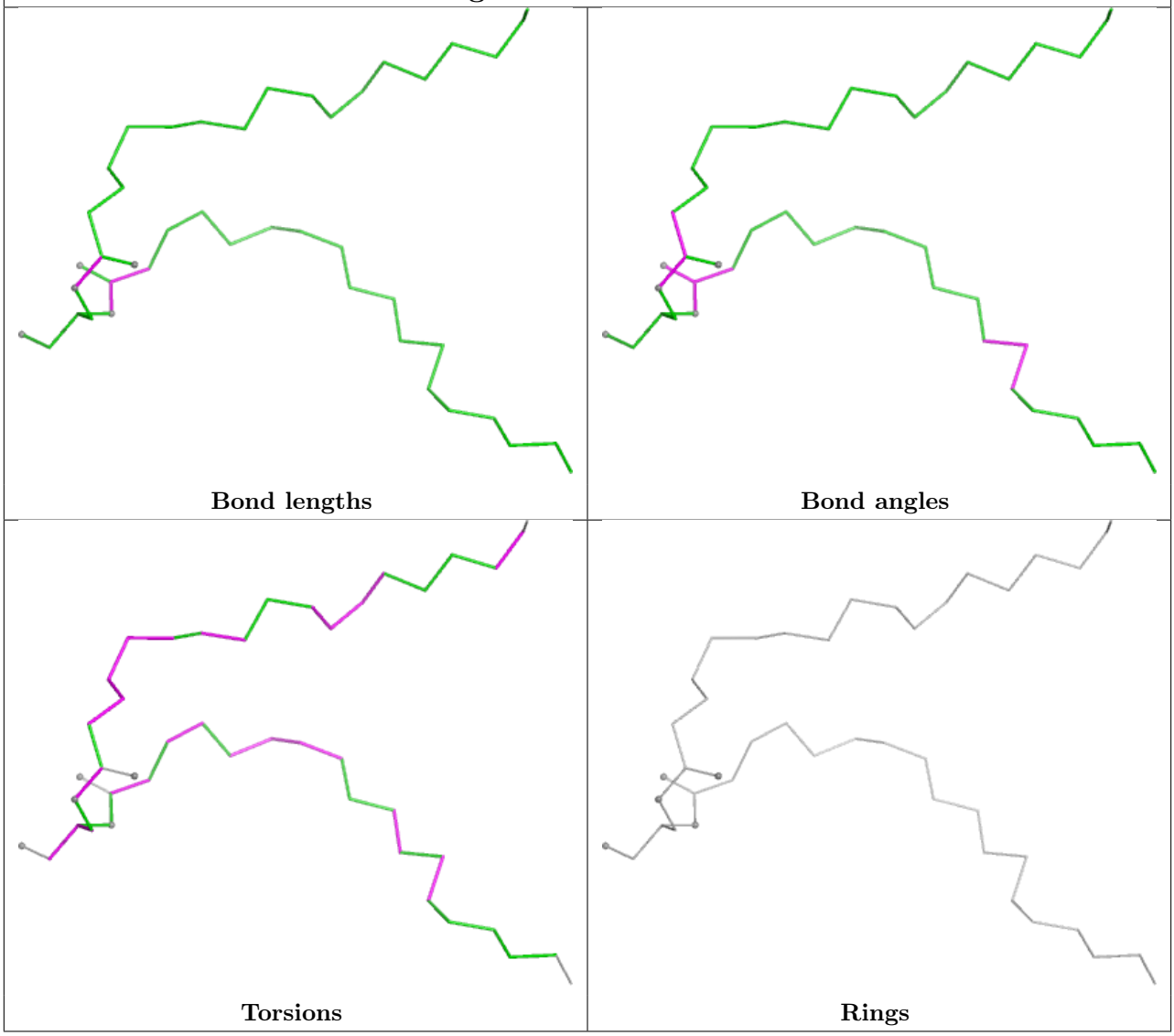


Torsions

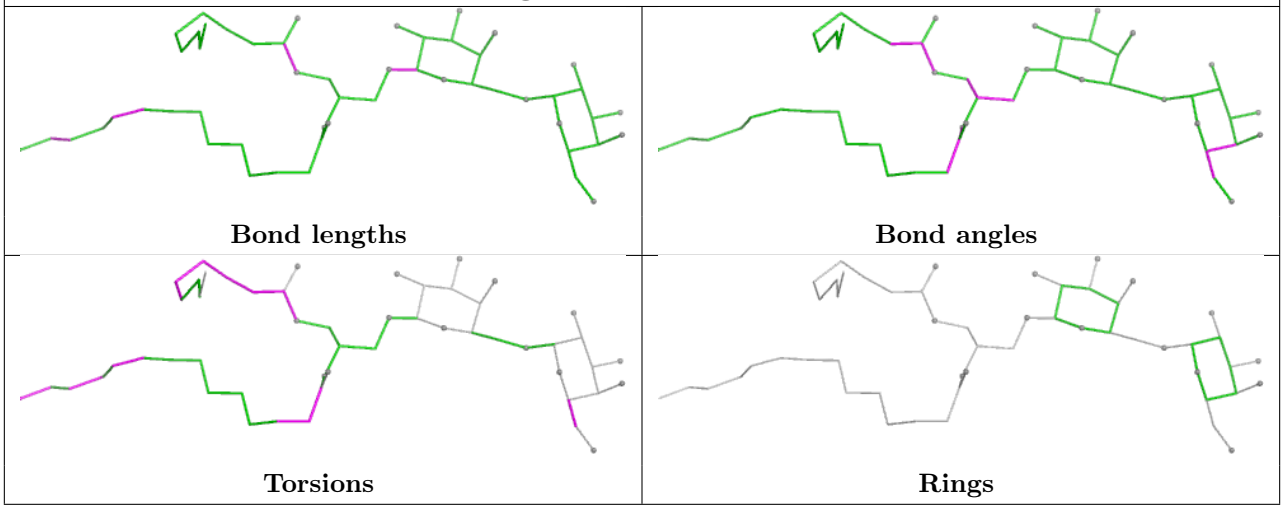


Rings

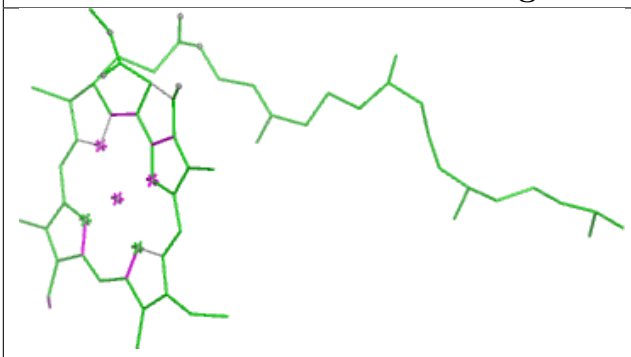
Ligand DGA C1 524



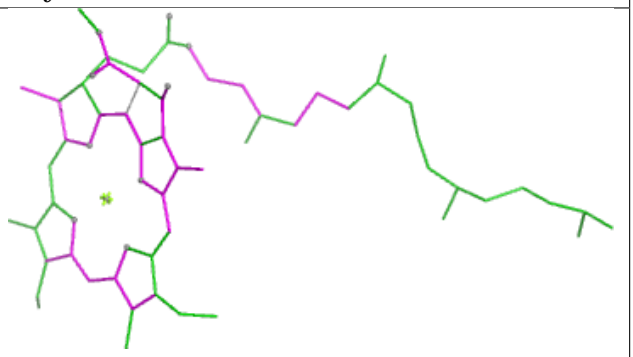
Ligand DGD c1 518



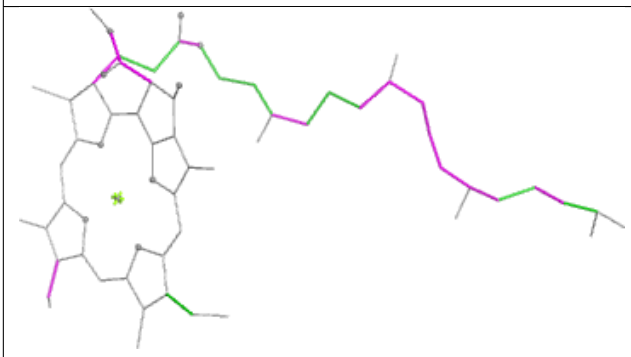
Ligand CLA y1 611



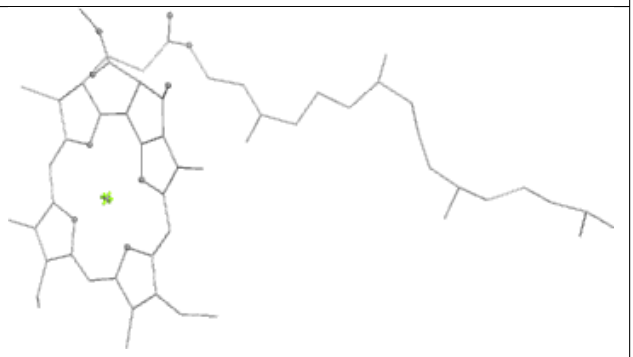
Bond lengths



Bond angles

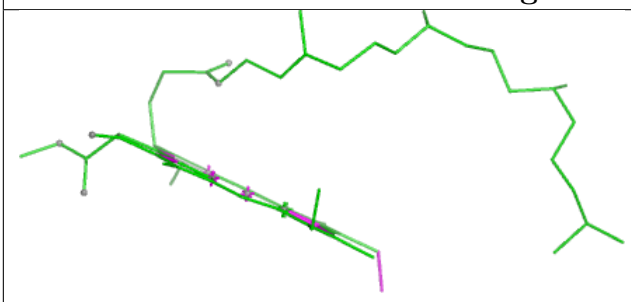


Torsions

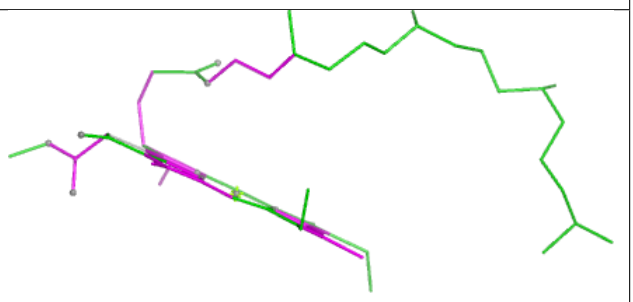


Rings

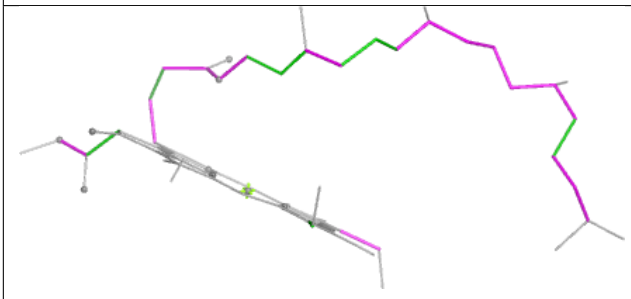
Ligand CLA c1 513



Bond lengths



Bond angles

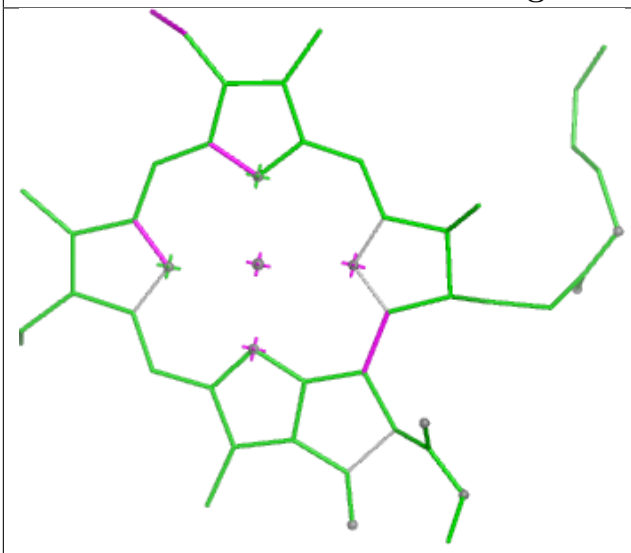


Torsions

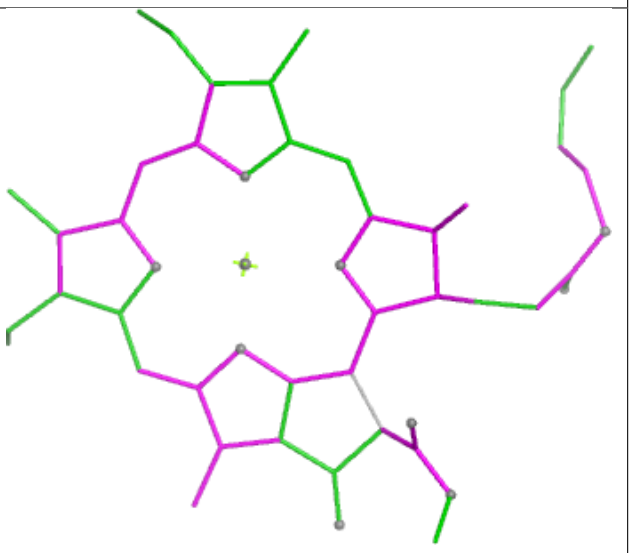


Rings

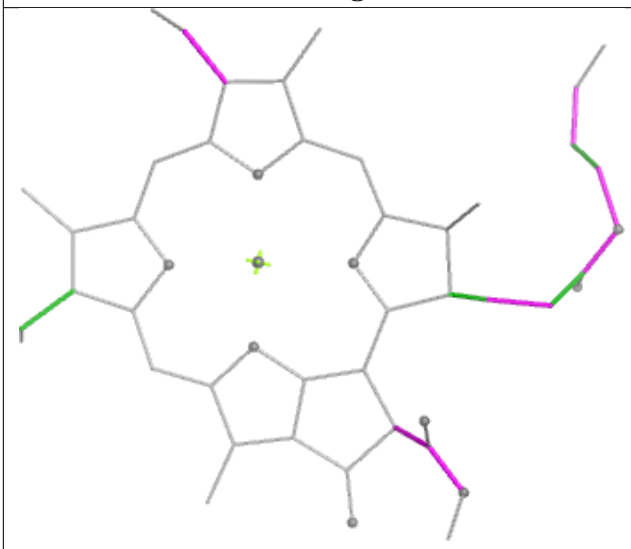
Ligand CLA n 611



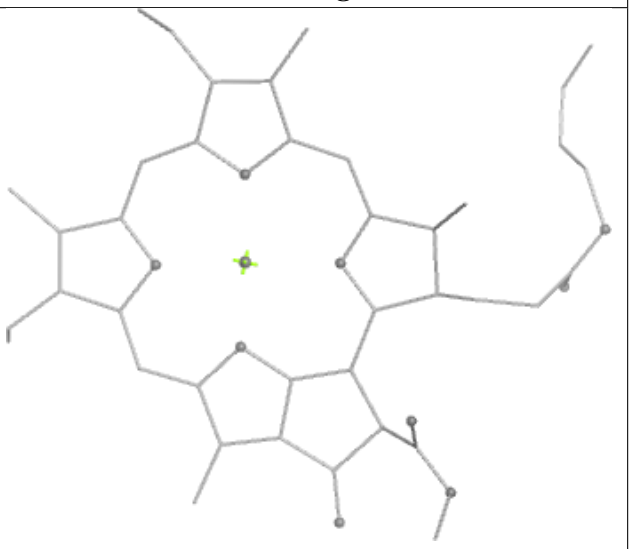
Bond lengths



Bond angles

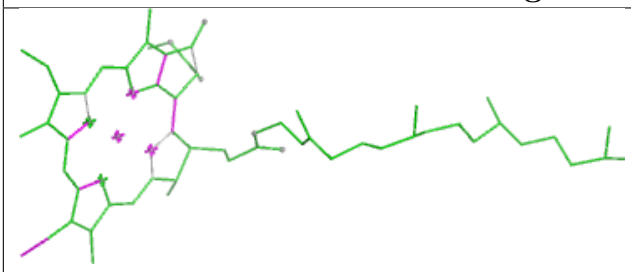


Torsions

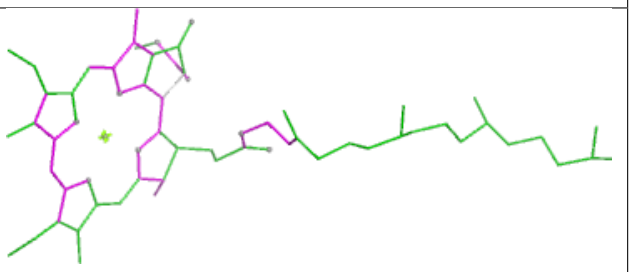


Rings

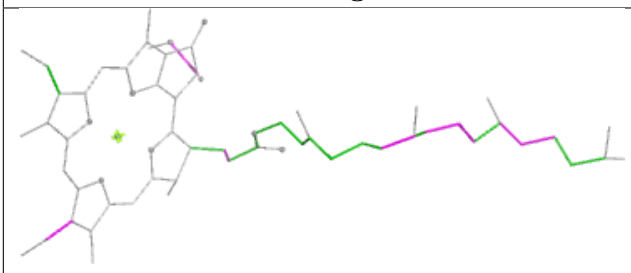
Ligand CLA C 502



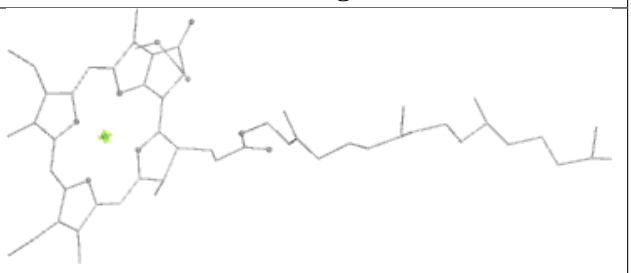
Bond lengths



Bond angles

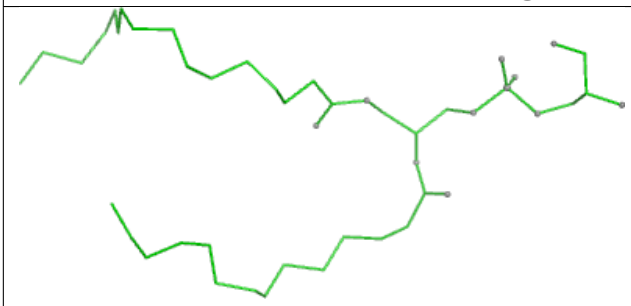


Torsions

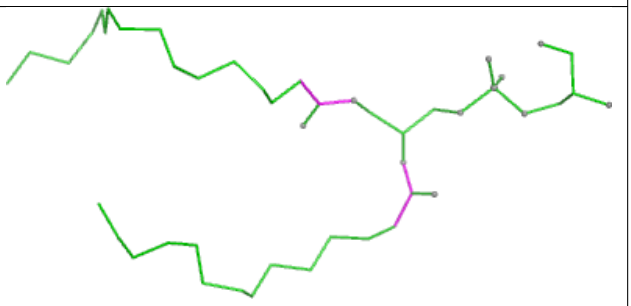


Rings

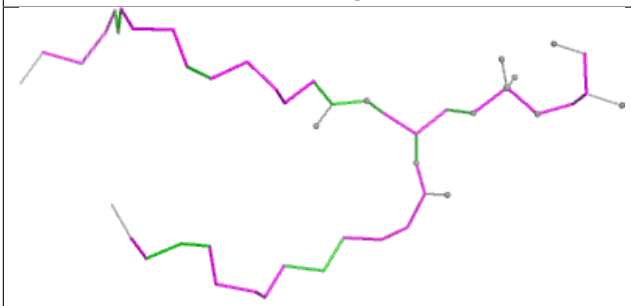
Ligand LHG c1 525



Bond lengths



Bond angles

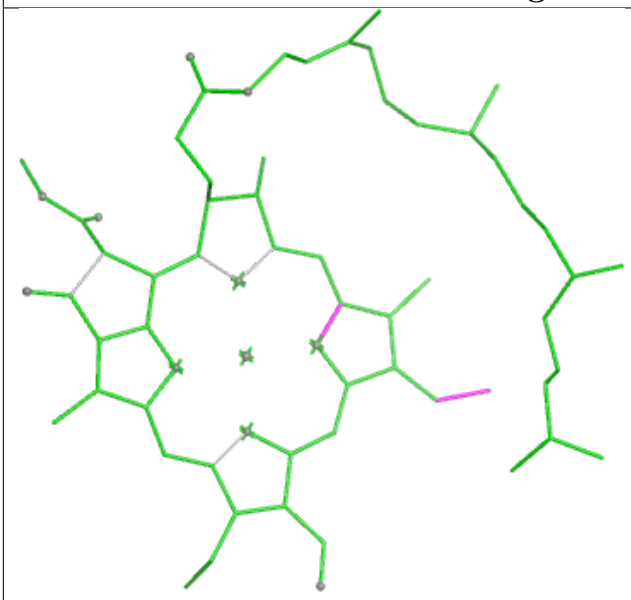


Torsions

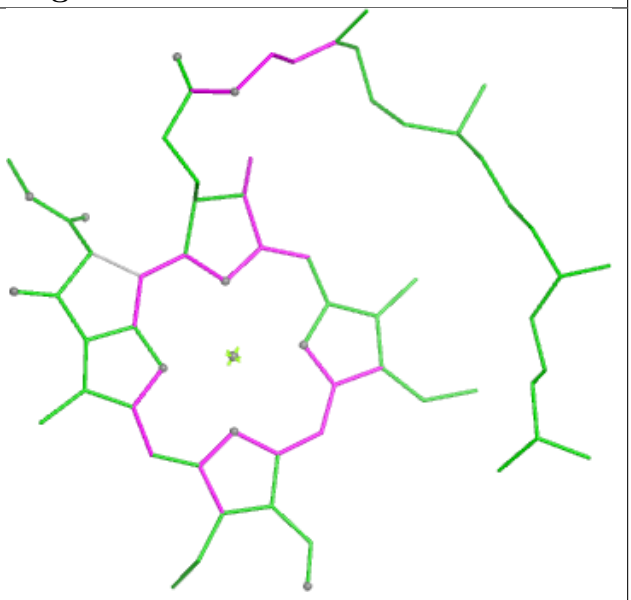


Rings

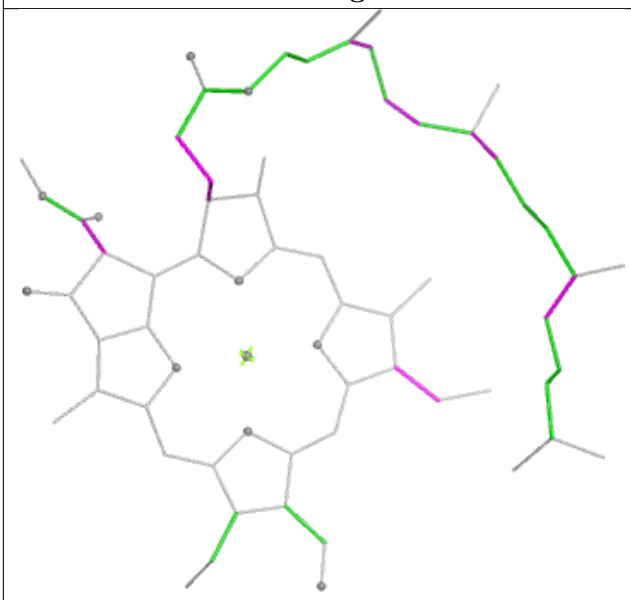
Ligand CHL g 607



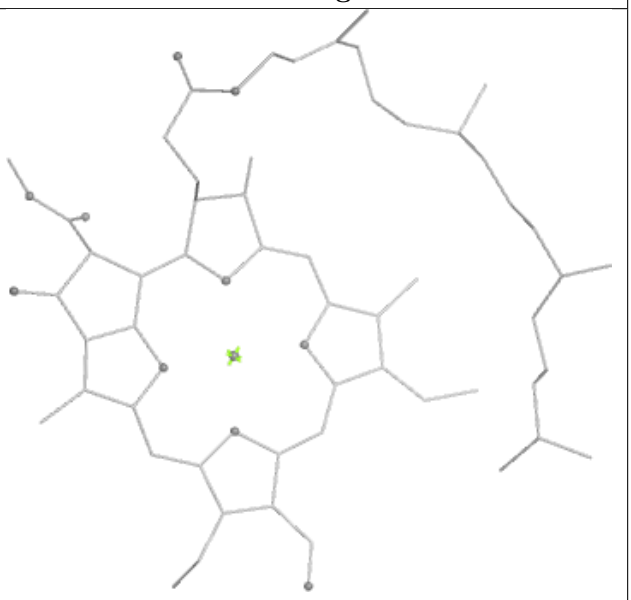
Bond lengths



Bond angles

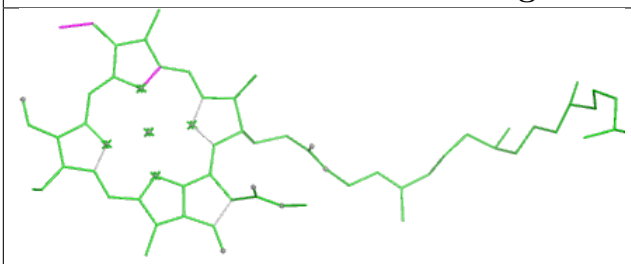


Torsions

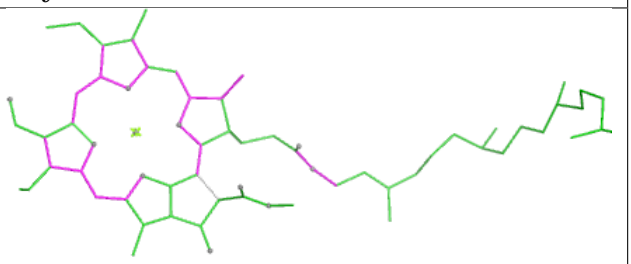


Rings

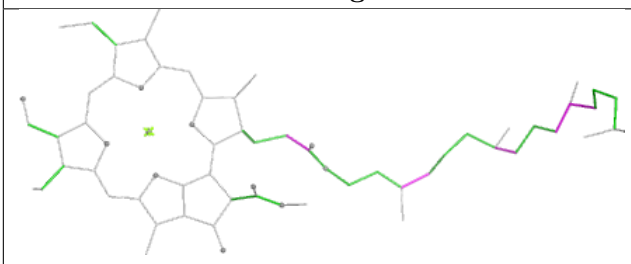
Ligand CHL y1 606



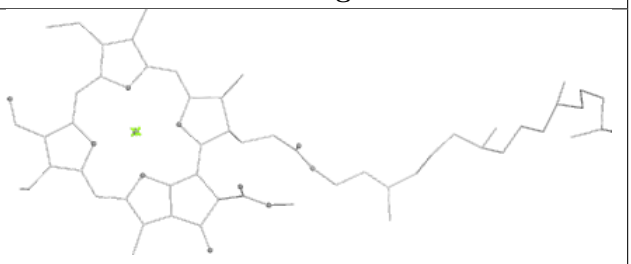
Bond lengths



Bond angles

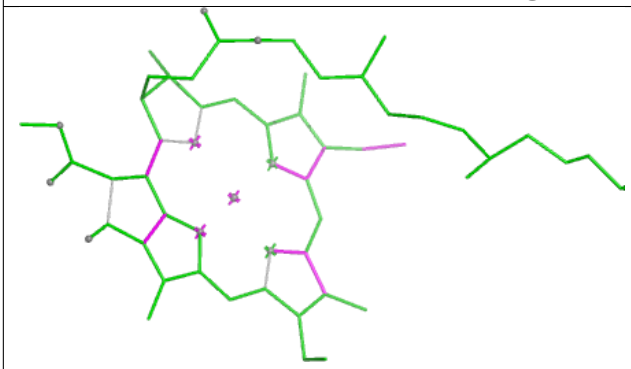


Torsions

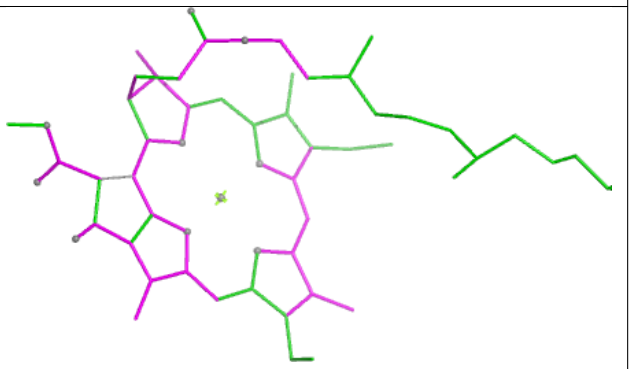


Rings

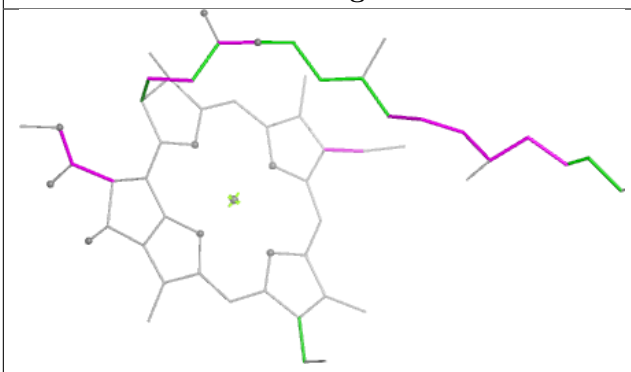
Ligand CLA R 610



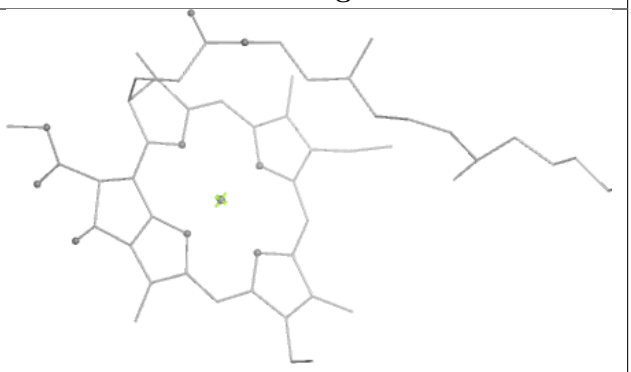
Bond lengths



Bond angles

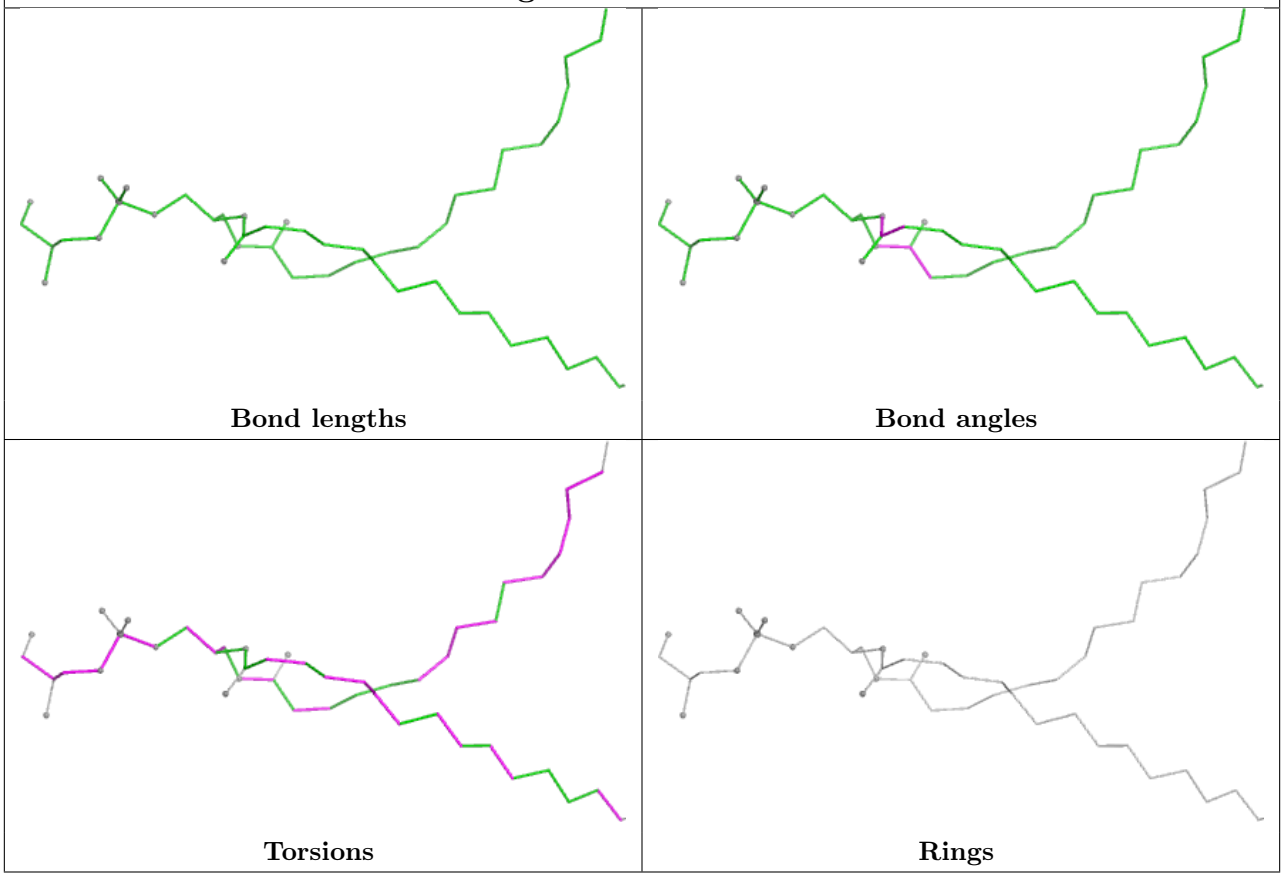


Torsions

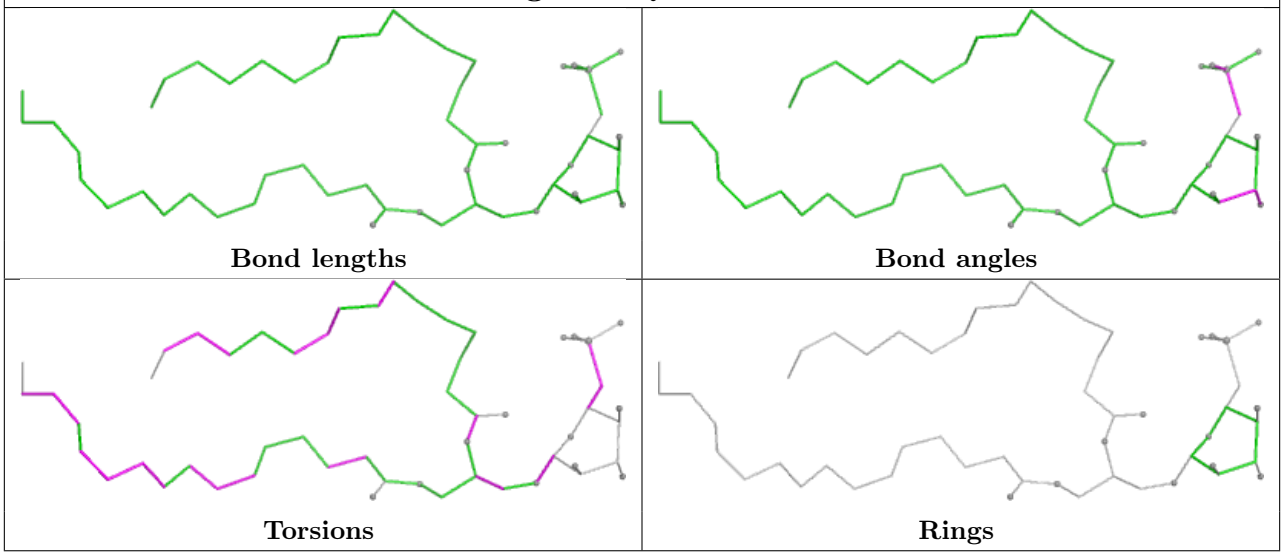


Rings

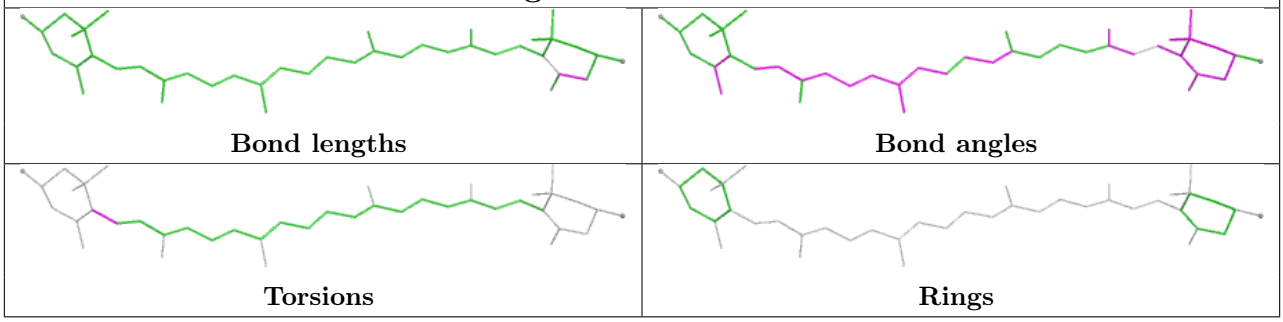
Ligand LHG d1 409



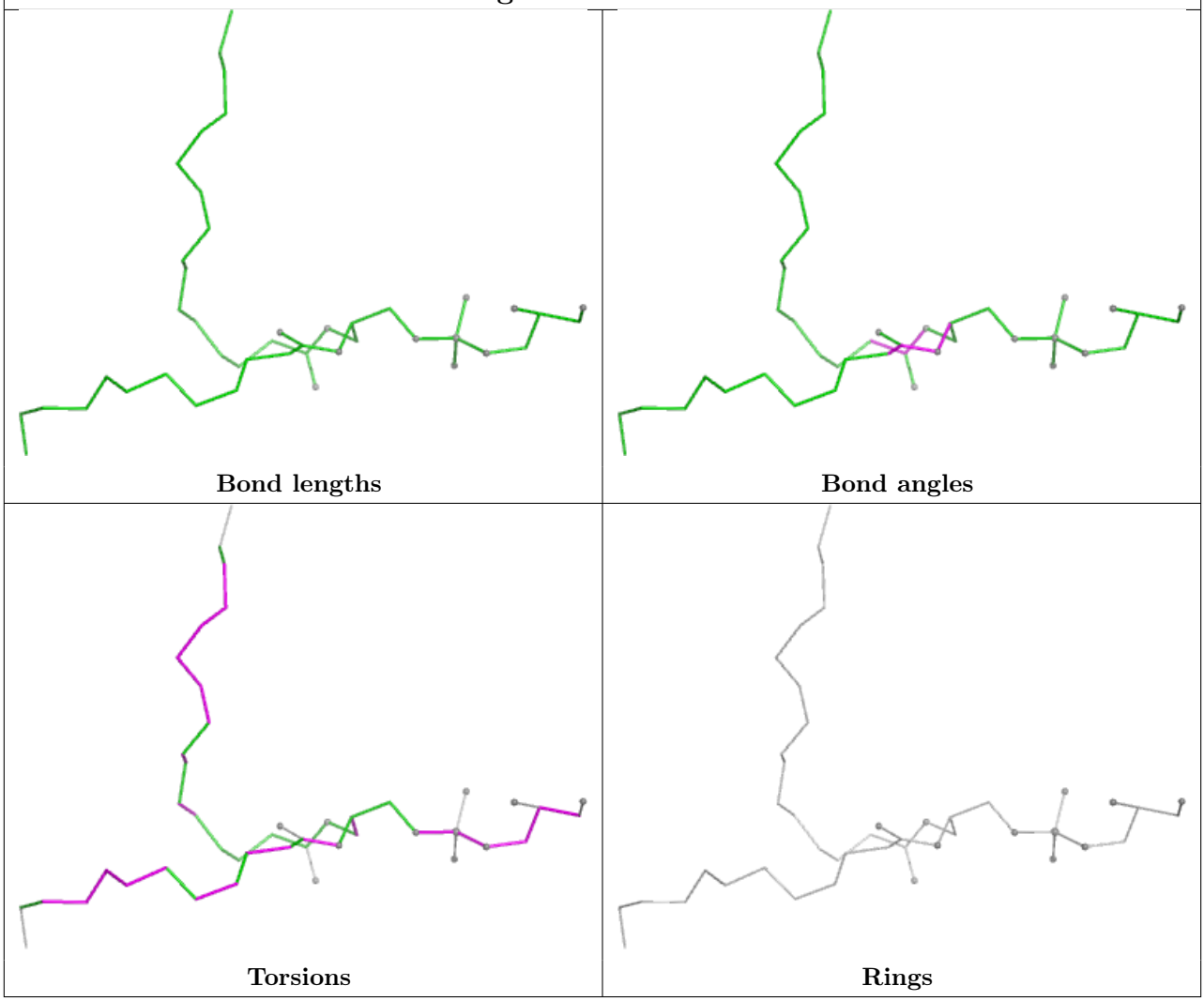
Ligand SQD B 626



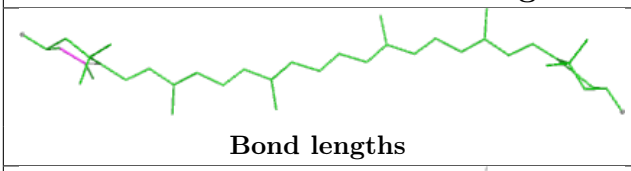
Ligand LUT N 620



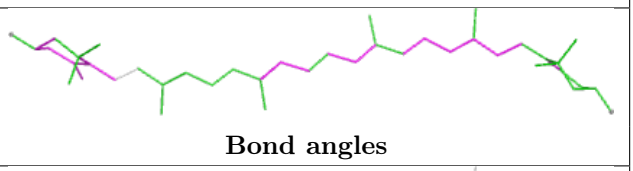
Ligand LHG s 624



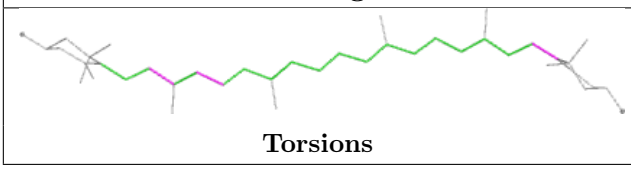
Ligand LUT n1 620



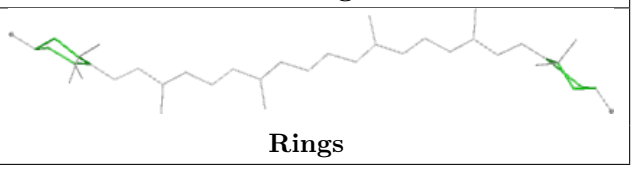
Bond lengths



Bond angles

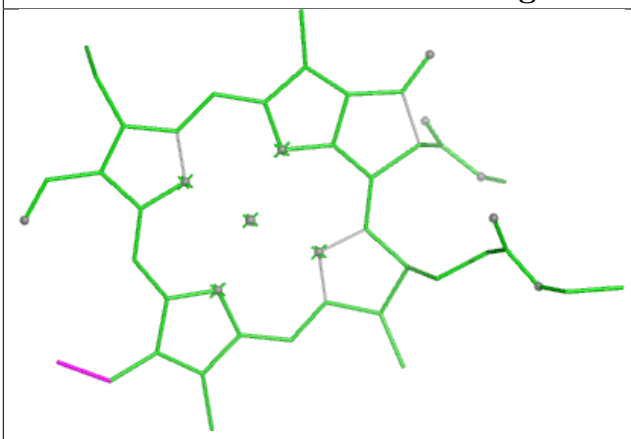


Torsions

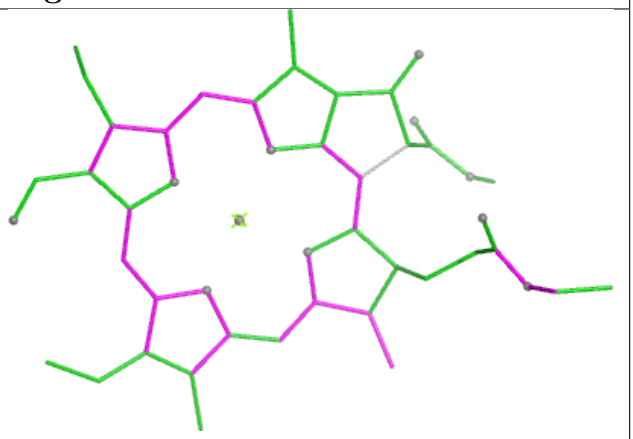


Rings

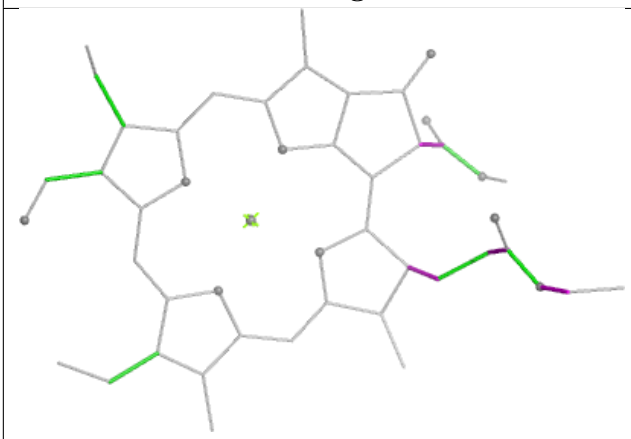
Ligand CHL g1 605



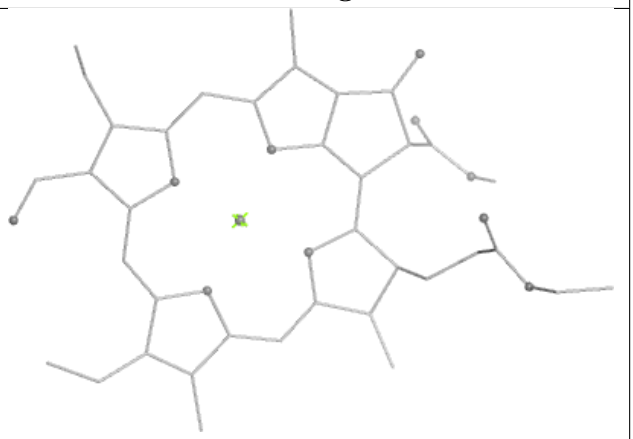
Bond lengths



Bond angles

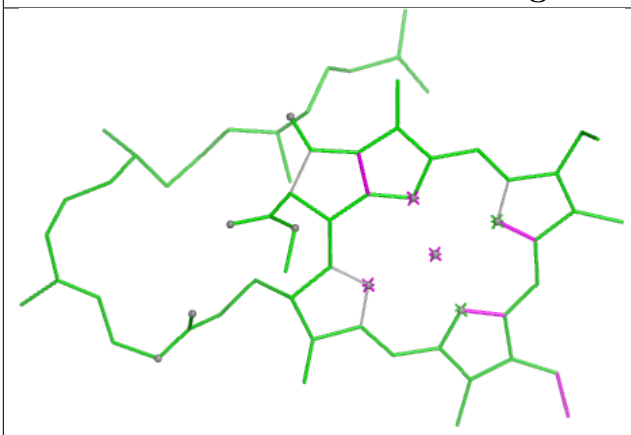


Torsions

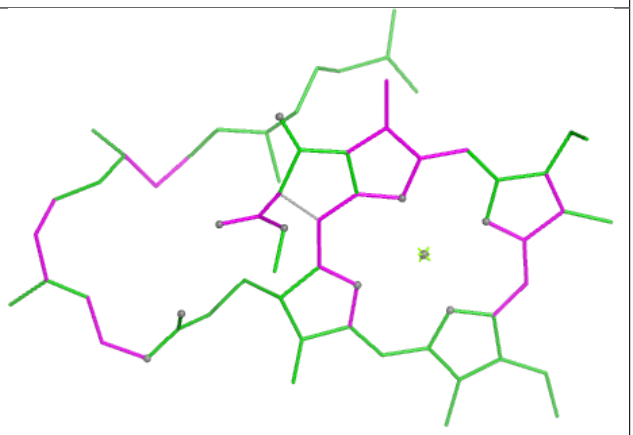


Rings

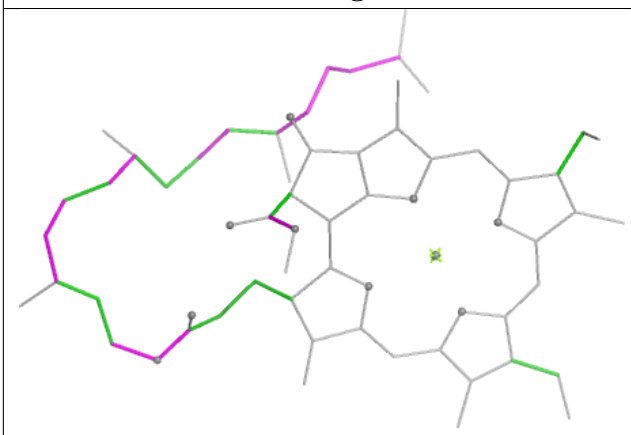
Ligand CLA c 509



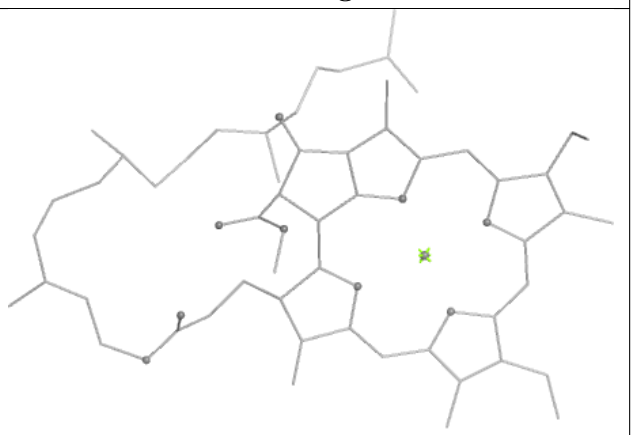
Bond lengths



Bond angles

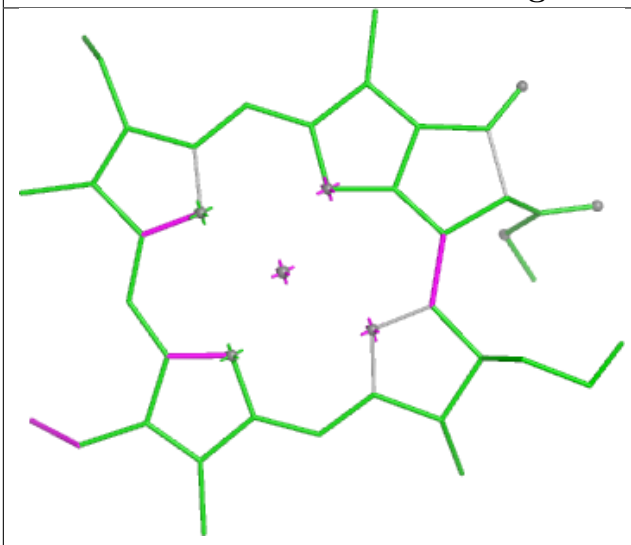


Torsions

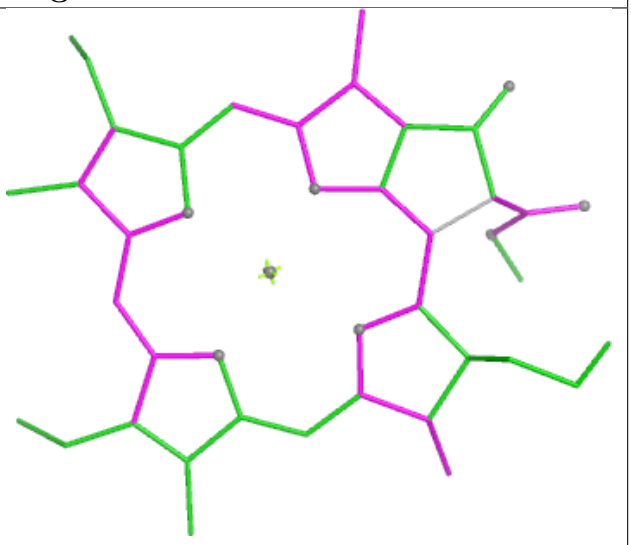


Rings

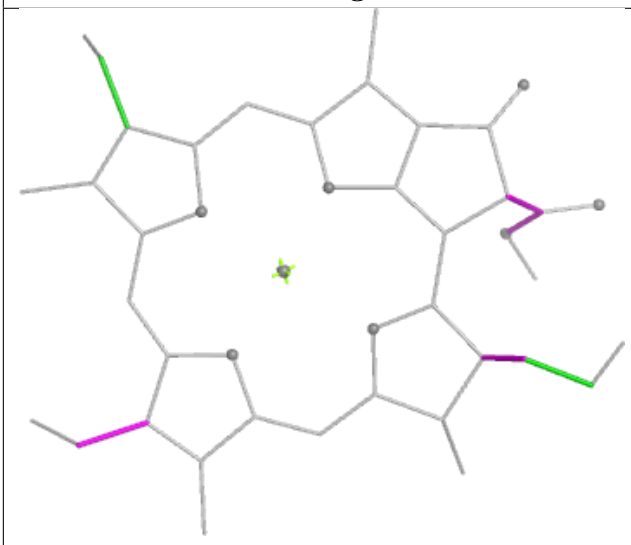
Ligand CLA g 612



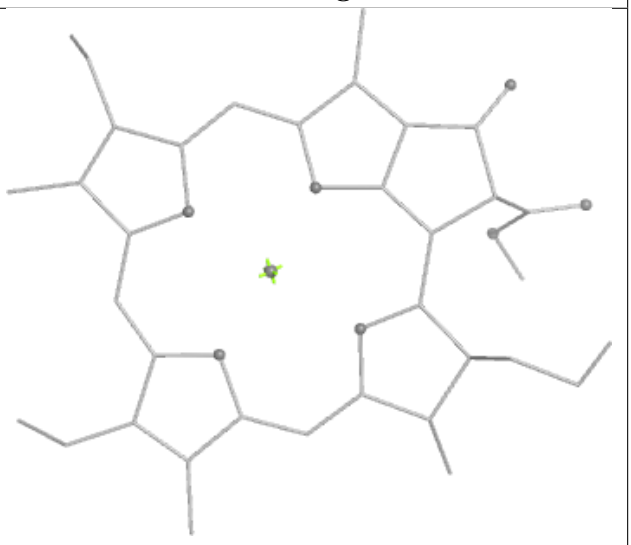
Bond lengths



Bond angles

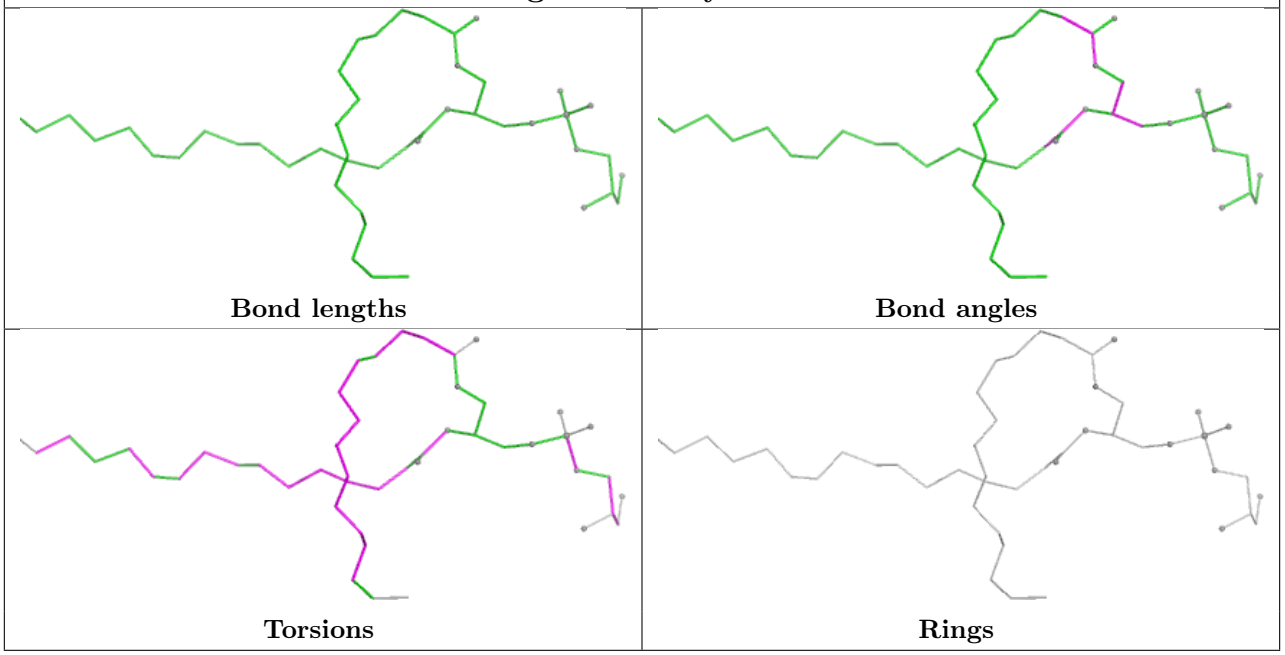


Torsions

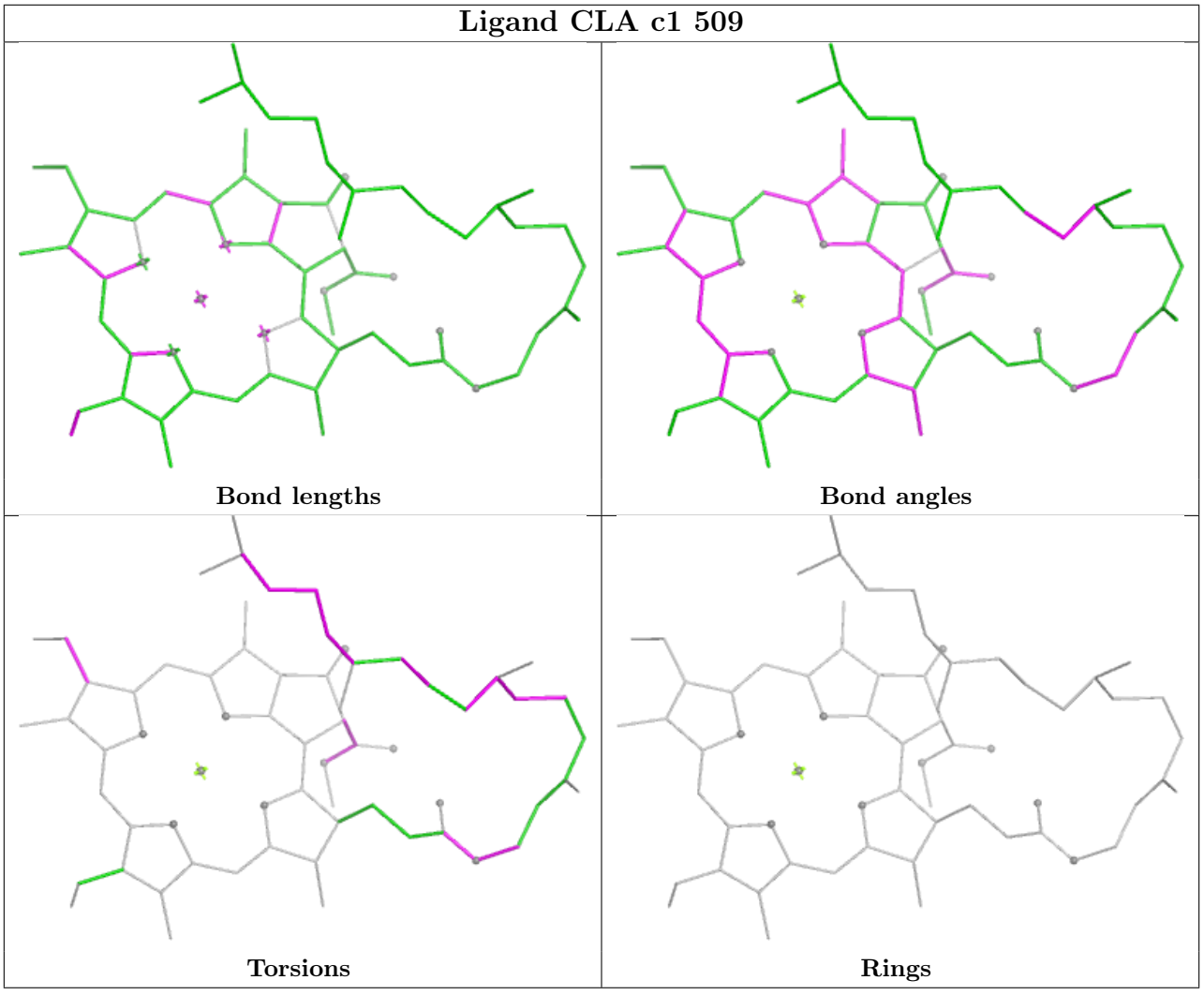


Rings

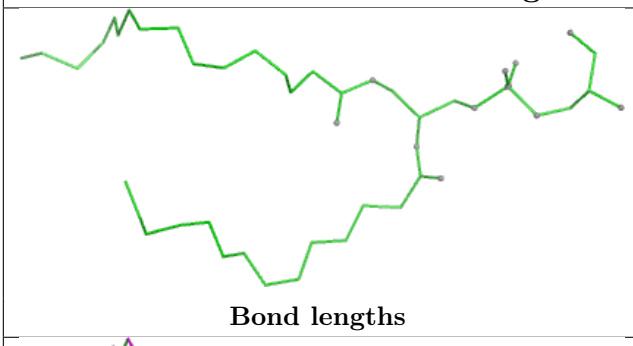
Ligand LHG y 624



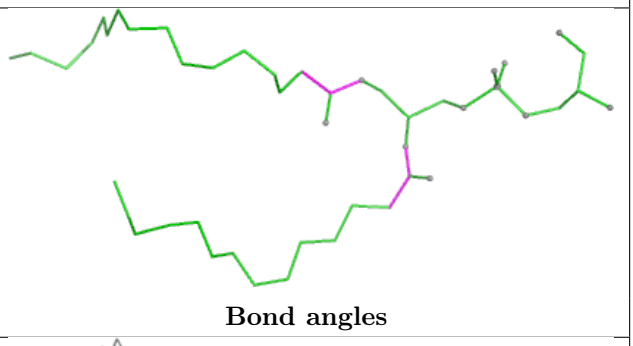
Ligand CLA c1 509



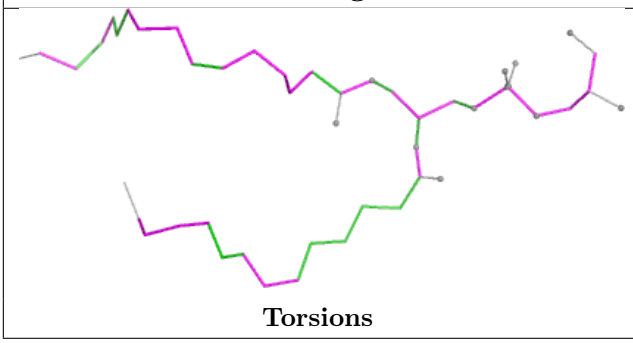
Ligand LHG C 525



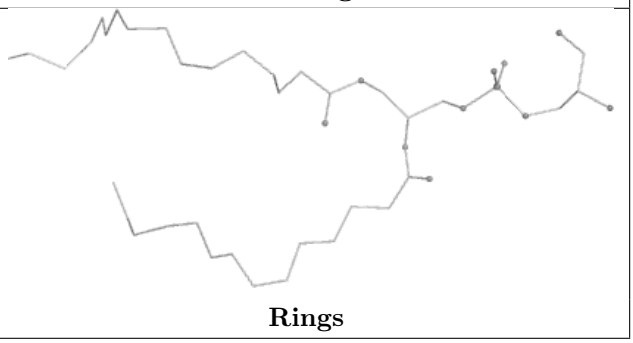
Bond lengths



Bond angles

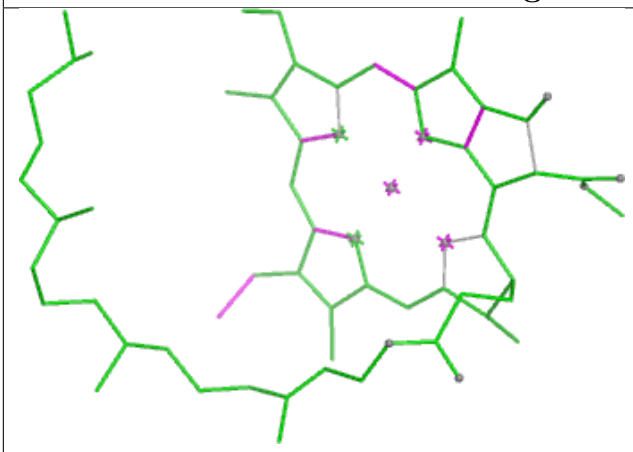


Torsions

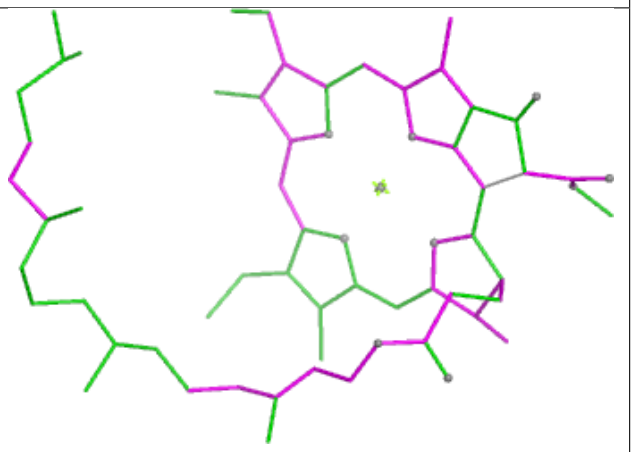


Rings

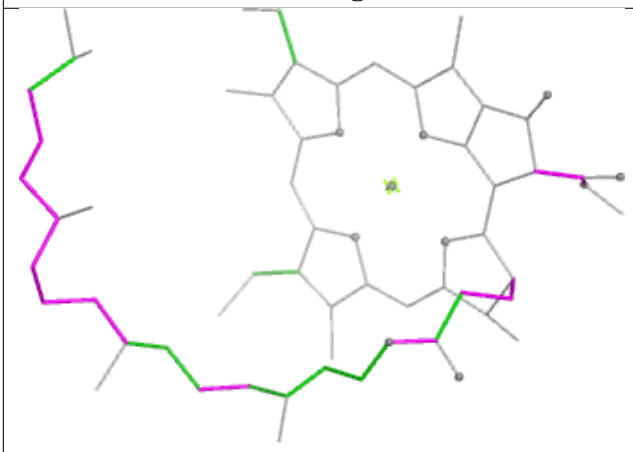
Ligand CLA Y 602



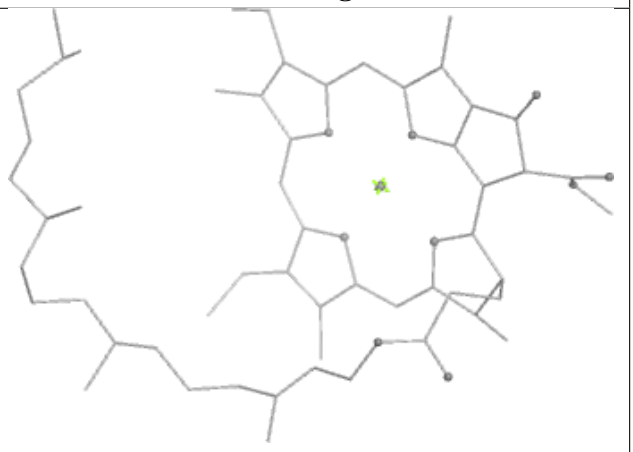
Bond lengths



Bond angles

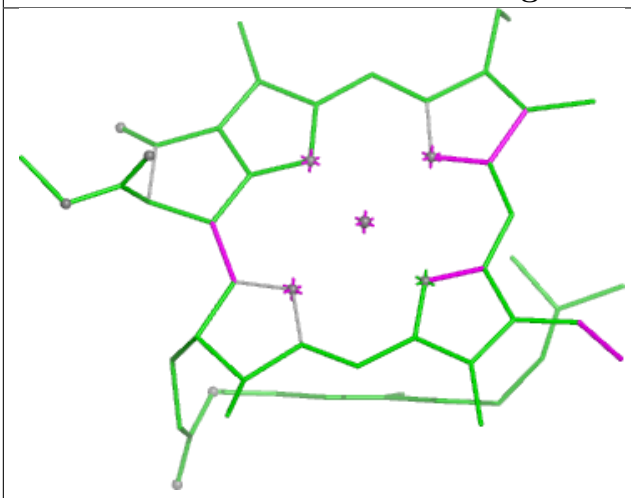


Torsions

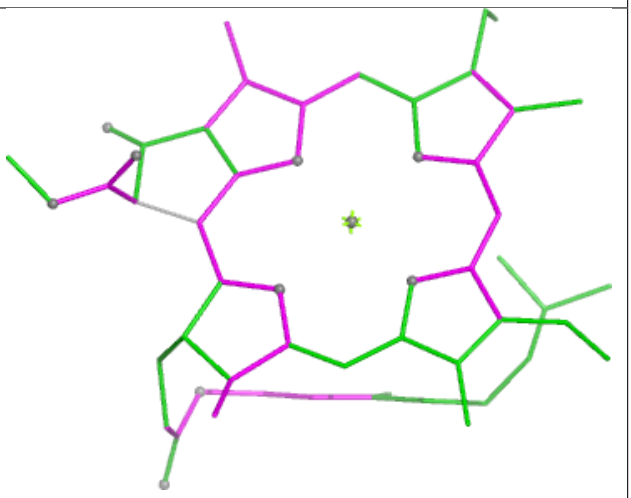


Rings

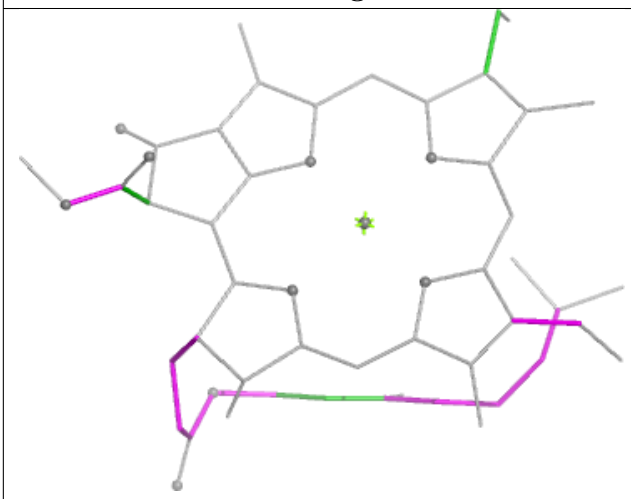
Ligand CLA s1 614



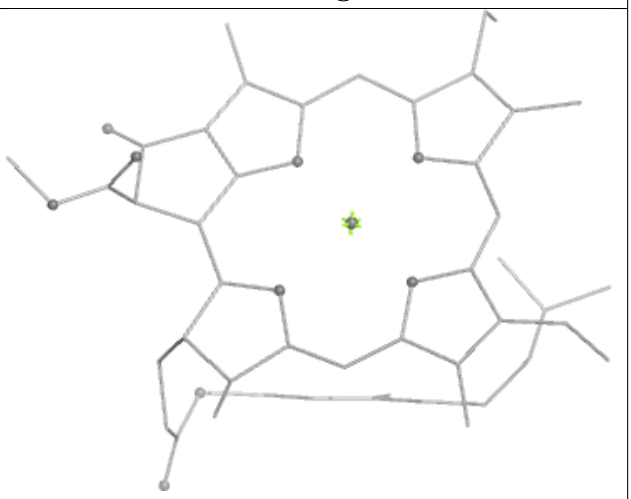
Bond lengths



Bond angles

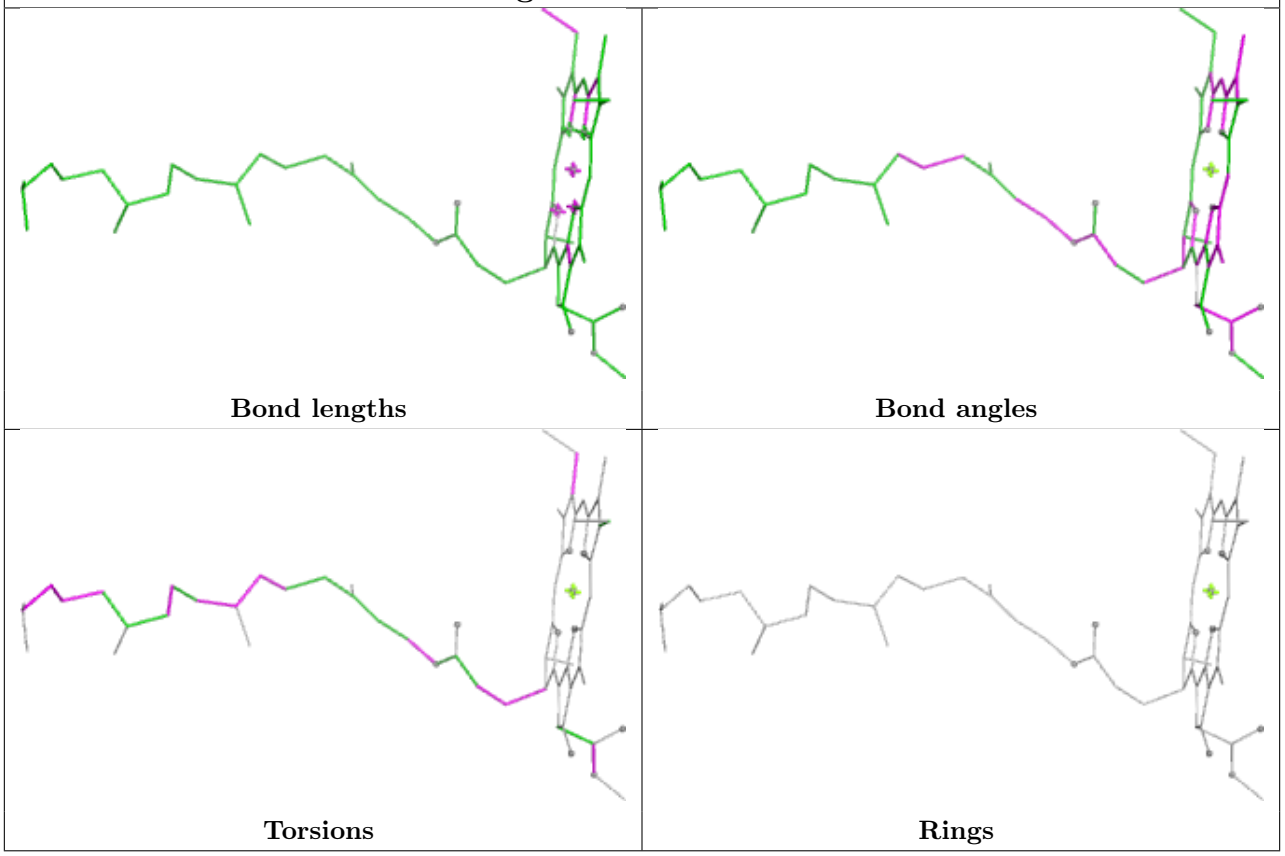


Torsions

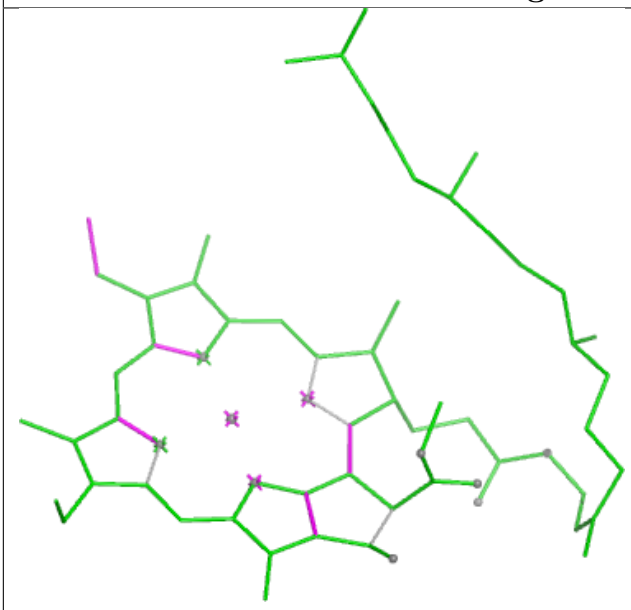


Rings

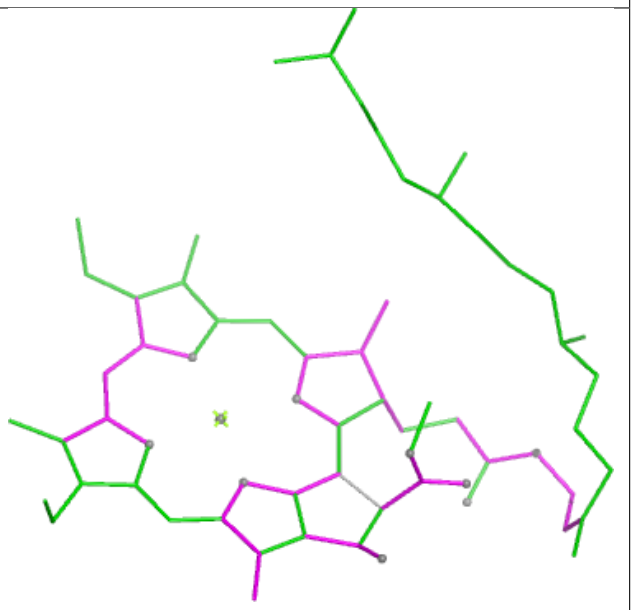
Ligand CLA B1 607



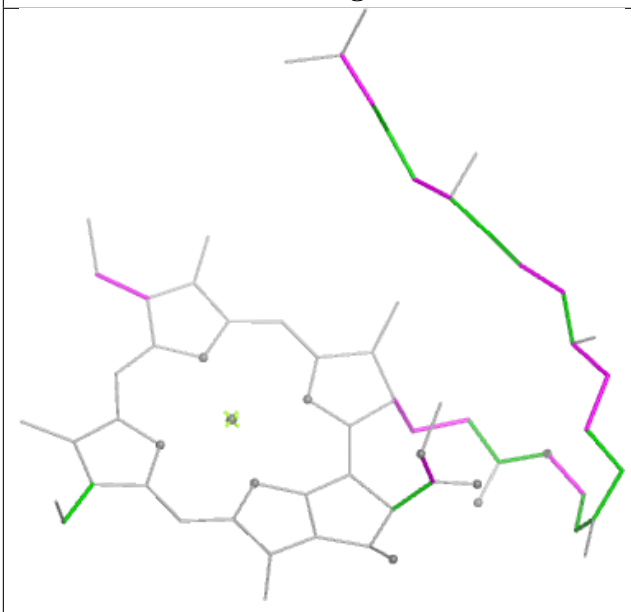
Ligand CLA b 617



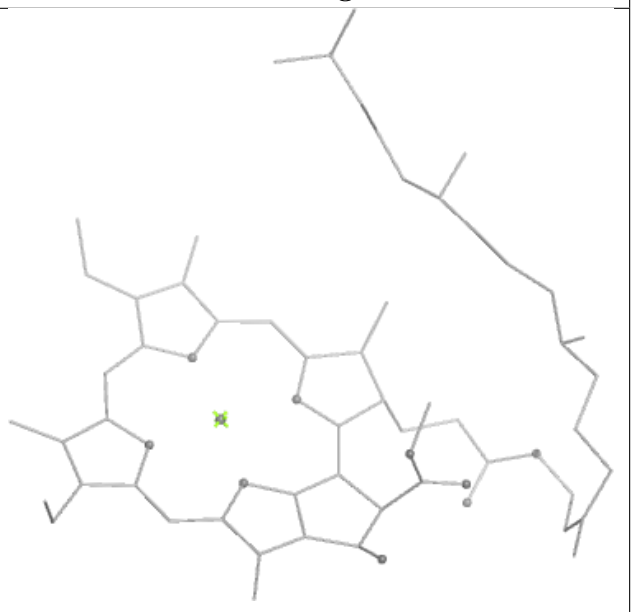
Bond lengths



Bond angles

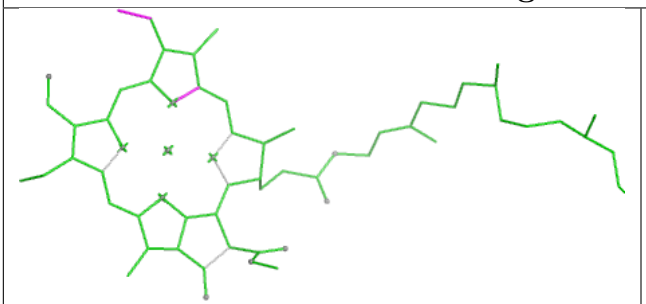


Torsions

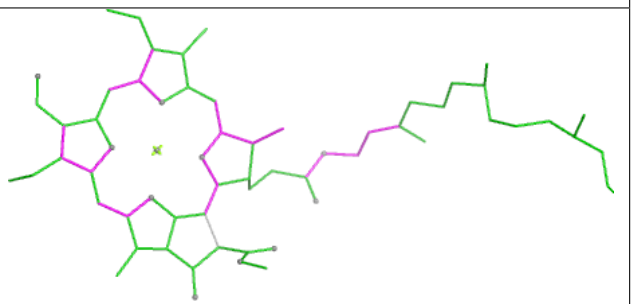


Rings

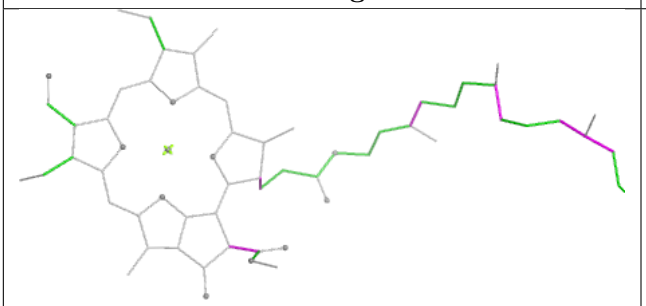
Ligand CHL n1 601



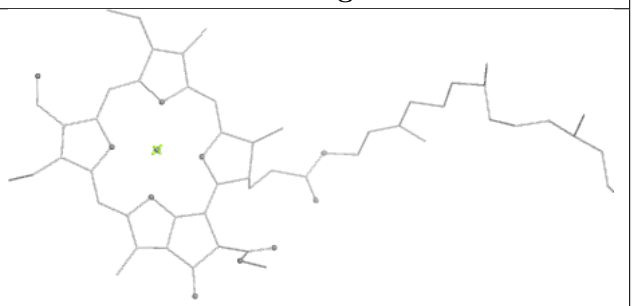
Bond lengths



Bond angles

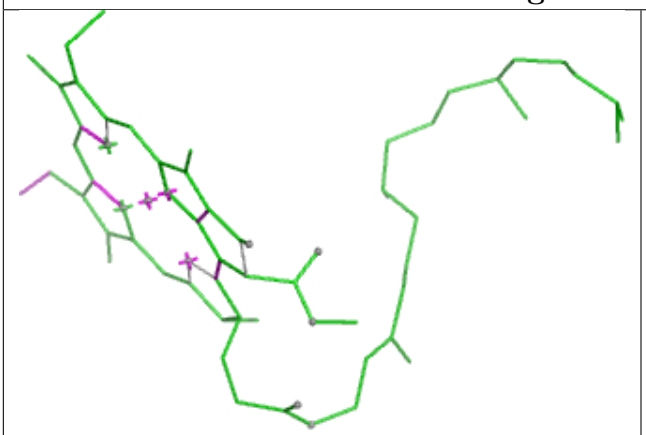


Torsions

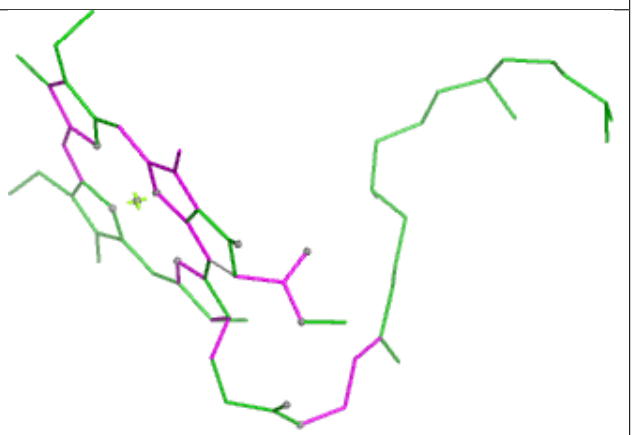


Rings

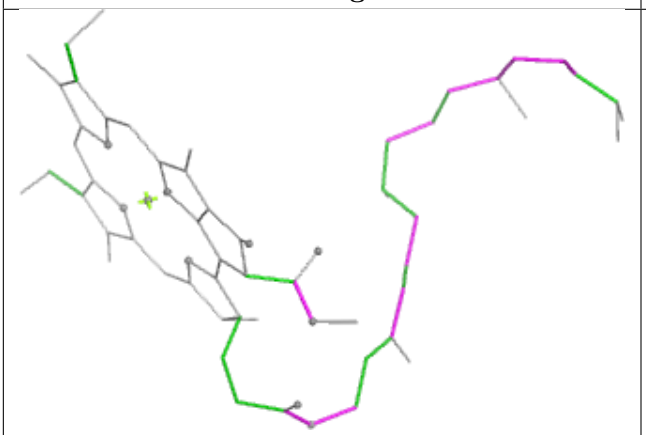
Ligand CLA b 614



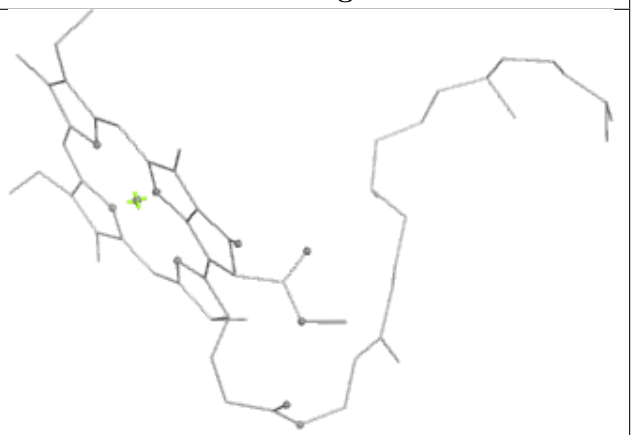
Bond lengths



Bond angles

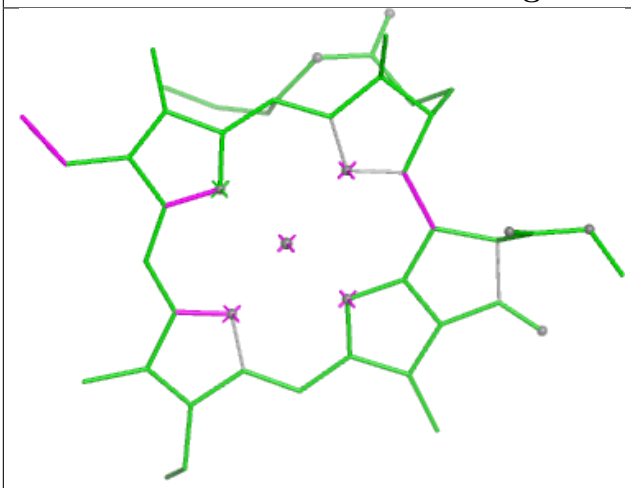


Torsions

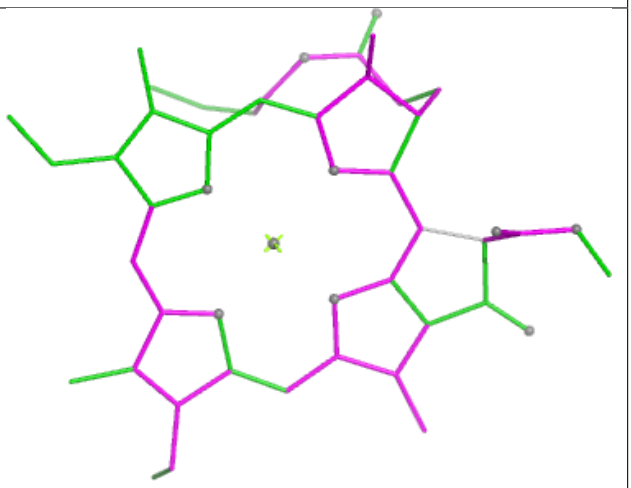


Rings

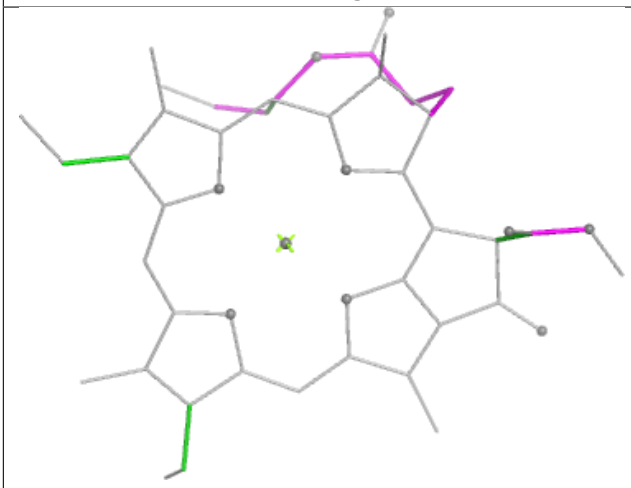
Ligand CLA G 614



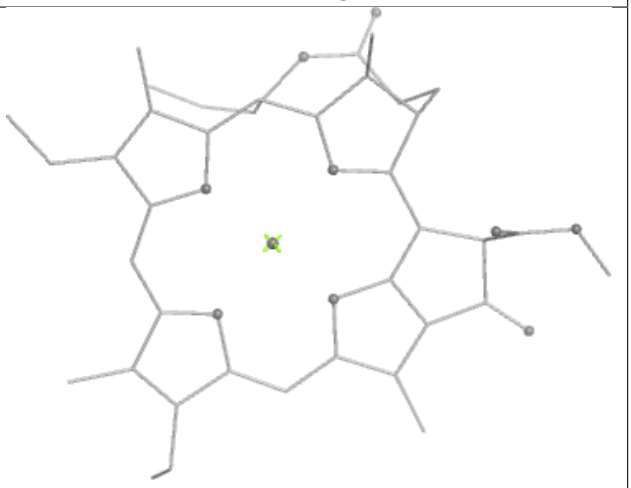
Bond lengths



Bond angles



Torsions



Rings

Ligand LPX S 625



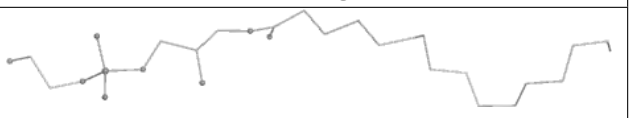
Bond lengths



Bond angles

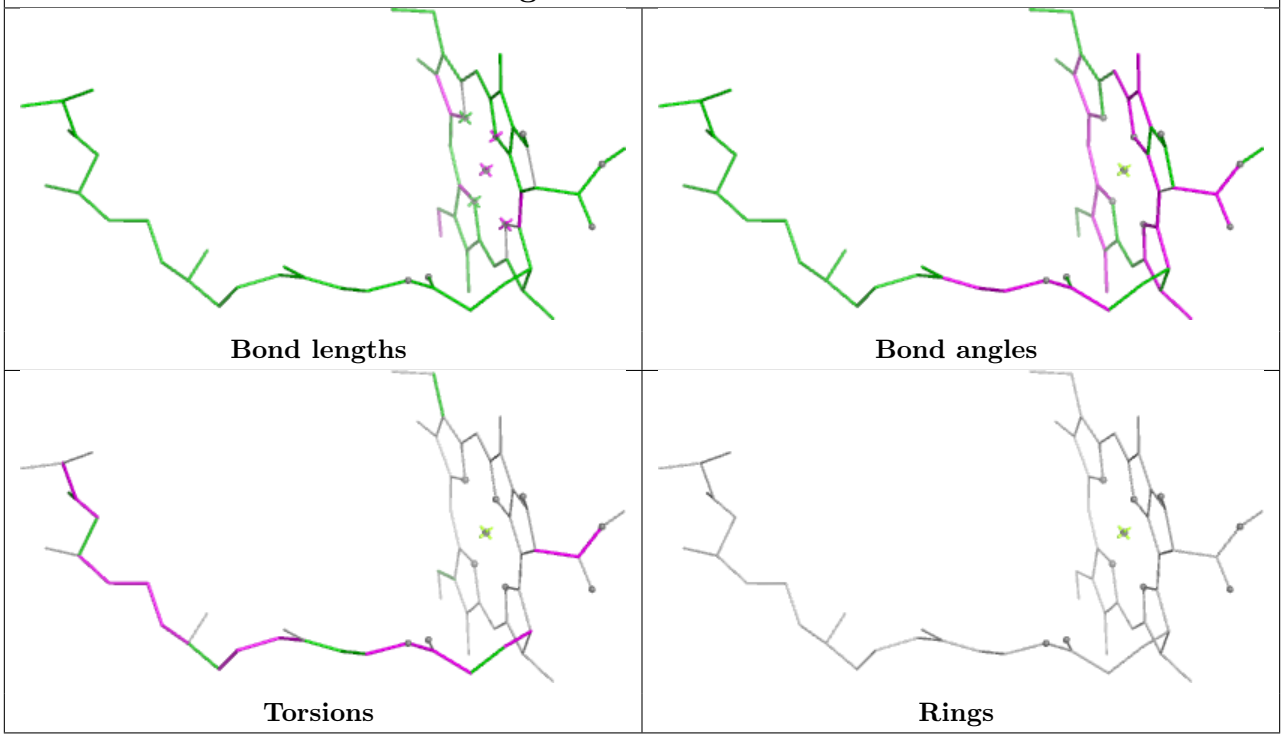


Torsions

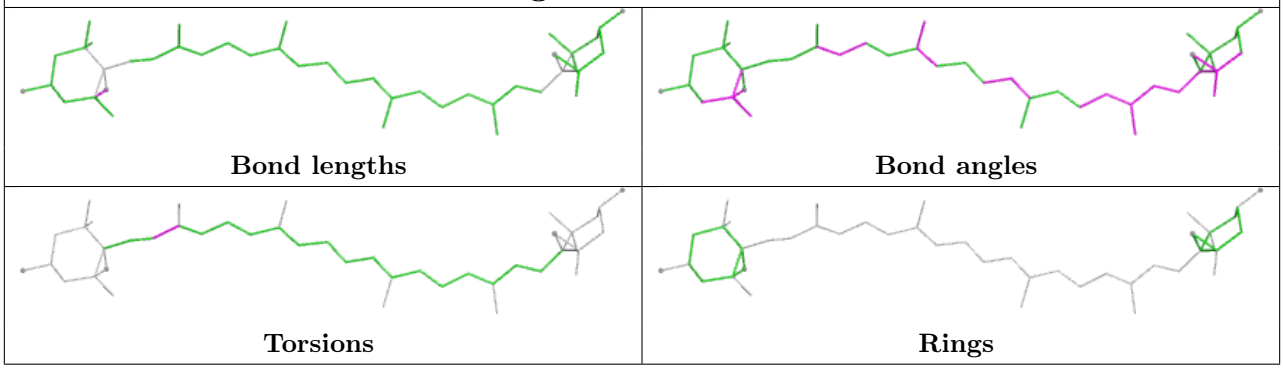


Rings

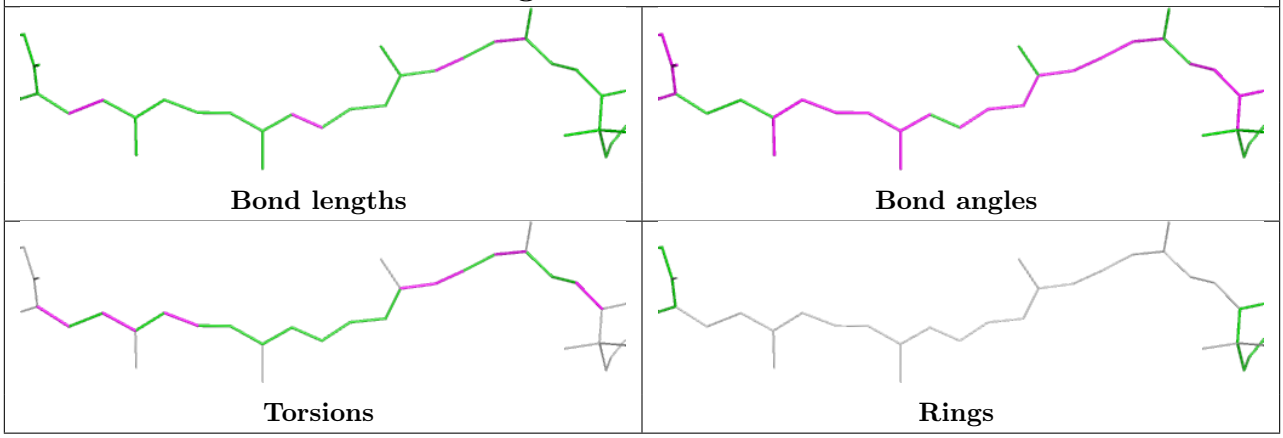
Ligand CLA b1 608



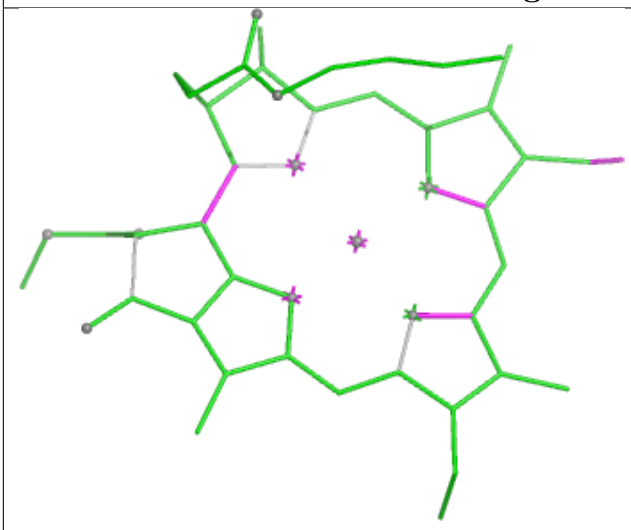
Ligand XAT r 621



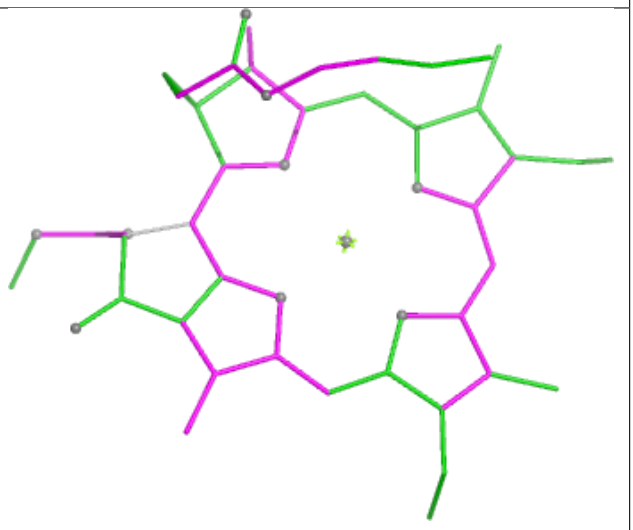
Ligand BCR b1 618



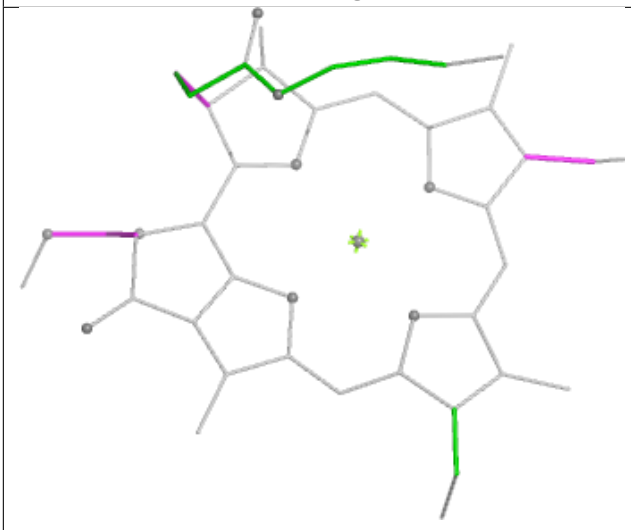
Ligand CLA N 614



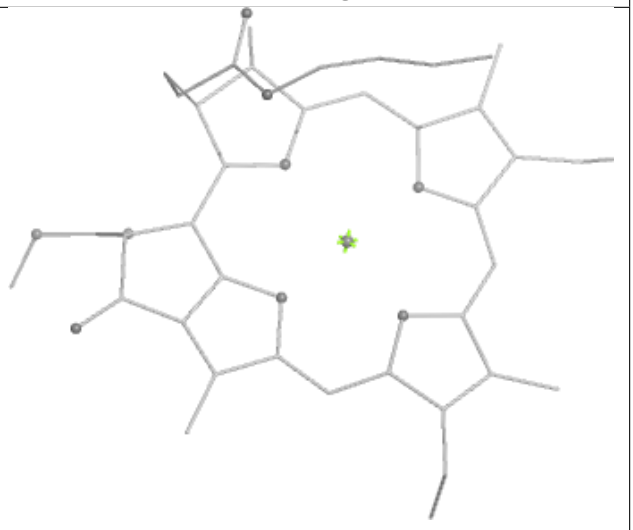
Bond lengths



Bond angles

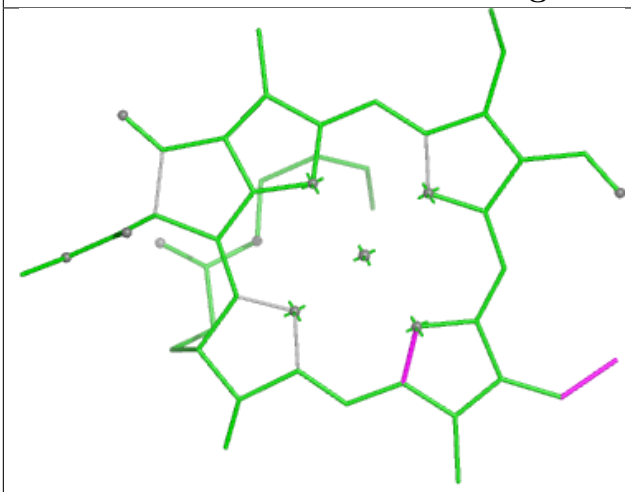


Torsions

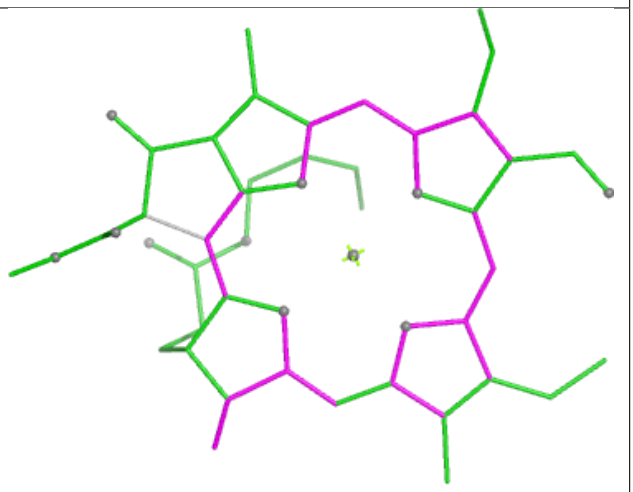


Rings

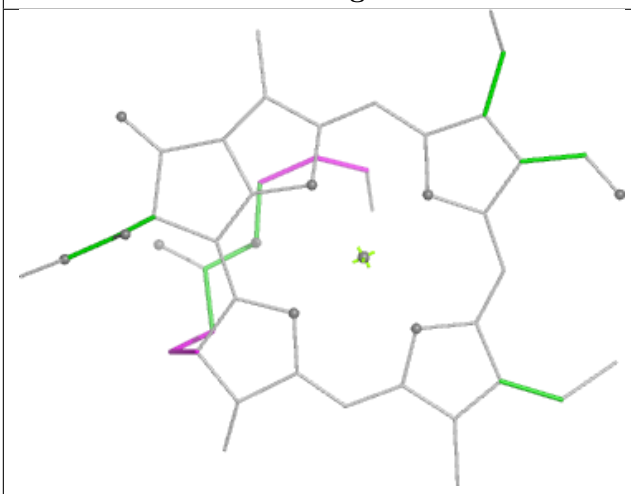
Ligand CHL r 607



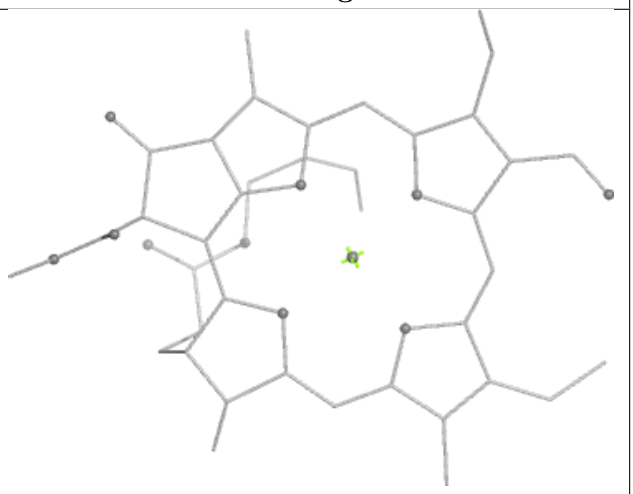
Bond lengths



Bond angles

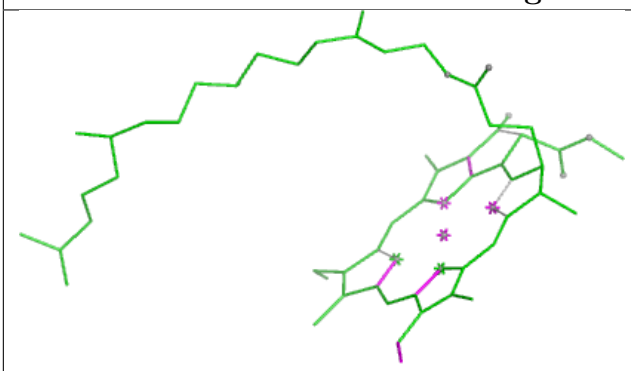


Torsions

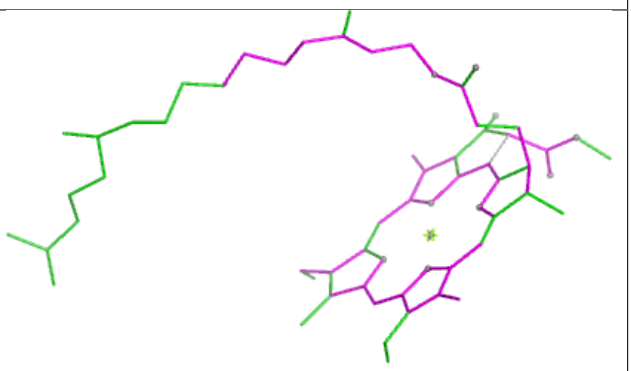


Rings

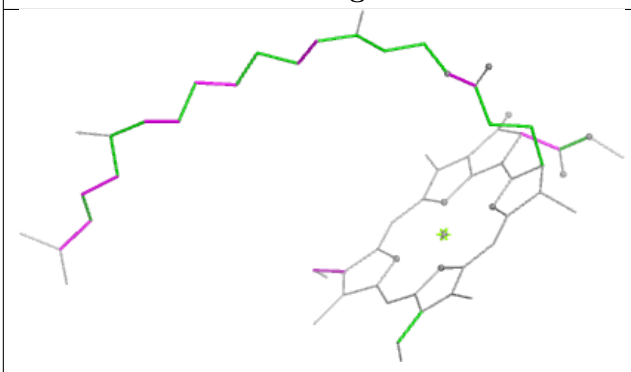
Ligand CLA C 508



Bond lengths



Bond angles

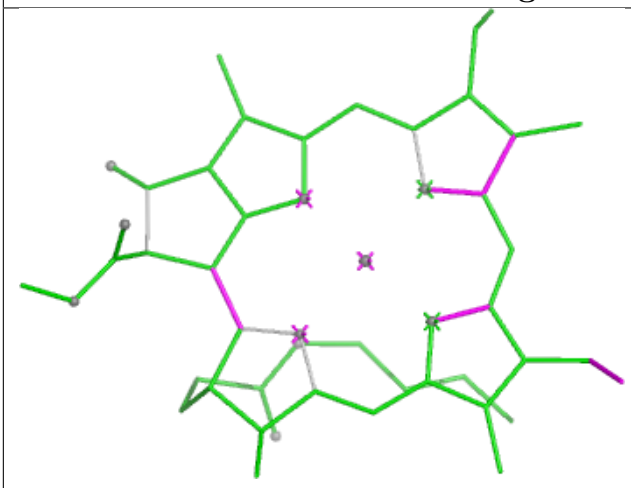


Torsions

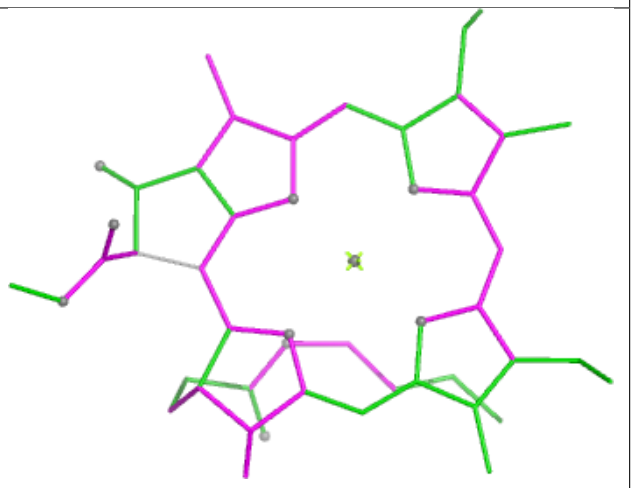


Rings

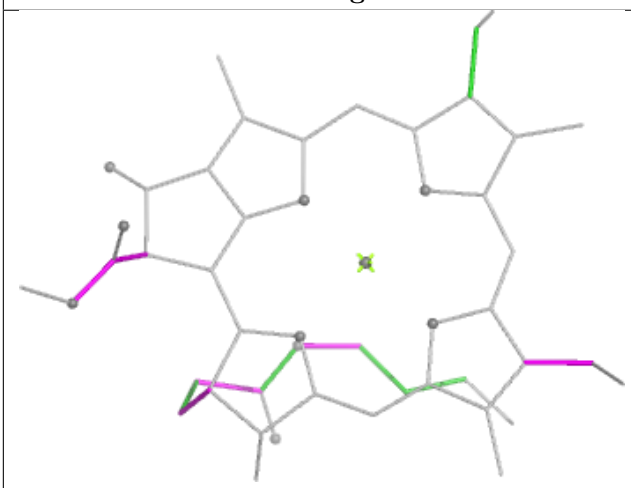
Ligand CLA n1 614



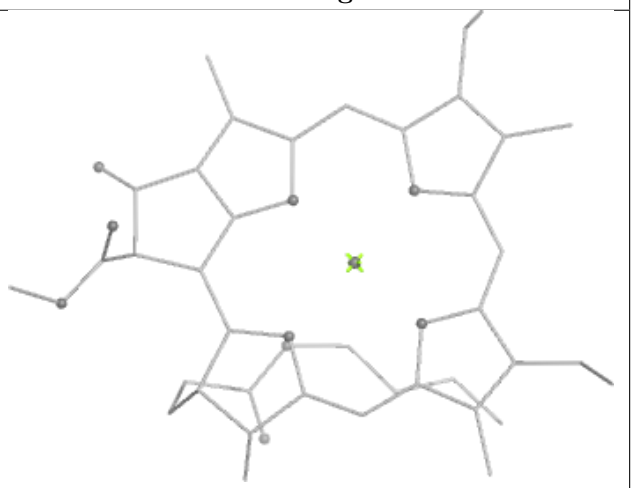
Bond lengths



Bond angles

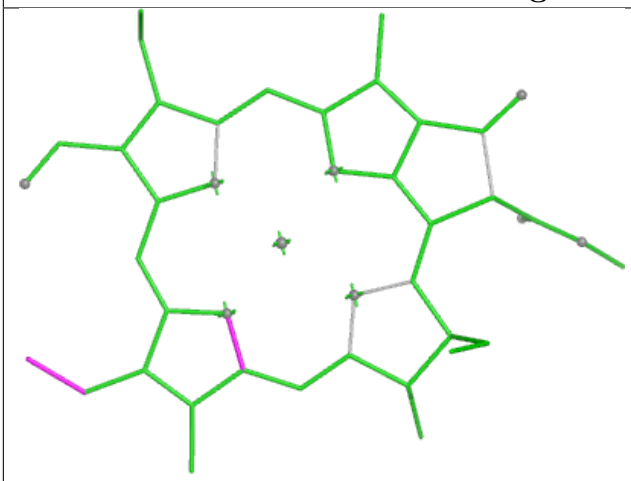


Torsions

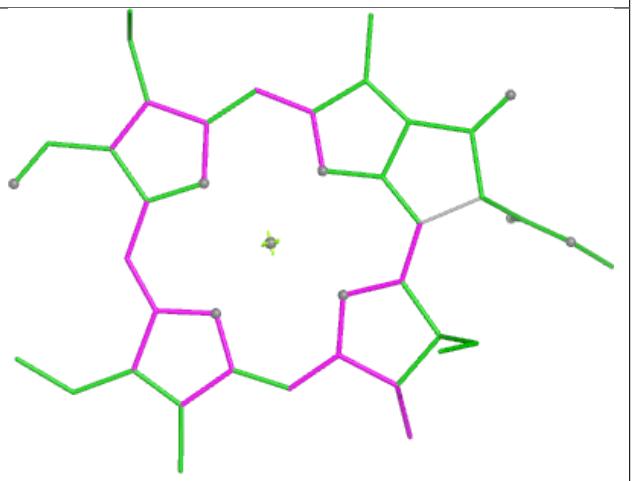


Rings

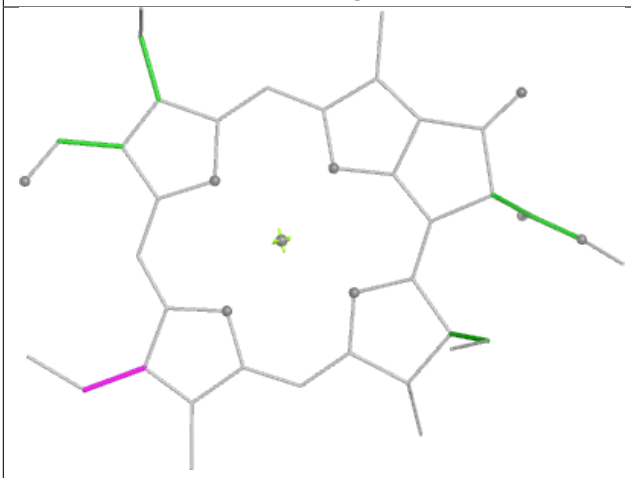
Ligand CHL s 607



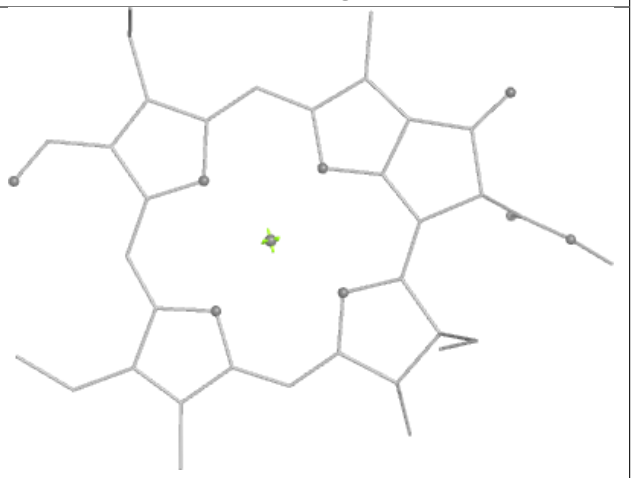
Bond lengths



Bond angles

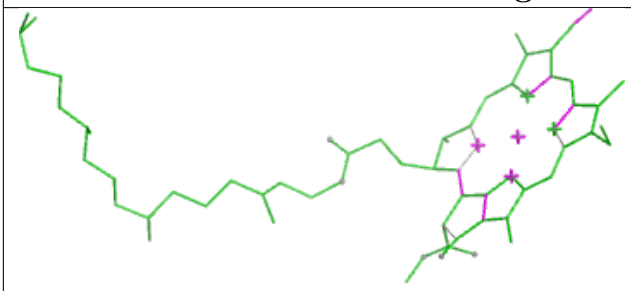


Torsions

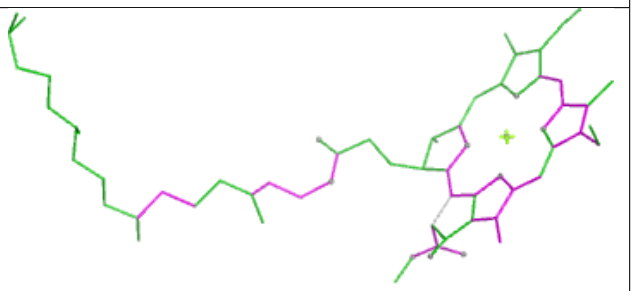


Rings

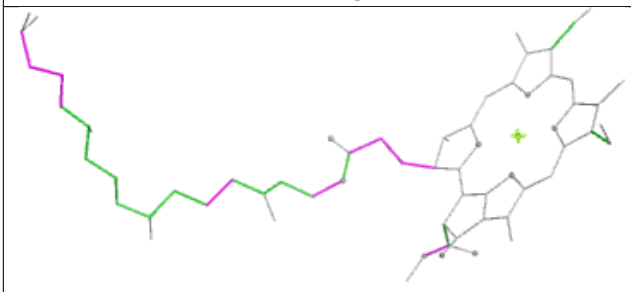
Ligand CLA A1 405



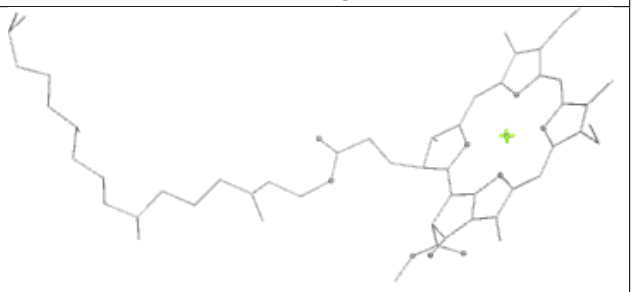
Bond lengths



Bond angles

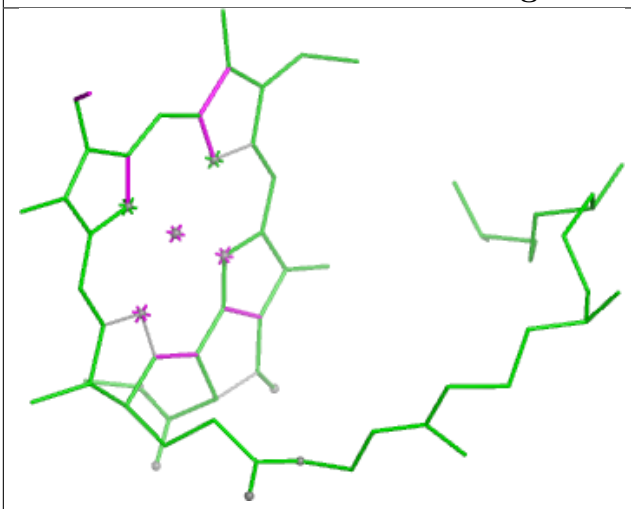


Torsions

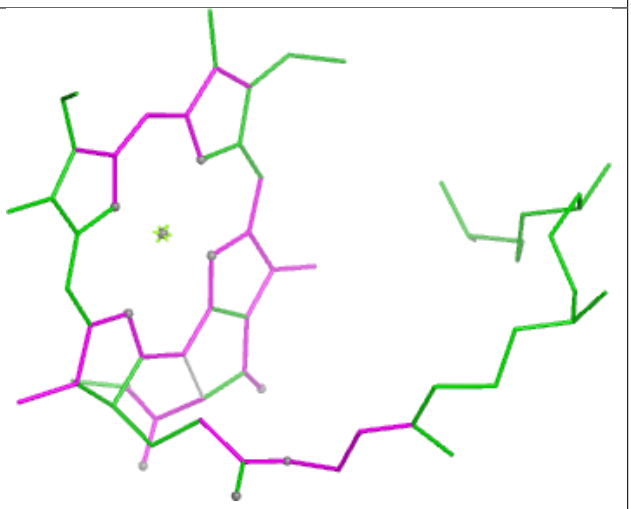


Rings

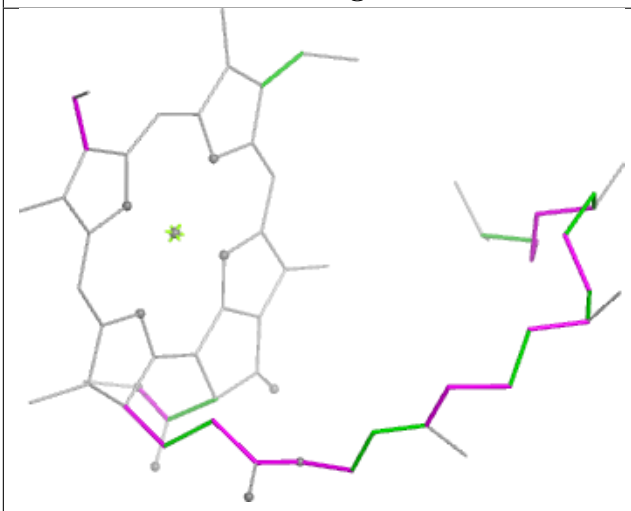
Ligand CLA c1 503



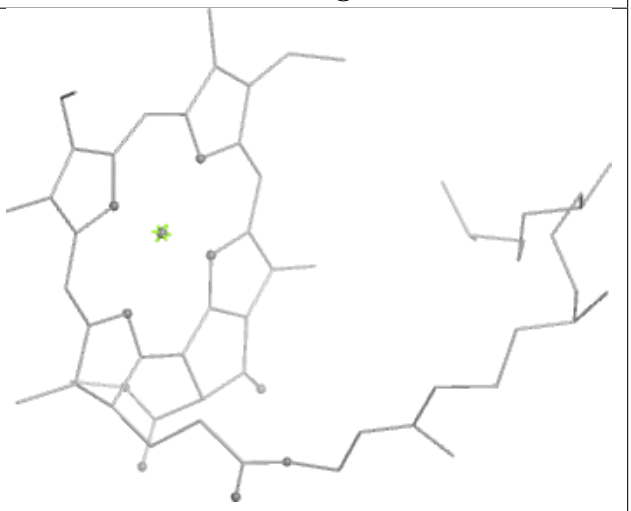
Bond lengths



Bond angles

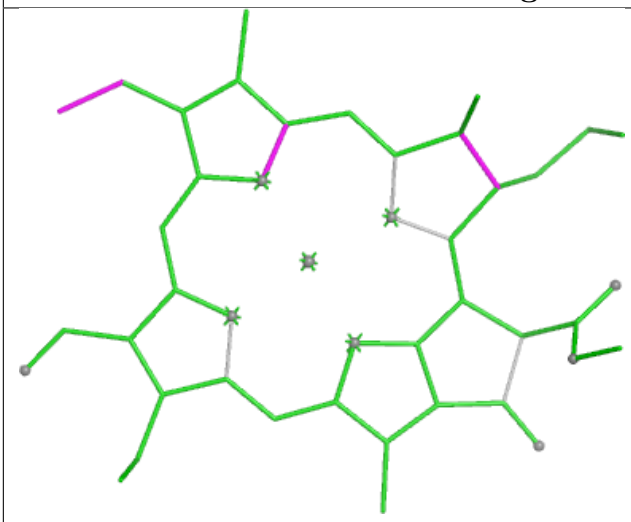


Torsions

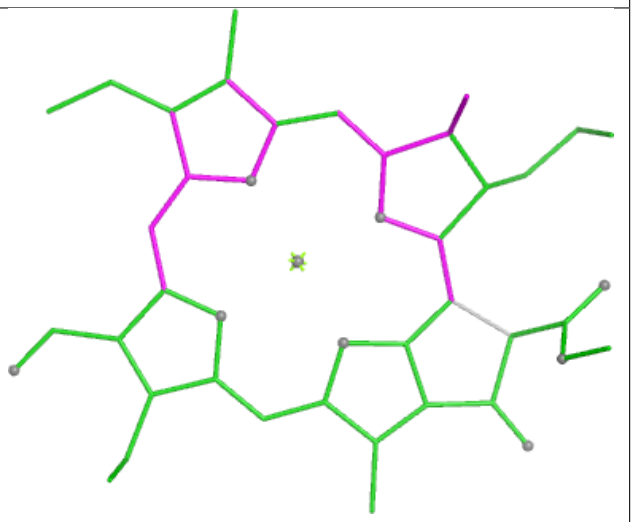


Rings

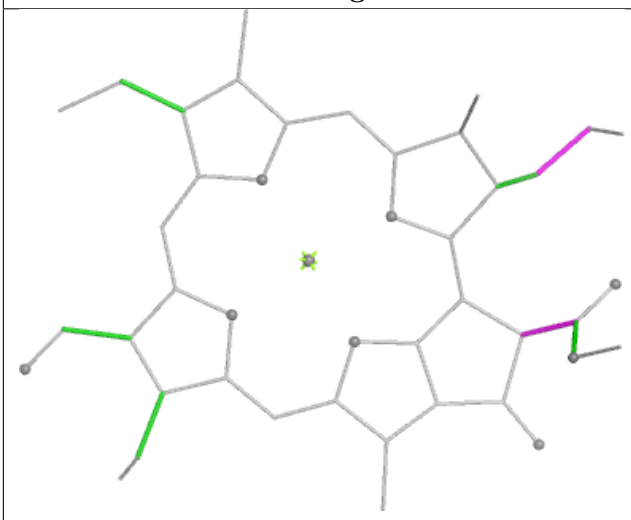
Ligand CHL r1 606



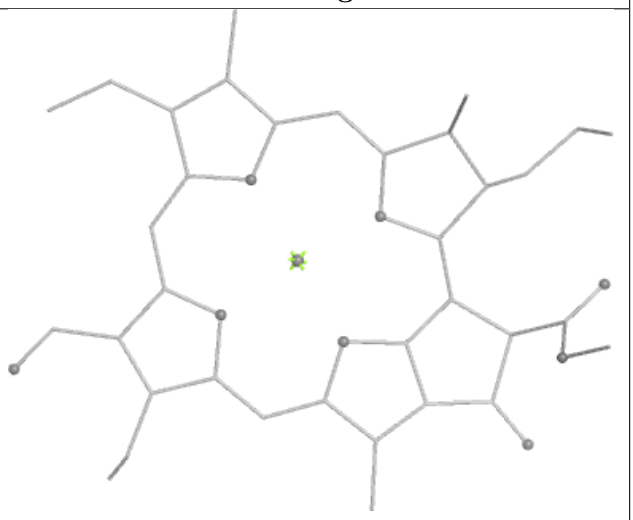
Bond lengths



Bond angles

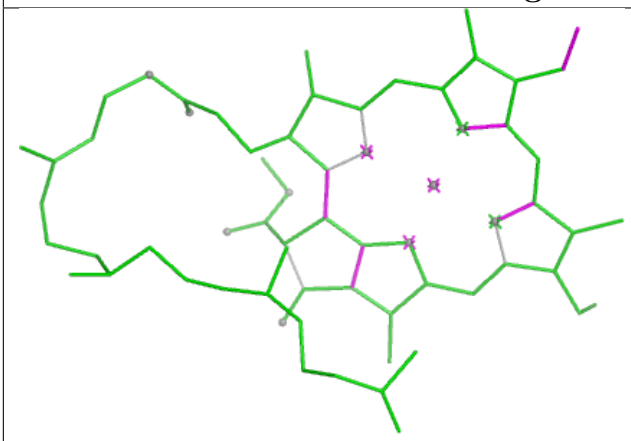


Torsions

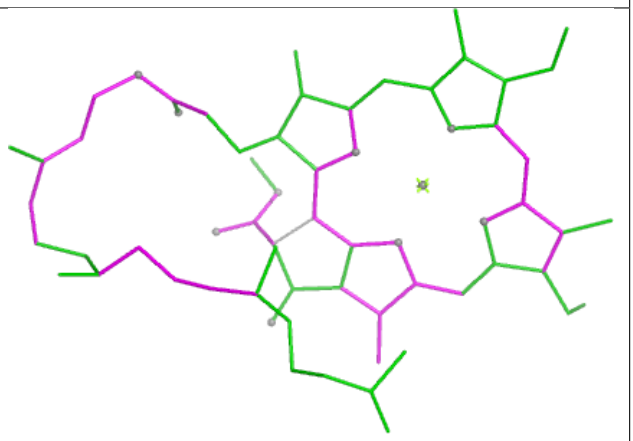


Rings

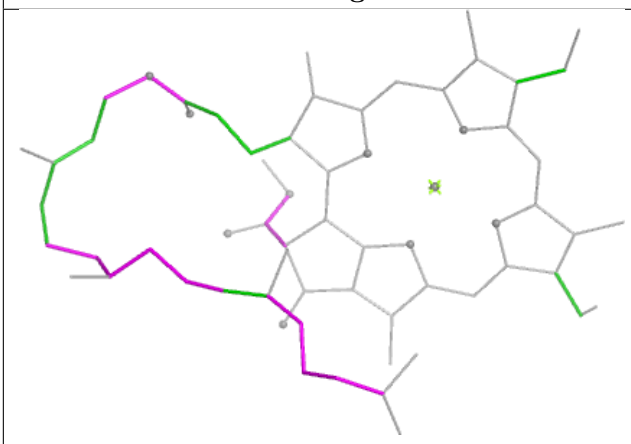
Ligand CLA C 509



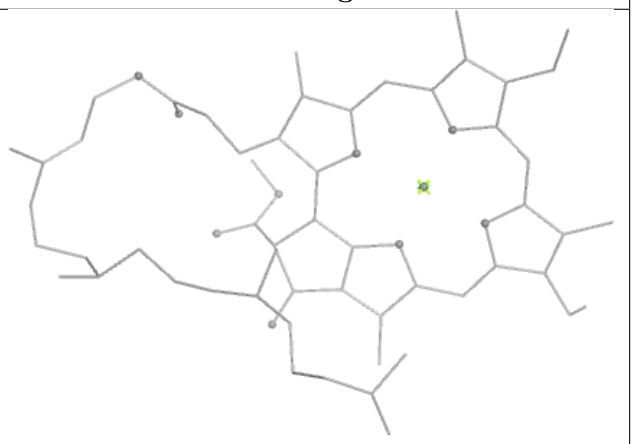
Bond lengths



Bond angles

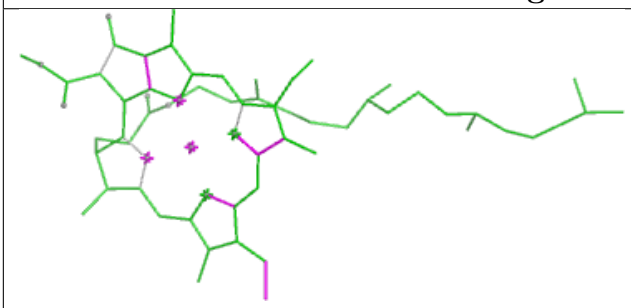


Torsions

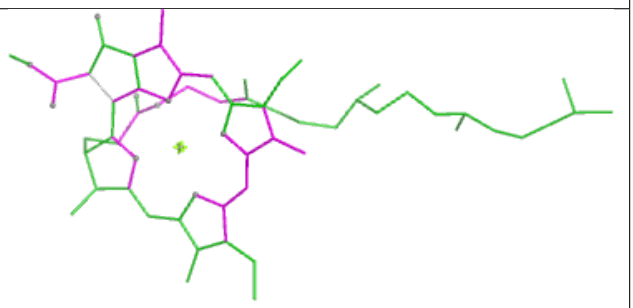


Rings

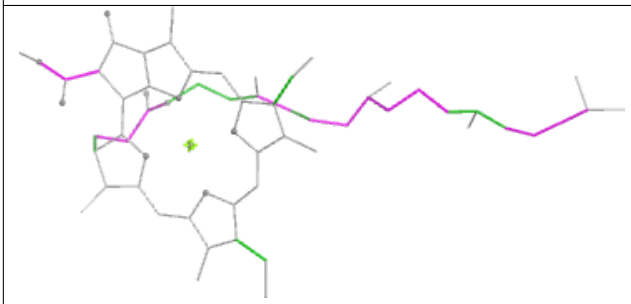
Ligand CLA b 615



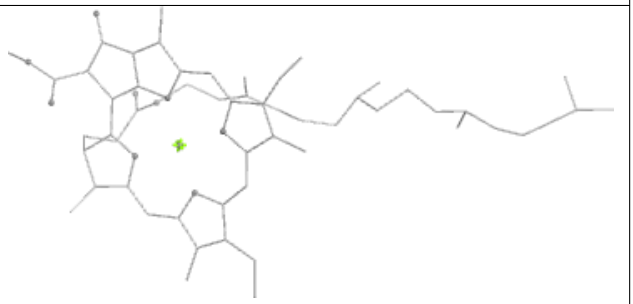
Bond lengths



Bond angles

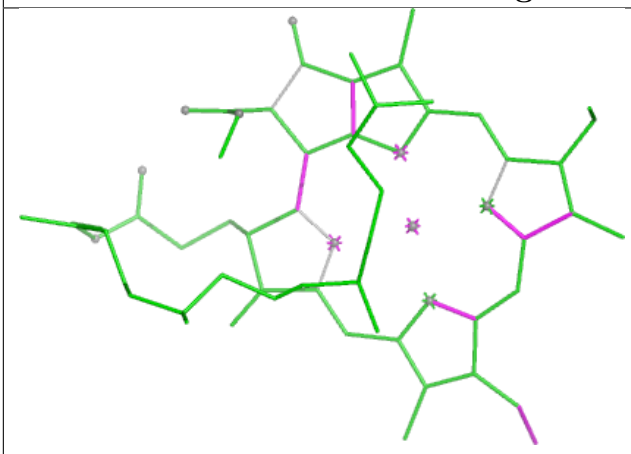


Torsions

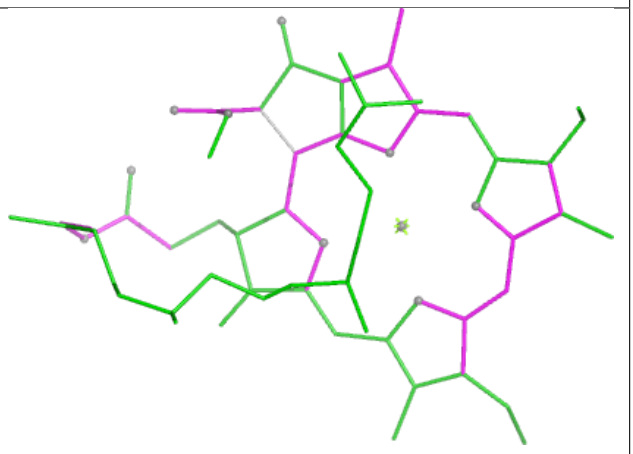


Rings

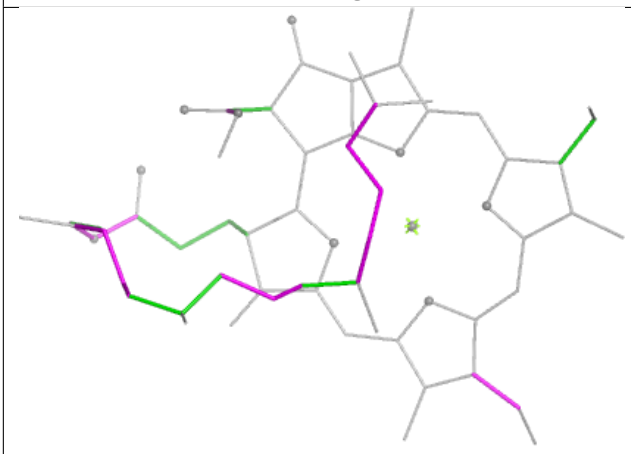
Ligand CLA C1 510



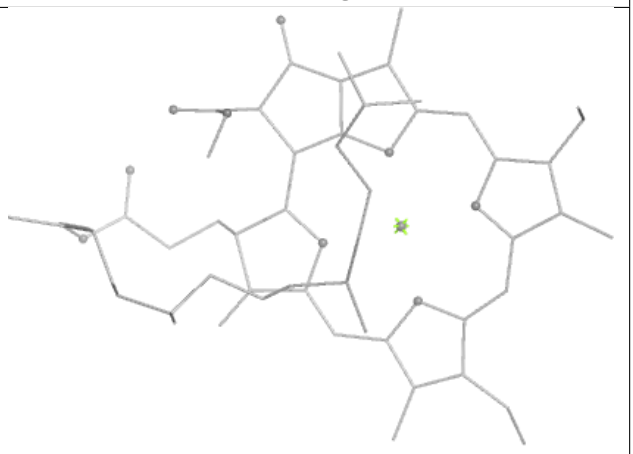
Bond lengths



Bond angles

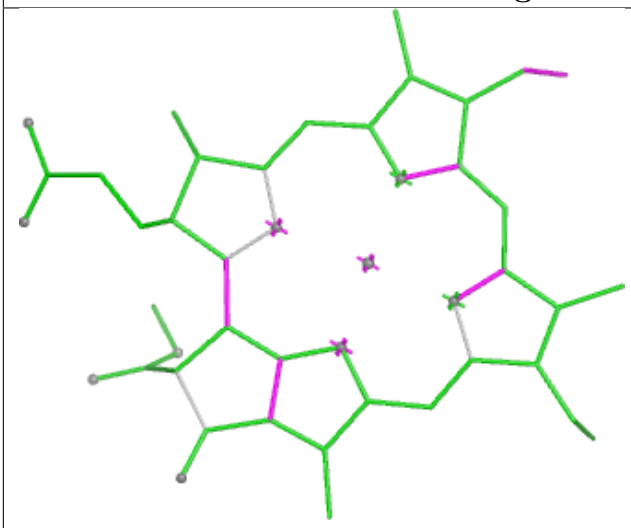


Torsions

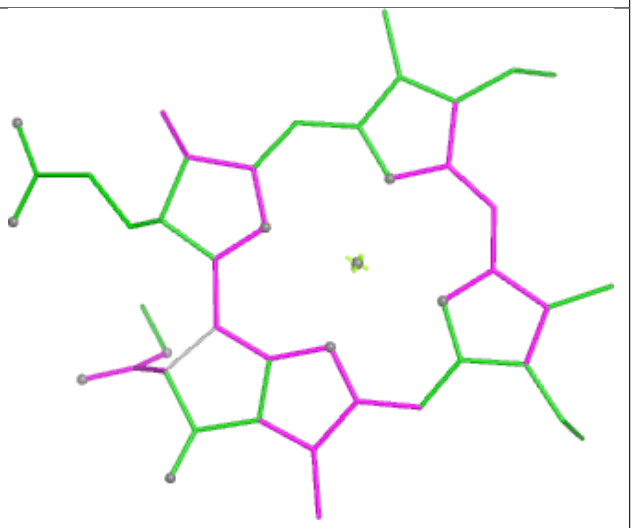


Rings

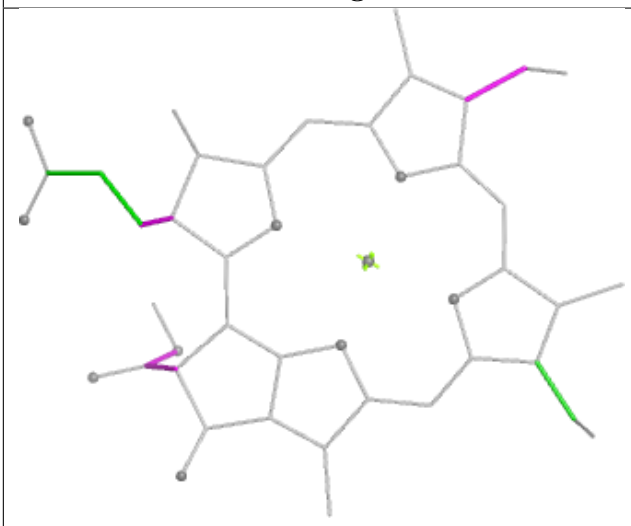
Ligand CLA N1 612



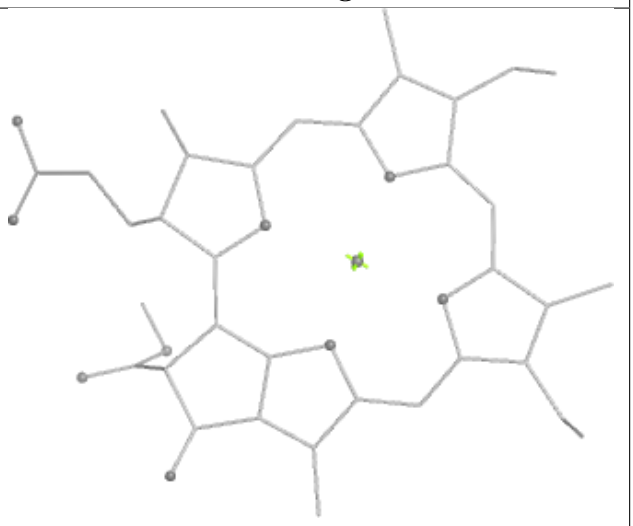
Bond lengths



Bond angles

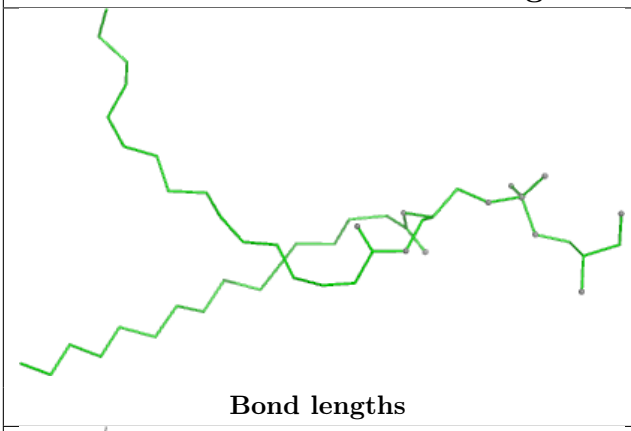


Torsions

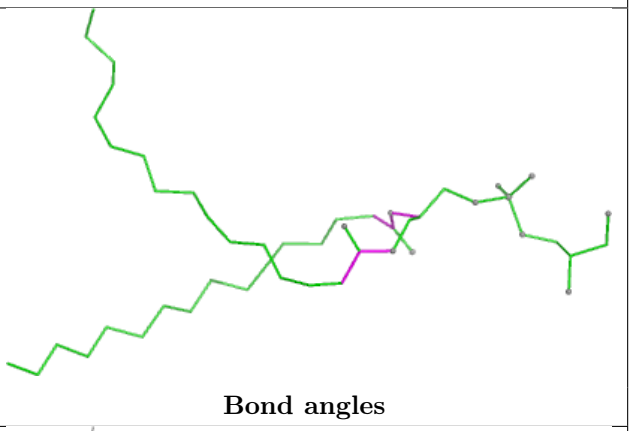


Rings

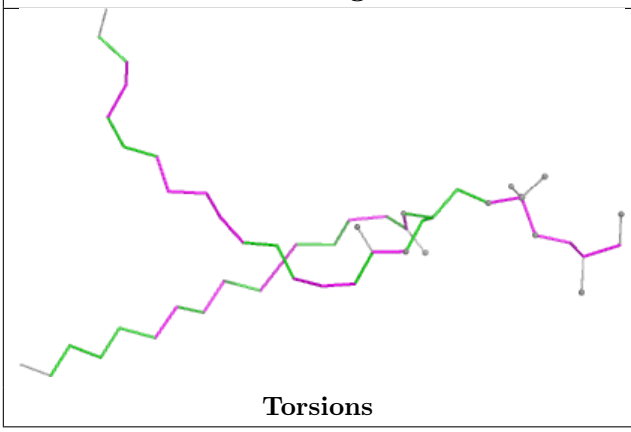
Ligand LHG d 409



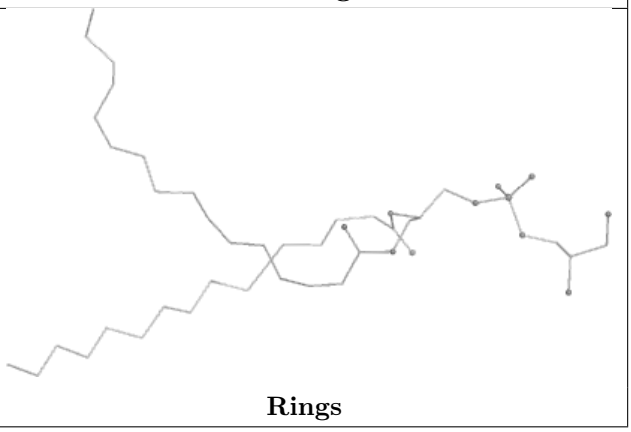
Bond lengths



Bond angles

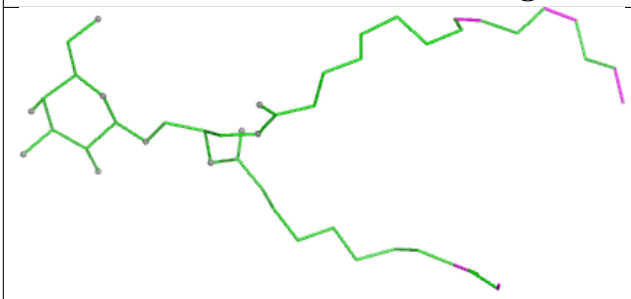


Torsions



Rings

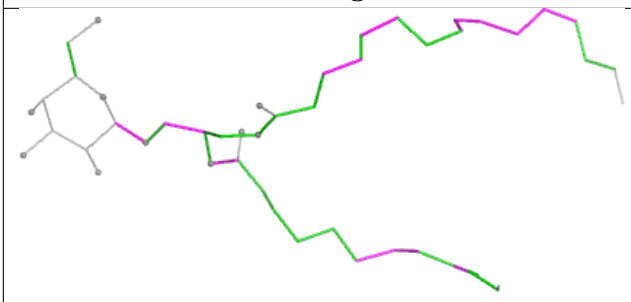
Ligand LMG A 413



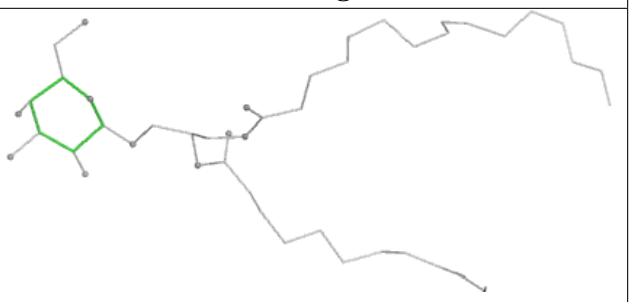
Bond lengths



Bond angles

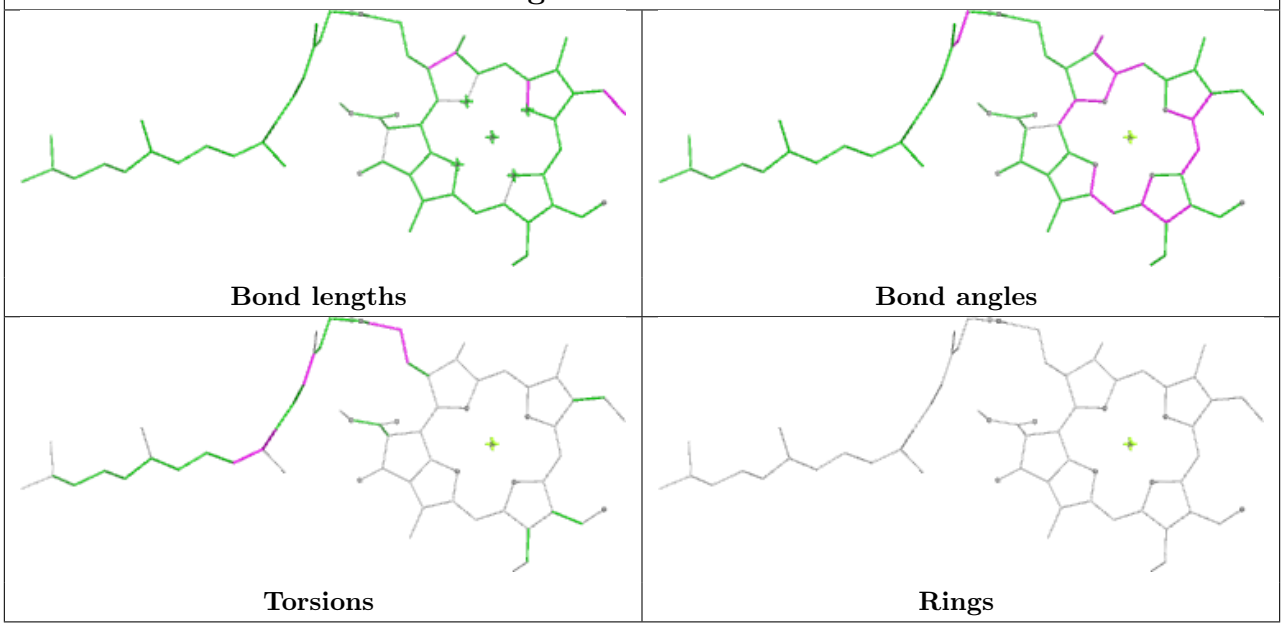


Torsions

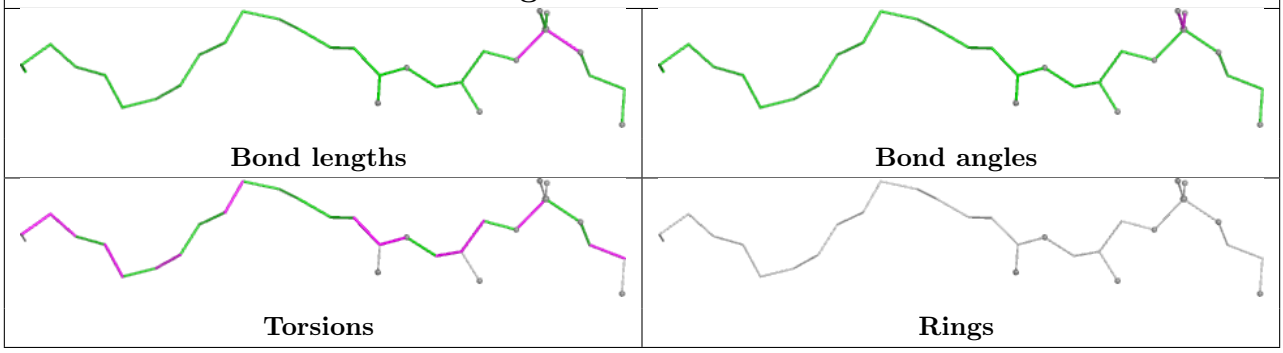


Rings

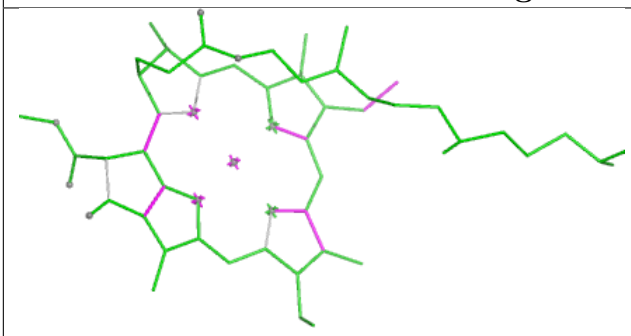
Ligand CHL n 605



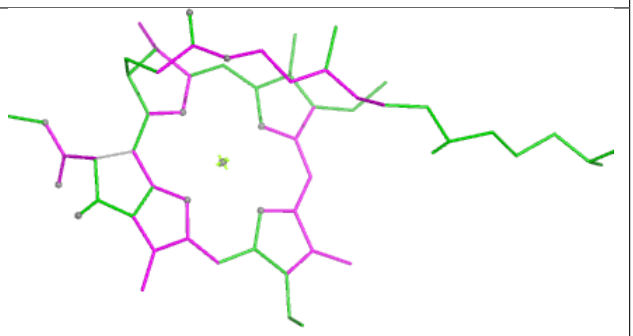
Ligand LPX S1 625



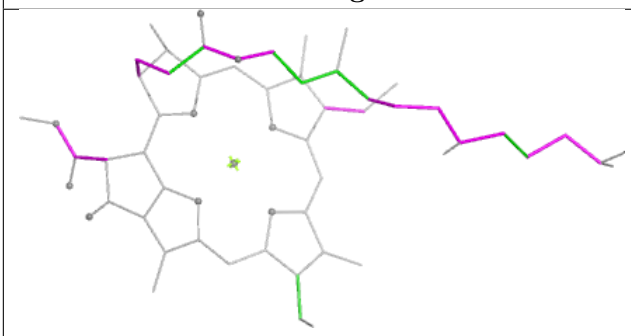
Ligand CLA R1 610



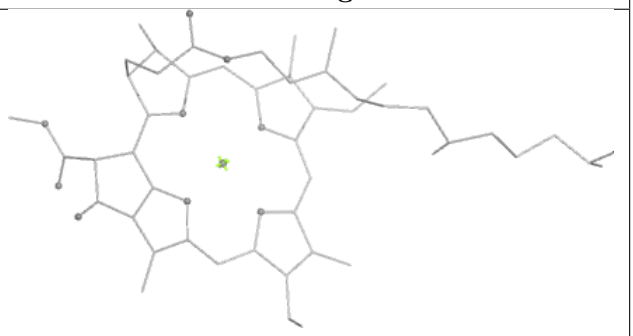
Bond lengths



Bond angles

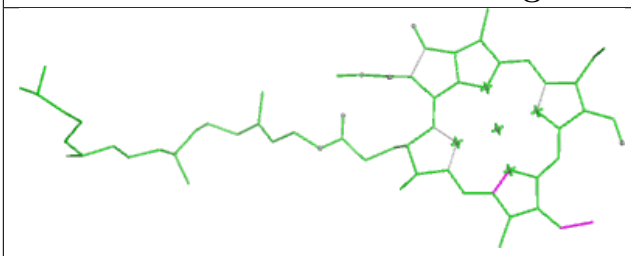


Torsions

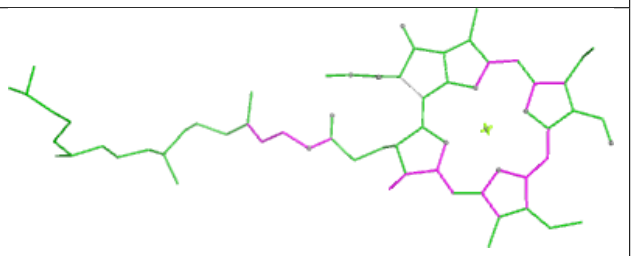


Rings

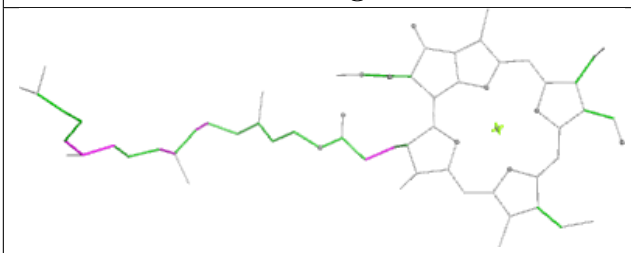
Ligand CHL Y 606



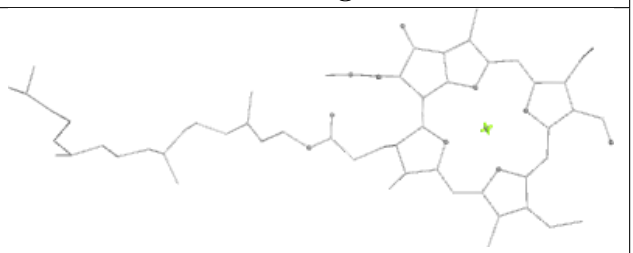
Bond lengths



Bond angles

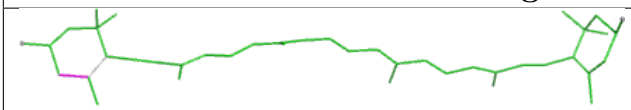


Torsions

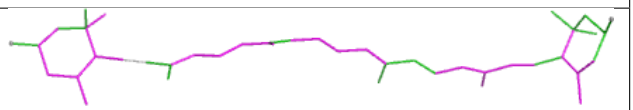


Rings

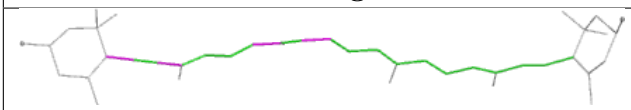
Ligand LUT s1 620



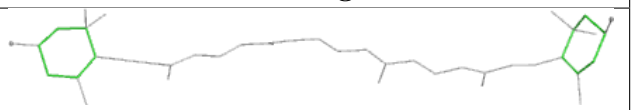
Bond lengths



Bond angles

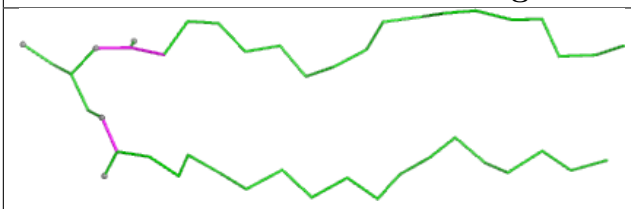


Torsions

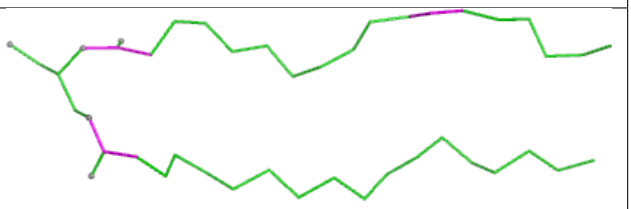


Rings

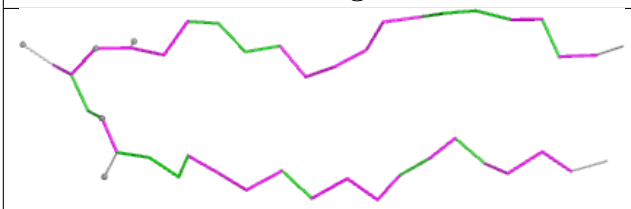
Ligand DGA B1 625



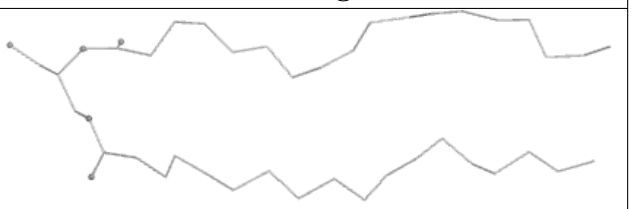
Bond lengths



Bond angles

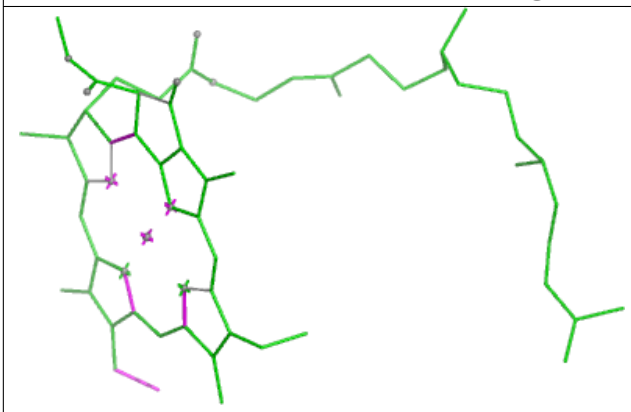


Torsions

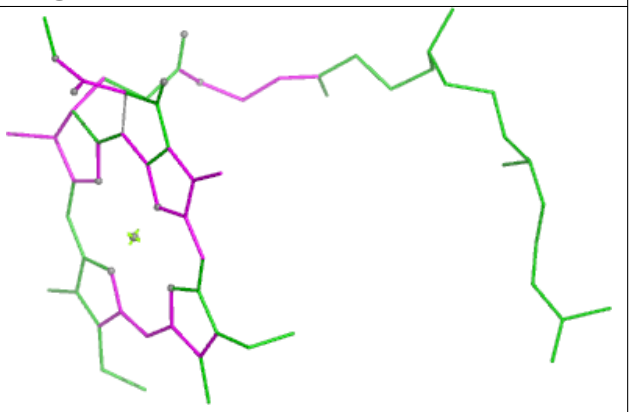


Rings

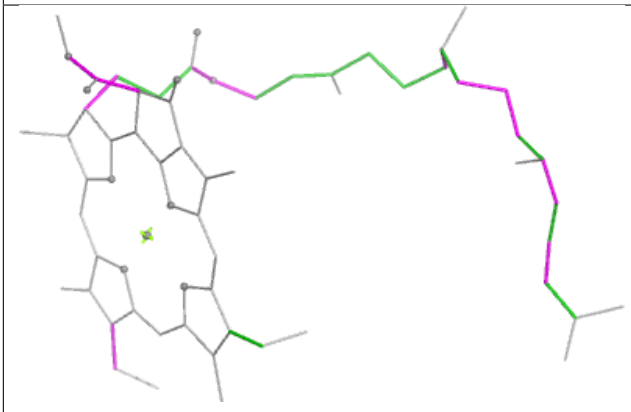
Ligand CLA g 611



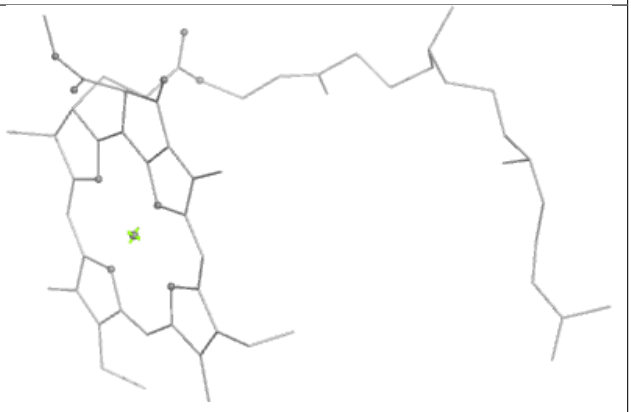
Bond lengths



Bond angles

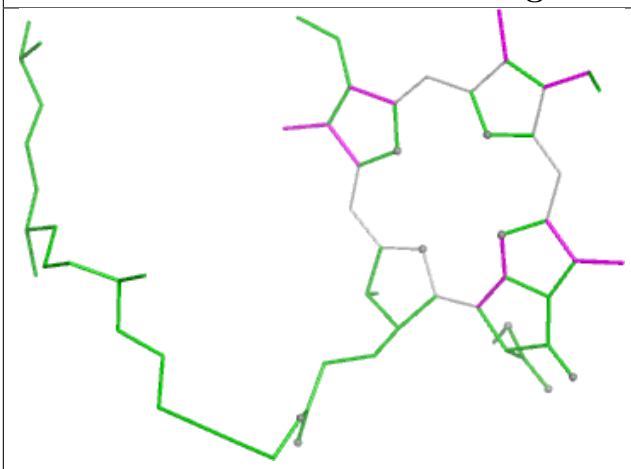


Torsions

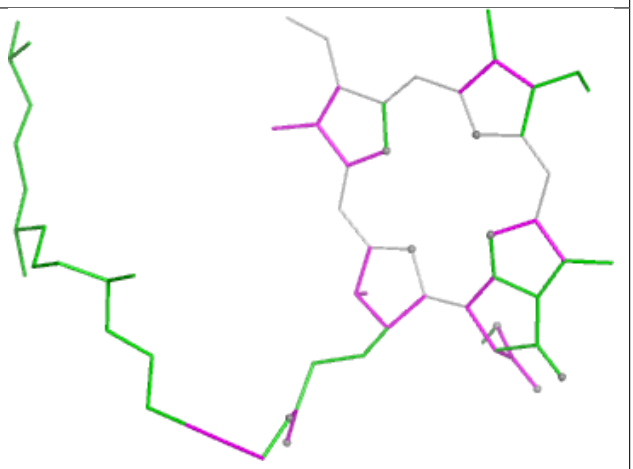


Rings

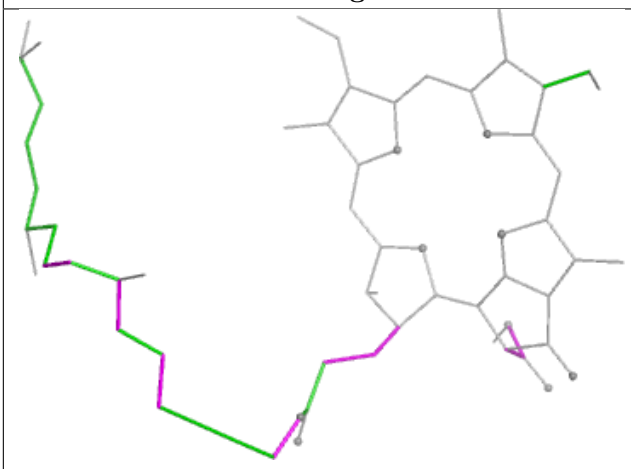
Ligand PHO a 409



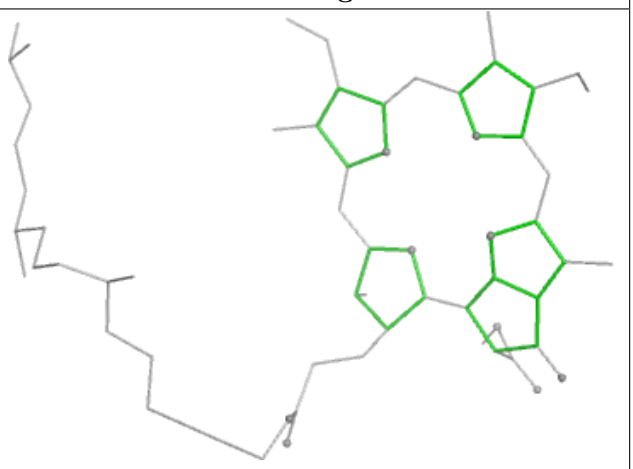
Bond lengths



Bond angles



Torsions

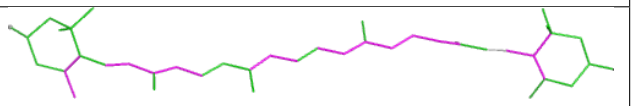


Rings

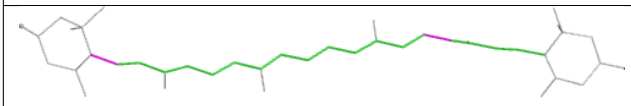
Ligand LUT G1 621



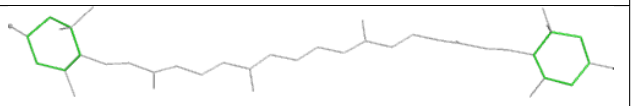
Bond lengths



Bond angles

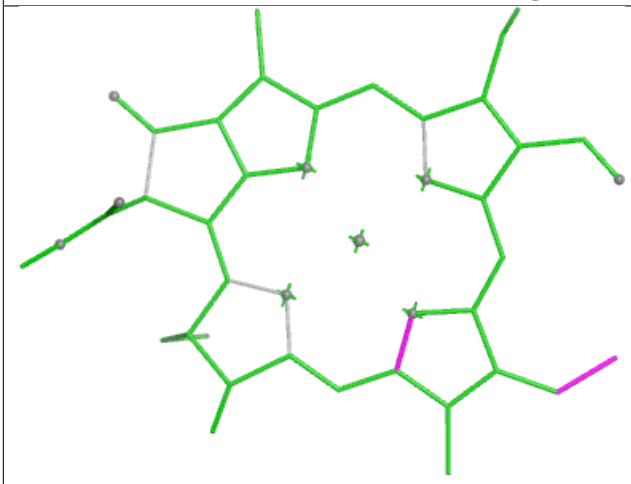


Torsions

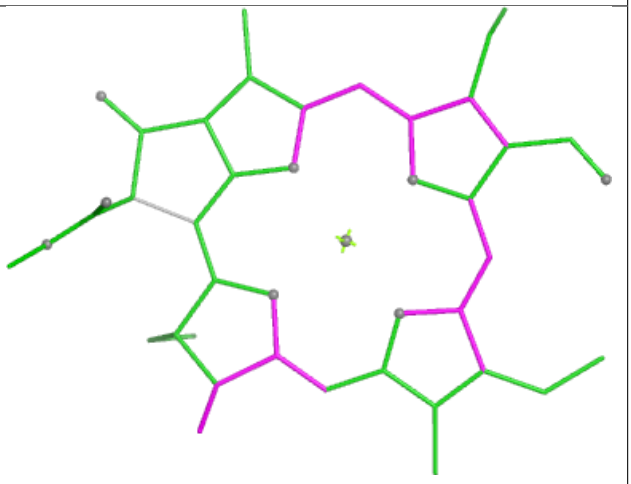


Rings

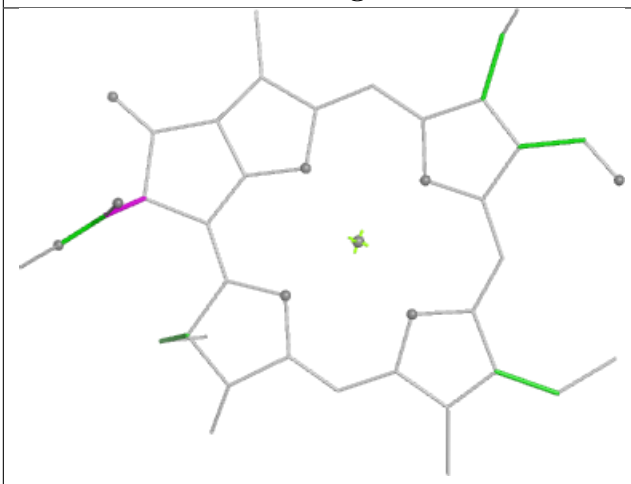
Ligand CHL S 607



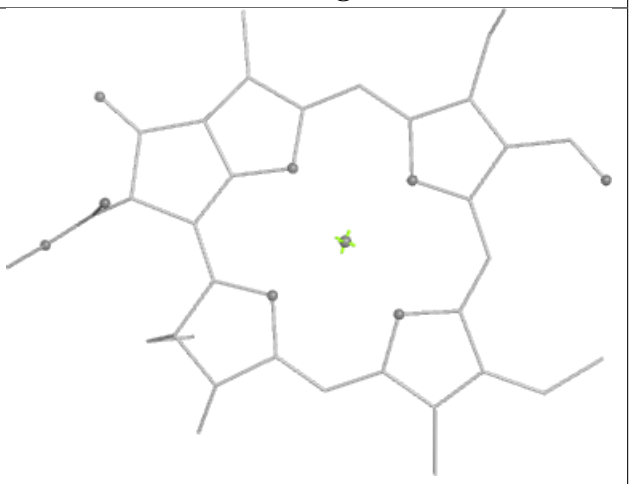
Bond lengths



Bond angles

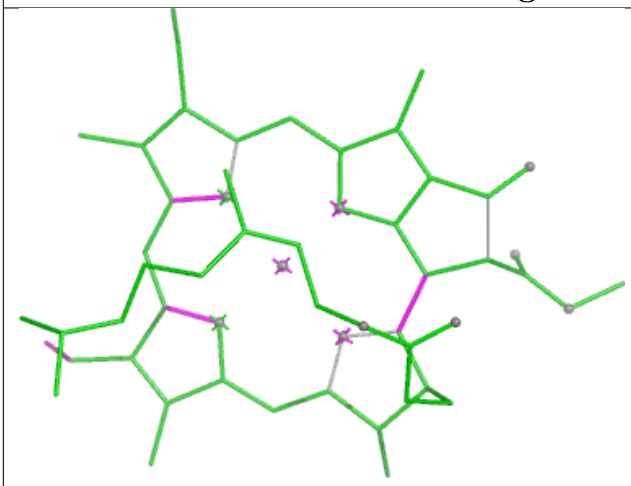


Torsions

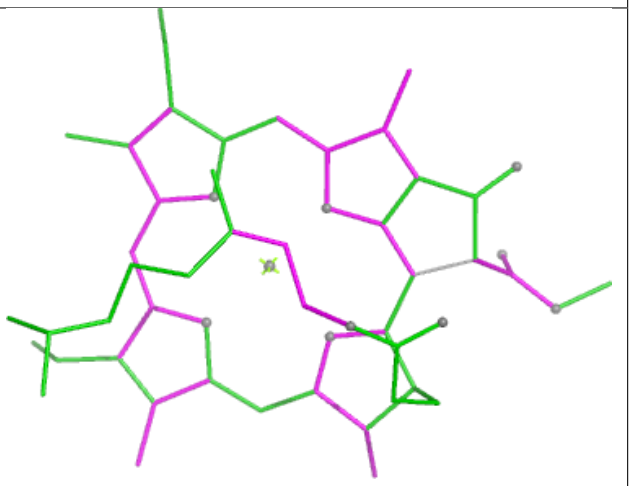


Rings

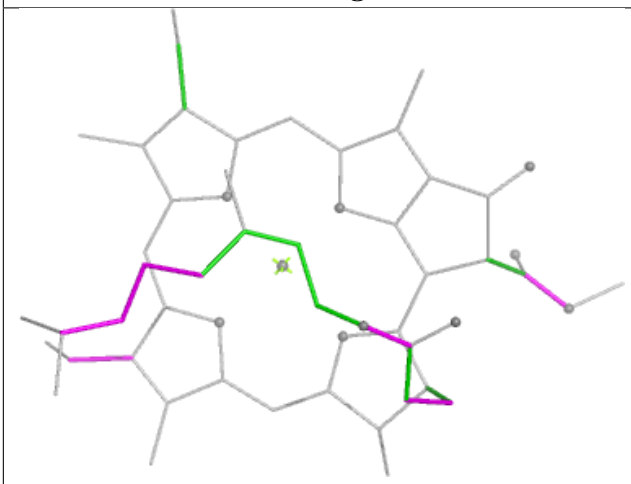
Ligand CLA S1 613



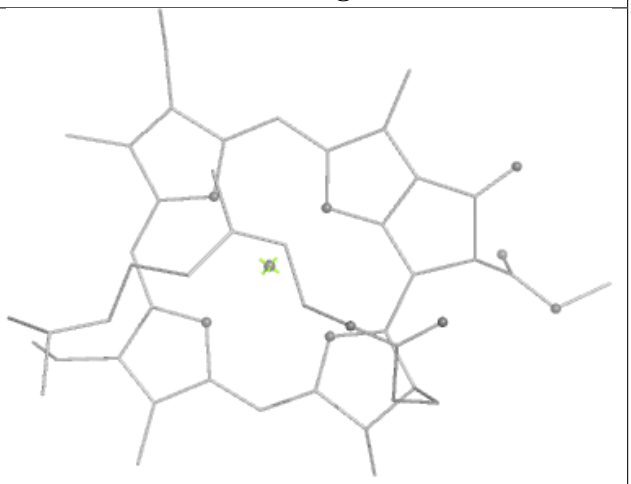
Bond lengths



Bond angles

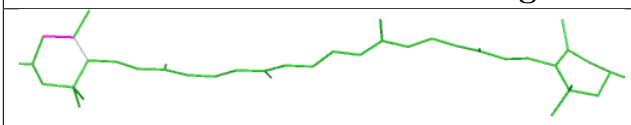


Torsions

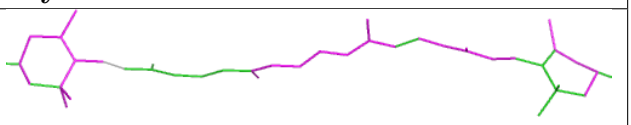


Rings

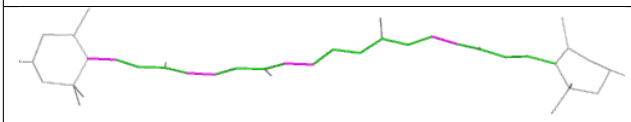
Ligand LUT y1 621



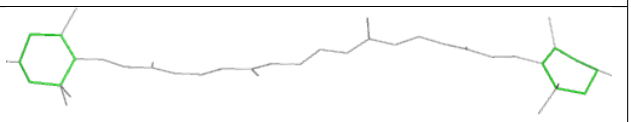
Bond lengths



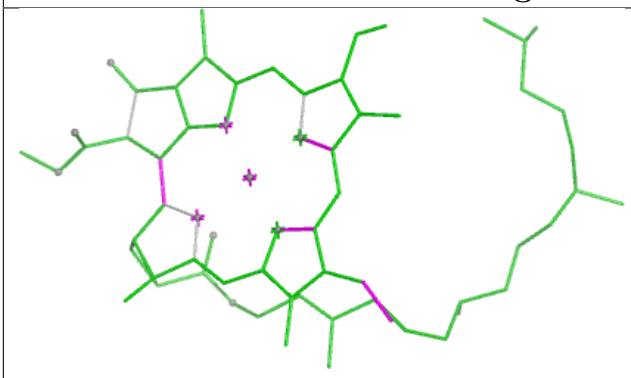
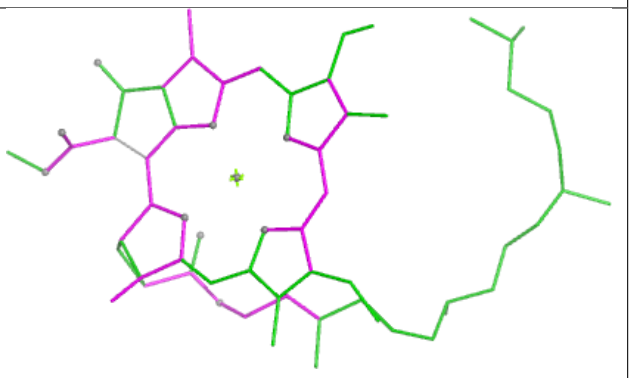
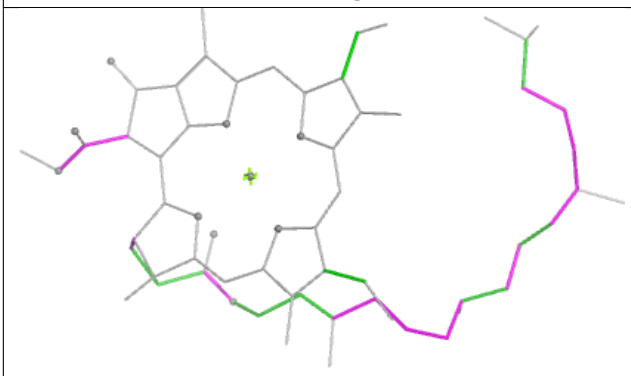
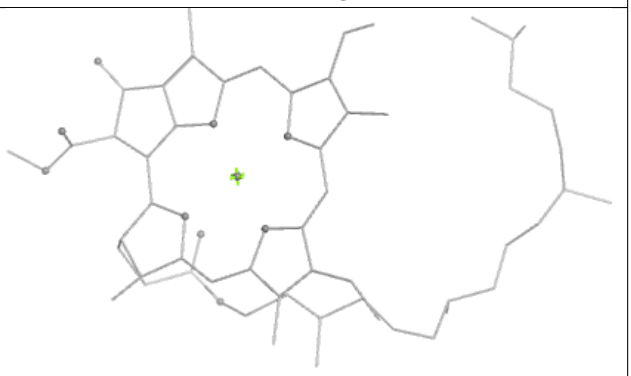
Bond angles



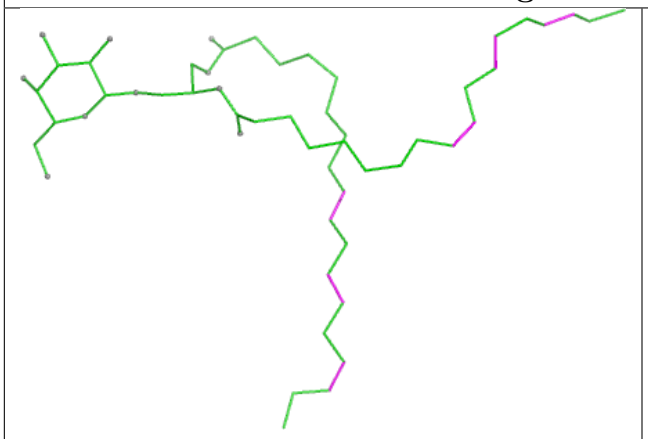
Torsions



Rings

Ligand CLA N1 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG c1 523



Bond lengths



Bond angles

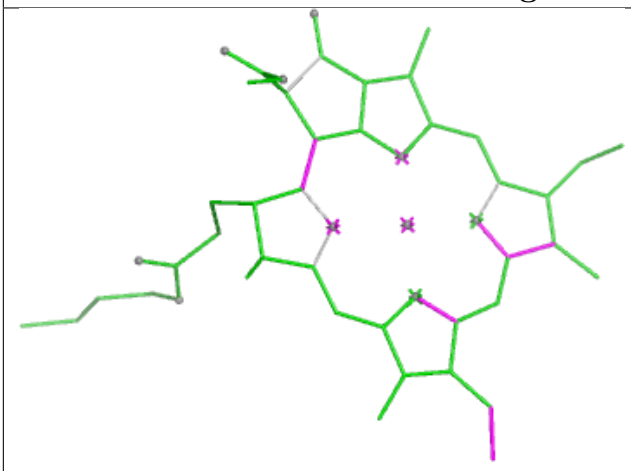


Torsions

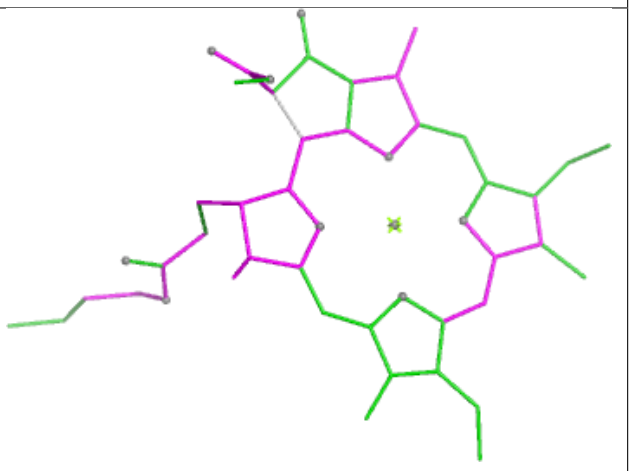


Rings

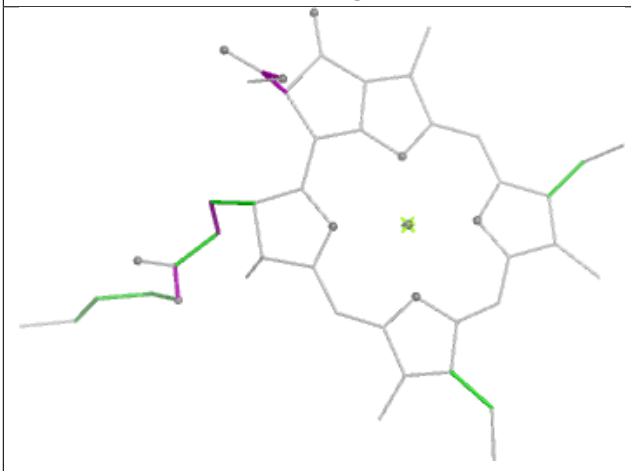
Ligand CLA a1 407



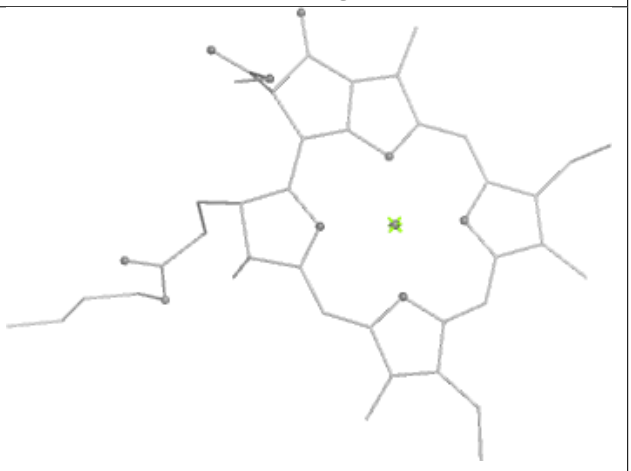
Bond lengths



Bond angles

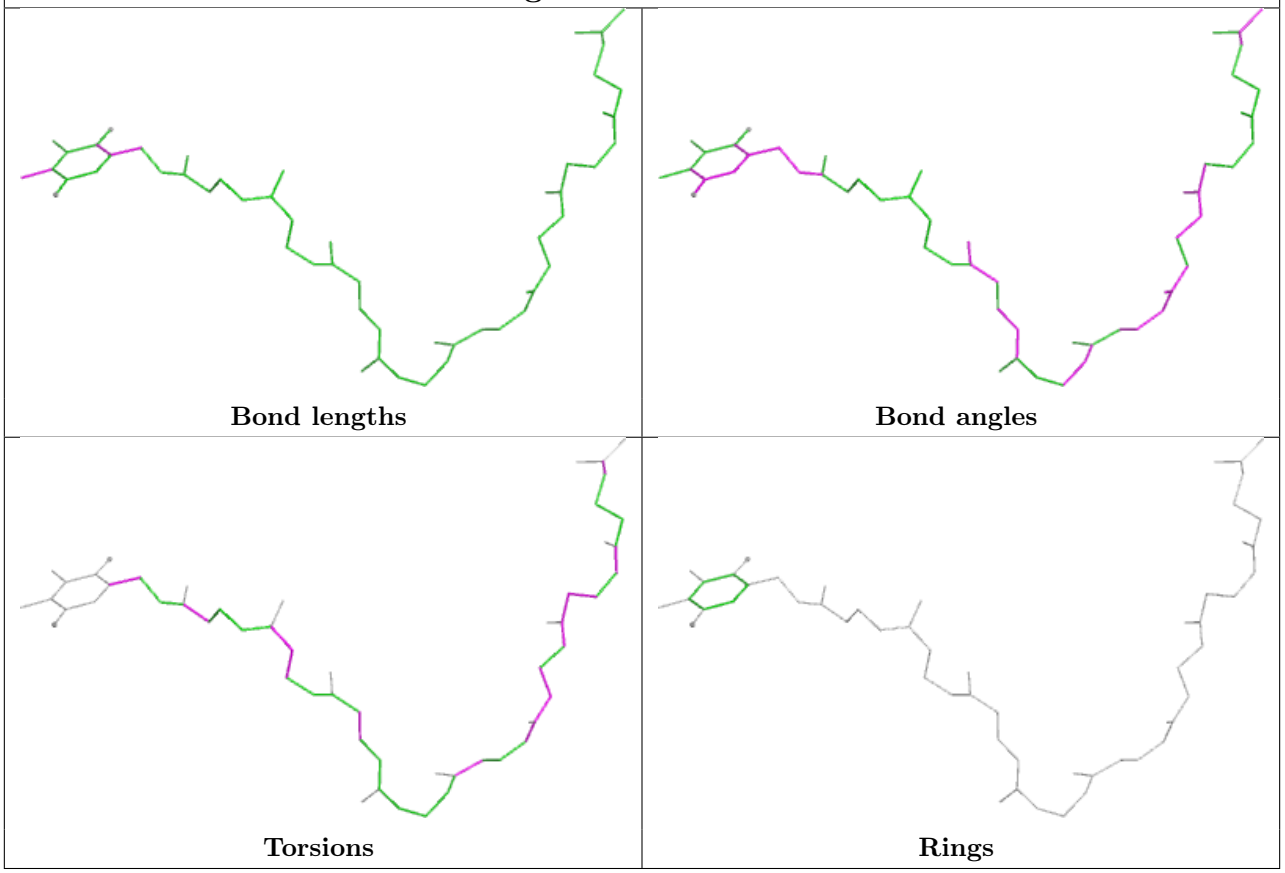


Torsions

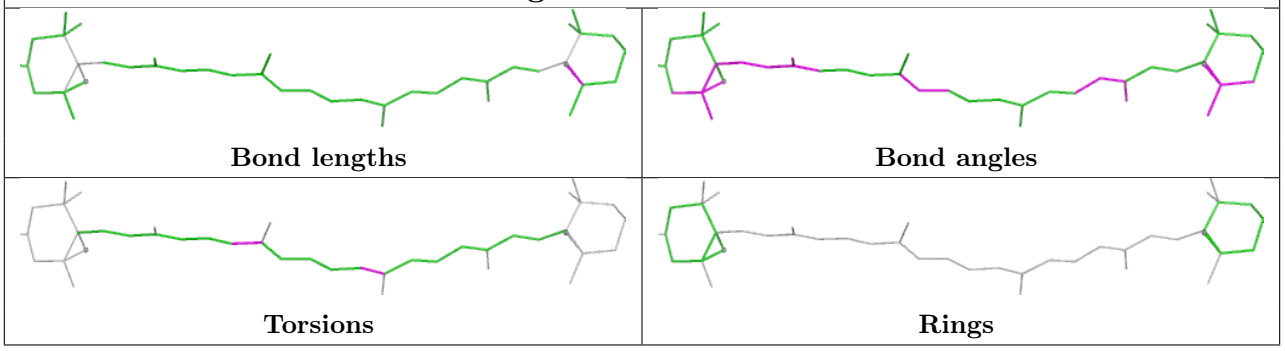


Rings

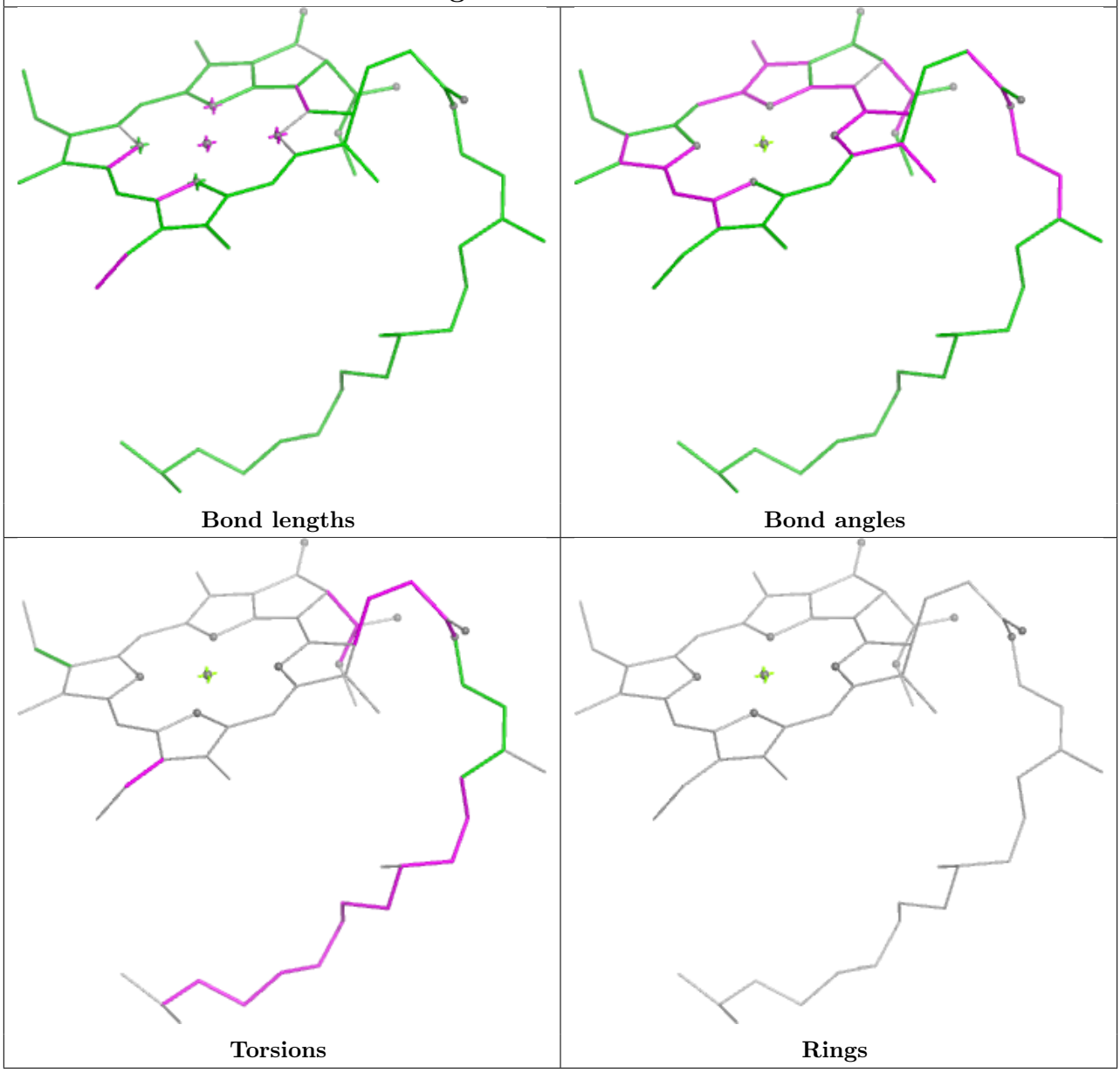
Ligand PL9 d1 405



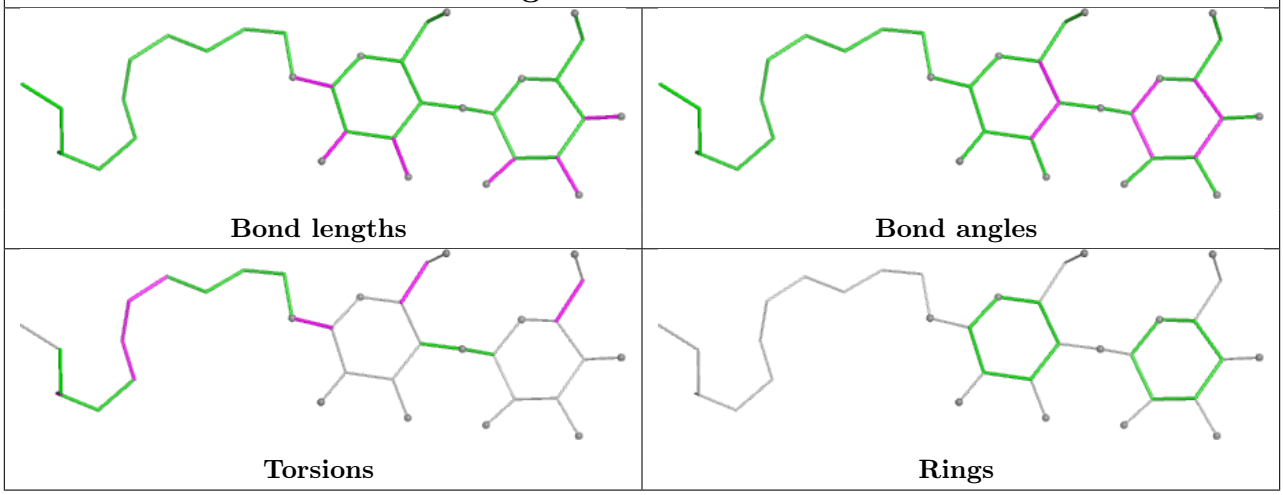
Ligand XAT n 622



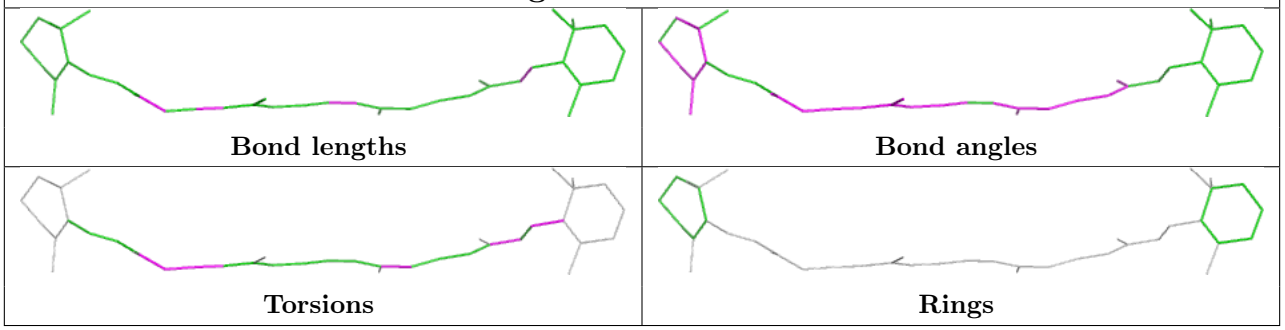
Ligand CLA G1 603



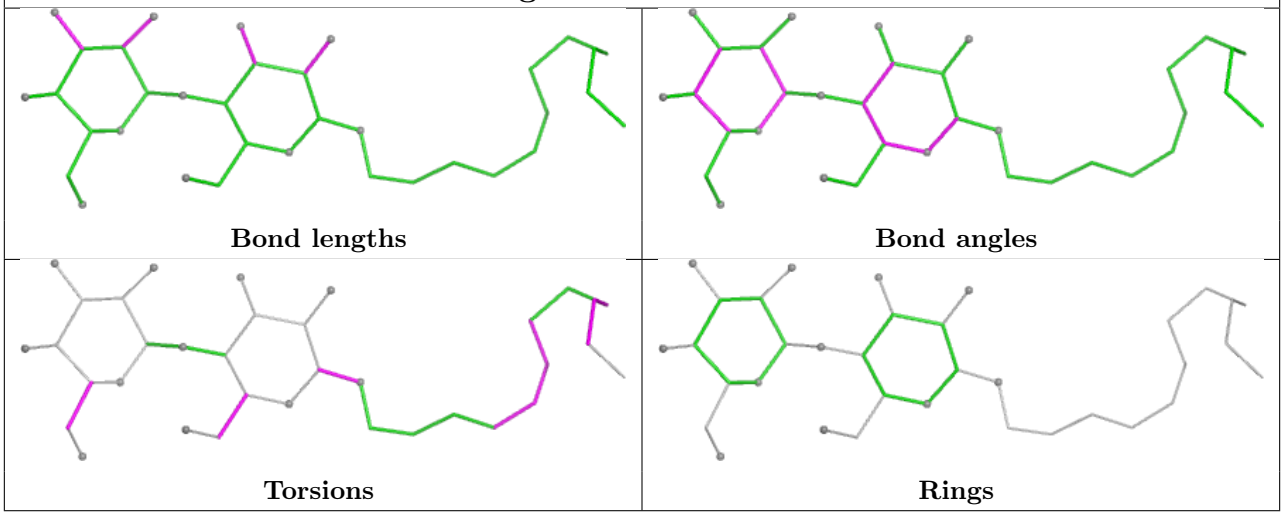
Ligand LMT R 625



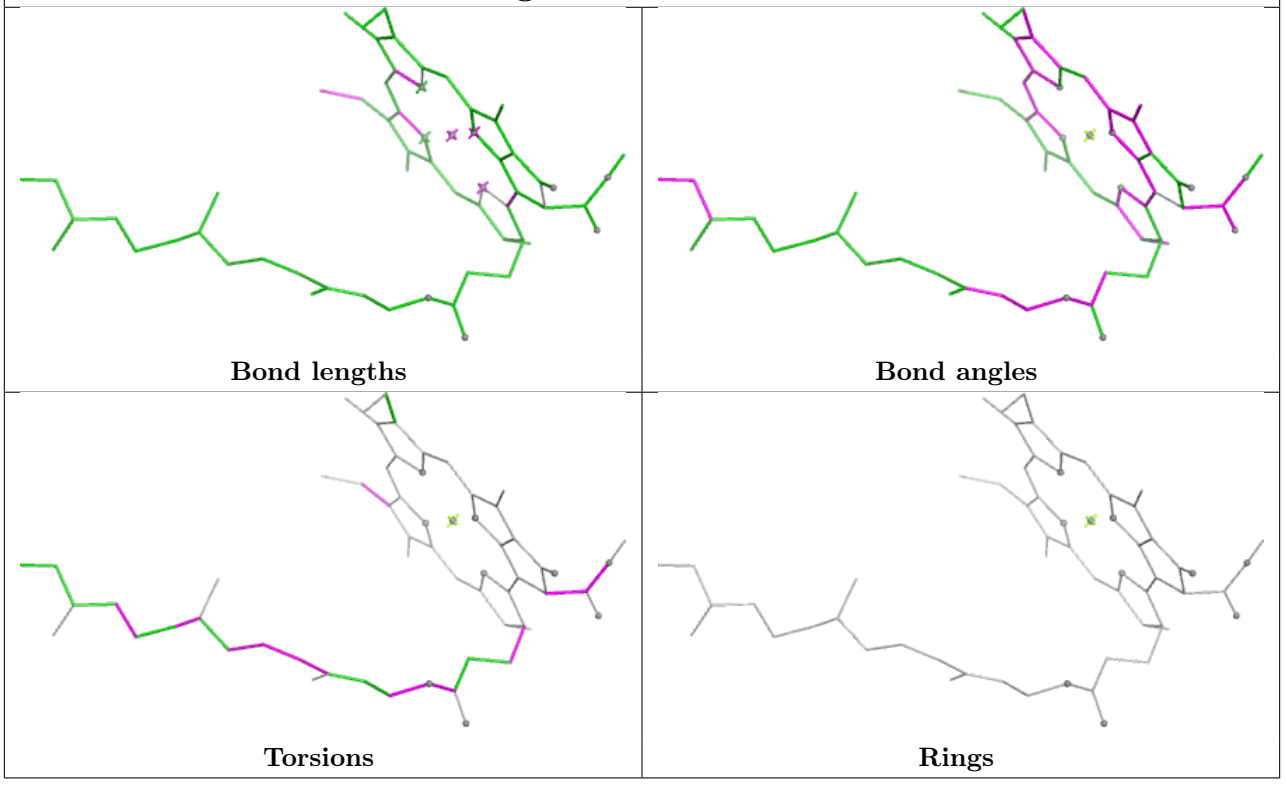
Ligand BCR c 517



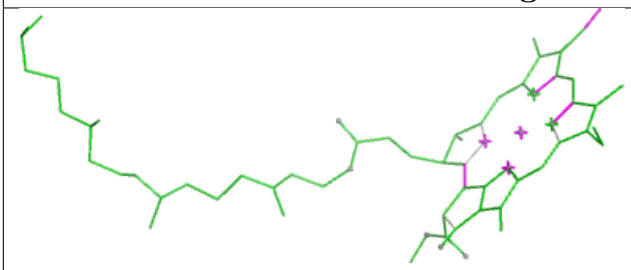
Ligand LMT r1 625



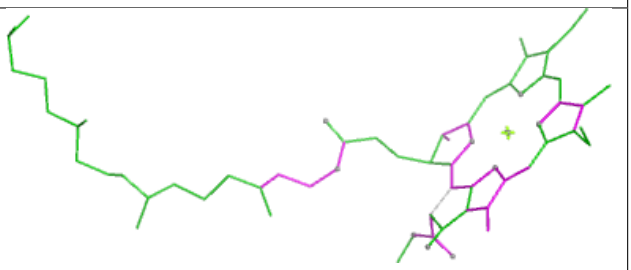
Ligand CLA C1 504



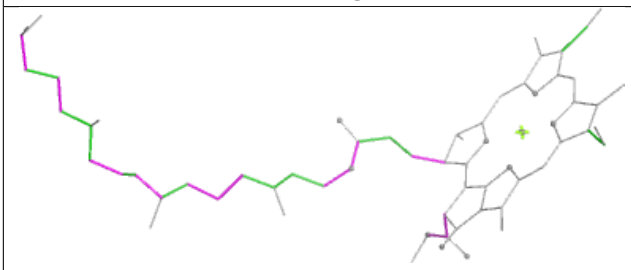
Ligand CLA a1 405



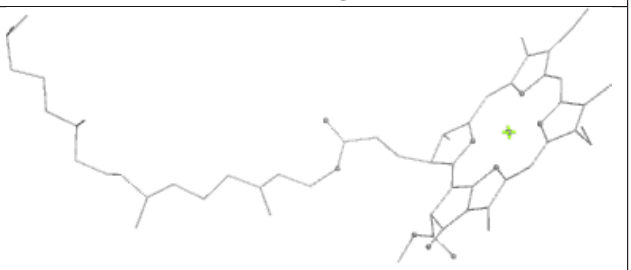
Bond lengths



Bond angles

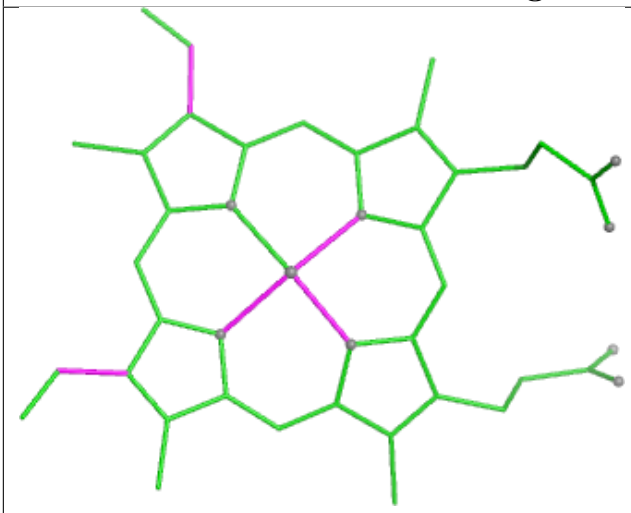


Torsions

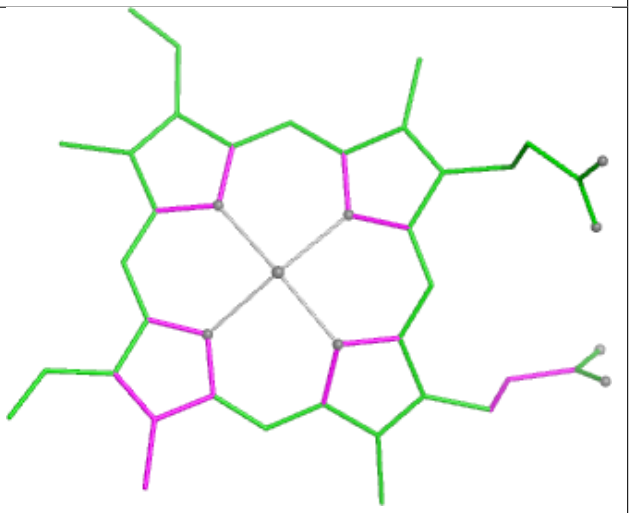


Rings

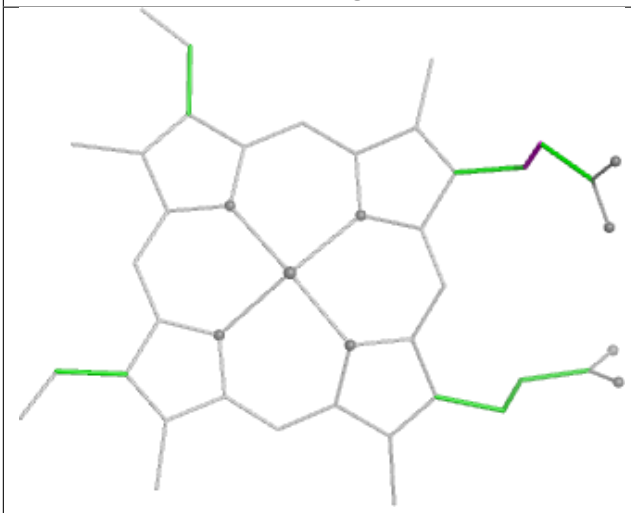
Ligand HEM f 101



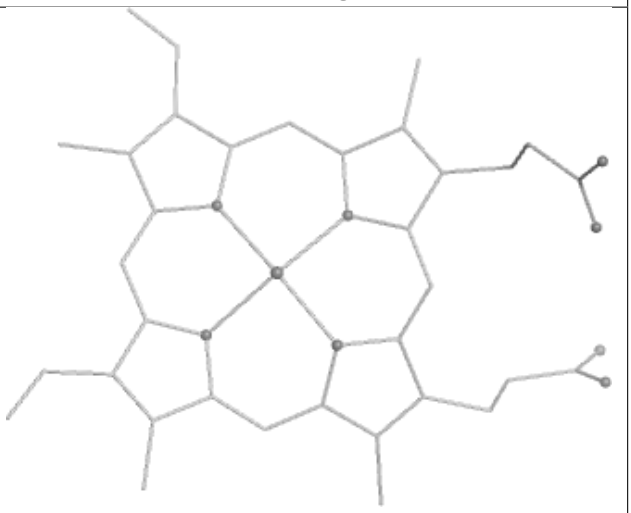
Bond lengths



Bond angles

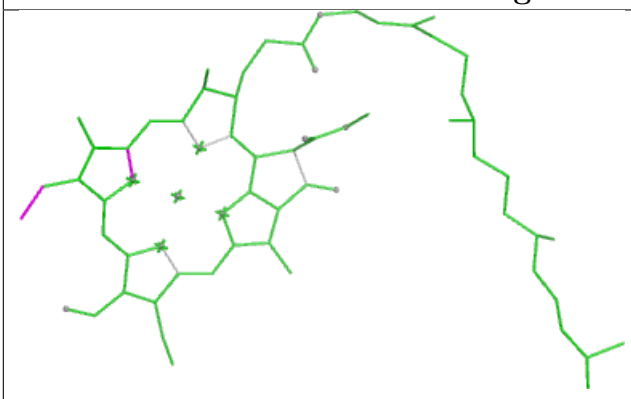


Torsions

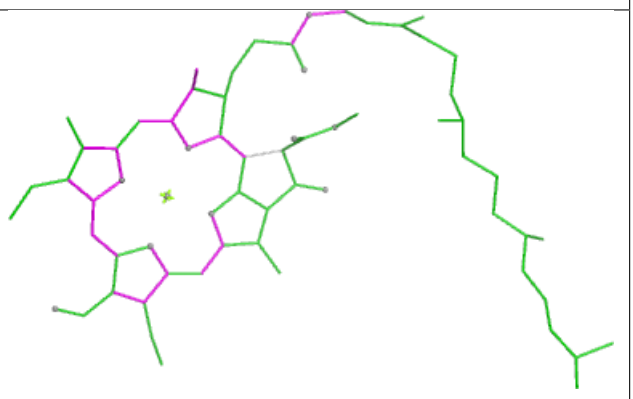


Rings

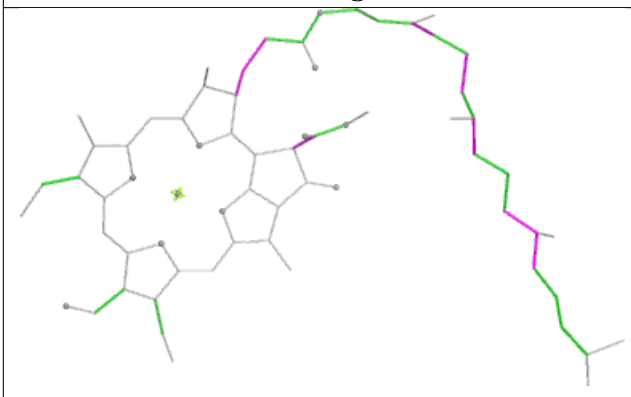
Ligand CHL N1 606



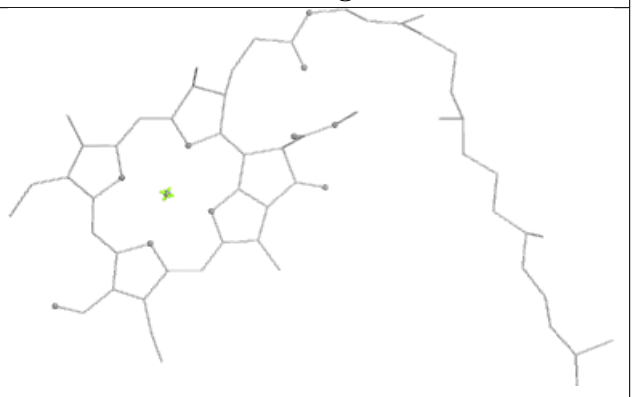
Bond lengths



Bond angles

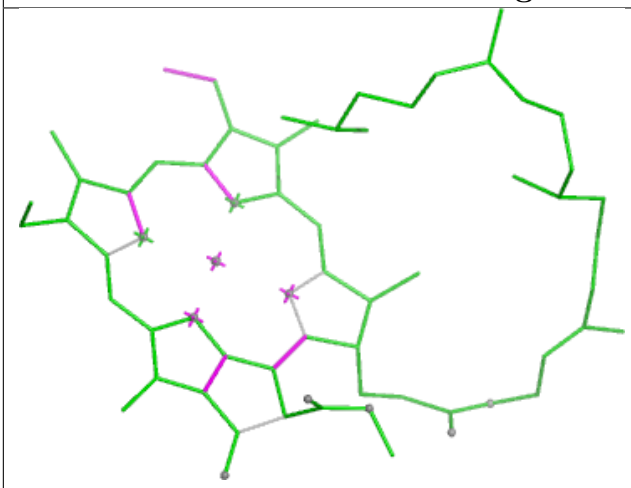


Torsions

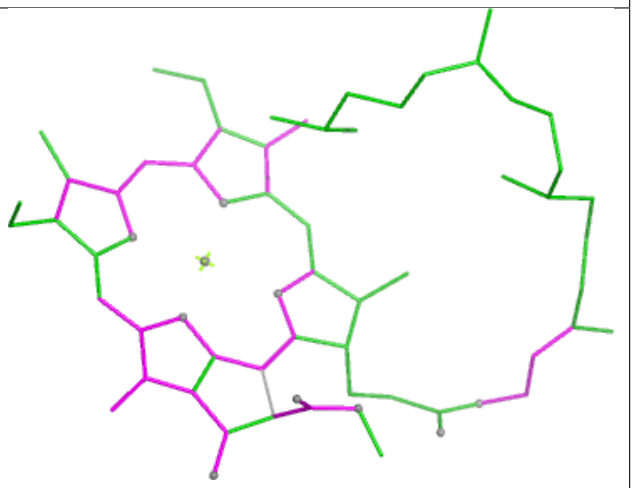


Rings

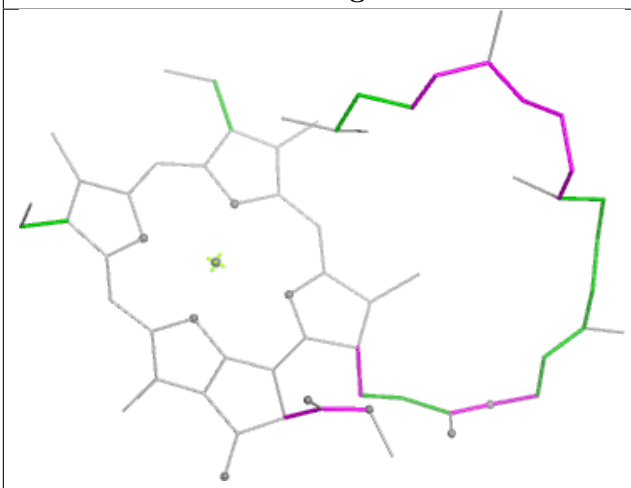
Ligand CLA B1 616



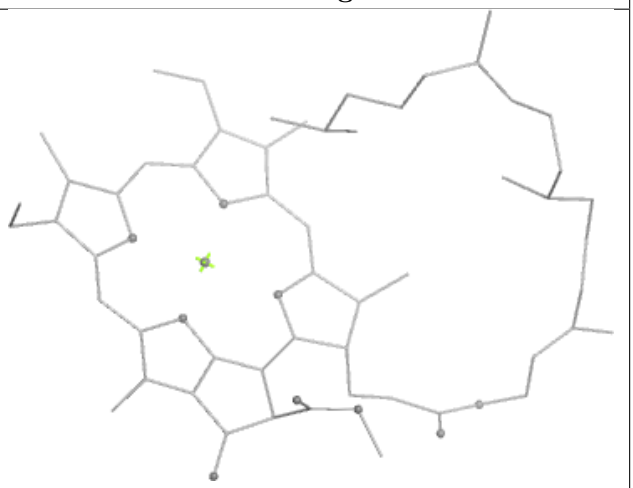
Bond lengths



Bond angles

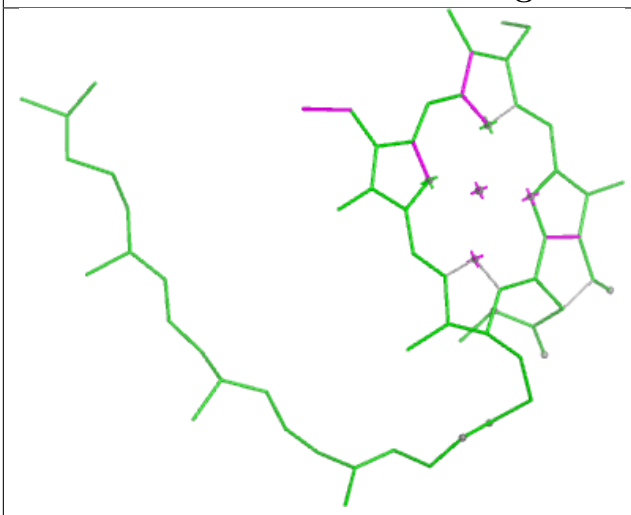


Torsions

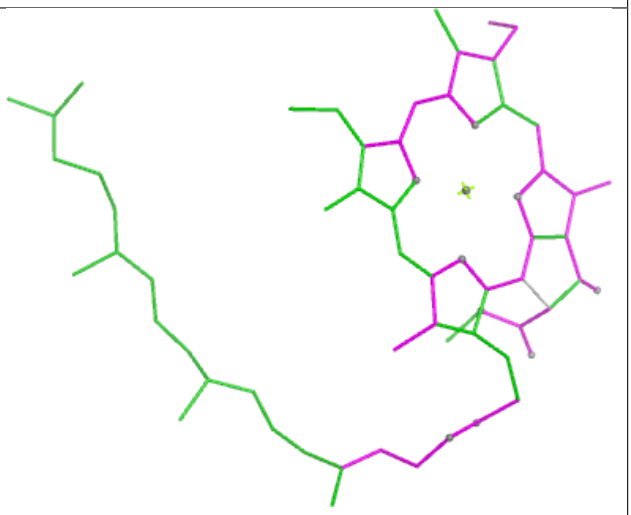


Rings

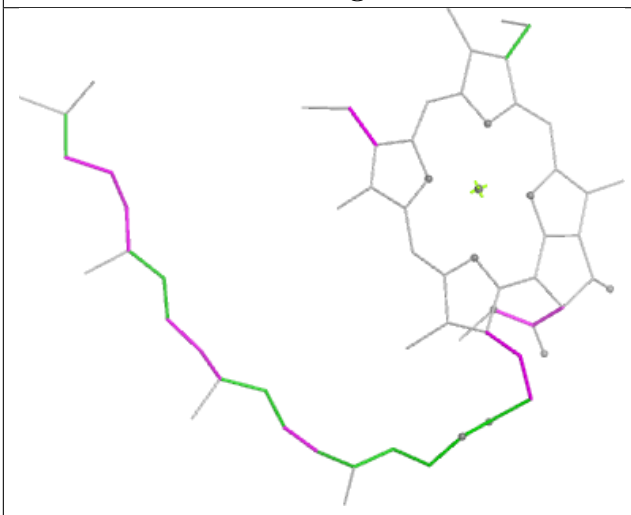
Ligand CLA C1 507



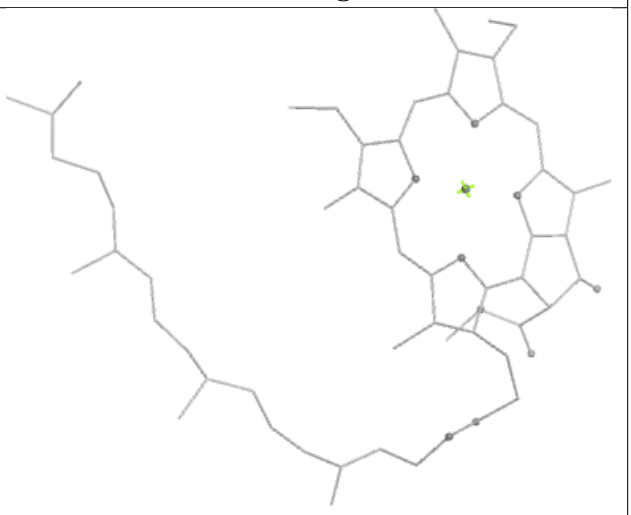
Bond lengths



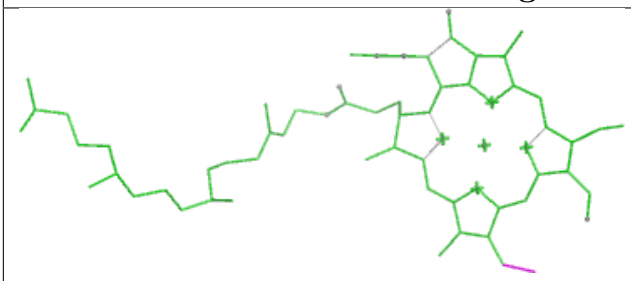
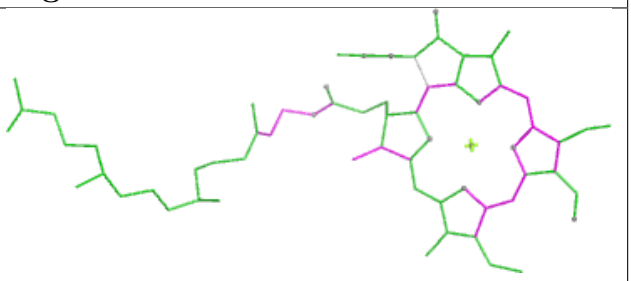
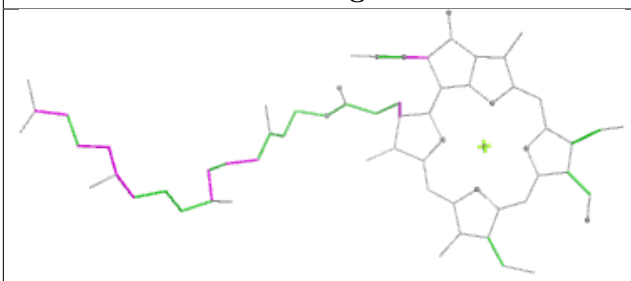
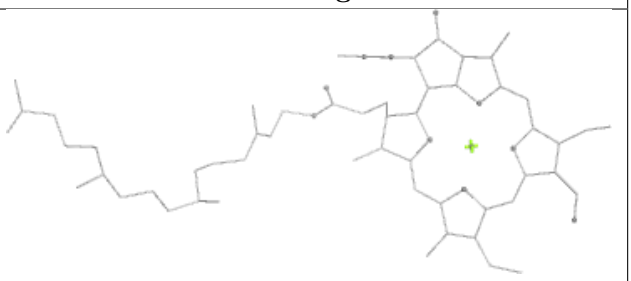
Bond angles

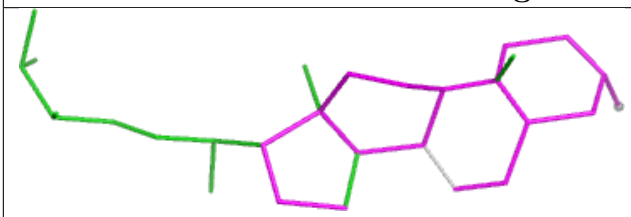
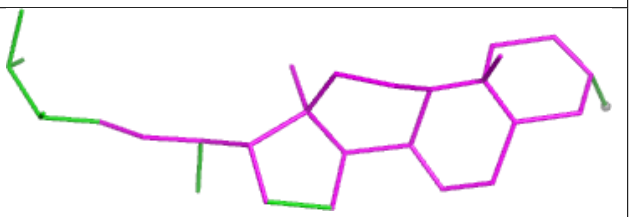
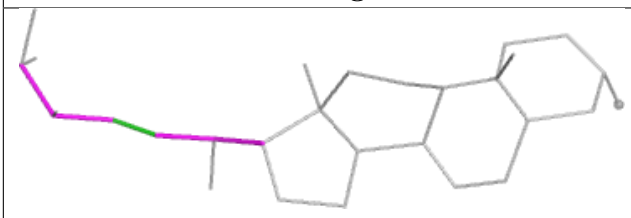
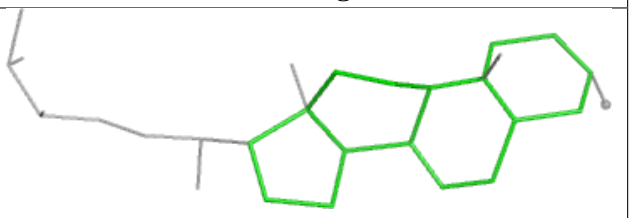


Torsions

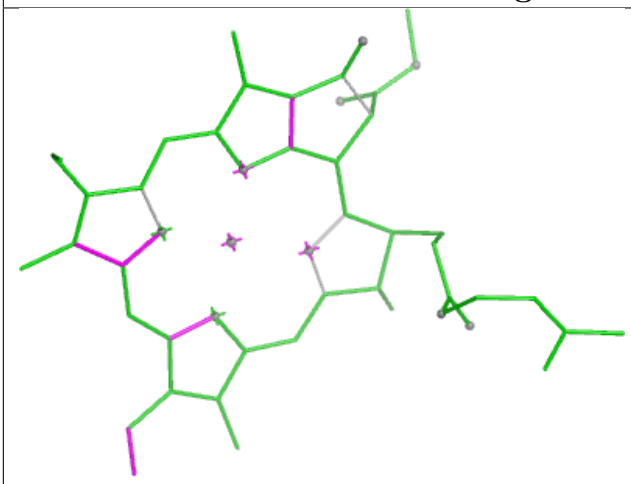


Rings

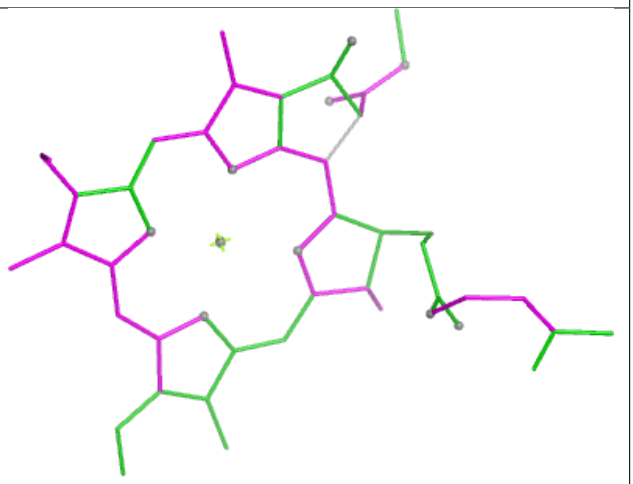
Ligand CHL g1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ERG R1 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

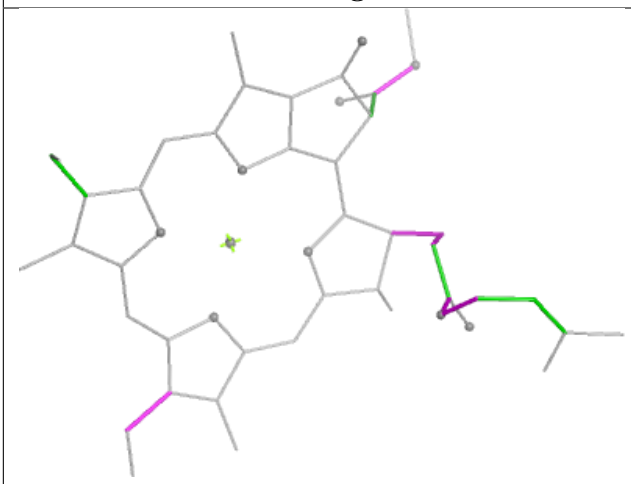
Ligand CLA Y1 608



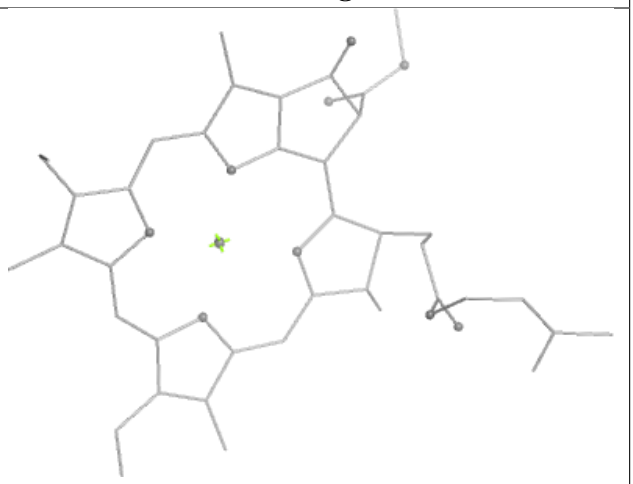
Bond lengths



Bond angles

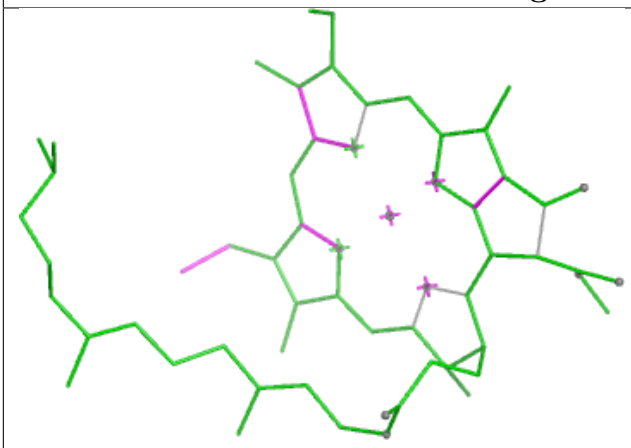


Torsions

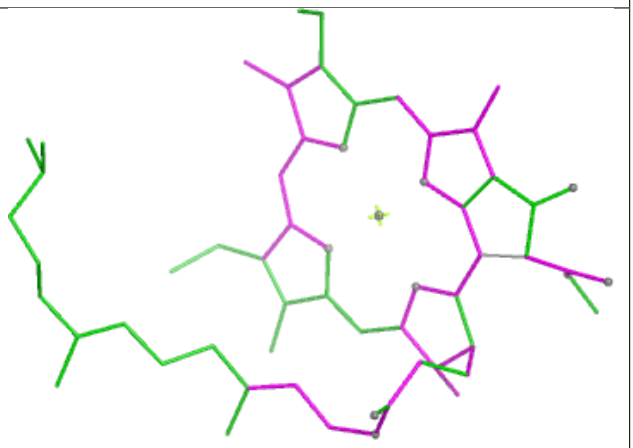


Rings

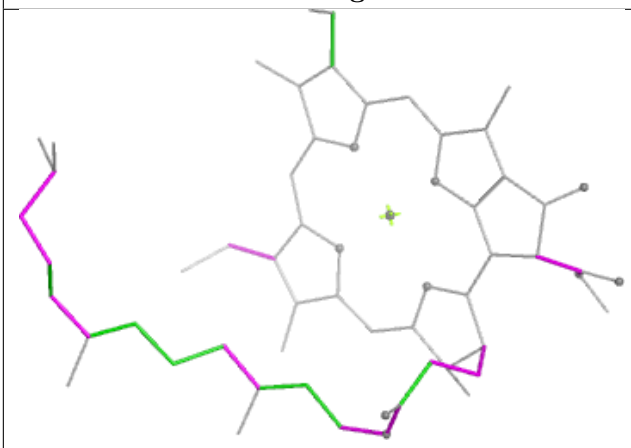
Ligand CLA s 602



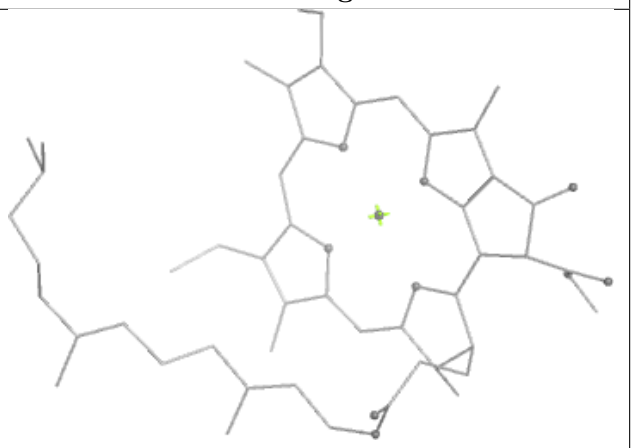
Bond lengths



Bond angles

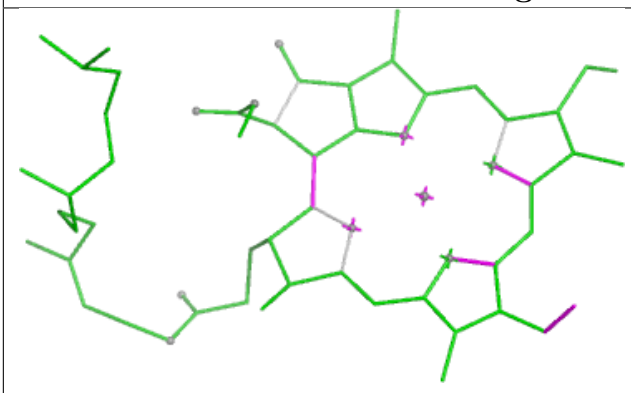


Torsions

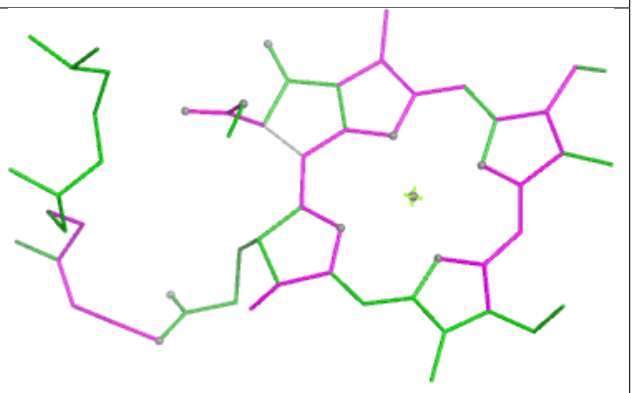


Rings

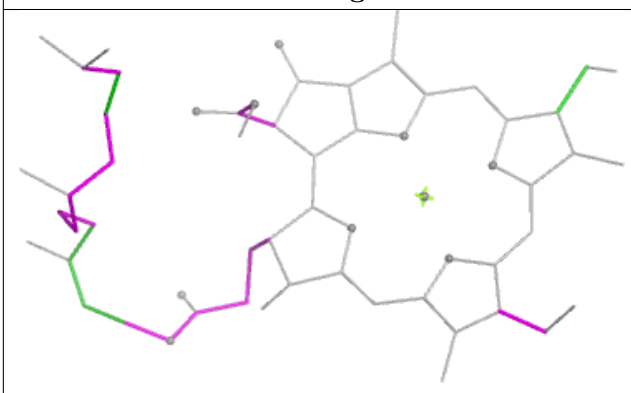
Ligand CLA R1 612



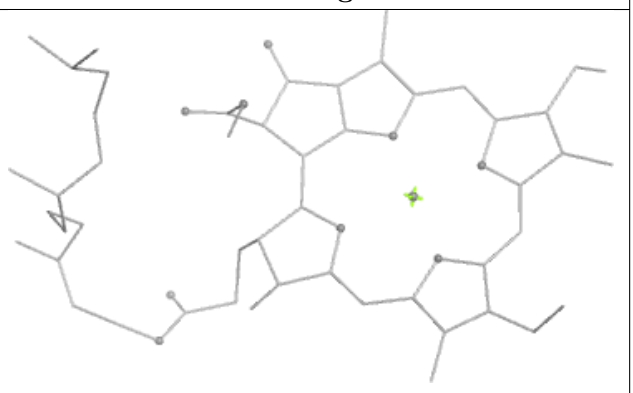
Bond lengths



Bond angles



Torsions

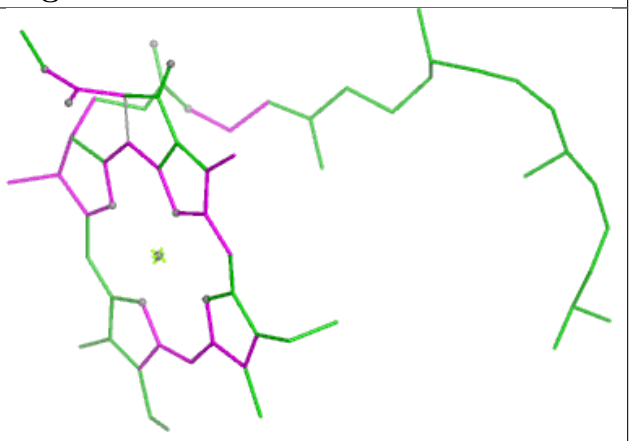


Rings

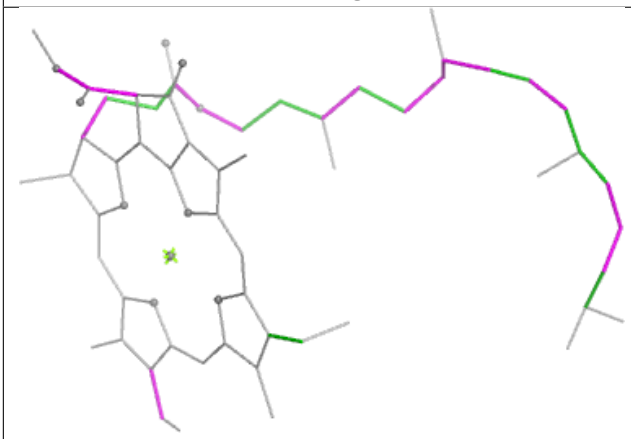
Ligand CLA g1 611



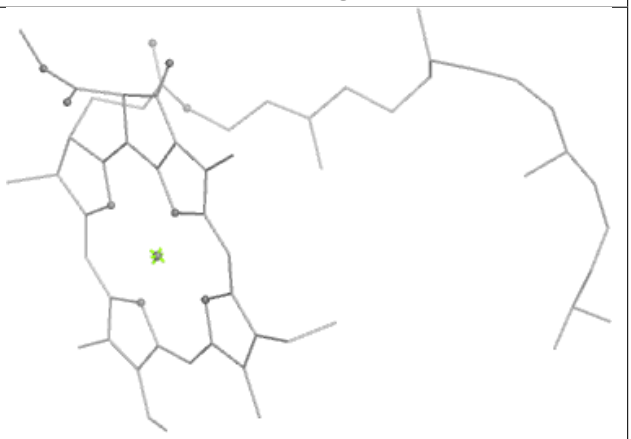
Bond lengths



Bond angles

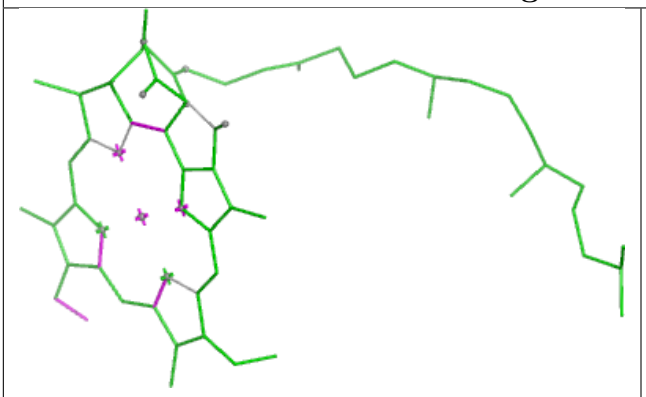


Torsions

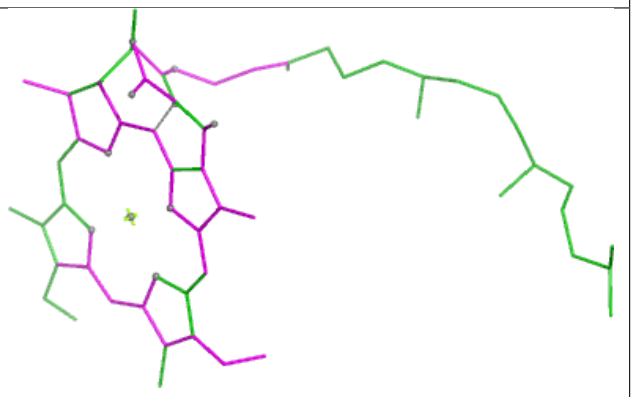


Rings

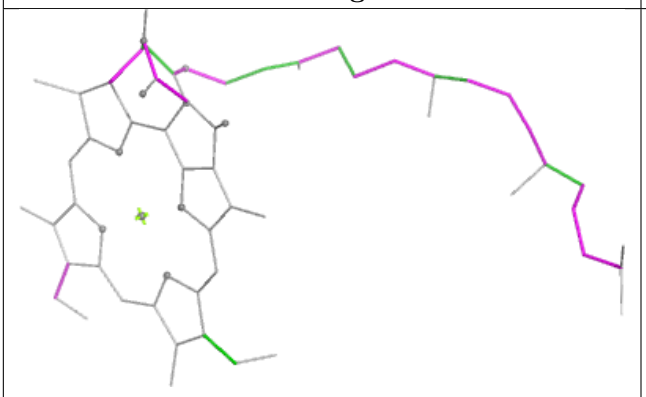
Ligand CLA s1 611



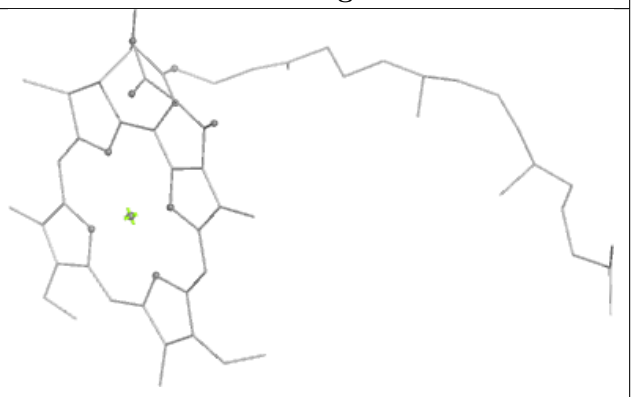
Bond lengths



Bond angles

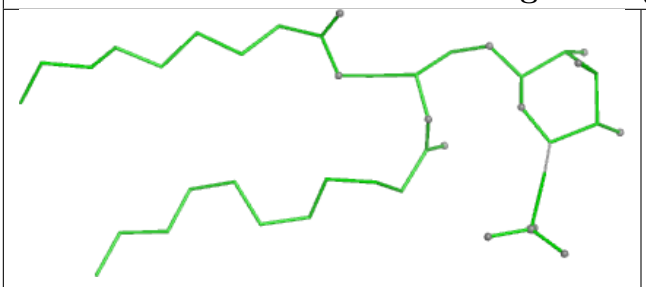


Torsions

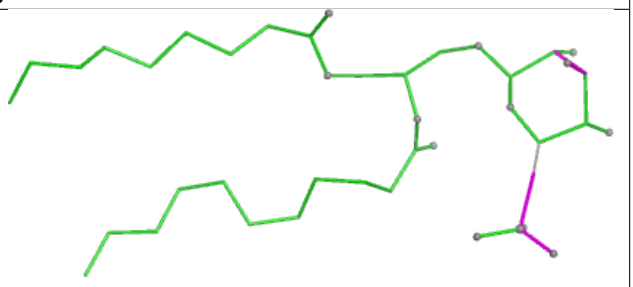


Rings

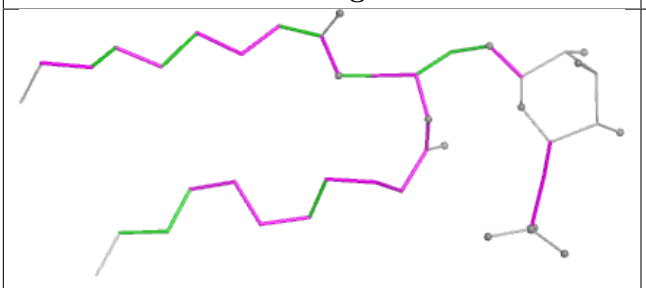
Ligand SQD M 101



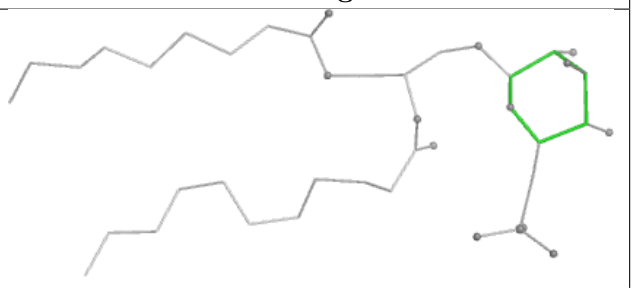
Bond lengths



Bond angles

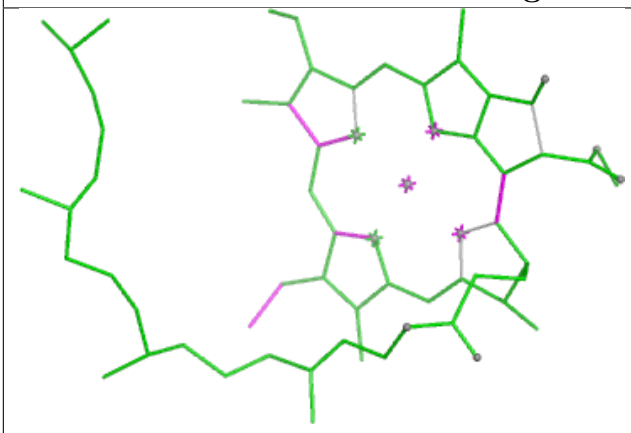


Torsions

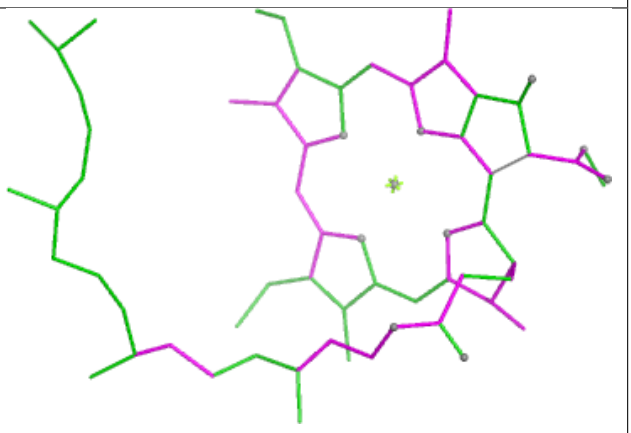


Rings

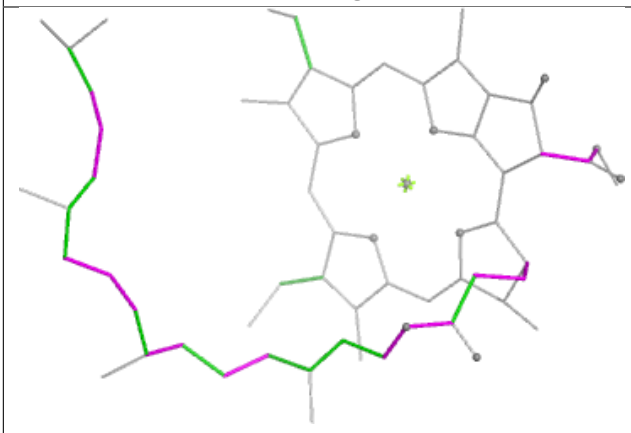
Ligand CLA N 602



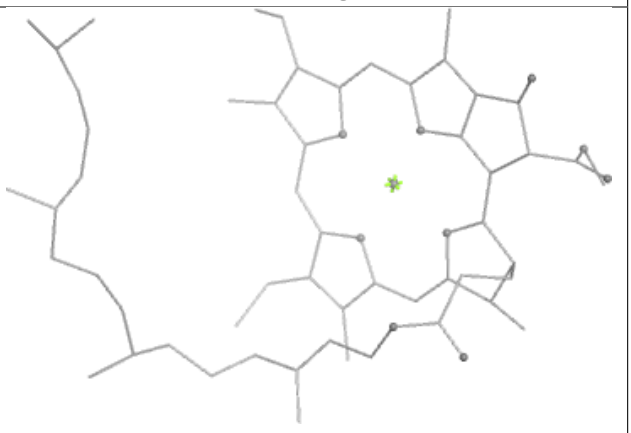
Bond lengths



Bond angles

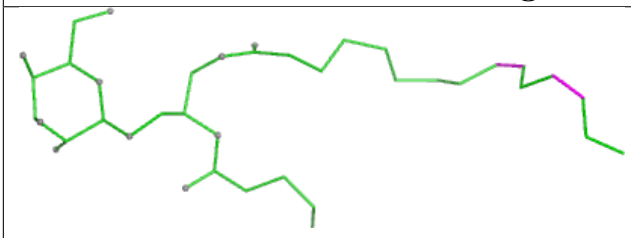


Torsions

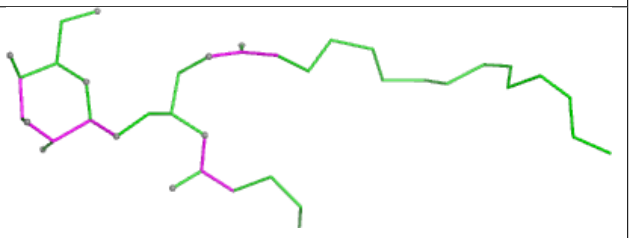


Rings

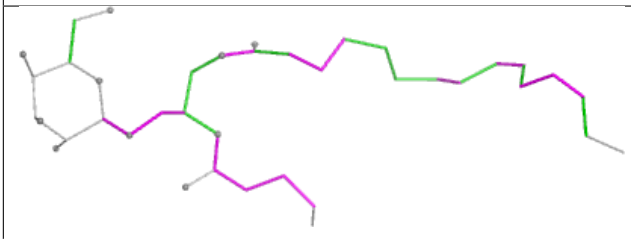
Ligand LMG w 201



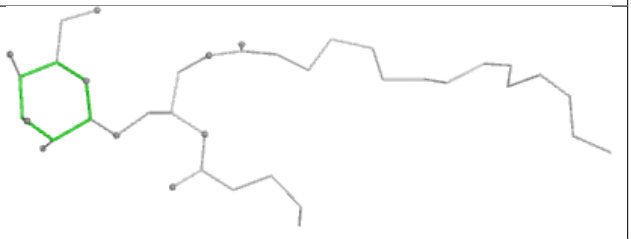
Bond lengths



Bond angles

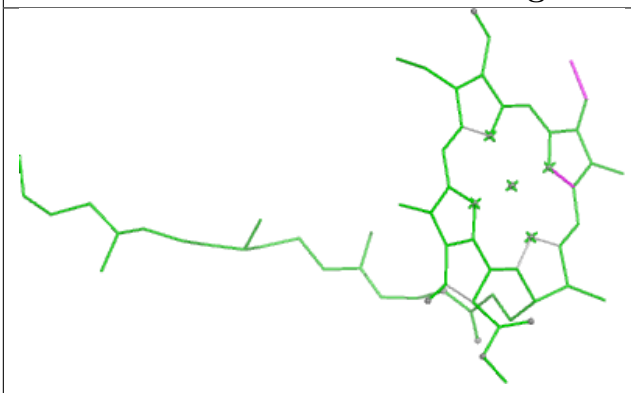


Torsions

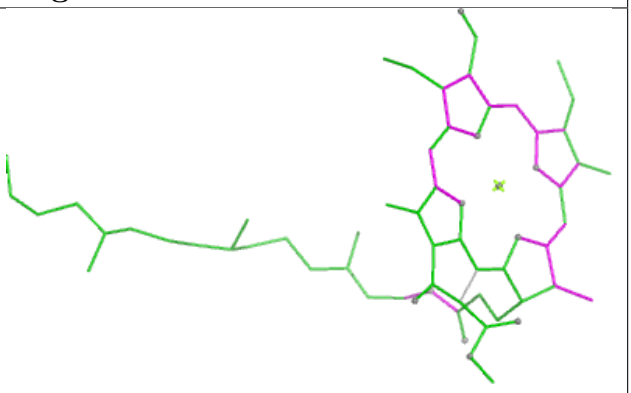


Rings

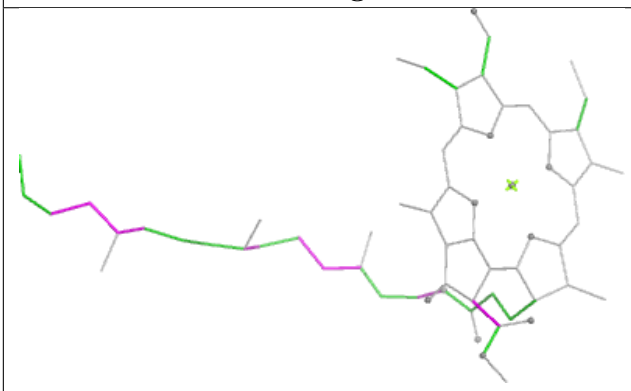
Ligand CHL g 609



Bond lengths



Bond angles

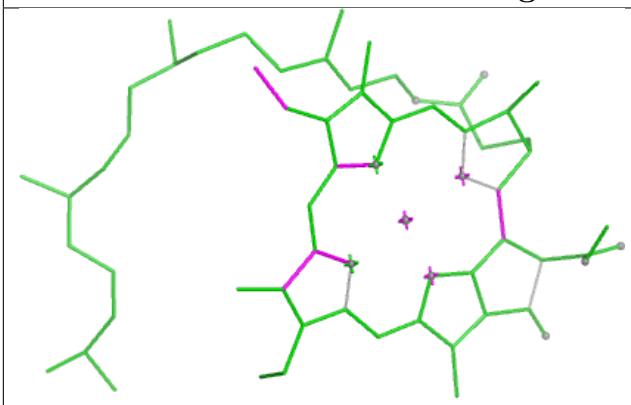


Torsions

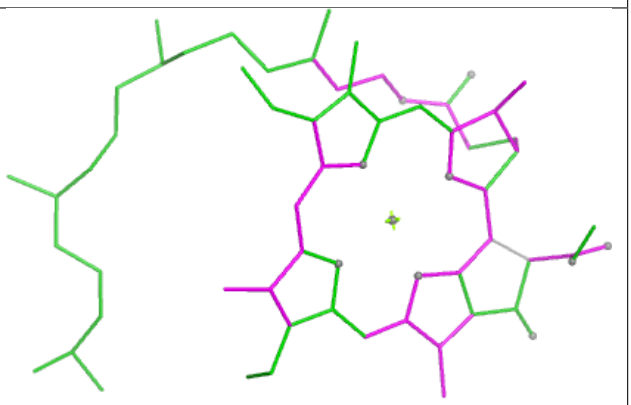


Rings

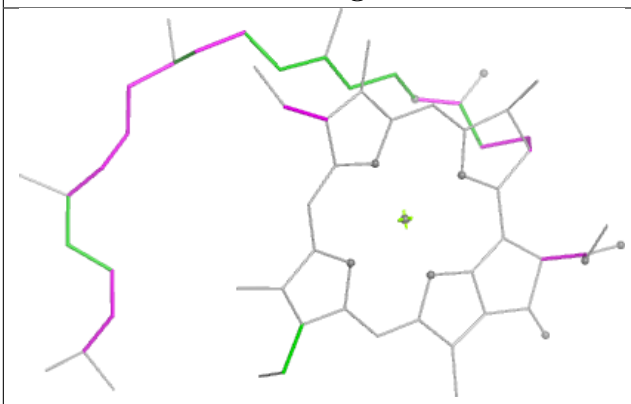
Ligand CLA n1 602



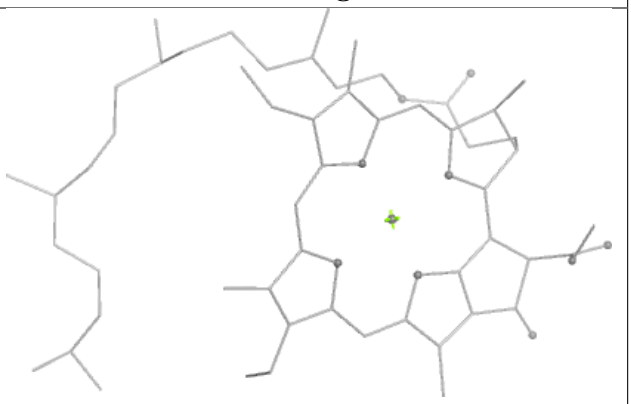
Bond lengths



Bond angles

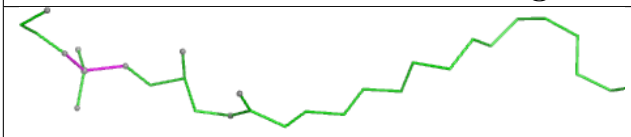


Torsions

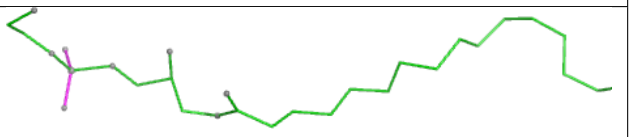


Rings

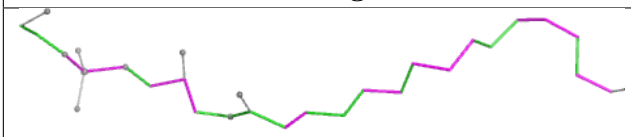
Ligand LPX s 625



Bond lengths



Bond angles

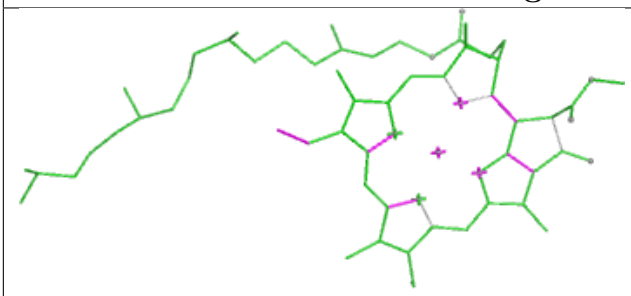


Torsions

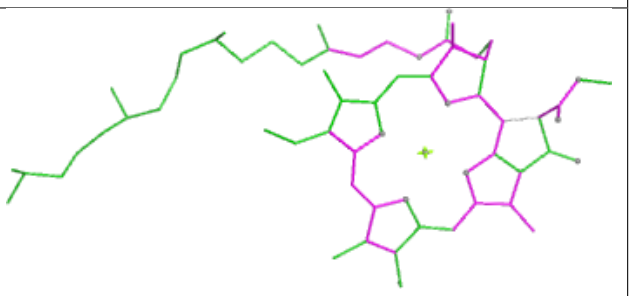


Rings

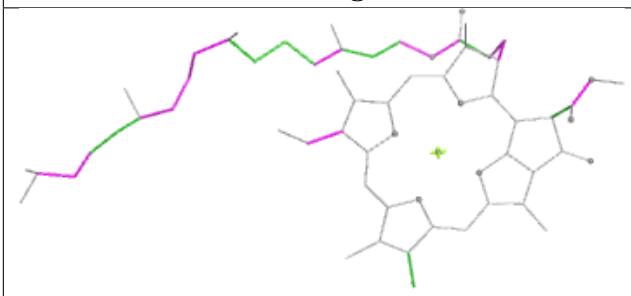
Ligand CLA C 501



Bond lengths



Bond angles

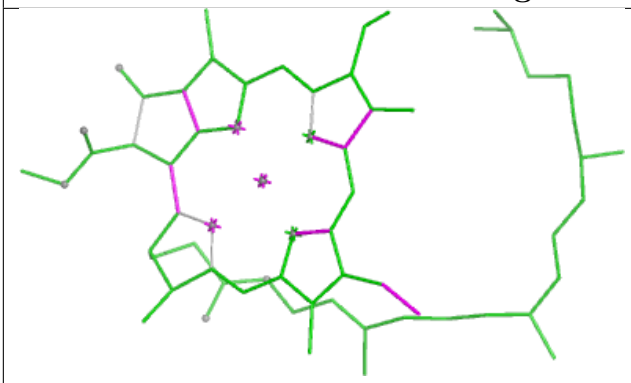


Torsions

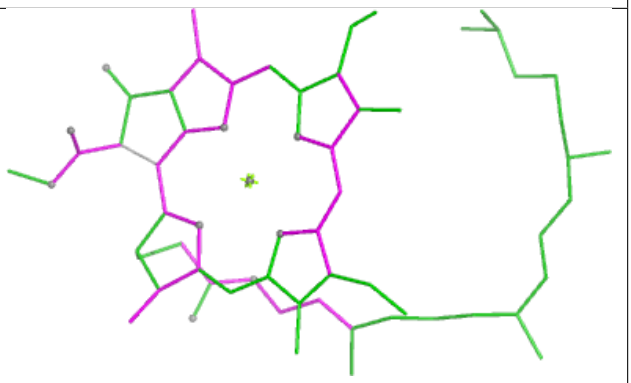


Rings

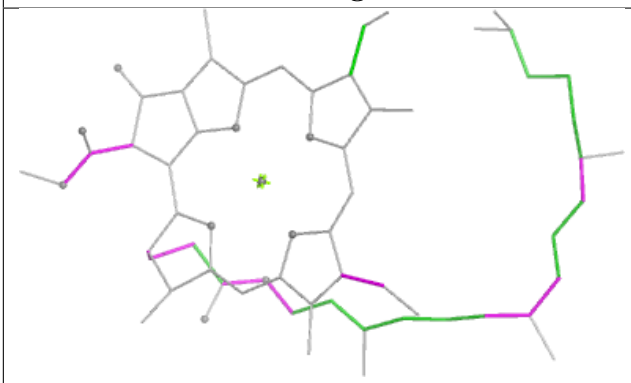
Ligand CLA G1 610



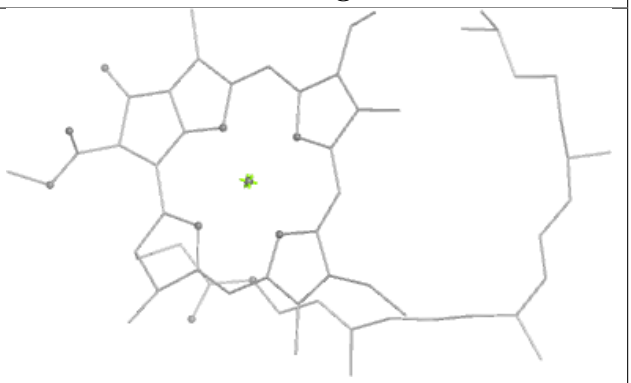
Bond lengths



Bond angles

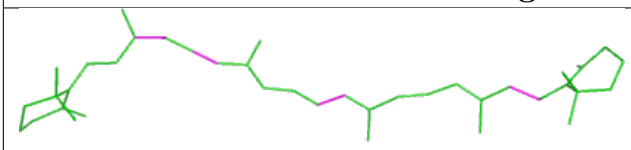


Torsions

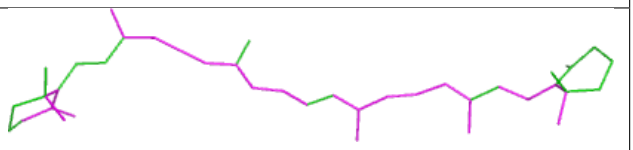


Rings

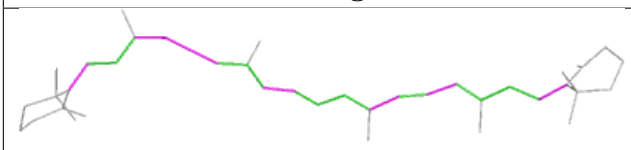
Ligand BCR c1 514



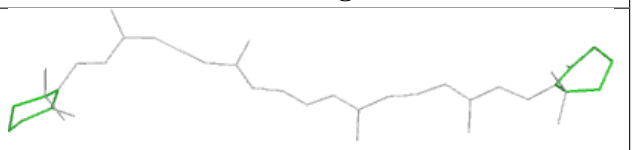
Bond lengths



Bond angles

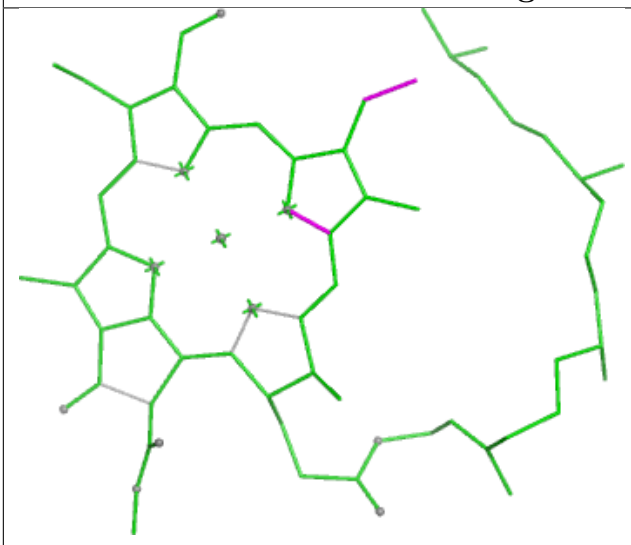


Torsions

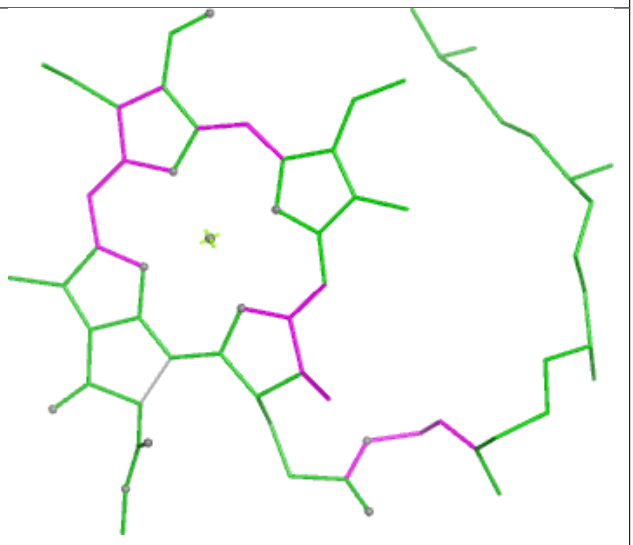


Rings

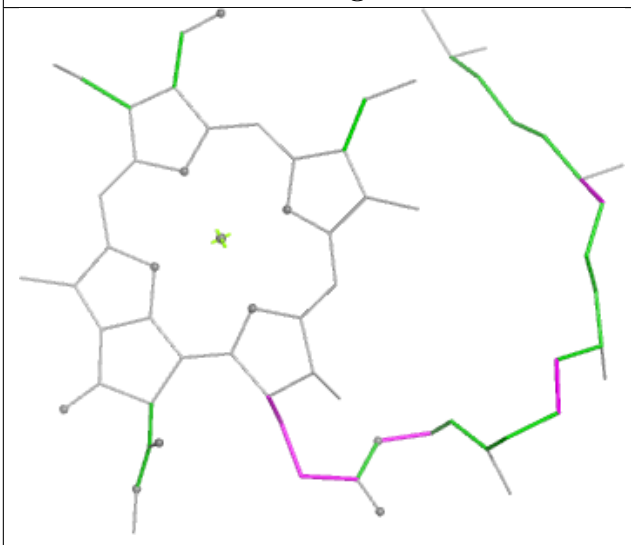
Ligand CHL n1 607



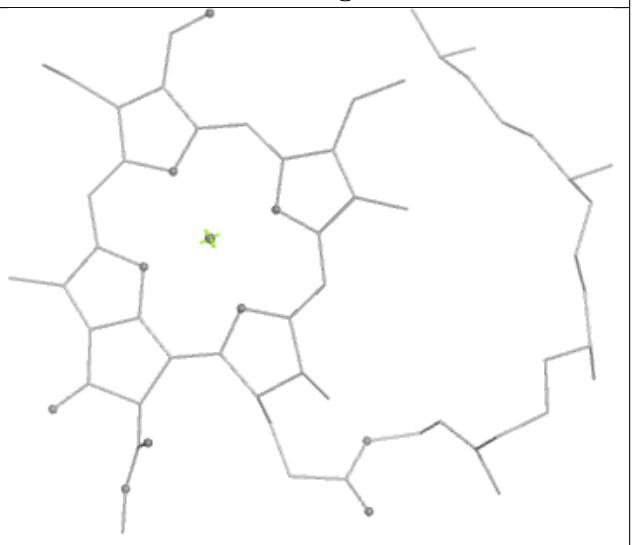
Bond lengths



Bond angles

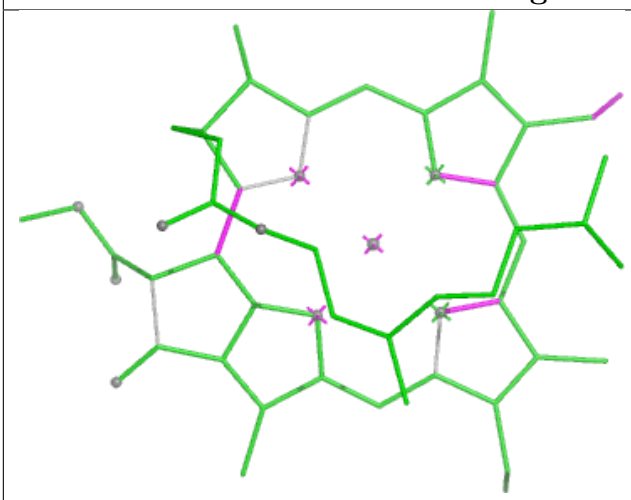


Torsions

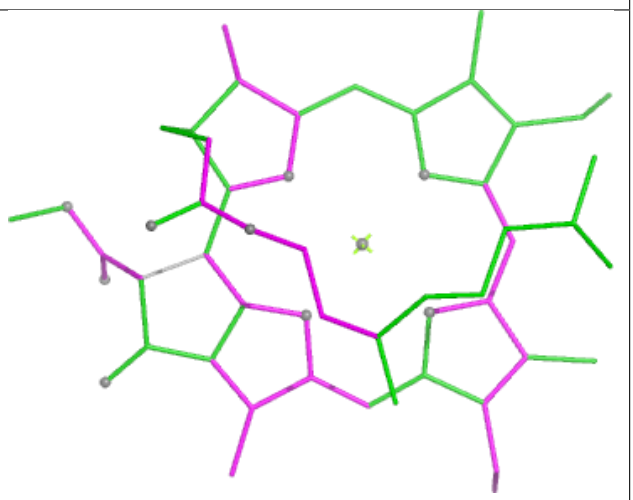


Rings

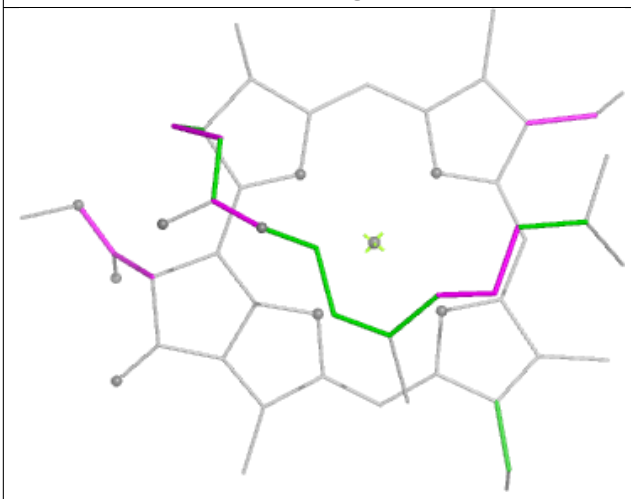
Ligand CLA s 613



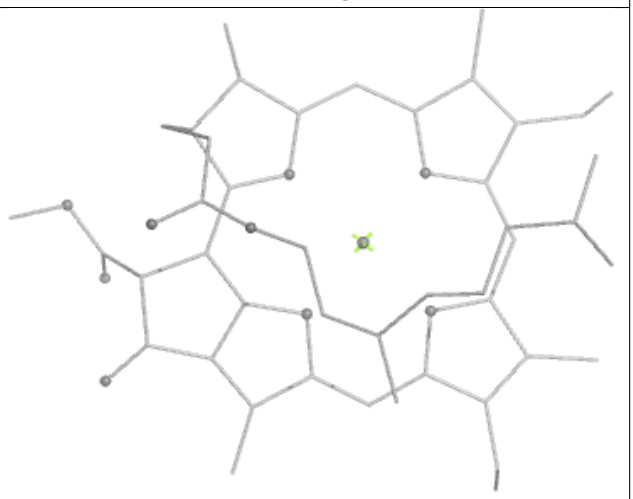
Bond lengths



Bond angles



Torsions

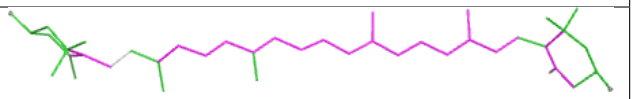


Rings

Ligand LUT r1 620



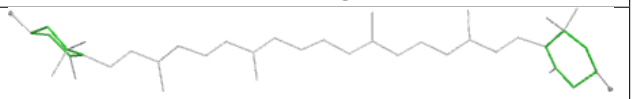
Bond lengths



Bond angles

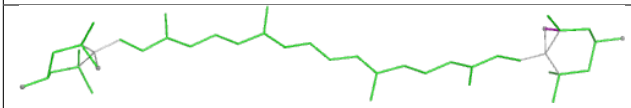


Torsions

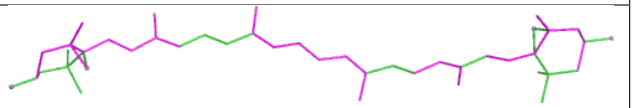


Rings

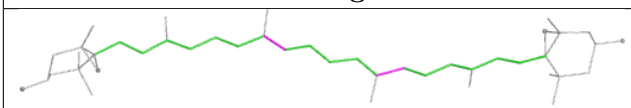
Ligand XAT R1 621



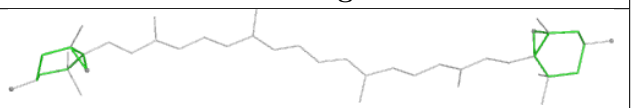
Bond lengths



Bond angles

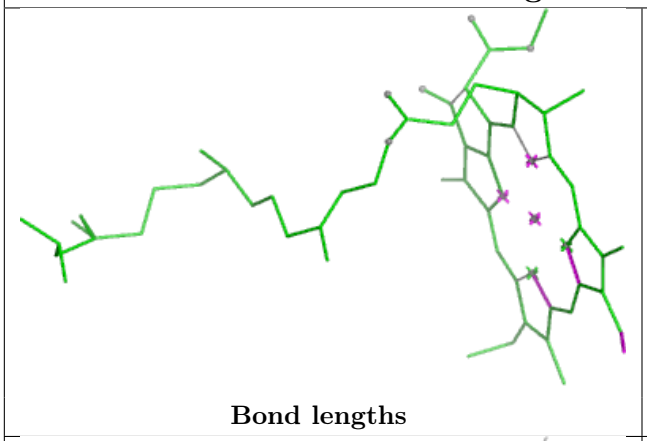


Torsions

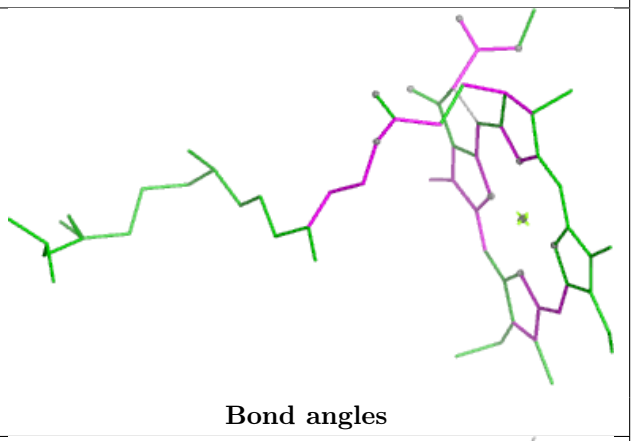


Rings

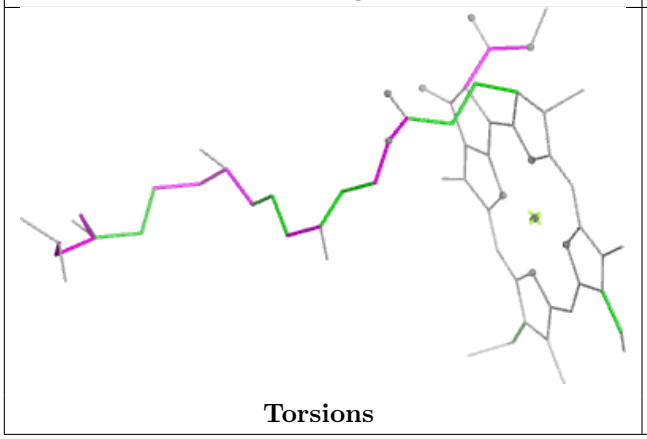
Ligand CLA Y 604



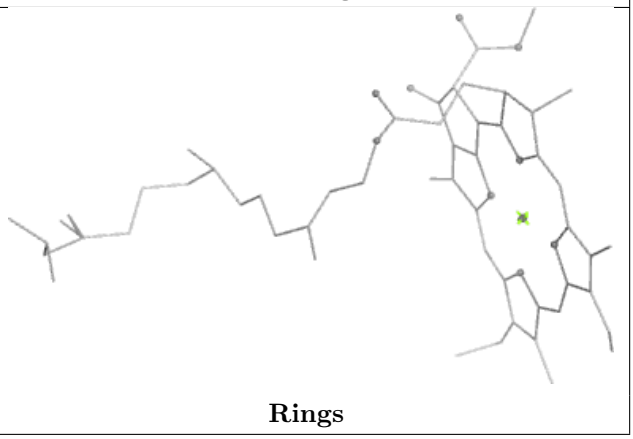
Bond lengths



Bond angles

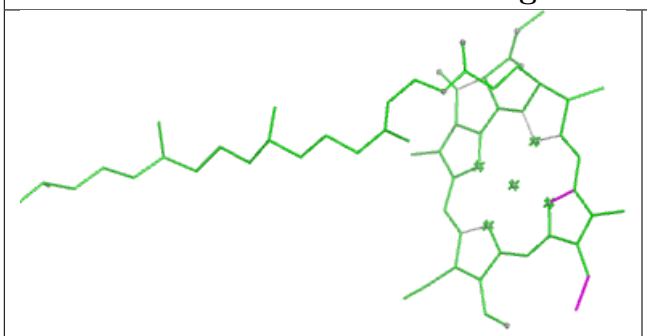


Torsions

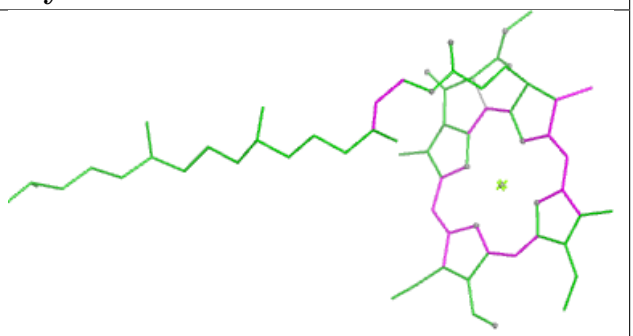


Rings

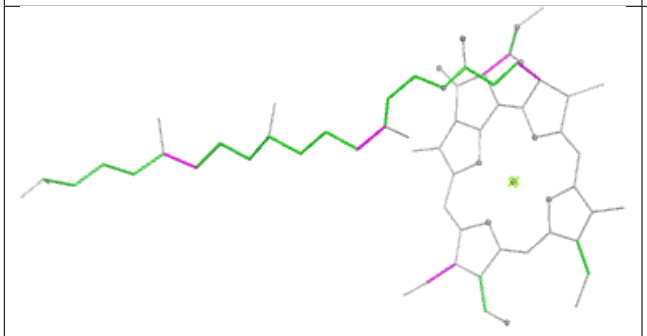
Ligand CHL y1 609



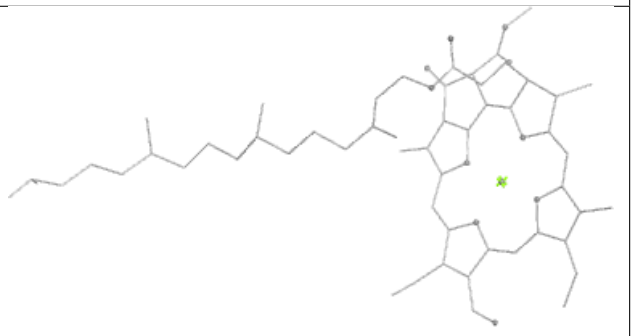
Bond lengths



Bond angles

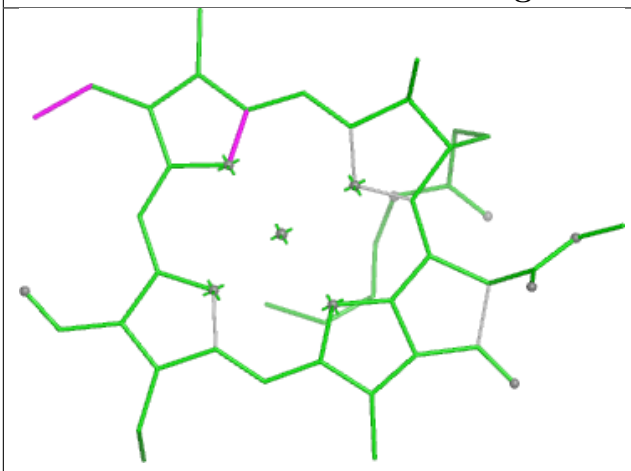


Torsions

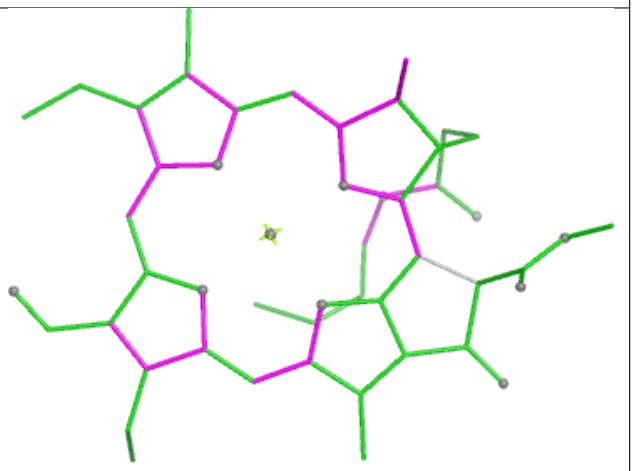


Rings

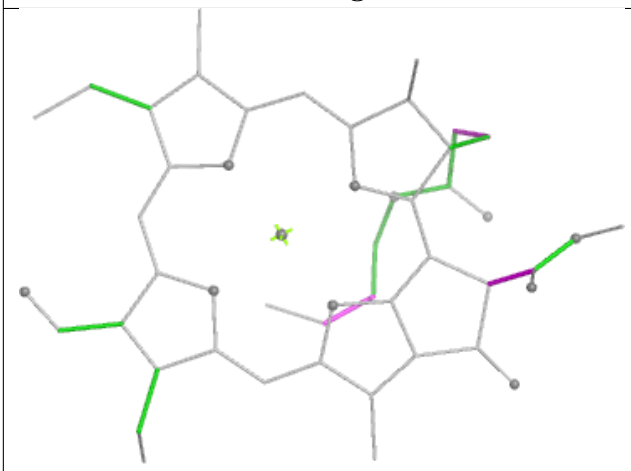
Ligand CHL R1 607



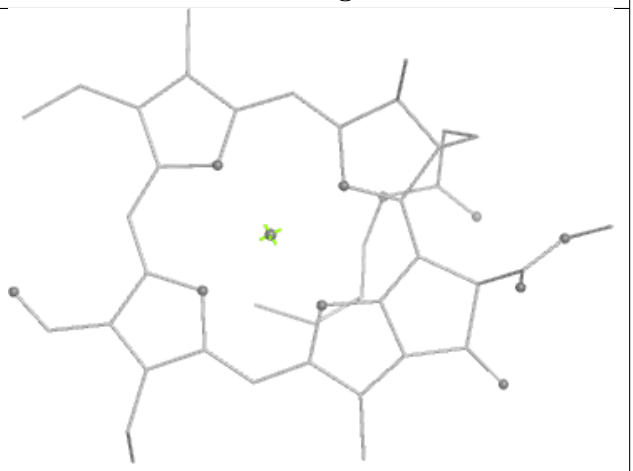
Bond lengths



Bond angles

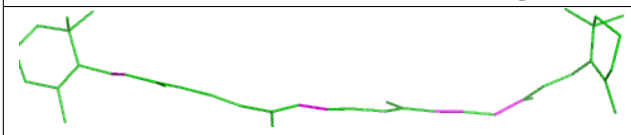


Torsions

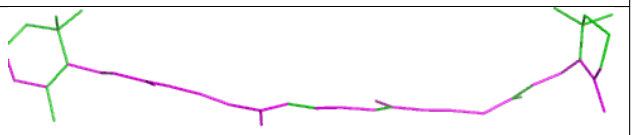


Rings

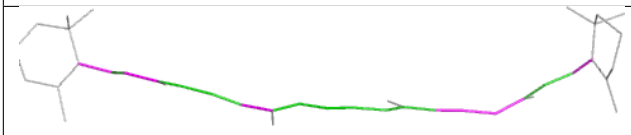
Ligand BCR C1 517



Bond lengths



Bond angles

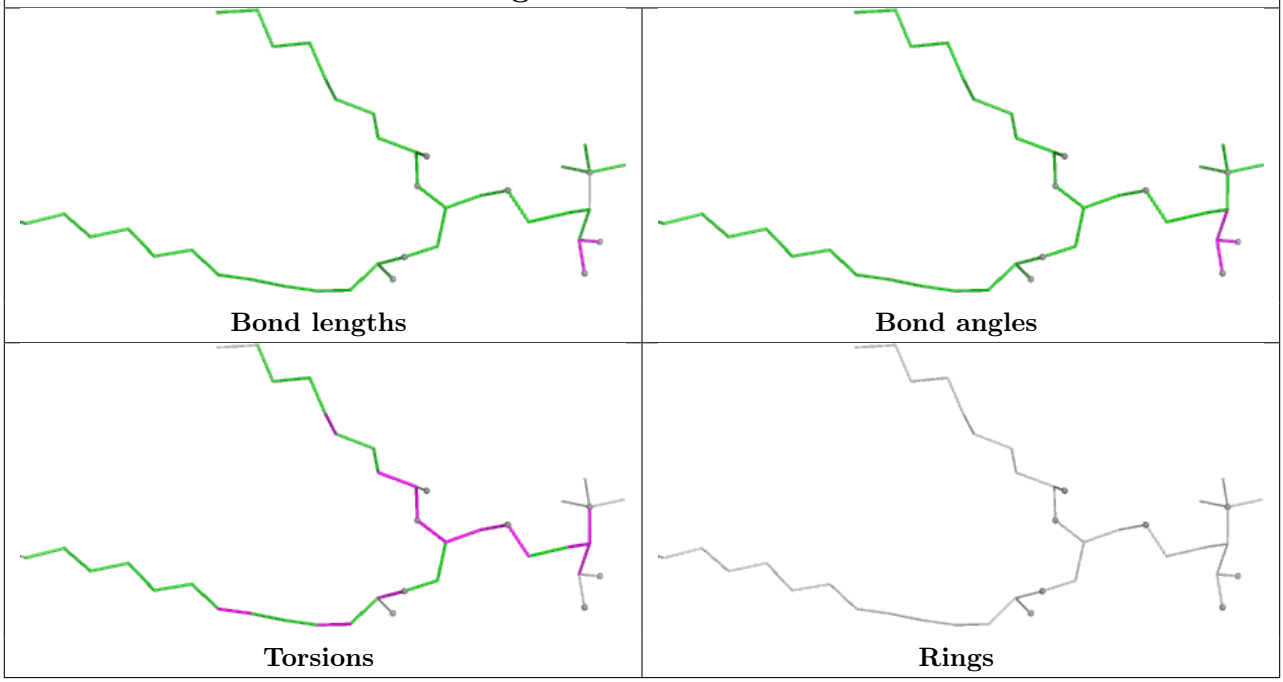


Torsions

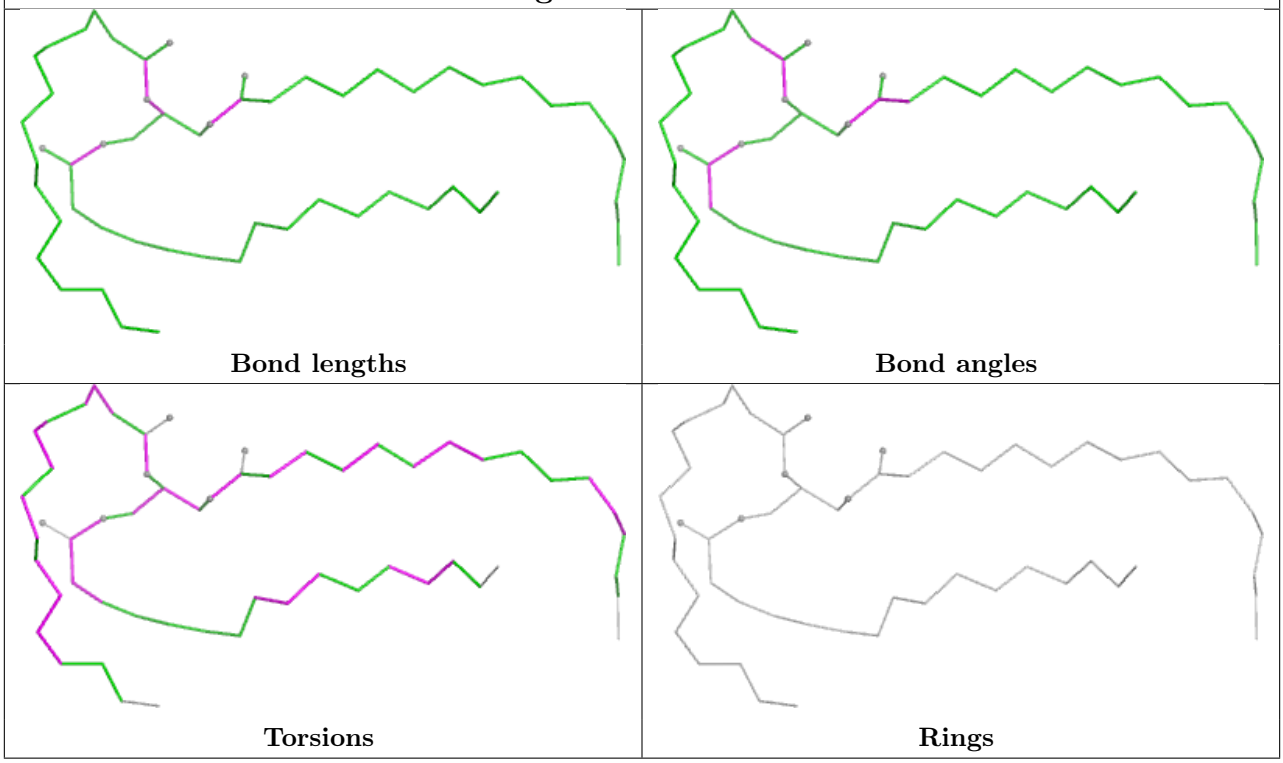


Rings

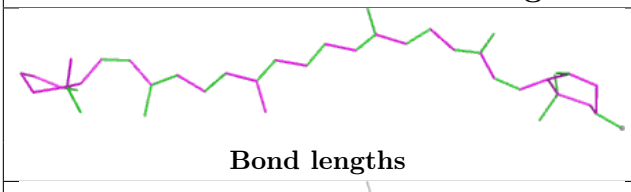
Ligand LMK C1 527



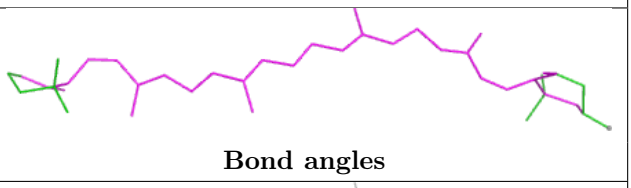
Ligand 4RF I 102



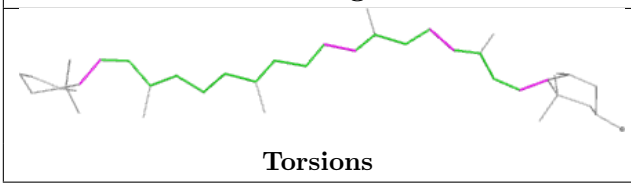
Ligand RRX h 101



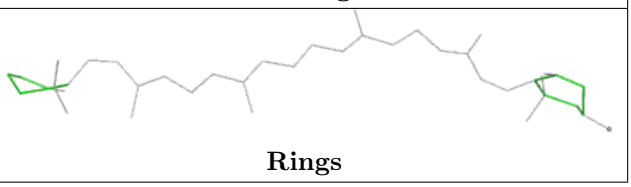
Bond lengths



Bond angles

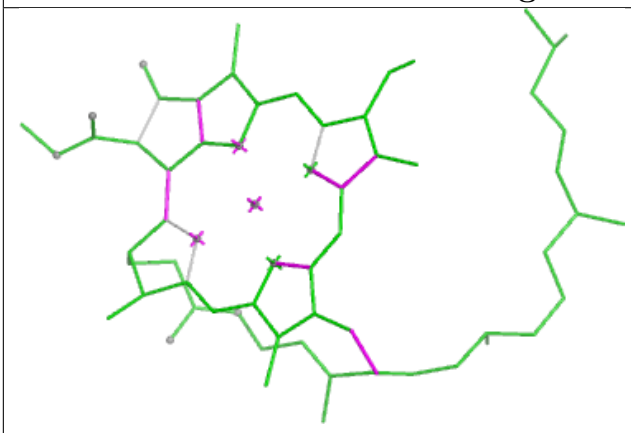


Torsions

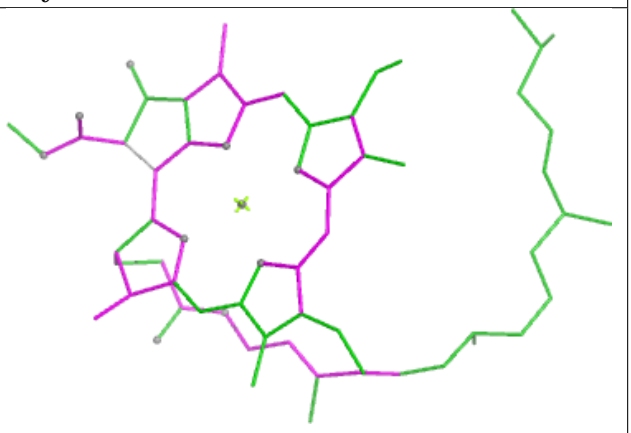


Rings

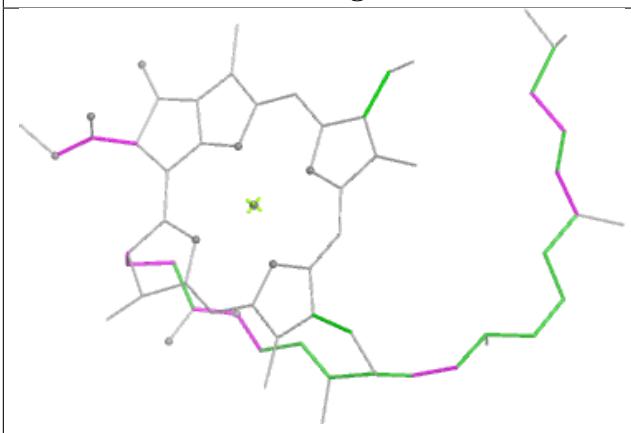
Ligand CLA y1 610



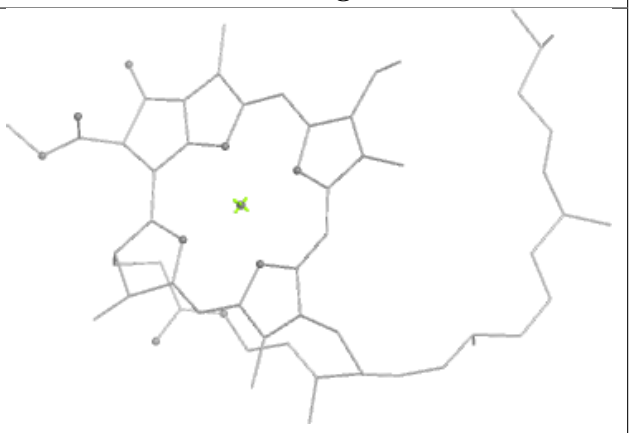
Bond lengths



Bond angles

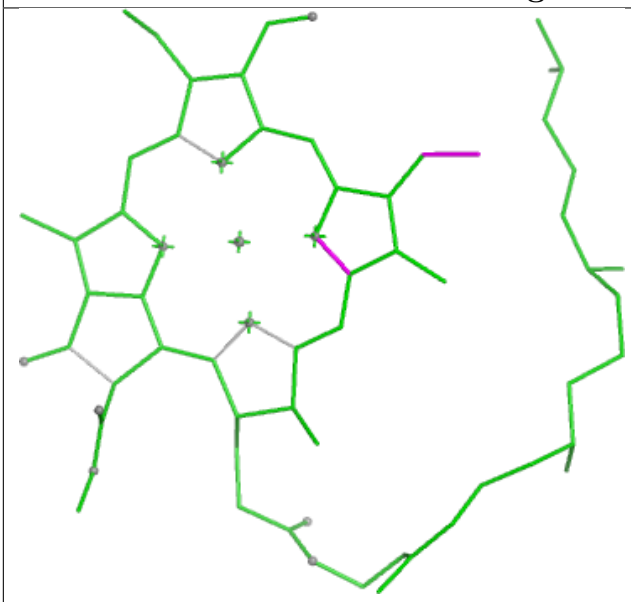


Torsions

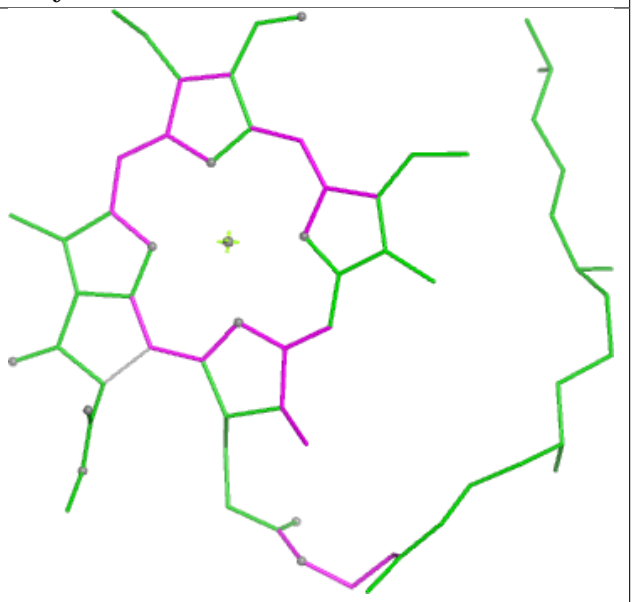


Rings

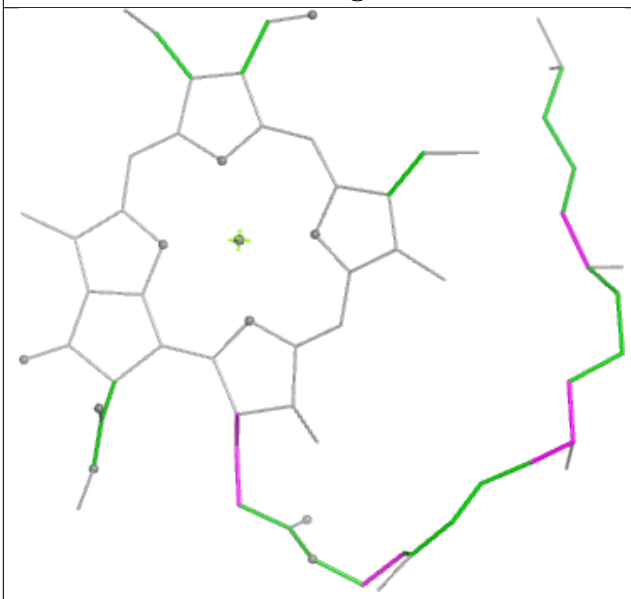
Ligand CHL y 607



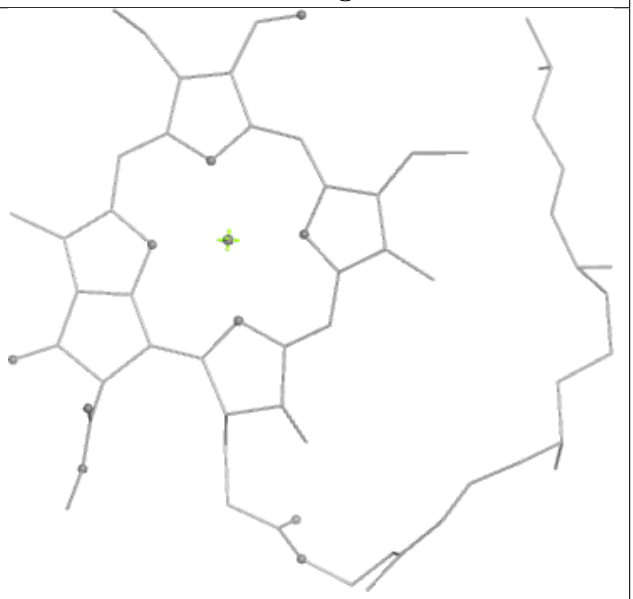
Bond lengths



Bond angles

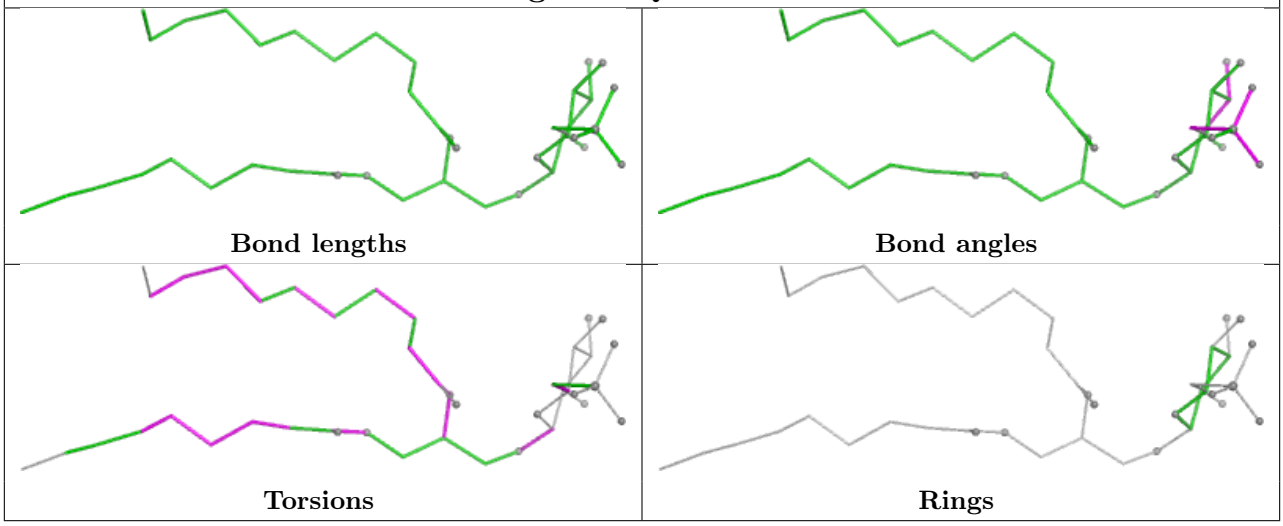


Torsions

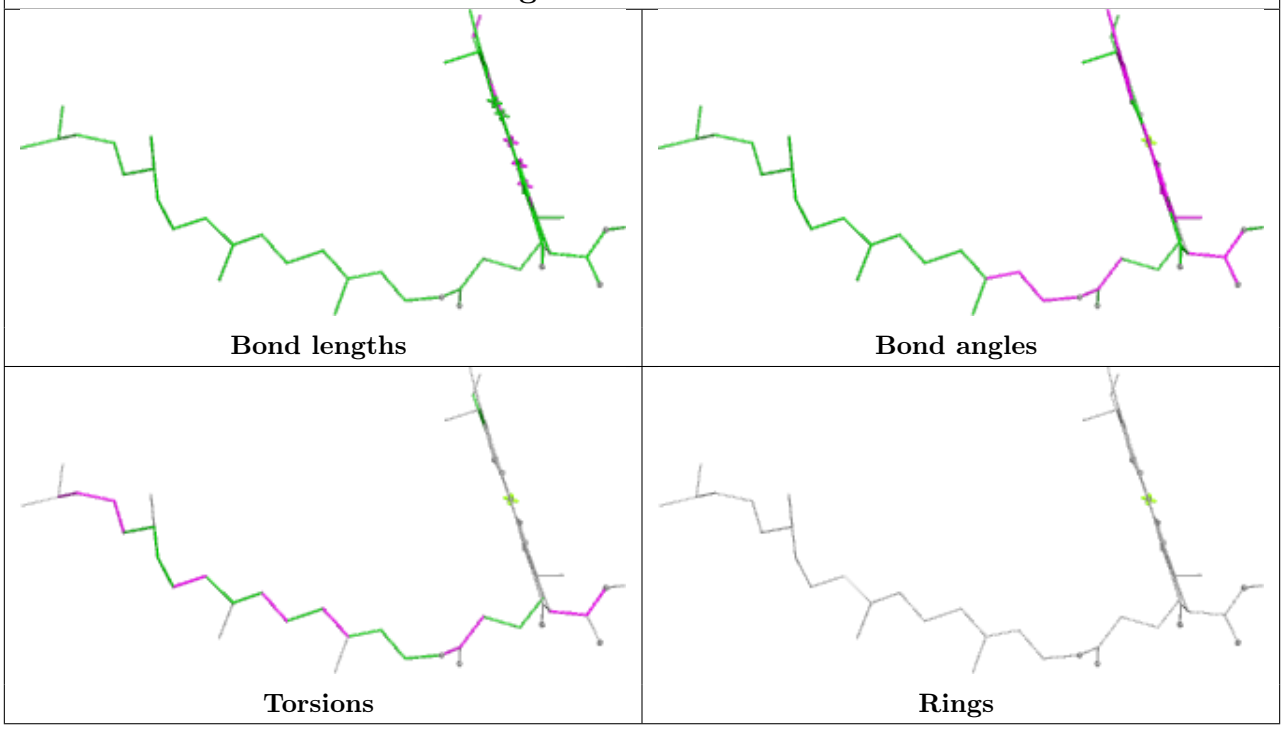


Rings

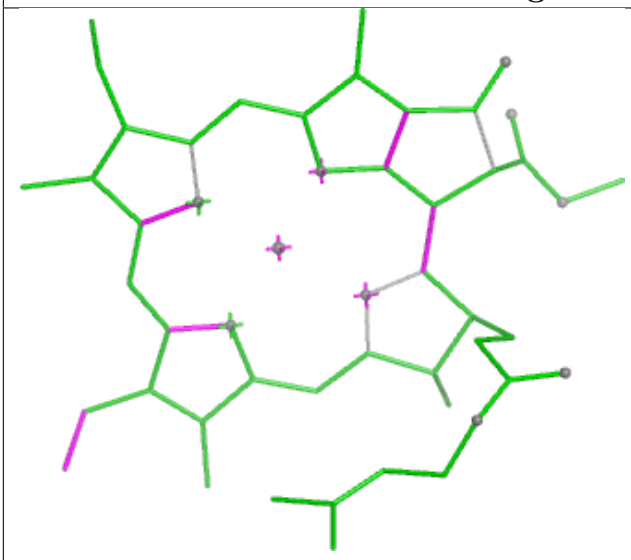
Ligand SQD b 621



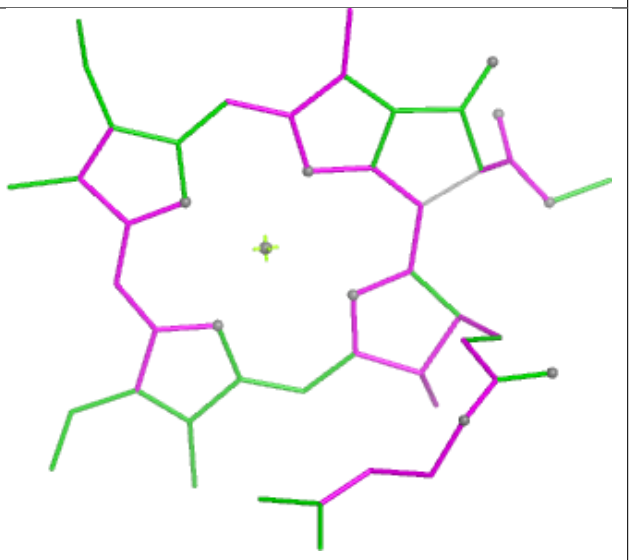
Ligand CLA b1 606



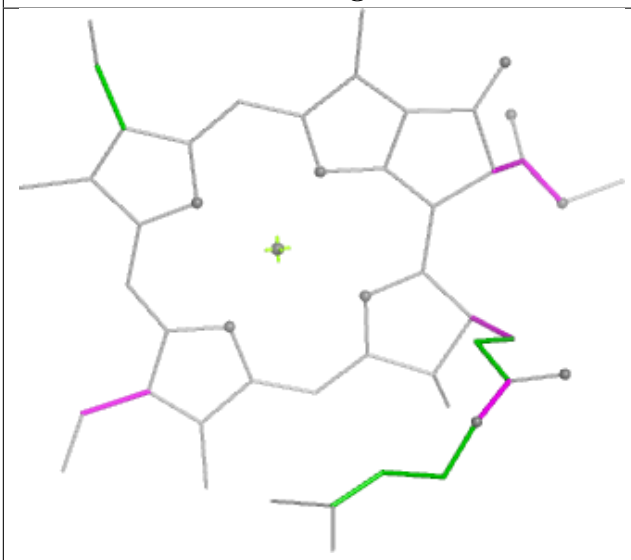
Ligand CLA S 617



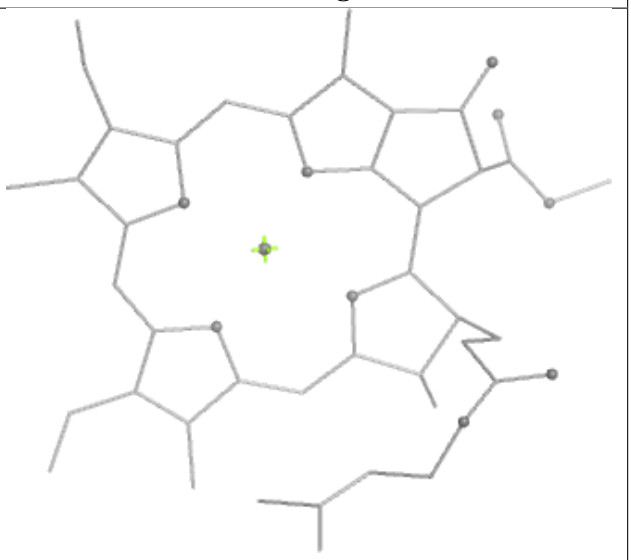
Bond lengths



Bond angles

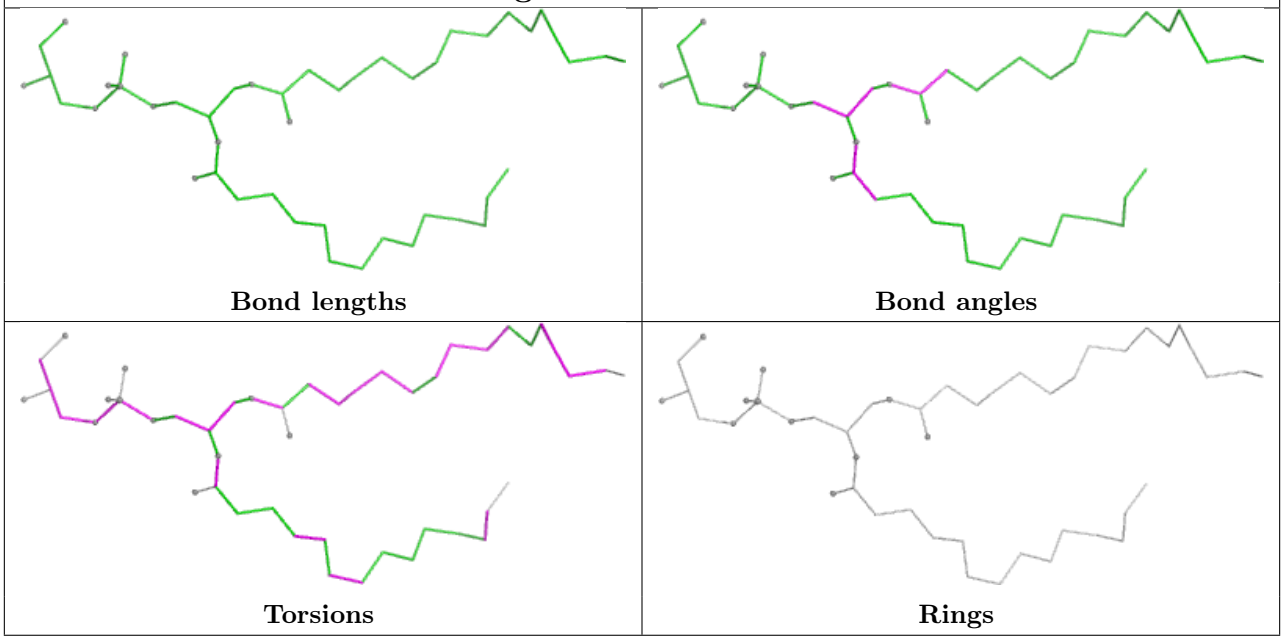


Torsions

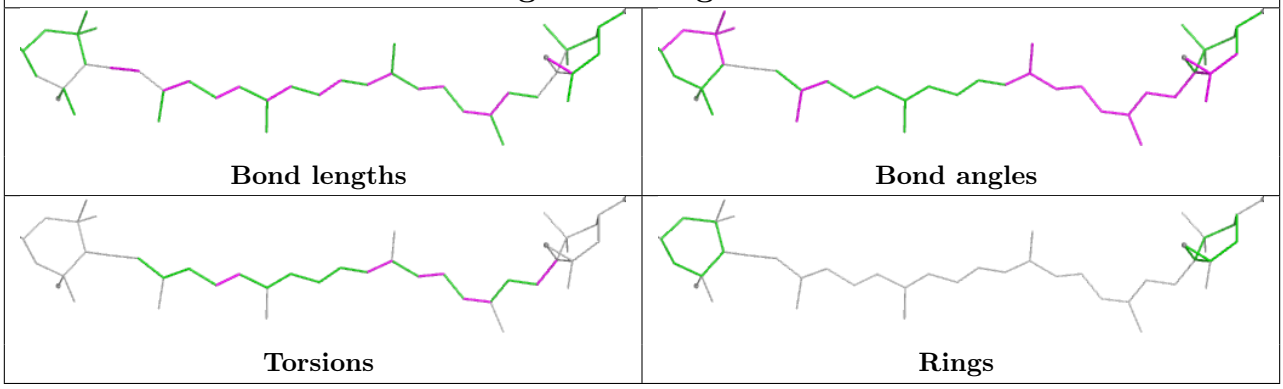


Rings

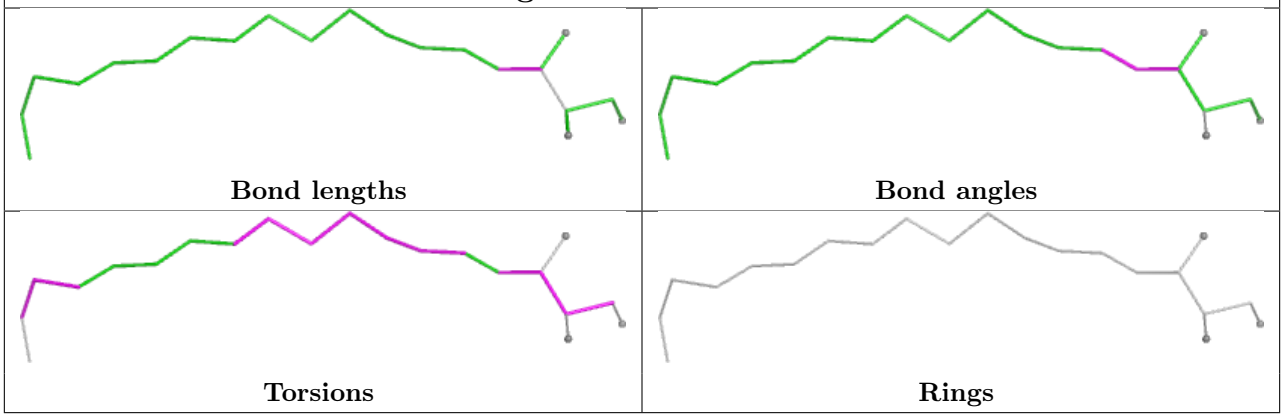
Ligand LHG C1 525



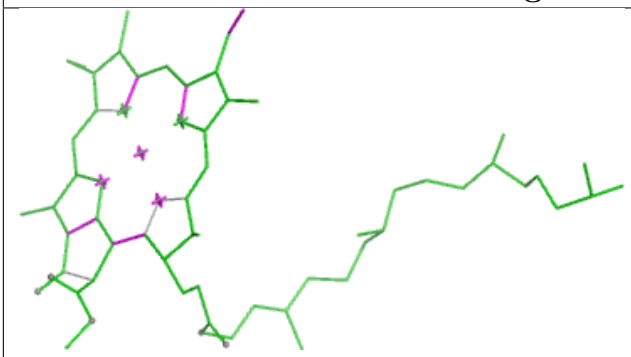
Ligand NEX g1 623



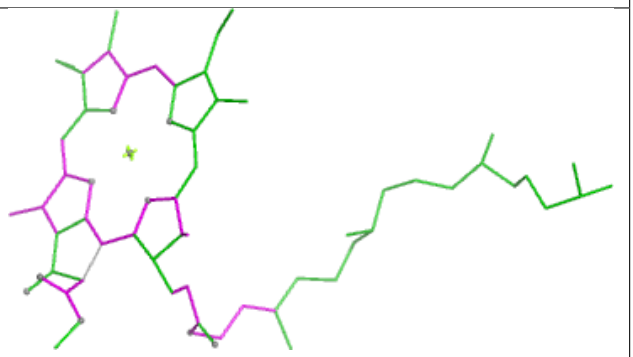
Ligand SPH A1 414



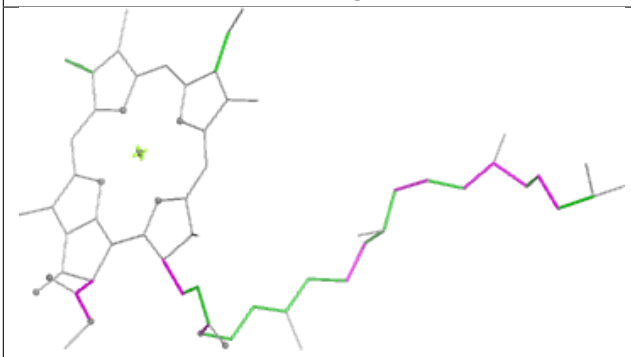
Ligand CLA C 511



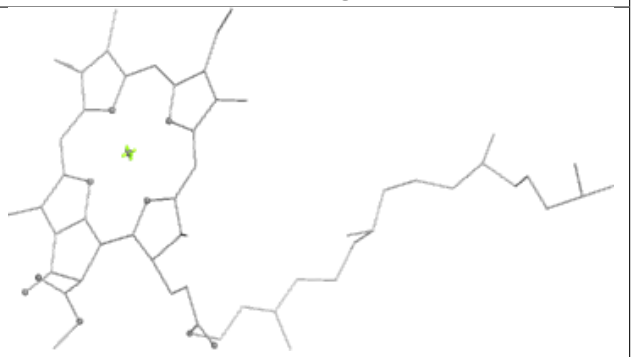
Bond lengths



Bond angles

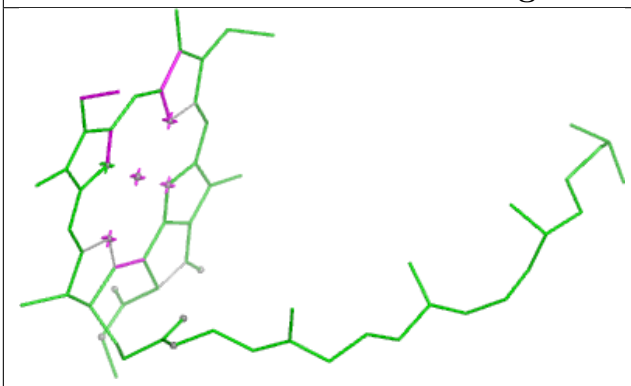


Torsions

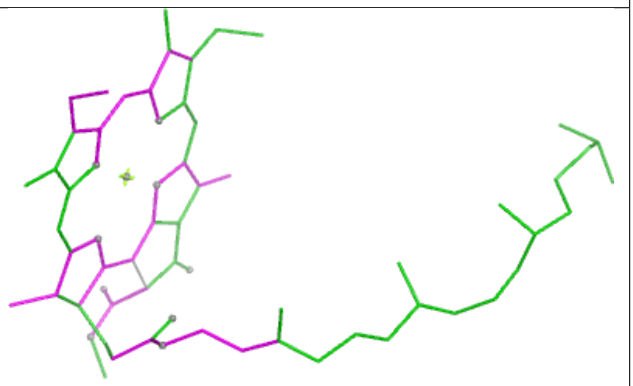


Rings

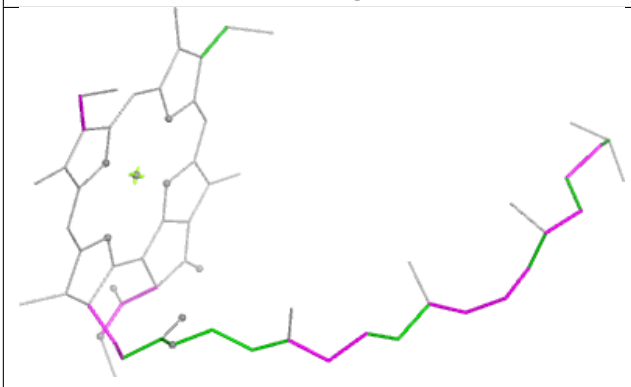
Ligand CLA S1 611



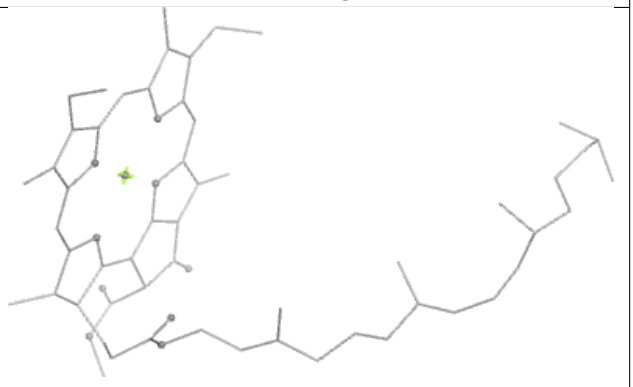
Bond lengths



Bond angles

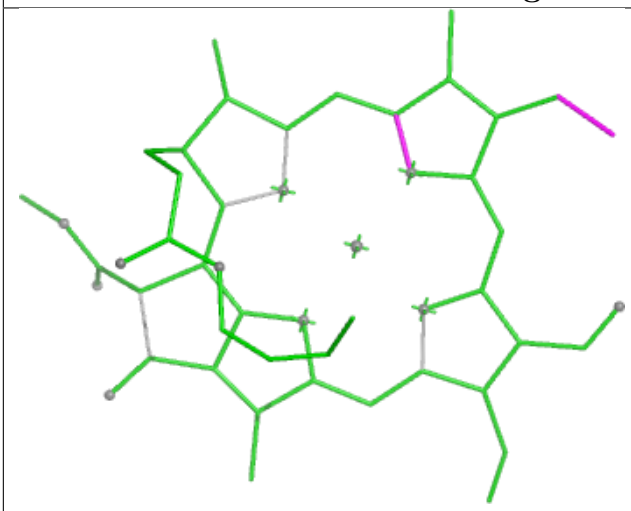


Torsions

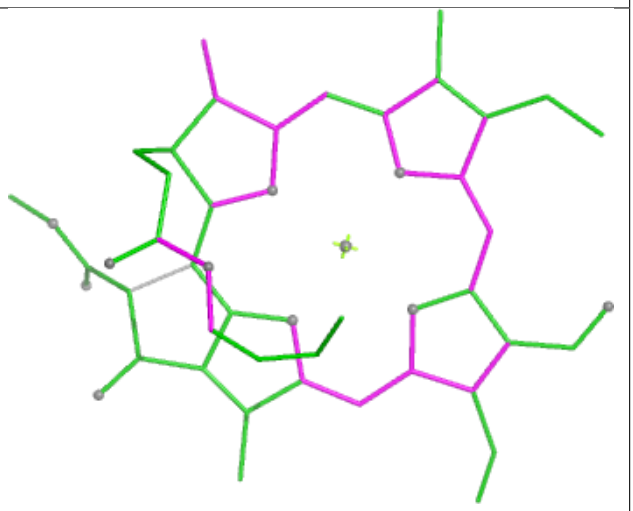


Rings

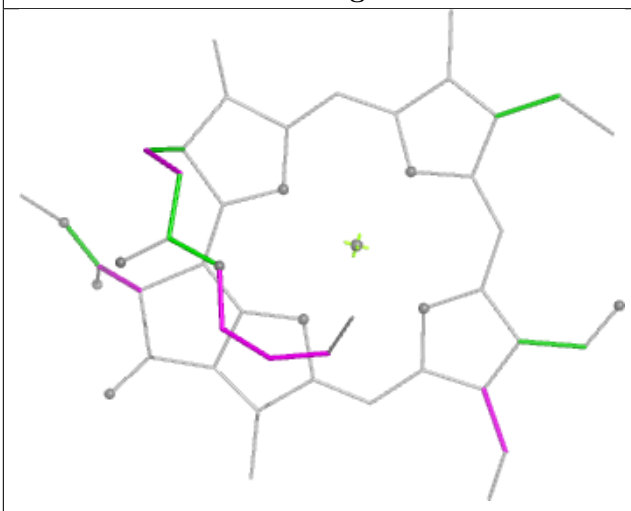
Ligand CHL R 607



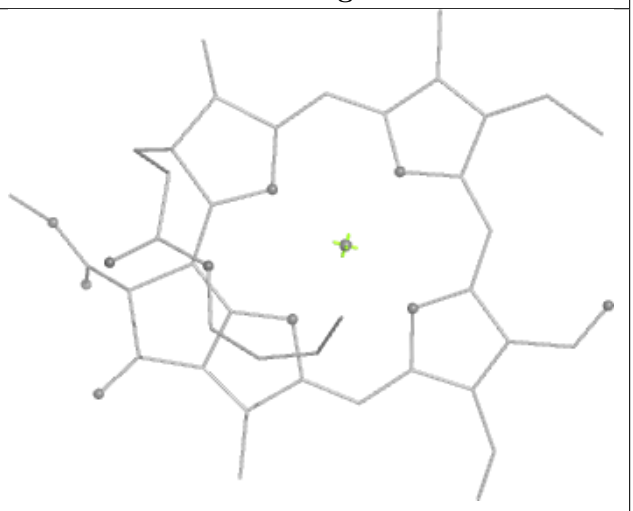
Bond lengths



Bond angles

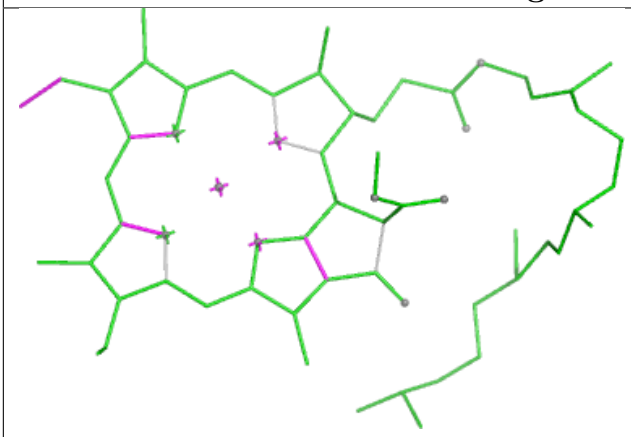


Torsions

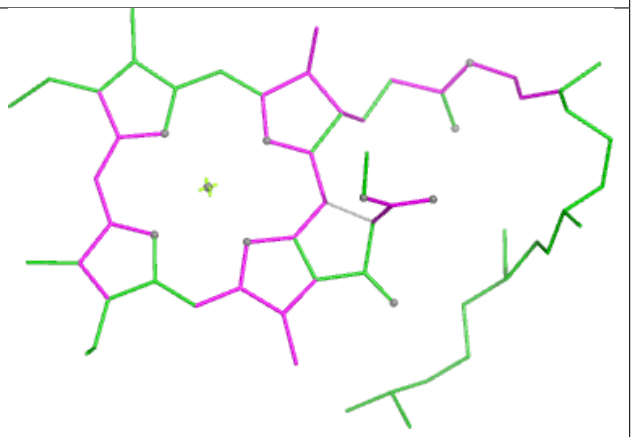


Rings

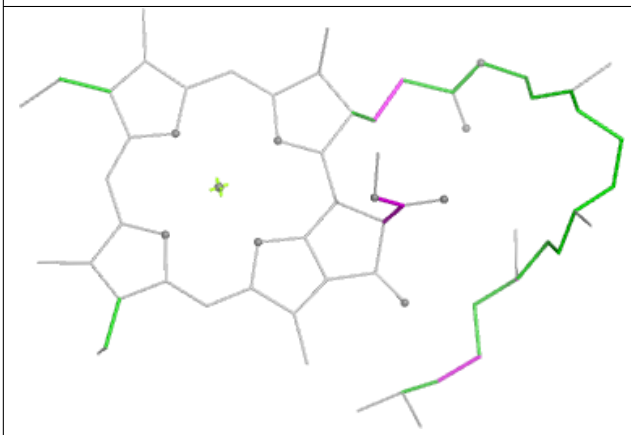
Ligand CLA b 611



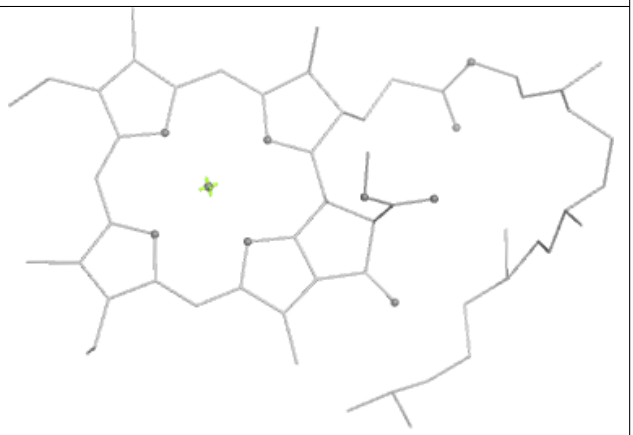
Bond lengths



Bond angles

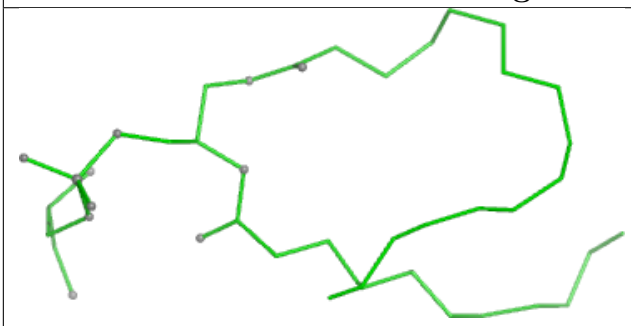


Torsions

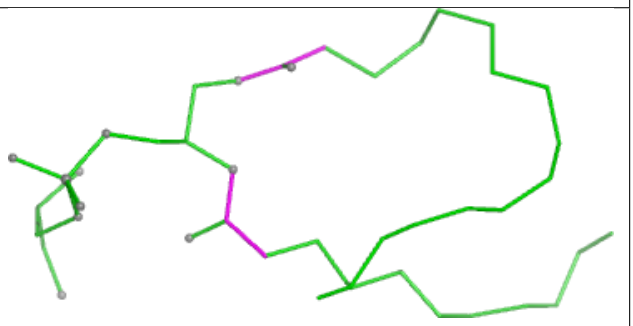


Rings

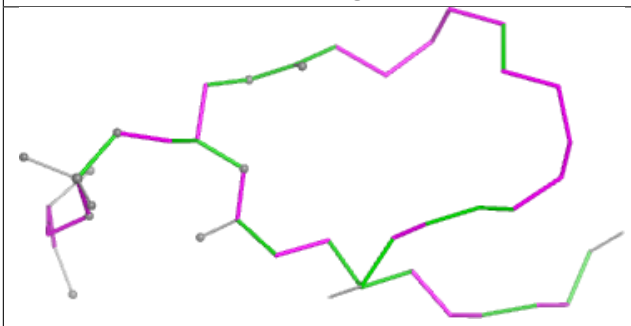
Ligand LHG D1 408



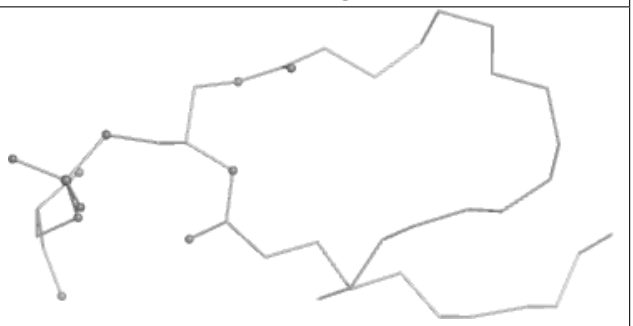
Bond lengths



Bond angles

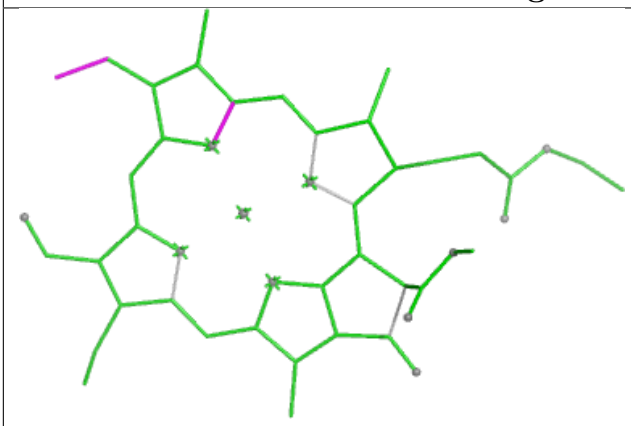


Torsions

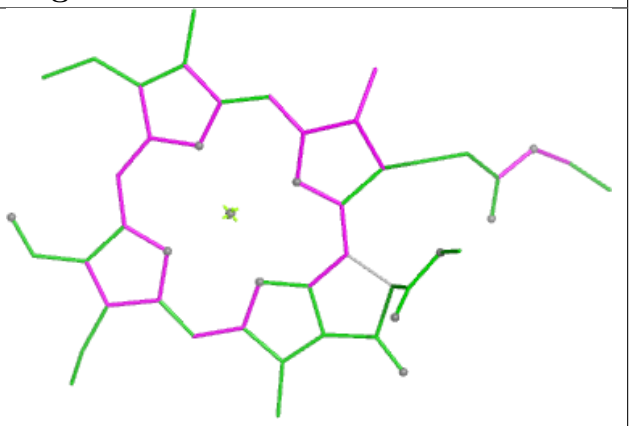


Rings

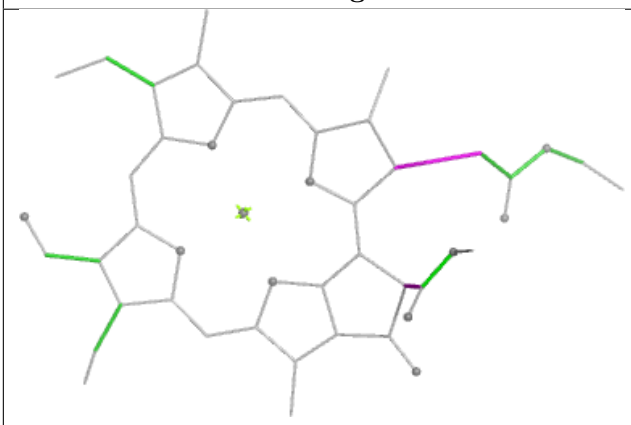
Ligand CHL g 605



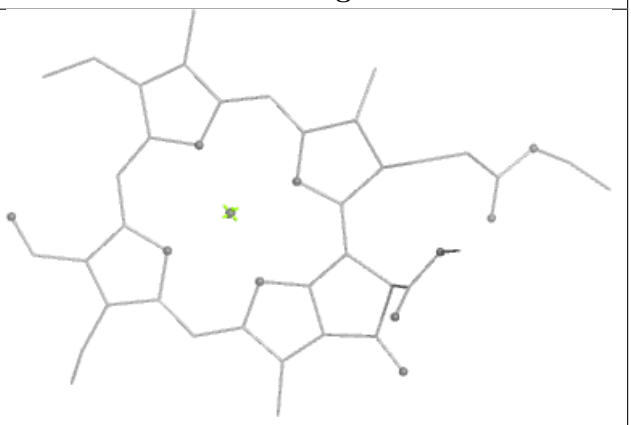
Bond lengths



Bond angles

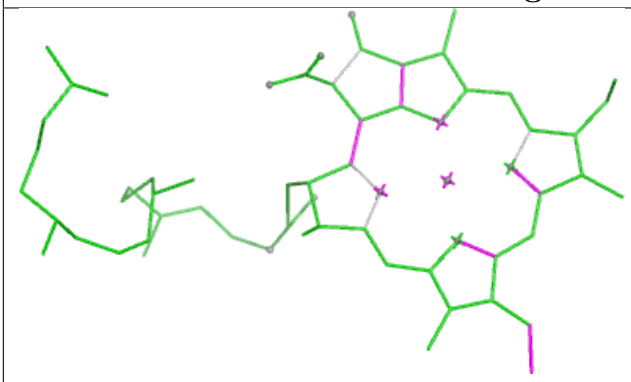


Torsions

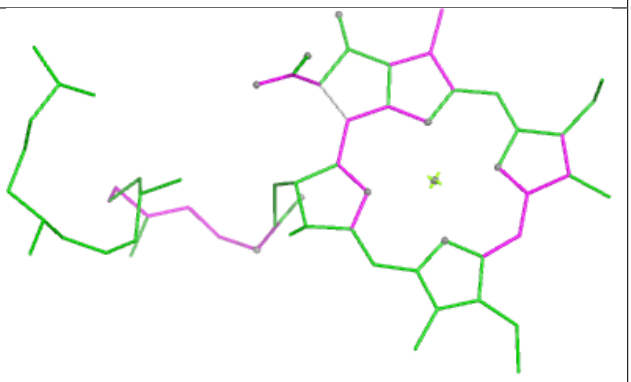


Rings

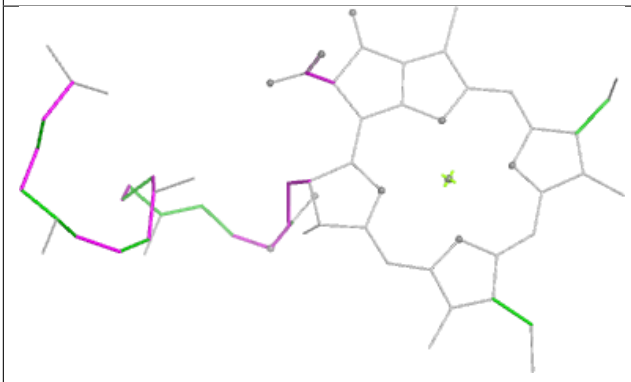
Ligand CLA B 613



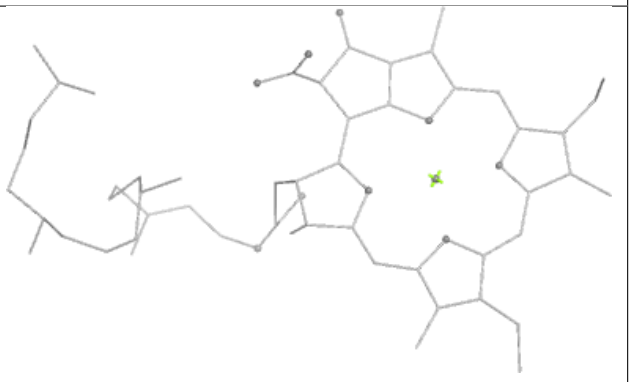
Bond lengths



Bond angles

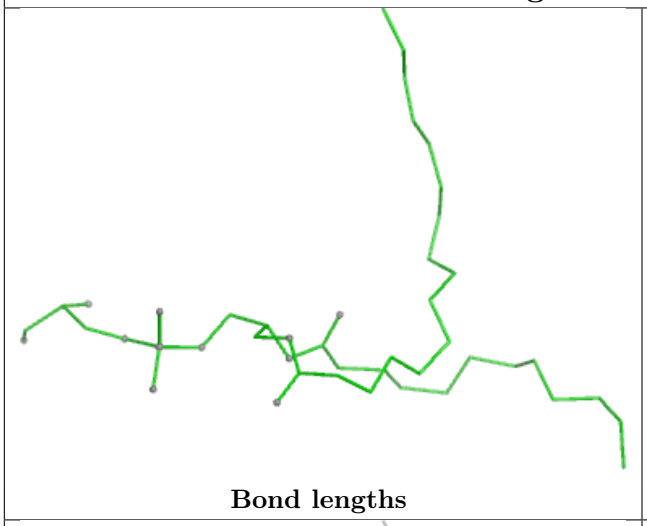


Torsions

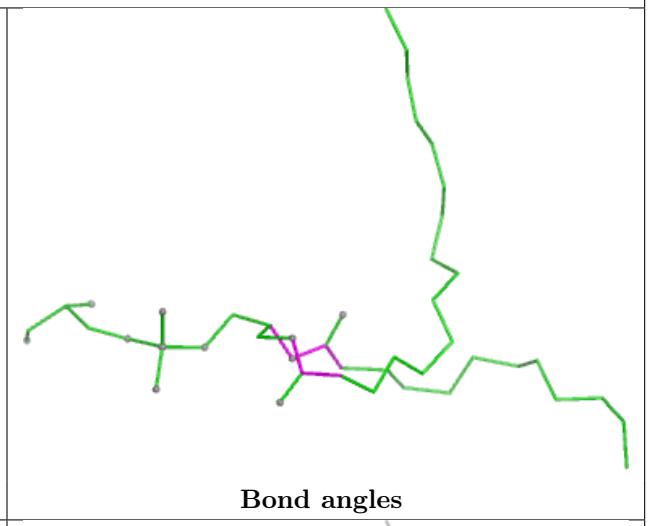


Rings

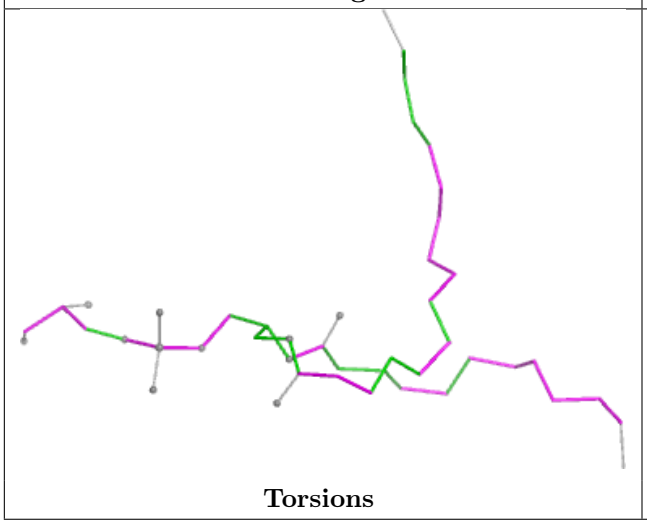
Ligand LHG S 624



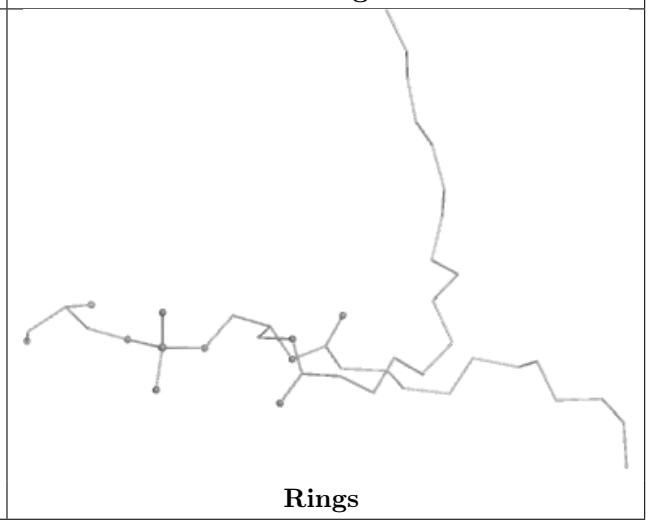
Bond lengths



Bond angles

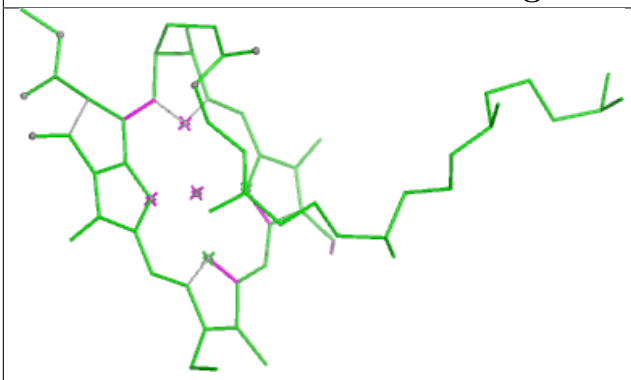


Torsions

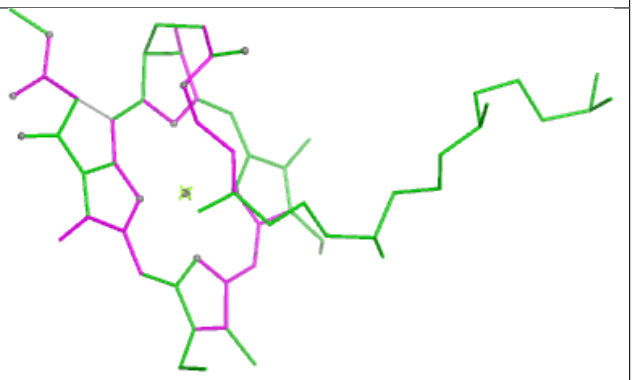


Rings

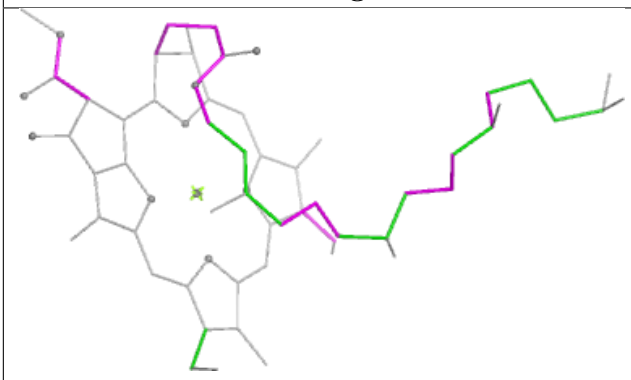
Ligand CLA N 613



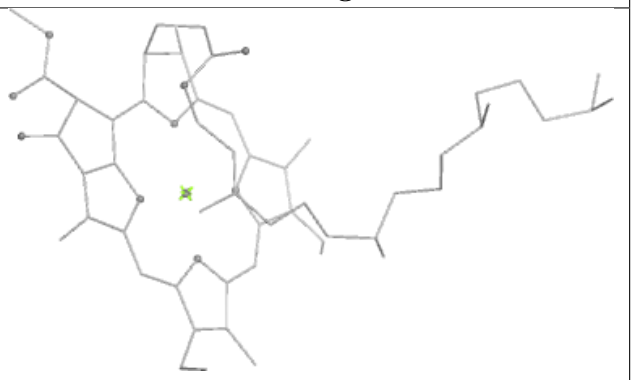
Bond lengths



Bond angles

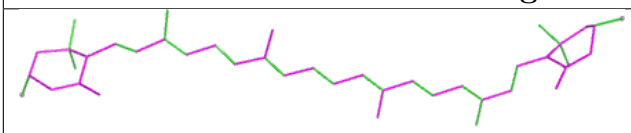


Torsions

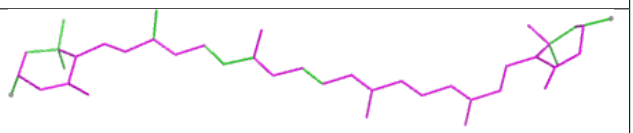


Rings

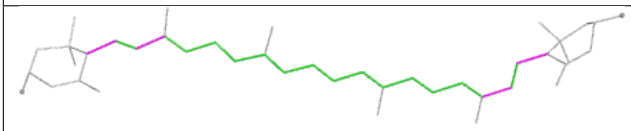
Ligand C7Z B1 620



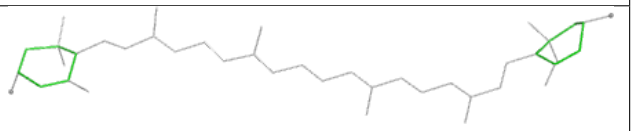
Bond lengths



Bond angles

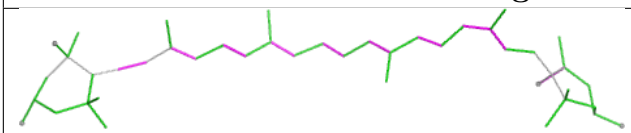


Torsions

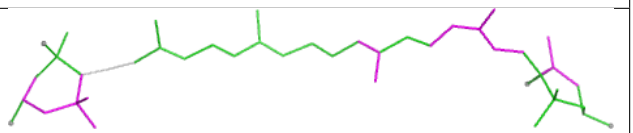


Rings

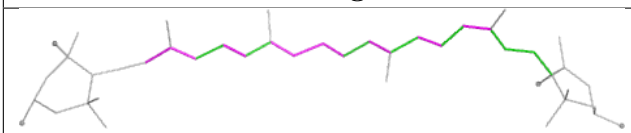
Ligand NEX G1 623



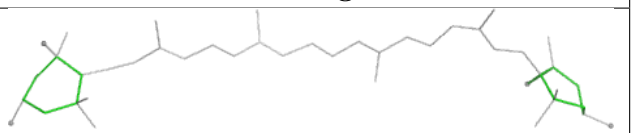
Bond lengths



Bond angles

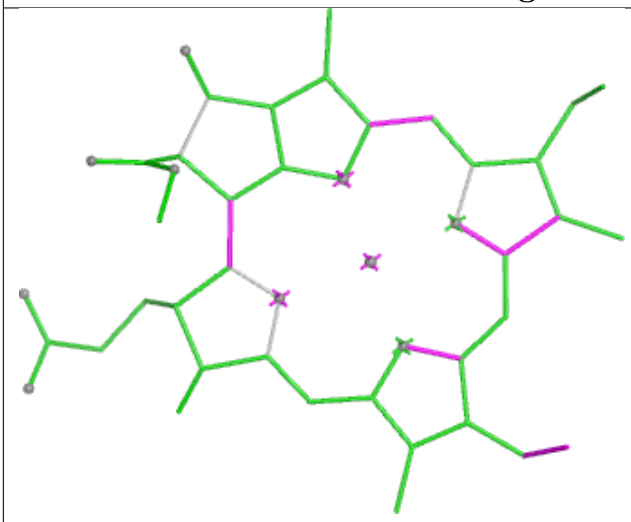


Torsions

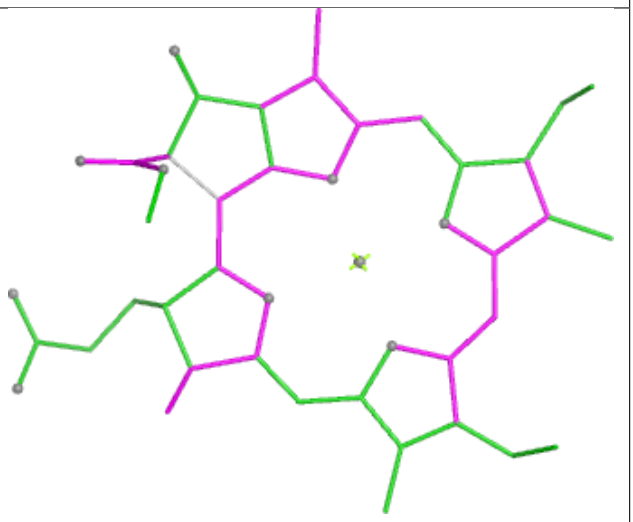


Rings

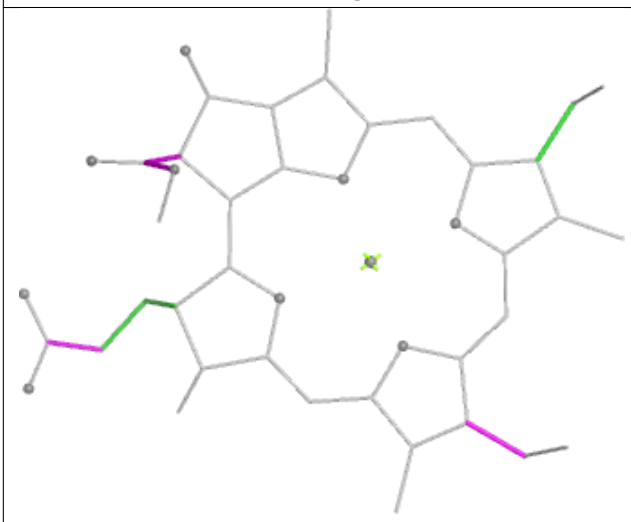
Ligand CLA n1 612



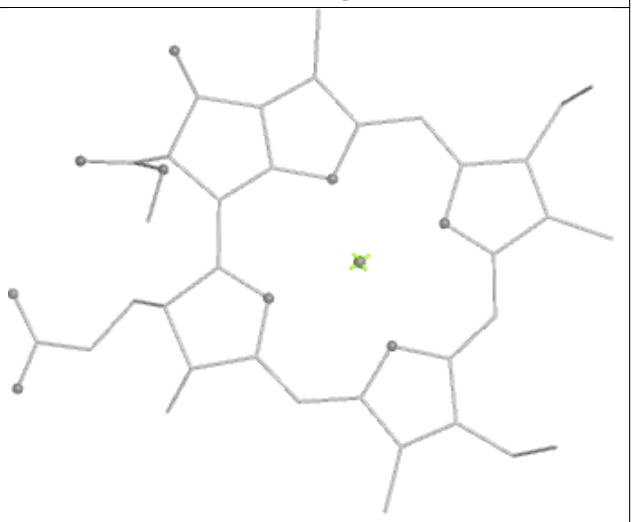
Bond lengths



Bond angles

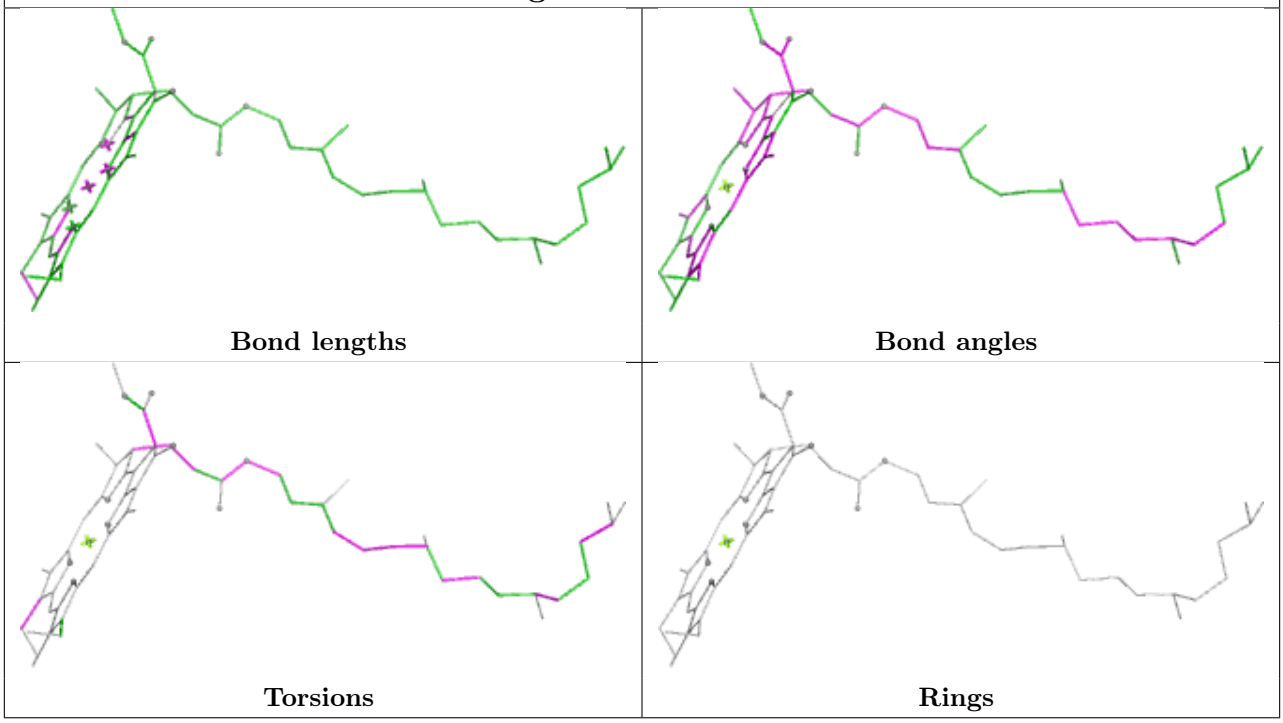


Torsions

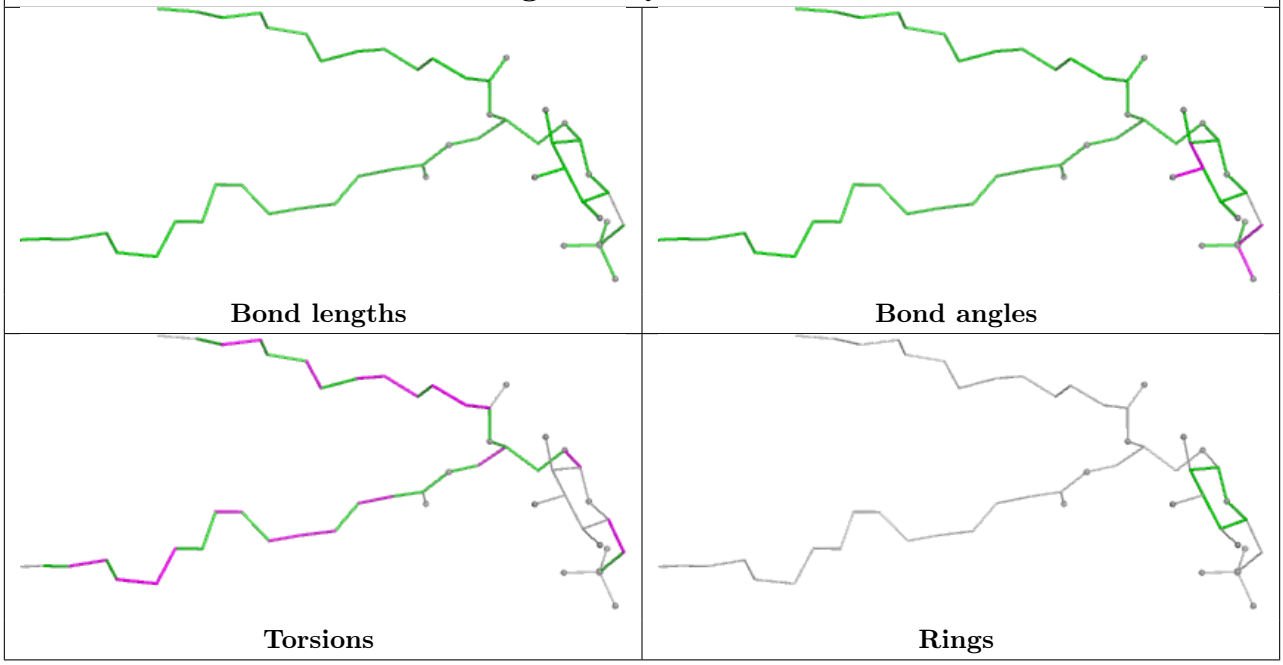


Rings

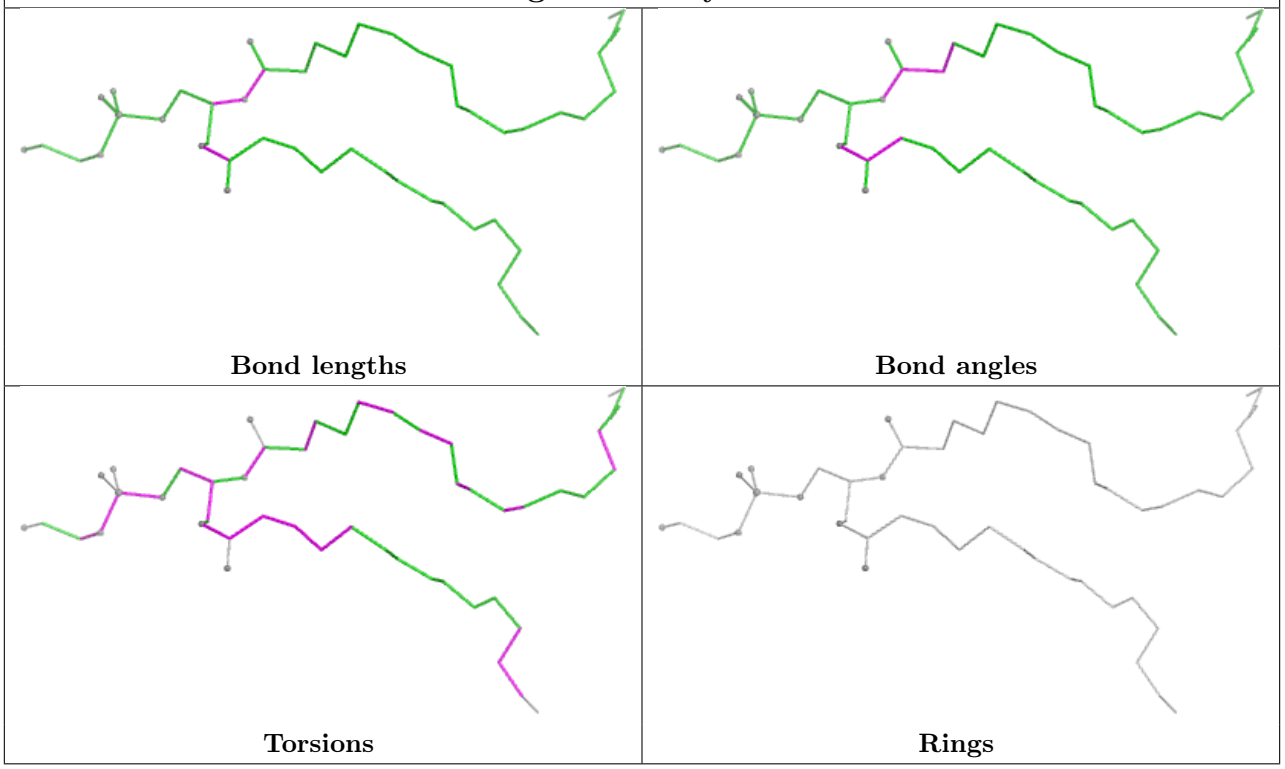
Ligand CLA b 605



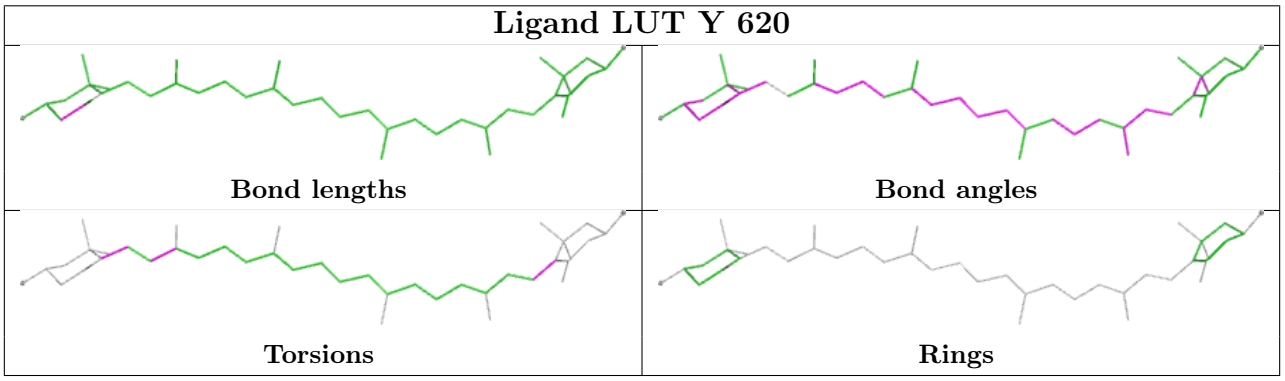
Ligand SQD a1 412



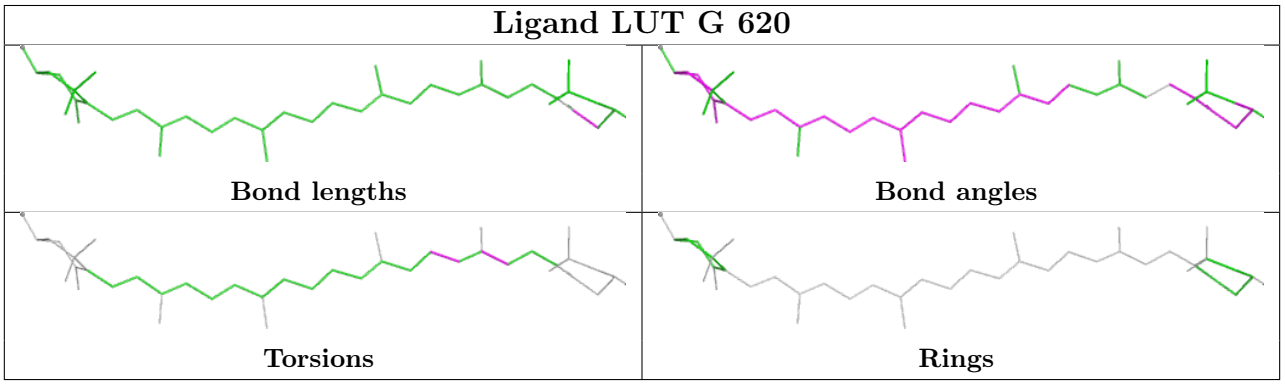
Ligand PTY y 626



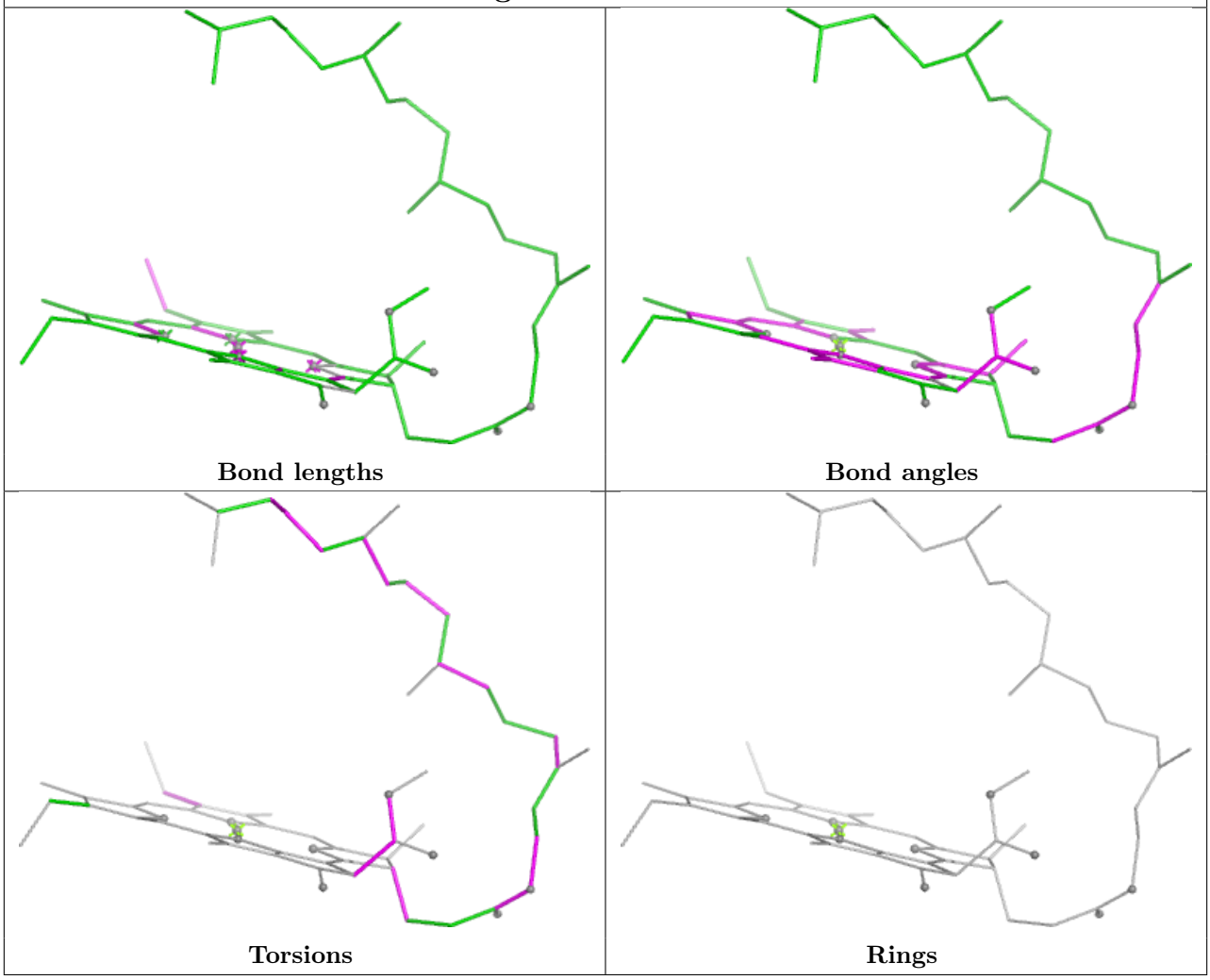
Ligand LUT Y 620



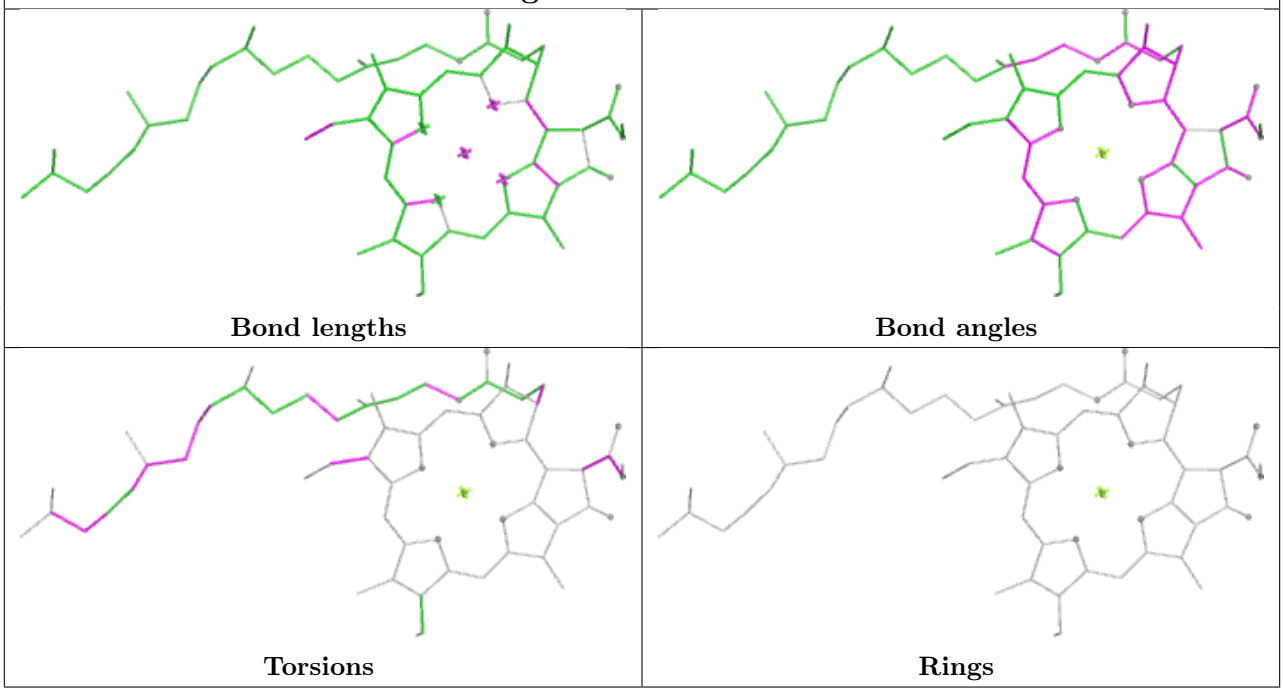
Ligand LUT G 620



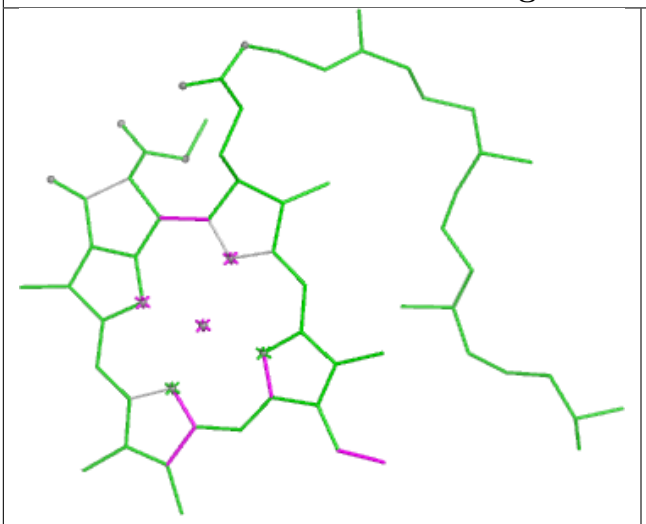
Ligand CLA Y 603



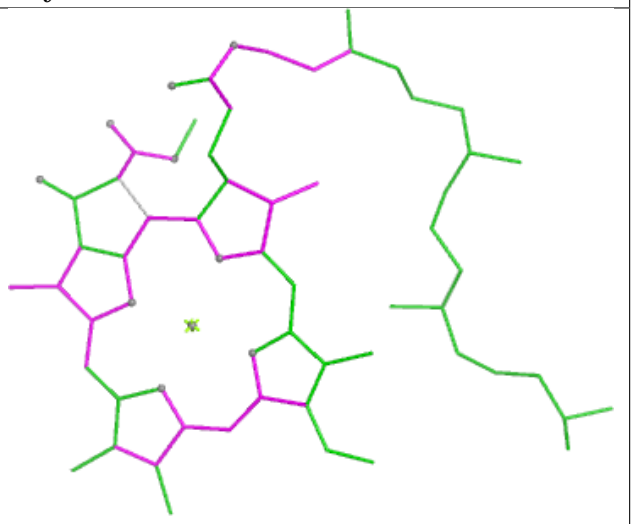
Ligand CLA c1 501



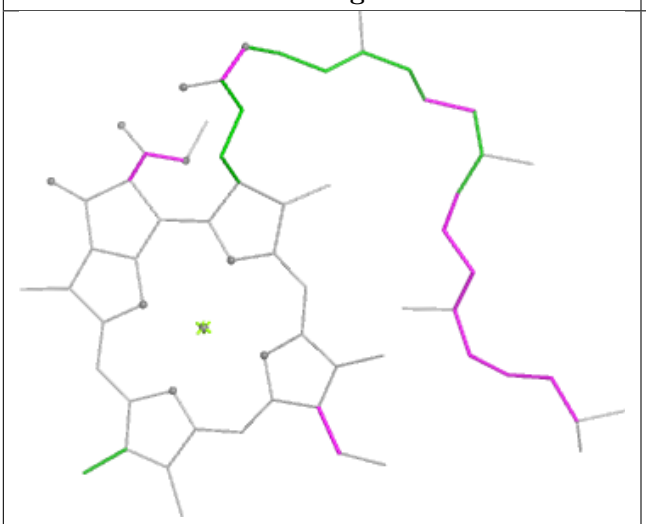
Ligand CLA y1 612



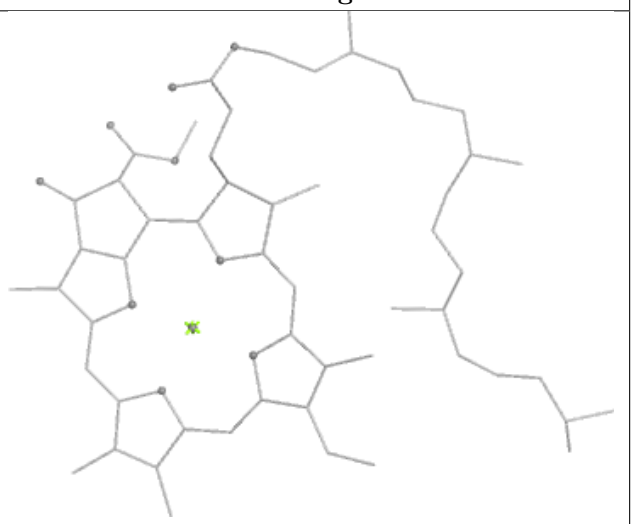
Bond lengths



Bond angles

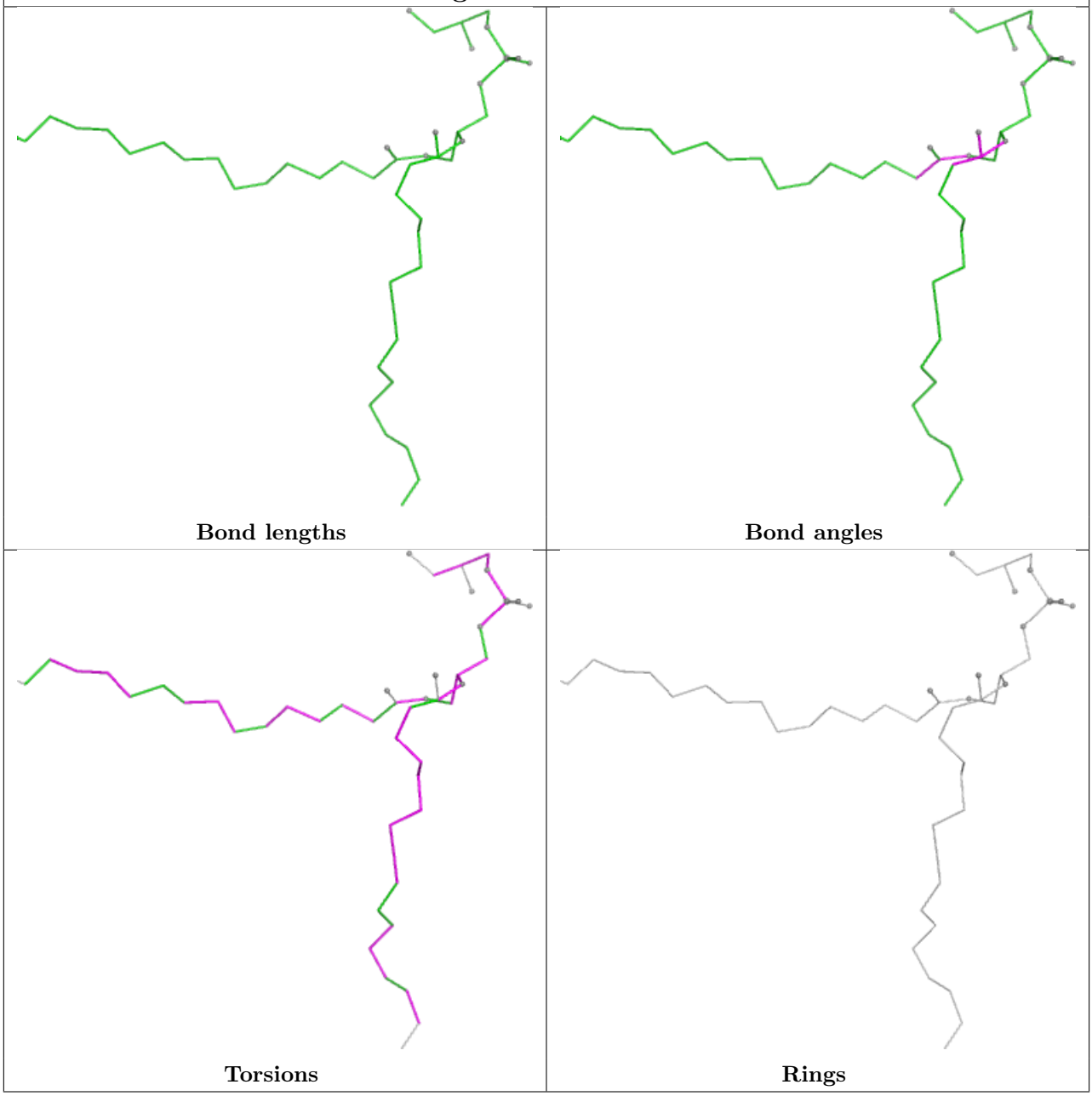


Torsions

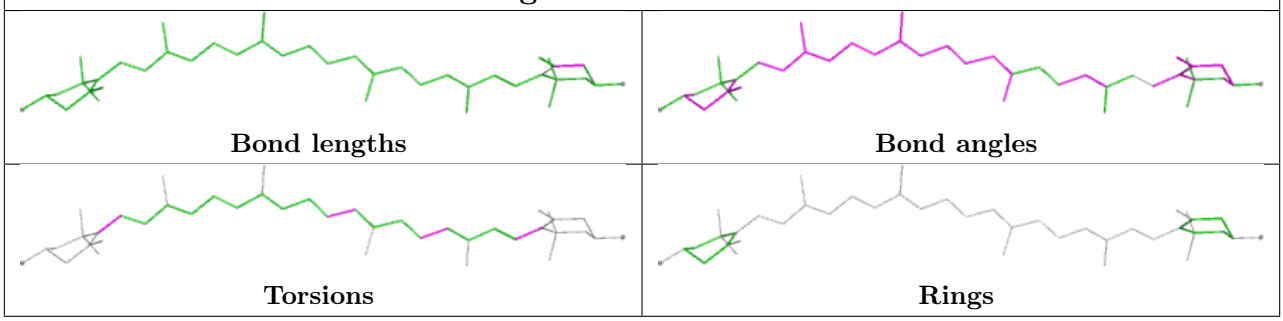


Rings

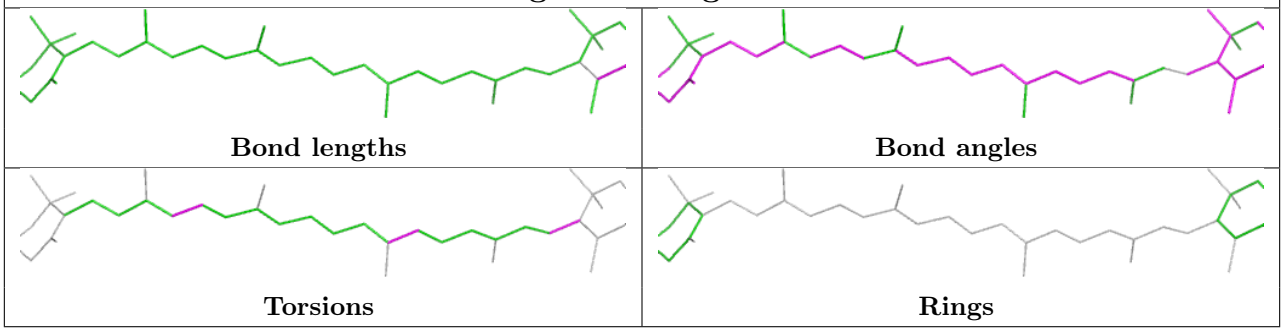
Ligand LHG l 101



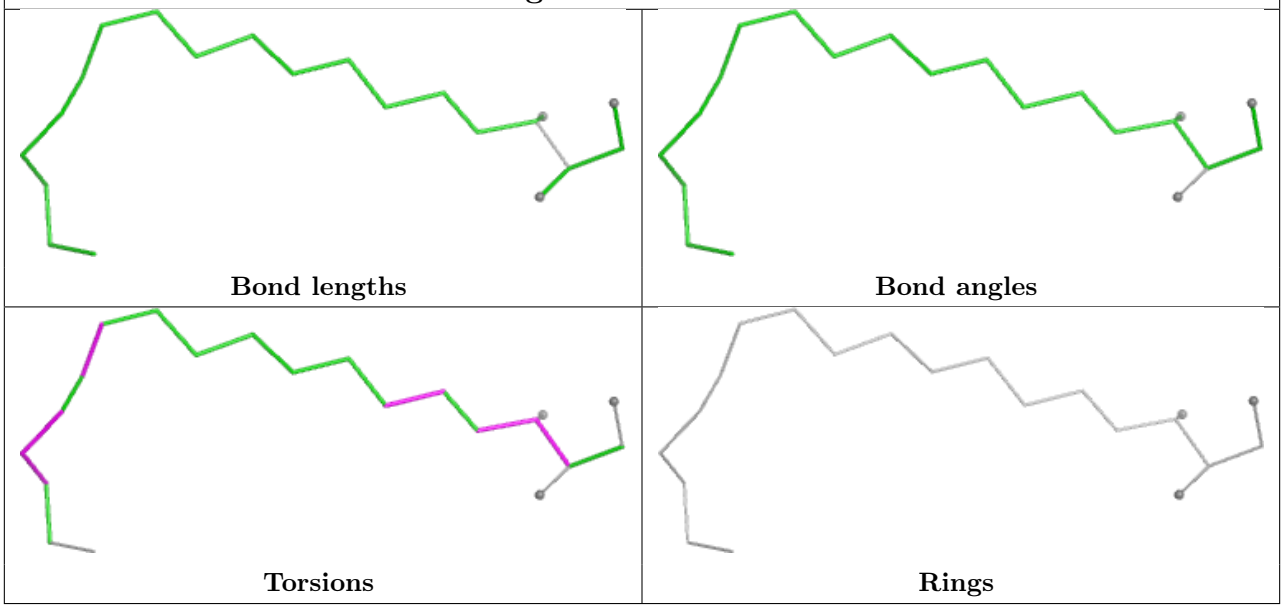
Ligand LUT n1 621



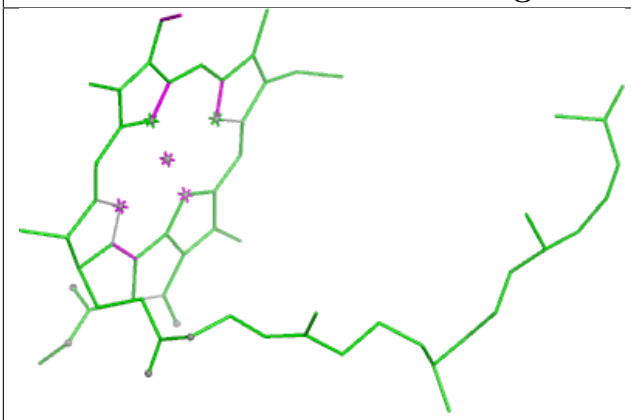
Ligand LUT g 620



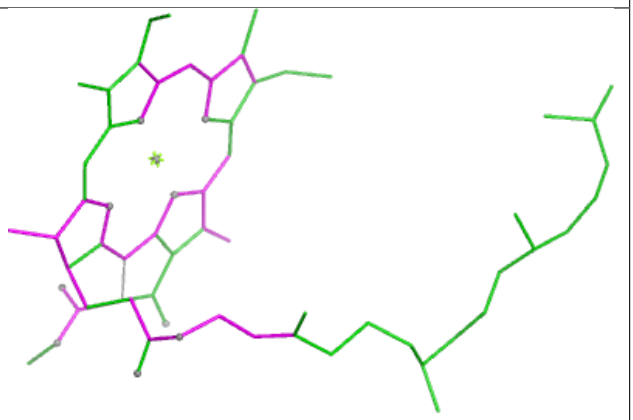
Ligand SPH Y 625



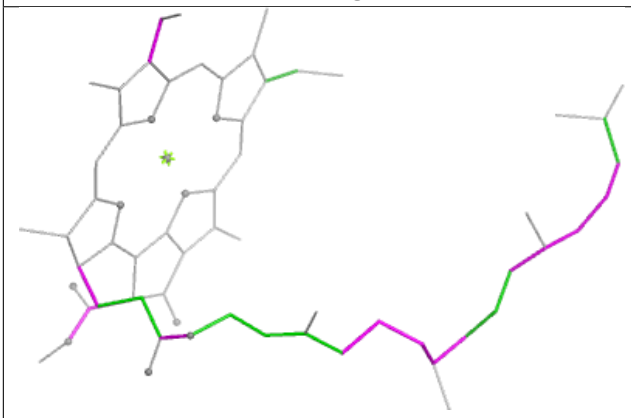
Ligand CLA G1 611



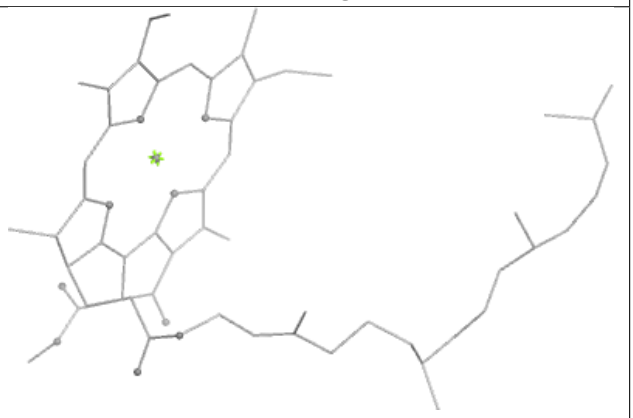
Bond lengths



Bond angles

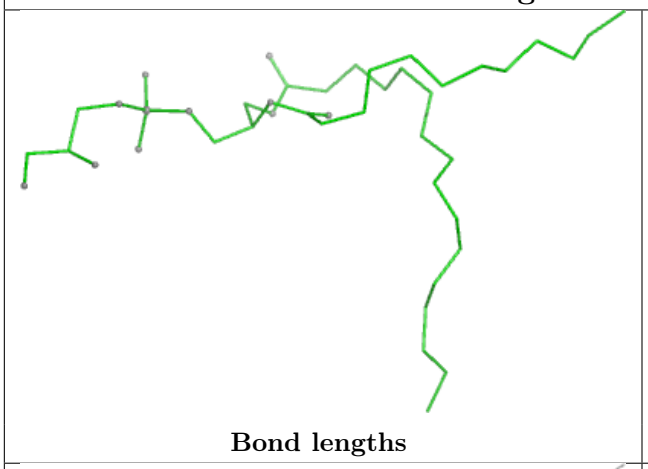


Torsions

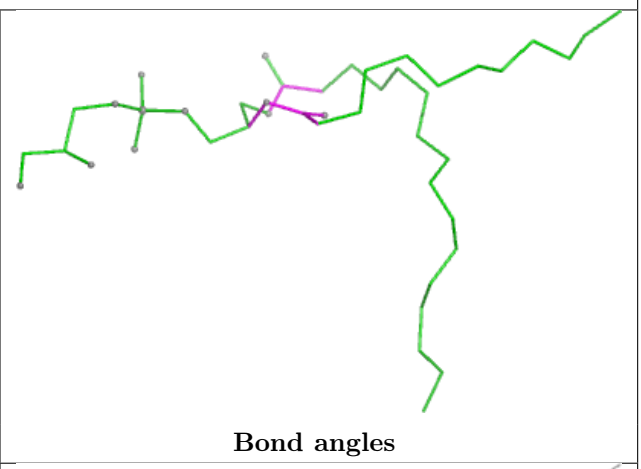


Rings

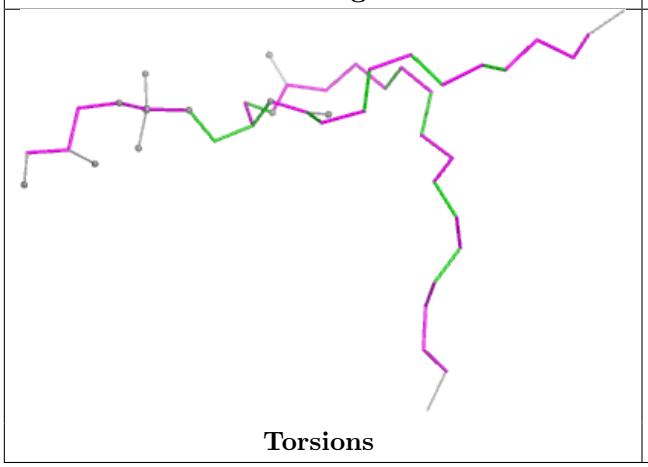
Ligand LHG S1 624



Bond lengths



Bond angles

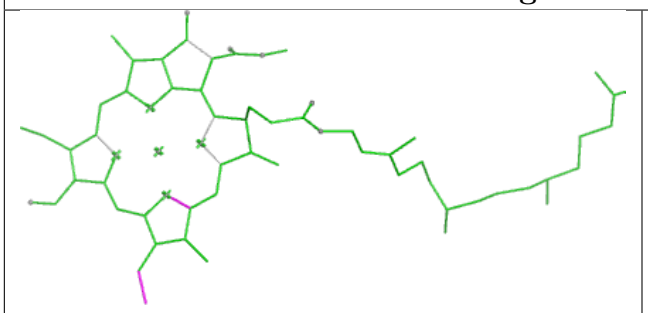


Torsions

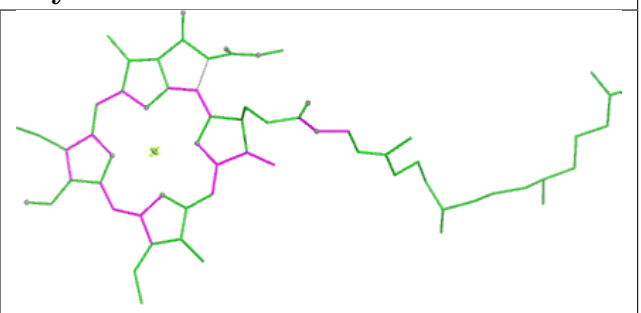


Rings

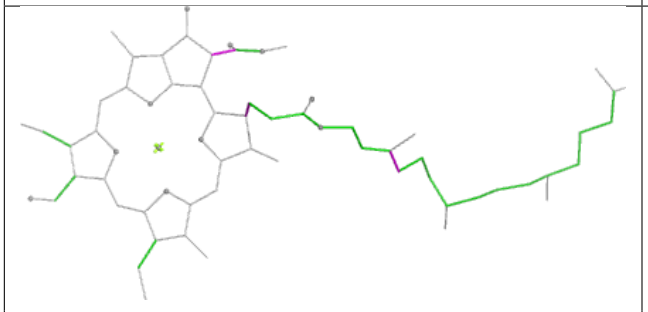
Ligand CHL y1 601



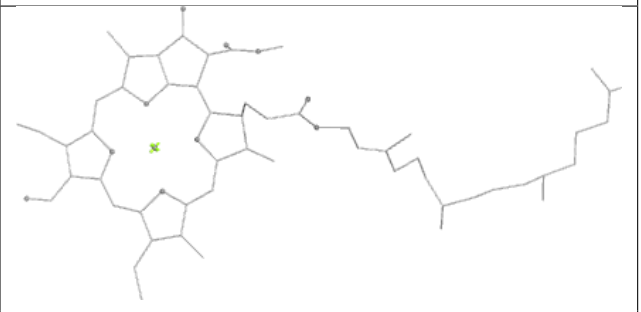
Bond lengths



Bond angles

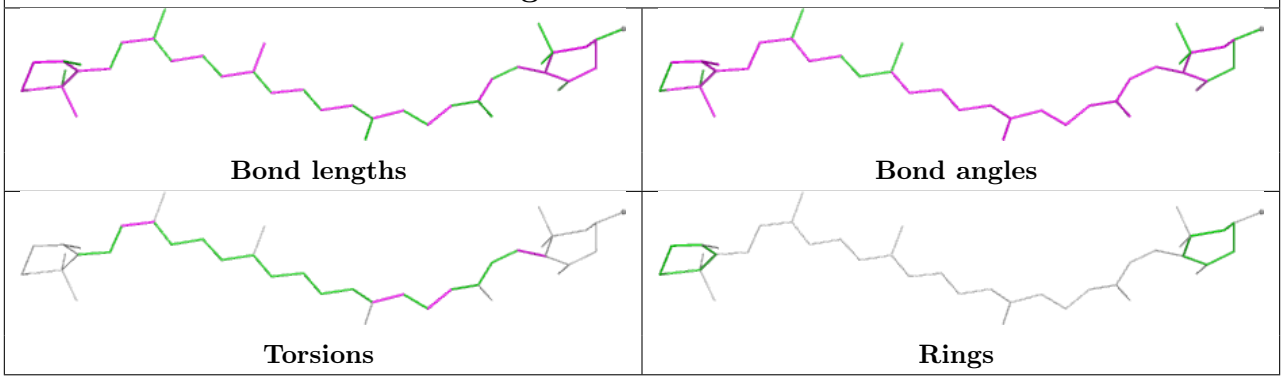


Torsions

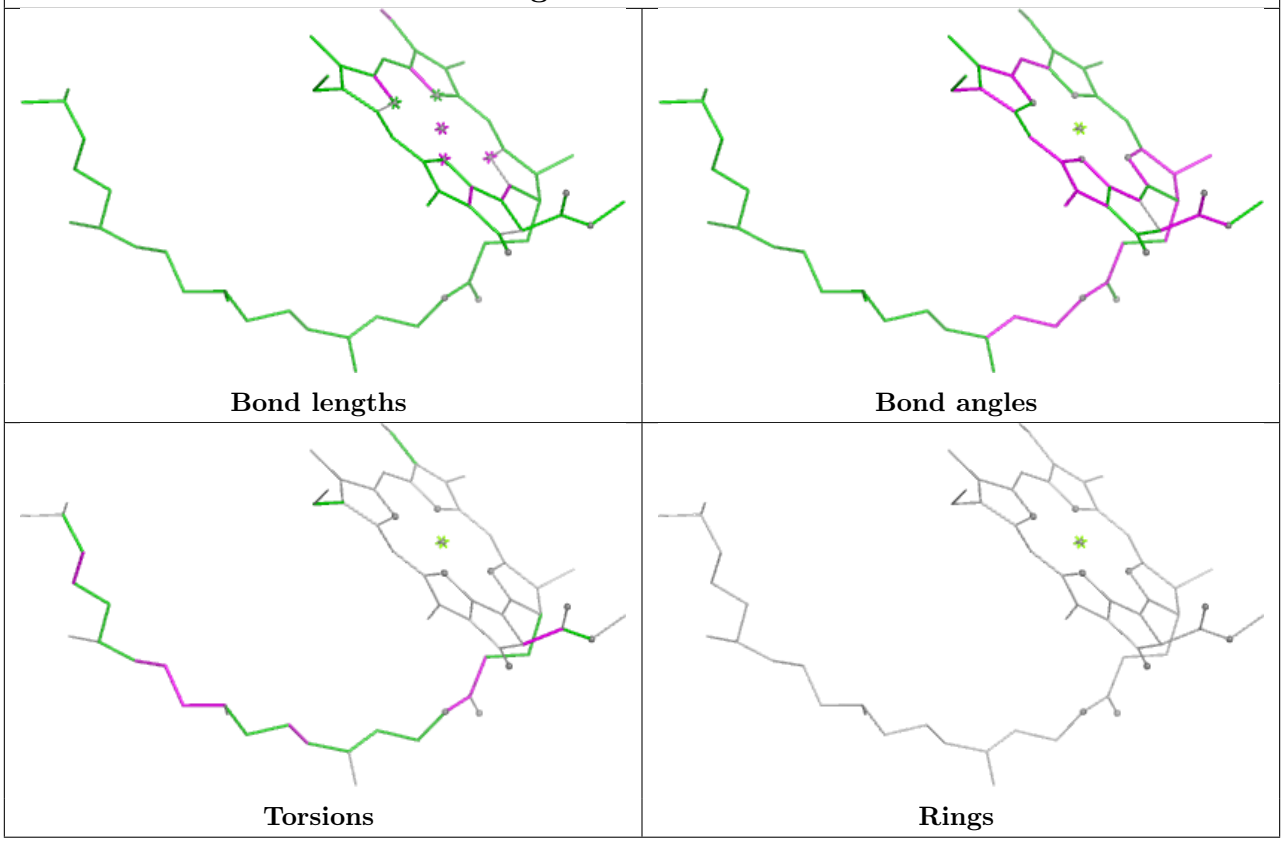


Rings

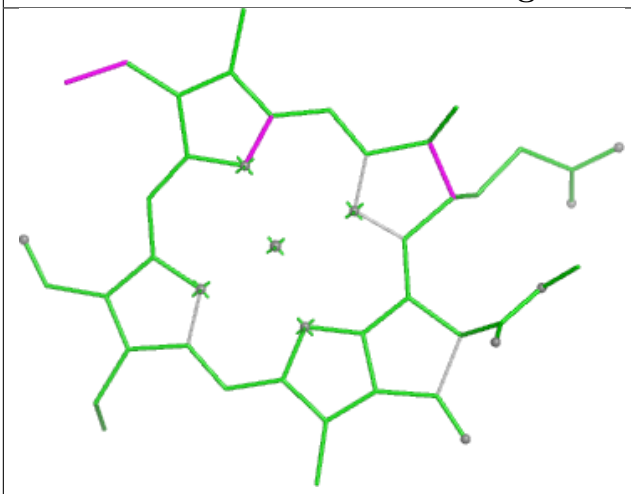
Ligand RRX H 101



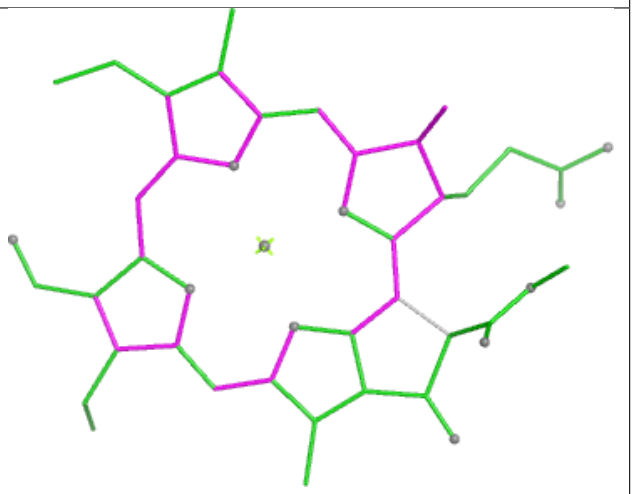
Ligand CLA c 508



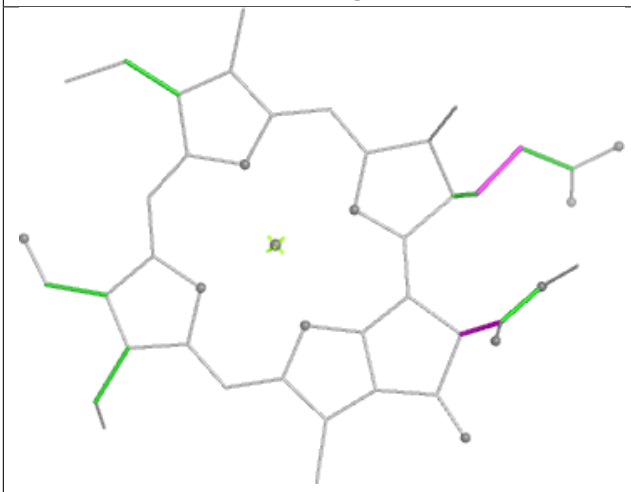
Ligand CHL S1 601



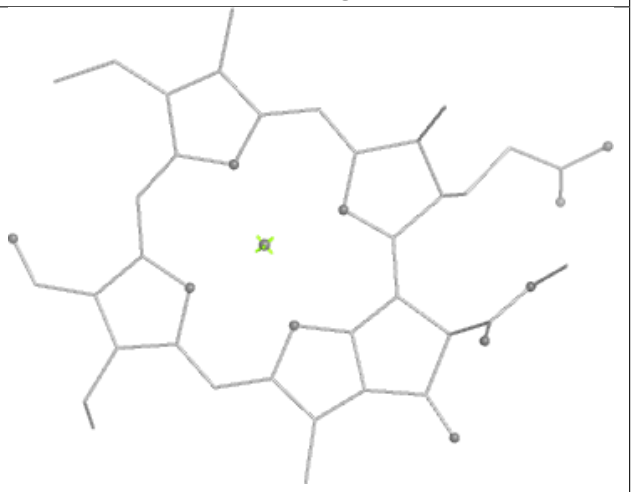
Bond lengths



Bond angles

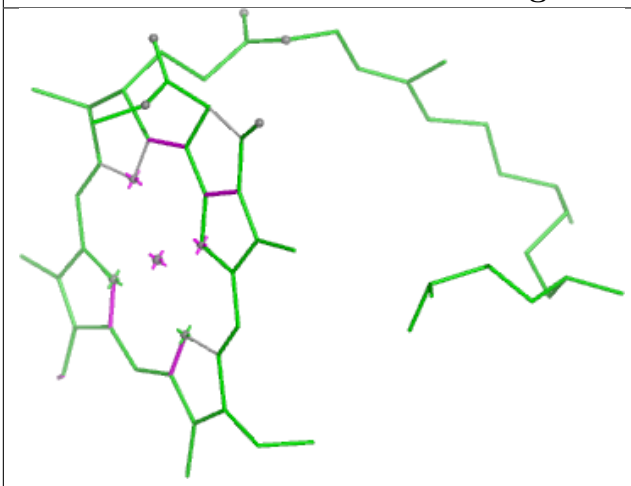


Torsions

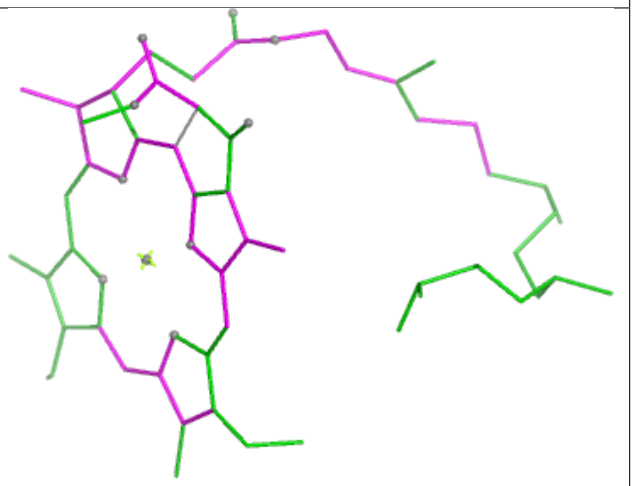


Rings

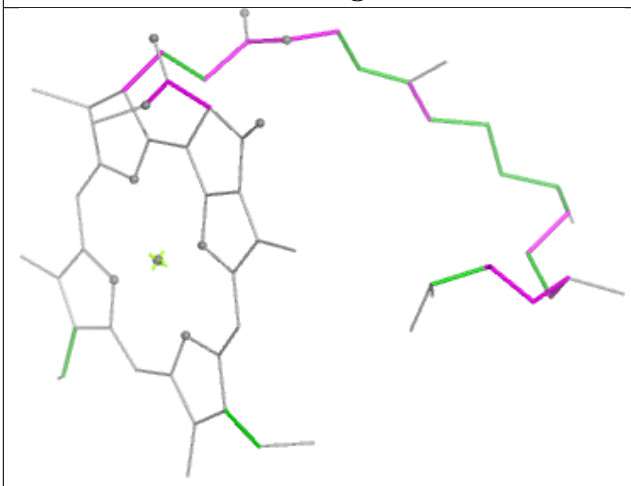
Ligand CLA c 503



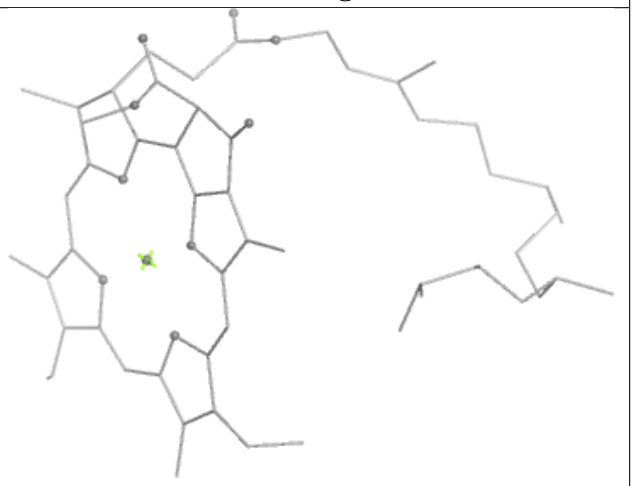
Bond lengths



Bond angles

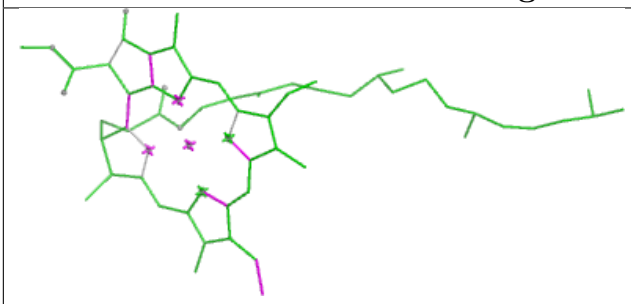


Torsions

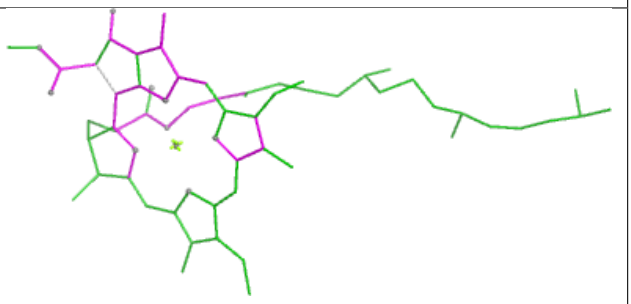


Rings

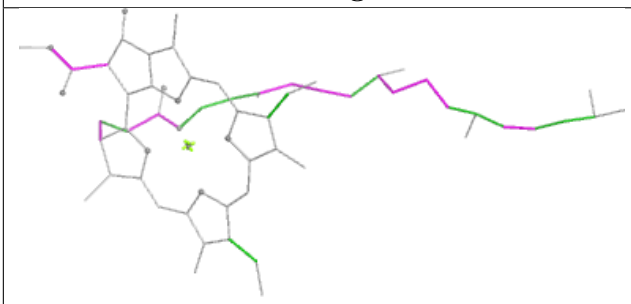
Ligand CLA b1 615



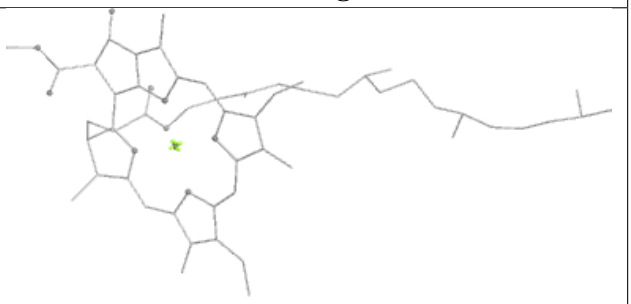
Bond lengths



Bond angles

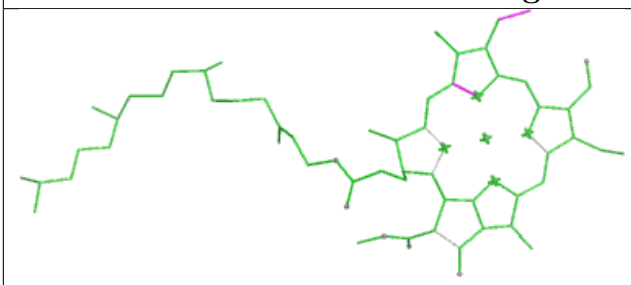


Torsions

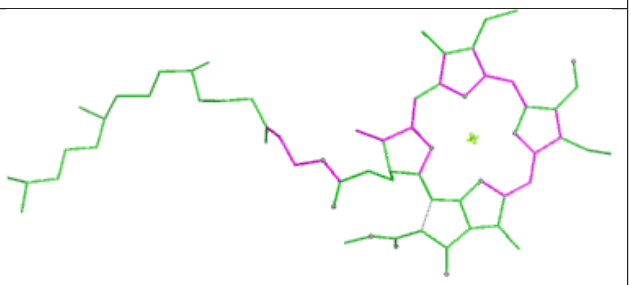


Rings

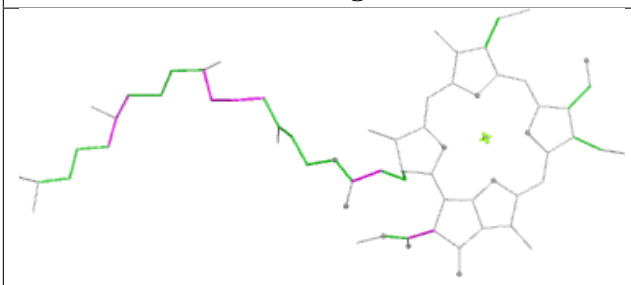
Ligand CHL G 601



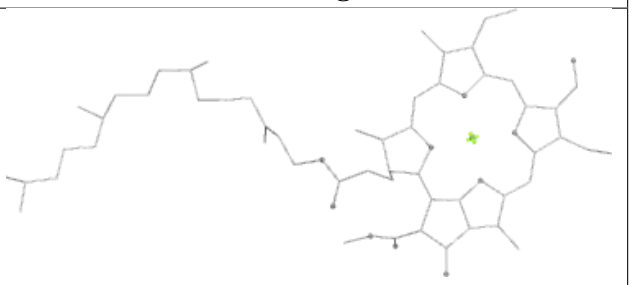
Bond lengths



Bond angles

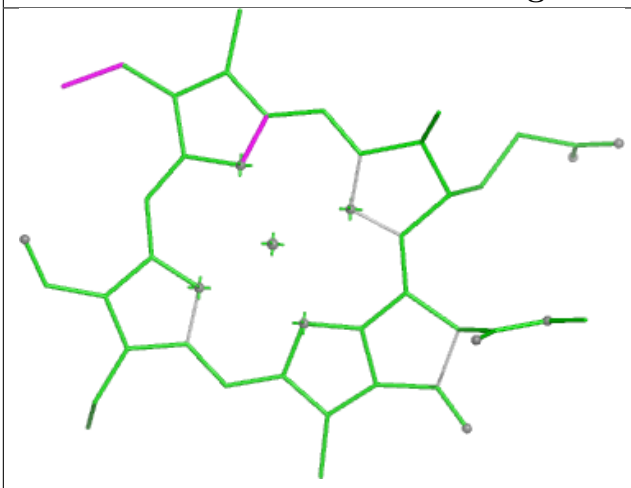


Torsions

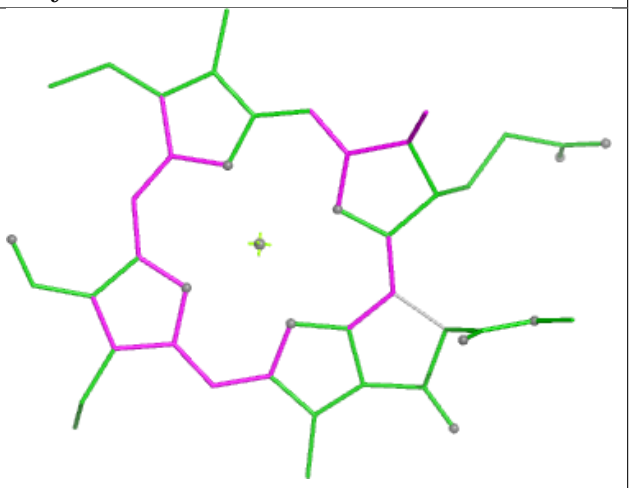


Rings

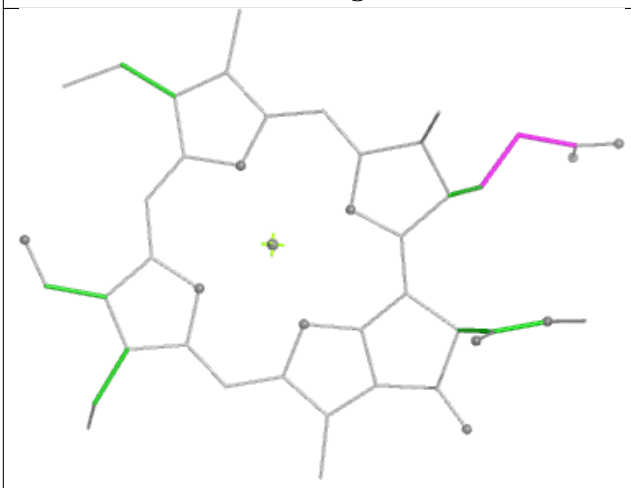
Ligand CHL y 605



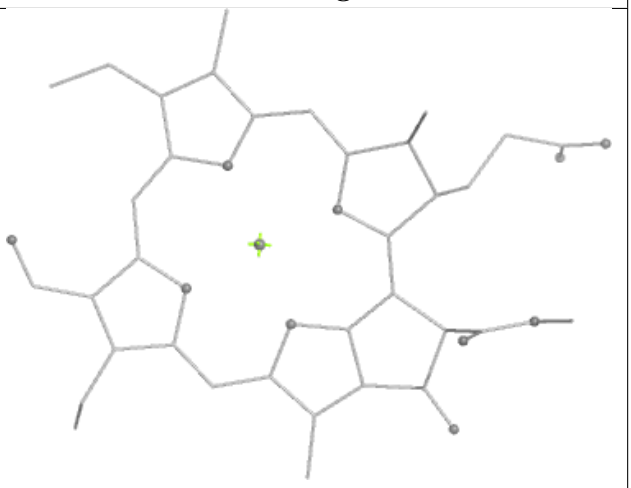
Bond lengths



Bond angles

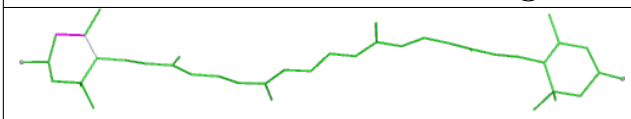


Torsions

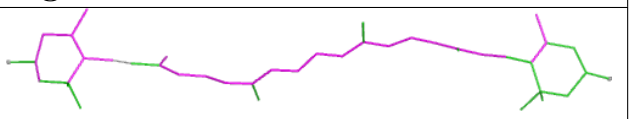


Rings

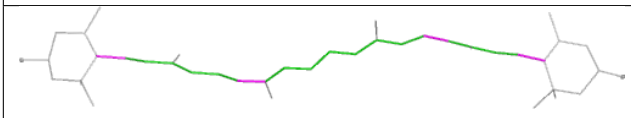
Ligand LUT g1 621



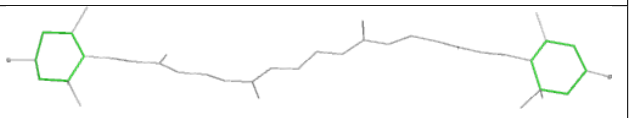
Bond lengths



Bond angles

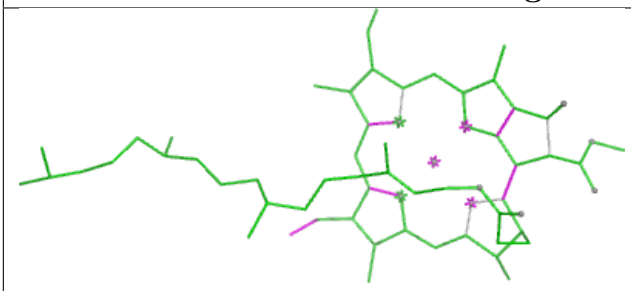


Torsions

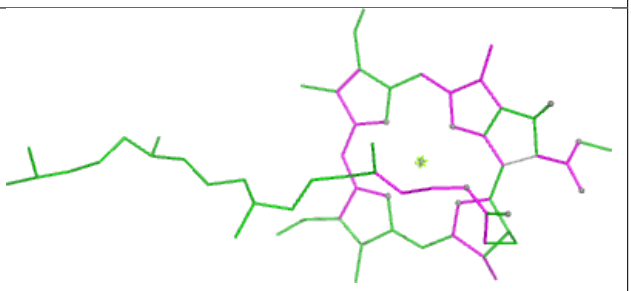


Rings

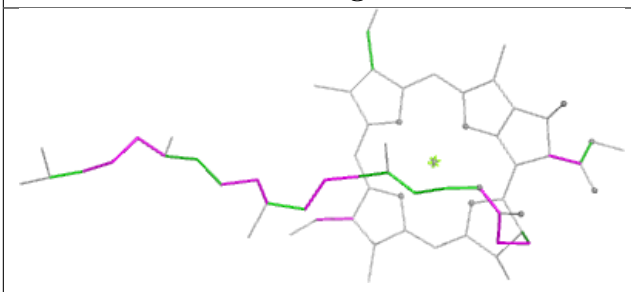
Ligand CLA C 505



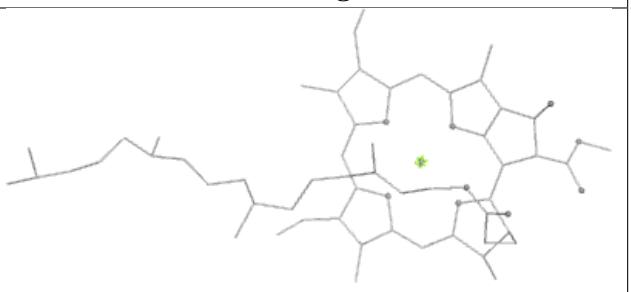
Bond lengths



Bond angles

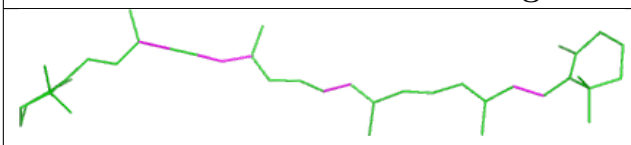


Torsions

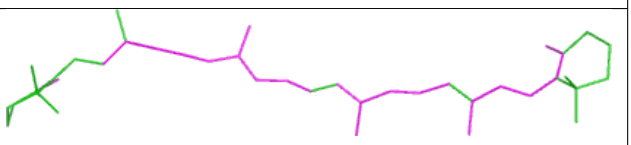


Rings

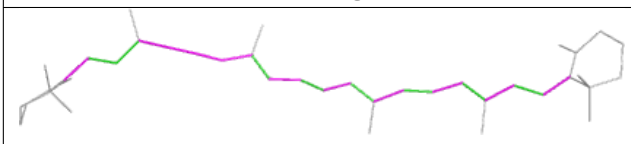
Ligand BCR C 514



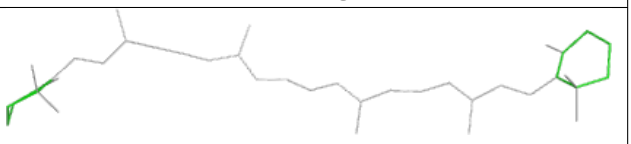
Bond lengths



Bond angles

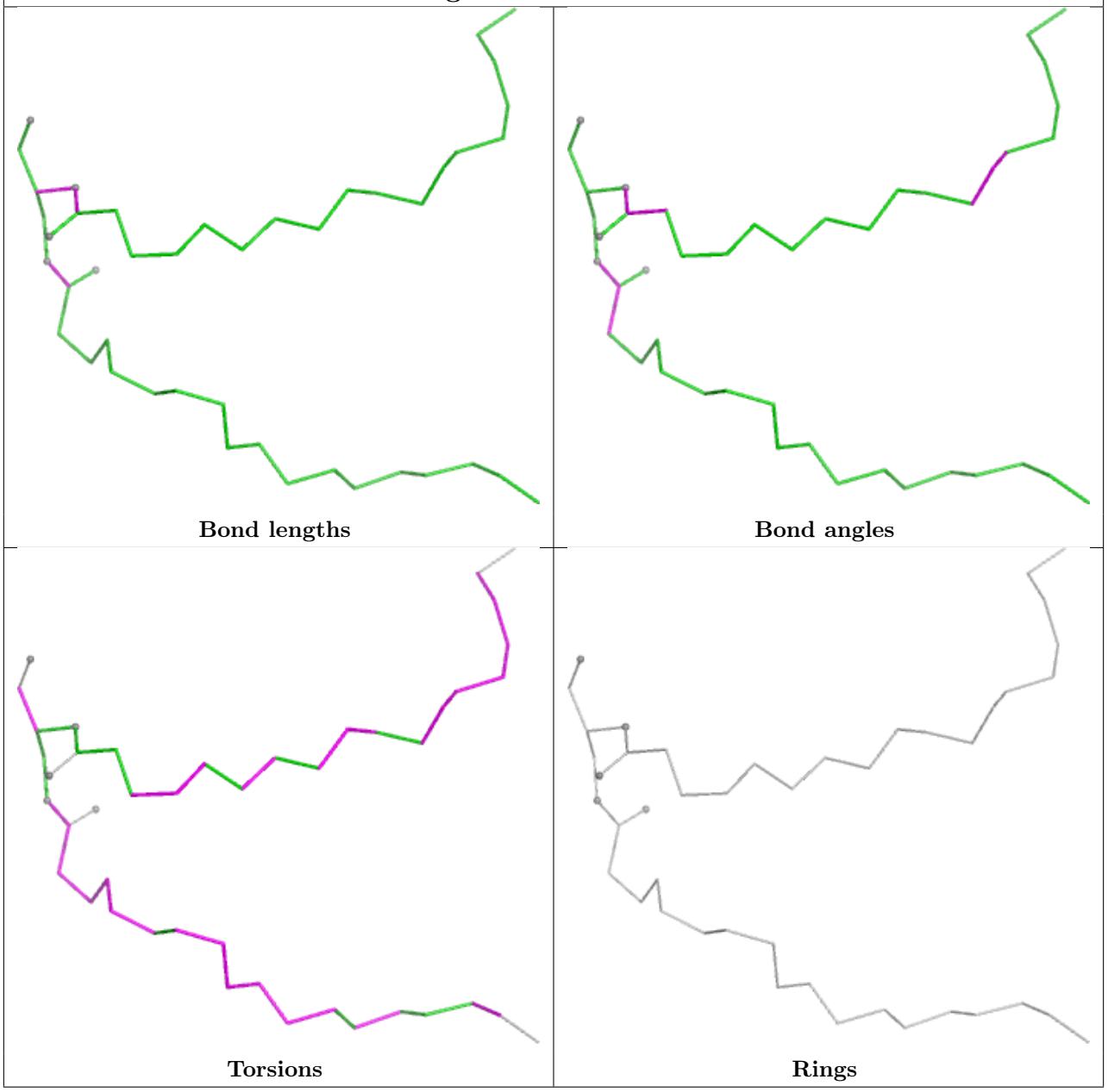


Torsions

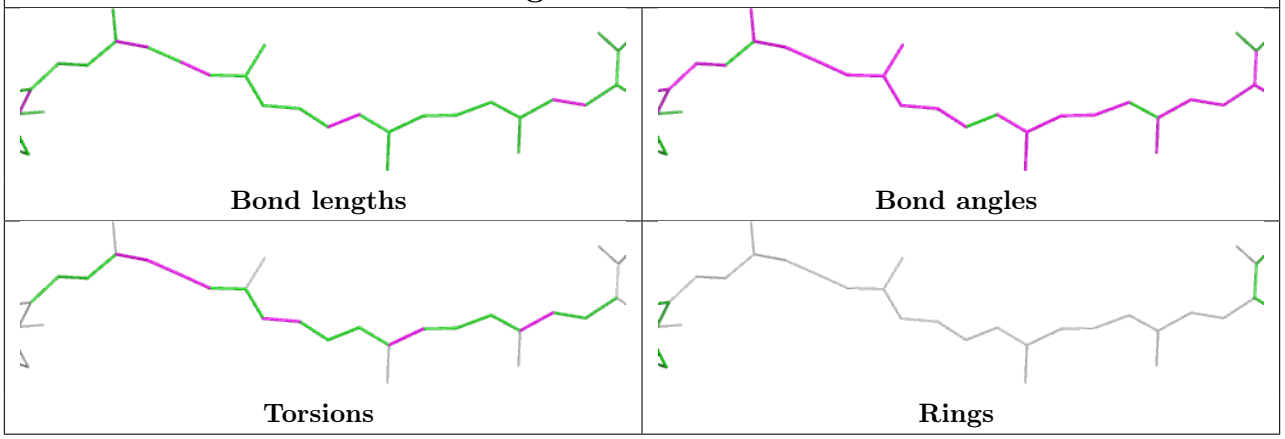


Rings

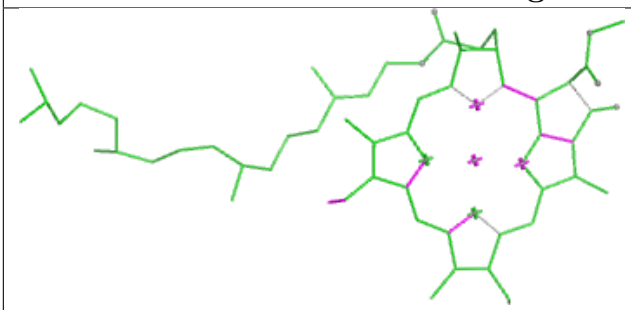
Ligand DGA c1 524



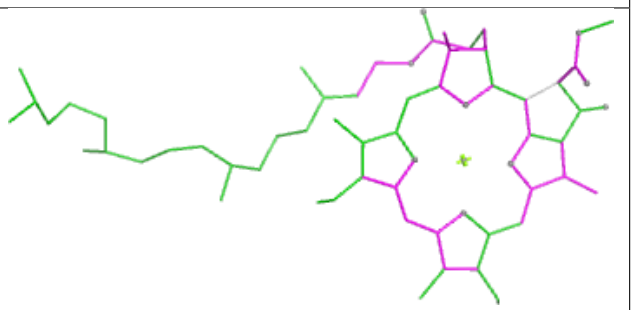
Ligand BCR b 618



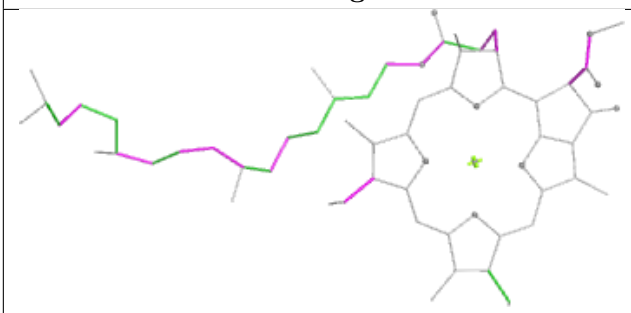
Ligand CLA b 604



Bond lengths



Bond angles

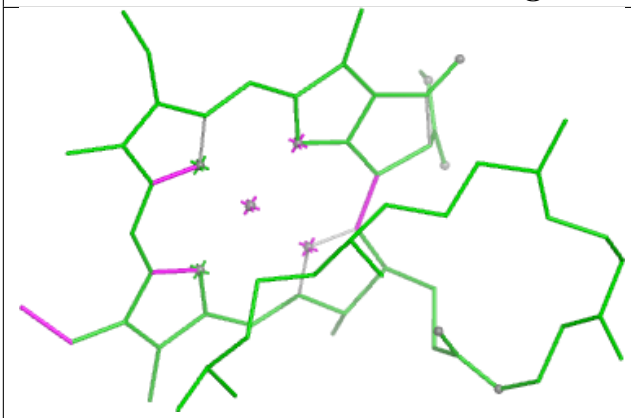


Torsions

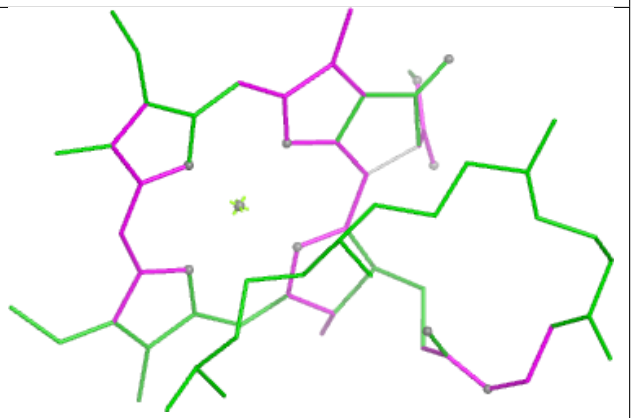


Rings

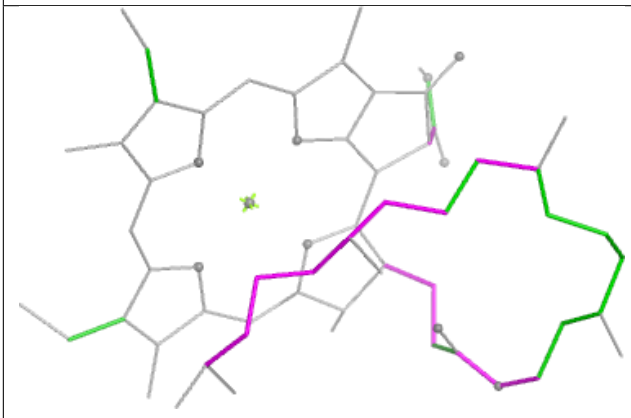
Ligand CLA B 602



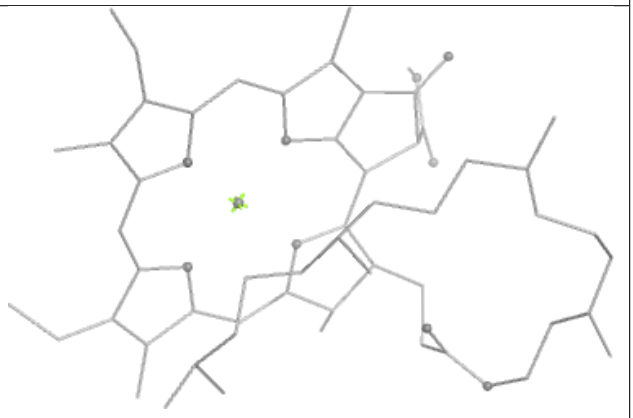
Bond lengths



Bond angles

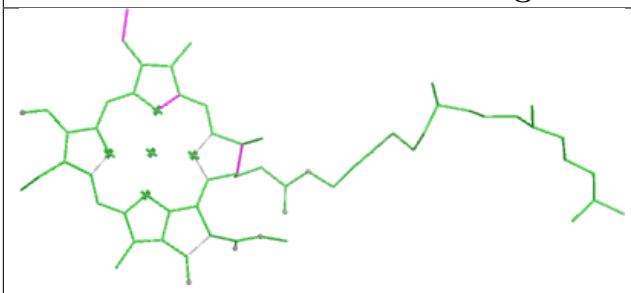


Torsions

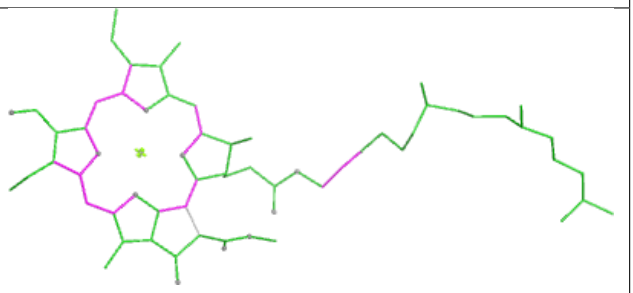


Rings

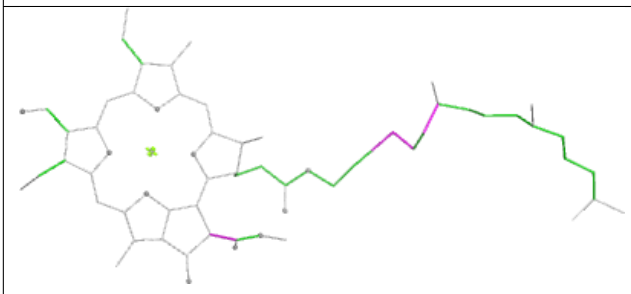
Ligand CHL Y1 601



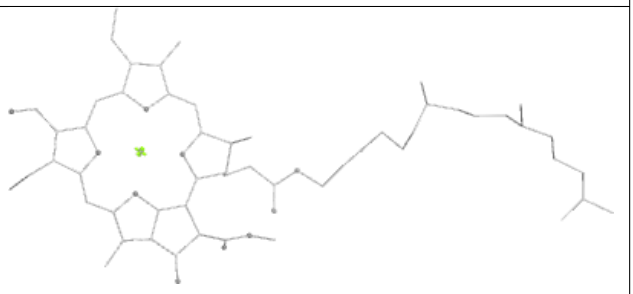
Bond lengths



Bond angles

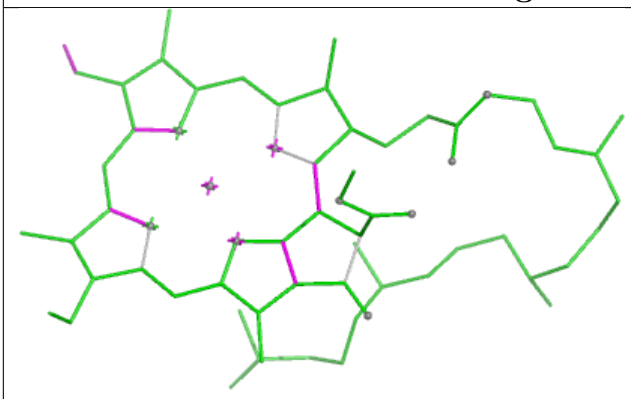


Torsions

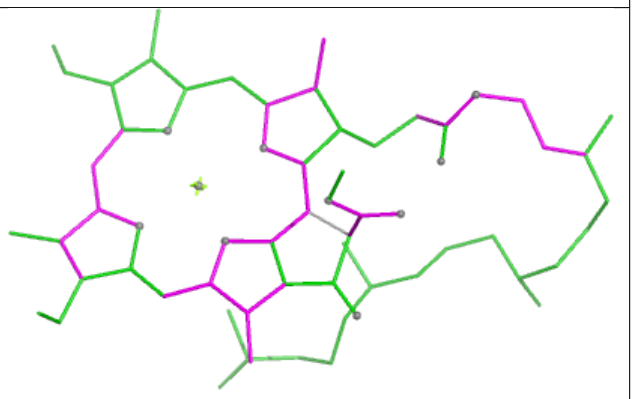


Rings

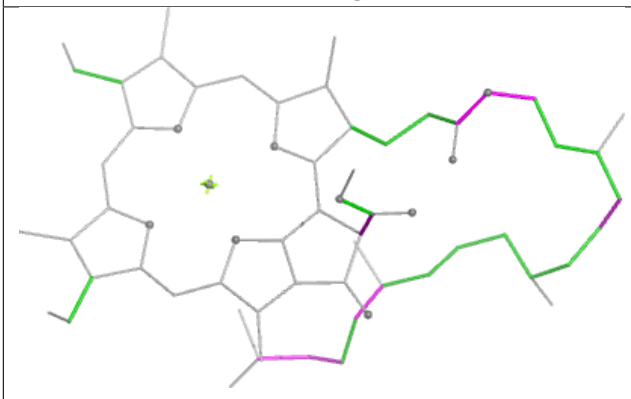
Ligand CLA C1 509



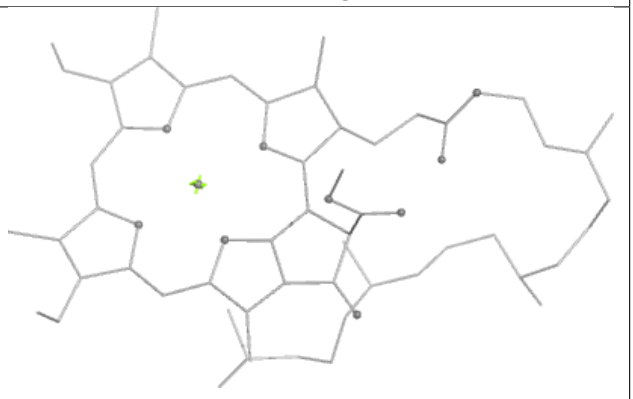
Bond lengths



Bond angles

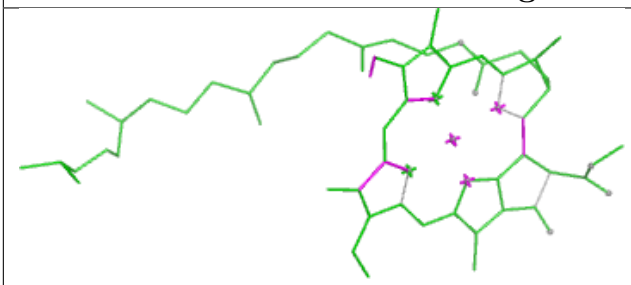


Torsions

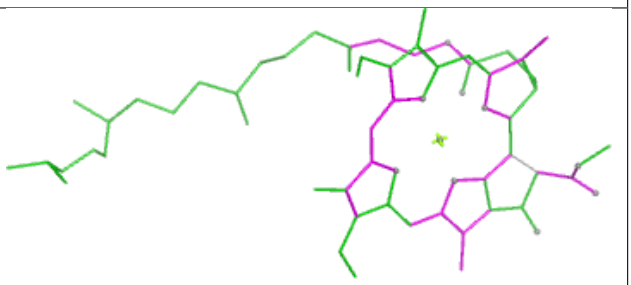


Rings

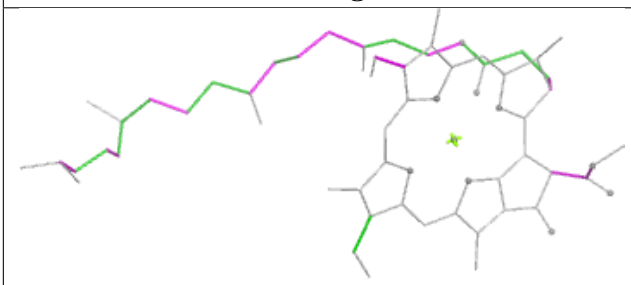
Ligand CLA b1 609



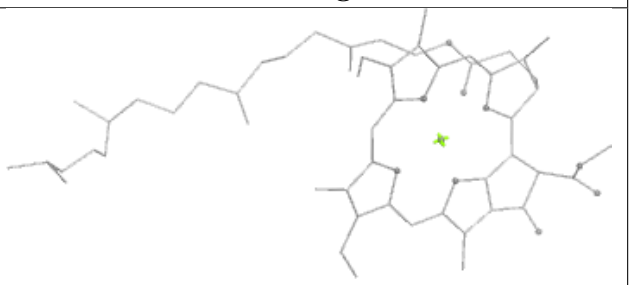
Bond lengths



Bond angles

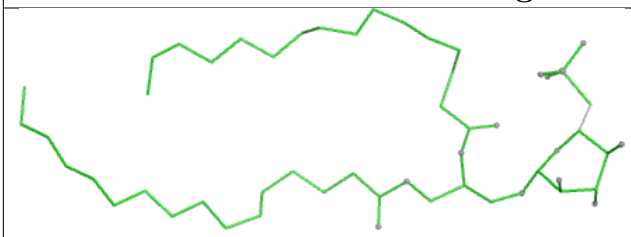


Torsions

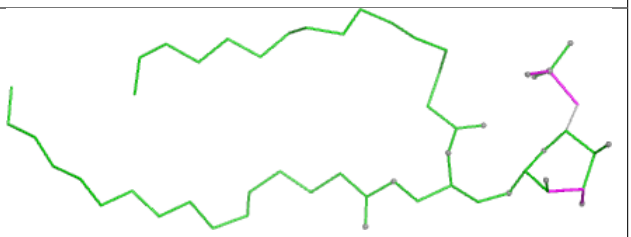


Rings

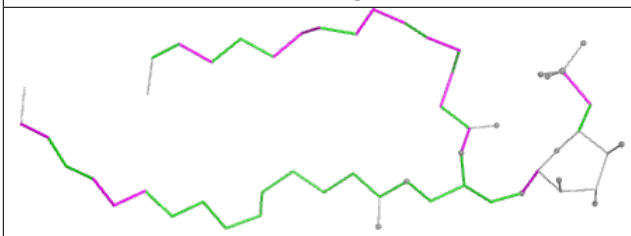
Ligand SQD B1 626



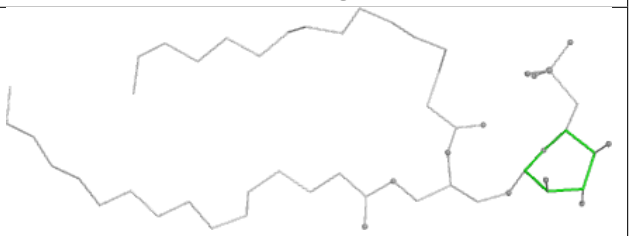
Bond lengths



Bond angles

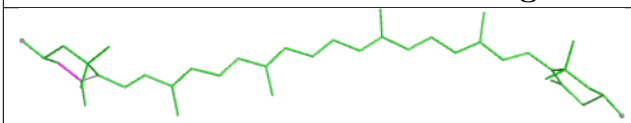


Torsions

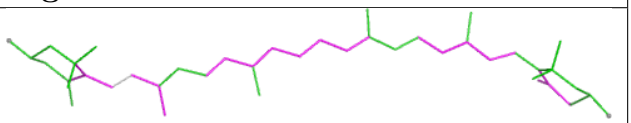


Rings

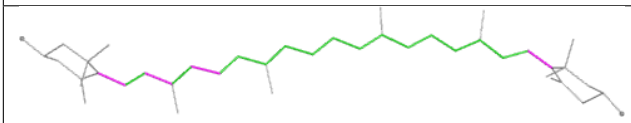
Ligand LUT g1 620



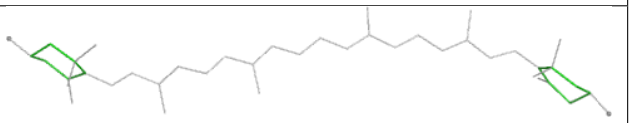
Bond lengths



Bond angles



Torsions

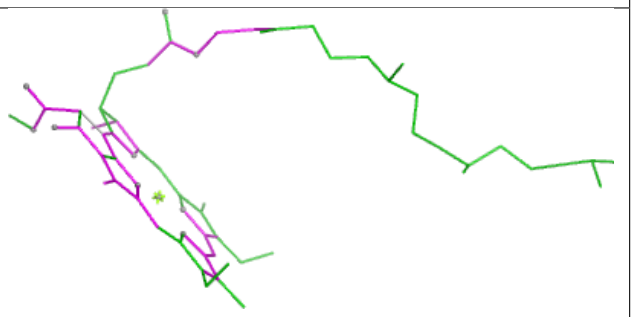


Rings

Ligand CLA N 604



Bond lengths



Bond angles

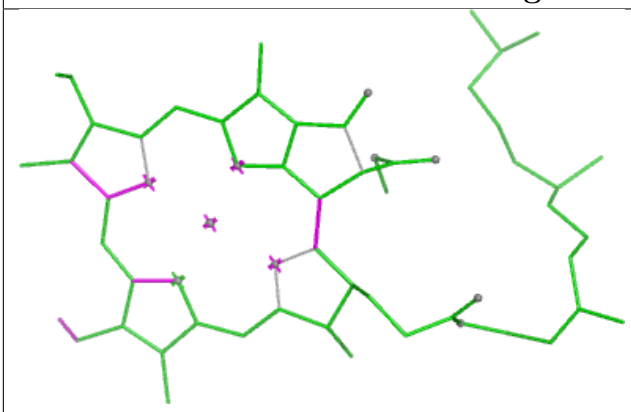


Torsions

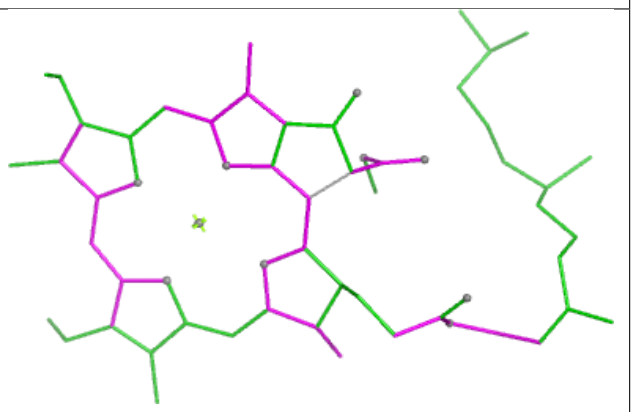


Rings

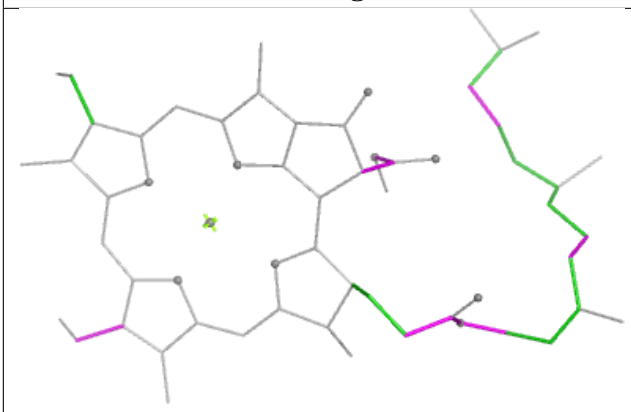
Ligand CLA R 612



Bond lengths



Bond angles

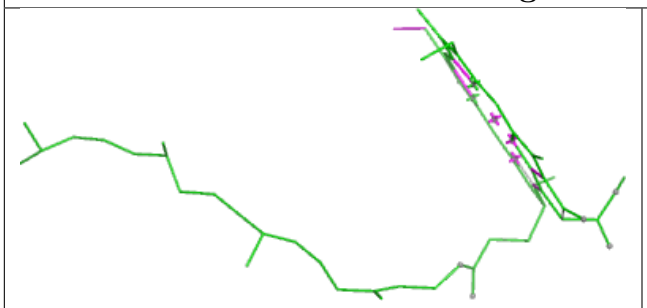


Torsions

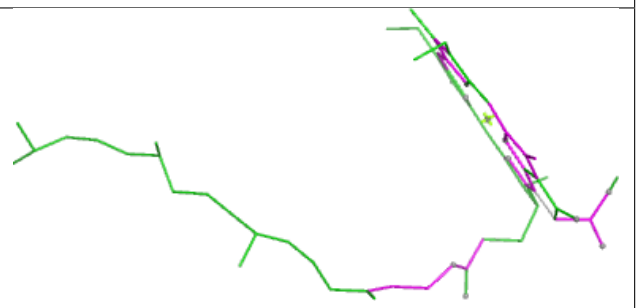


Rings

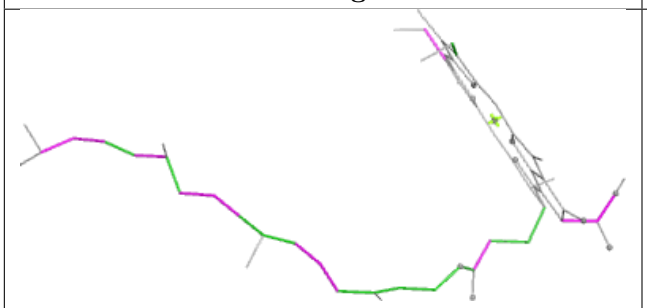
Ligand CLA n1 604



Bond lengths



Bond angles

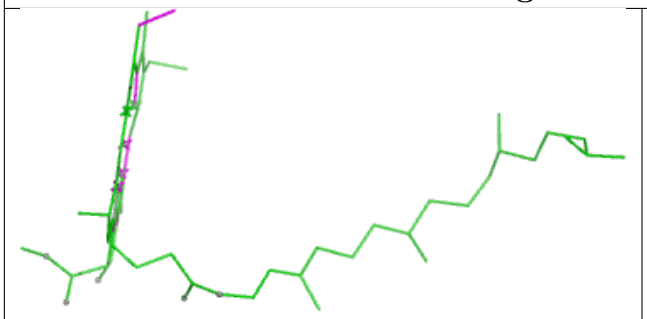


Torsions

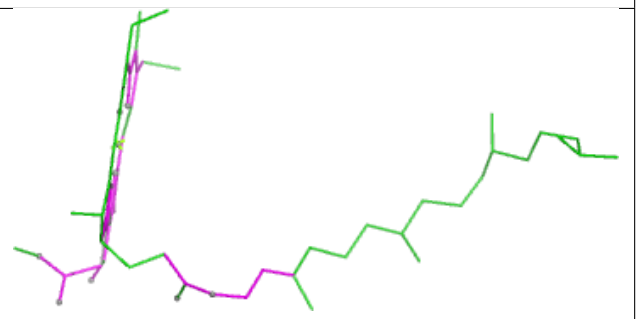


Rings

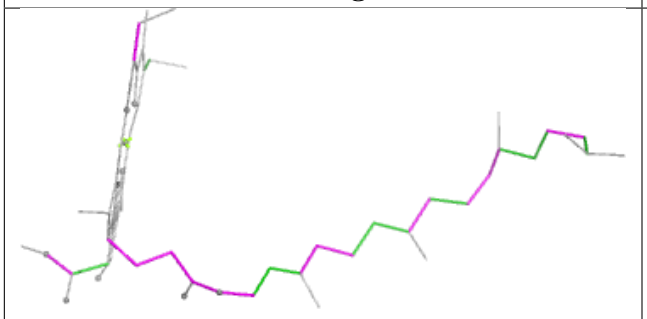
Ligand CLA B1 606



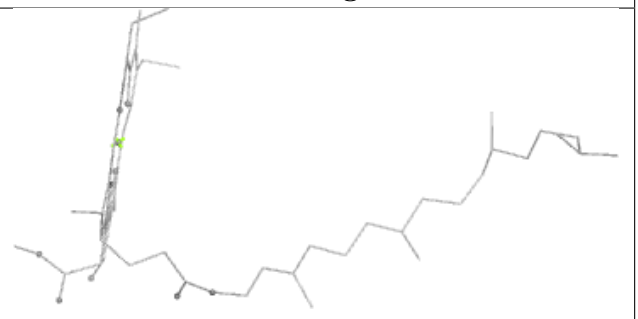
Bond lengths



Bond angles

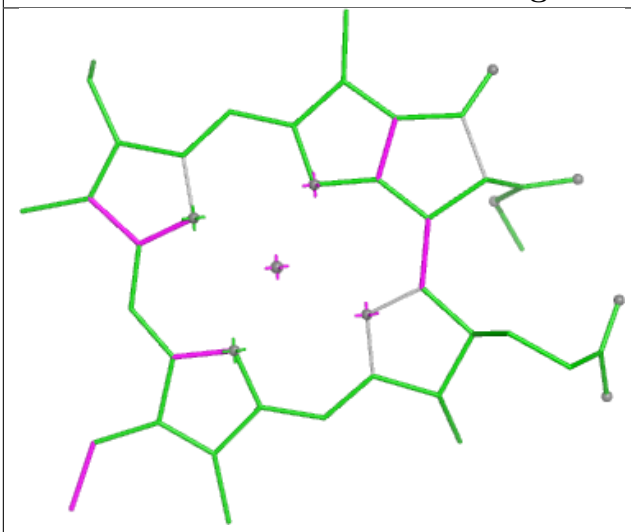


Torsions

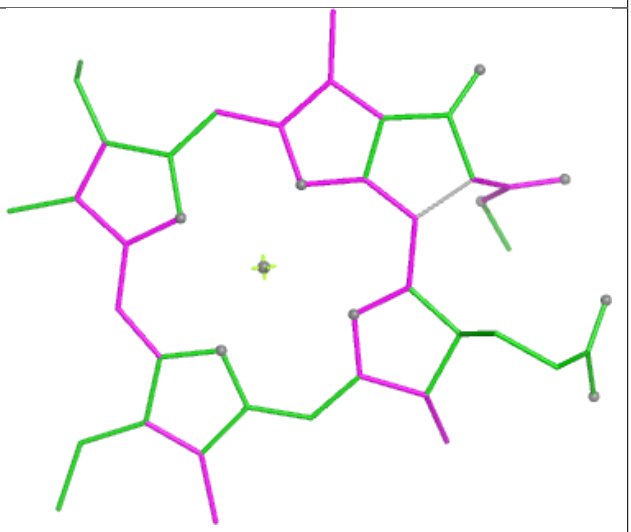


Rings

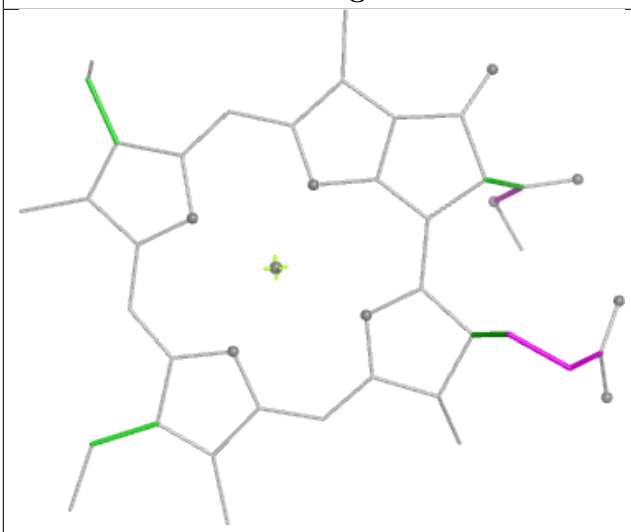
Ligand CLA s 612



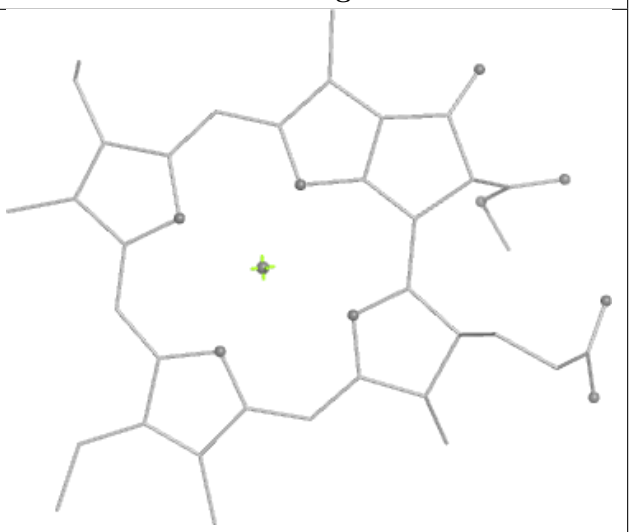
Bond lengths



Bond angles

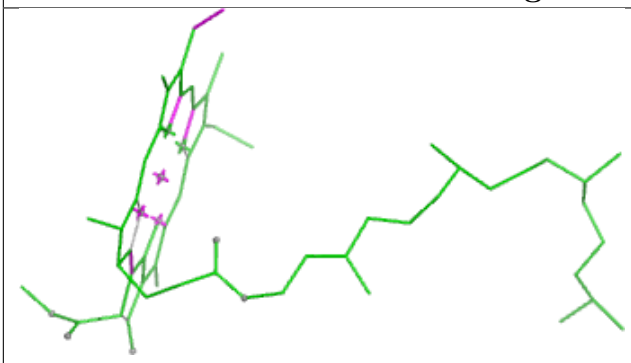


Torsions

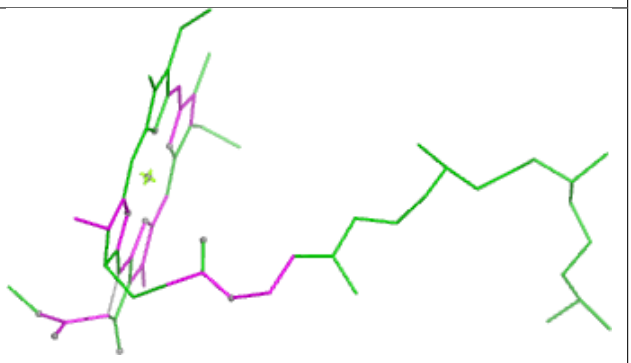


Rings

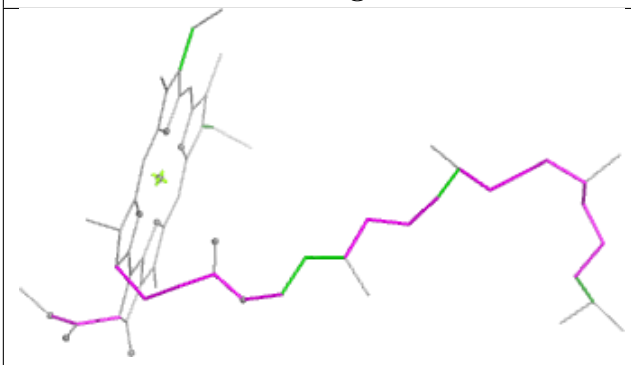
Ligand CLA B 608



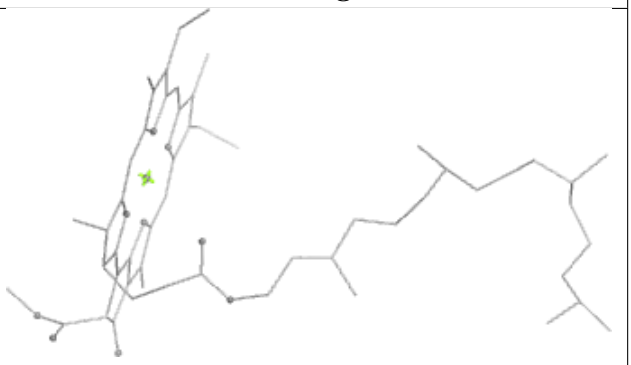
Bond lengths



Bond angles

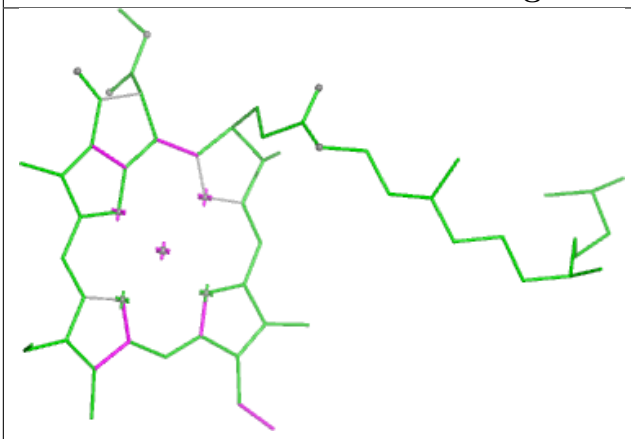


Torsions

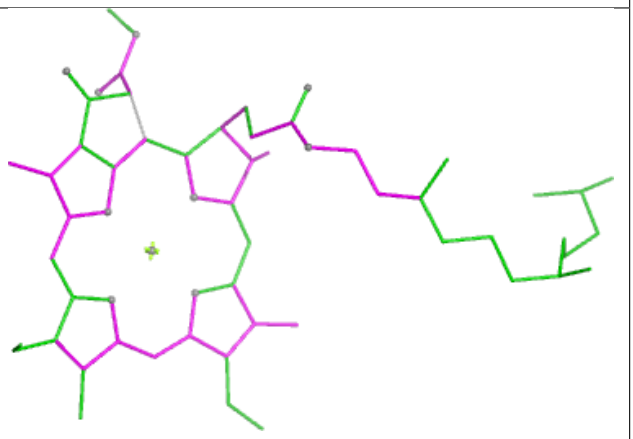


Rings

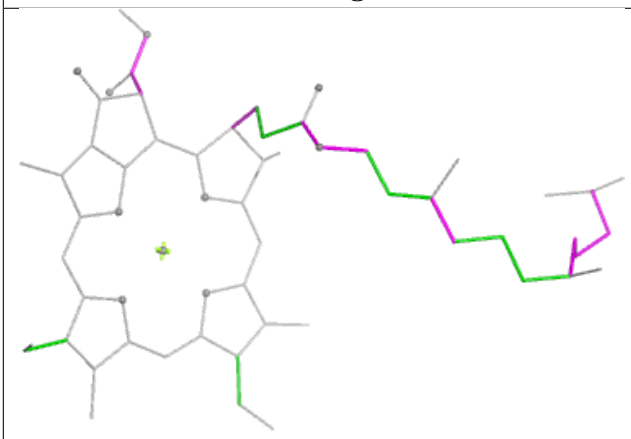
Ligand CLA A 410



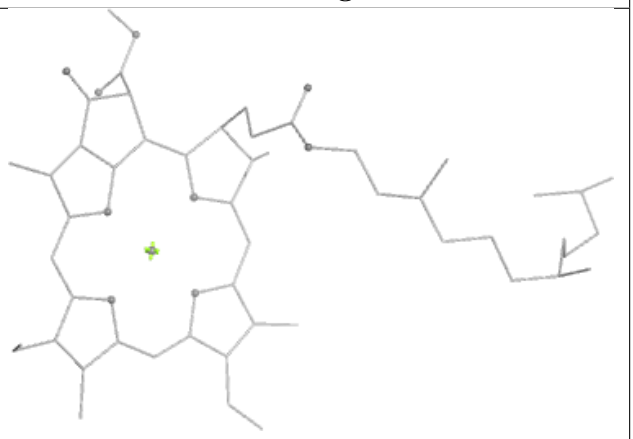
Bond lengths



Bond angles

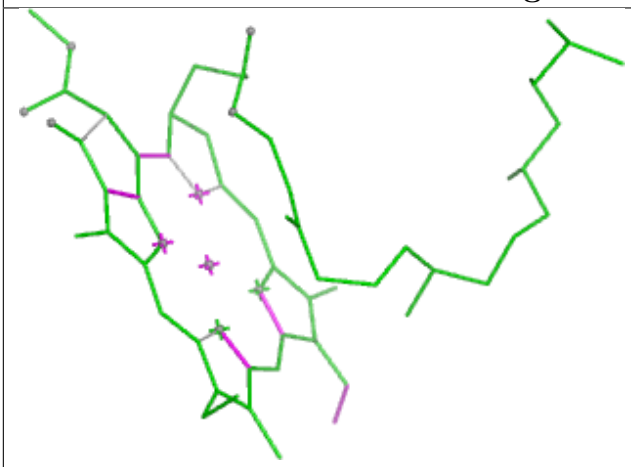


Torsions

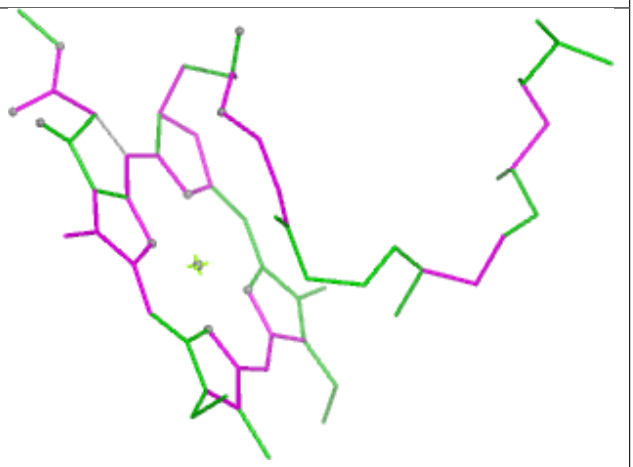


Rings

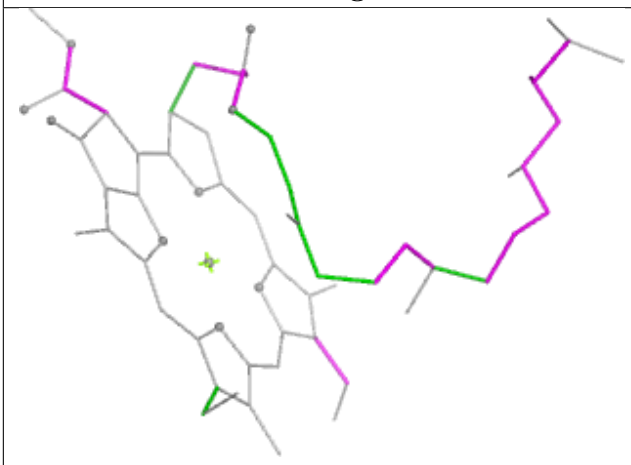
Ligand CLA Y 613



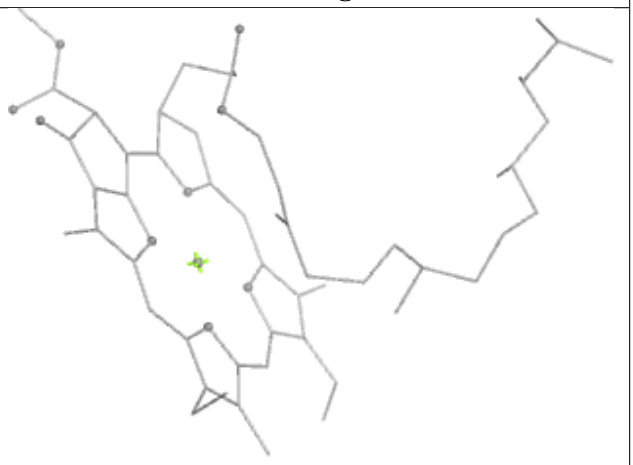
Bond lengths



Bond angles

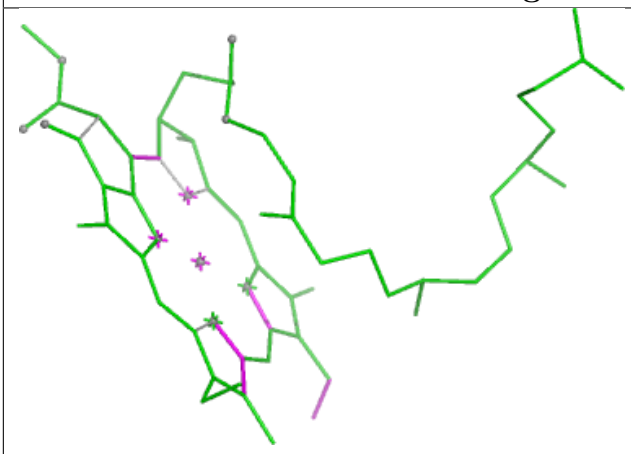


Torsions

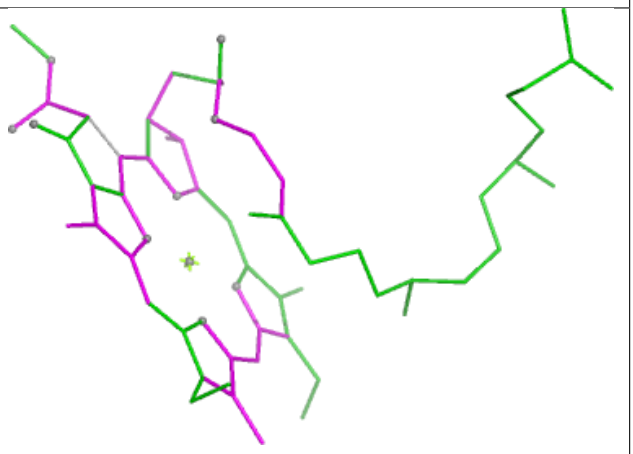


Rings

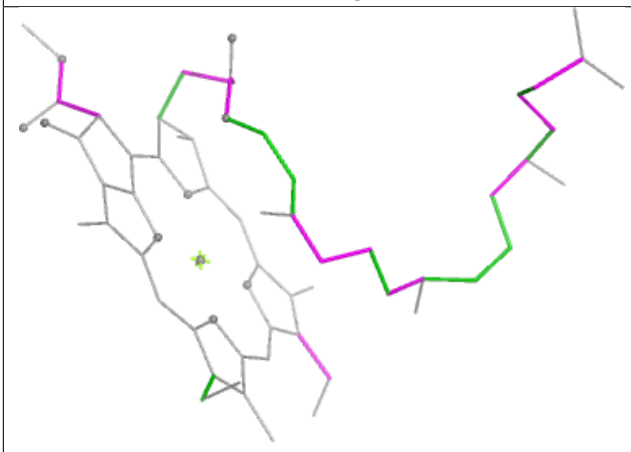
Ligand CLA G 613



Bond lengths



Bond angles

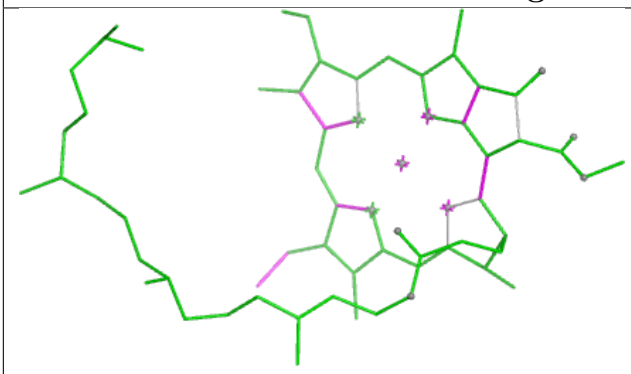


Torsions

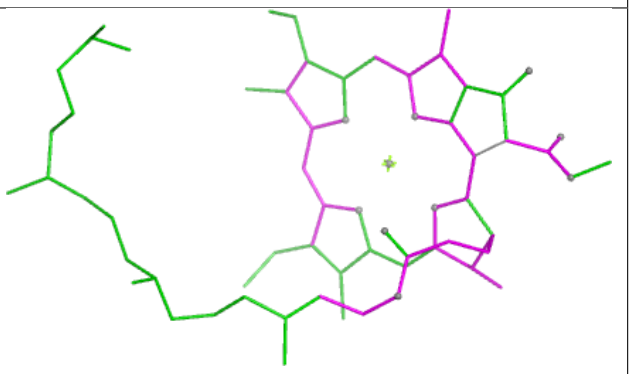


Rings

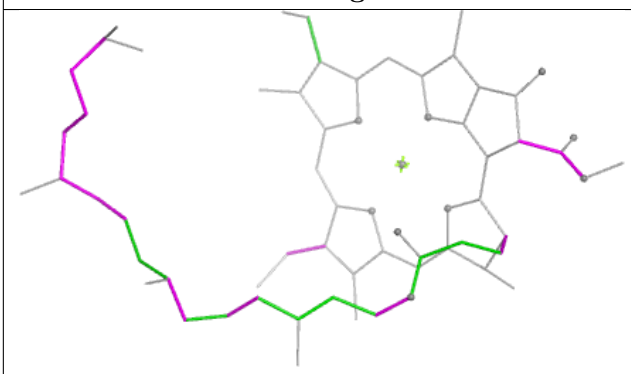
Ligand CLA n 610



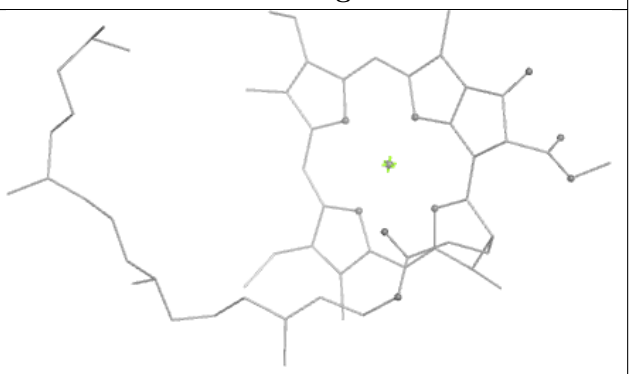
Bond lengths



Bond angles

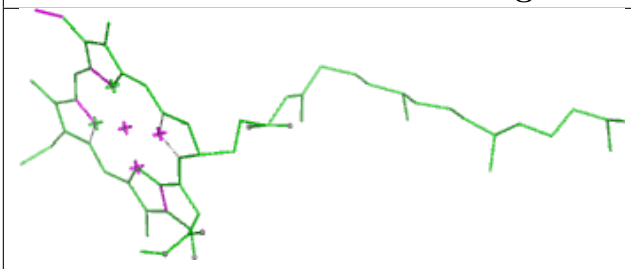


Torsions

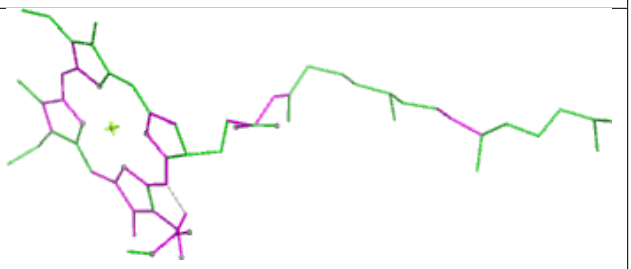


Rings

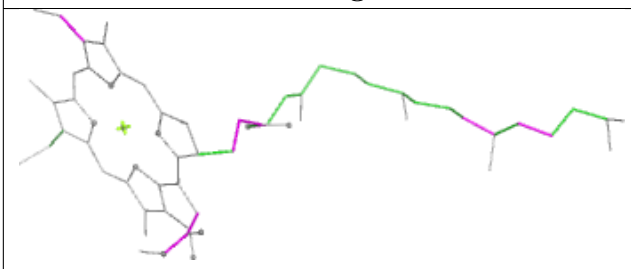
Ligand CLA C1 502



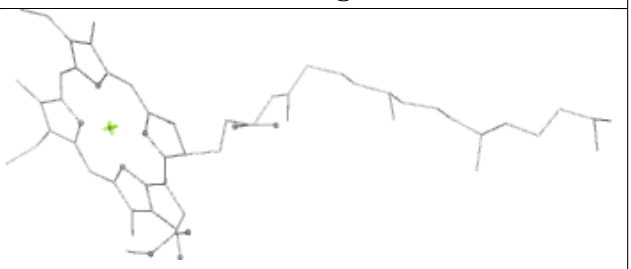
Bond lengths



Bond angles

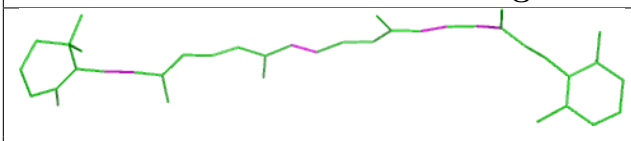


Torsions

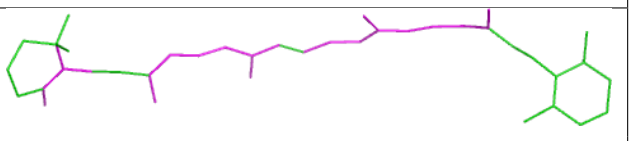


Rings

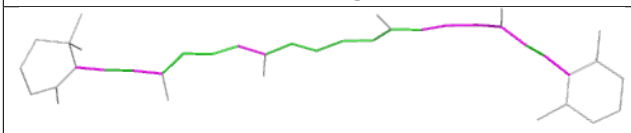
Ligand BCR D1 404



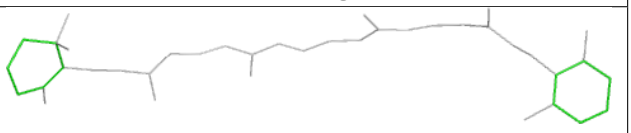
Bond lengths



Bond angles

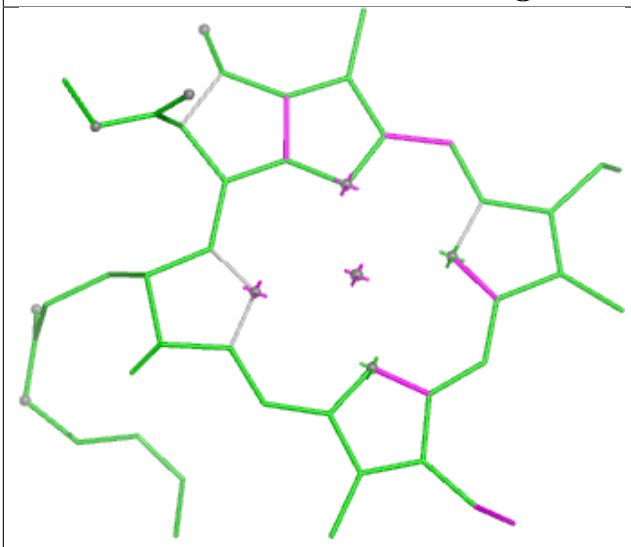


Torsions

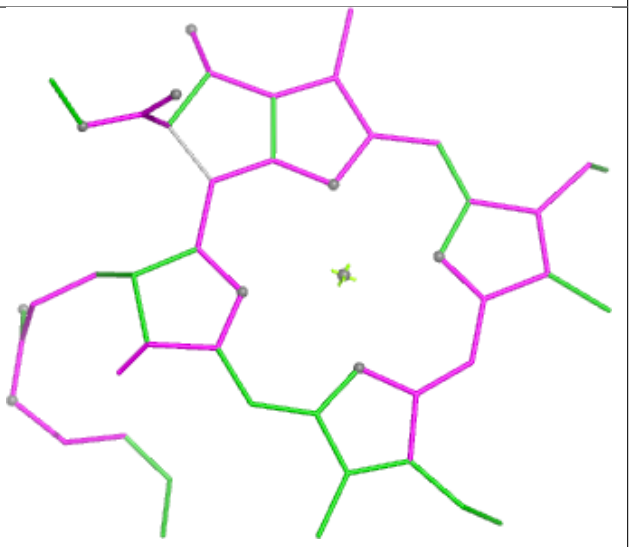


Rings

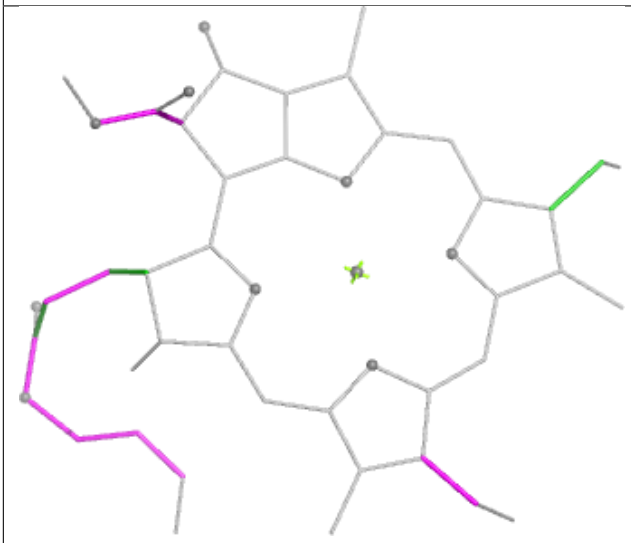
Ligand CLA N1 611



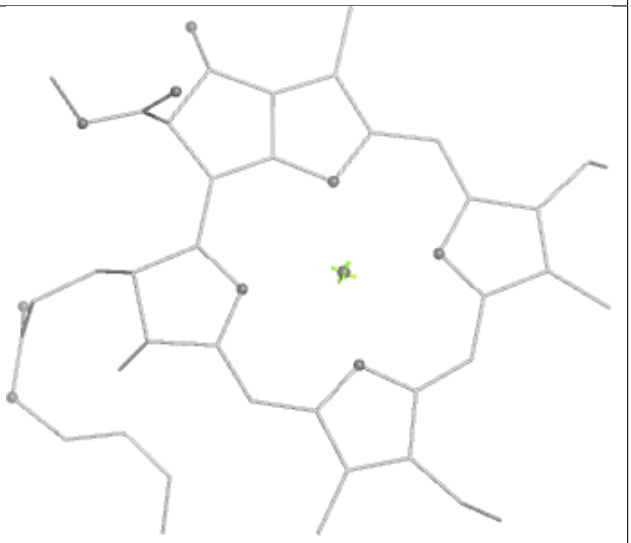
Bond lengths



Bond angles

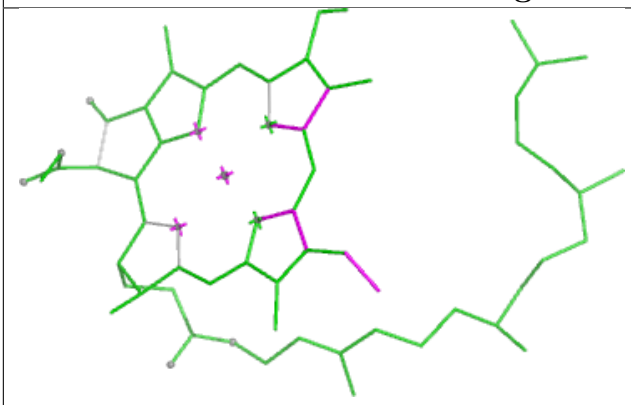


Torsions

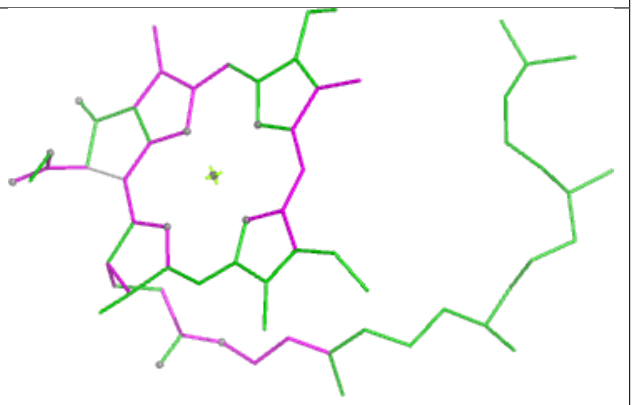


Rings

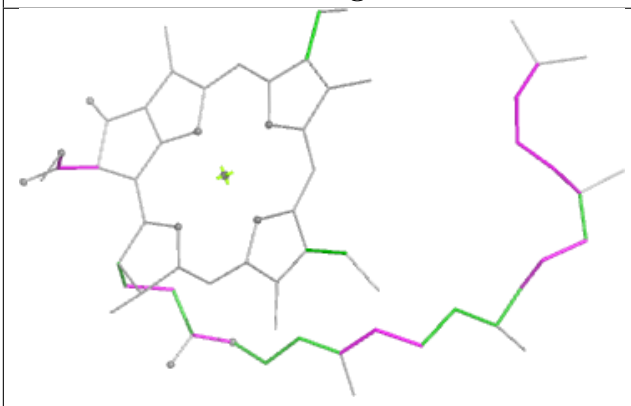
Ligand CLA N1 602



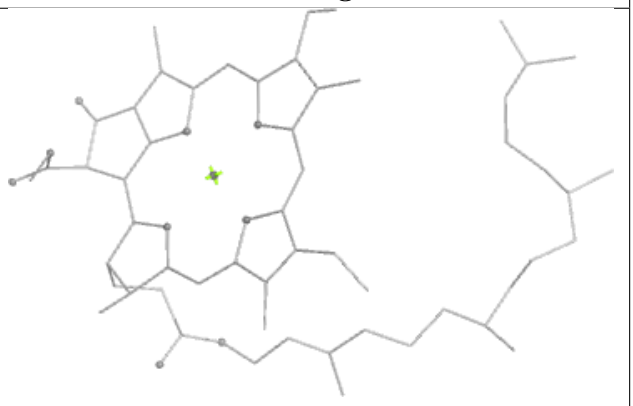
Bond lengths



Bond angles

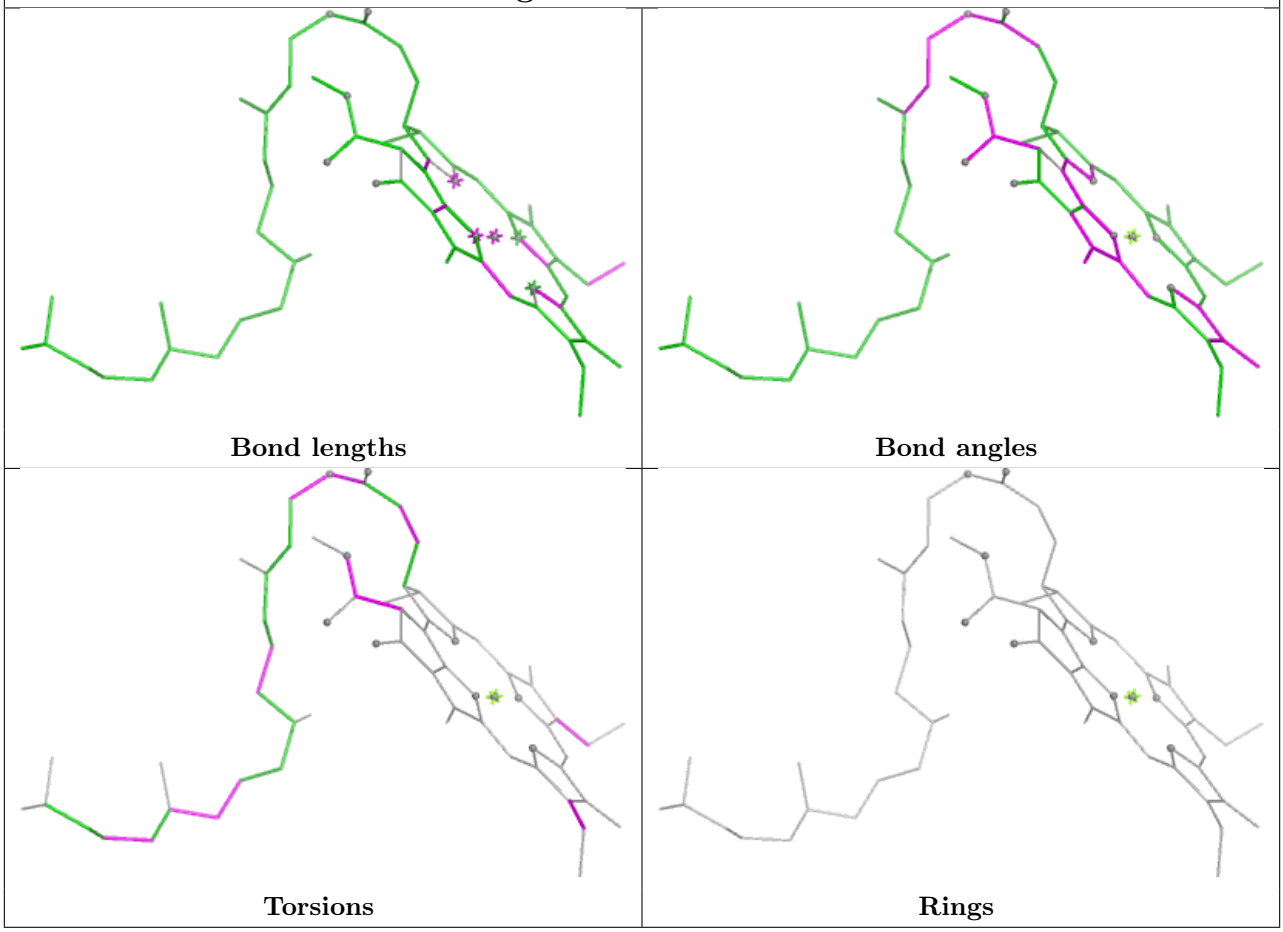


Torsions

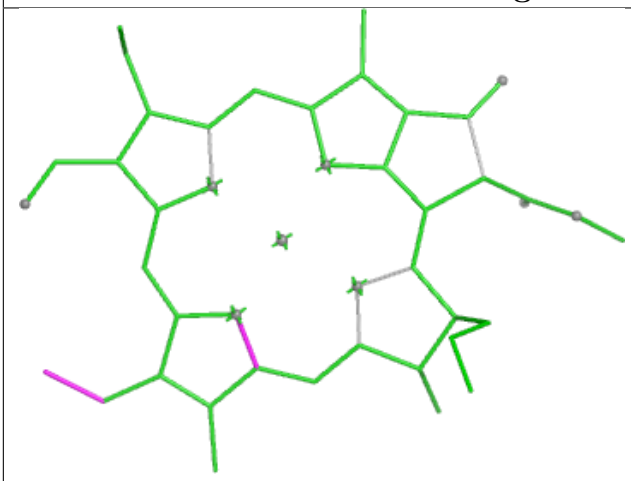


Rings

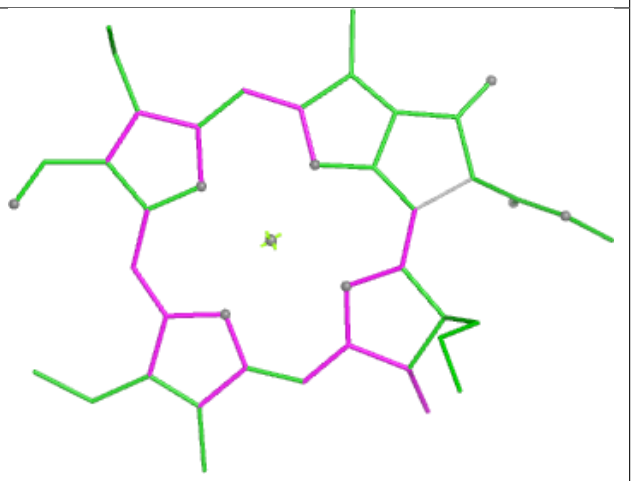
Ligand CLA B1 614



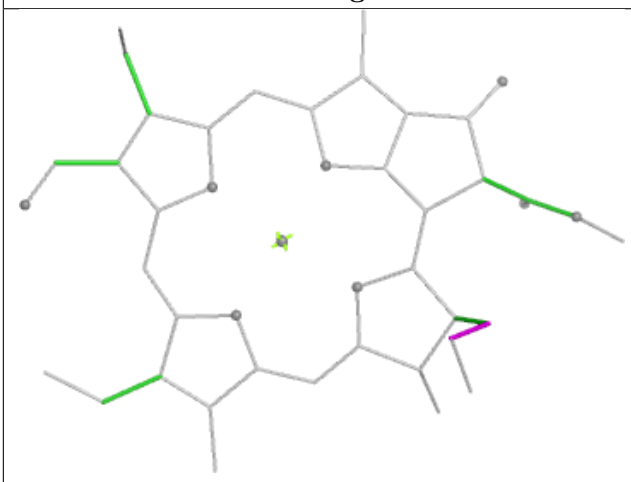
Ligand CHL G1 608



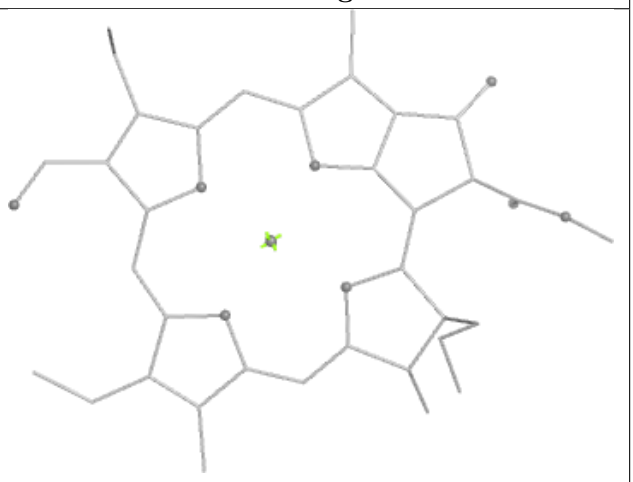
Bond lengths



Bond angles

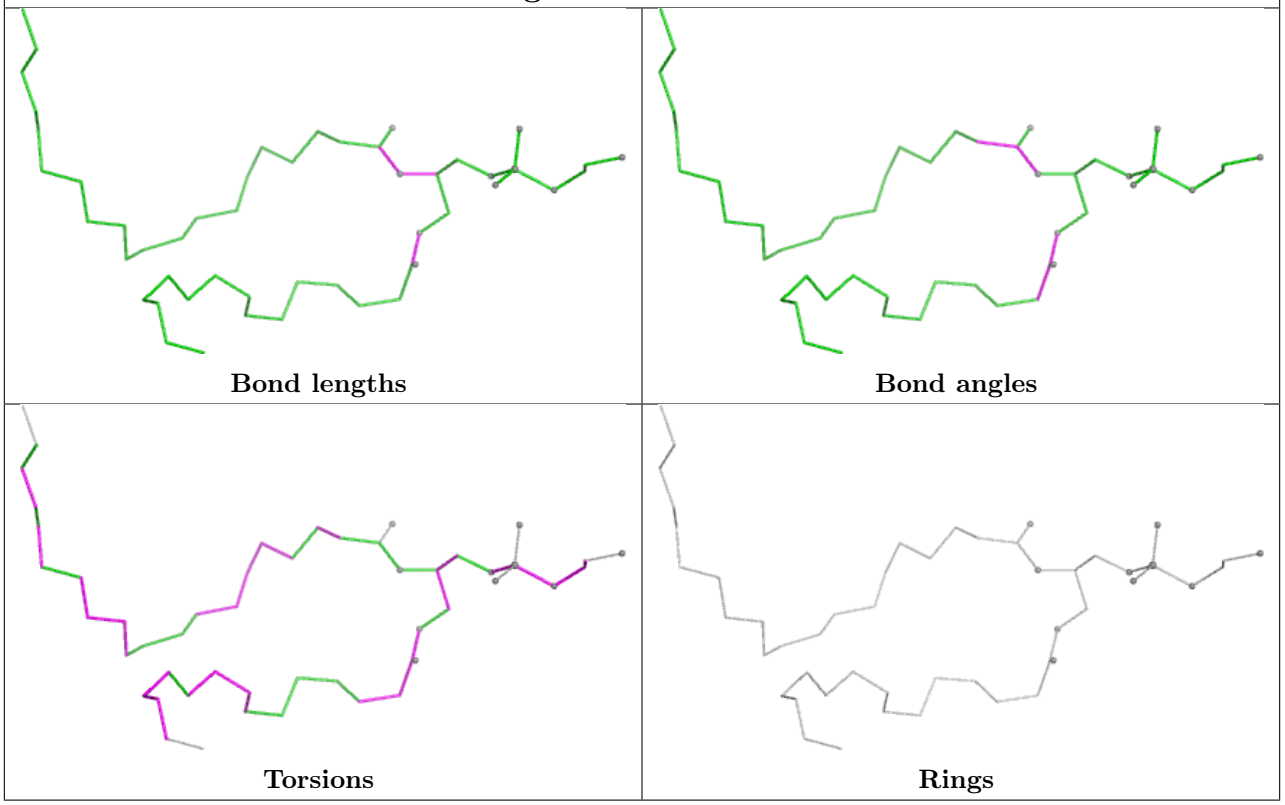


Torsions

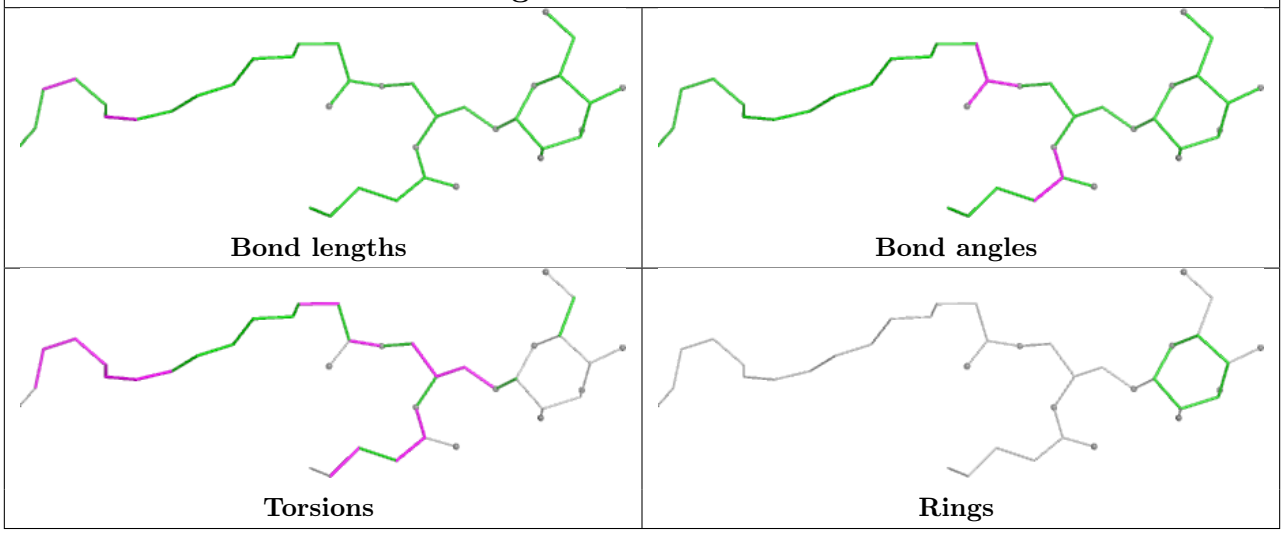


Rings

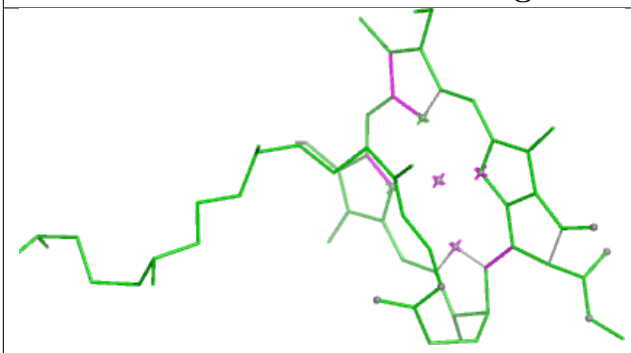
Ligand PTY Y 626



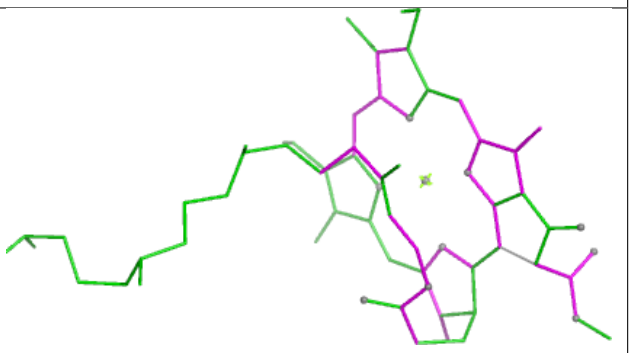
Ligand LMG w1 201



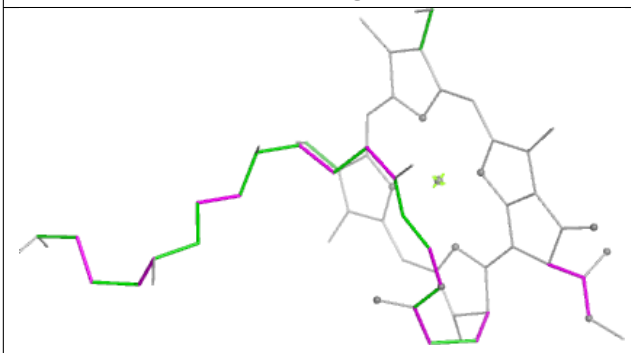
Ligand CLA N1 613



Bond lengths



Bond angles

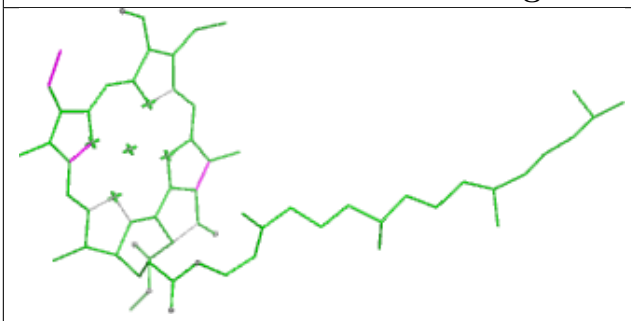


Torsions

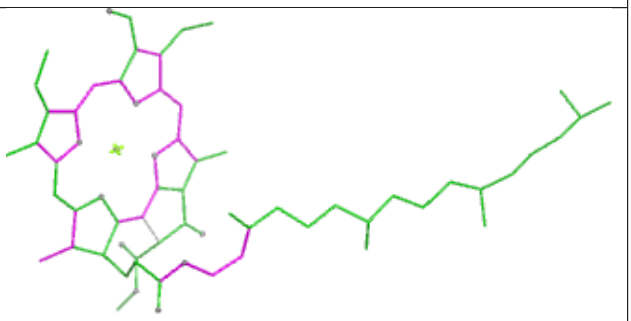


Rings

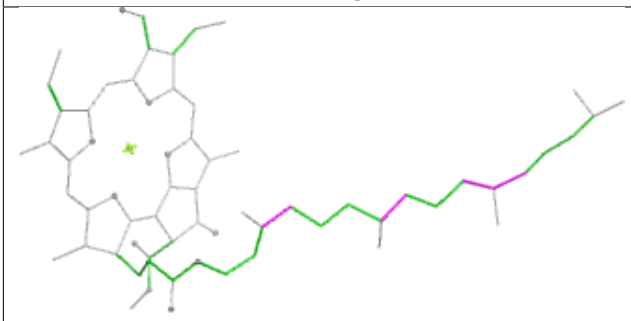
Ligand CHL Y 609



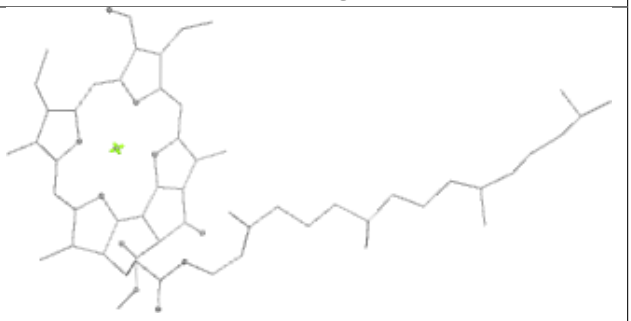
Bond lengths



Bond angles

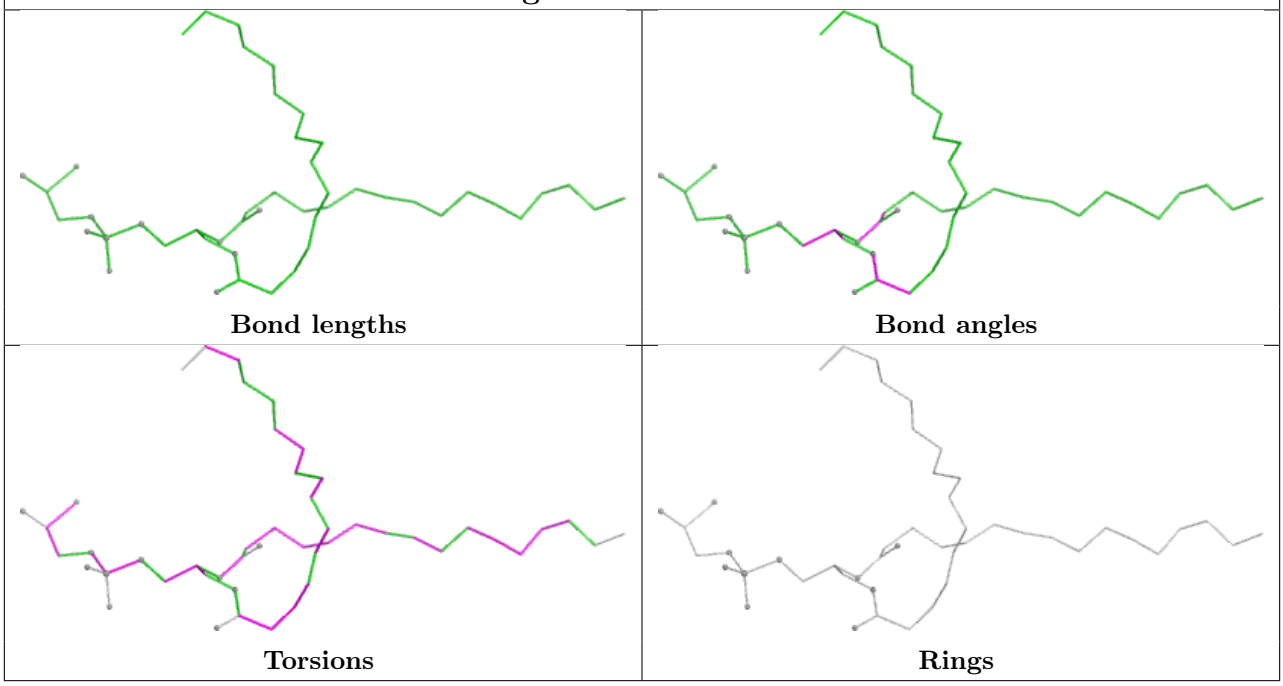


Torsions

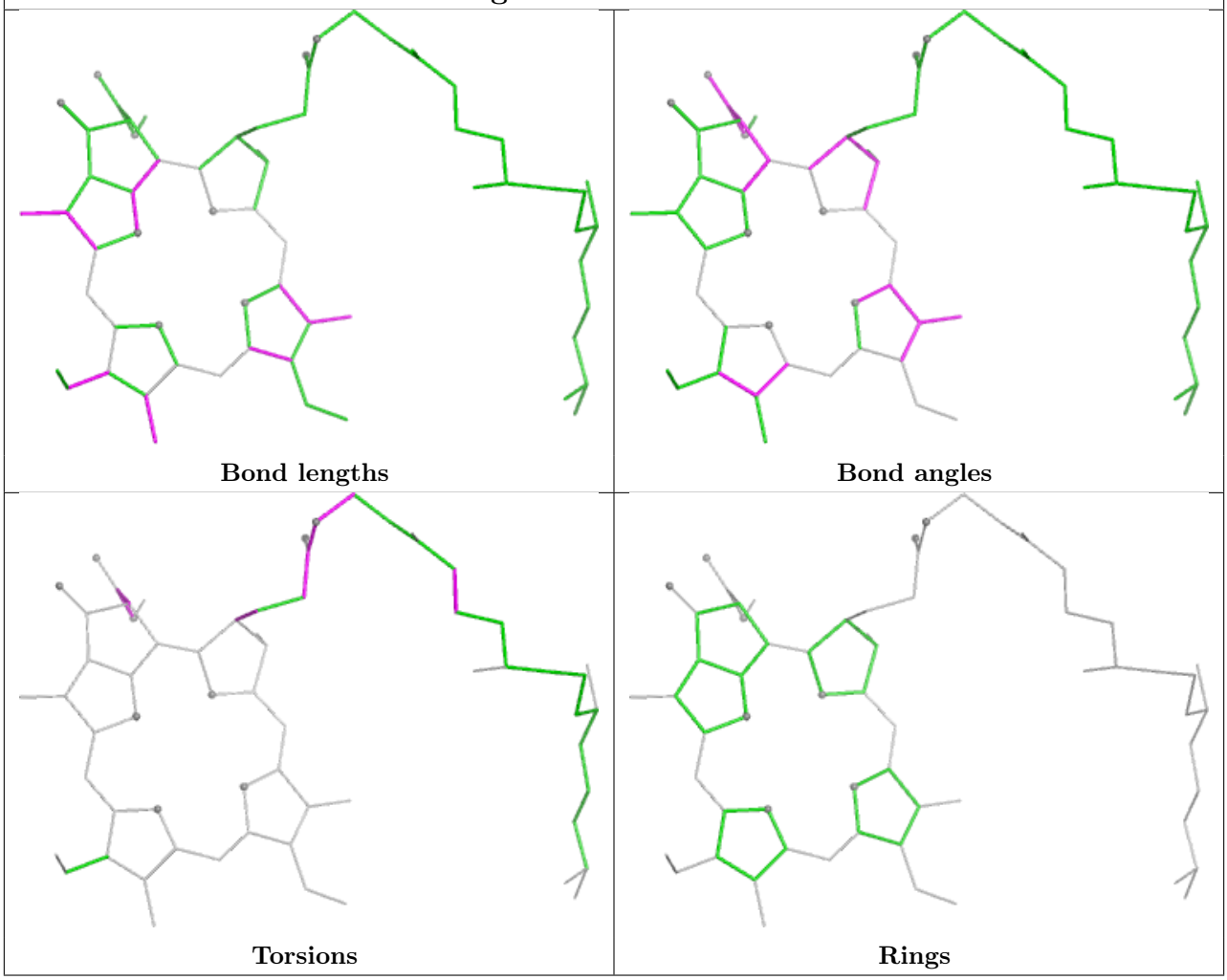


Rings

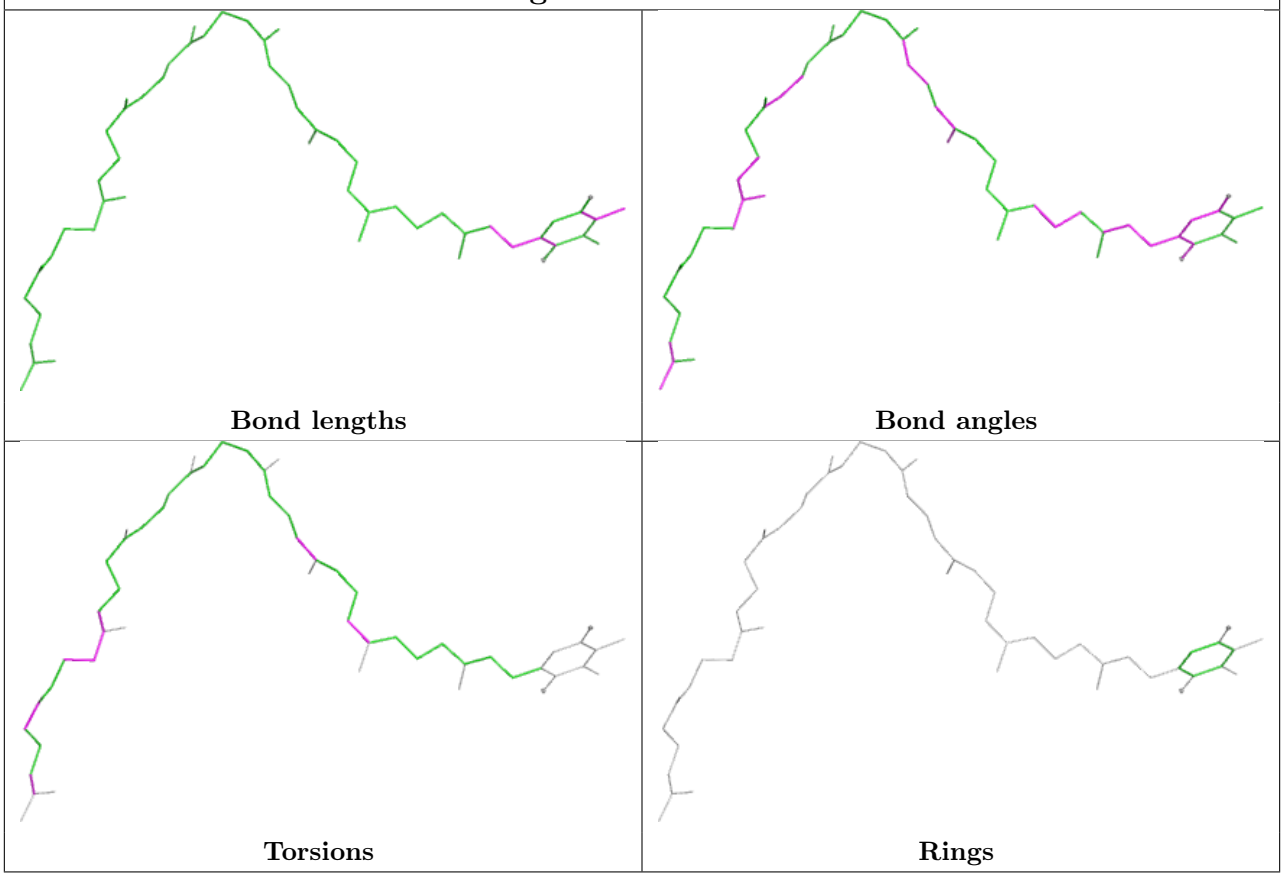
Ligand LHG G 624



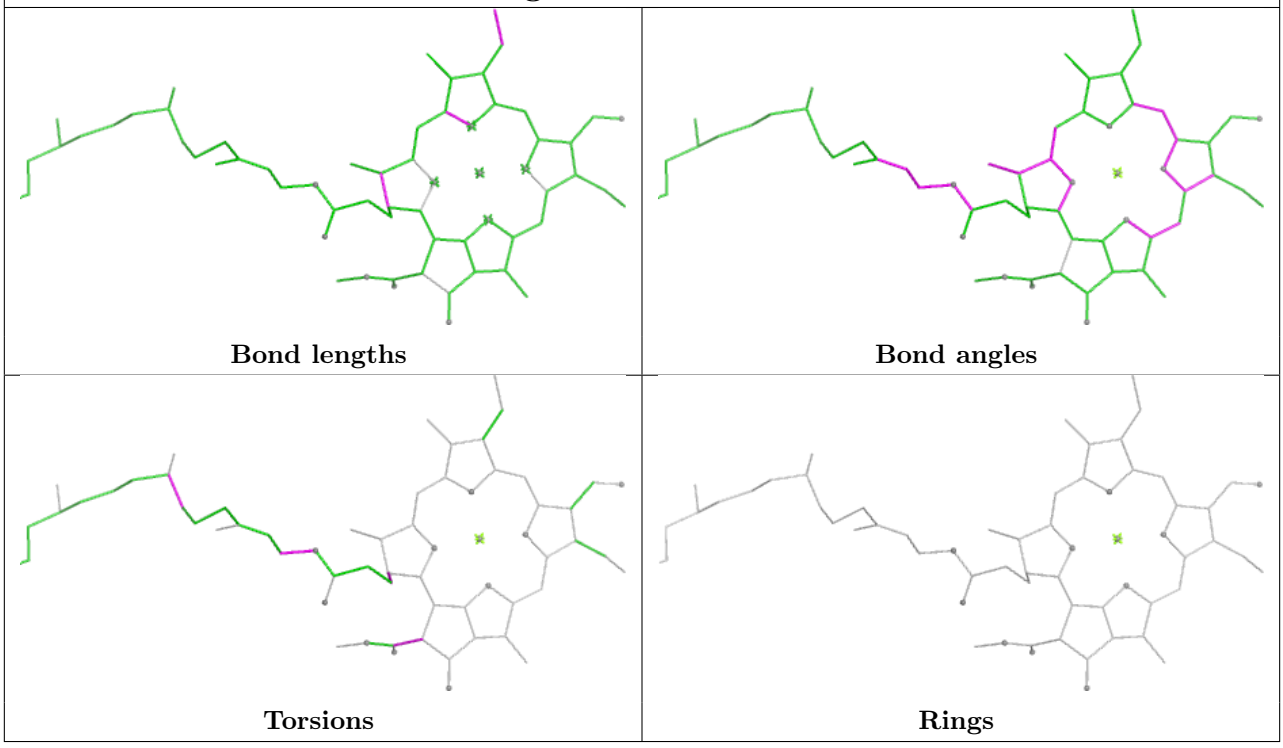
Ligand PHO A1 409



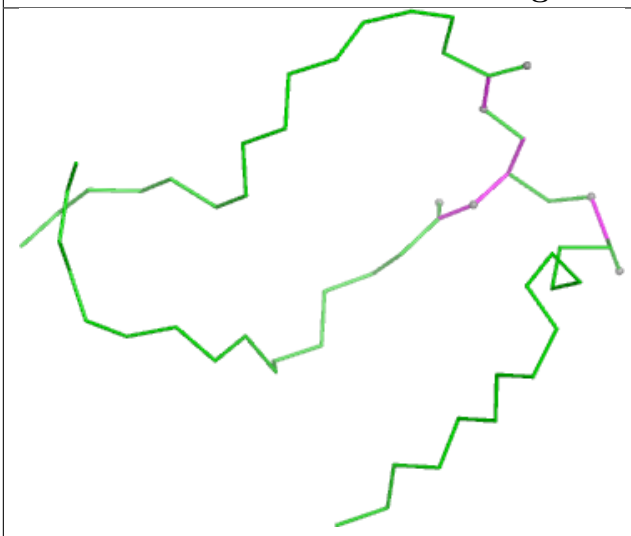
Ligand PL9 D 405



Ligand CHL Y 601



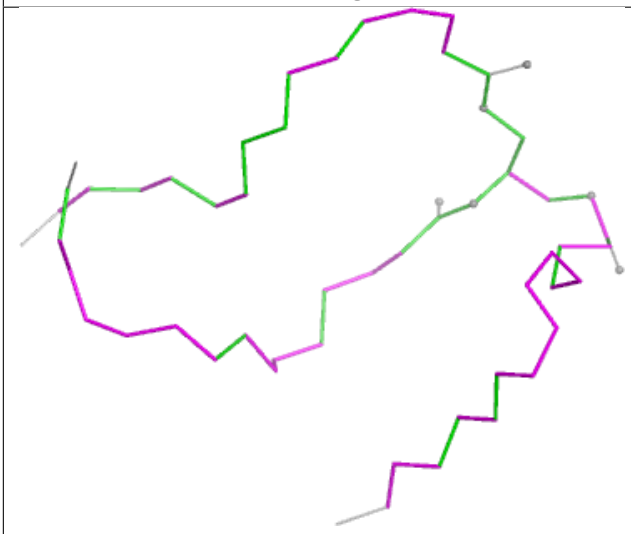
Ligand 4RF k 101



Bond lengths



Bond angles

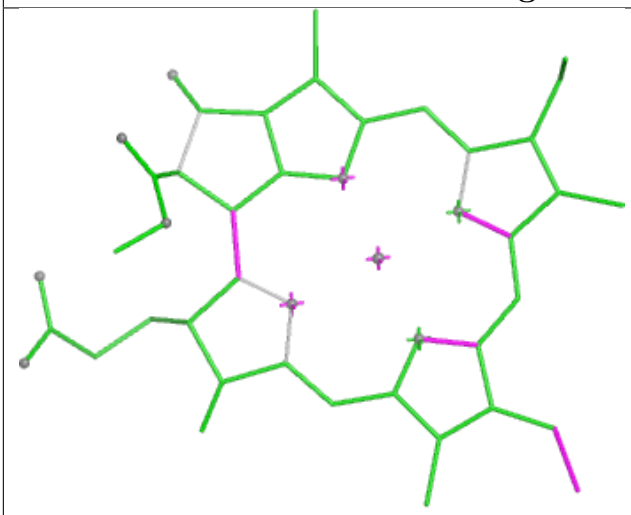


Torsions

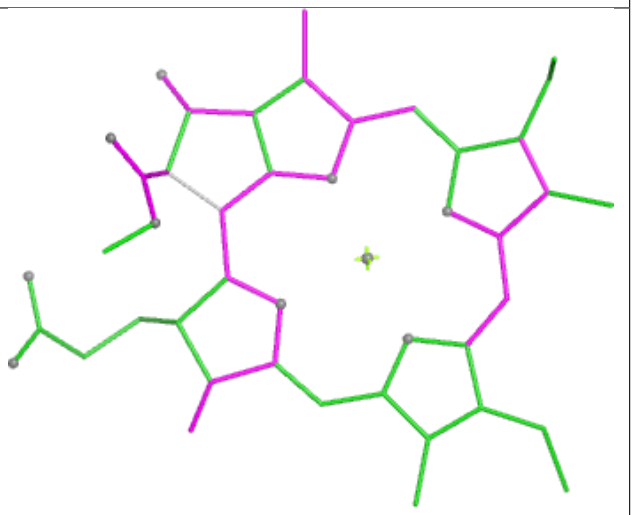


Rings

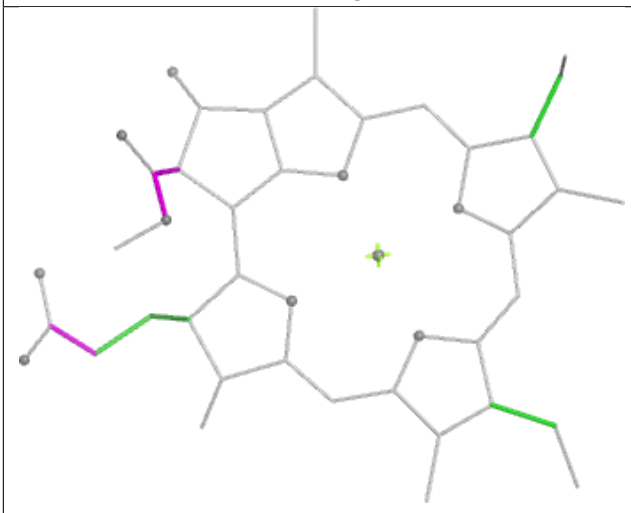
Ligand CLA S1 612



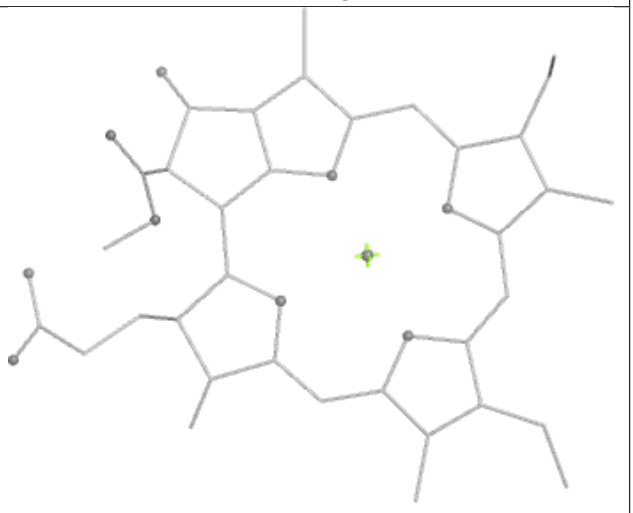
Bond lengths



Bond angles

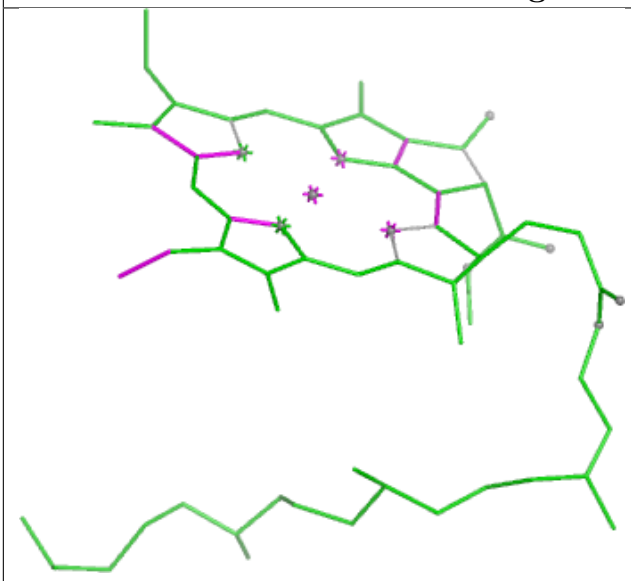


Torsions

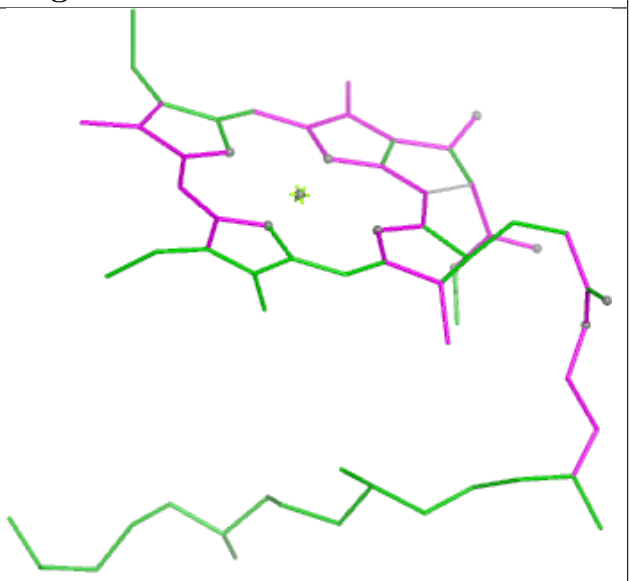


Rings

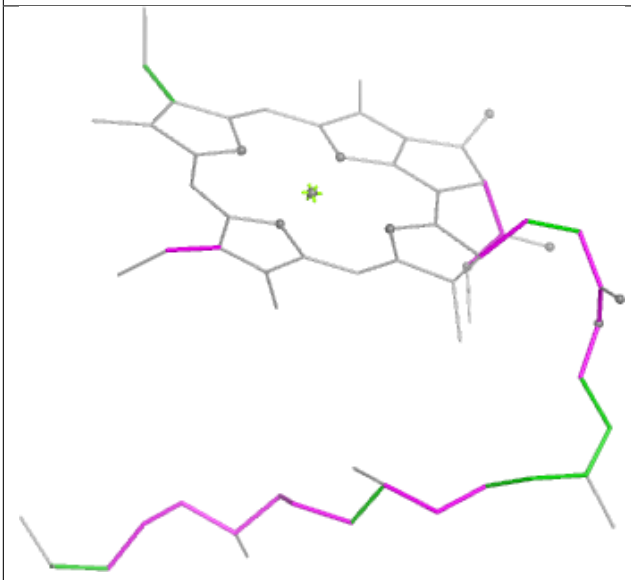
Ligand CLA g 603



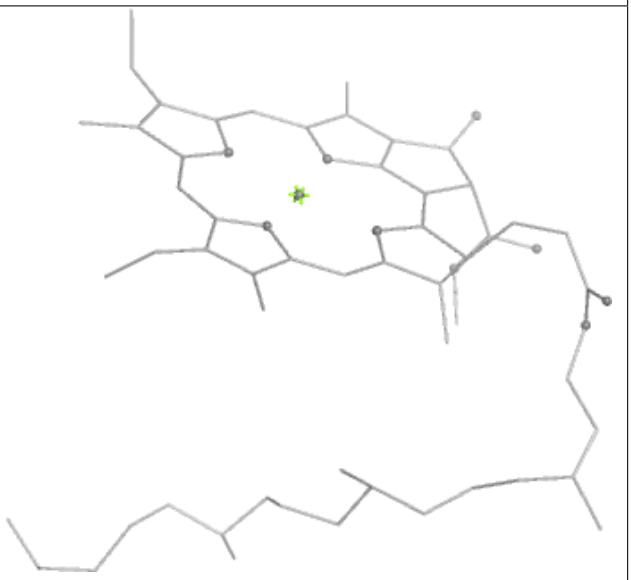
Bond lengths



Bond angles

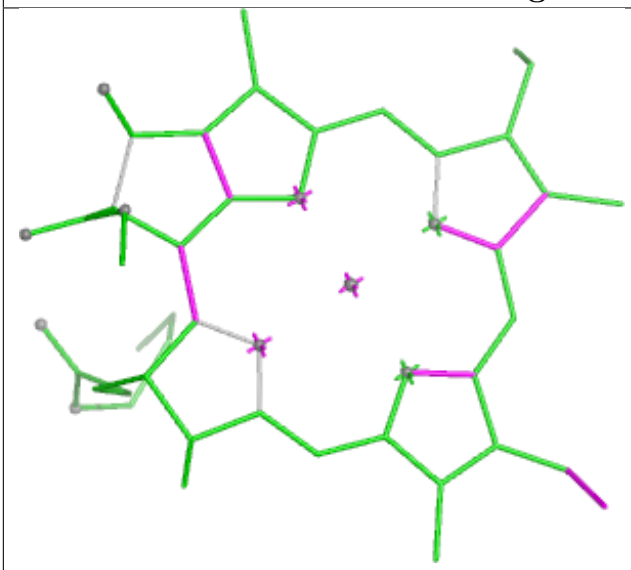


Torsions

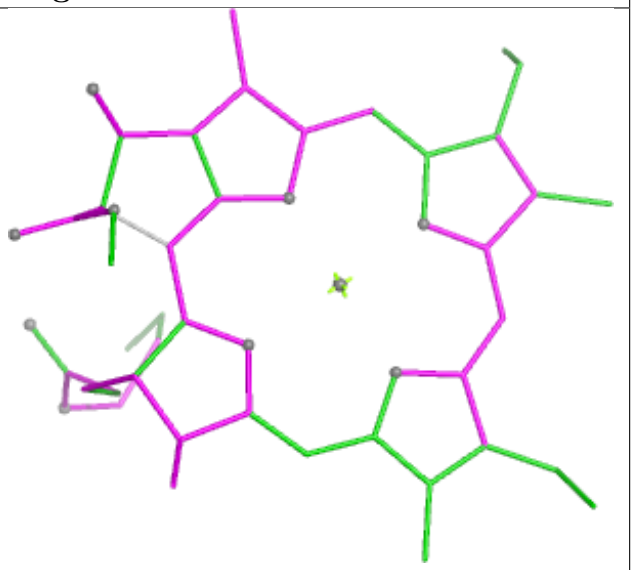


Rings

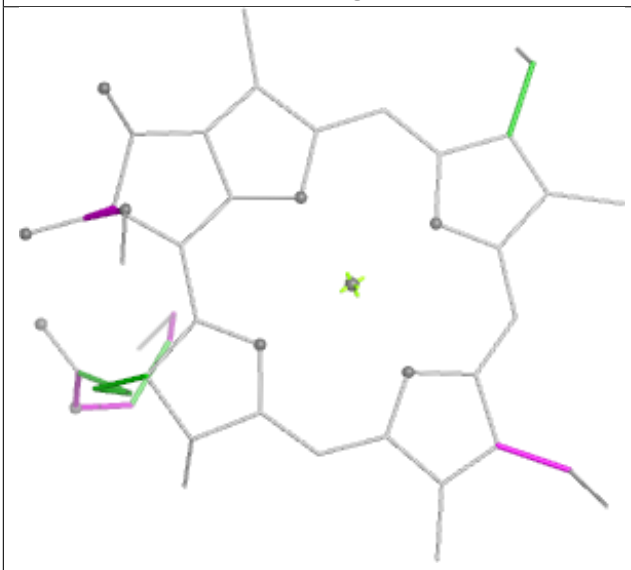
Ligand CLA g 604



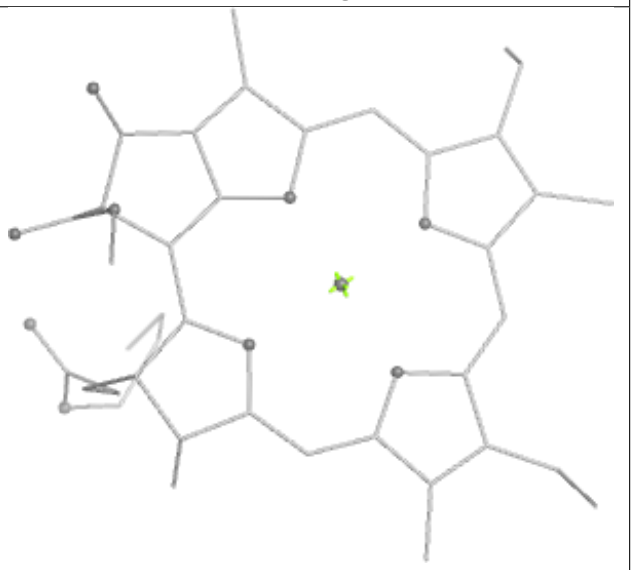
Bond lengths



Bond angles

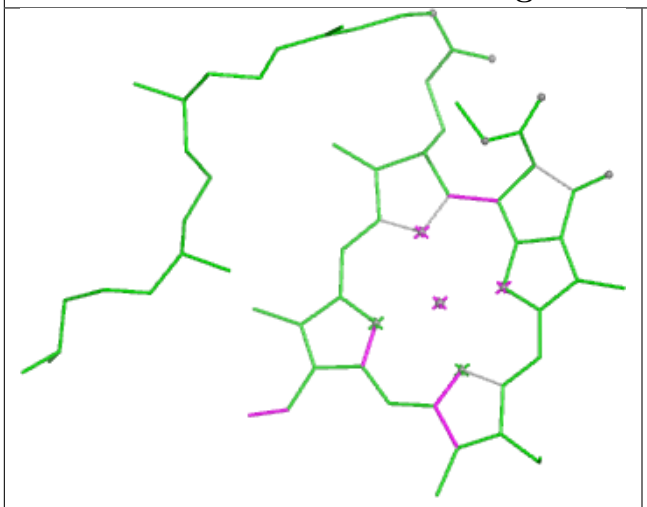


Torsions

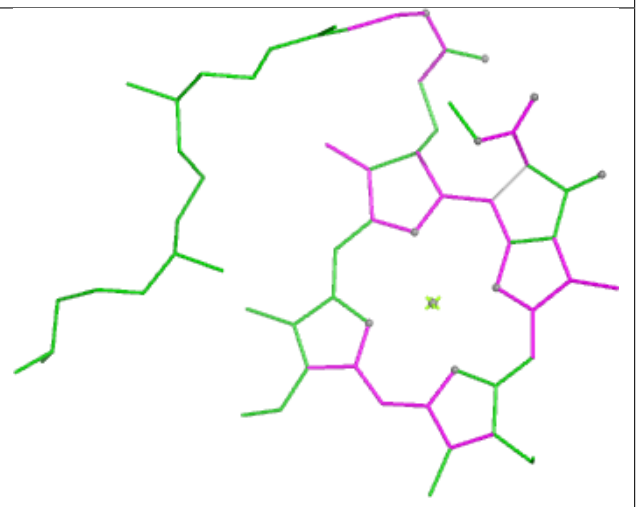


Rings

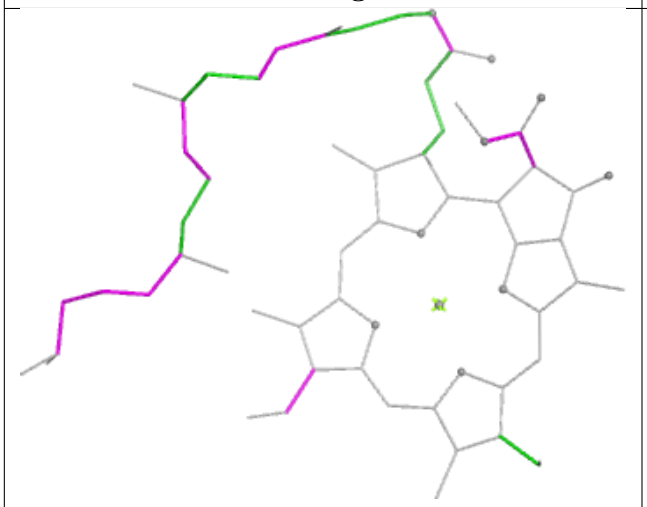
Ligand CLA Y1 612



Bond lengths



Bond angles

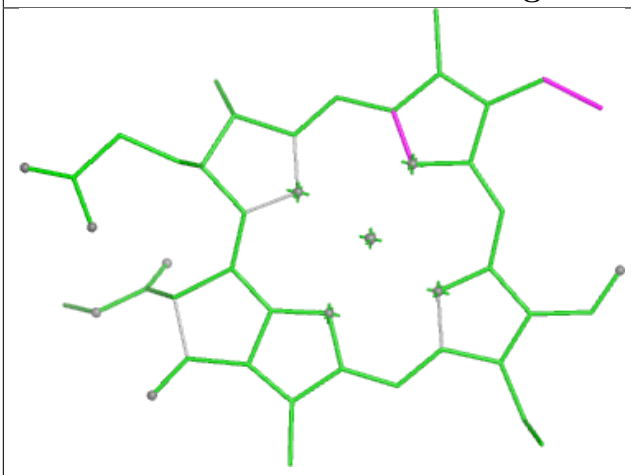


Torsions

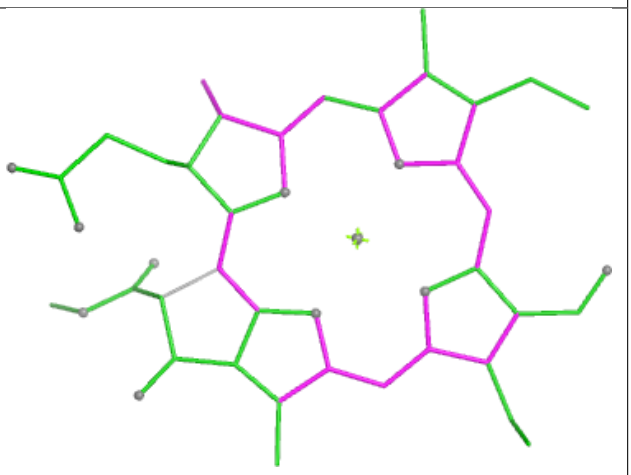


Rings

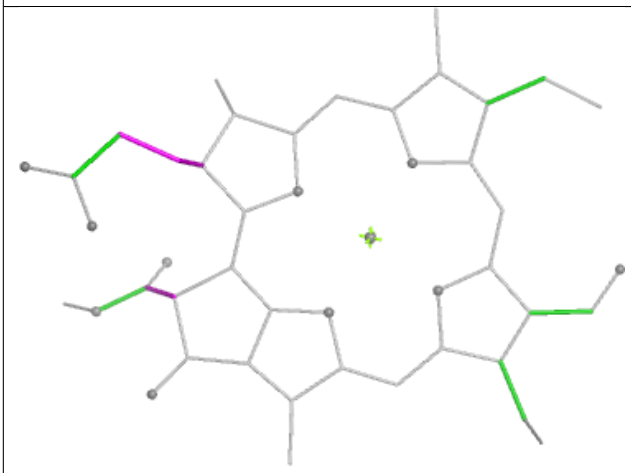
Ligand CHL Y 605



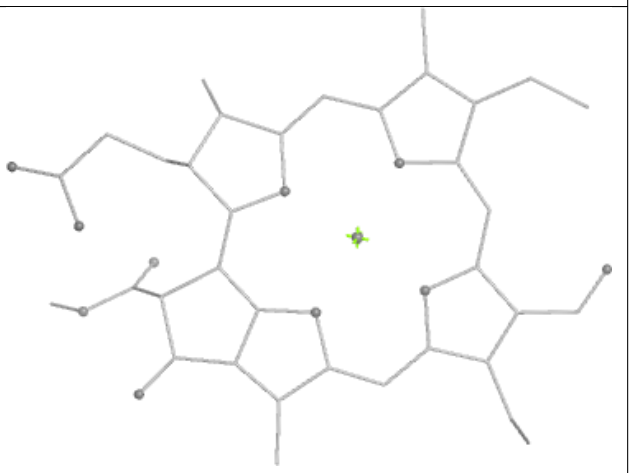
Bond lengths



Bond angles

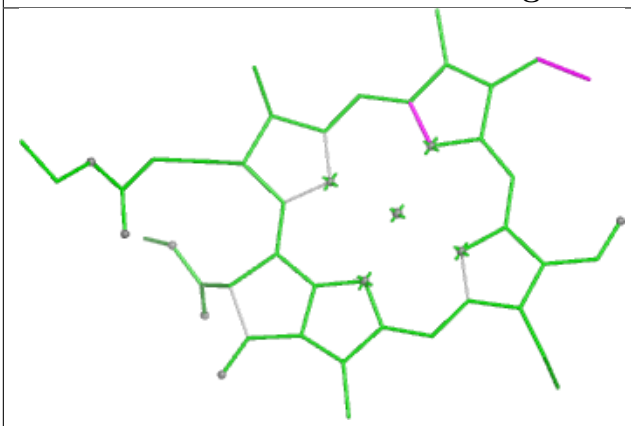


Torsions

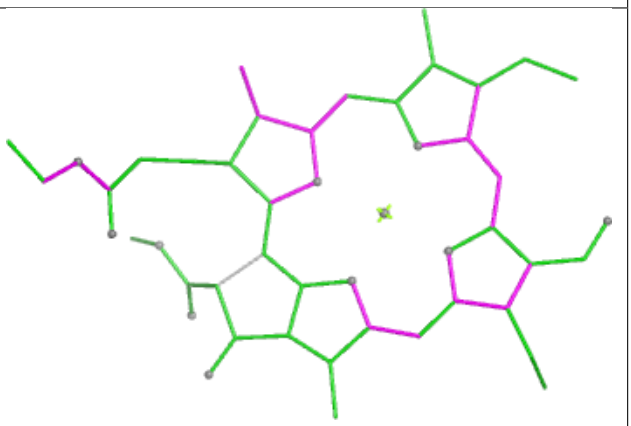


Rings

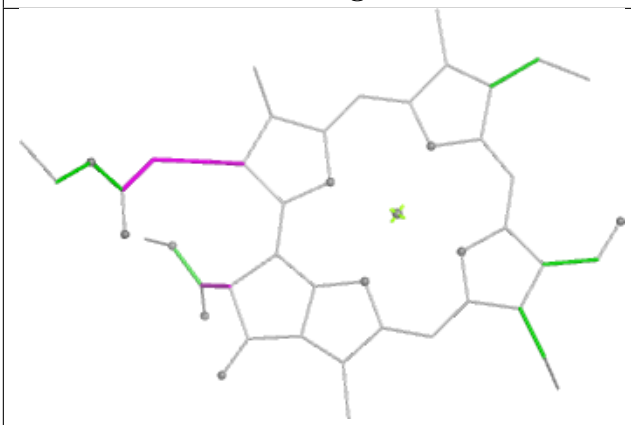
Ligand CHL G 605



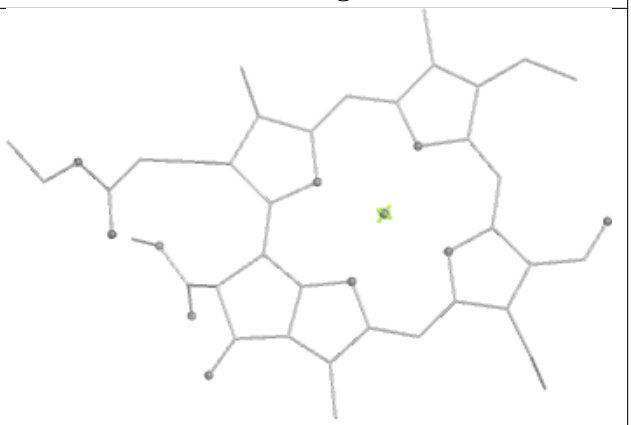
Bond lengths



Bond angles

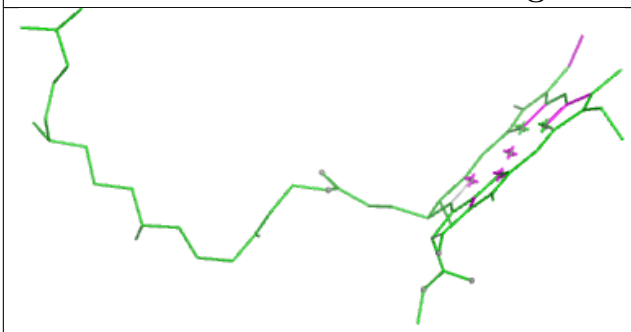


Torsions

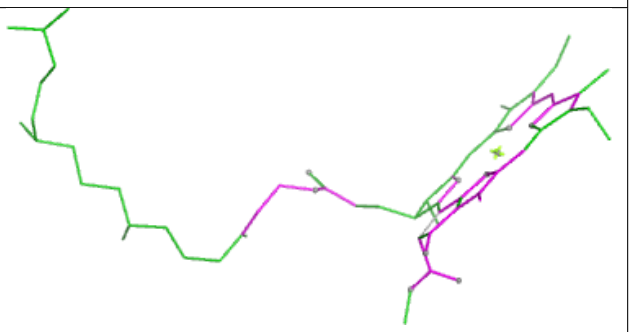


Rings

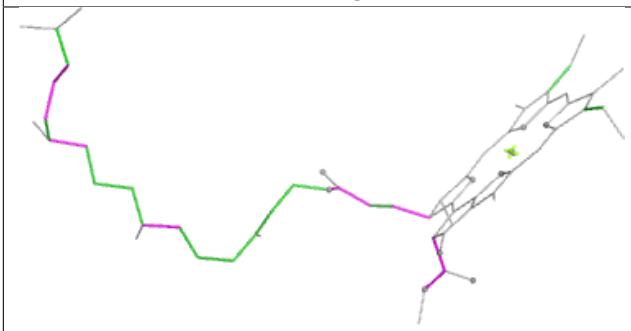
Ligand CLA d 402



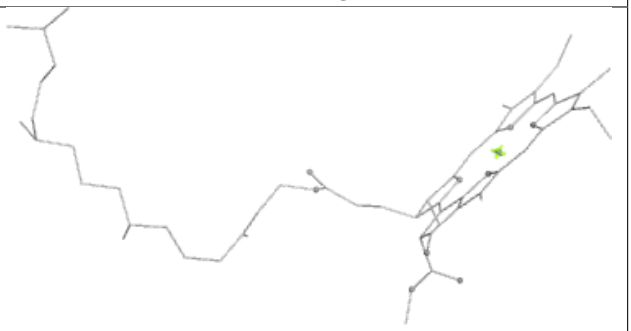
Bond lengths



Bond angles

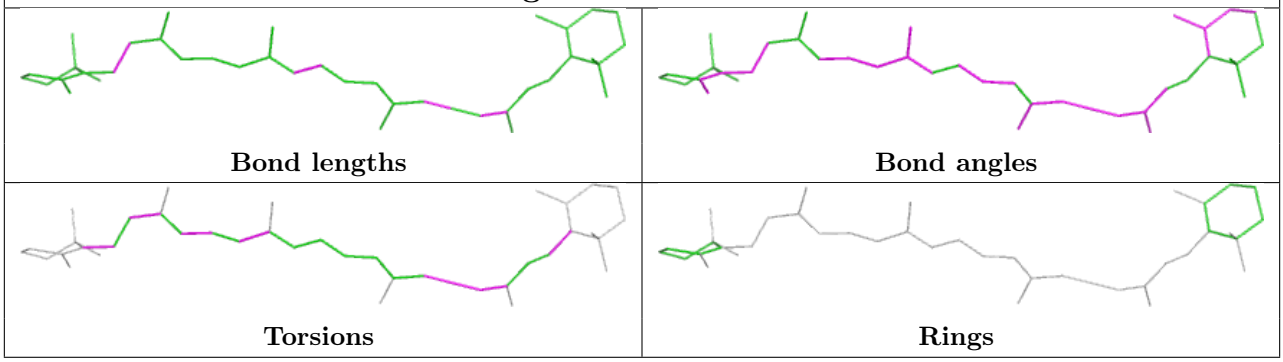


Torsions

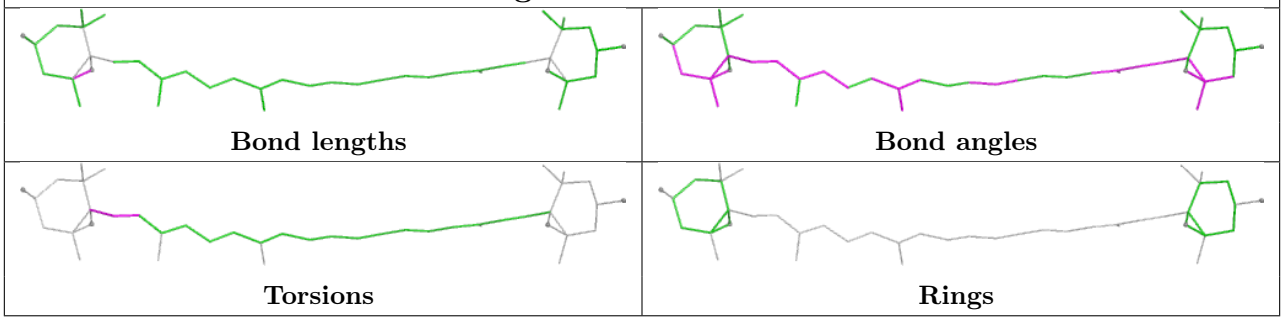


Rings

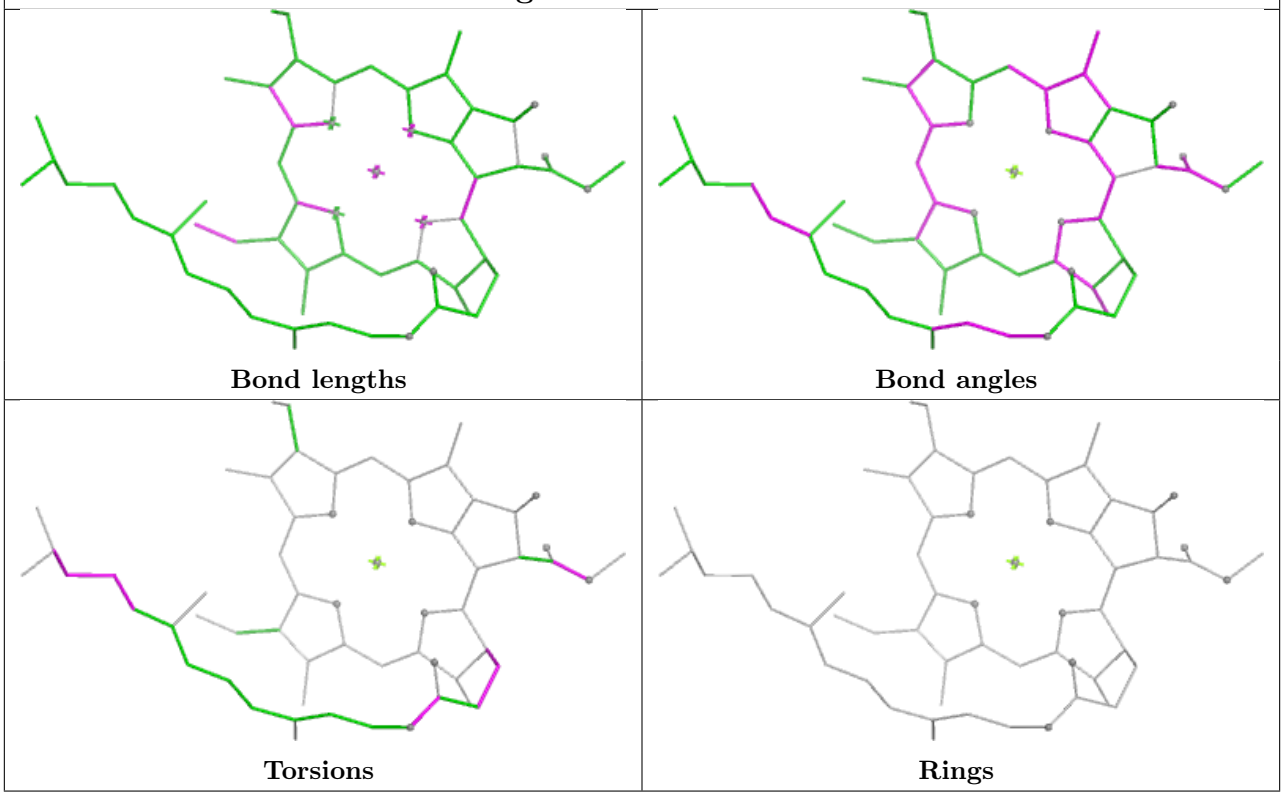
Ligand BCR D 404



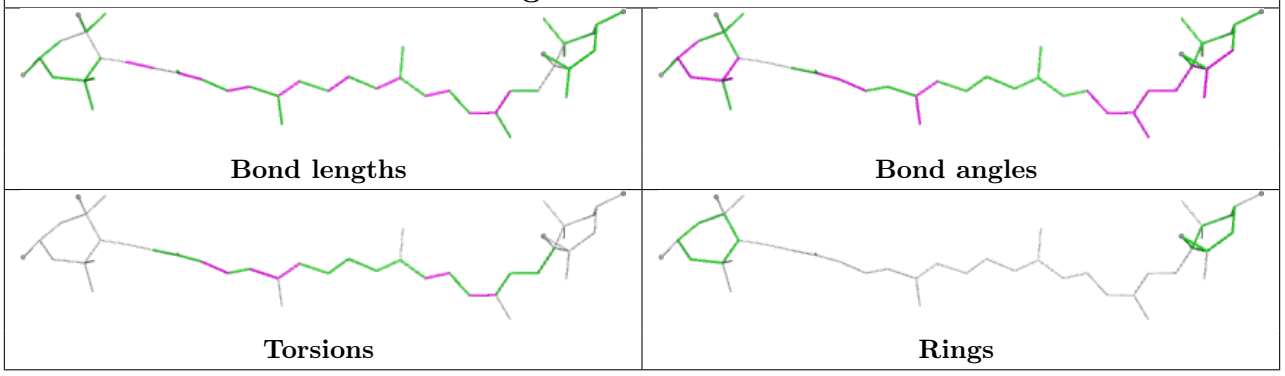
Ligand XAT G1 622



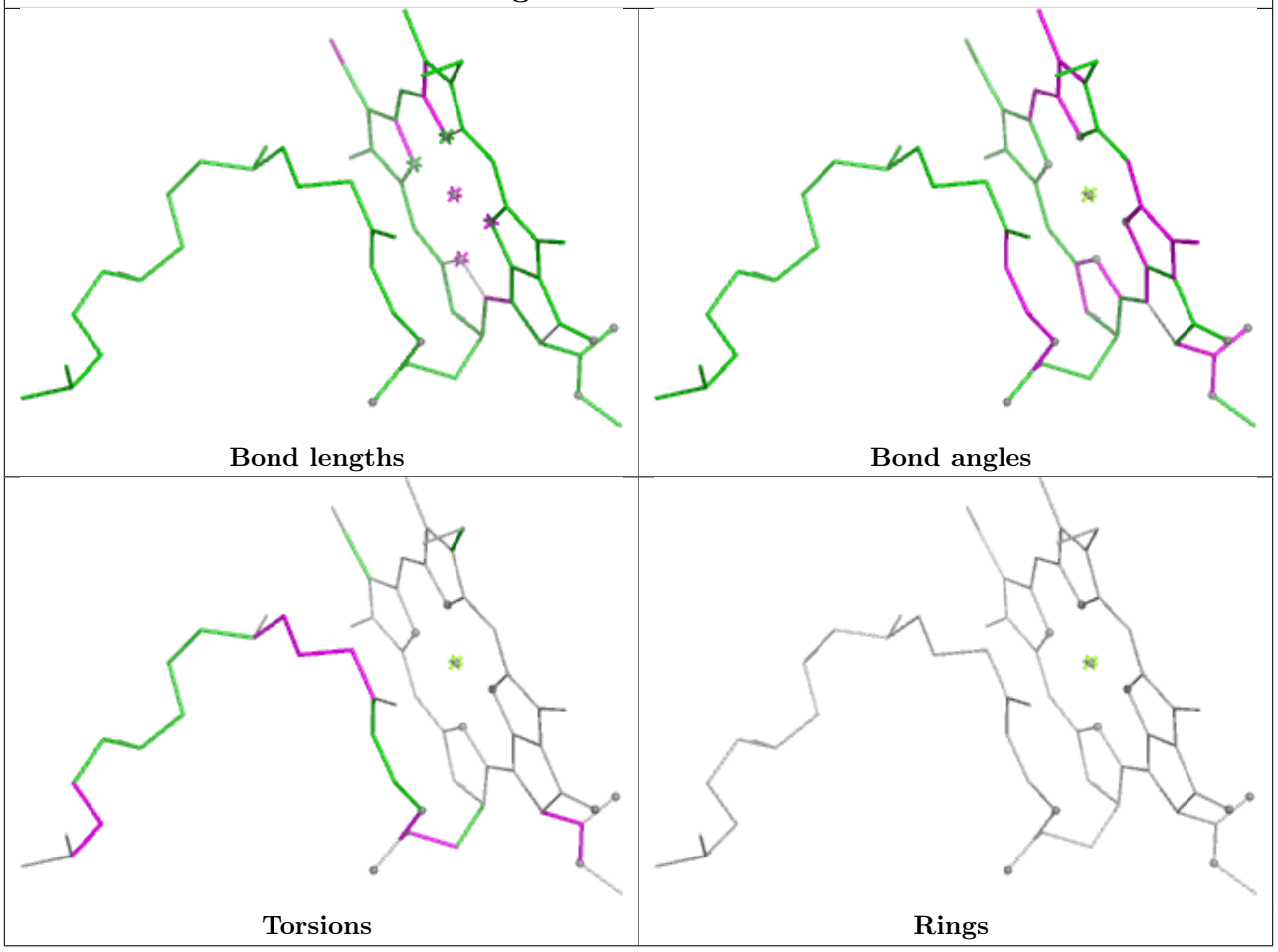
Ligand CLA R1 608



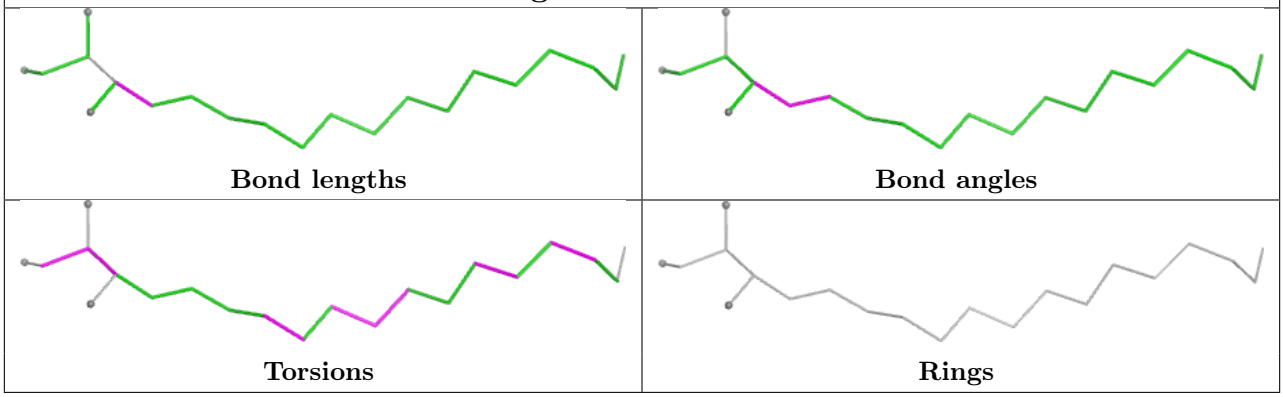
Ligand NEX Y 623



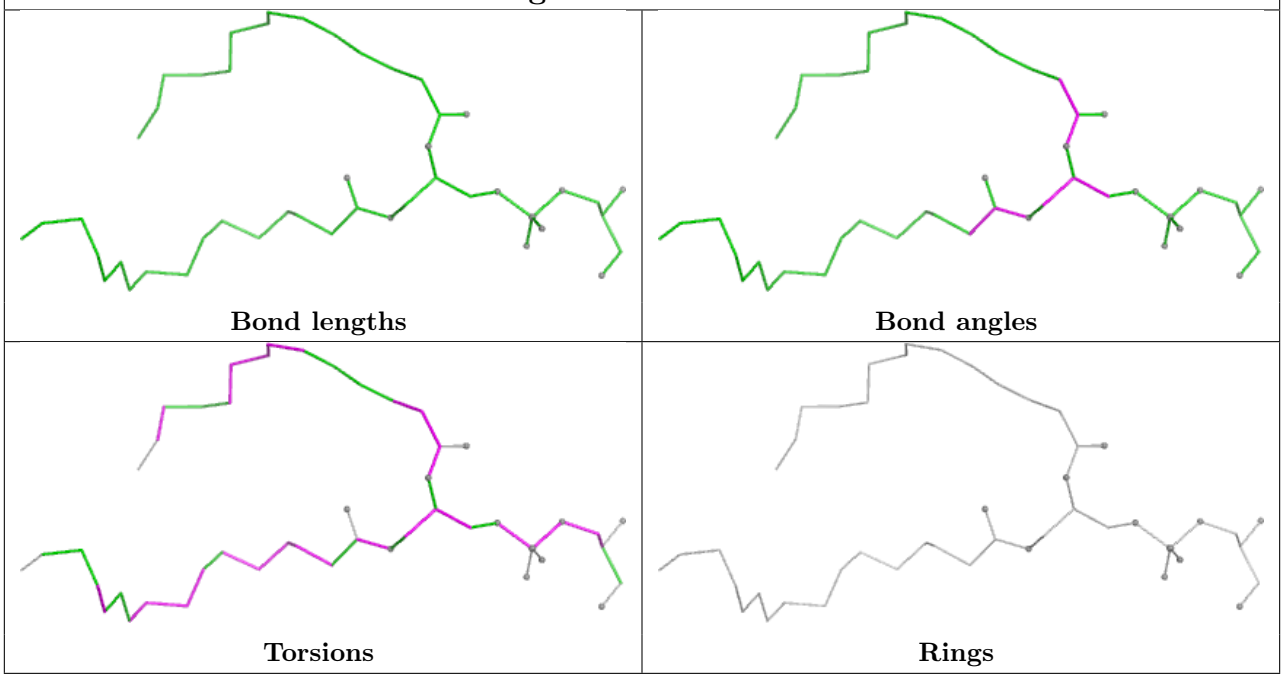
Ligand CLA G1 613



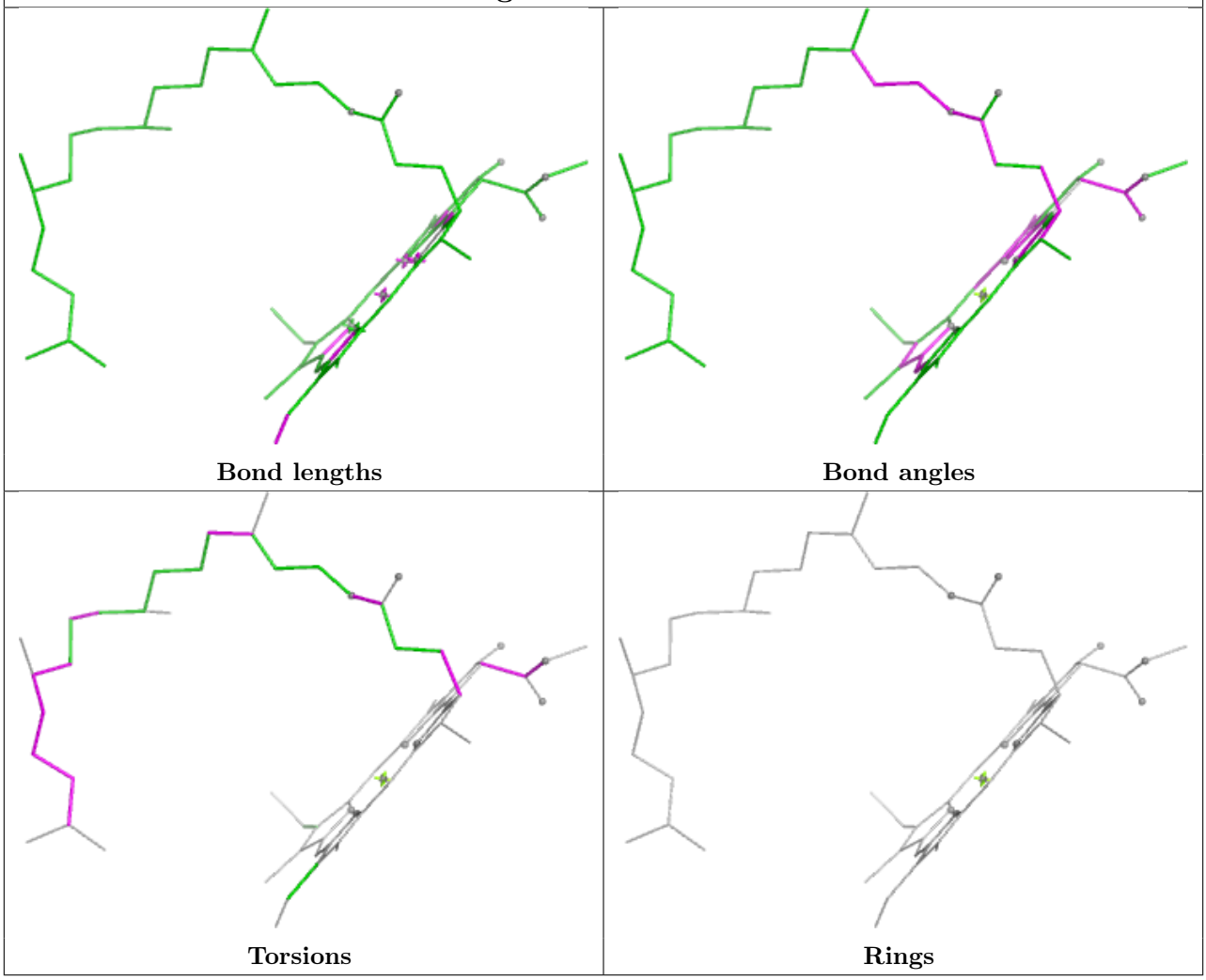
Ligand SPH a 414



Ligand LHG c 525



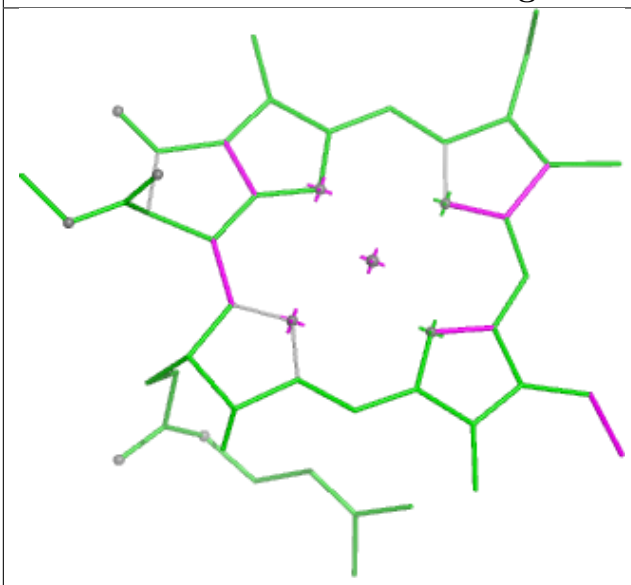
Ligand CLA b 612



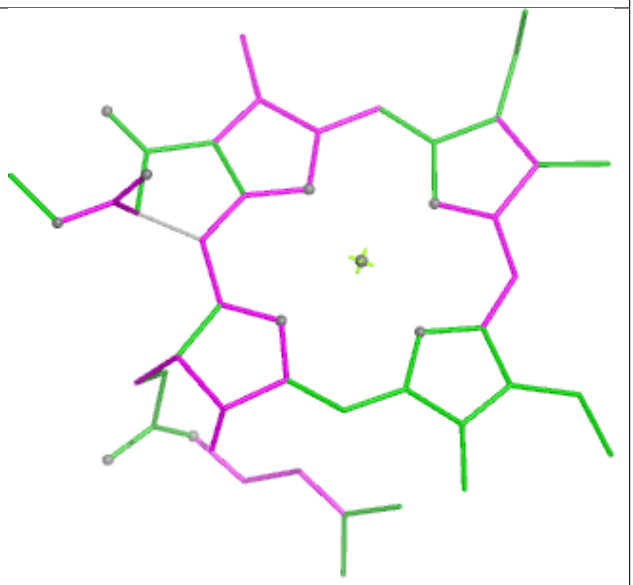
Bond lengths | **Bond angles**

Torsions | **Rings**

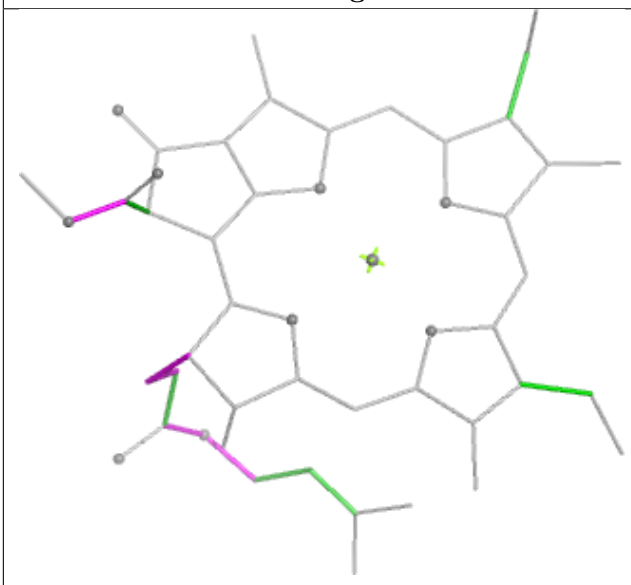
Ligand CLA S1 617



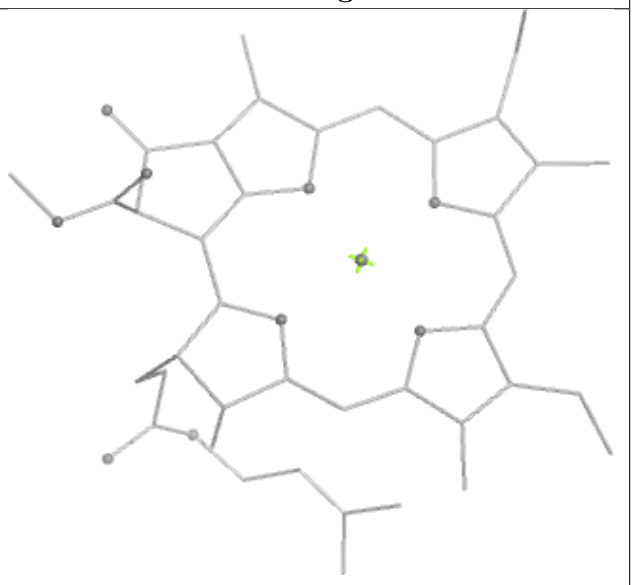
Bond lengths



Bond angles

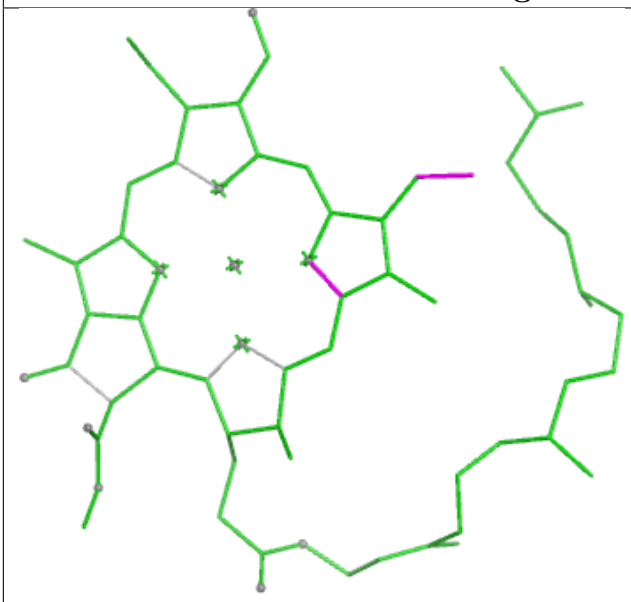


Torsions

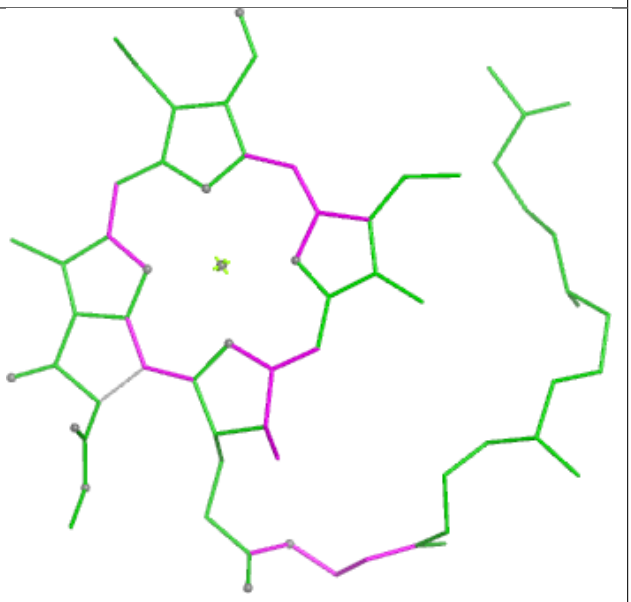


Rings

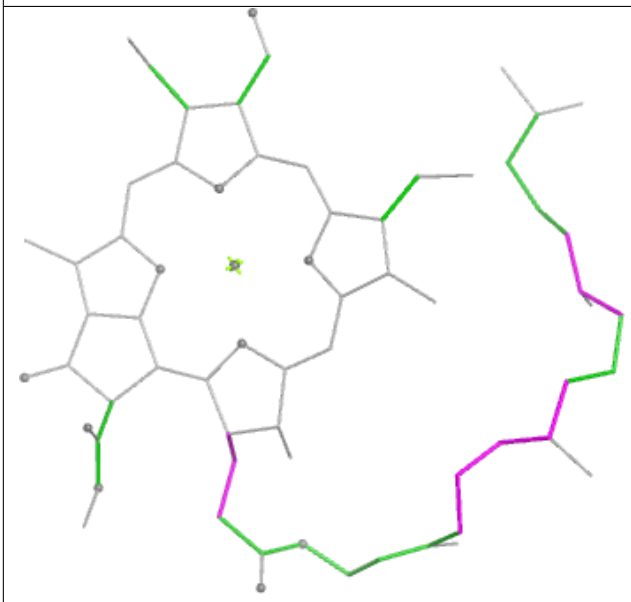
Ligand CHL G1 607



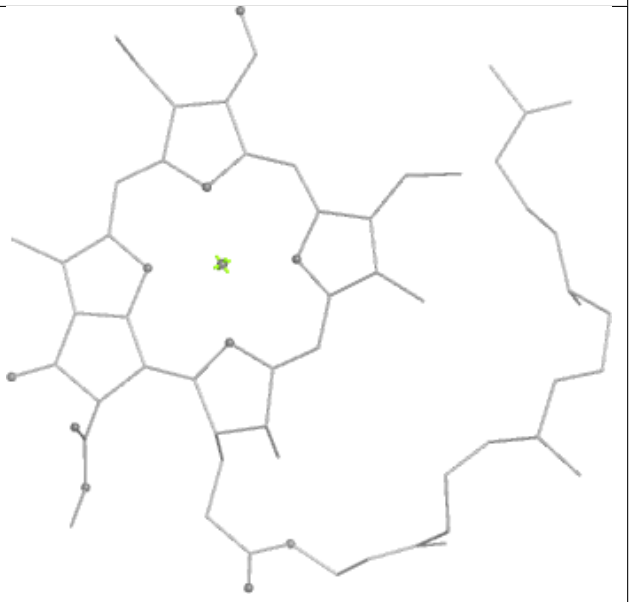
Bond lengths



Bond angles

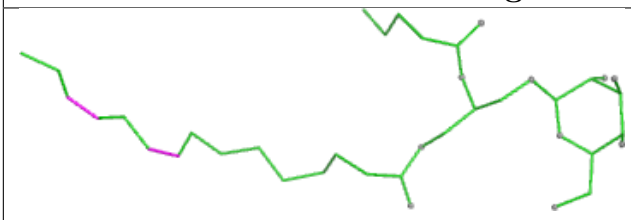


Torsions

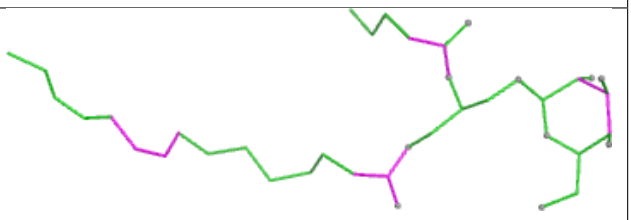


Rings

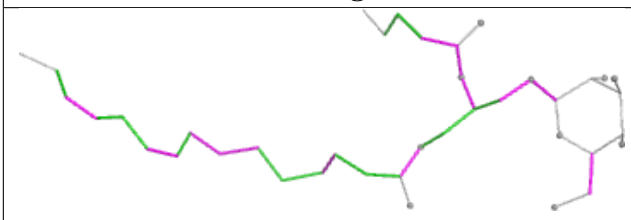
Ligand LMG W1 201



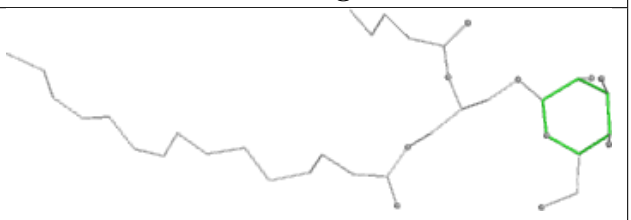
Bond lengths



Bond angles

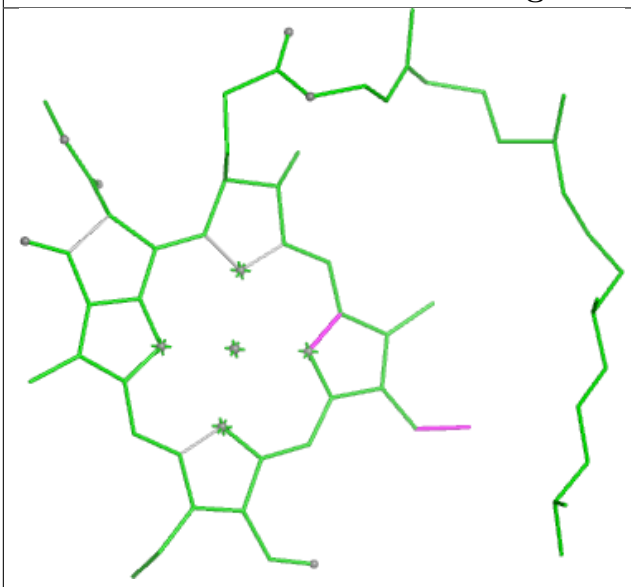


Torsions

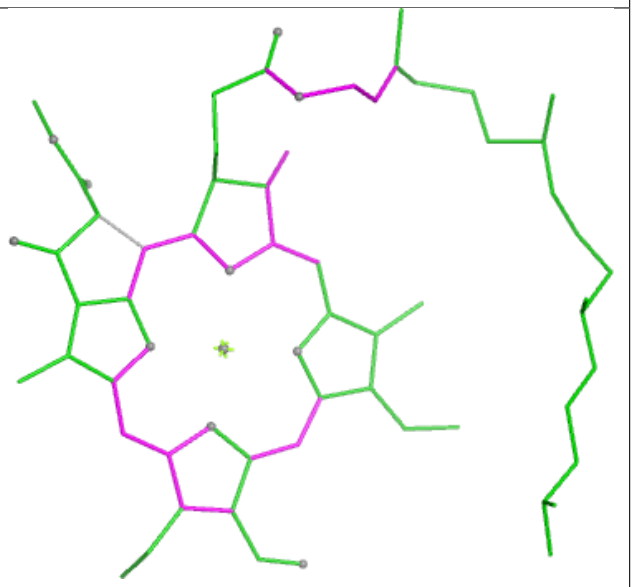


Rings

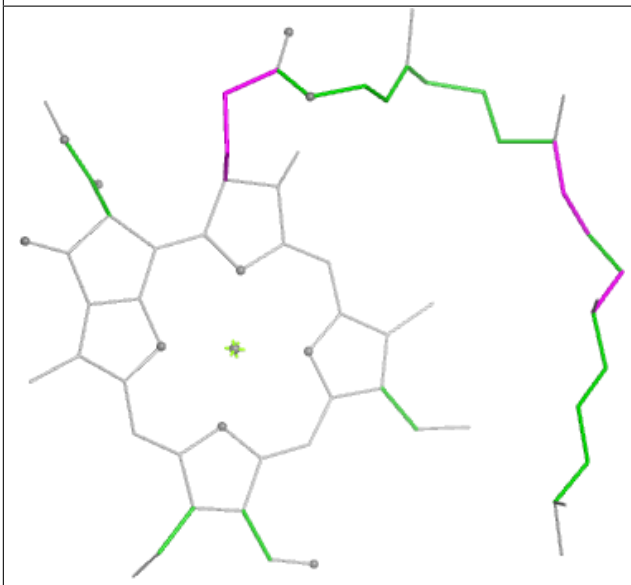
Ligand CHL n 607



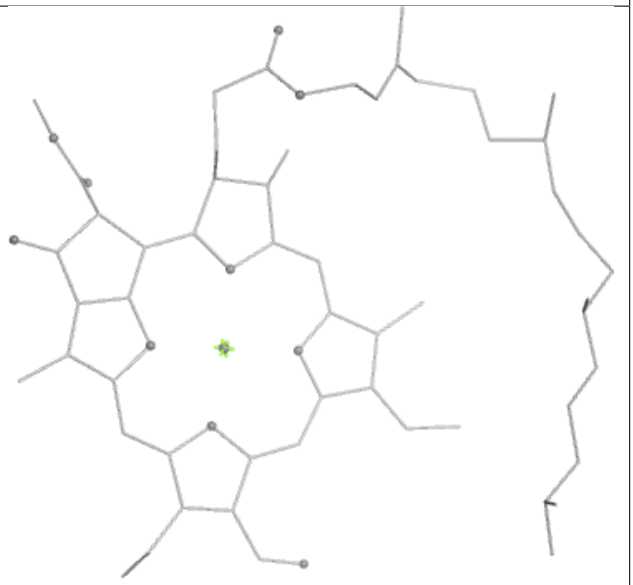
Bond lengths



Bond angles

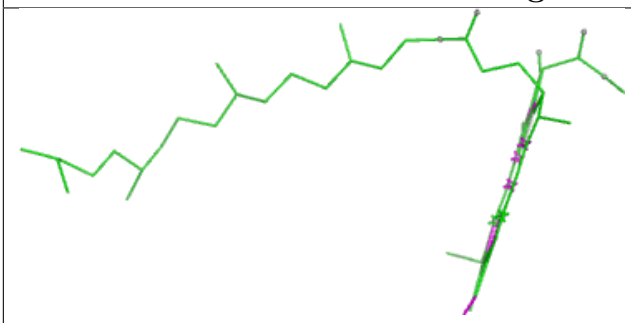


Torsions

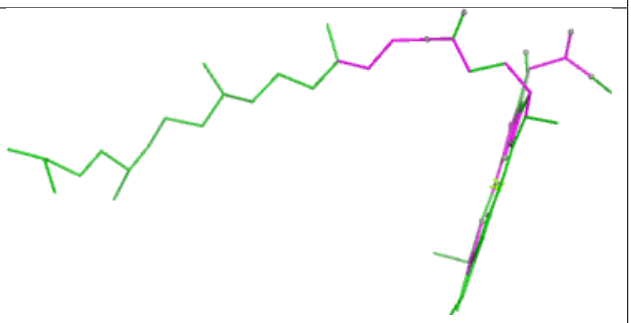


Rings

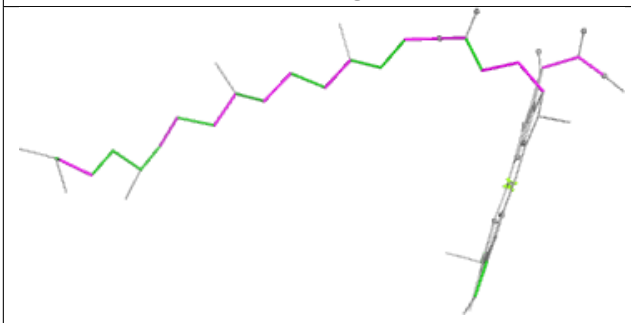
Ligand CLA b 606



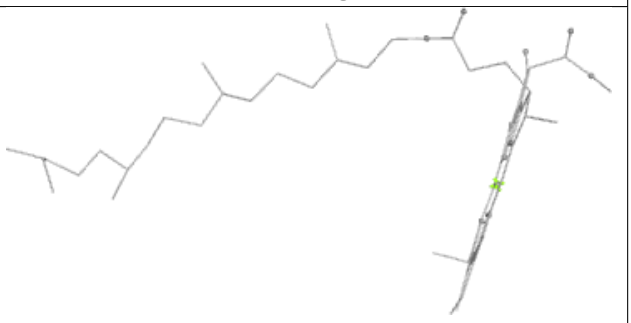
Bond lengths



Bond angles

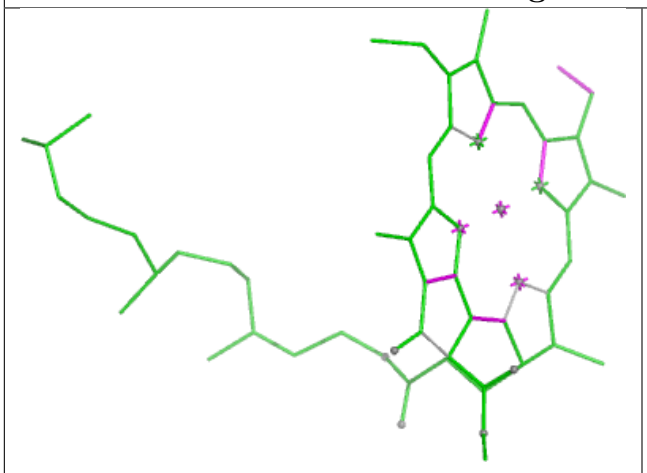


Torsions

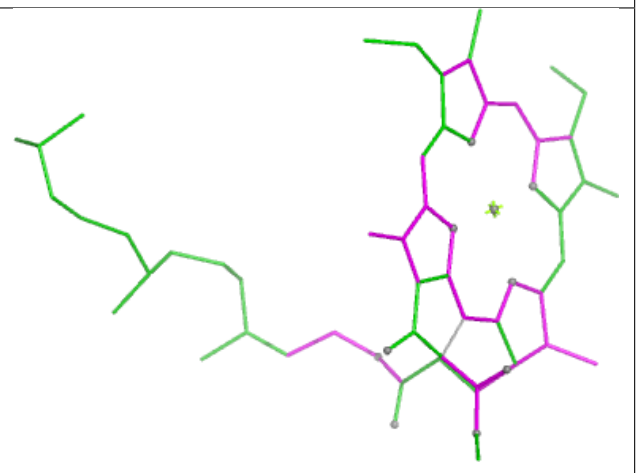


Rings

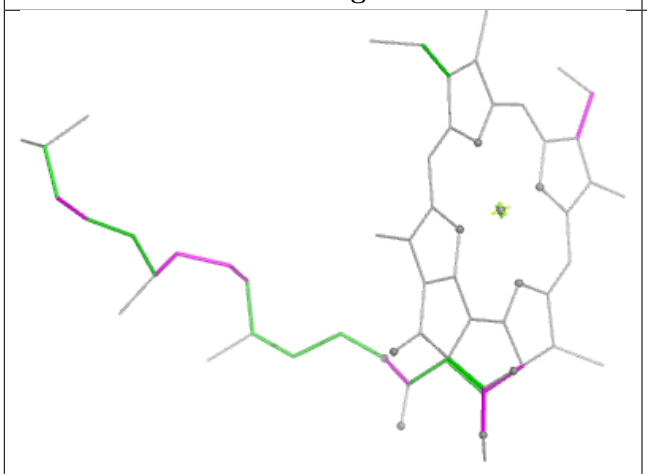
Ligand CLA S 609



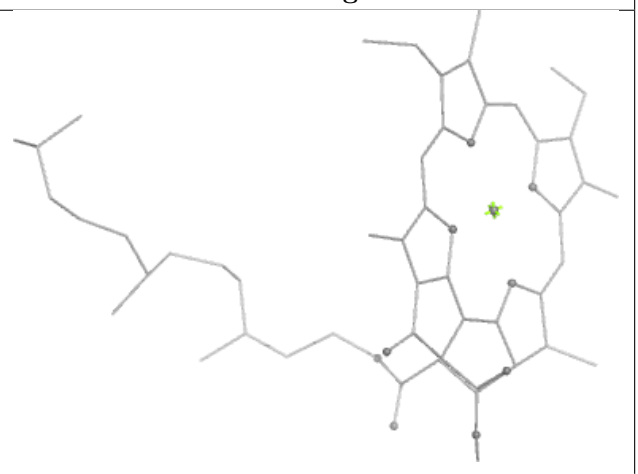
Bond lengths



Bond angles

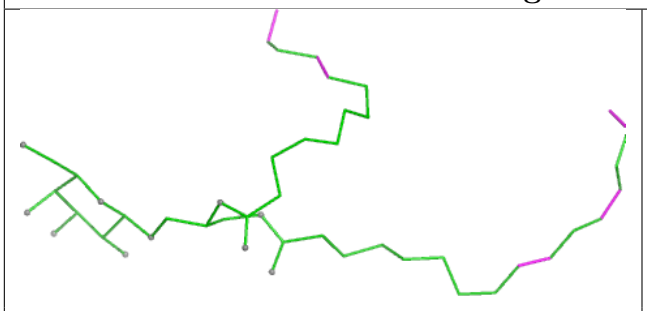


Torsions

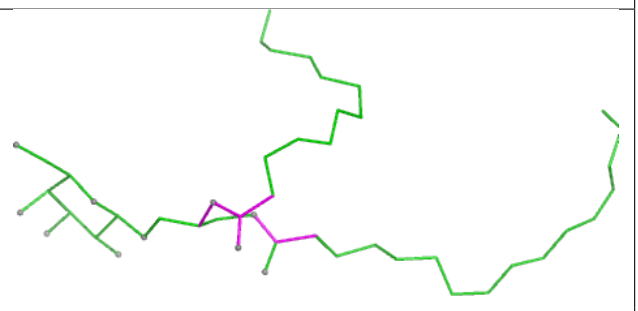


Rings

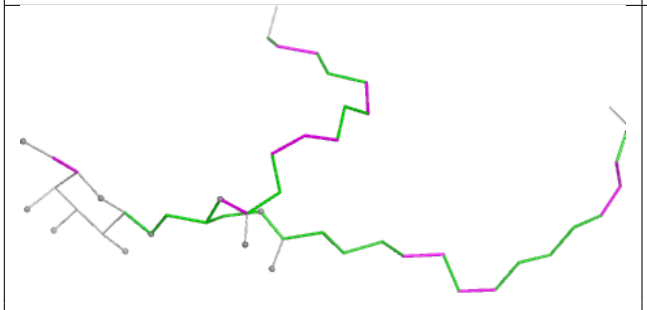
Ligand LMG h 102



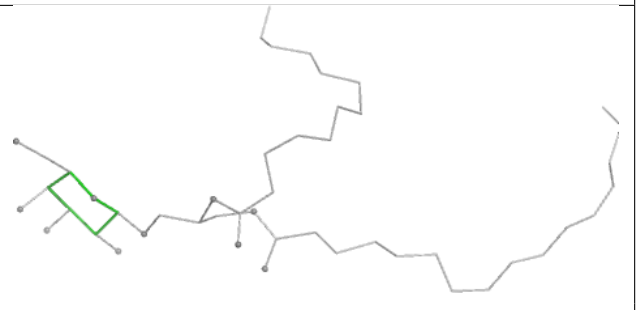
Bond lengths



Bond angles

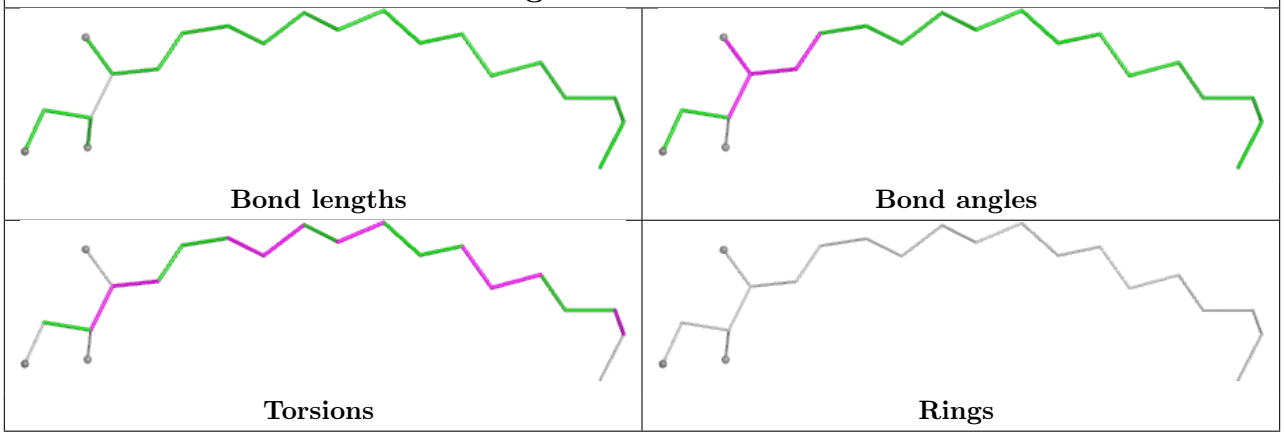


Torsions

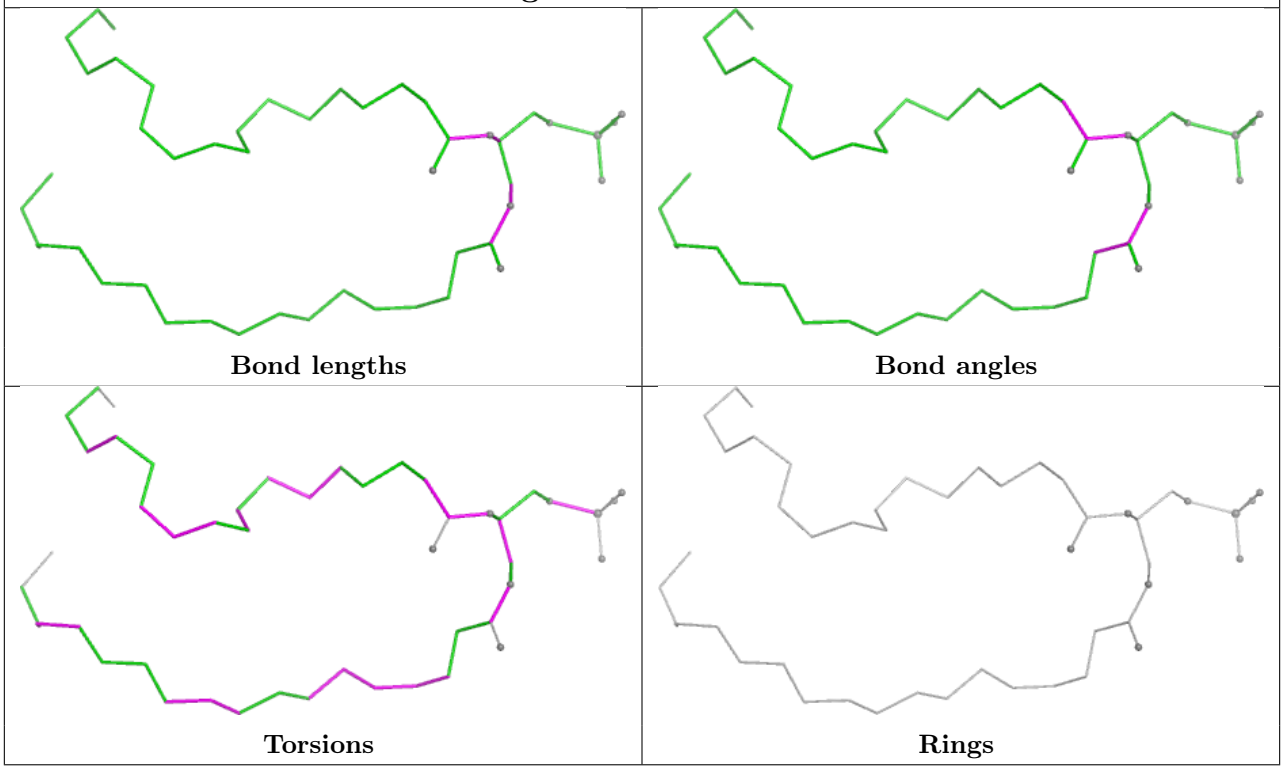


Rings

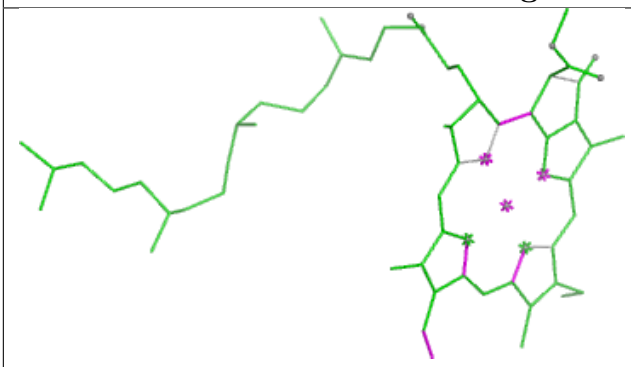
Ligand SPH A 414



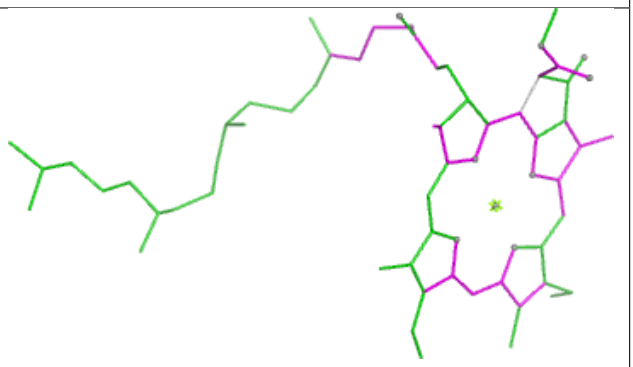
Ligand 3PH b1 624



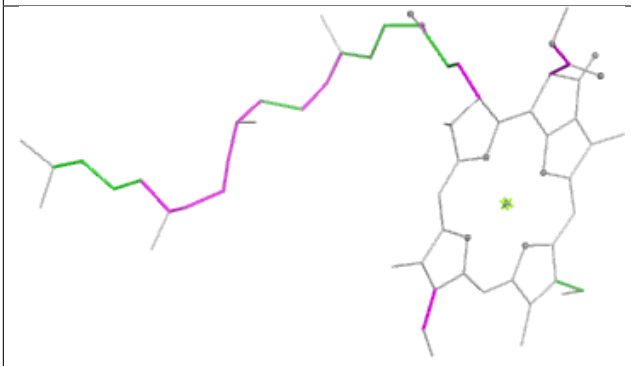
Ligand CLA c1 511



Bond lengths



Bond angles

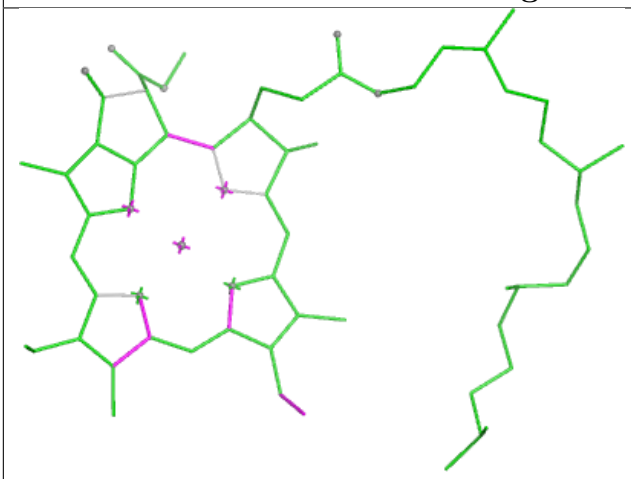


Torsions

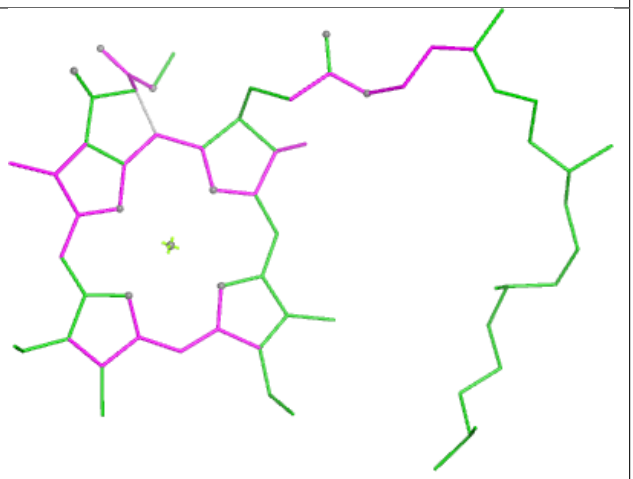


Rings

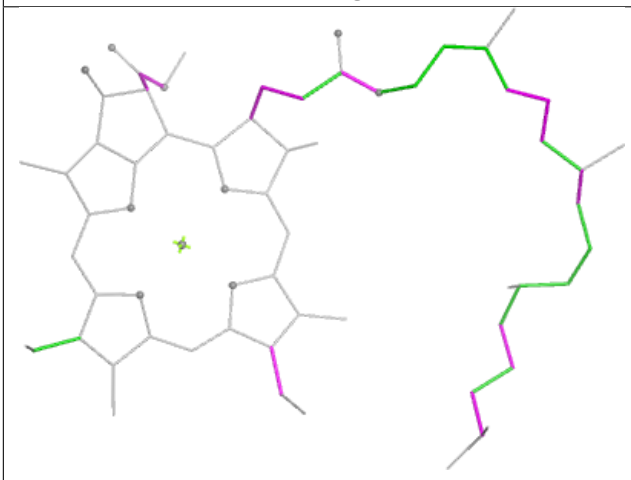
Ligand CLA s1 603



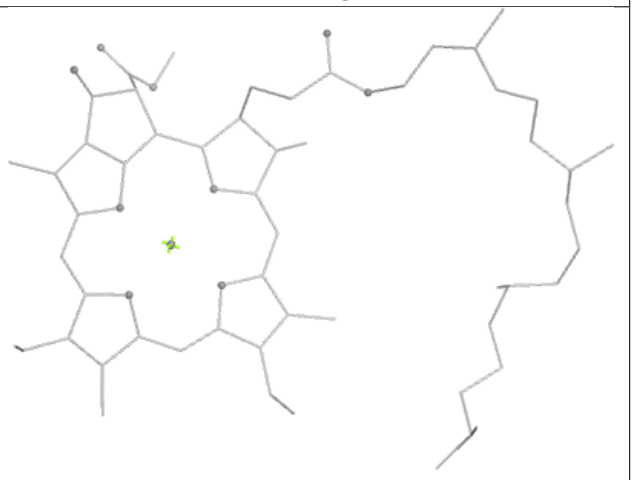
Bond lengths



Bond angles

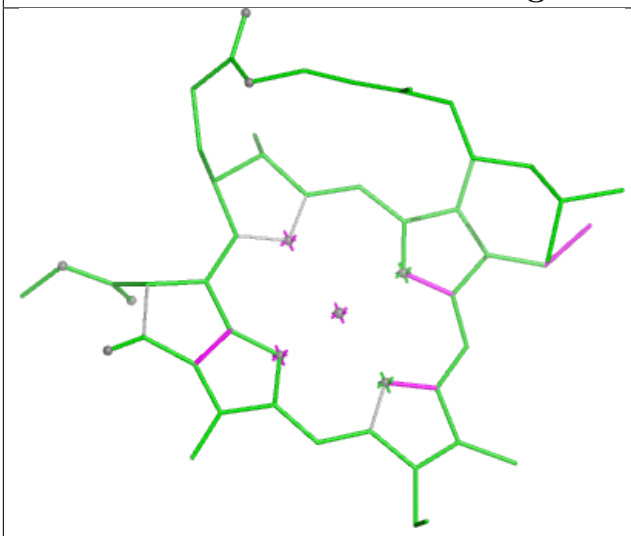


Torsions

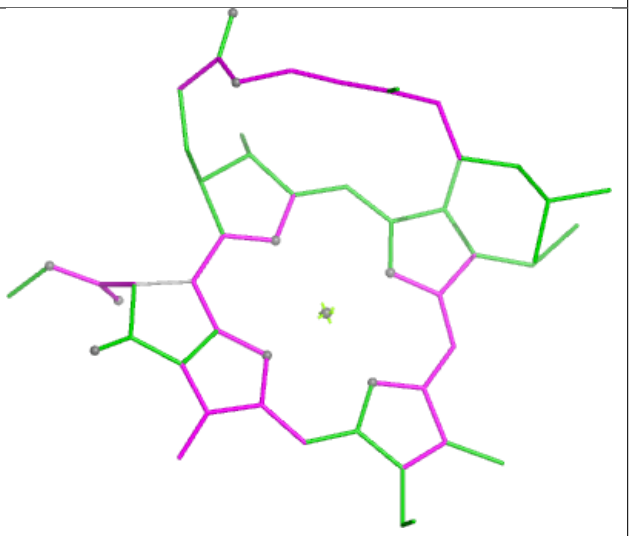


Rings

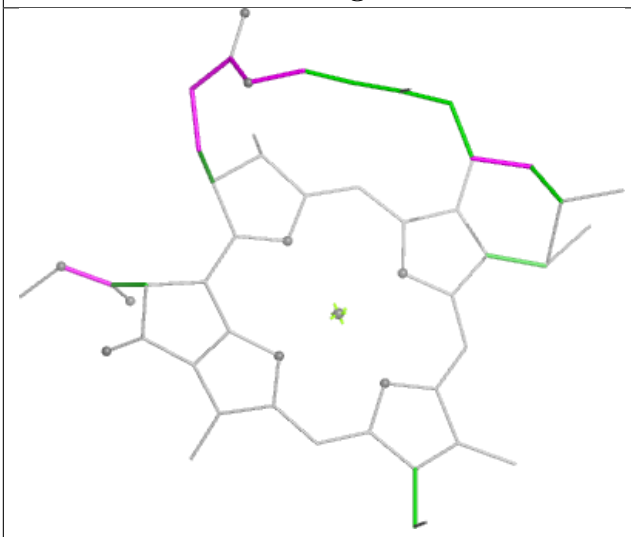
Ligand CLA S 614



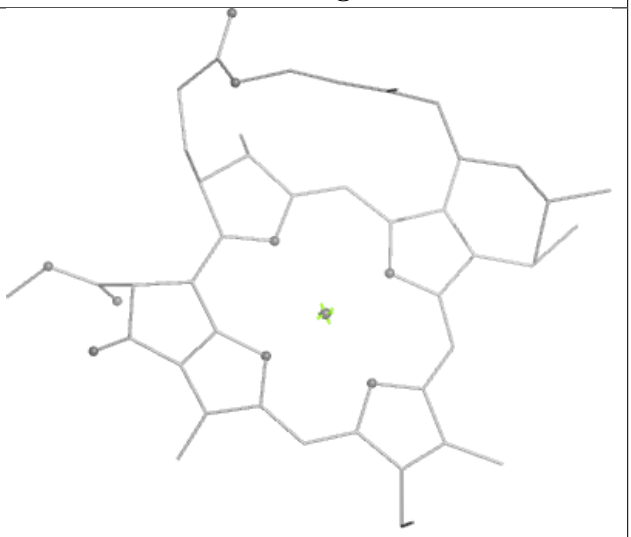
Bond lengths



Bond angles

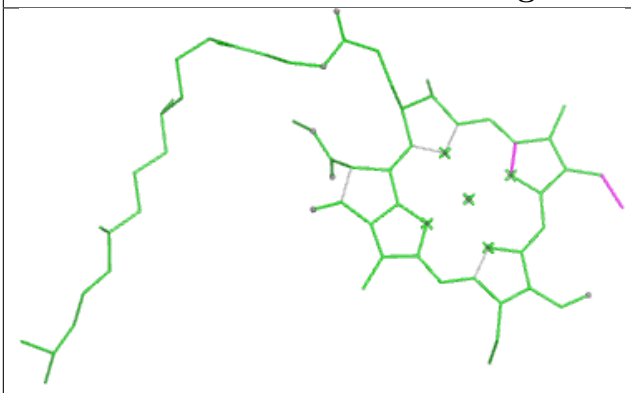


Torsions

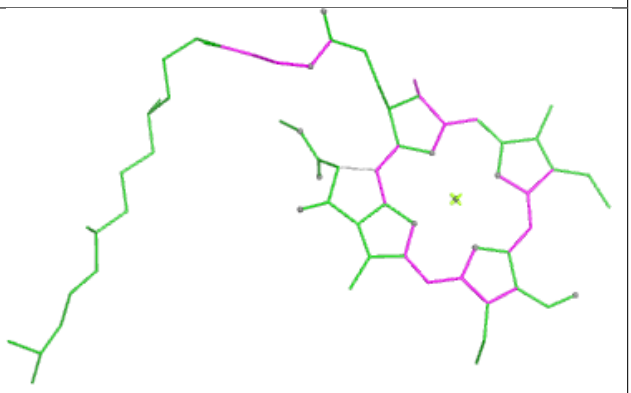


Rings

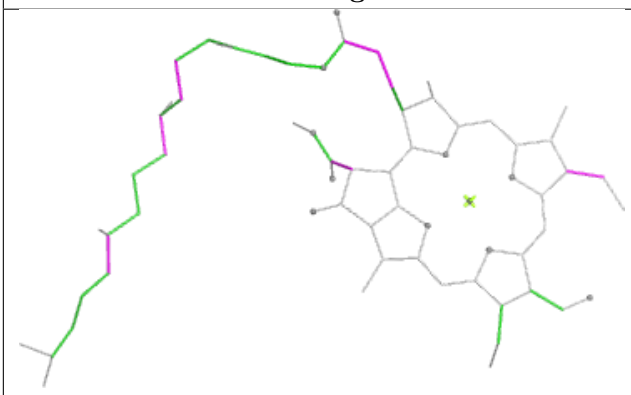
Ligand CHL n1 606



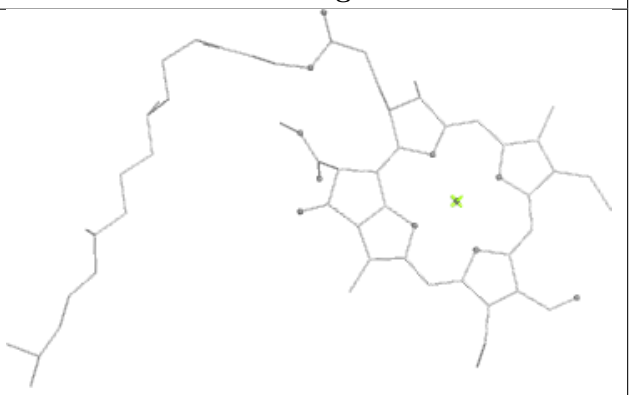
Bond lengths



Bond angles

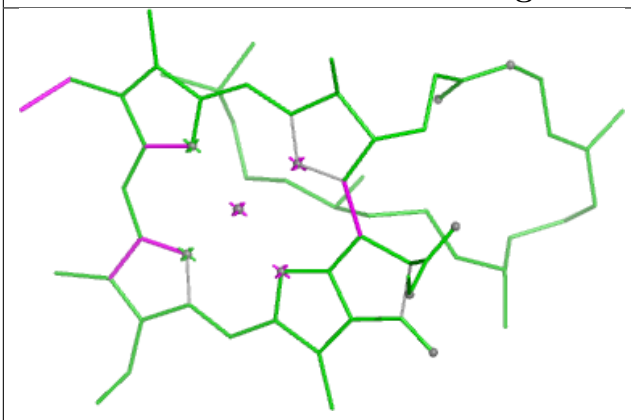


Torsions

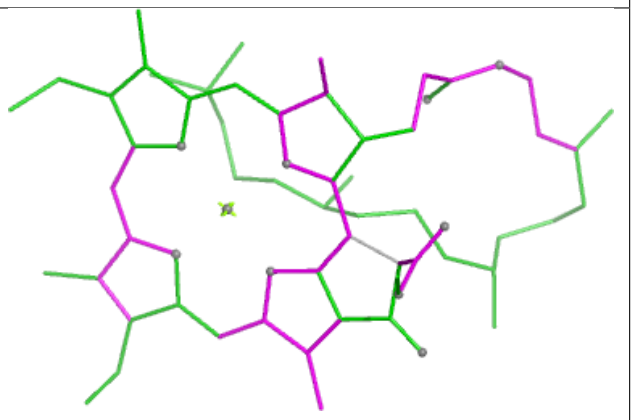


Rings

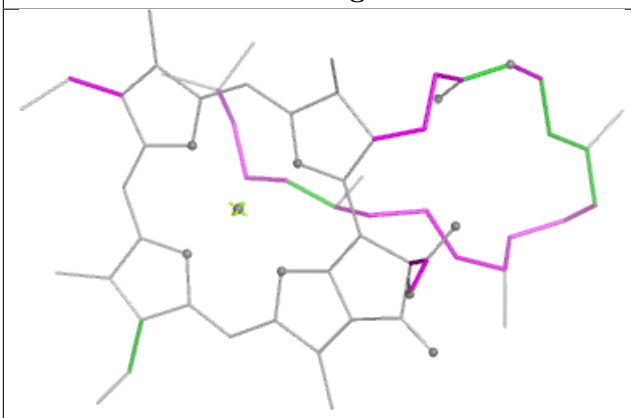
Ligand CLA B1 602



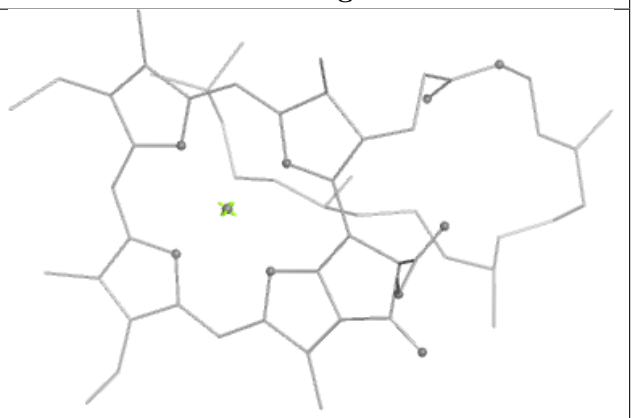
Bond lengths



Bond angles

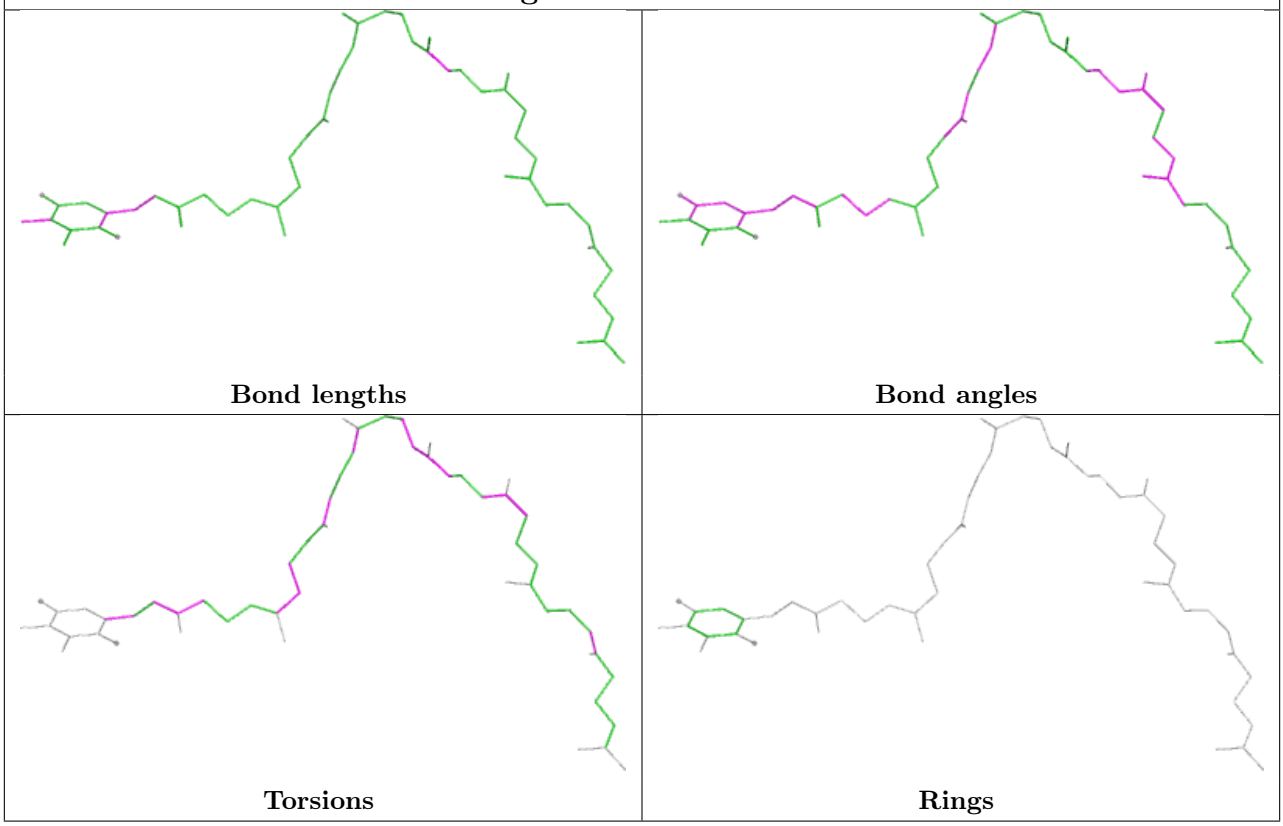


Torsions

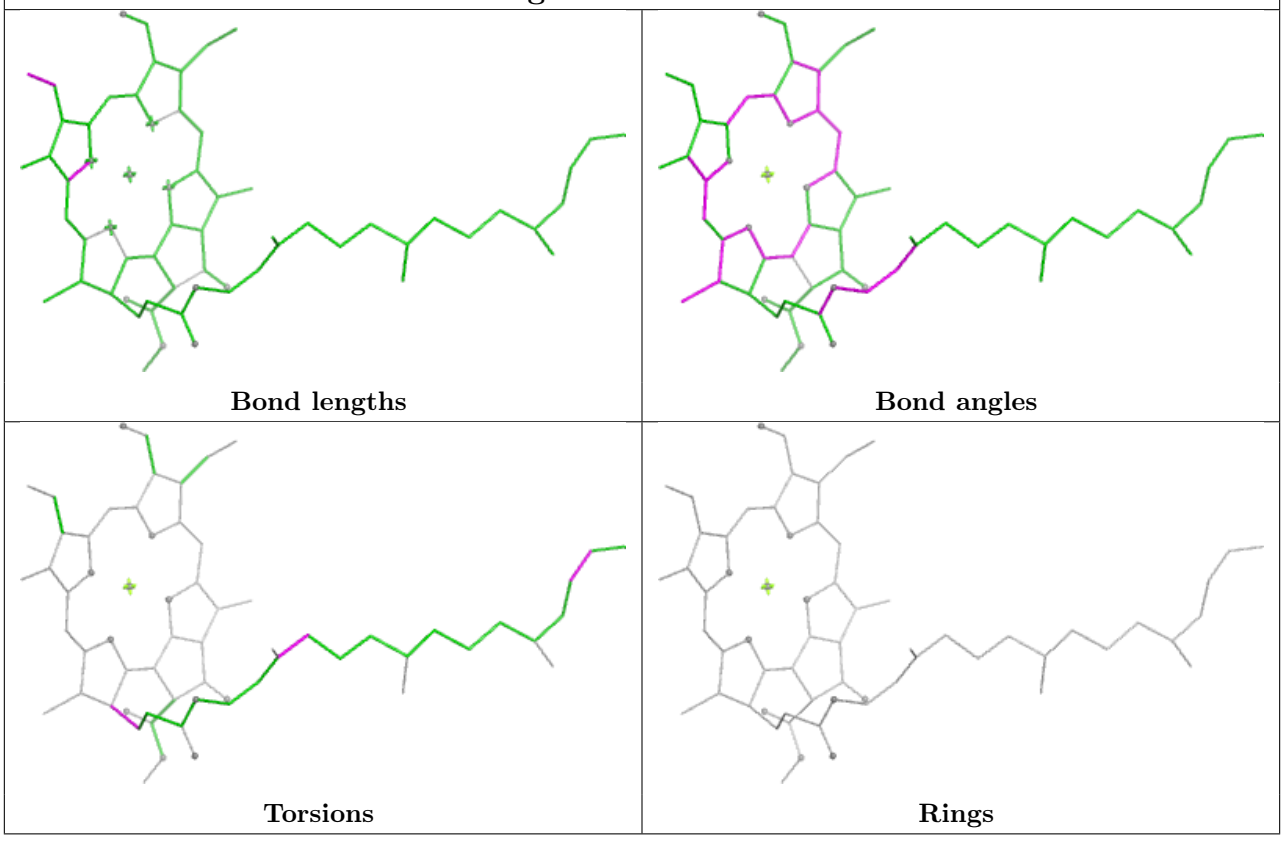


Rings

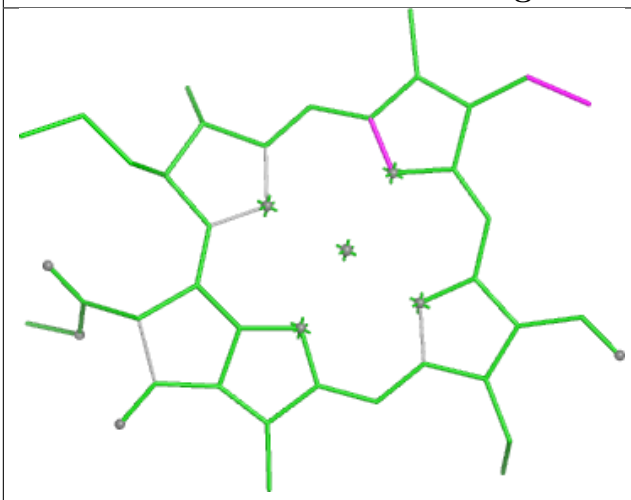
Ligand PL9 D1 405



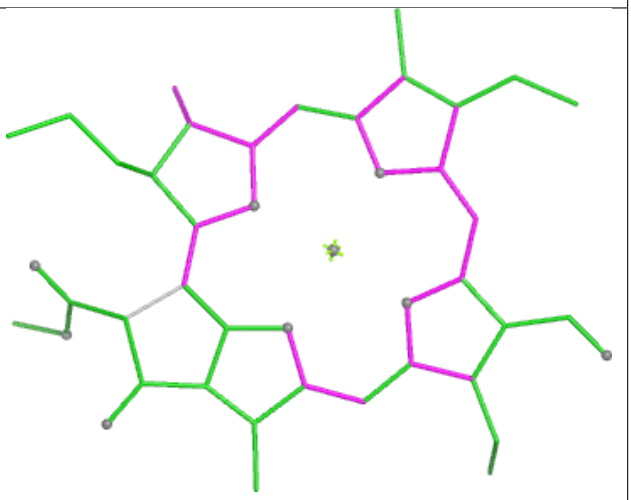
Ligand CHL n 609



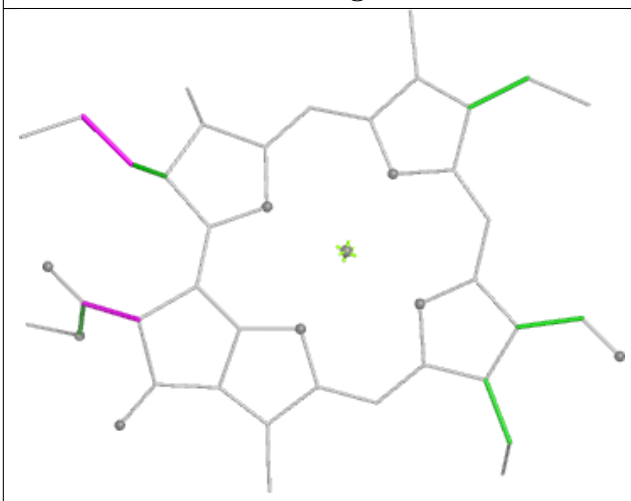
Ligand CHL R1 606



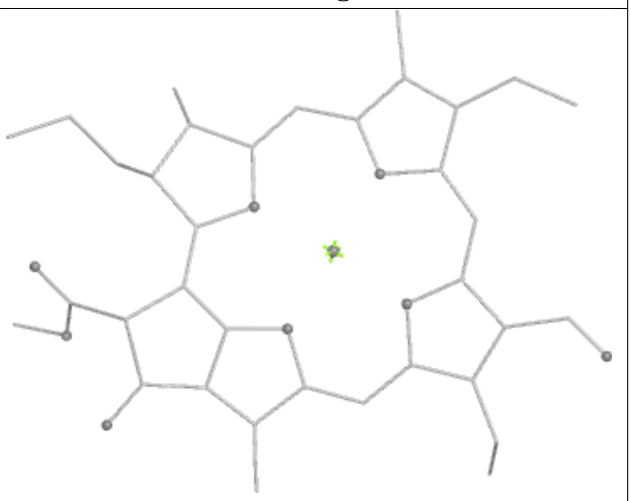
Bond lengths



Bond angles

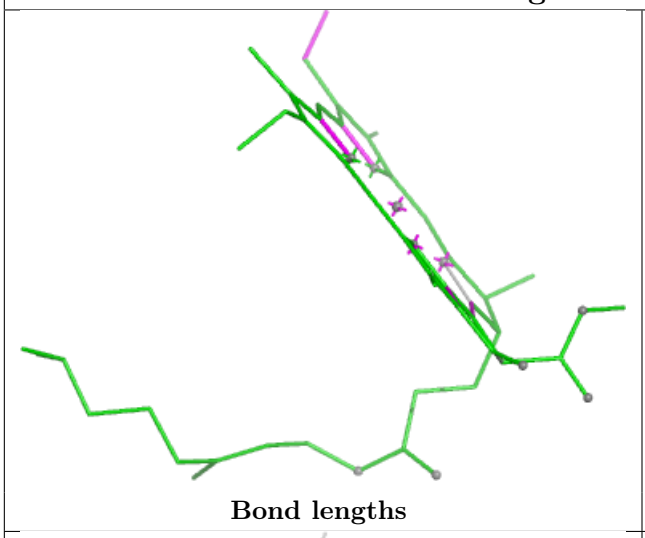


Torsions

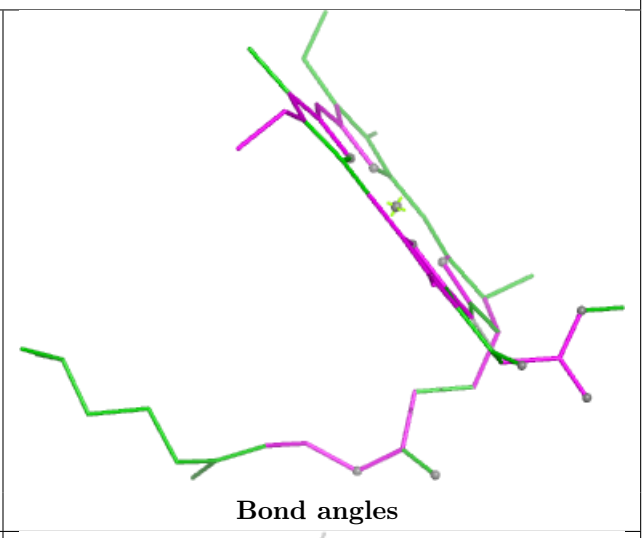


Rings

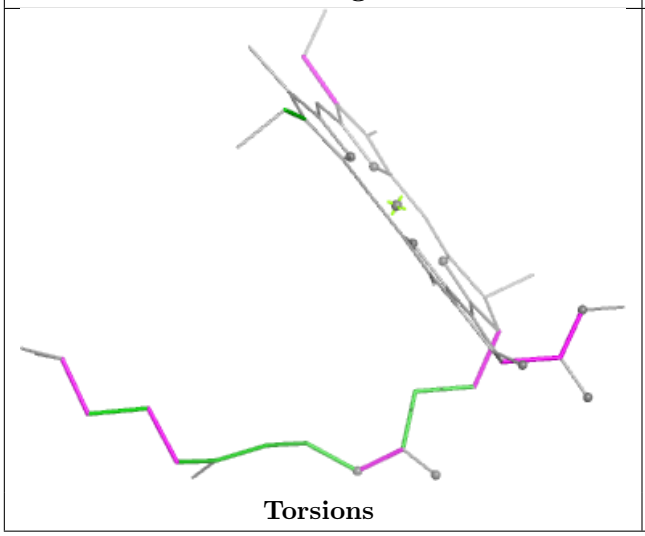
Ligand CLA S 604



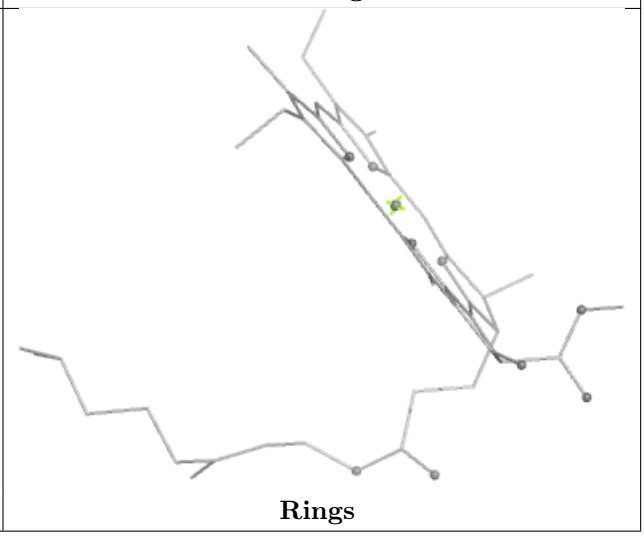
Bond lengths



Bond angles

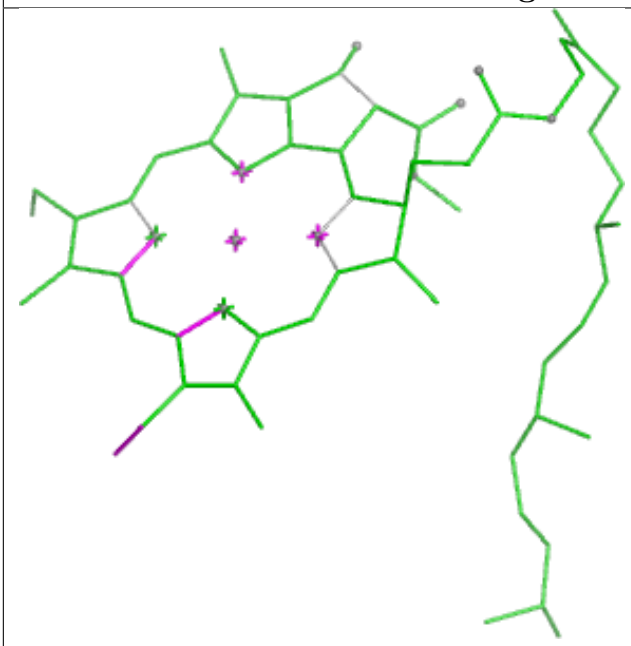


Torsions

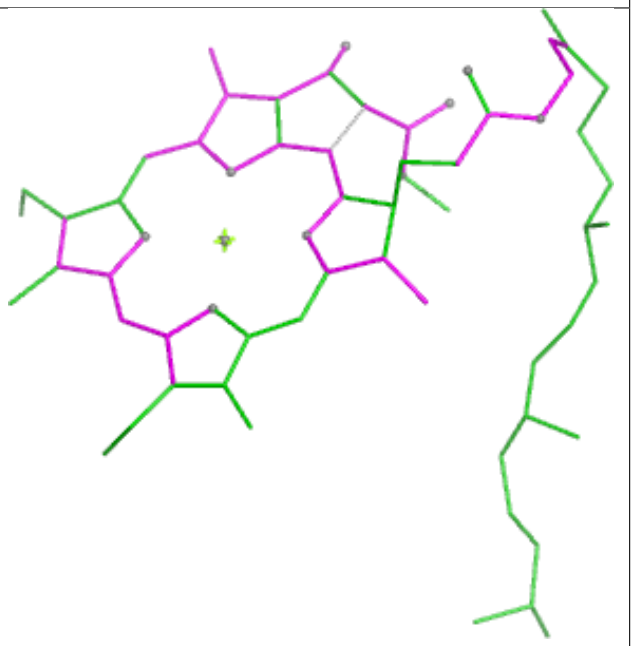


Rings

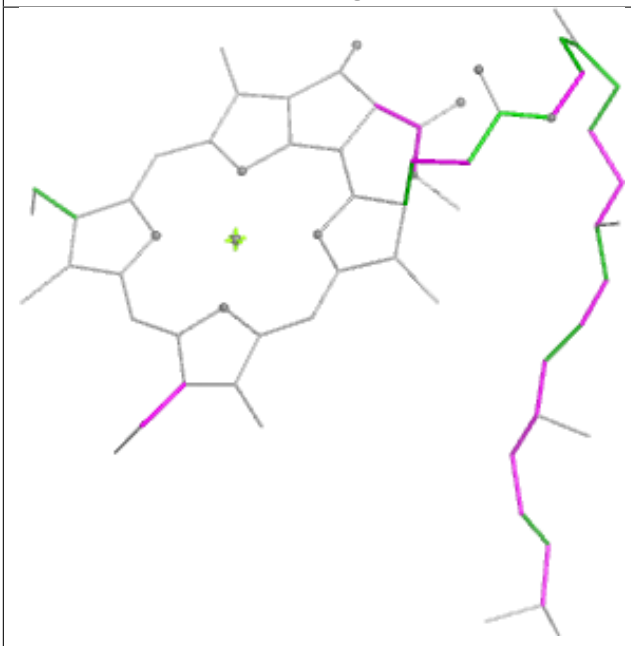
Ligand CLA b1 617



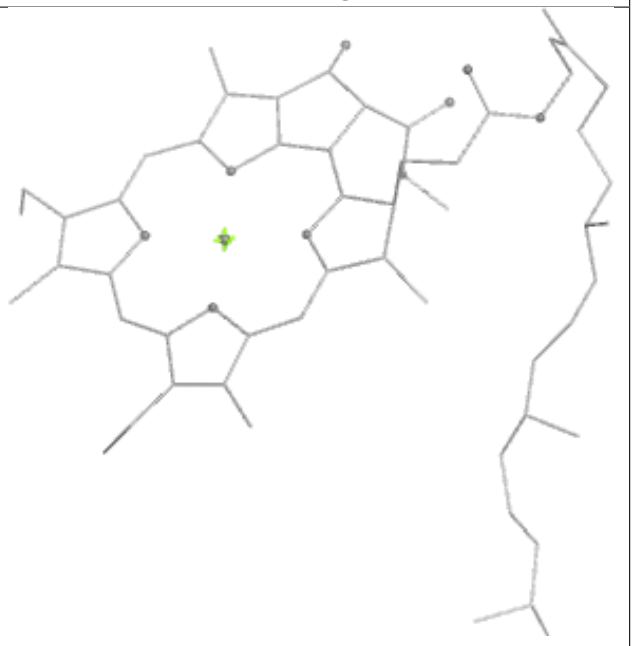
Bond lengths



Bond angles

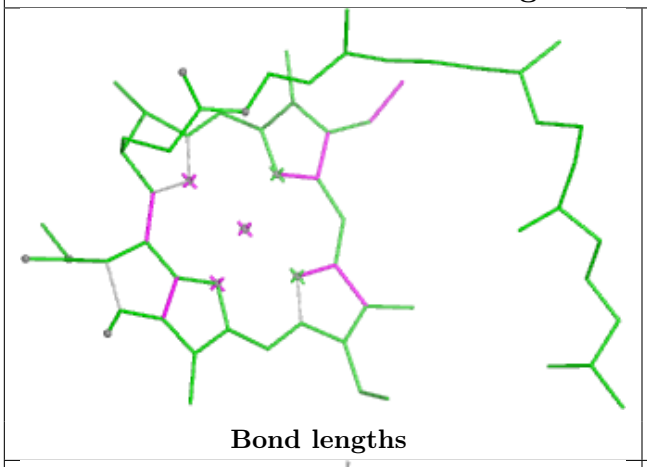


Torsions

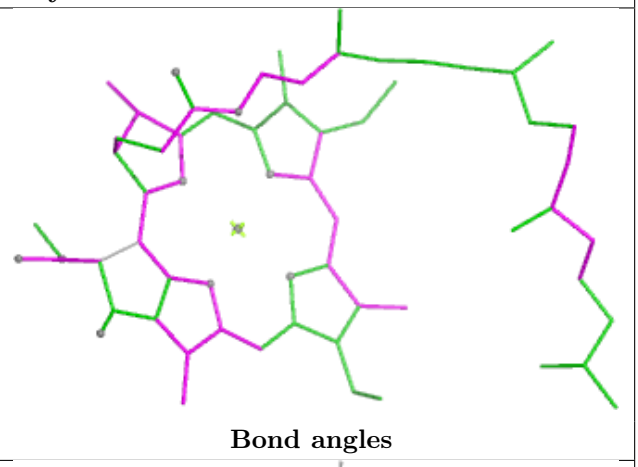


Rings

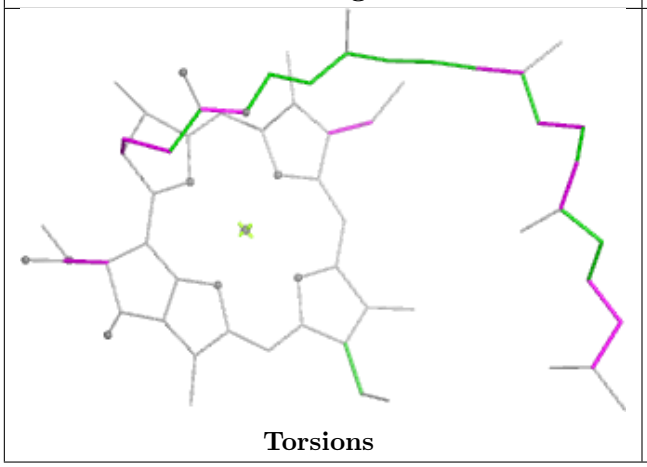
Ligand CLA y1 602



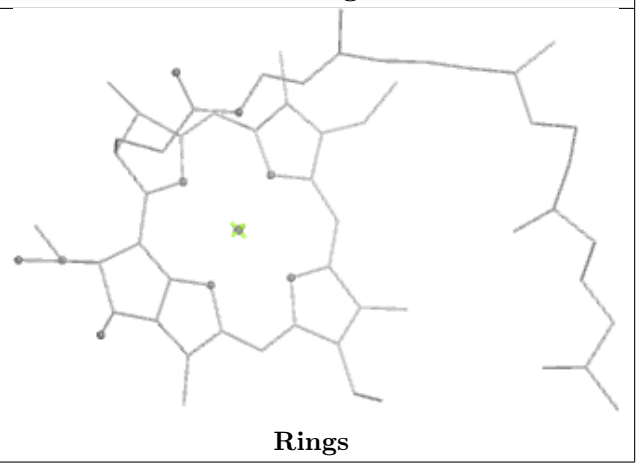
Bond lengths



Bond angles

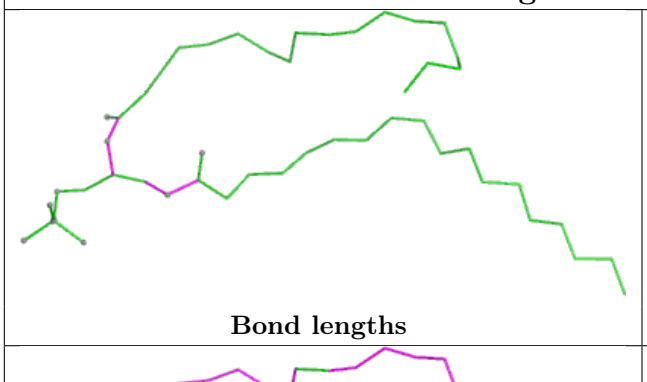


Torsions

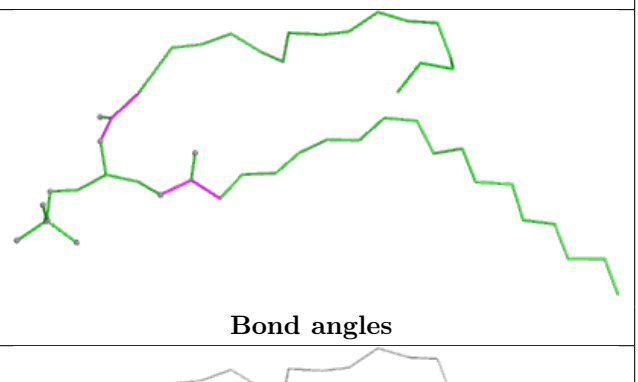


Rings

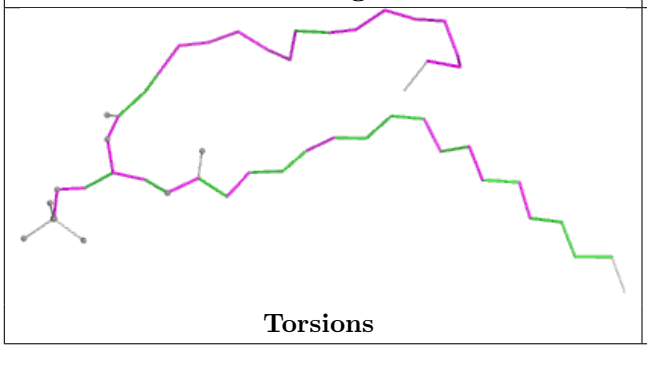
Ligand 3PH T1 101



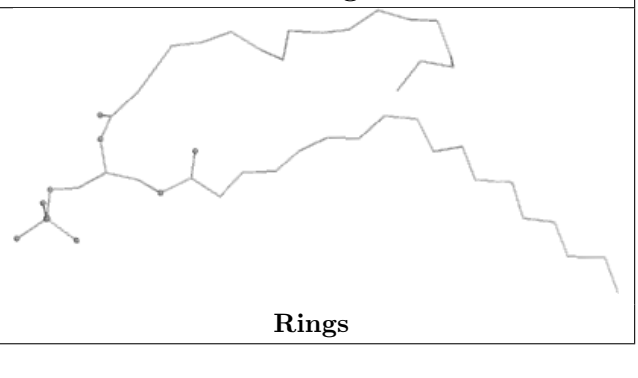
Bond lengths



Bond angles

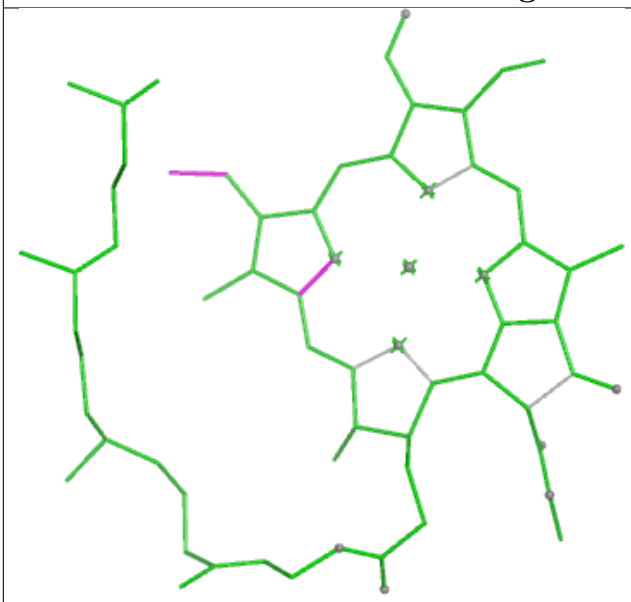


Torsions

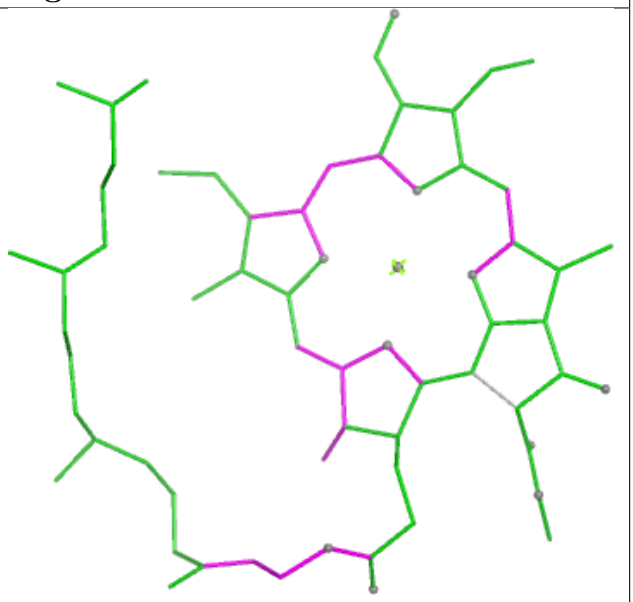


Rings

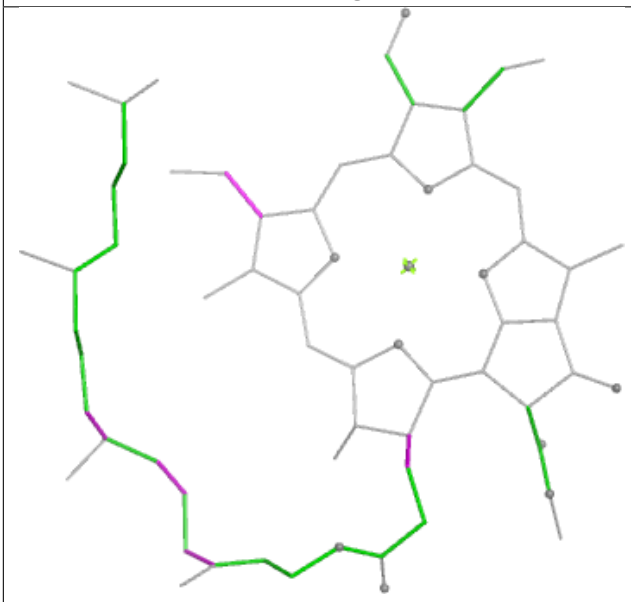
Ligand CHL g1 607



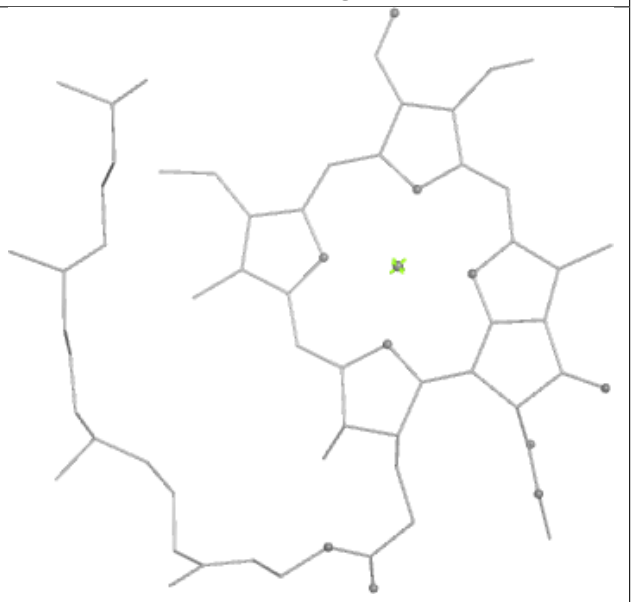
Bond lengths



Bond angles

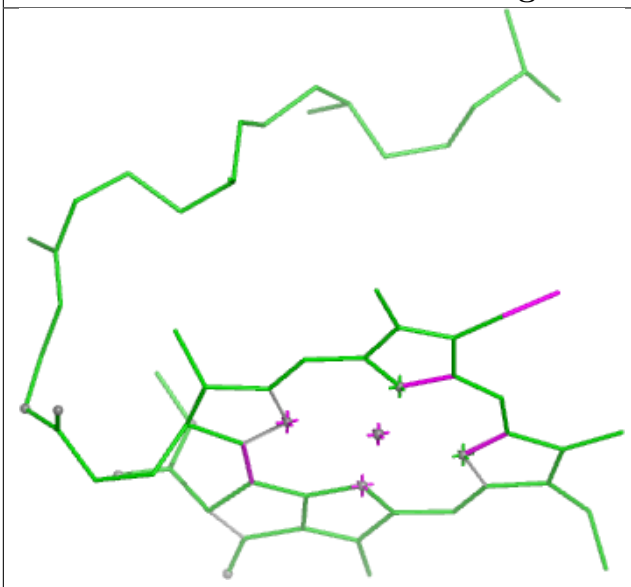


Torsions

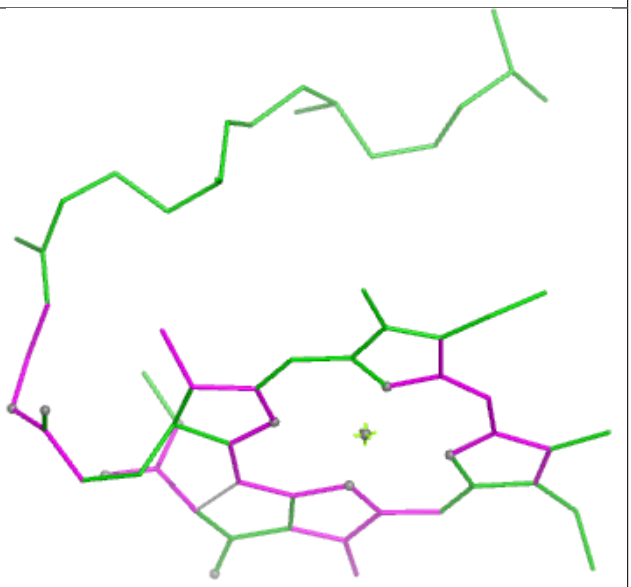


Rings

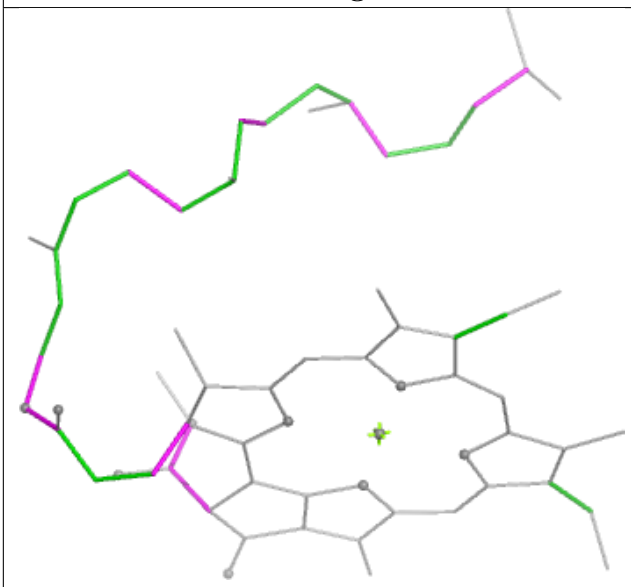
Ligand CLA n1 603



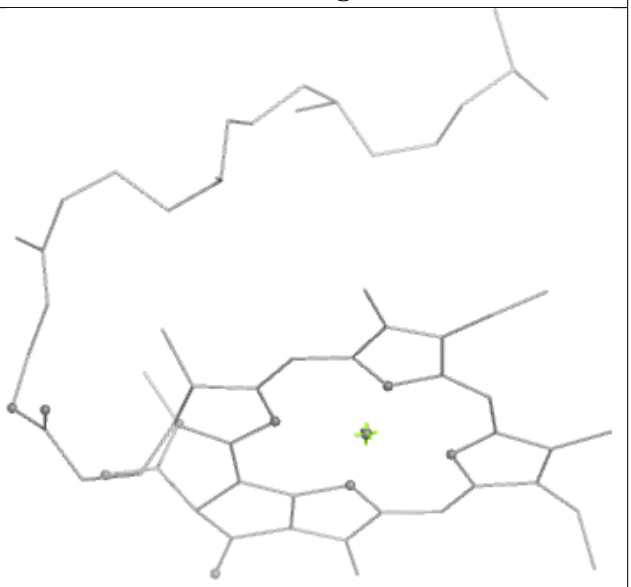
Bond lengths



Bond angles

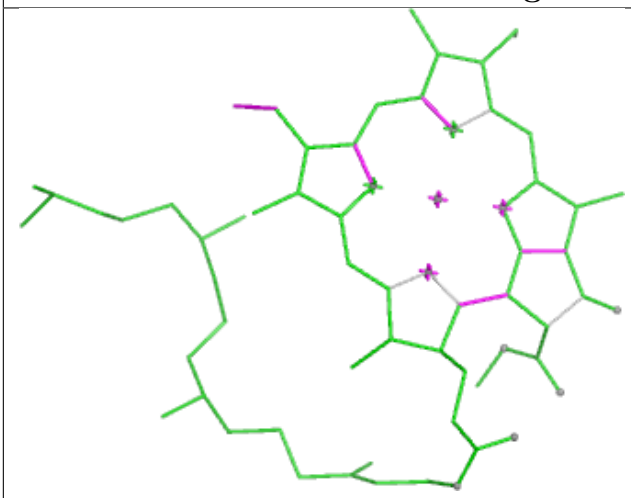


Torsions

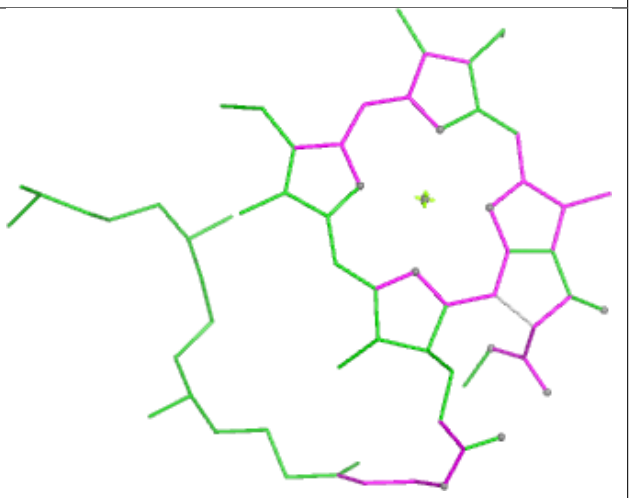


Rings

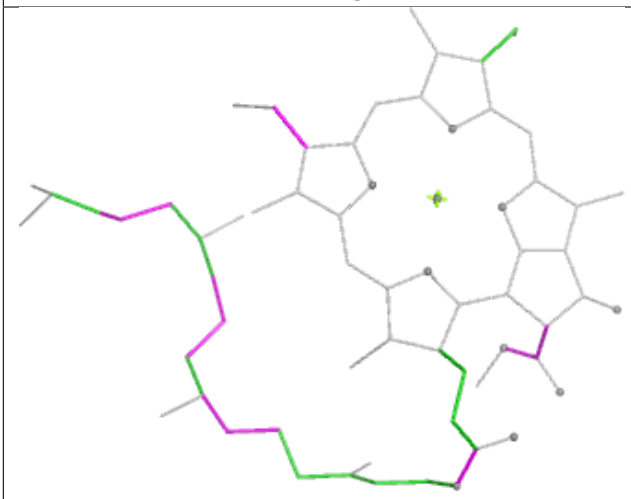
Ligand CLA Y 612



Bond lengths



Bond angles

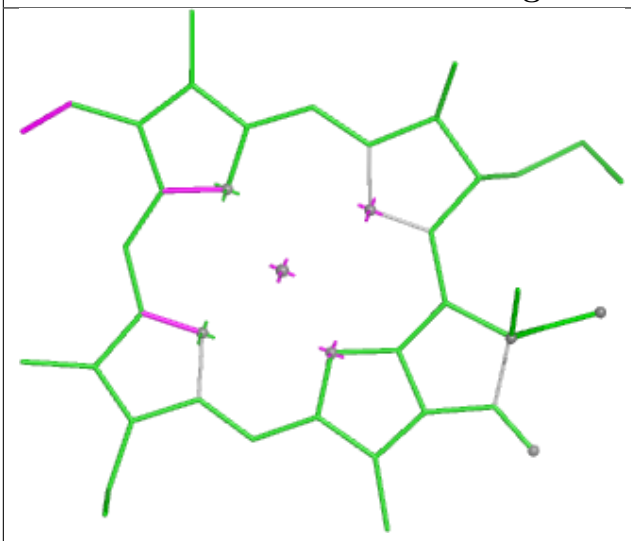


Torsions

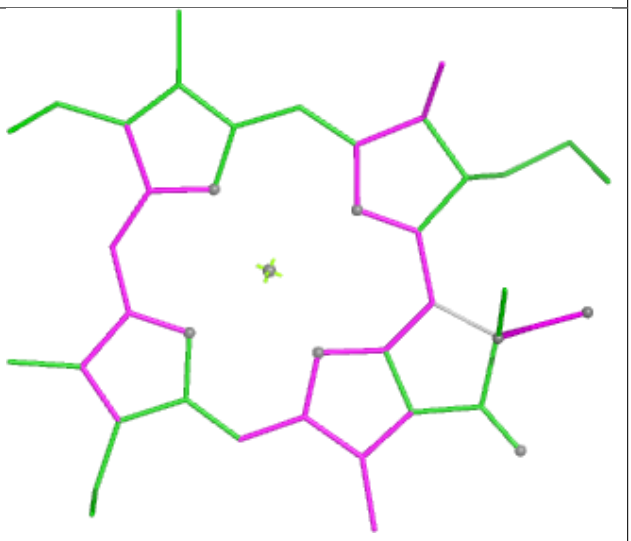


Rings

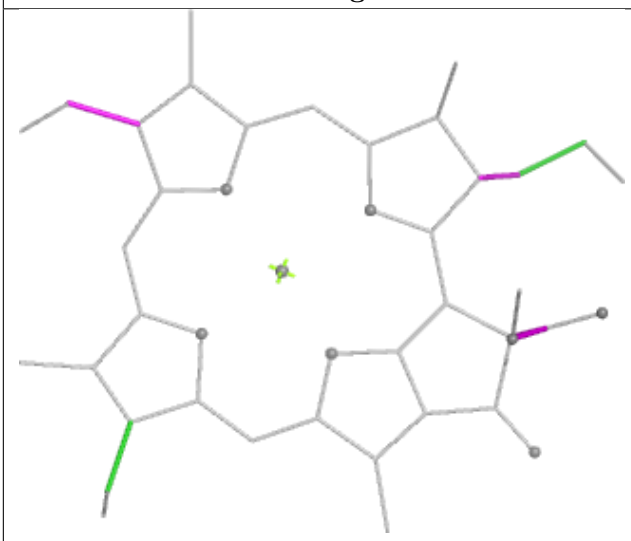
Ligand CLA G 612



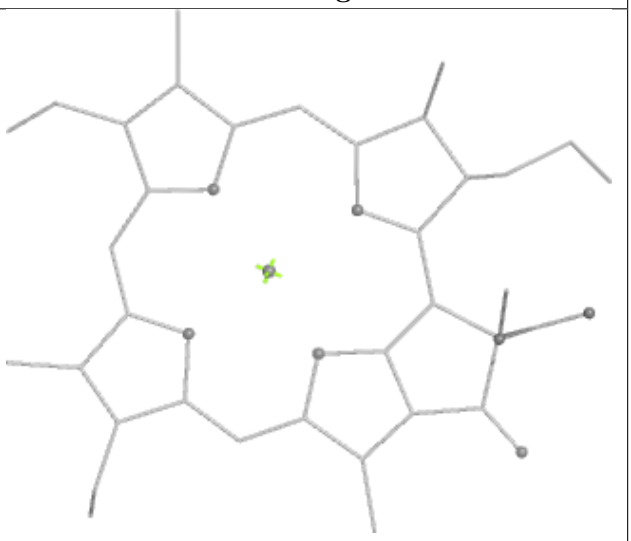
Bond lengths



Bond angles

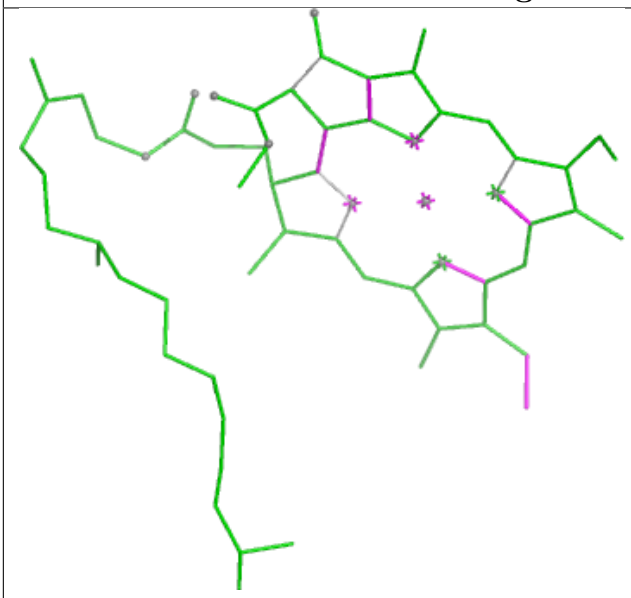


Torsions

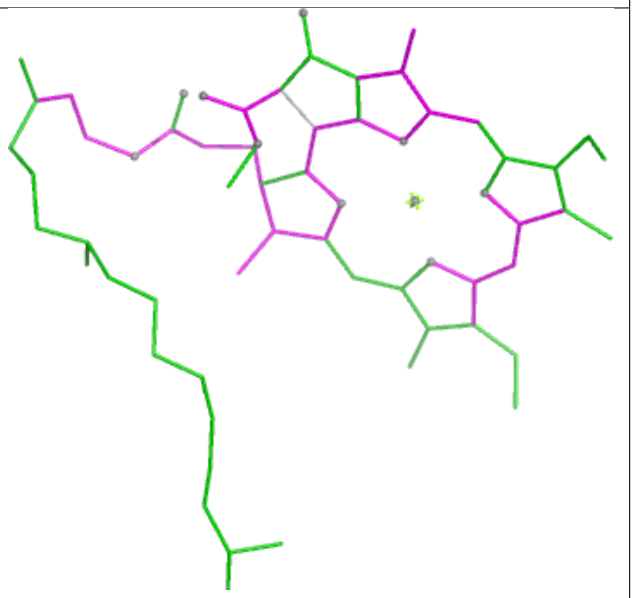


Rings

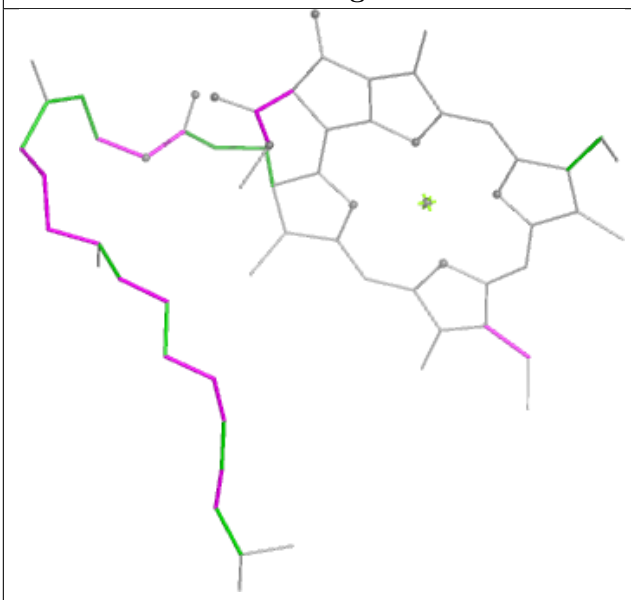
Ligand CLA B1 617



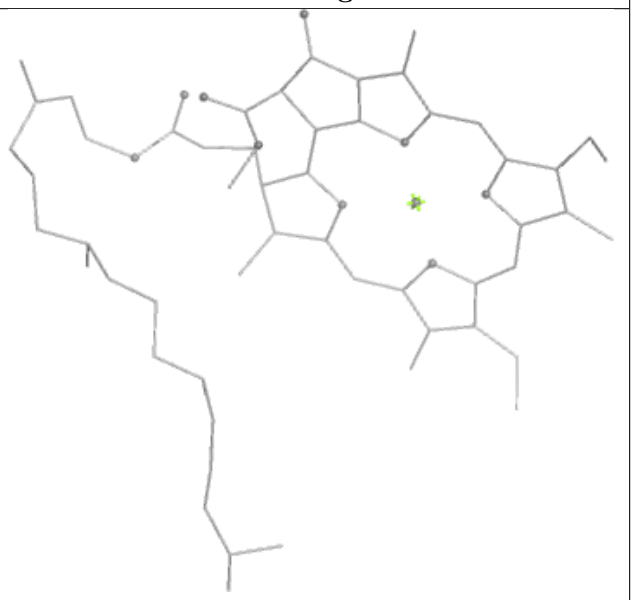
Bond lengths



Bond angles

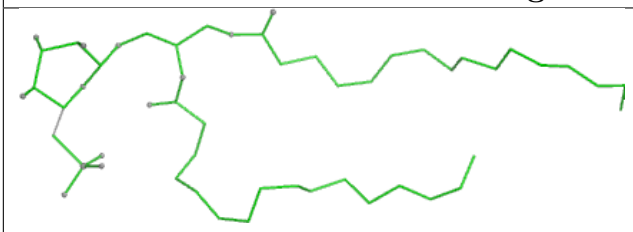


Torsions

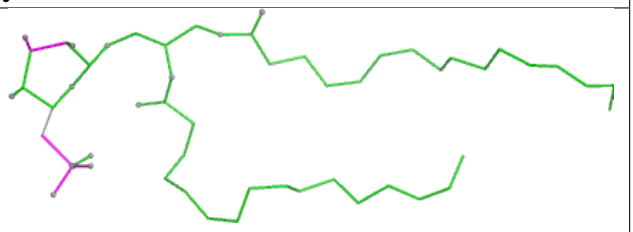


Rings

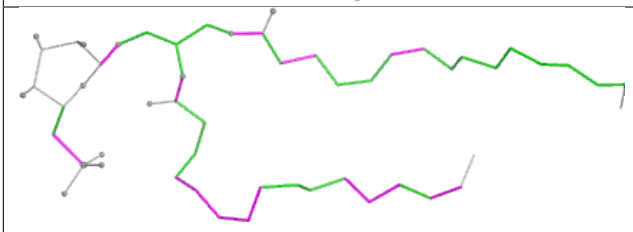
Ligand SQD b 626



Bond lengths



Bond angles

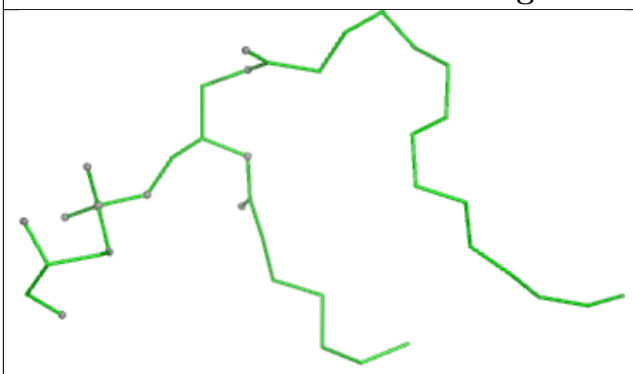


Torsions

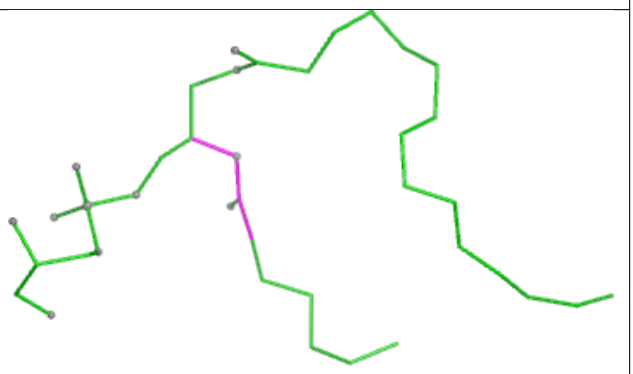


Rings

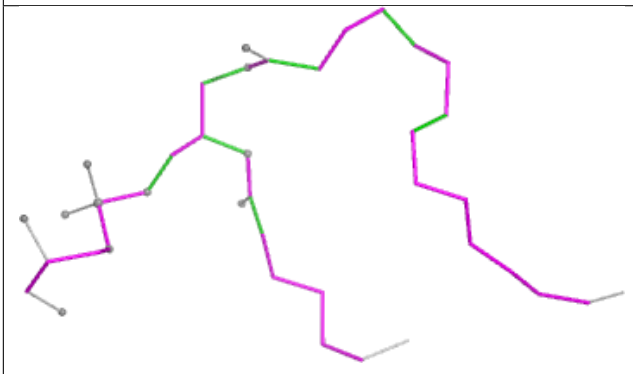
Ligand LHG d1 410



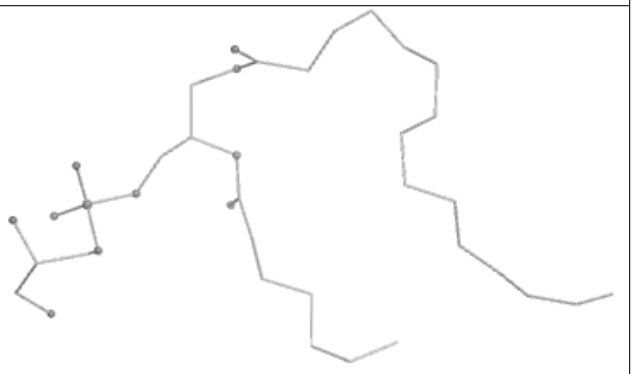
Bond lengths



Bond angles

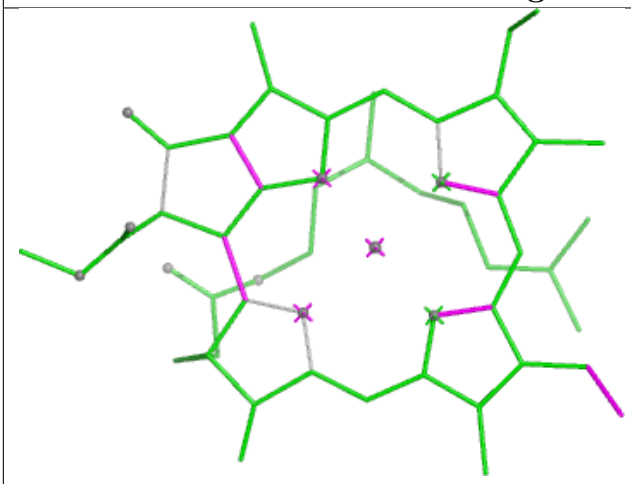


Torsions

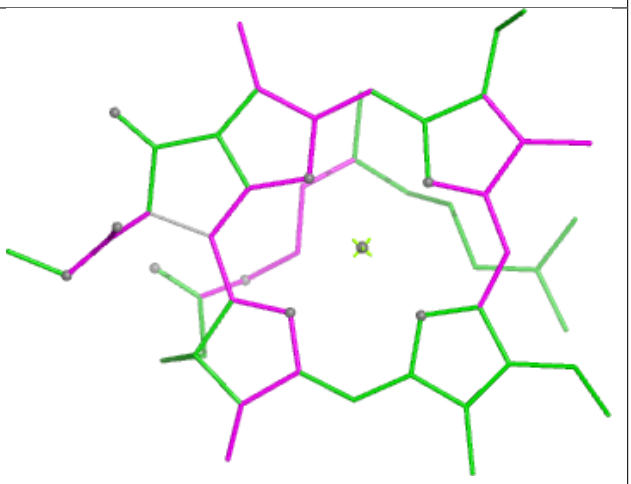


Rings

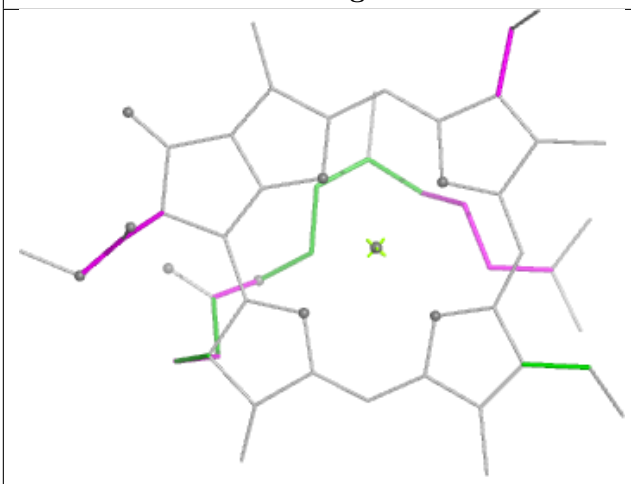
Ligand CLA S 613



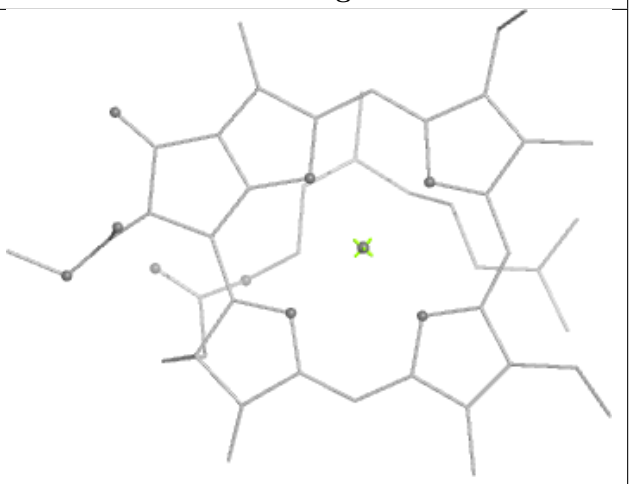
Bond lengths



Bond angles

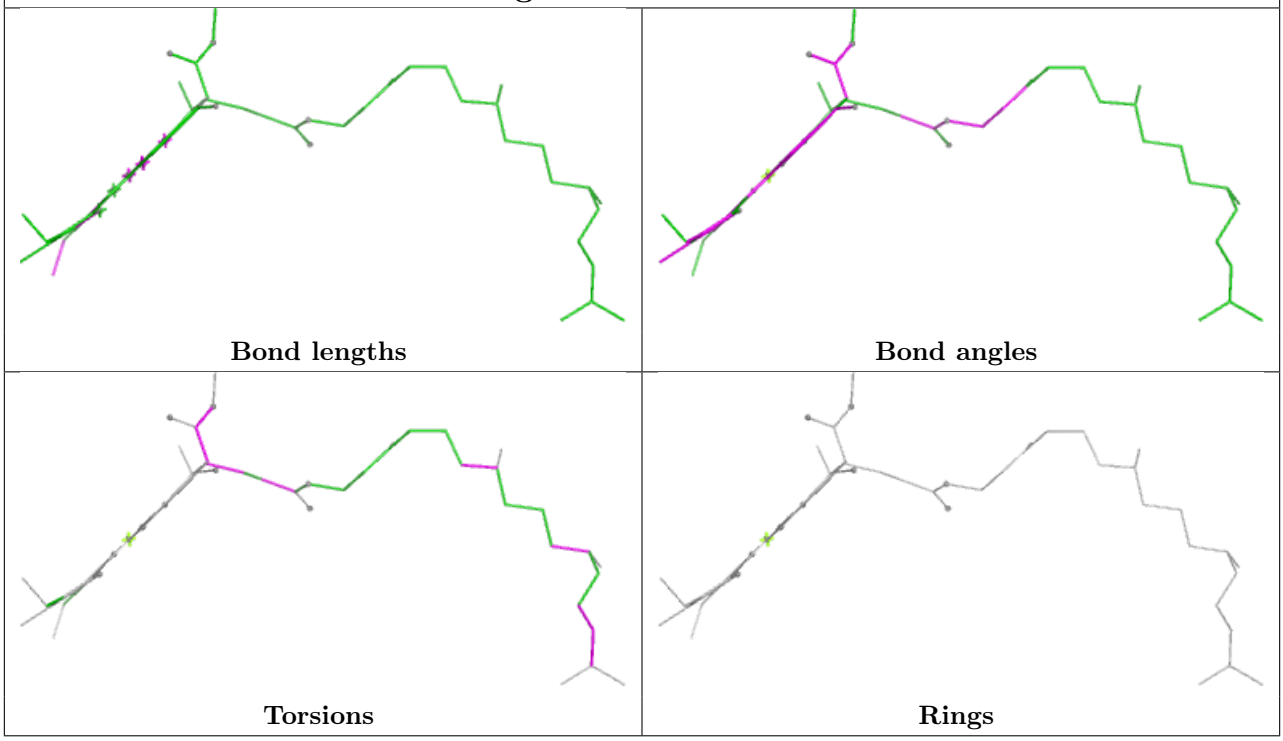


Torsions

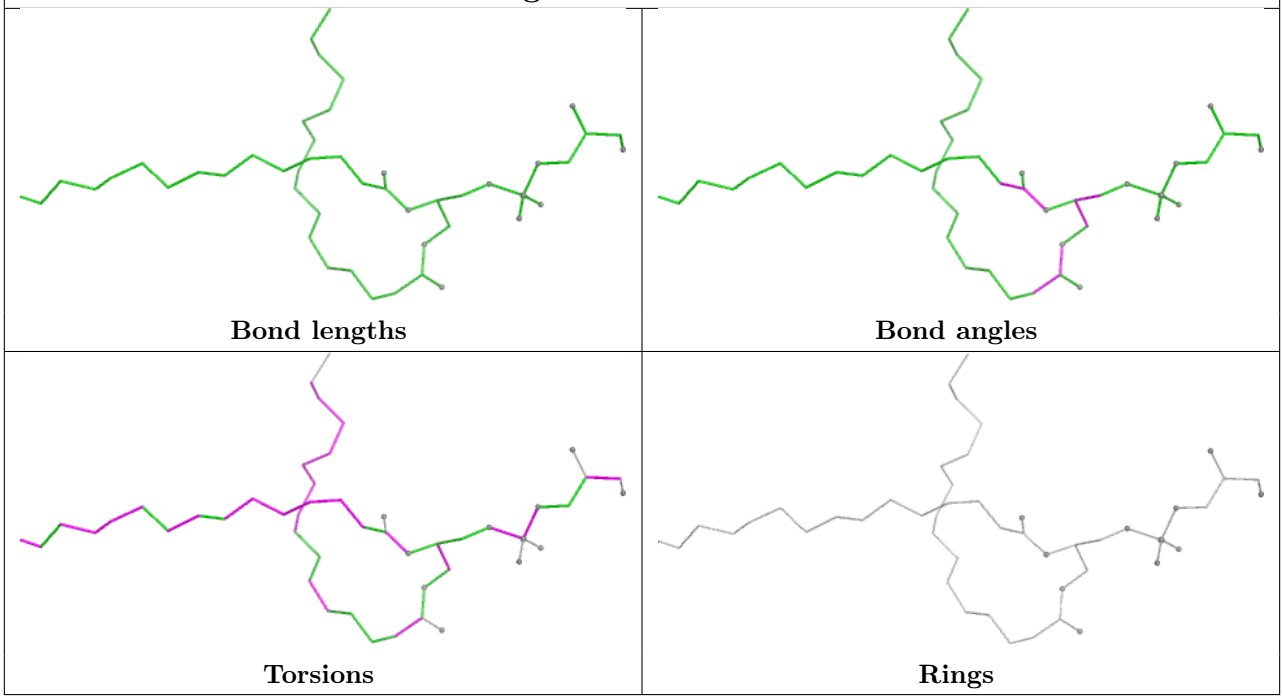


Rings

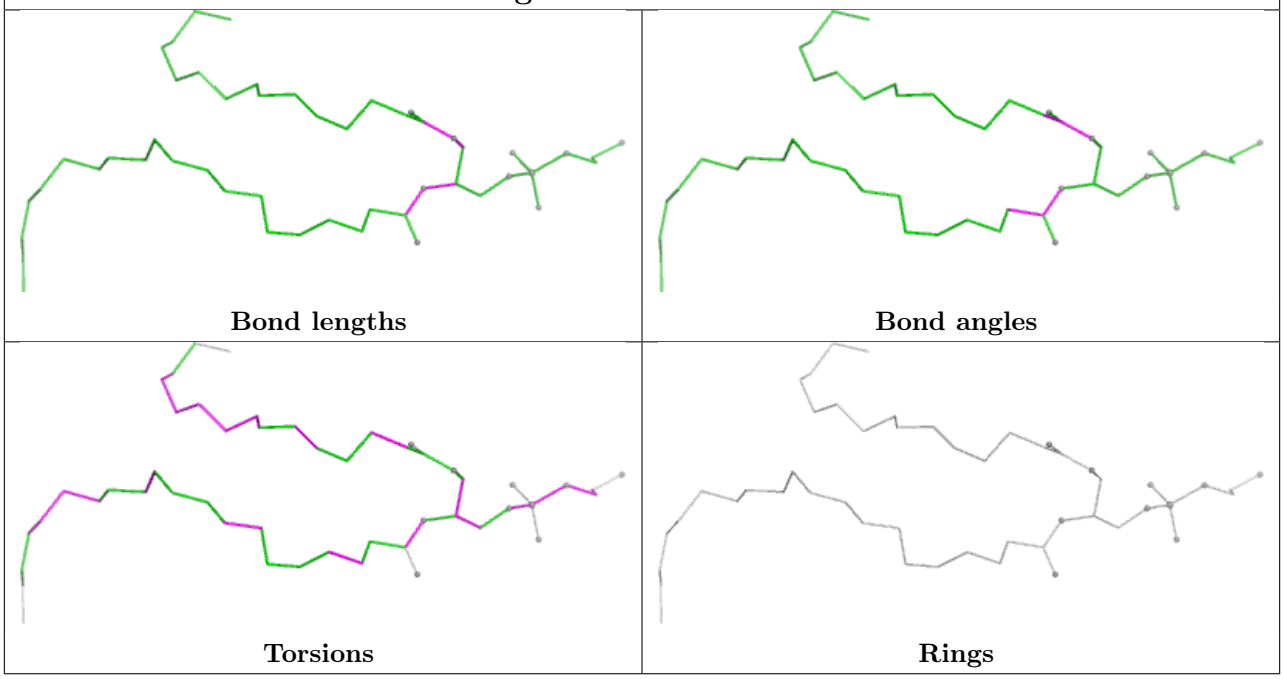
Ligand CLA D1 402



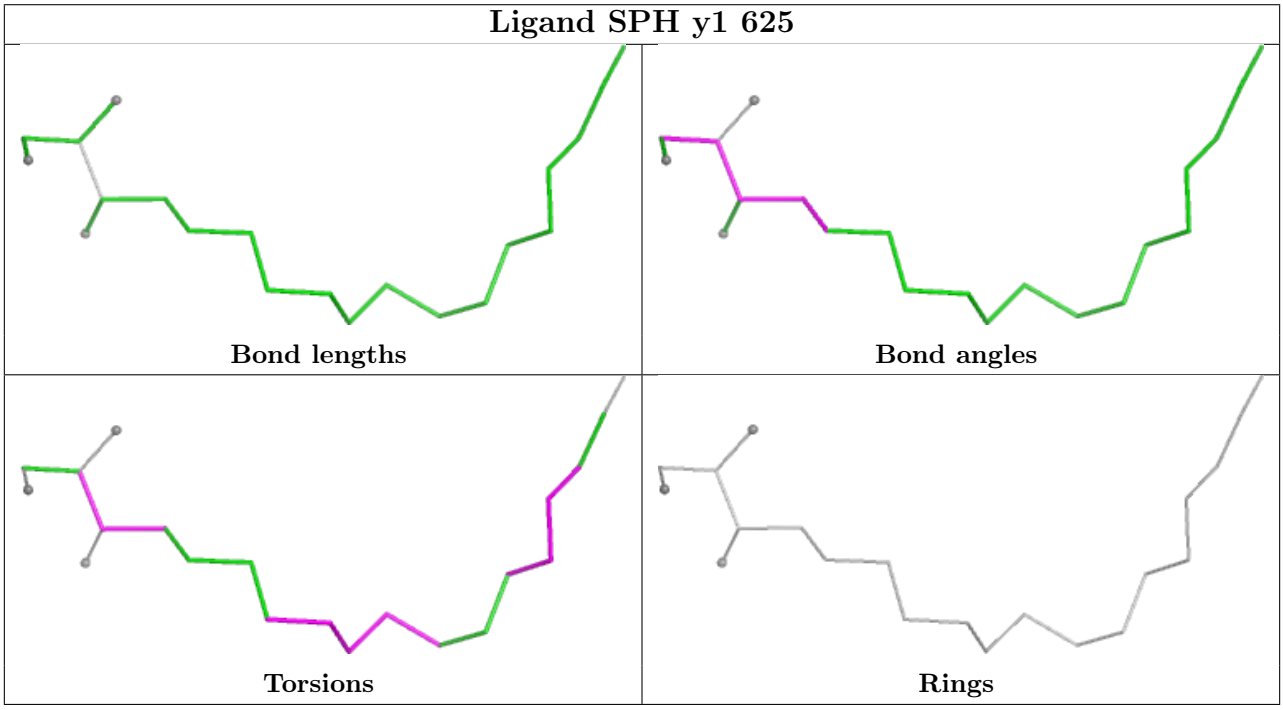
Ligand LHG Y 624



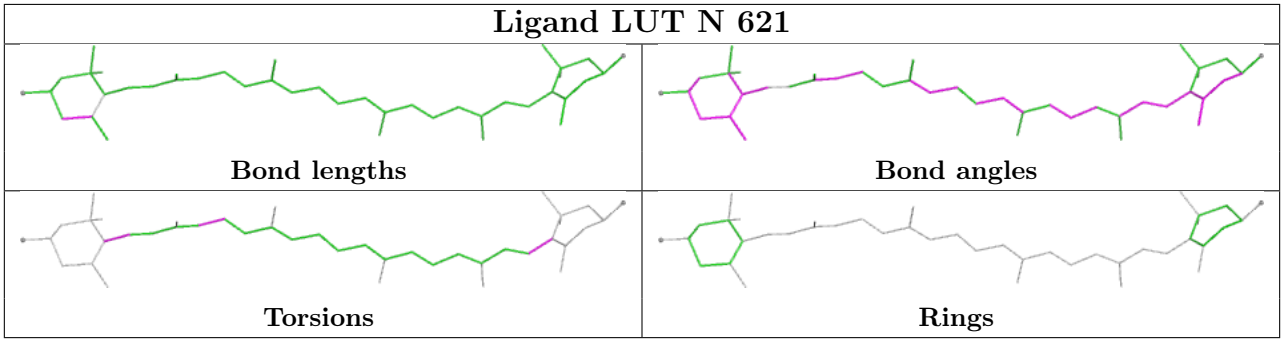
Ligand PTY Y1 626

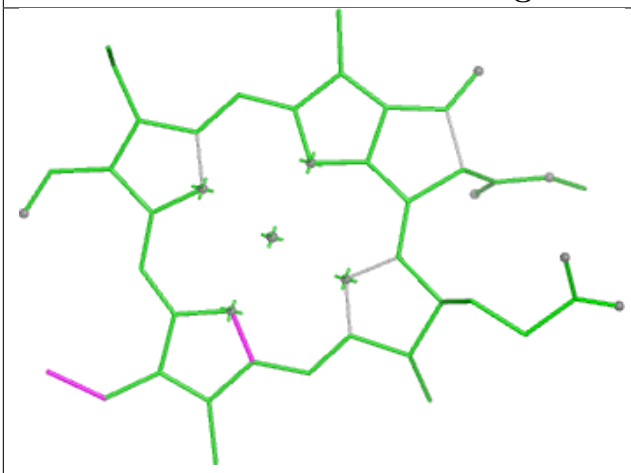
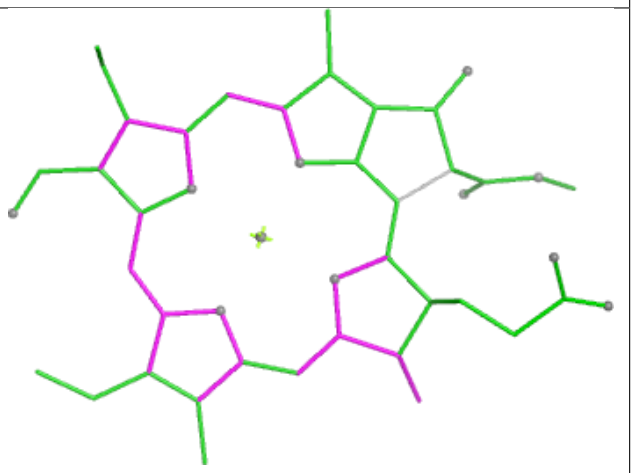
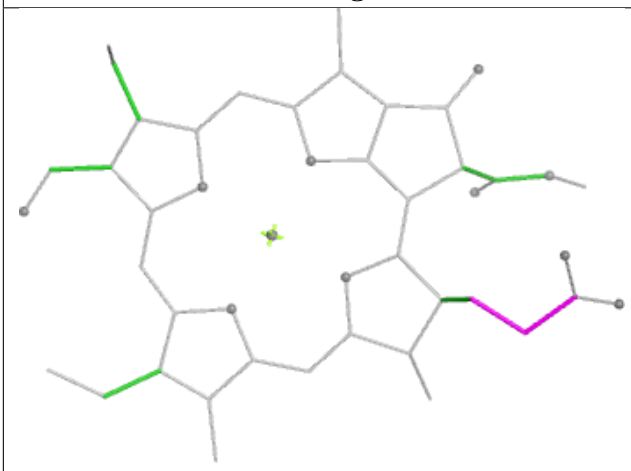
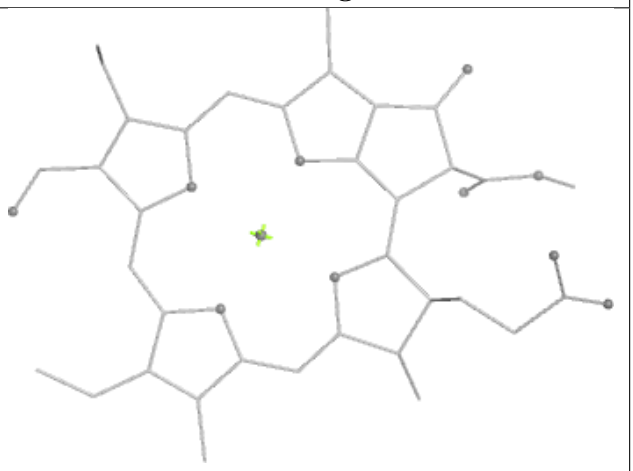


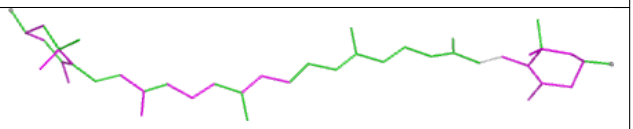
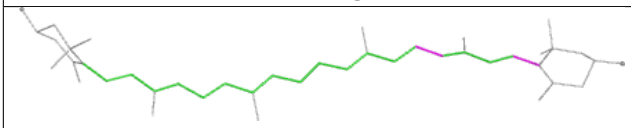
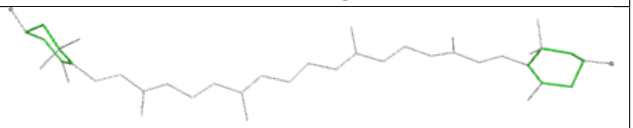
Ligand SPH y1 625



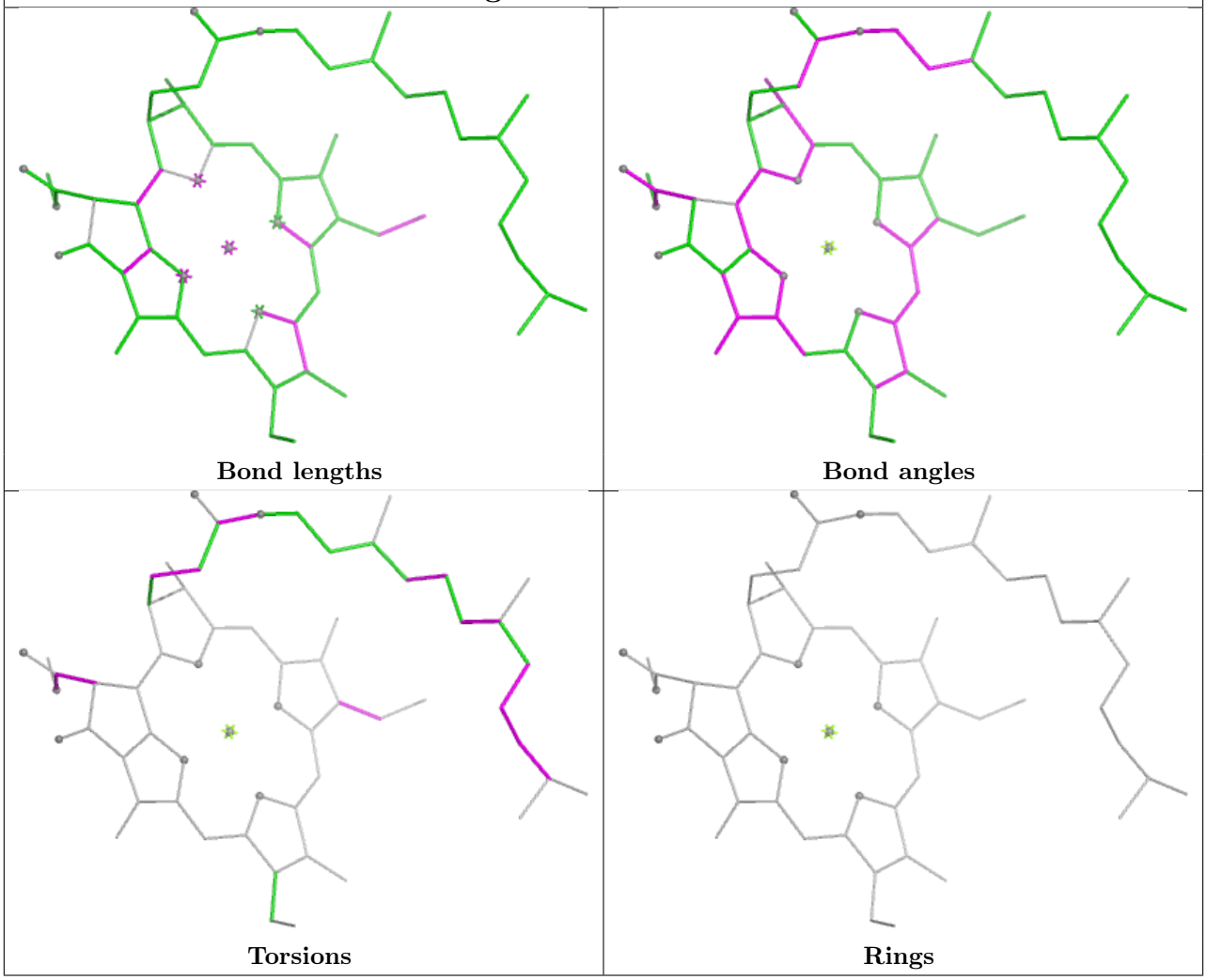
Ligand LUT N 621



Ligand CHL Y1 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT n 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

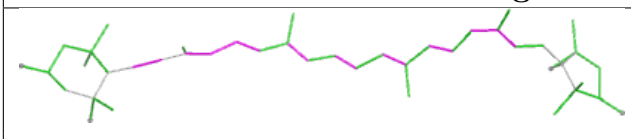
Ligand CLA R1 602



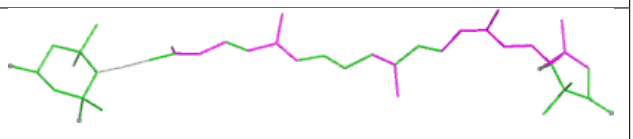
Ligand BCR A1 411



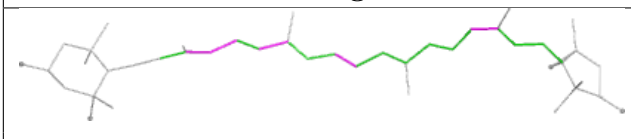
Ligand NEX Y1 623



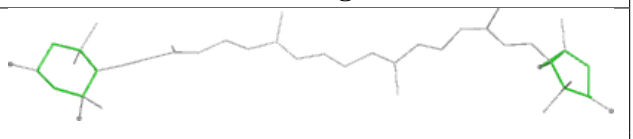
Bond lengths



Bond angles

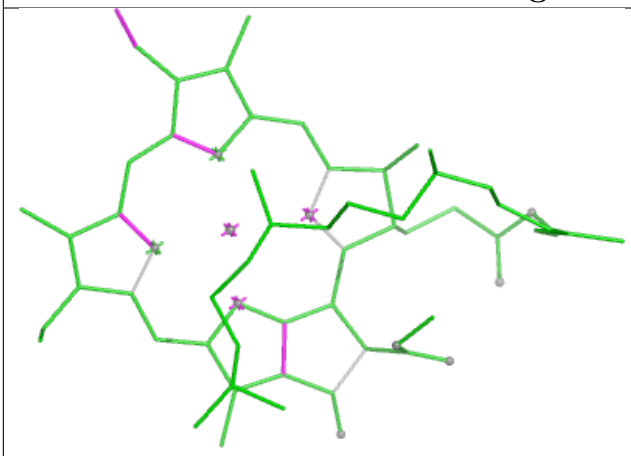


Torsions

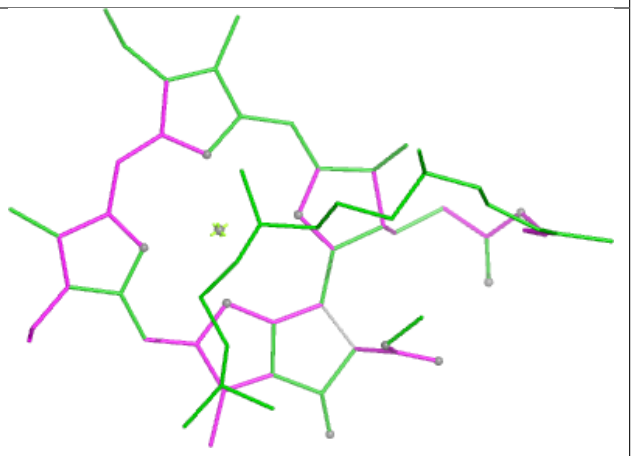


Rings

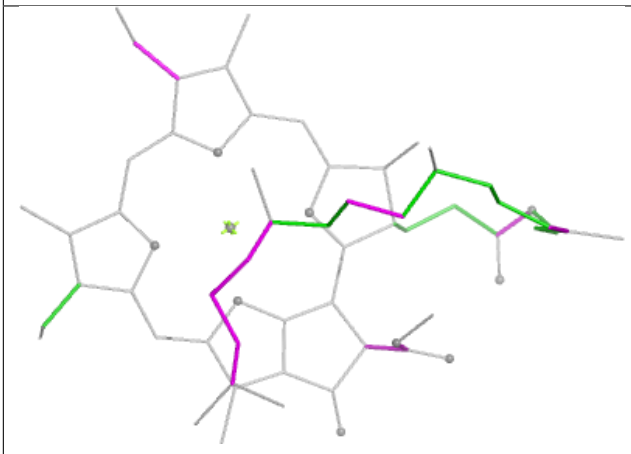
Ligand CLA c 510



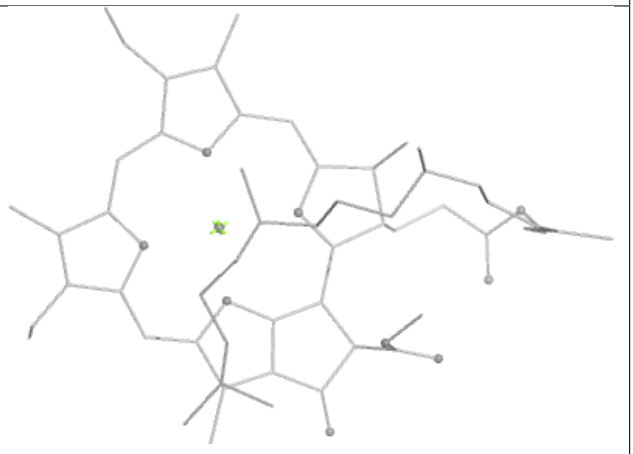
Bond lengths



Bond angles

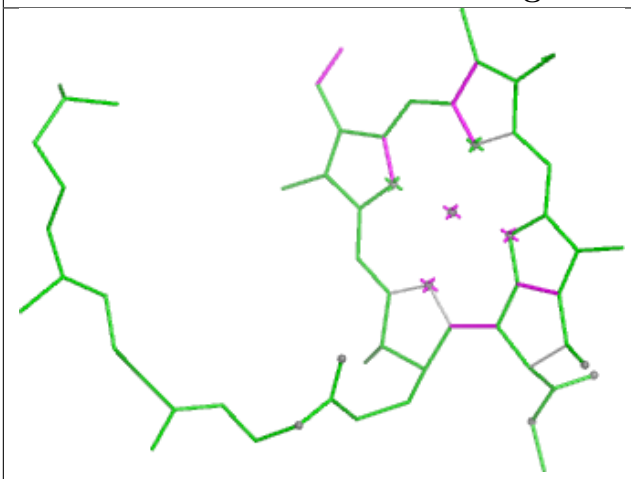


Torsions

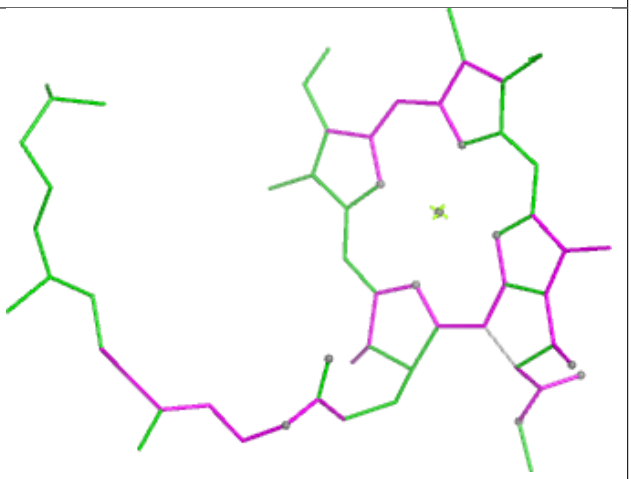


Rings

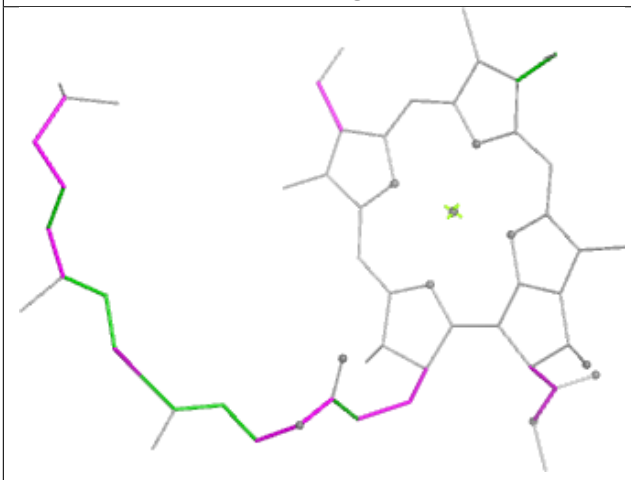
Ligand CLA R 603



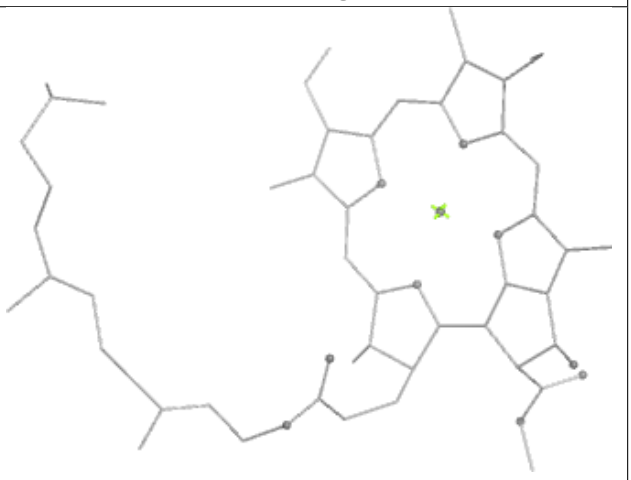
Bond lengths



Bond angles

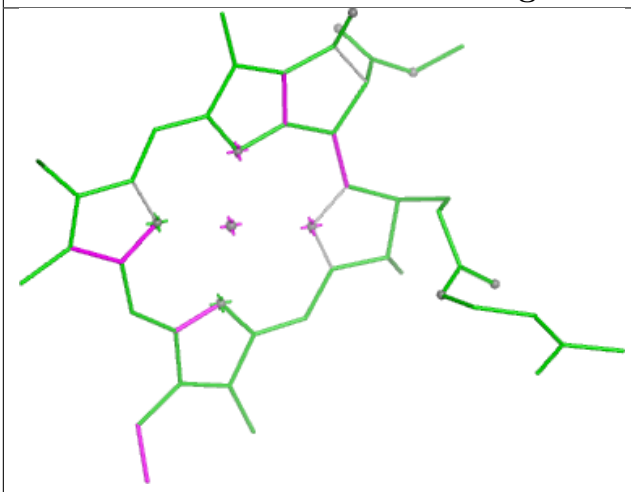


Torsions

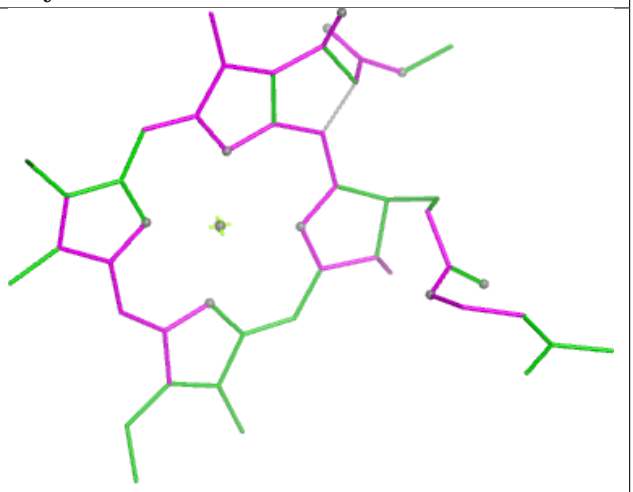


Rings

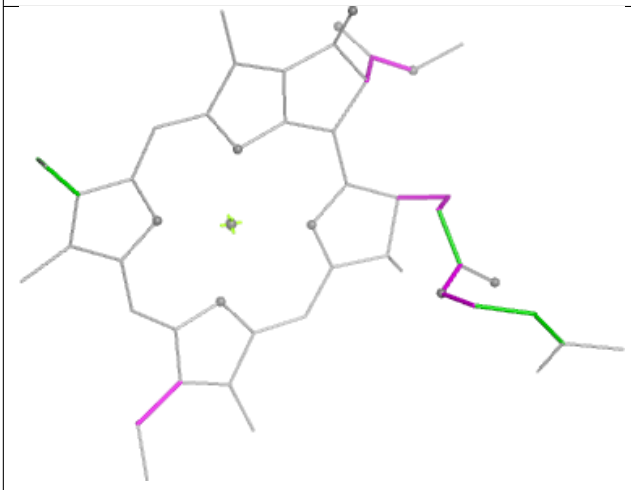
Ligand CLA y1 608



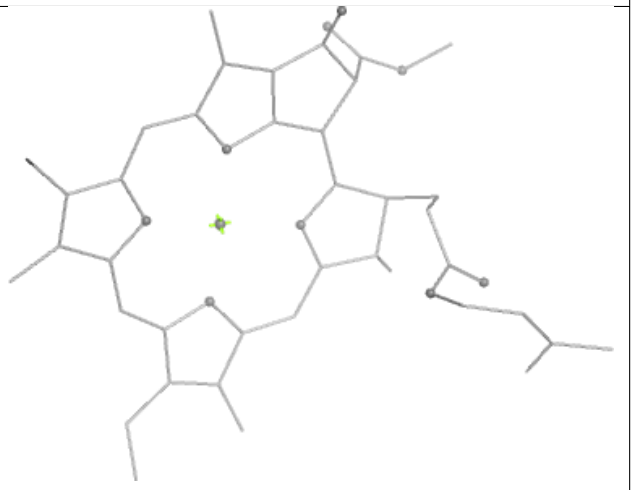
Bond lengths



Bond angles

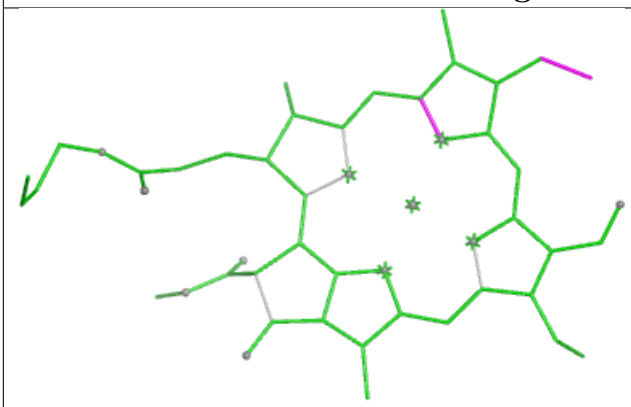


Torsions

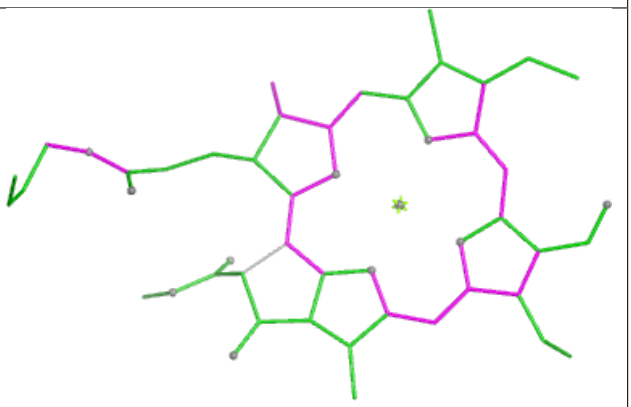


Rings

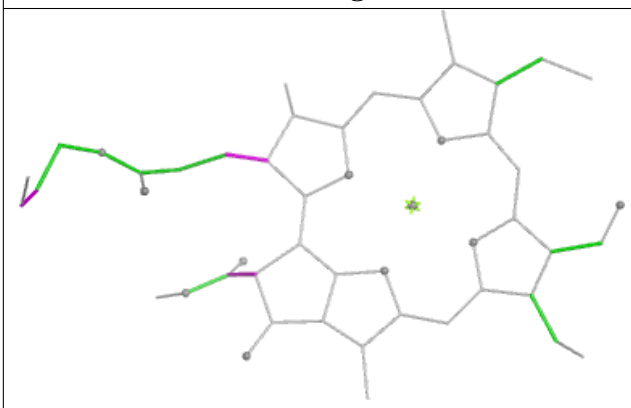
Ligand CHL G1 606



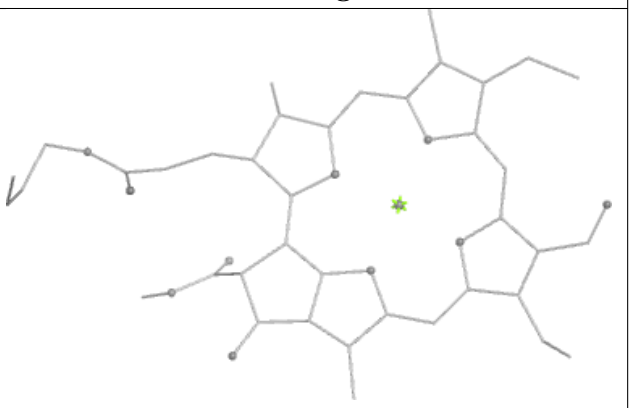
Bond lengths



Bond angles

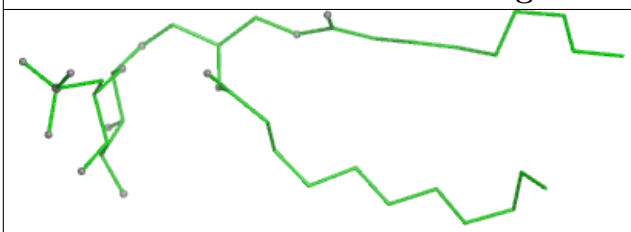


Torsions

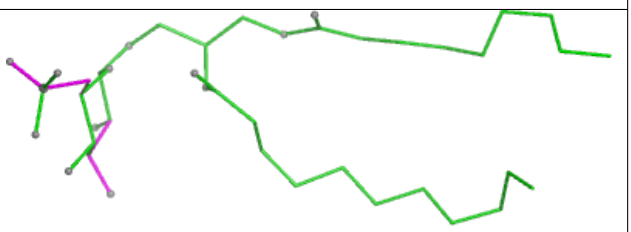


Rings

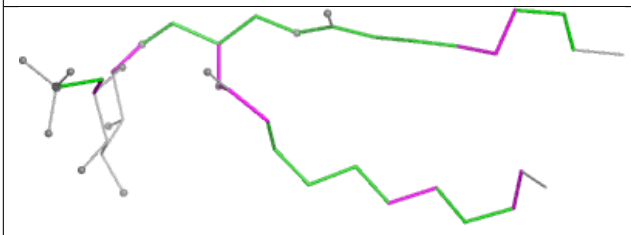
Ligand SQD B1 621



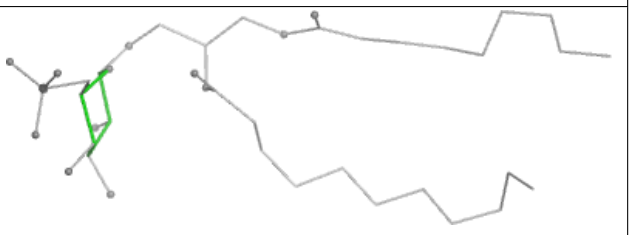
Bond lengths



Bond angles

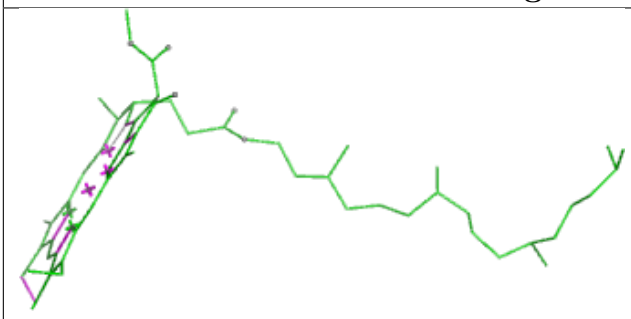


Torsions

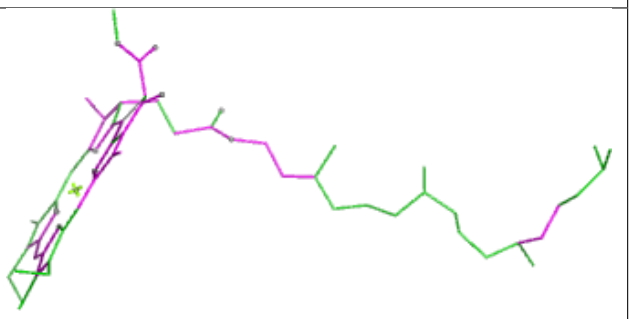


Rings

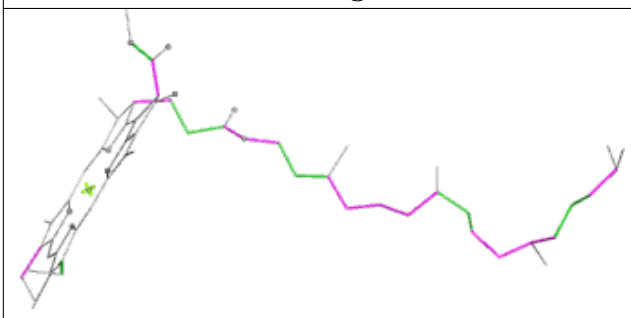
Ligand CLA B 605



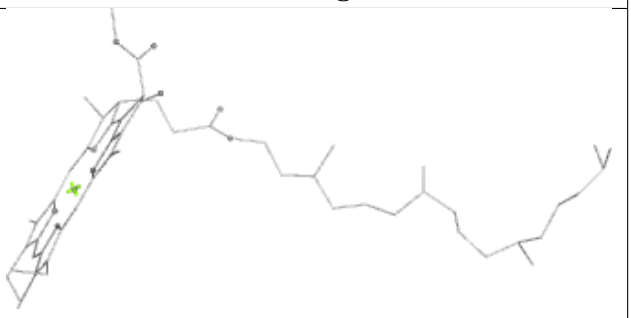
Bond lengths



Bond angles

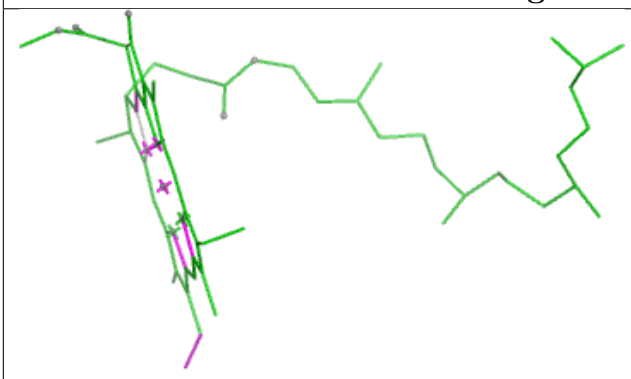


Torsions

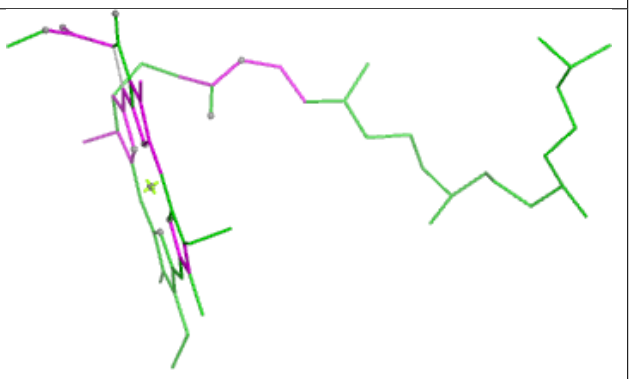


Rings

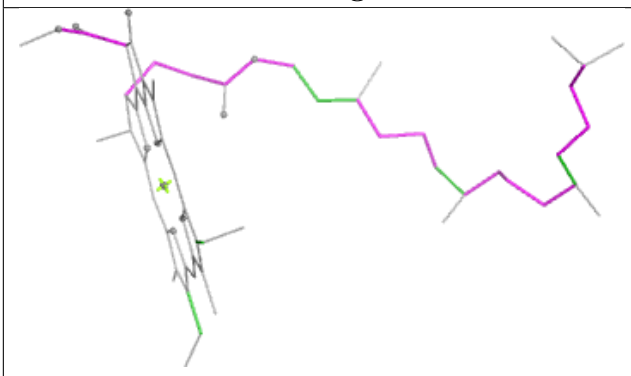
Ligand CLA b 608



Bond lengths



Bond angles

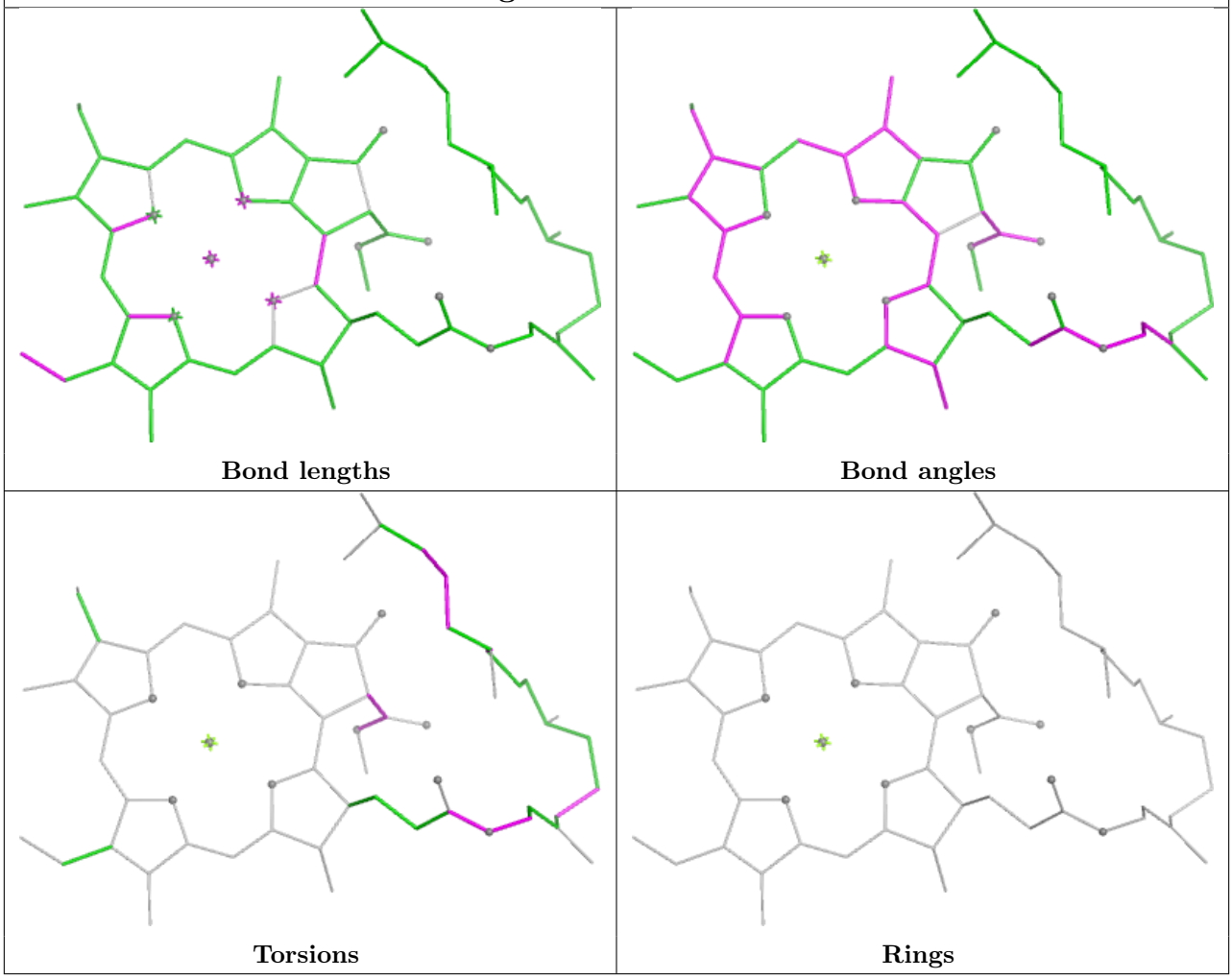


Torsions

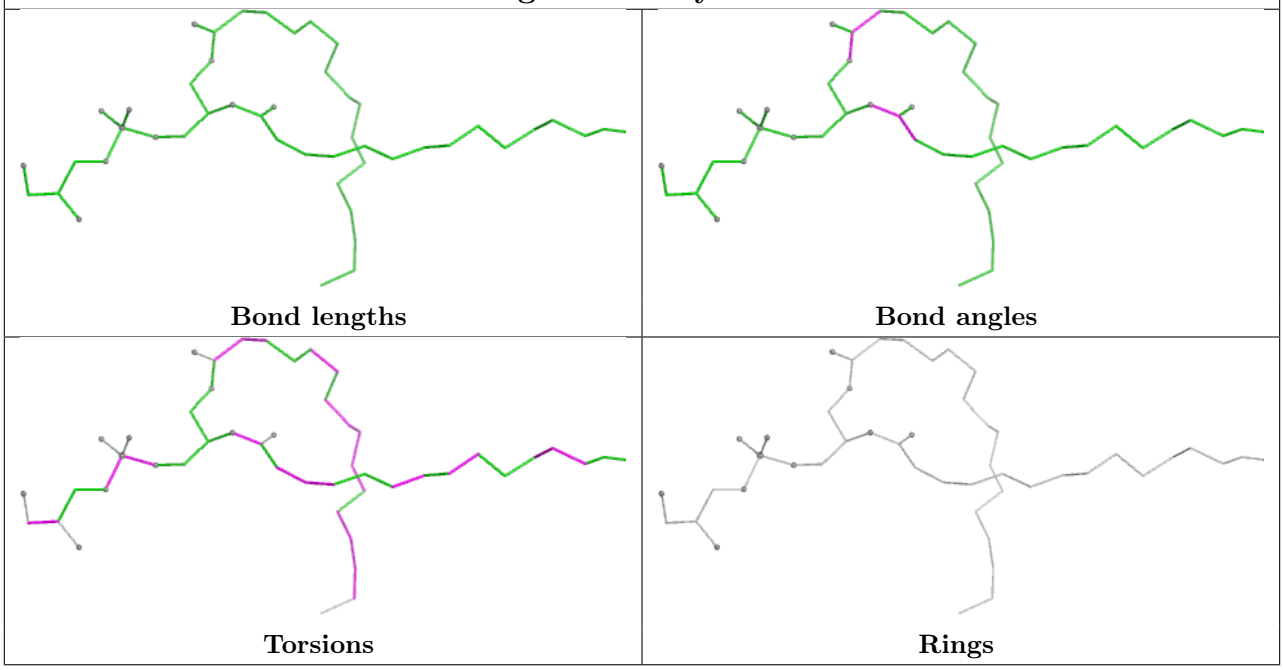


Rings

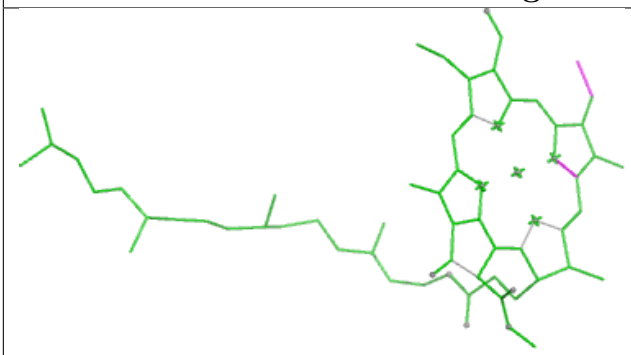
Ligand CLA b1 611



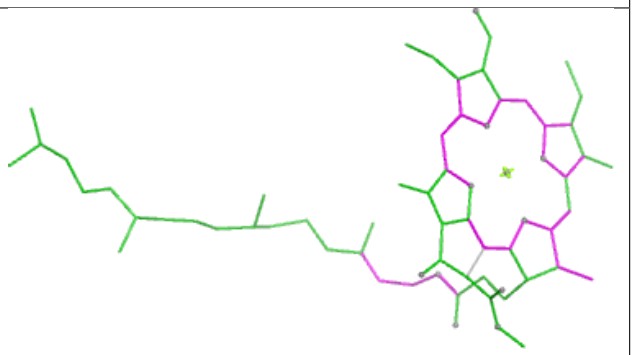
Ligand LHG y1 624



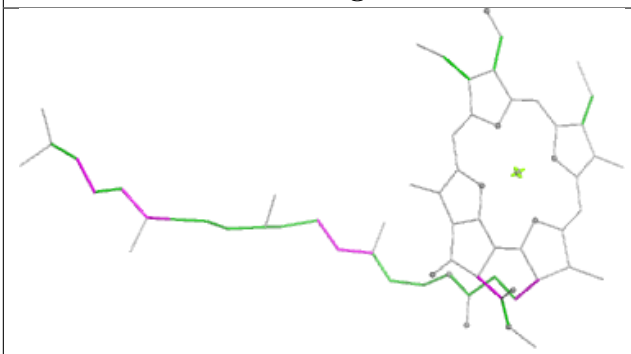
Ligand CHL G 609



Bond lengths



Bond angles

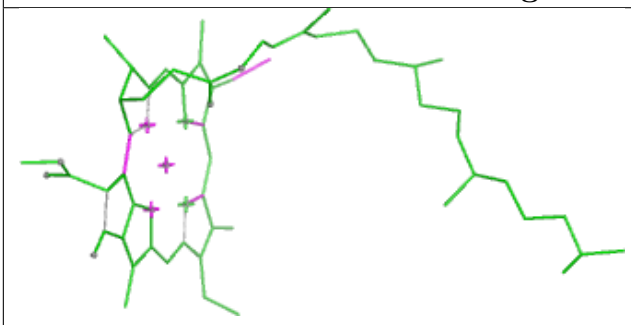


Torsions

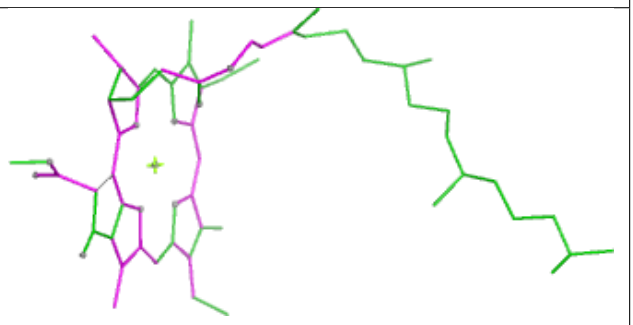


Rings

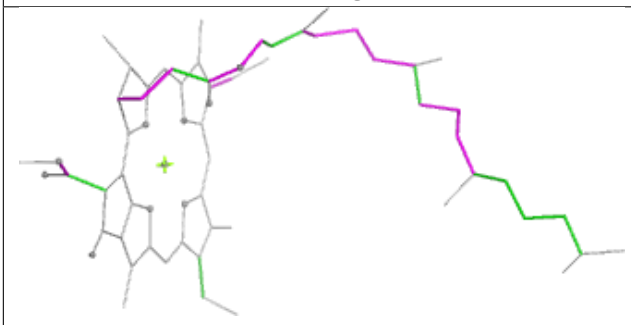
Ligand CLA s1 610



Bond lengths



Bond angles

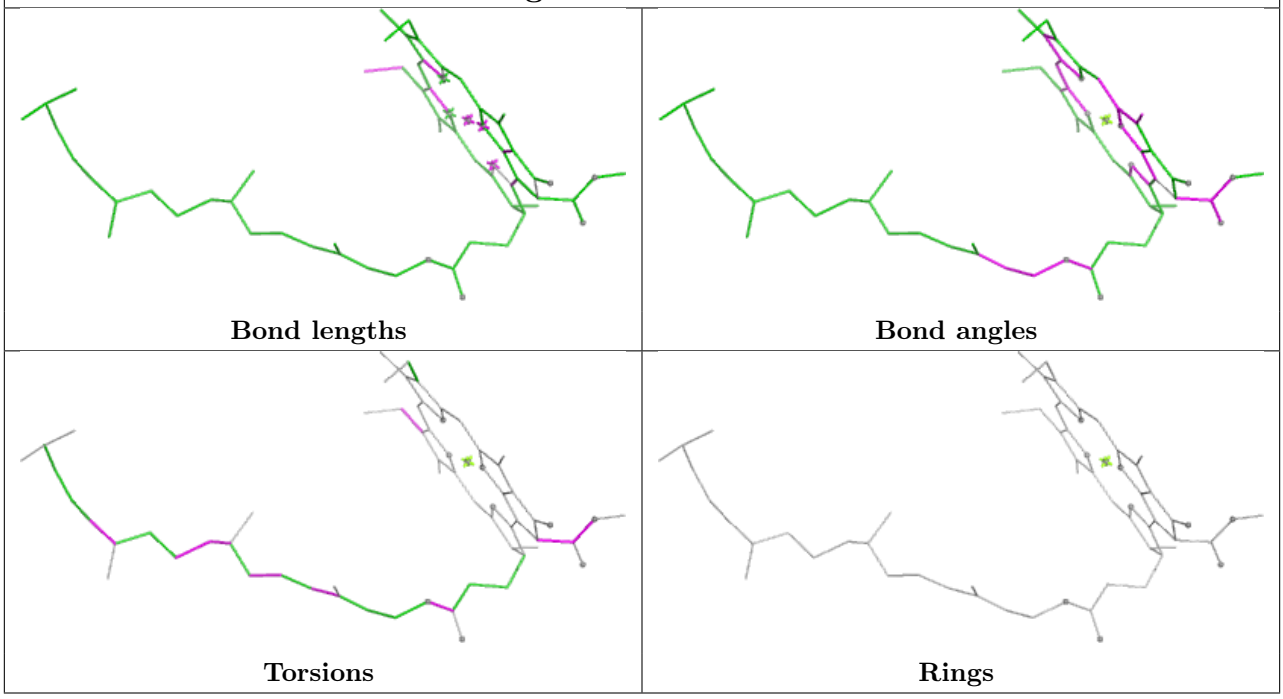


Torsions

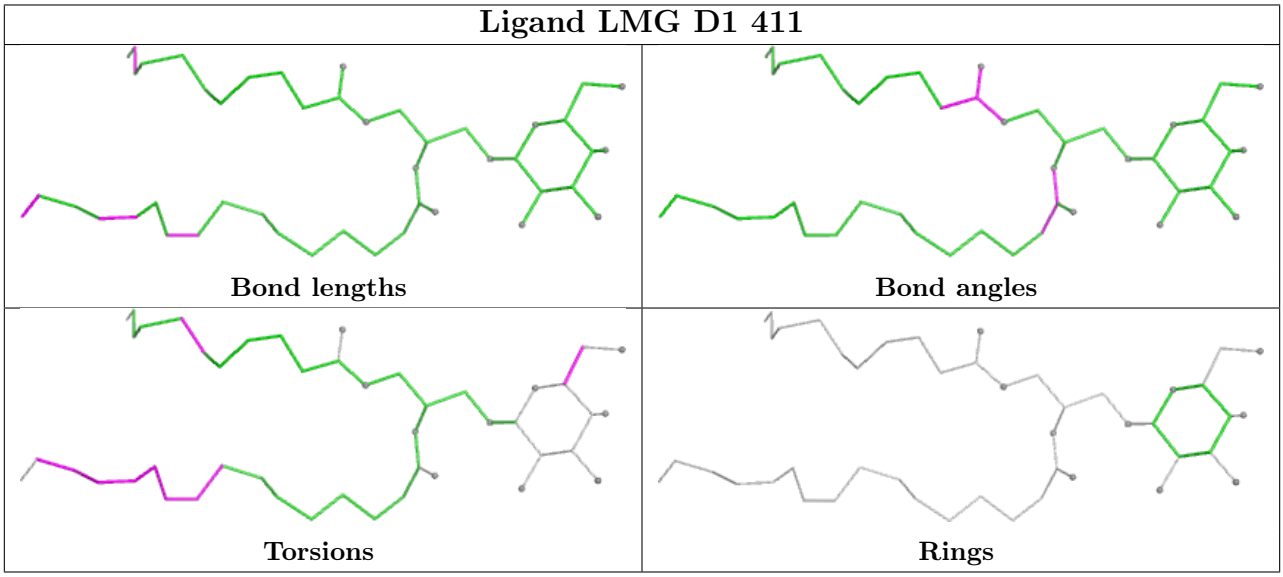


Rings

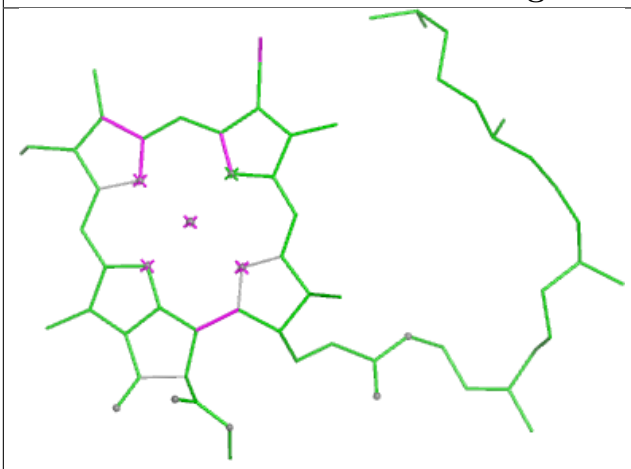
Ligand CLA C 504



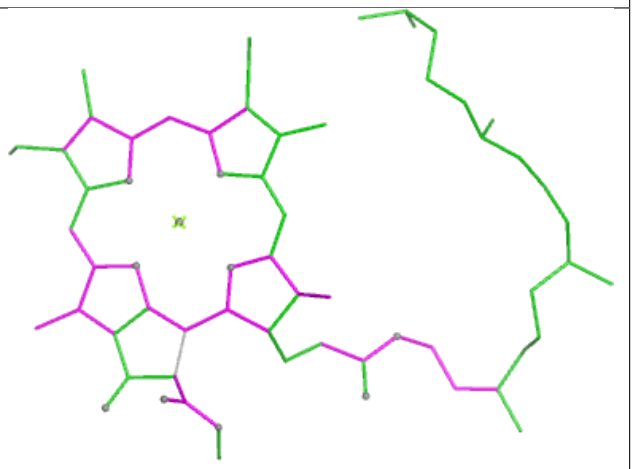
Ligand LMG D1 411



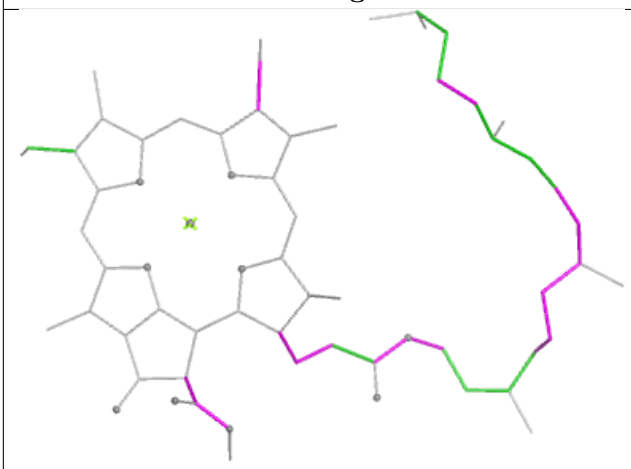
Ligand CLA S 603



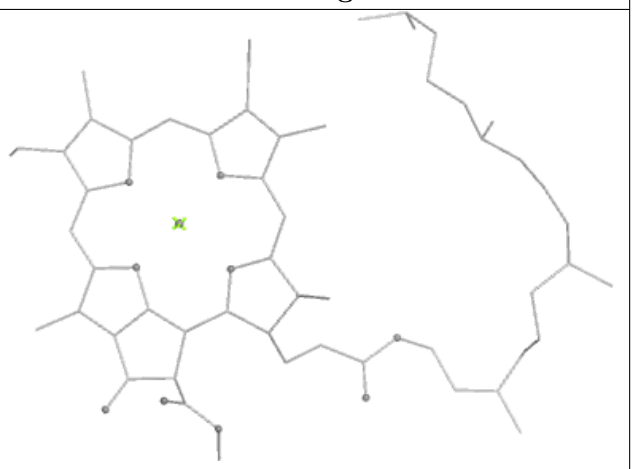
Bond lengths



Bond angles

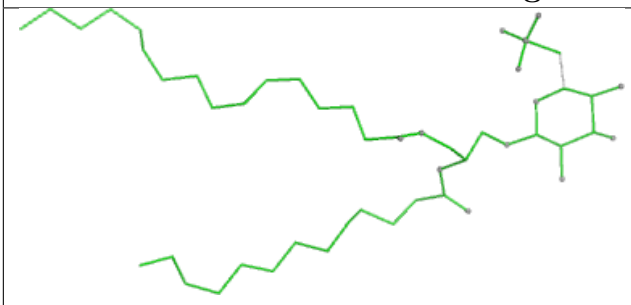


Torsions

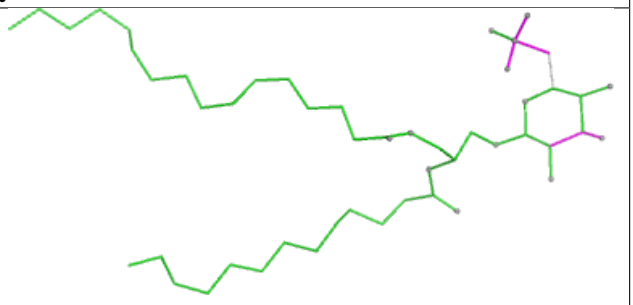


Rings

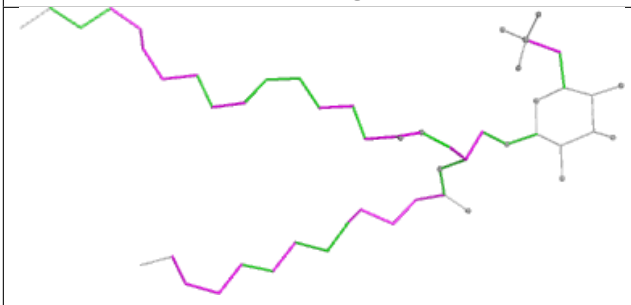
Ligand SQD A 412



Bond lengths



Bond angles

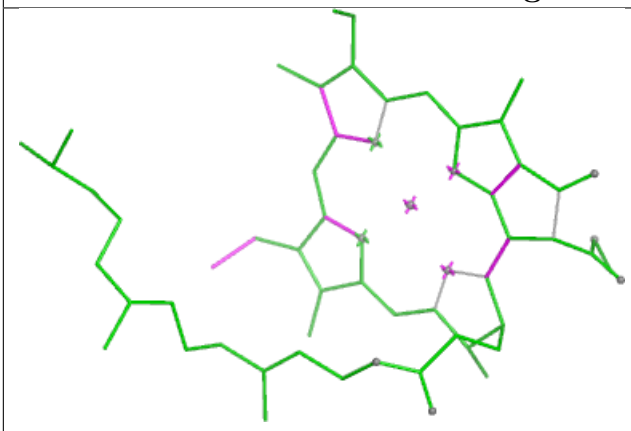


Torsions

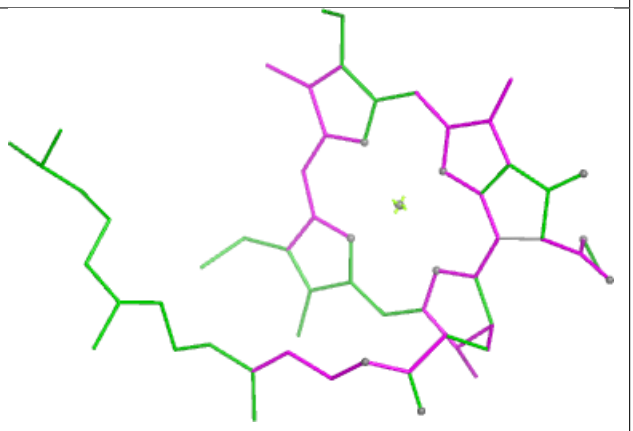


Rings

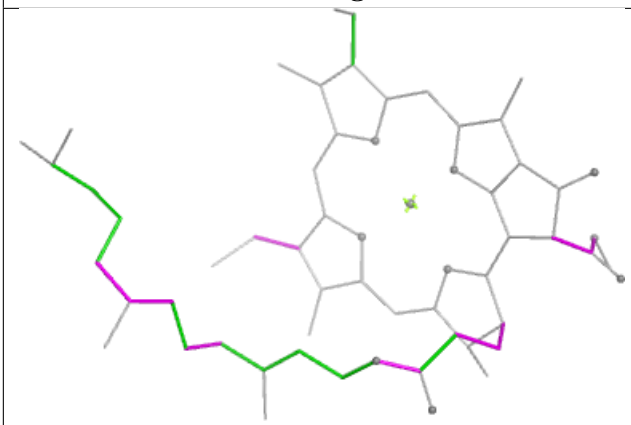
Ligand CLA R 602



Bond lengths



Bond angles

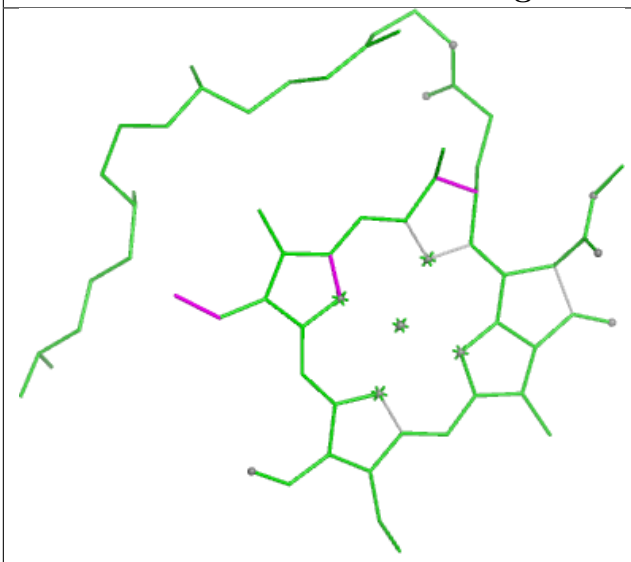


Torsions

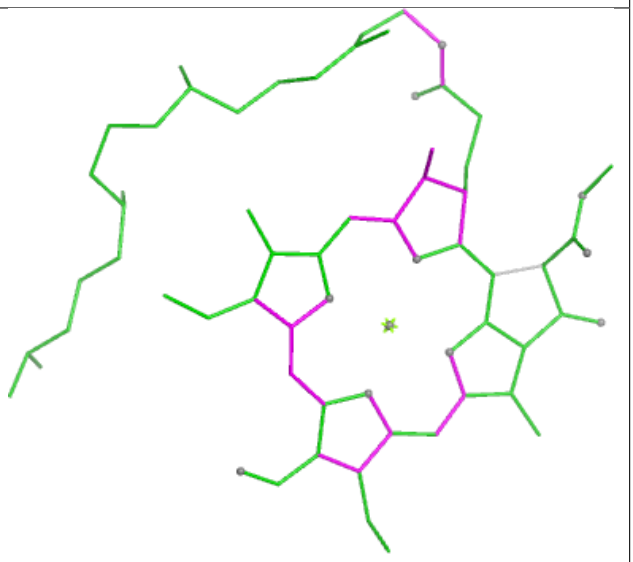


Rings

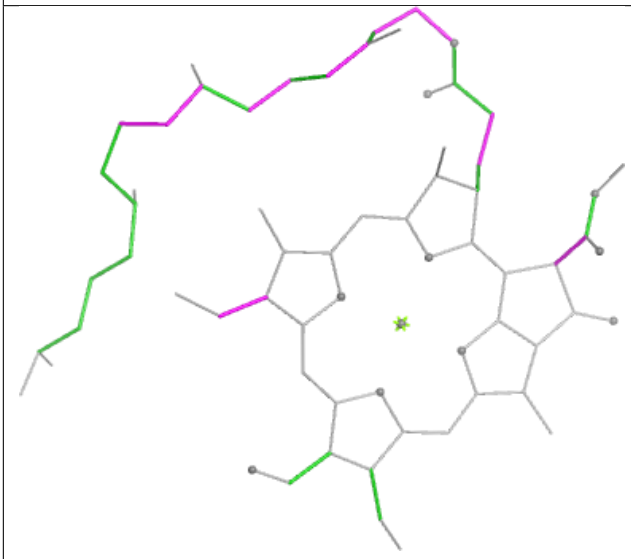
Ligand CHL Y1 607



Bond lengths



Bond angles

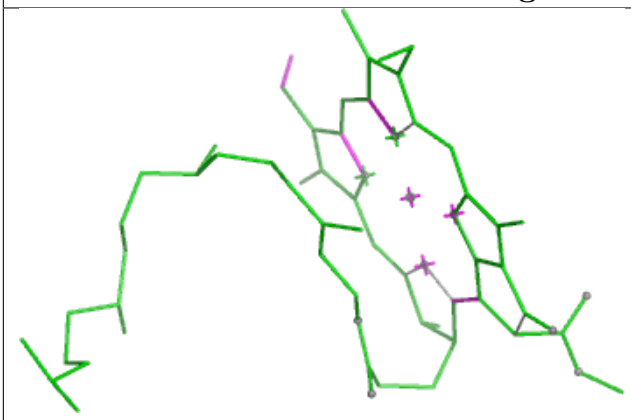


Torsions

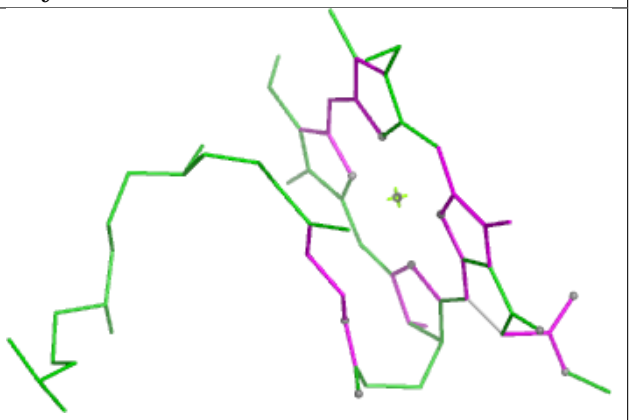


Rings

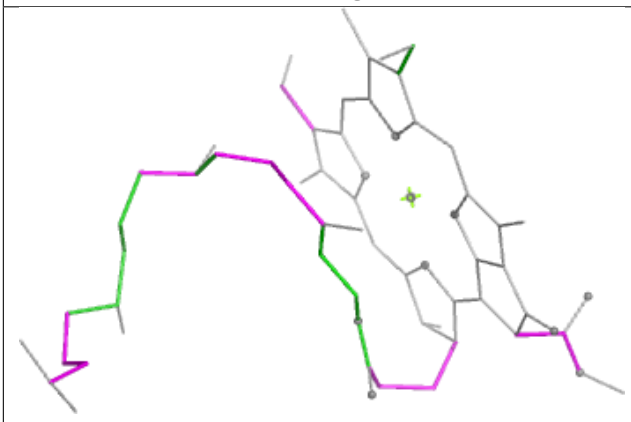
Ligand CLA y1 613



Bond lengths



Bond angles

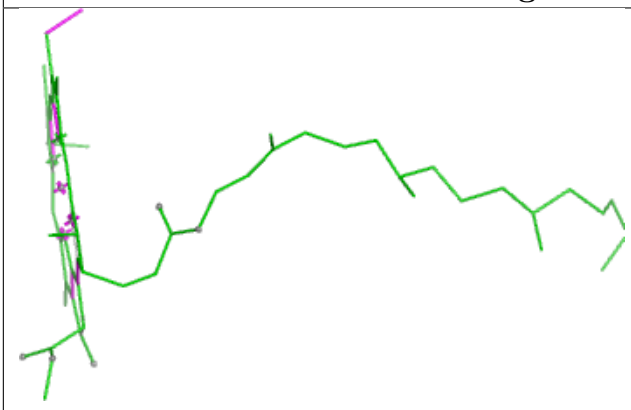


Torsions

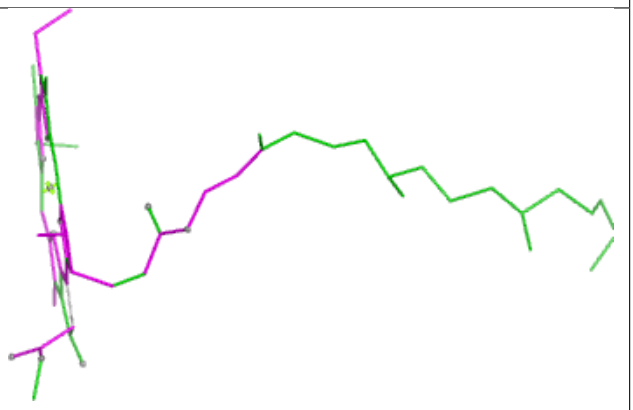


Rings

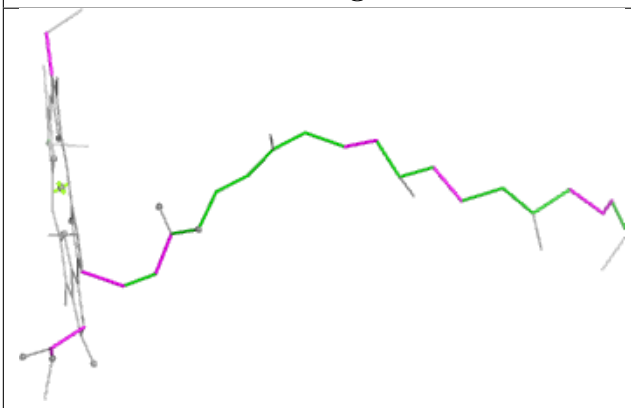
Ligand CLA b1 607



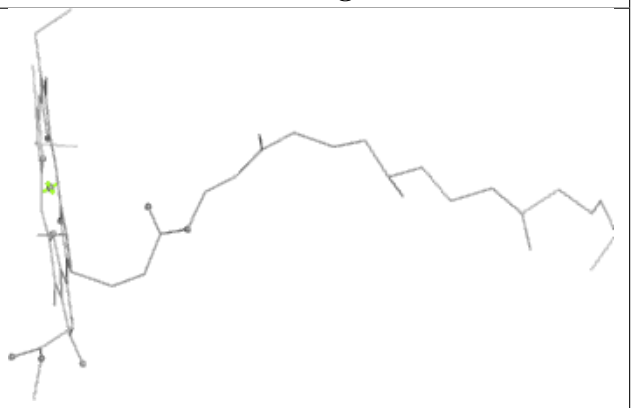
Bond lengths



Bond angles

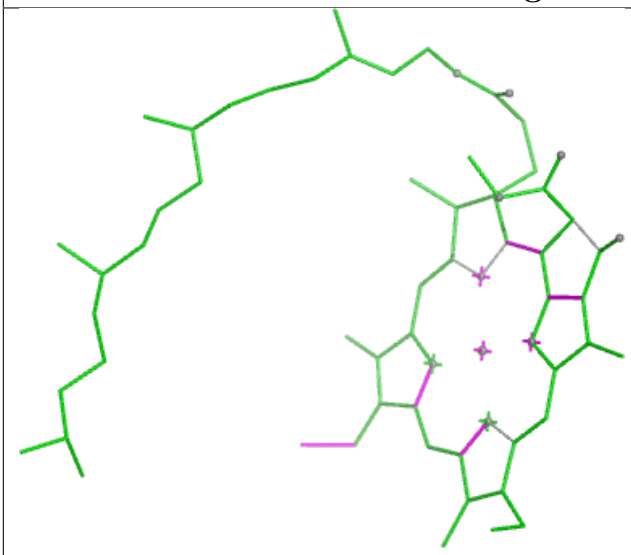


Torsions

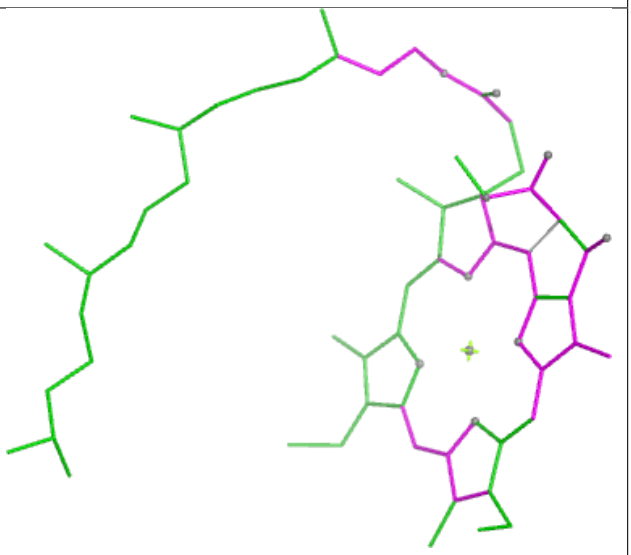


Rings

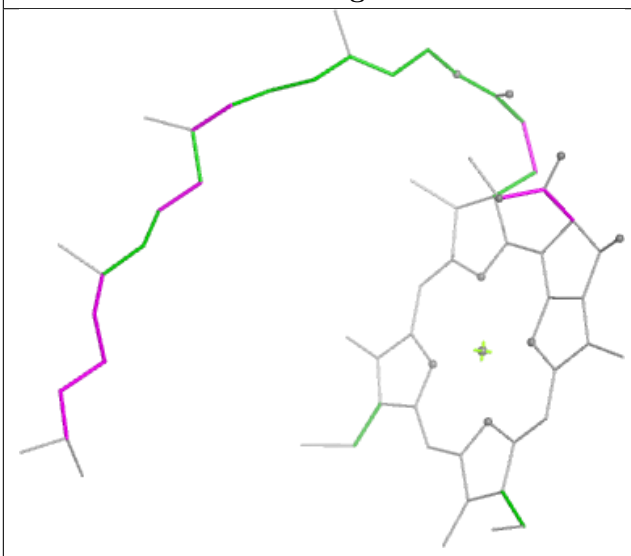
Ligand CLA C 507



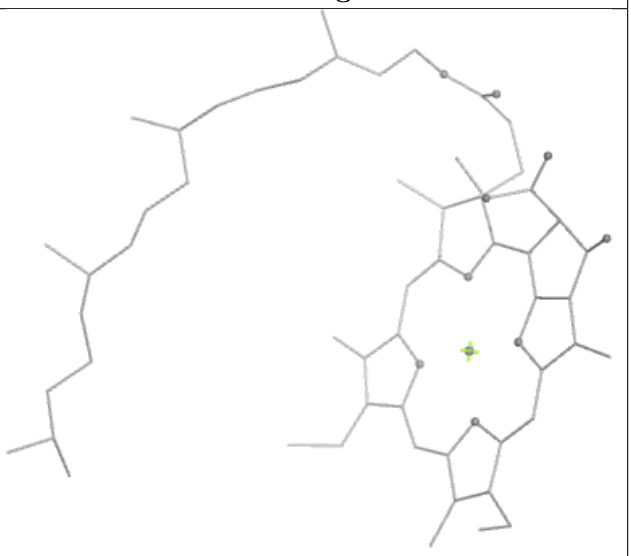
Bond lengths



Bond angles

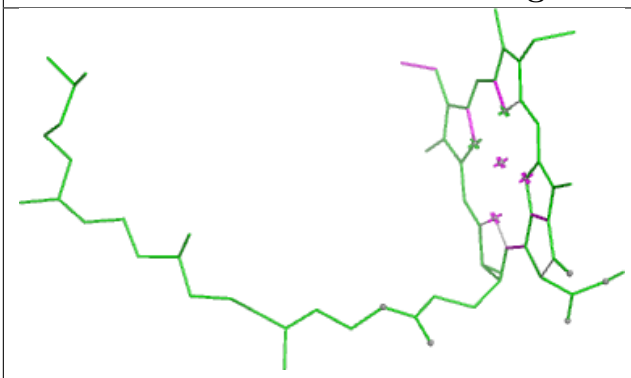


Torsions

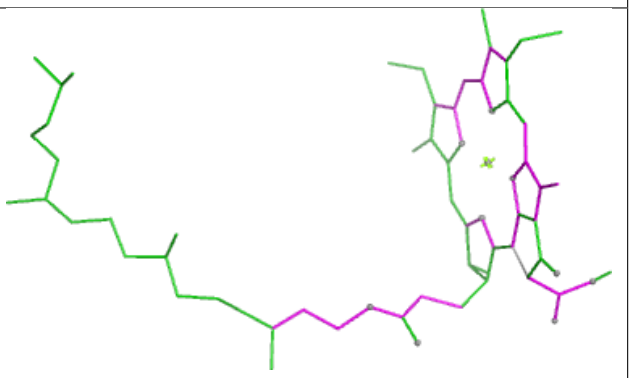


Rings

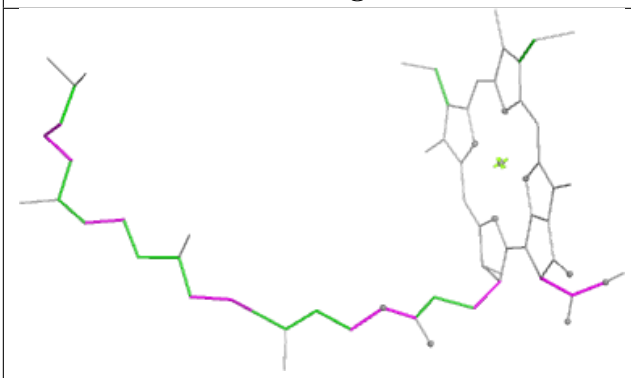
Ligand CLA b 610



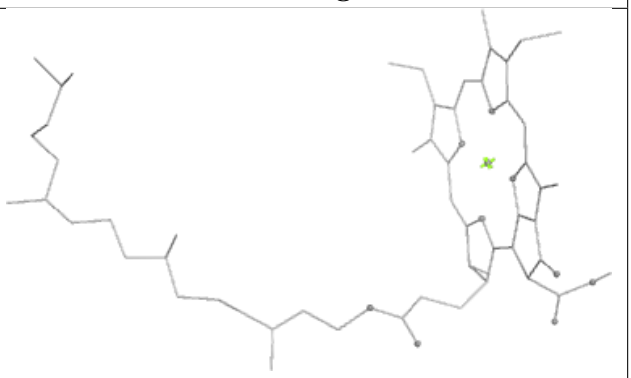
Bond lengths



Bond angles

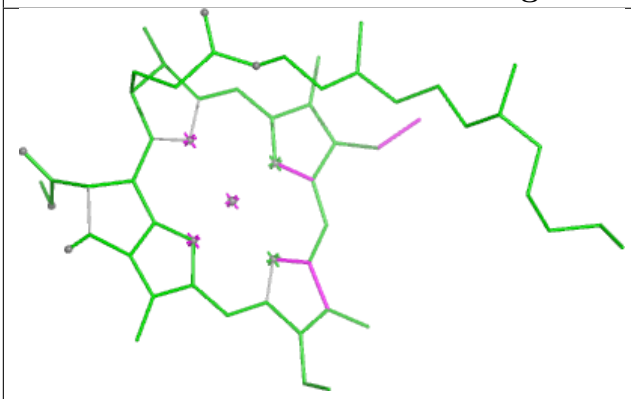


Torsions

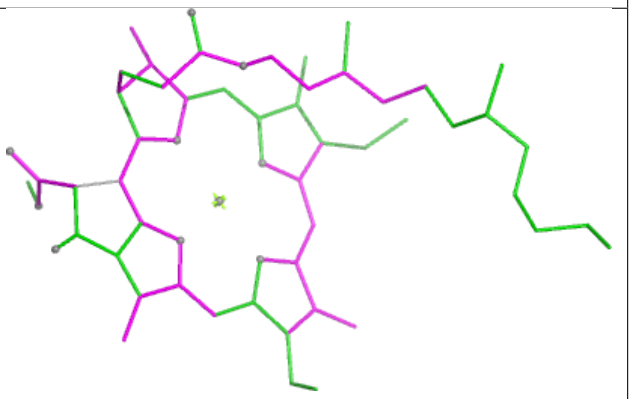


Rings

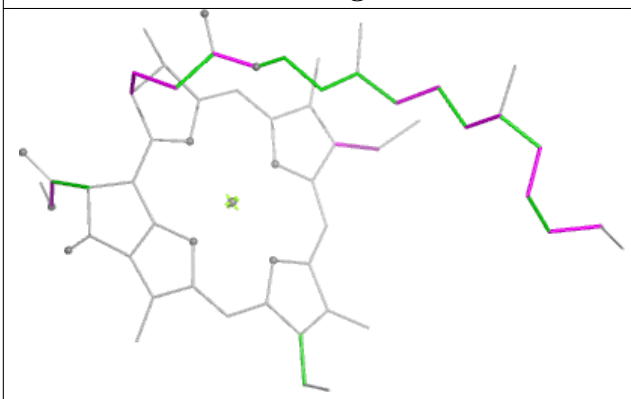
Ligand CLA r1 602



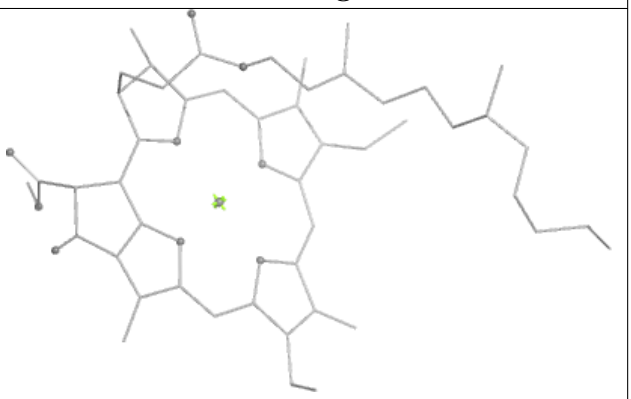
Bond lengths



Bond angles

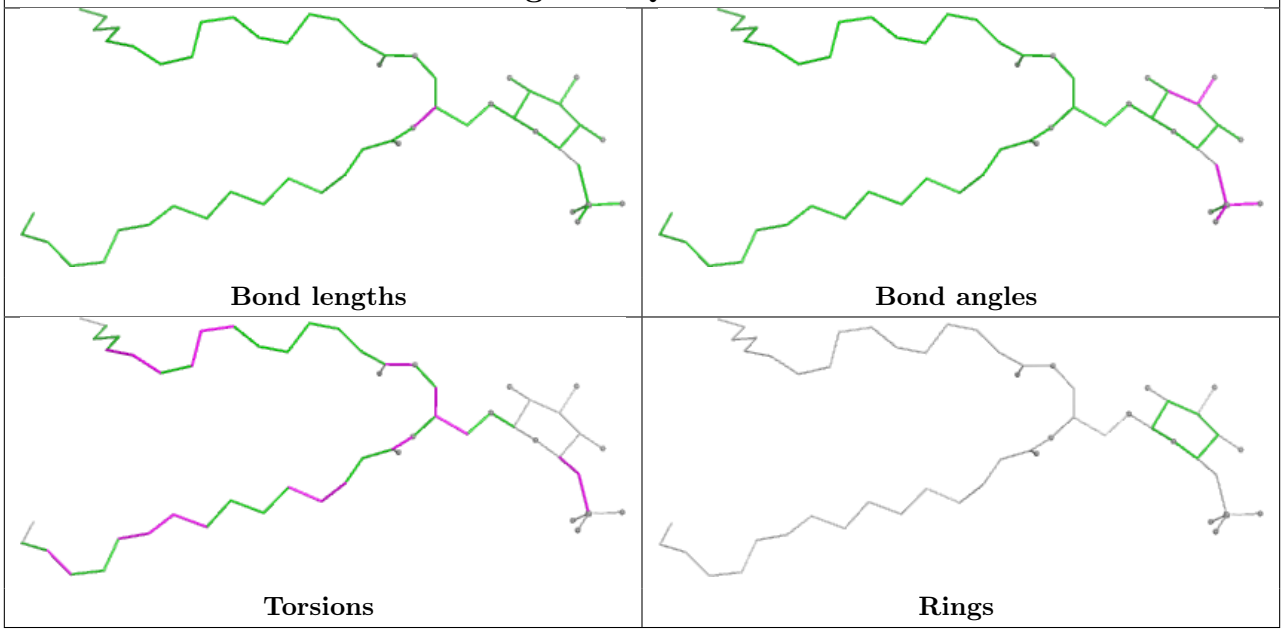


Torsions

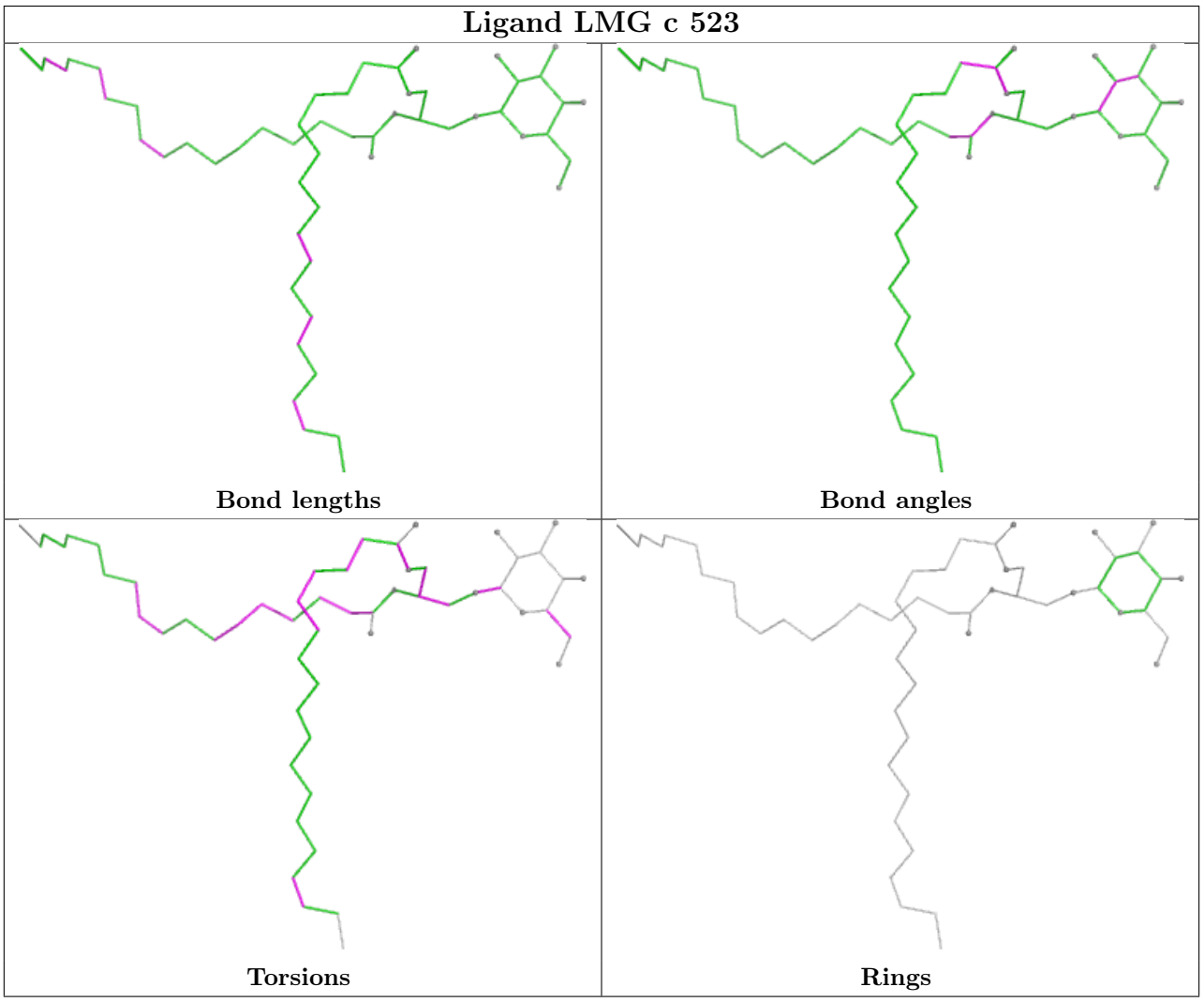


Rings

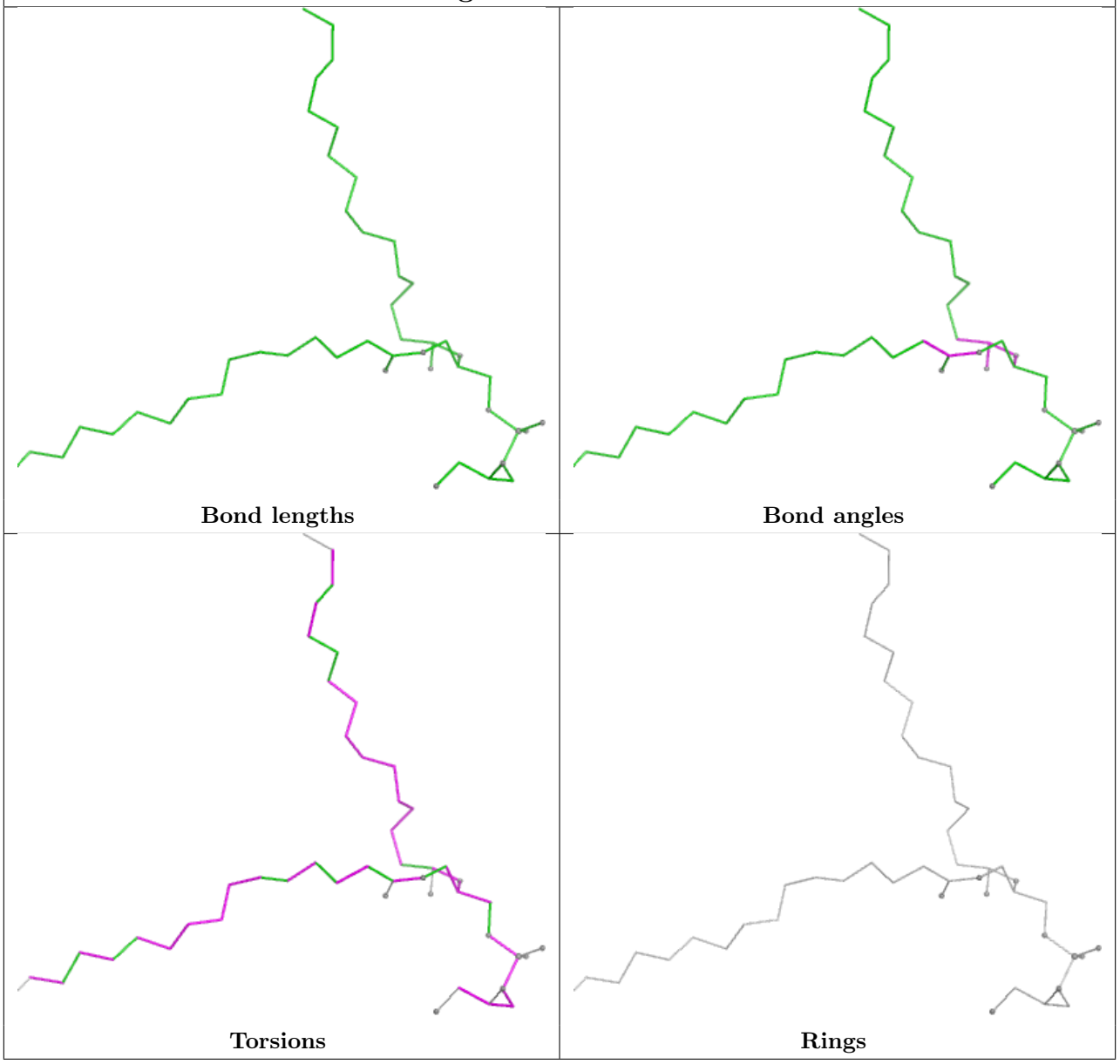
Ligand SQD C 526



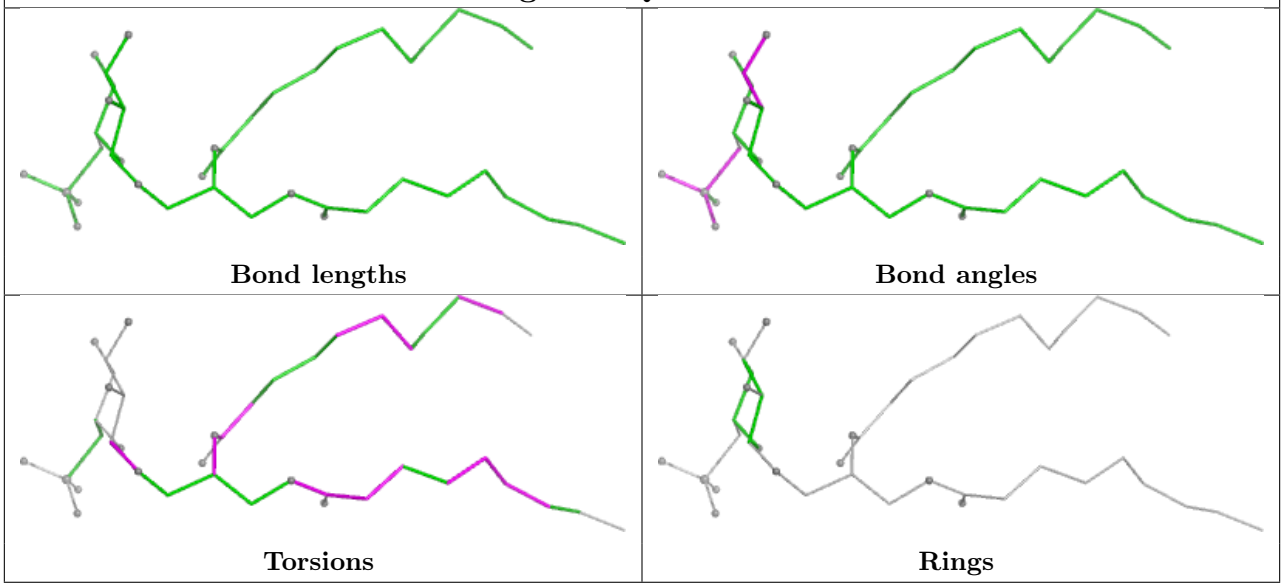
Ligand LMG c 523



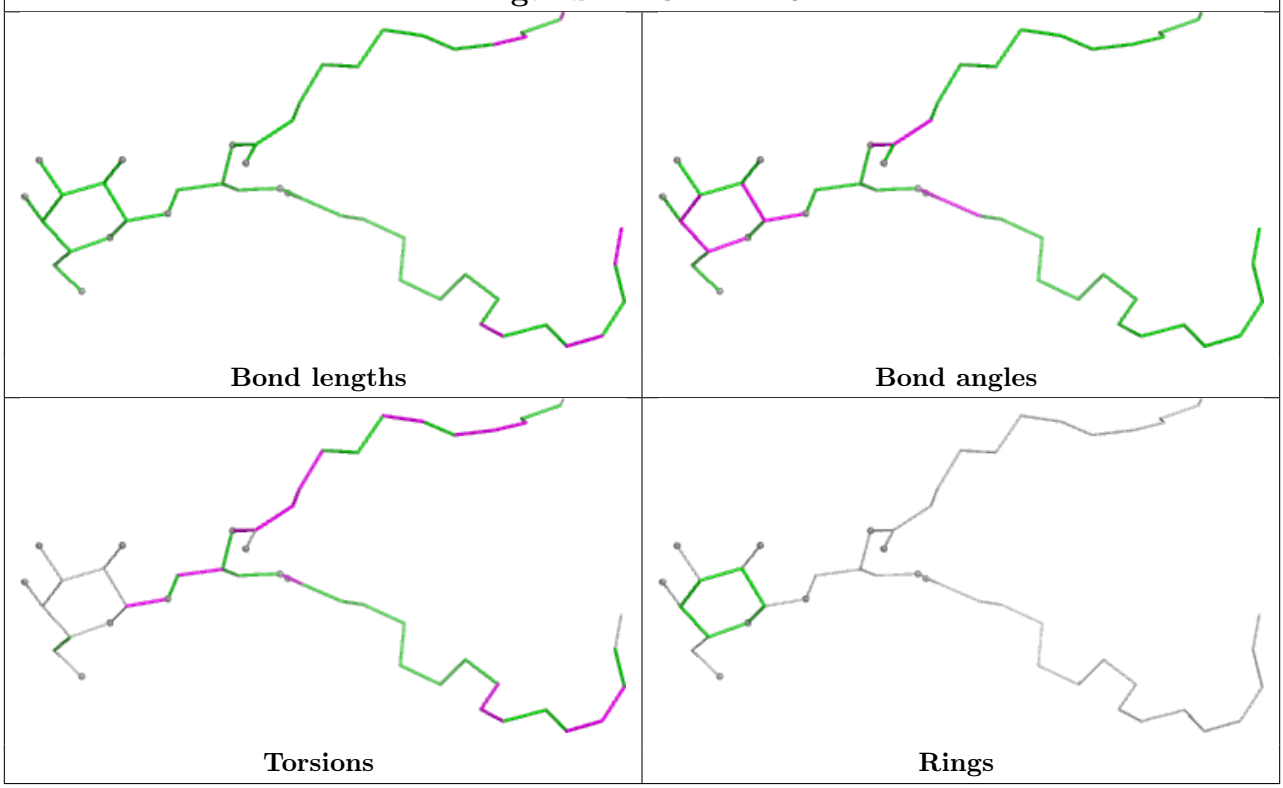
Ligand LHG L 101



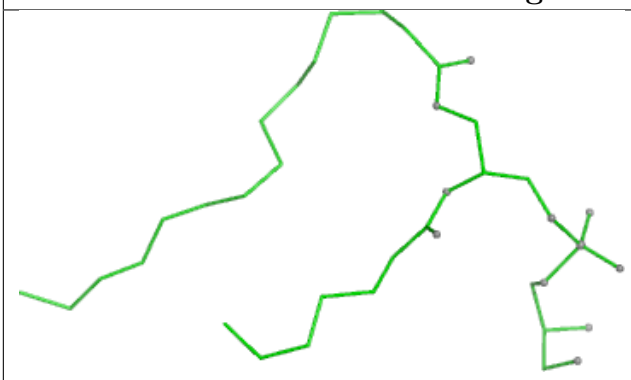
Ligand SQD b1 621



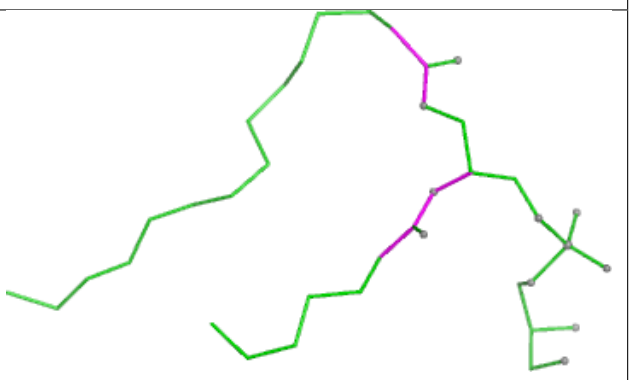
Ligand LMG A1 413



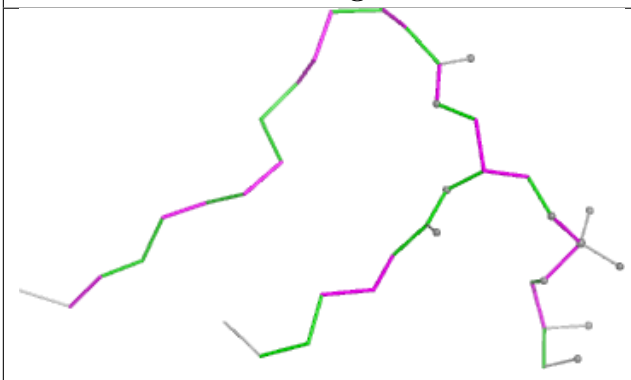
Ligand LHG d 410



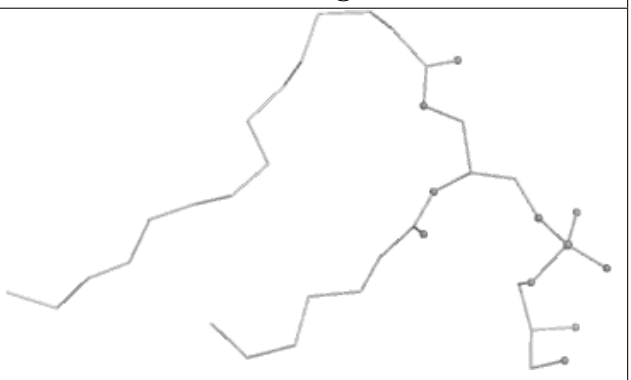
Bond lengths



Bond angles

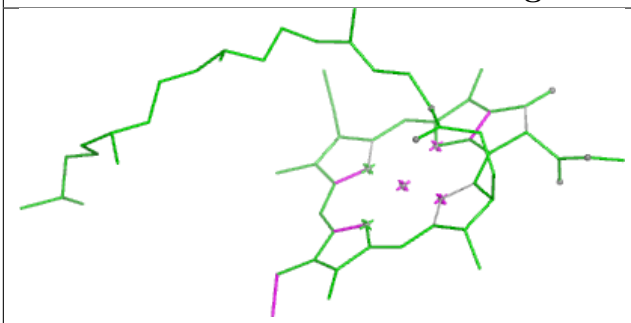


Torsions

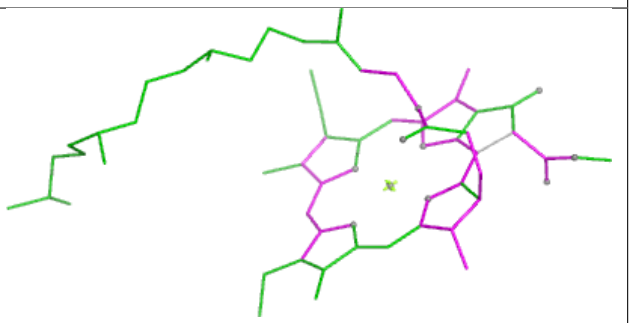


Rings

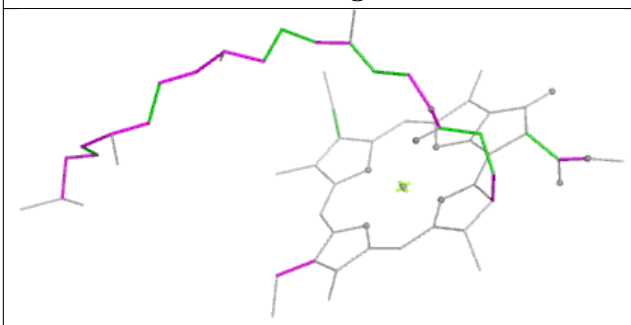
Ligand CLA C 513



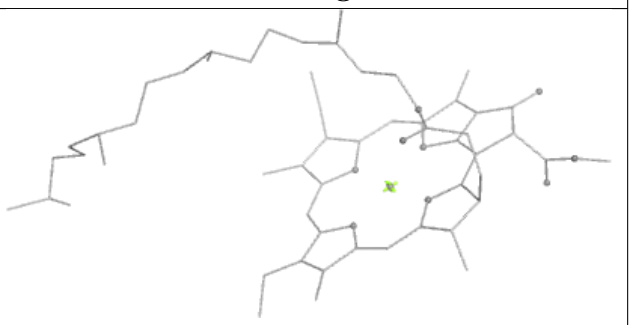
Bond lengths



Bond angles

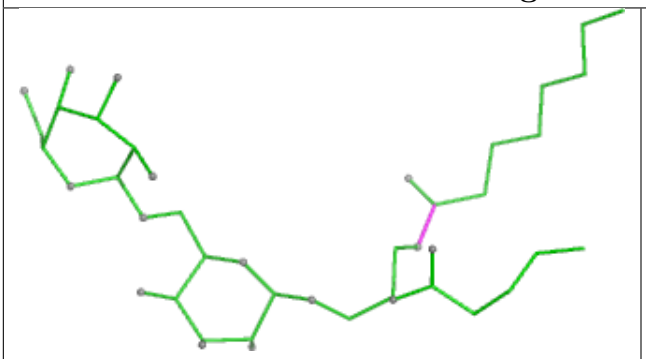


Torsions

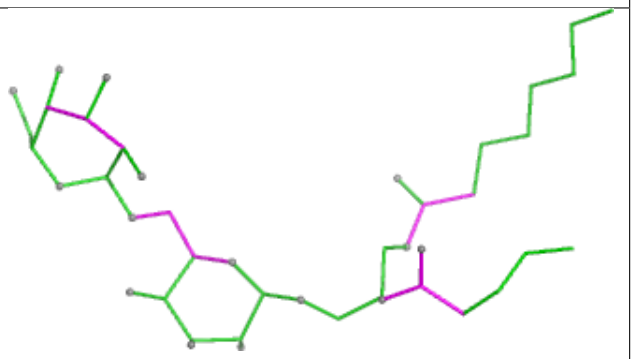


Rings

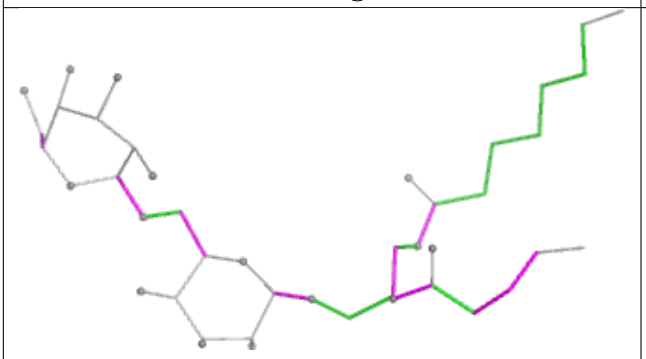
Ligand DGD B 623



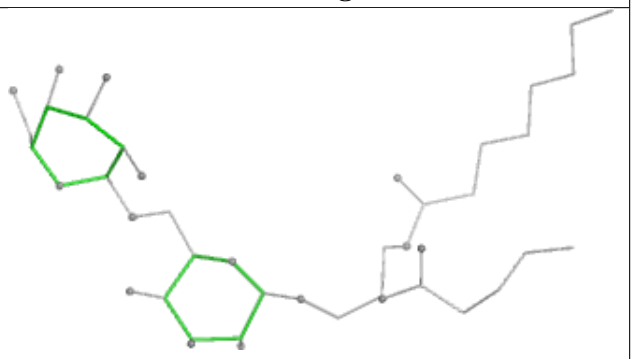
Bond lengths



Bond angles

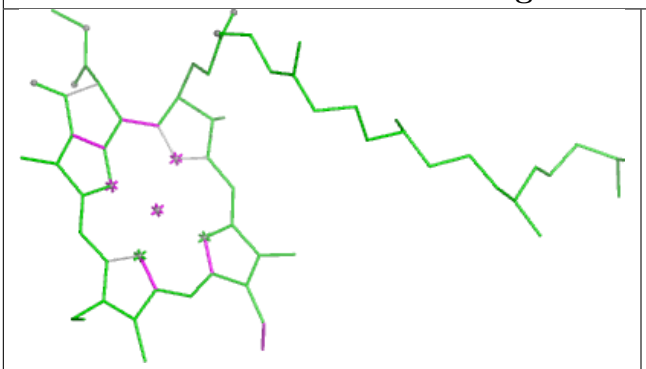


Torsions

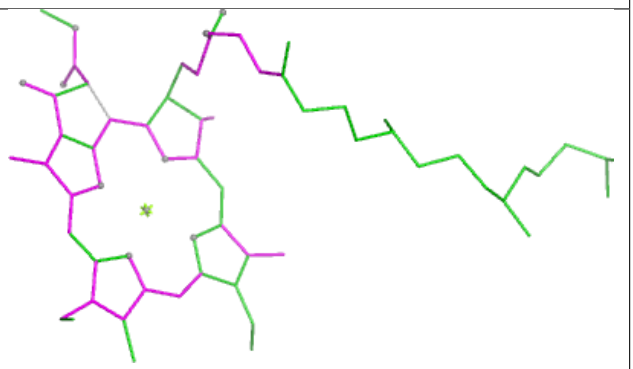


Rings

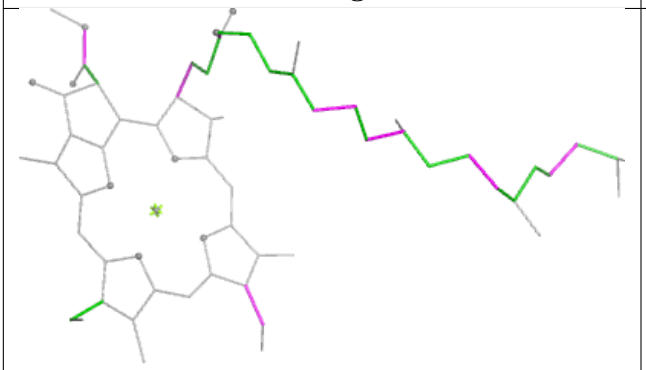
Ligand CLA C1 511



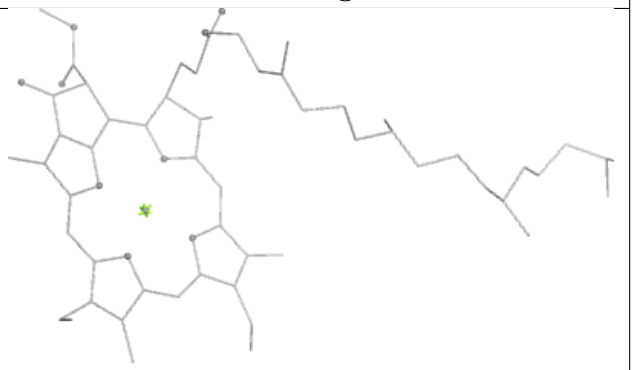
Bond lengths



Bond angles

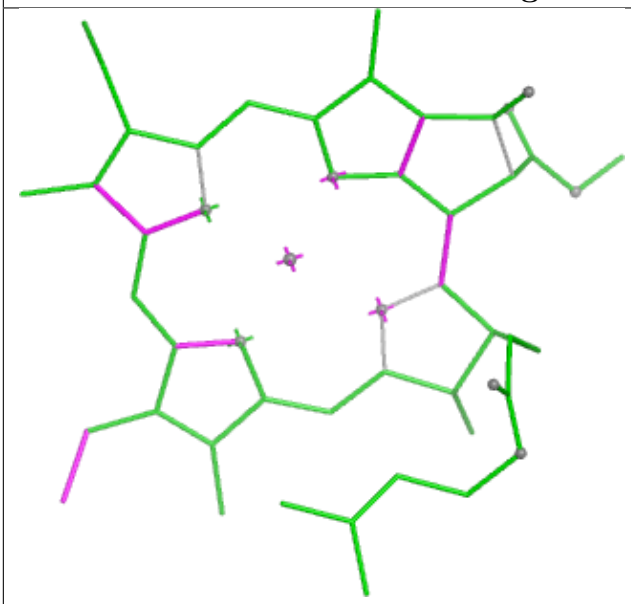


Torsions

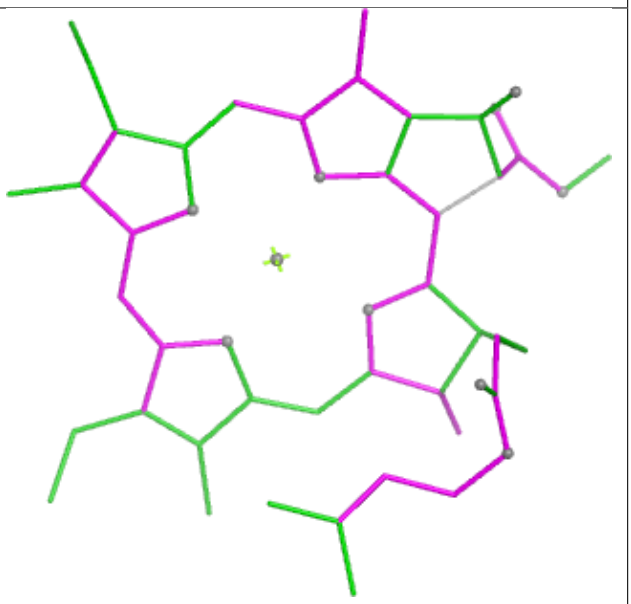


Rings

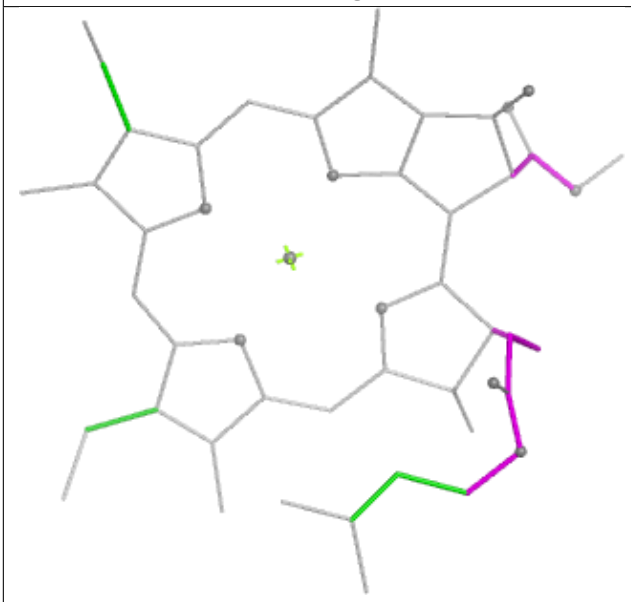
Ligand CLA s1 617



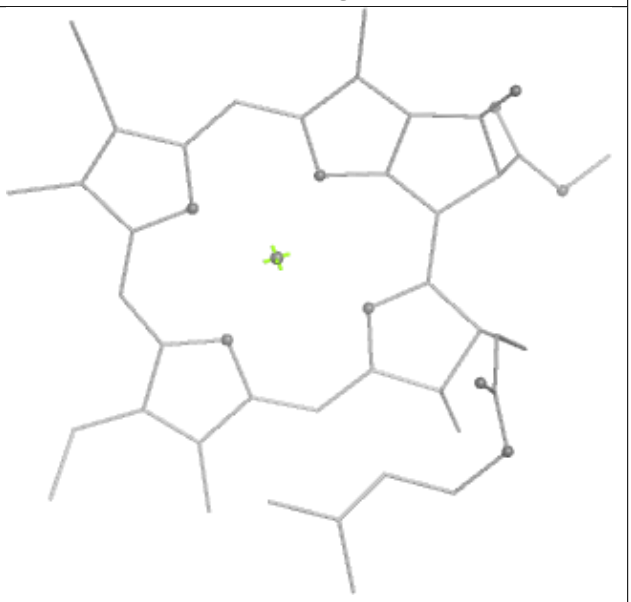
Bond lengths



Bond angles

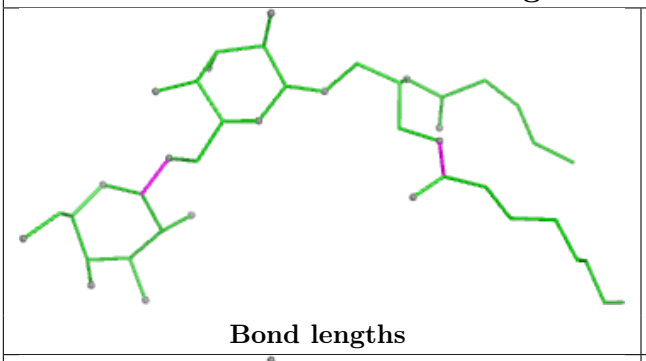


Torsions

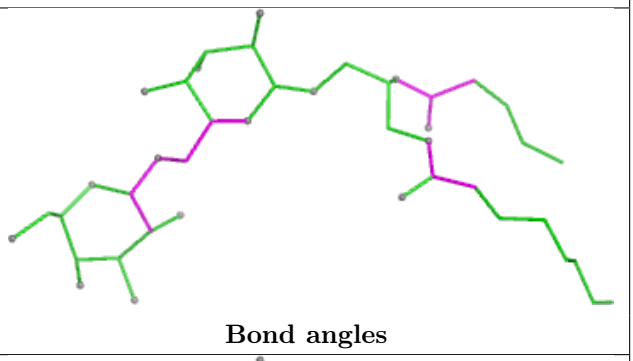


Rings

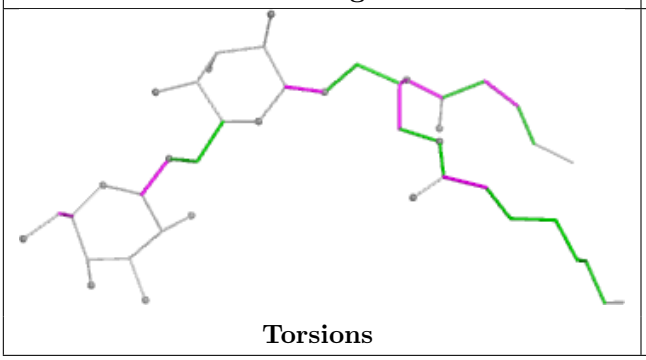
Ligand DGD b 623



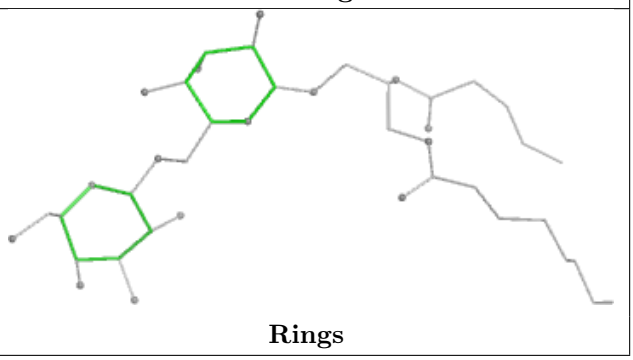
Bond lengths



Bond angles

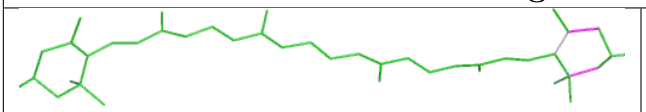


Torsions

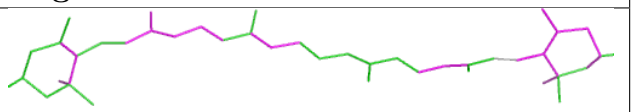


Rings

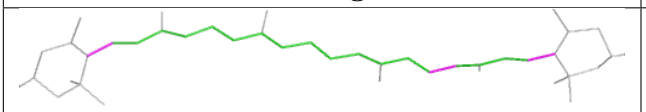
Ligand LUT g 621



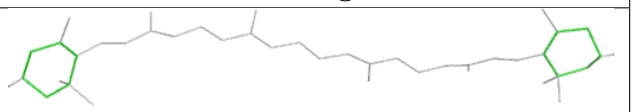
Bond lengths



Bond angles

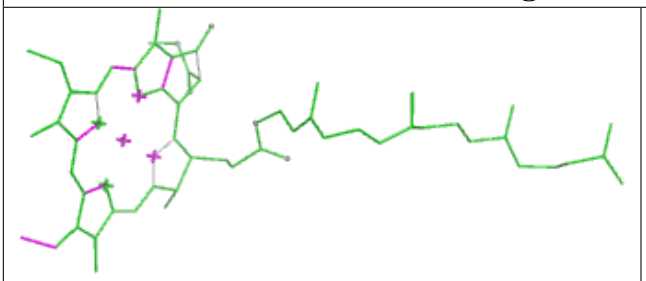


Torsions

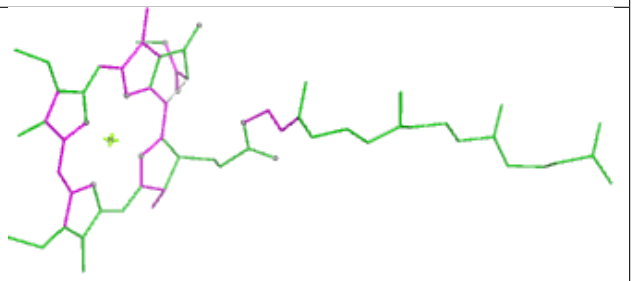


Rings

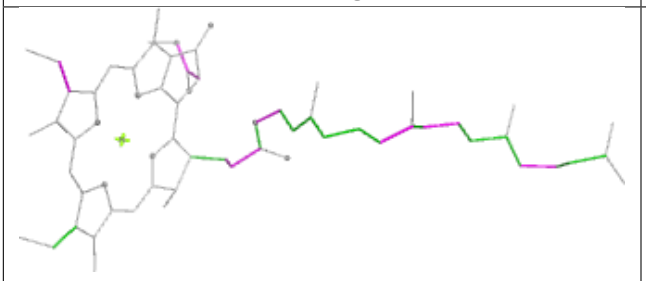
Ligand CLA c1 502



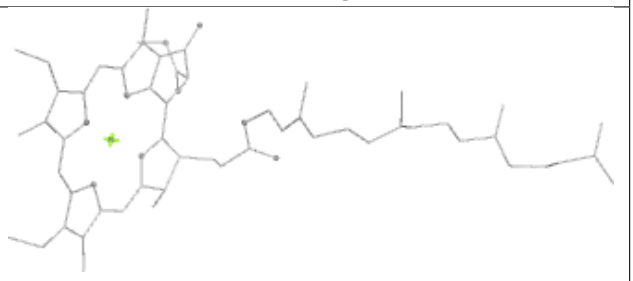
Bond lengths



Bond angles

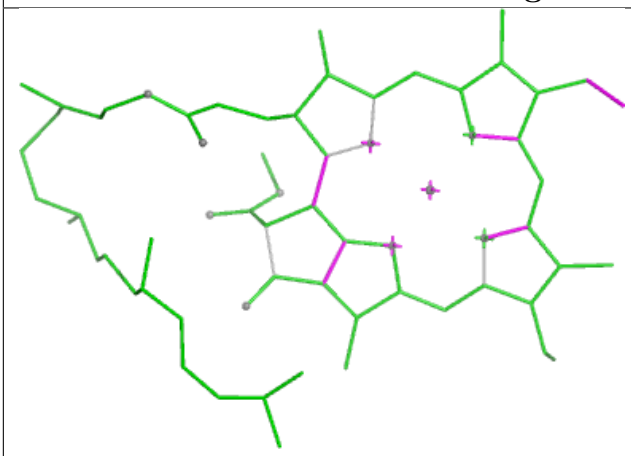


Torsions

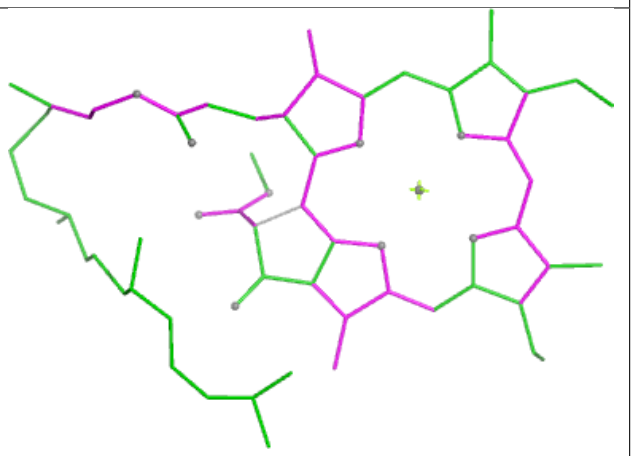


Rings

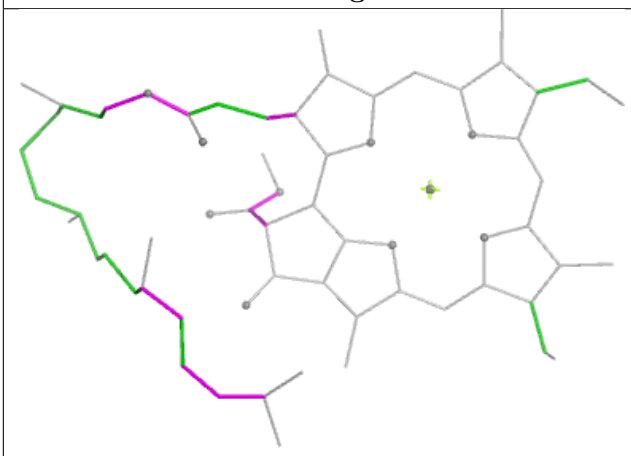
Ligand CLA B 611



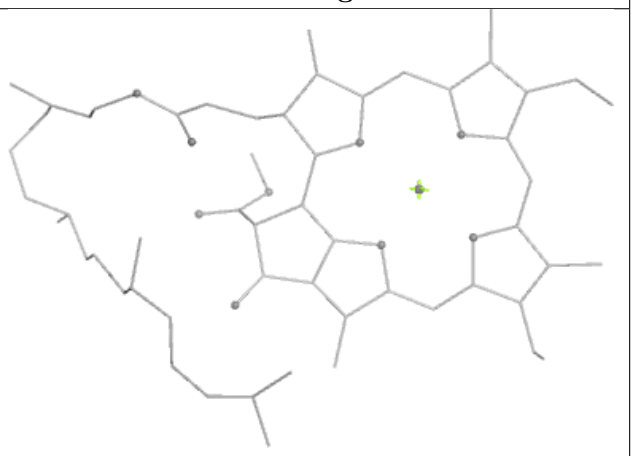
Bond lengths



Bond angles



Torsions

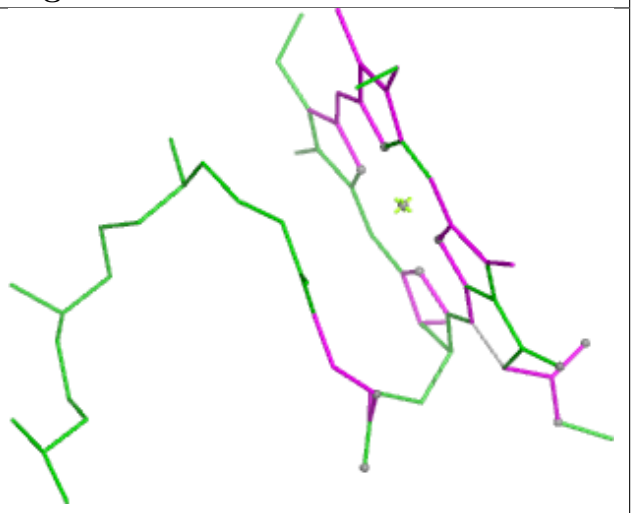


Rings

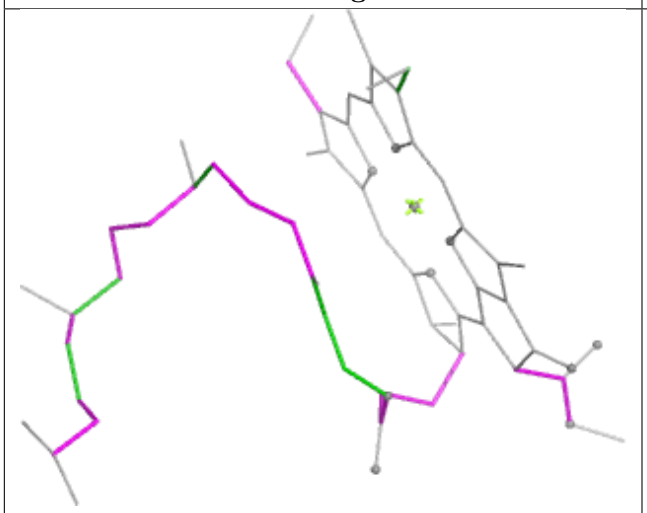
Ligand CLA g1 613



Bond lengths



Bond angles

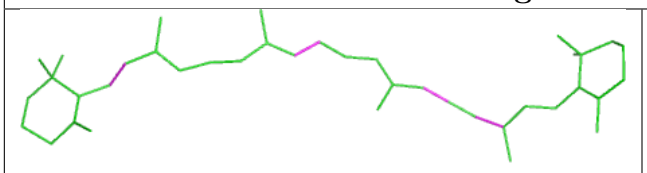


Torsions

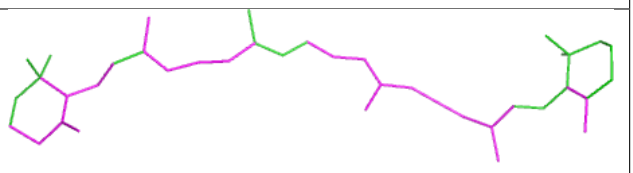


Rings

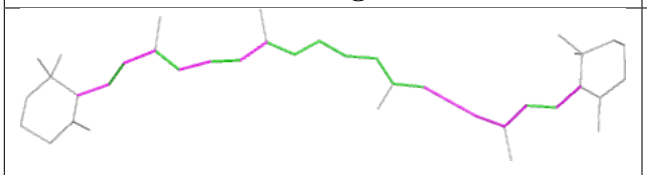
Ligand BCR C1 516



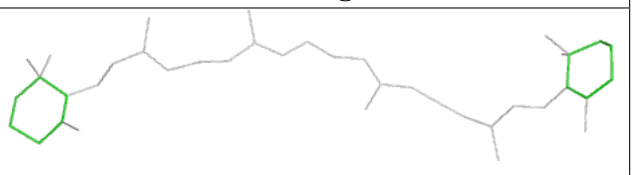
Bond lengths



Bond angles

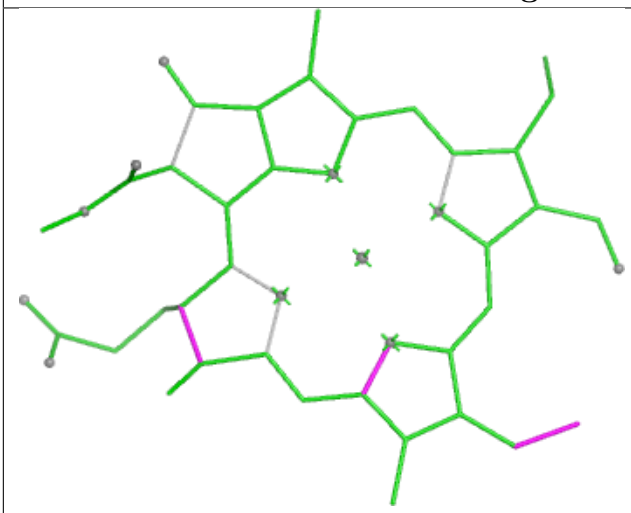


Torsions

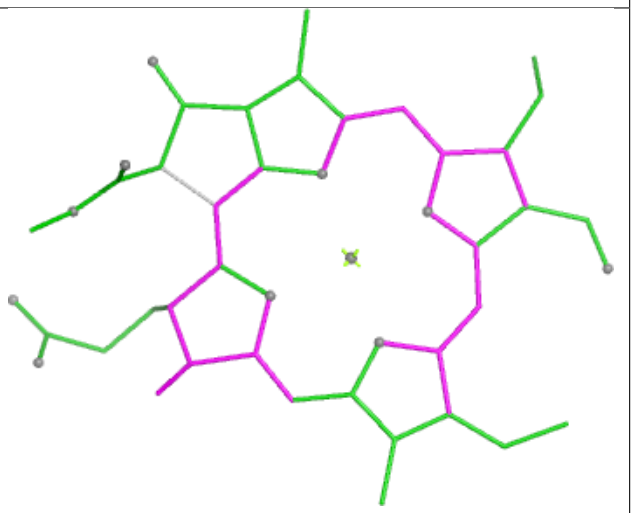


Rings

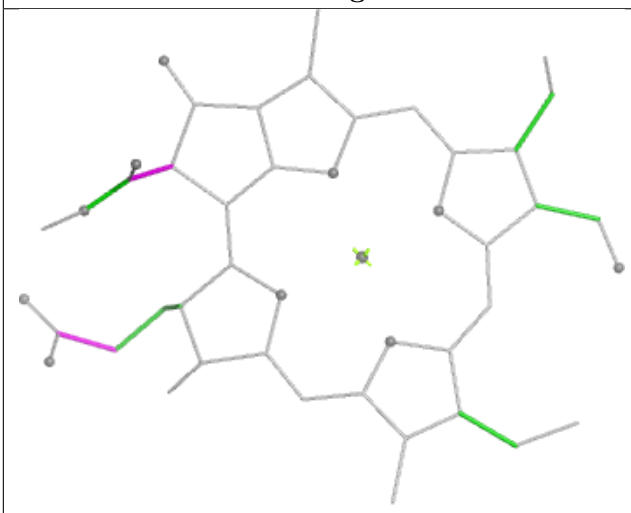
Ligand CHL s1 601



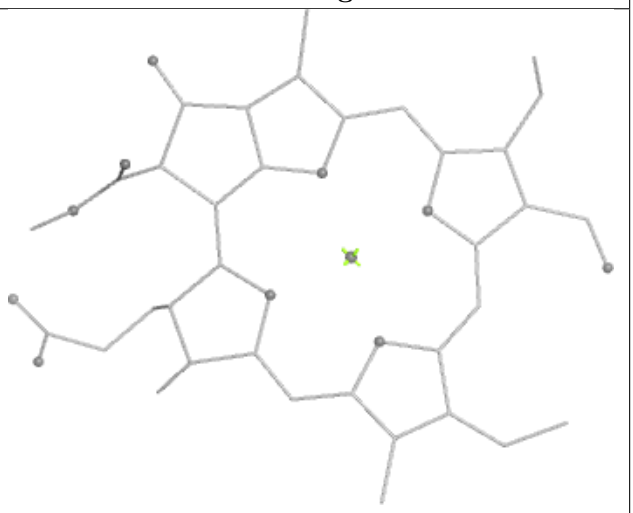
Bond lengths



Bond angles

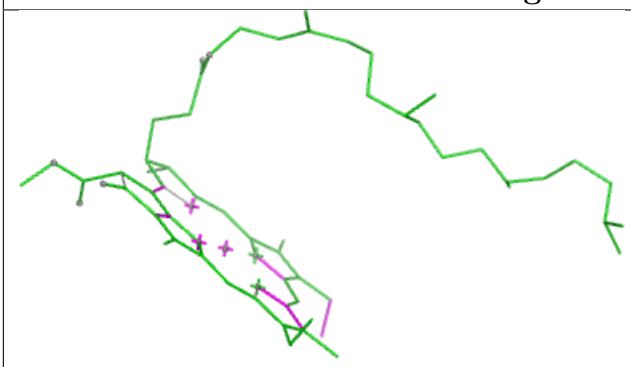


Torsions



Rings

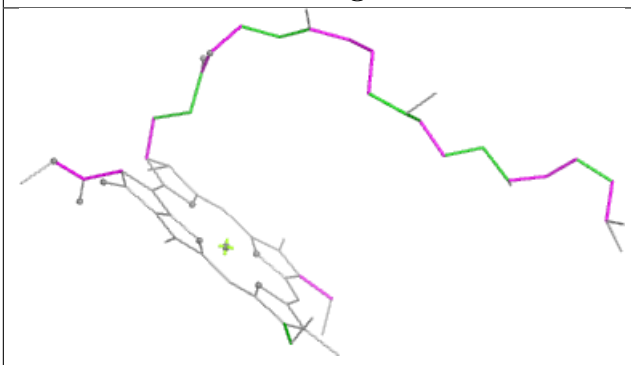
Ligand CLA Y 614



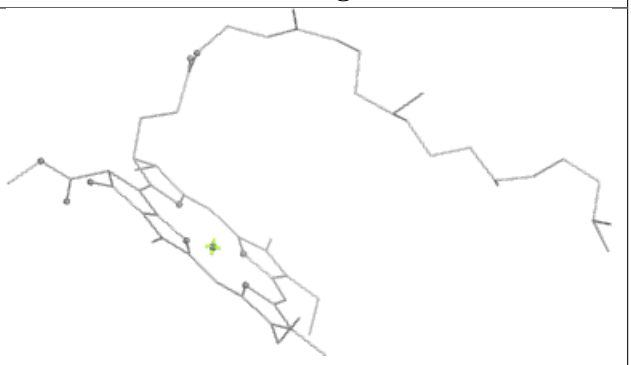
Bond lengths



Bond angles

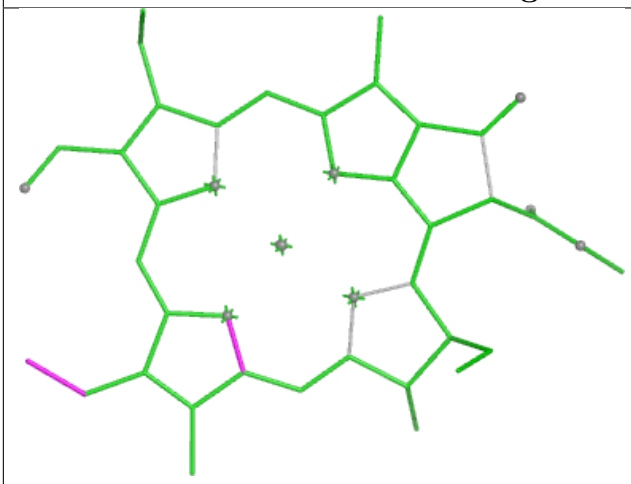


Torsions

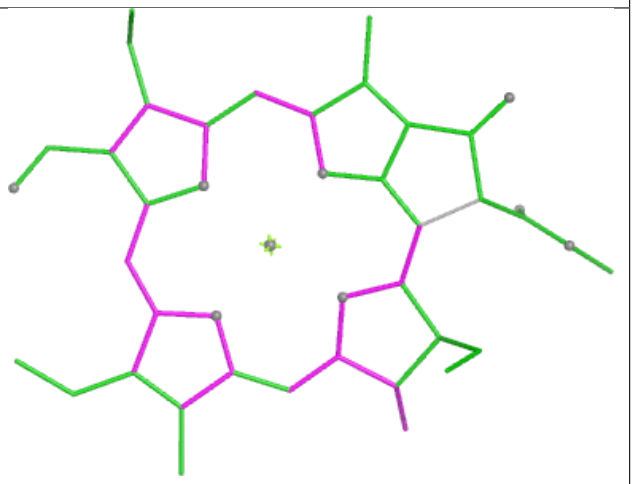


Rings

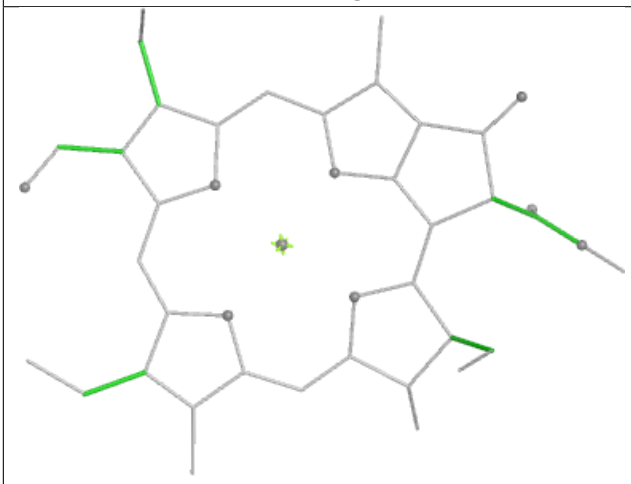
Ligand CHL s1 607



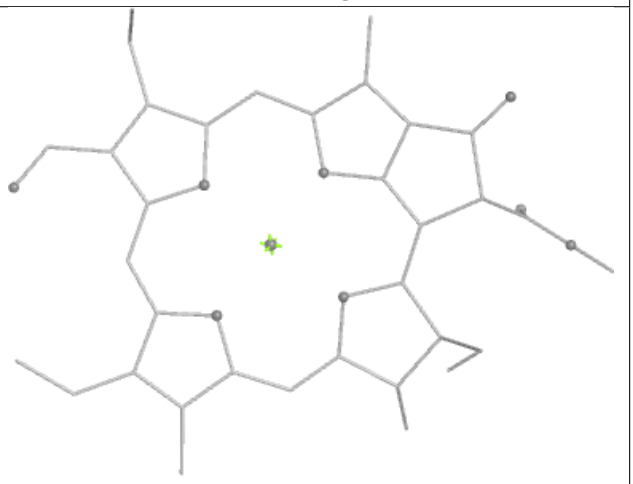
Bond lengths



Bond angles

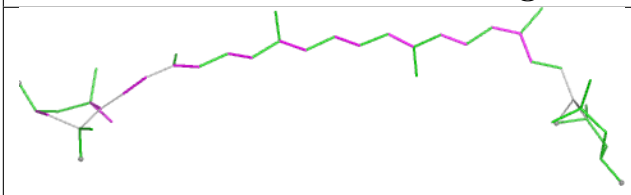


Torsions

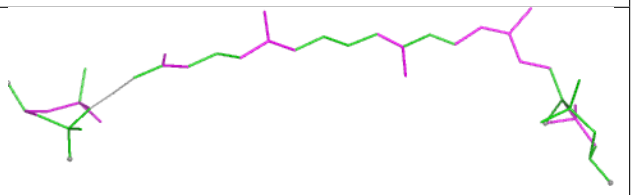


Rings

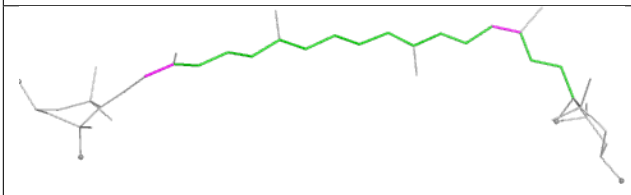
Ligand NEX s1 623



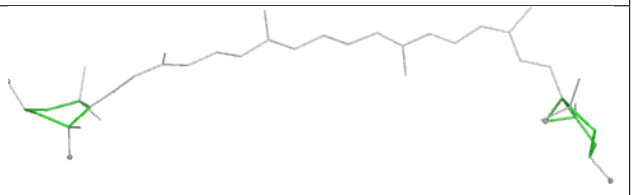
Bond lengths



Bond angles

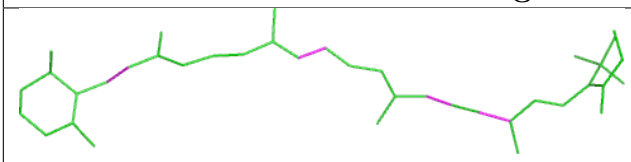


Torsions

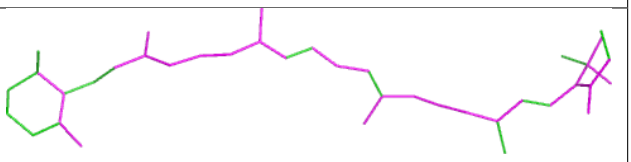


Rings

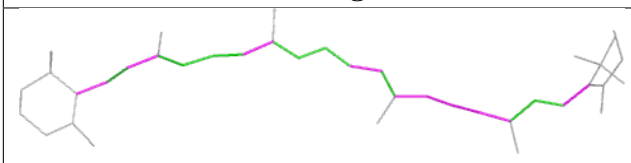
Ligand BCR B1 618



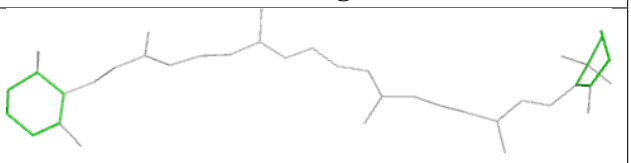
Bond lengths



Bond angles

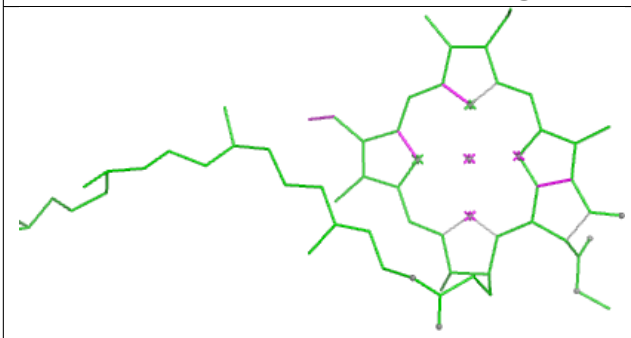


Torsions

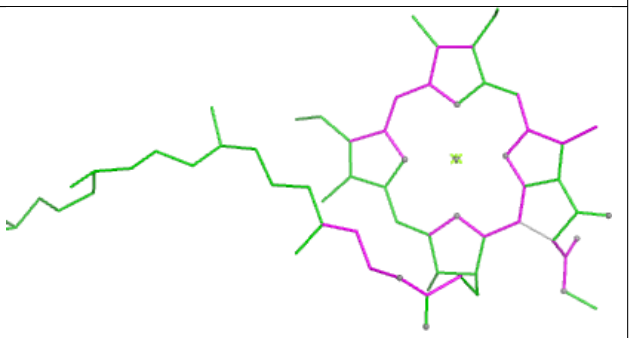


Rings

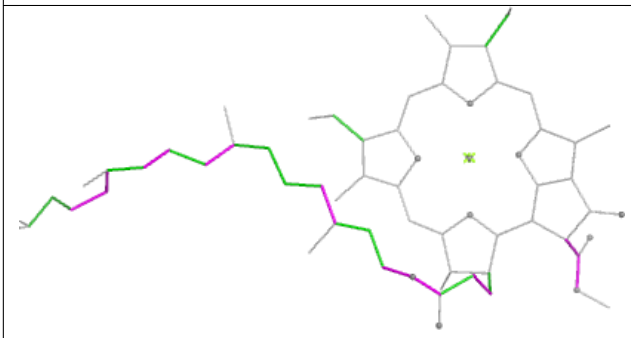
Ligand CLA B1 604



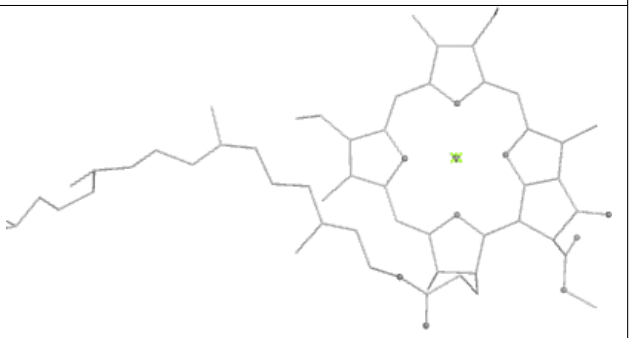
Bond lengths



Bond angles

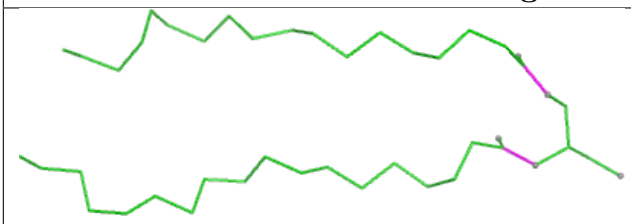


Torsions

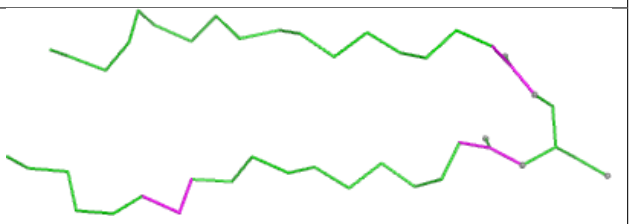


Rings

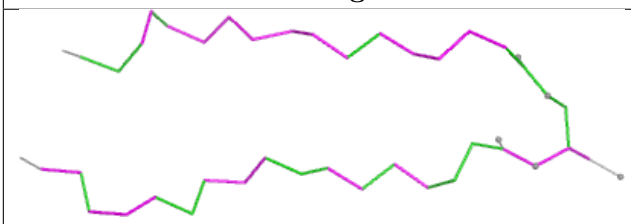
Ligand DGA B 625



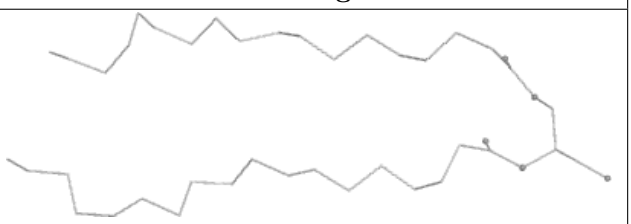
Bond lengths



Bond angles

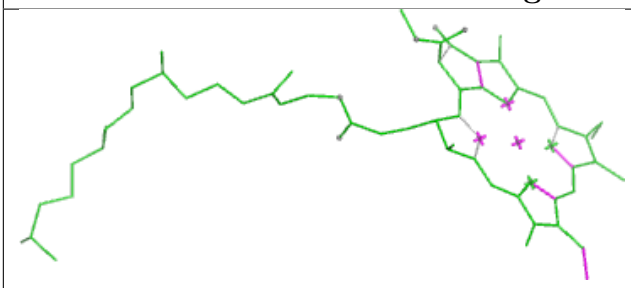


Torsions

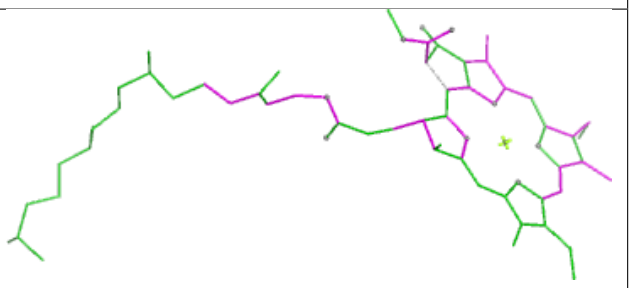


Rings

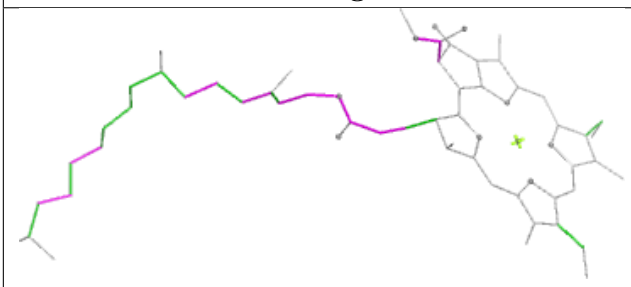
Ligand CLA A 405



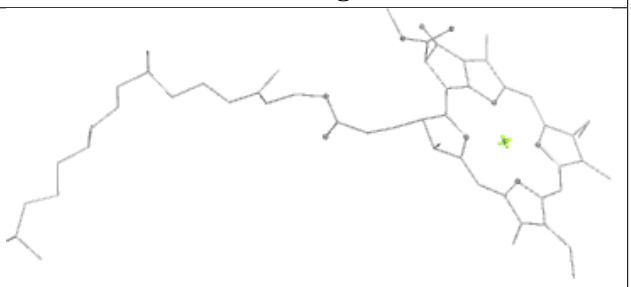
Bond lengths



Bond angles

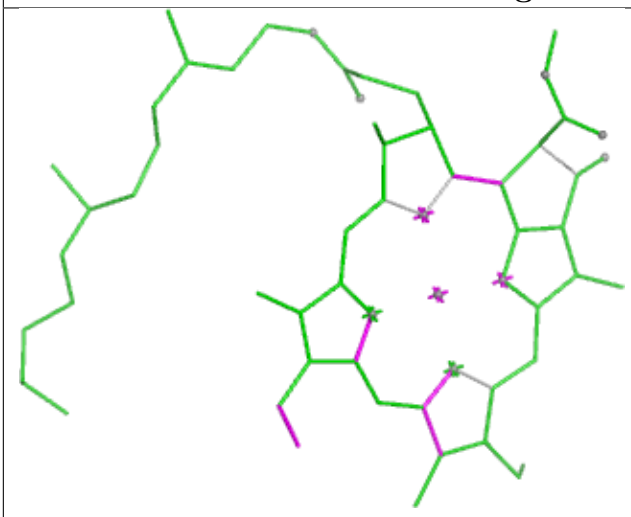


Torsions

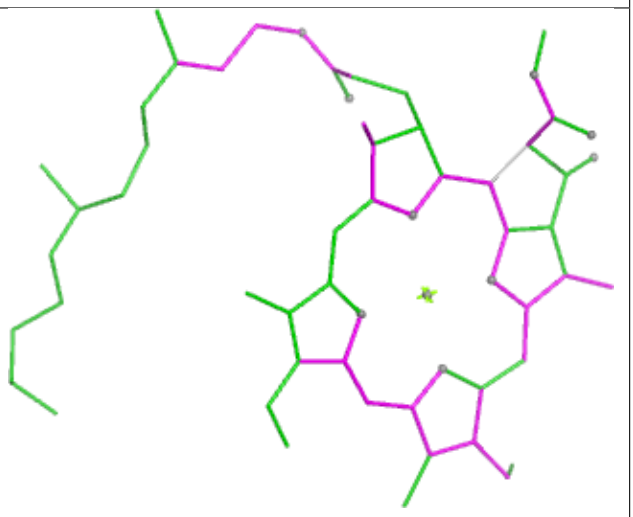


Rings

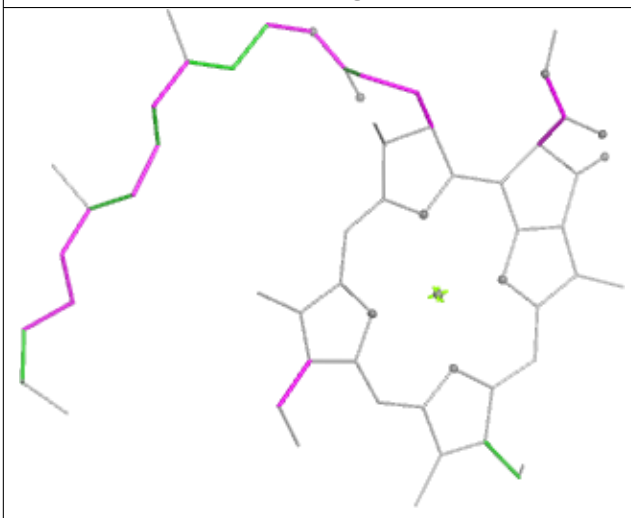
Ligand CLA R1 603



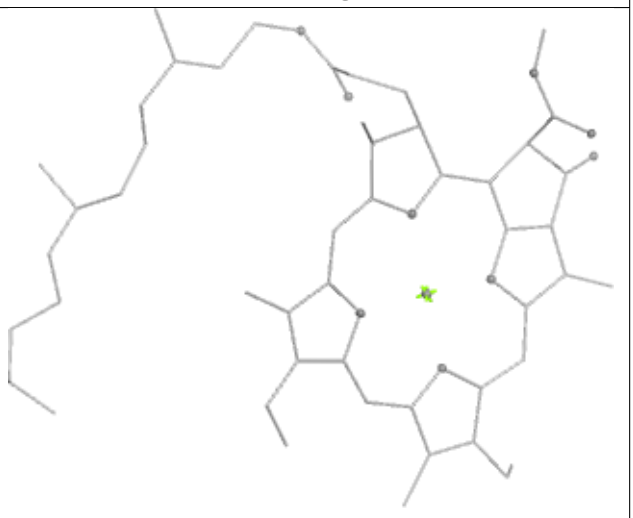
Bond lengths



Bond angles

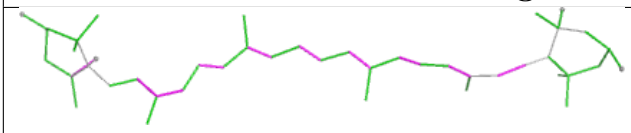


Torsions

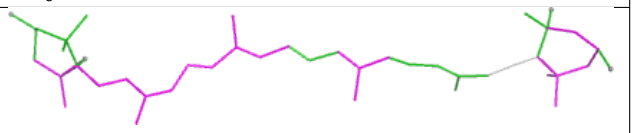


Rings

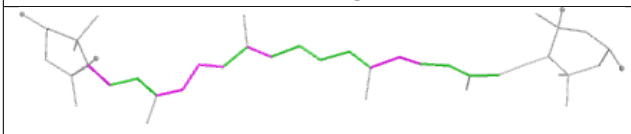
Ligand NEX y1 623



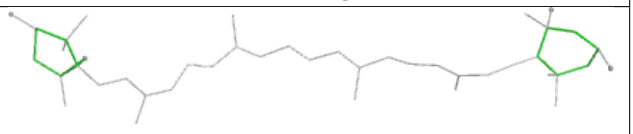
Bond lengths



Bond angles

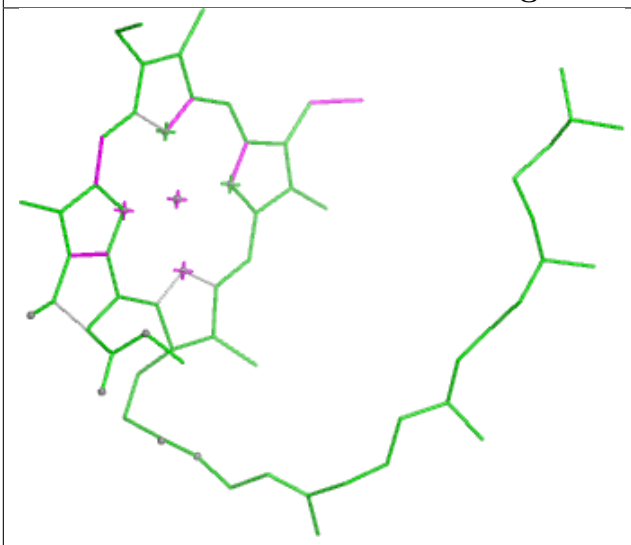


Torsions

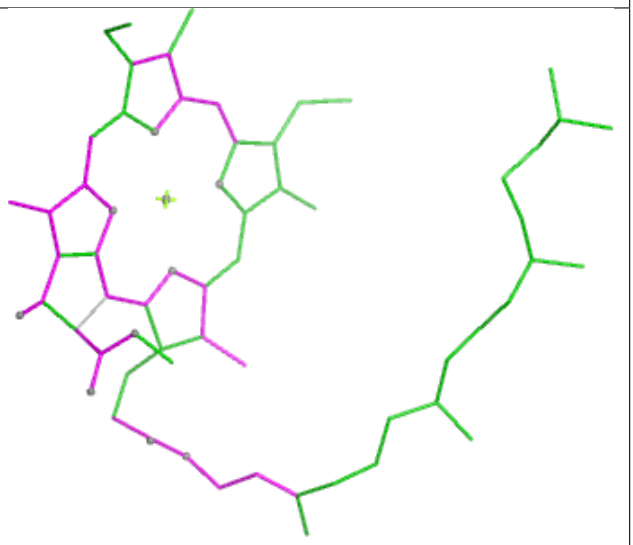


Rings

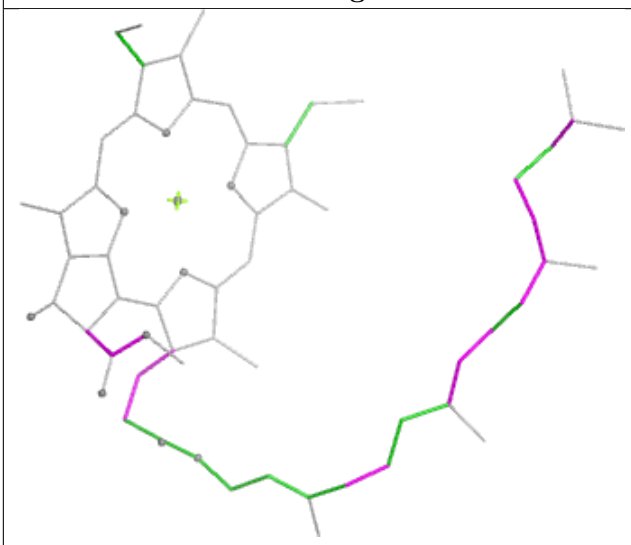
Ligand CLA c1 507



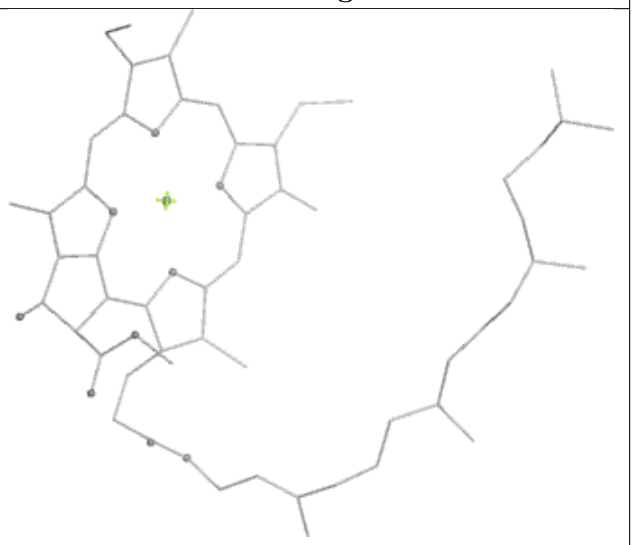
Bond lengths



Bond angles

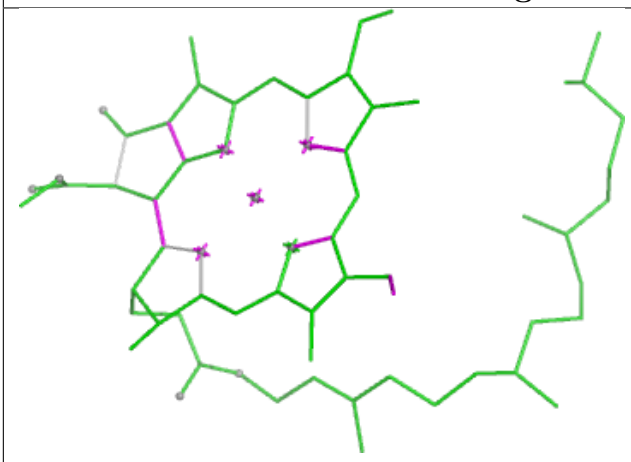


Torsions

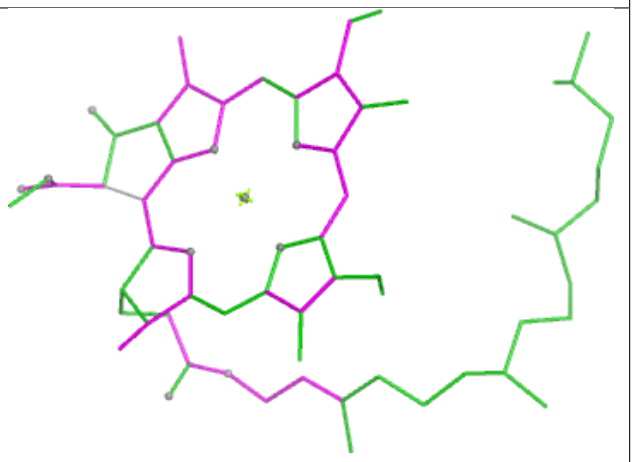


Rings

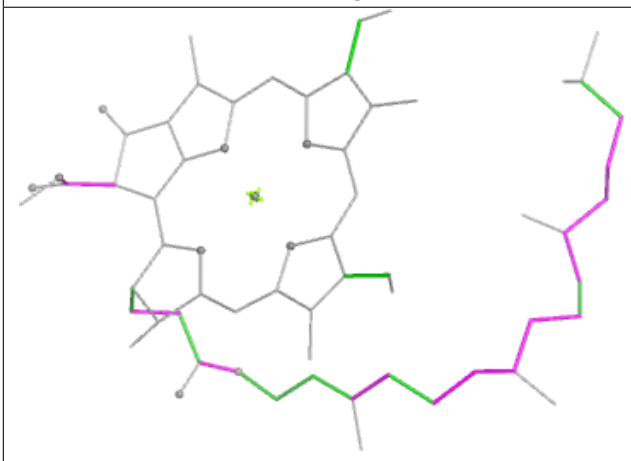
Ligand CLA Y1 602



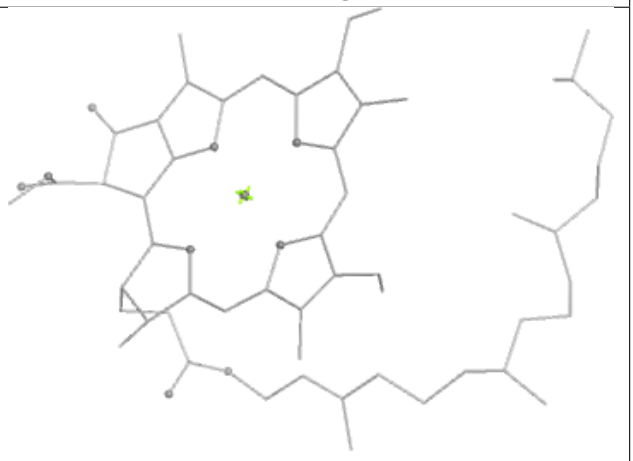
Bond lengths



Bond angles

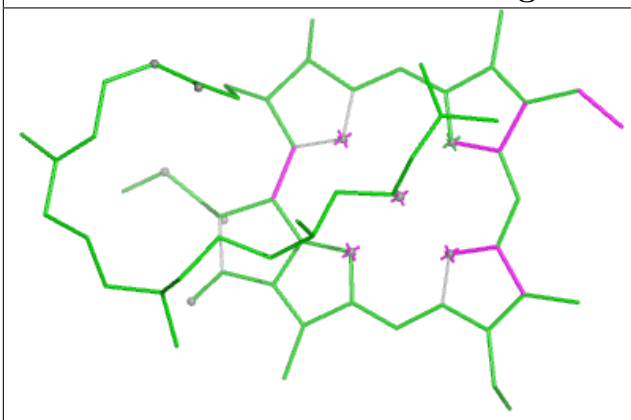


Torsions

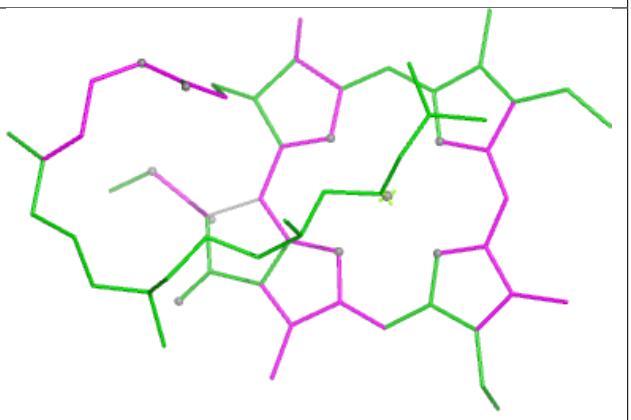


Rings

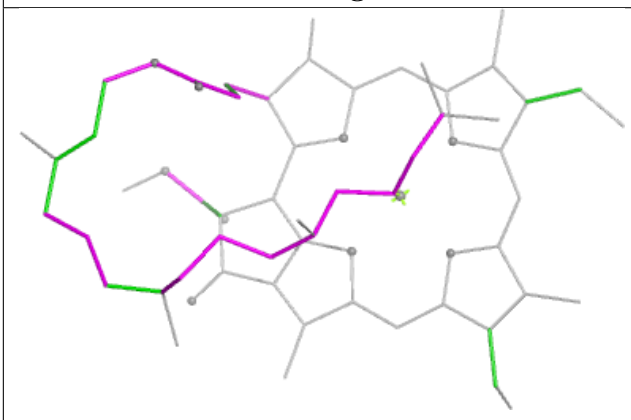
Ligand CLA b1 602



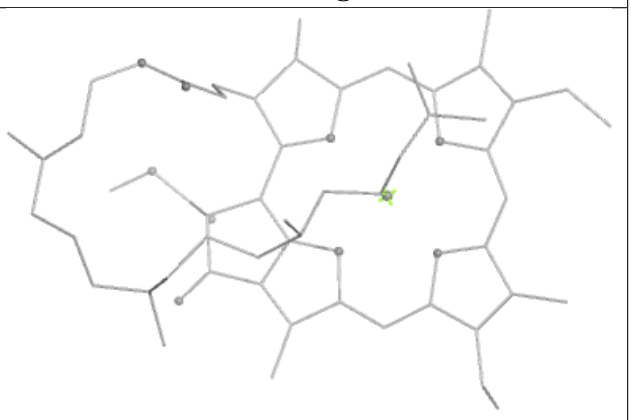
Bond lengths



Bond angles

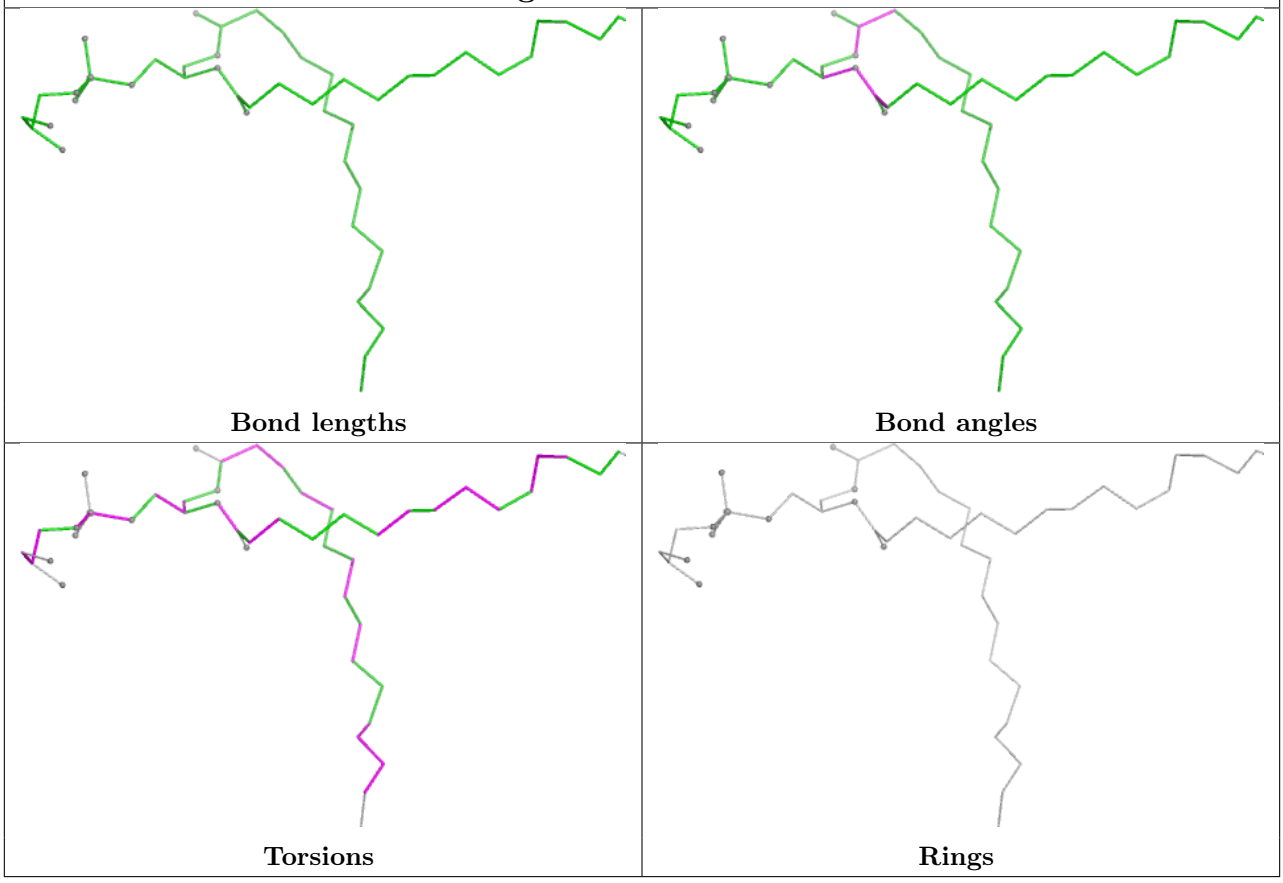


Torsions

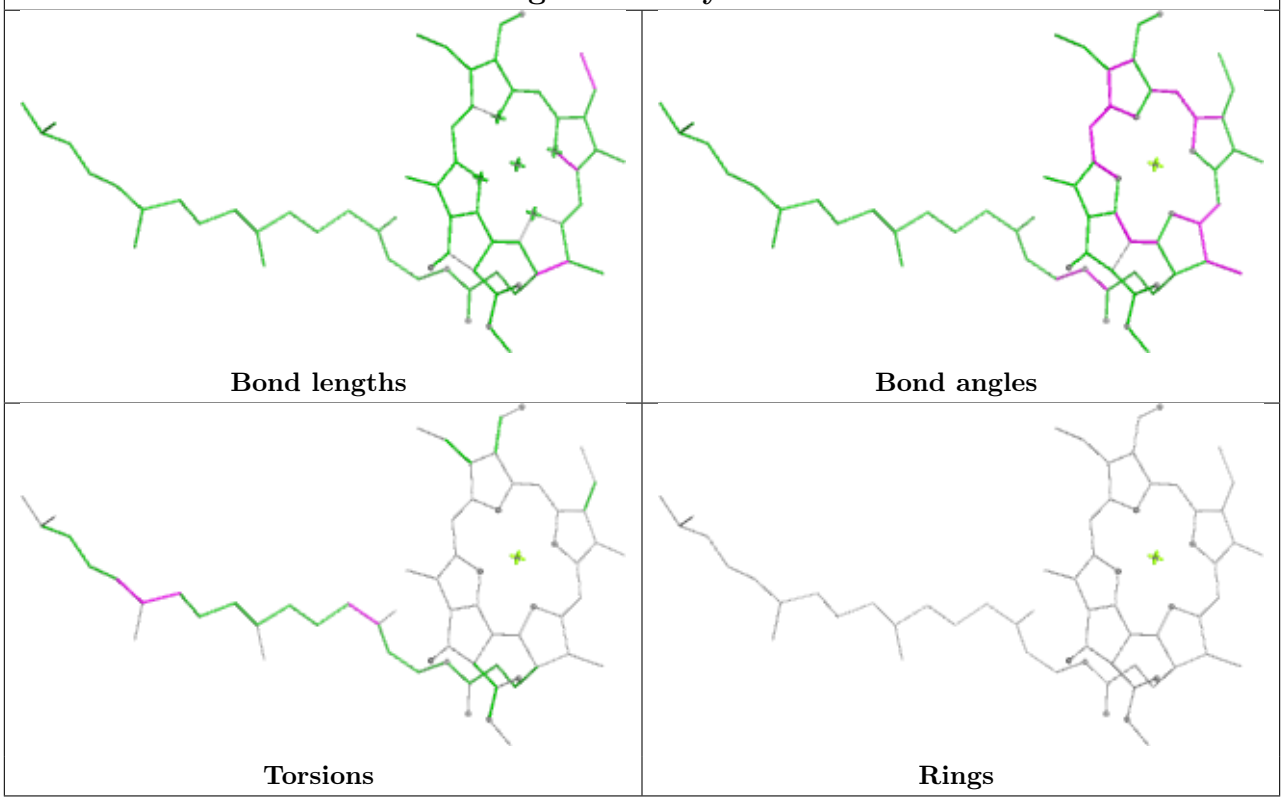


Rings

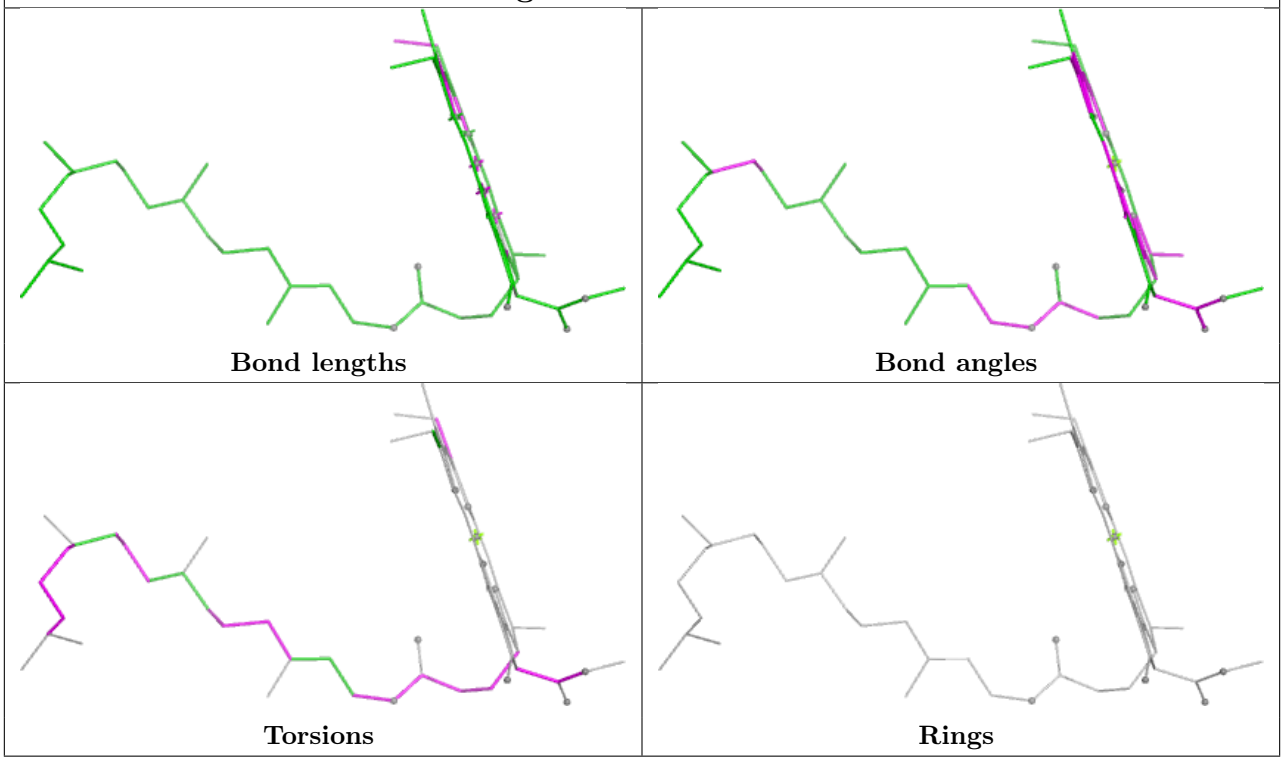
Ligand LHG n1 624



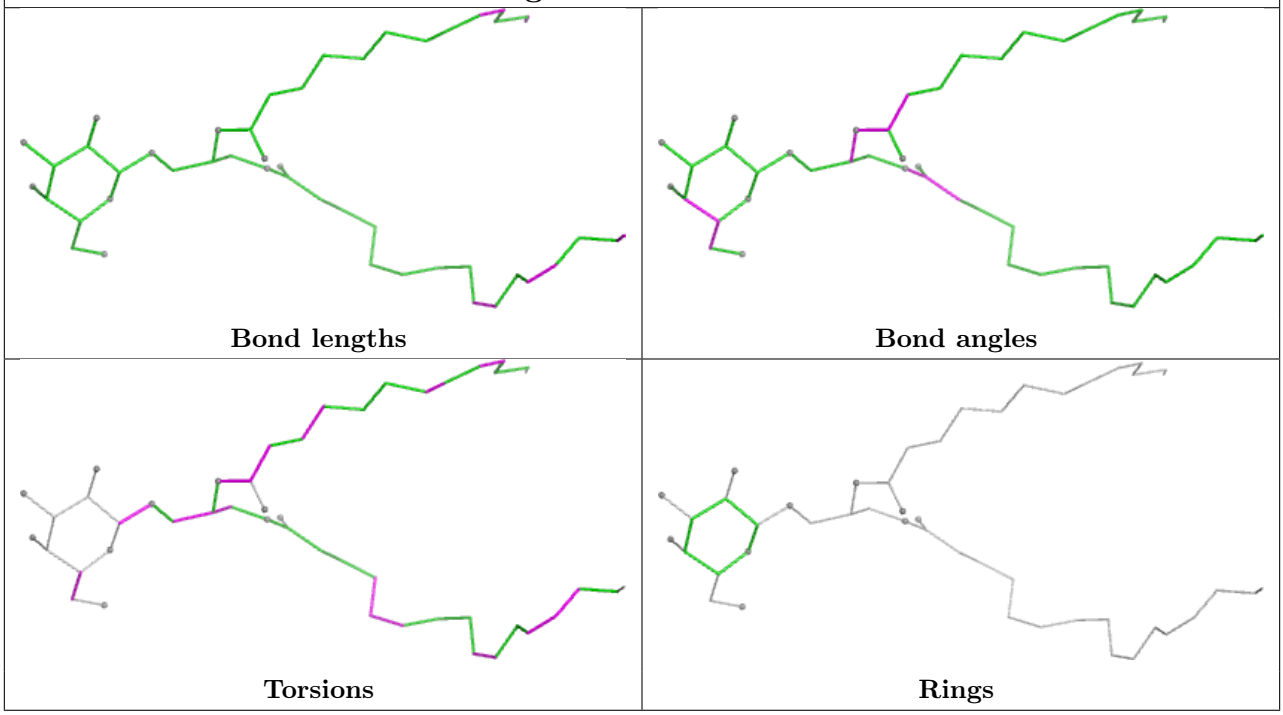
Ligand CHL y 609



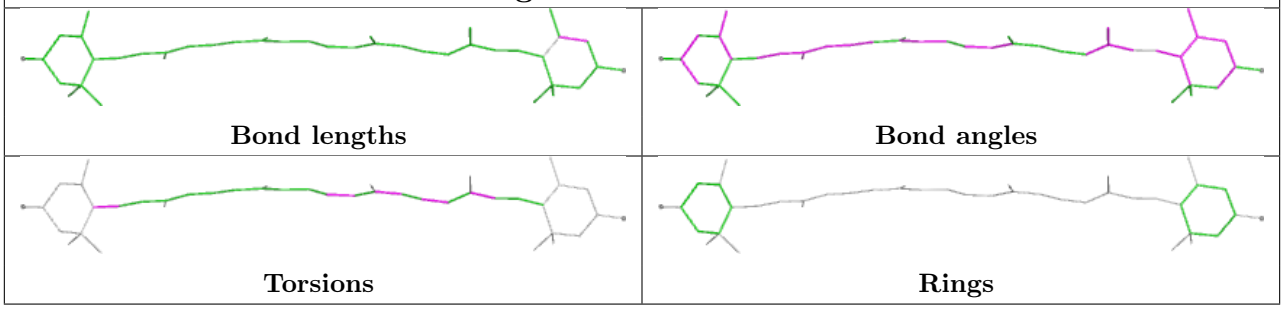
Ligand CLA B1 608



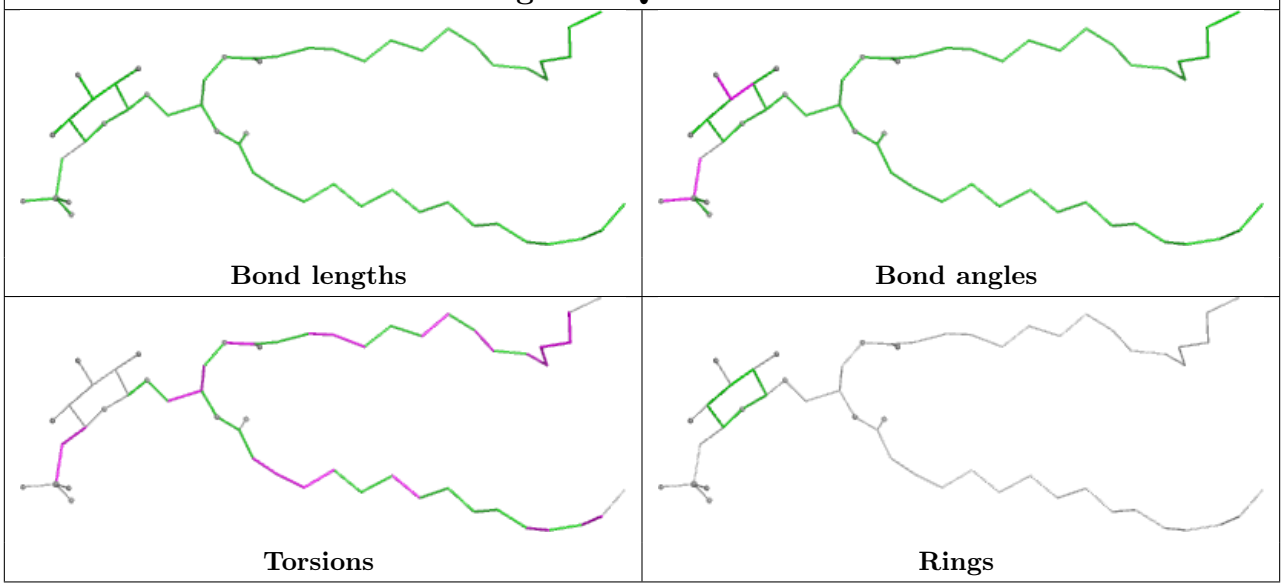
Ligand LMG a 413



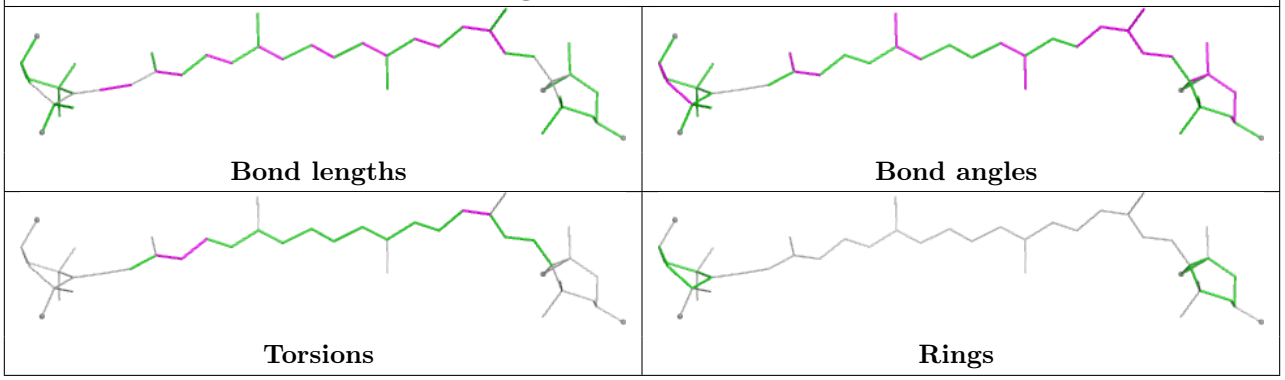
Ligand LUT N1 620



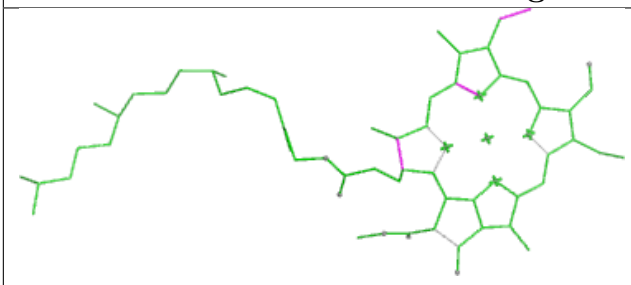
Ligand SQD C1 526



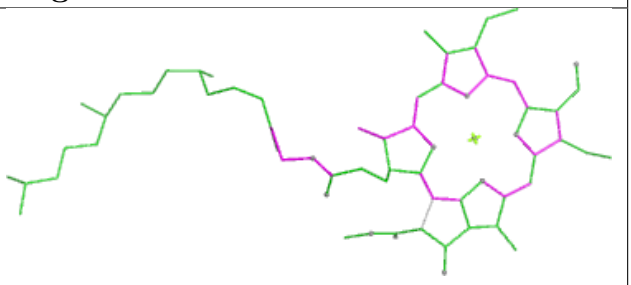
Ligand NEX n1 623



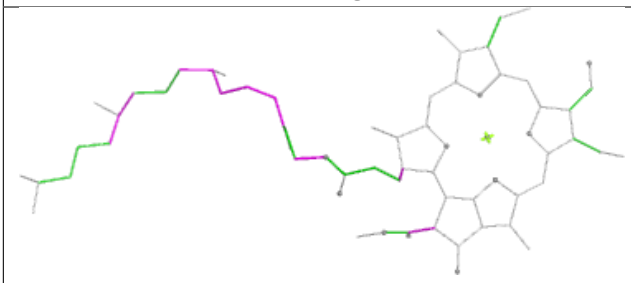
Ligand CHL g 601



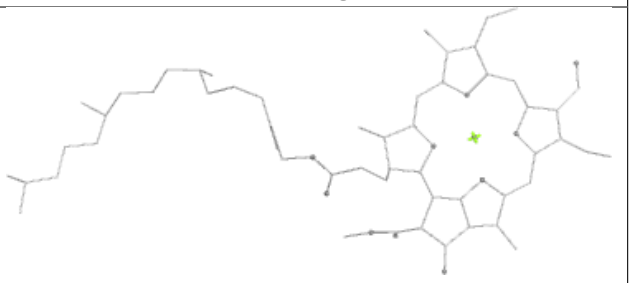
Bond lengths



Bond angles

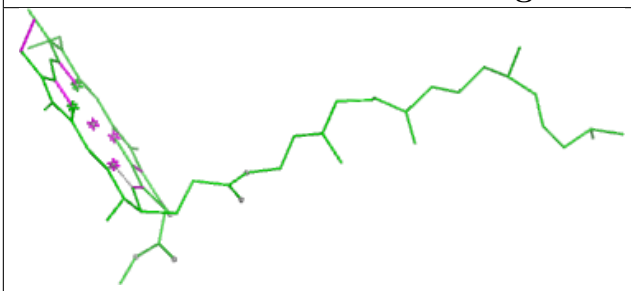


Torsions

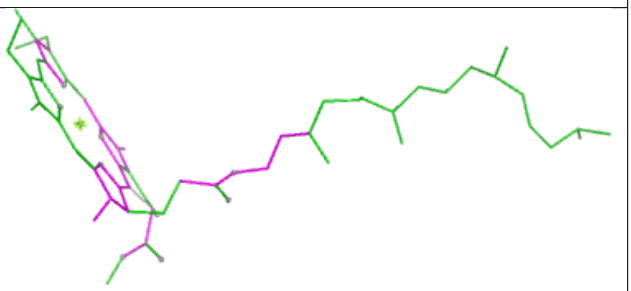


Rings

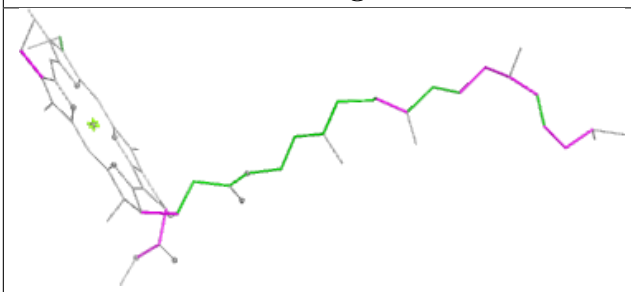
Ligand CLA B1 605



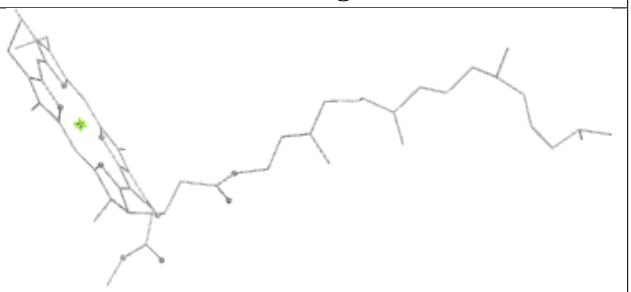
Bond lengths



Bond angles

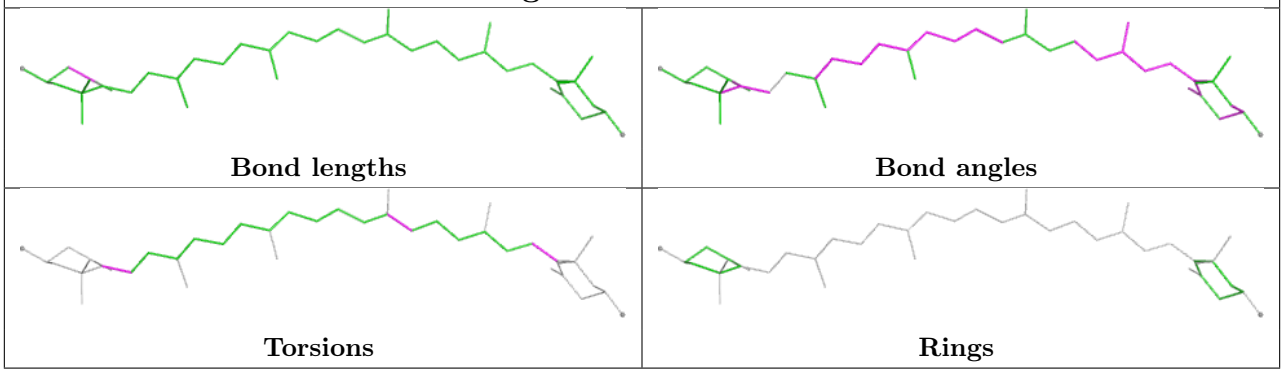


Torsions

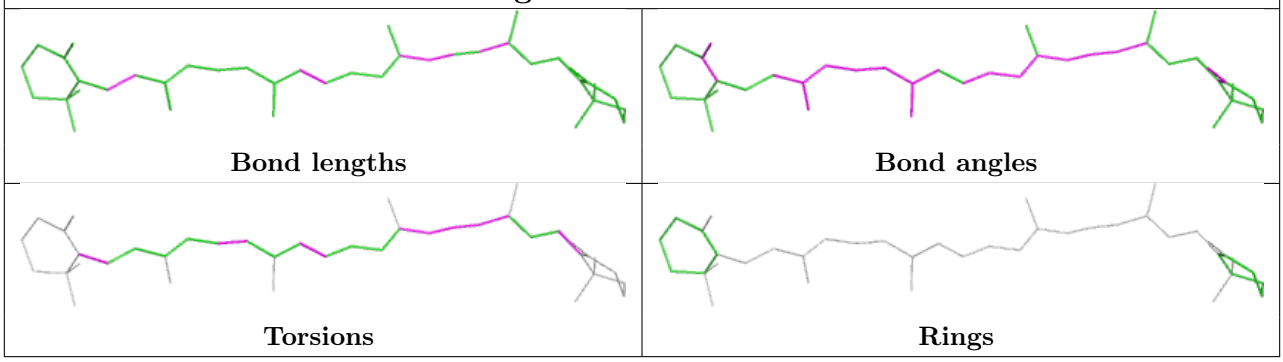


Rings

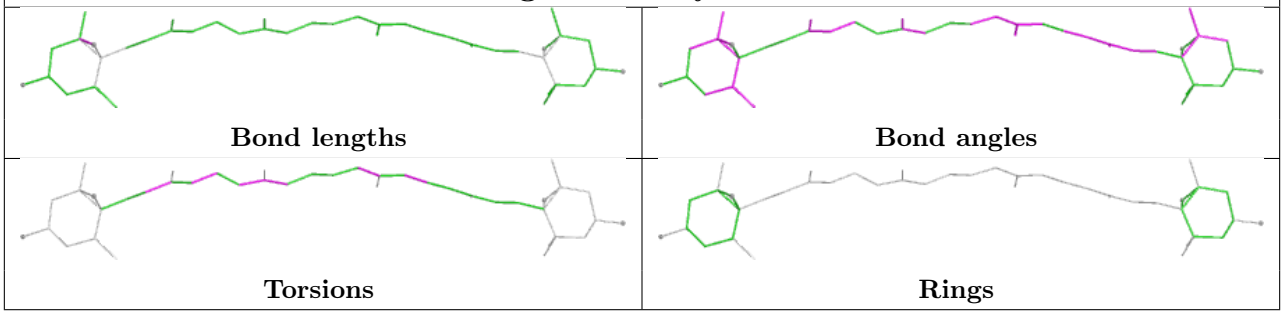
Ligand LUT s1 621



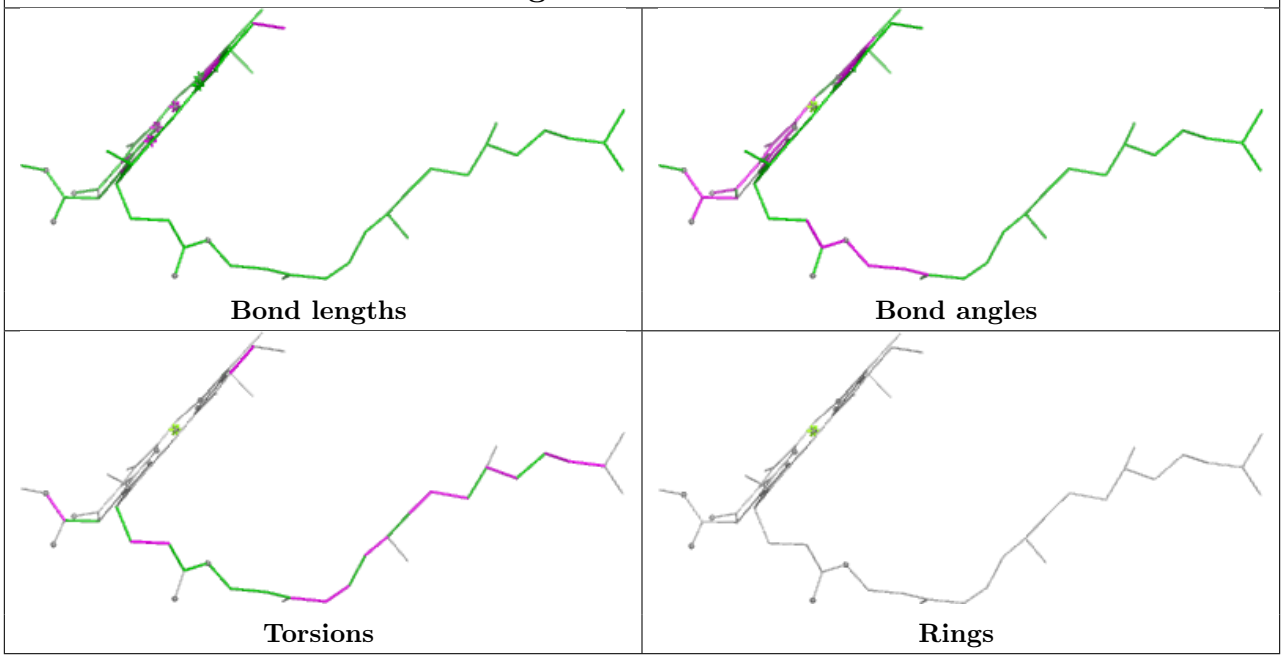
Ligand BCR C1 514



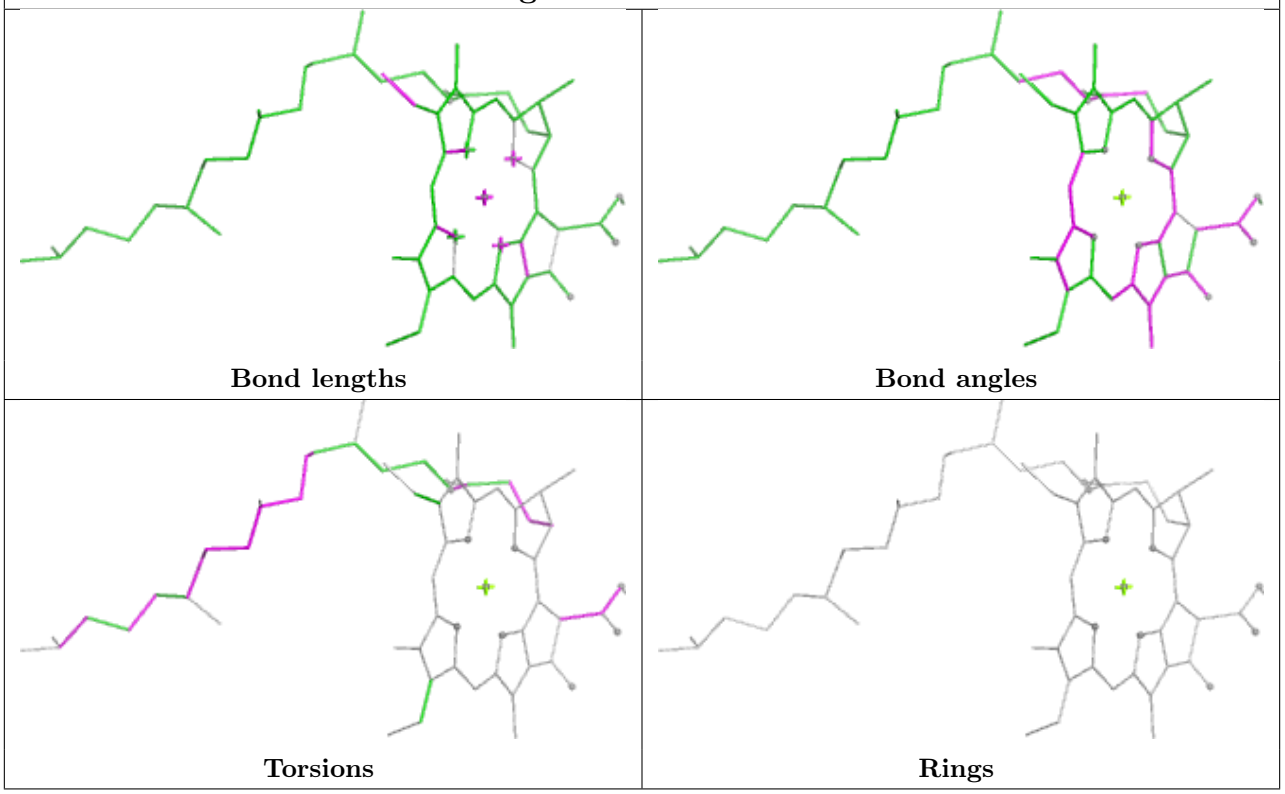
Ligand XAT y1 622



Ligand CLA n 604



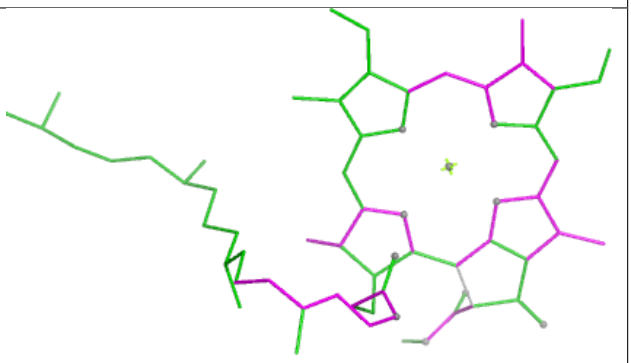
Ligand CLA S1 610



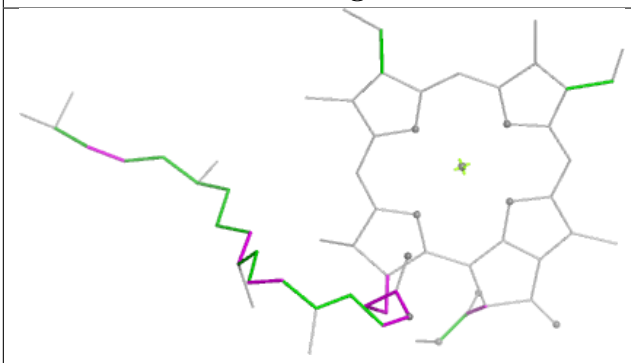
Ligand CLA A 406



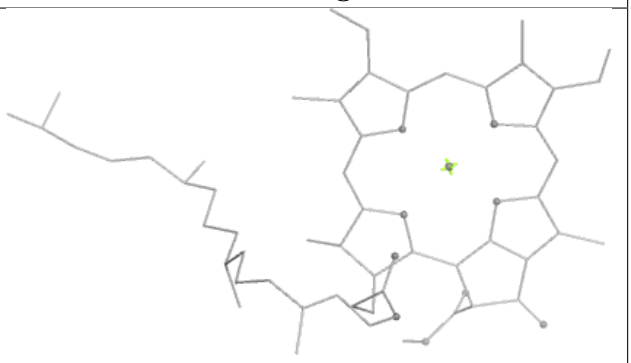
Bond lengths



Bond angles

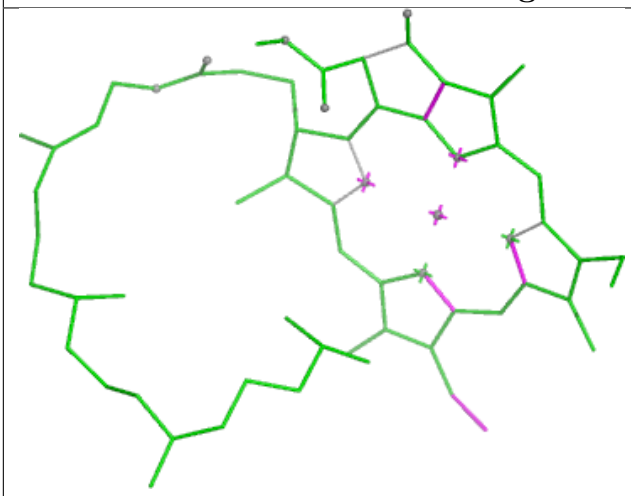


Torsions

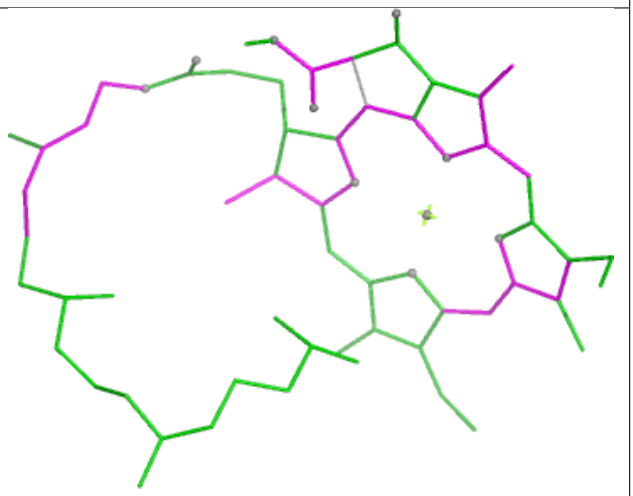


Rings

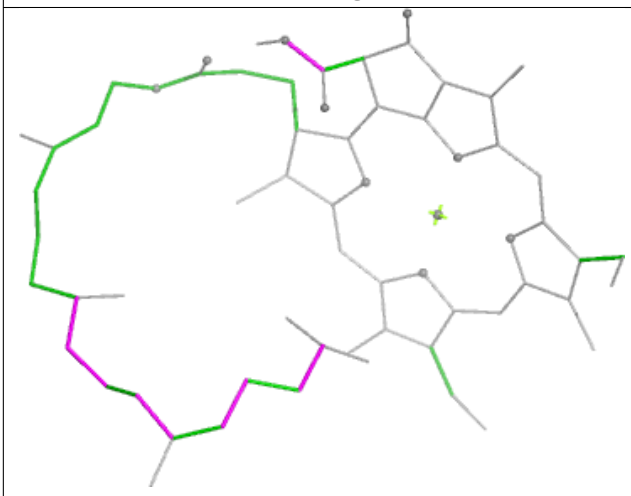
Ligand CLA b1 616



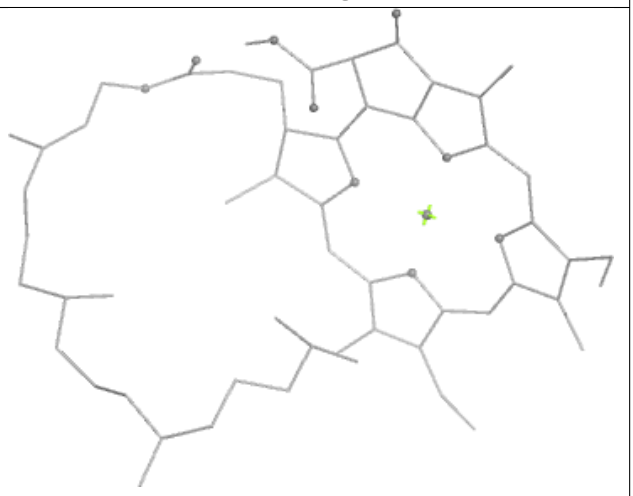
Bond lengths



Bond angles

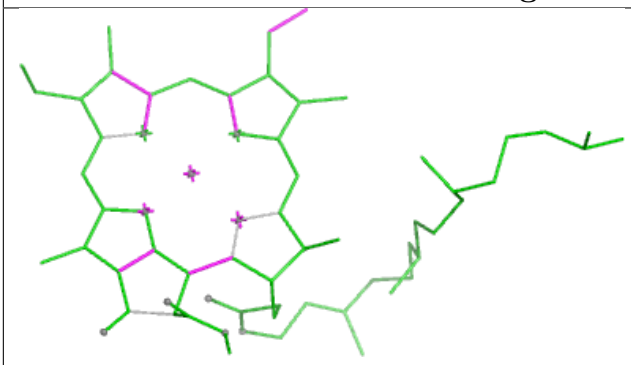


Torsions

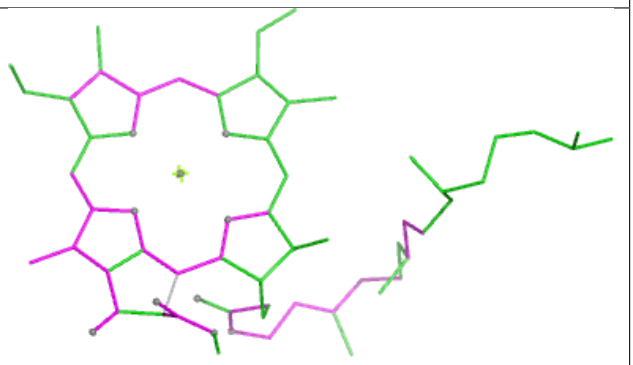


Rings

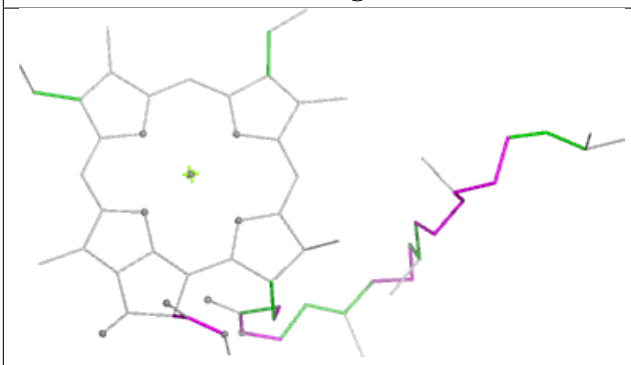
Ligand CLA a1 406



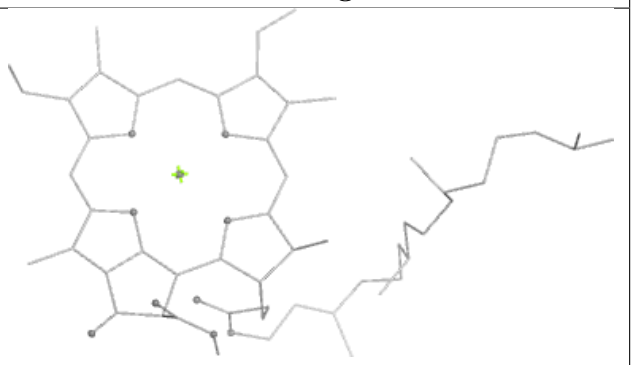
Bond lengths



Bond angles

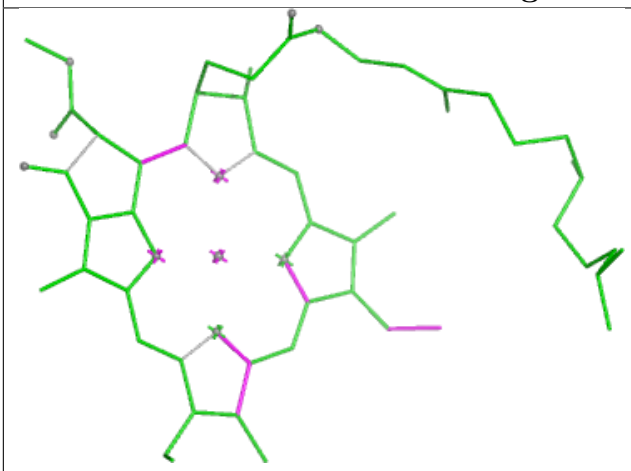


Torsions

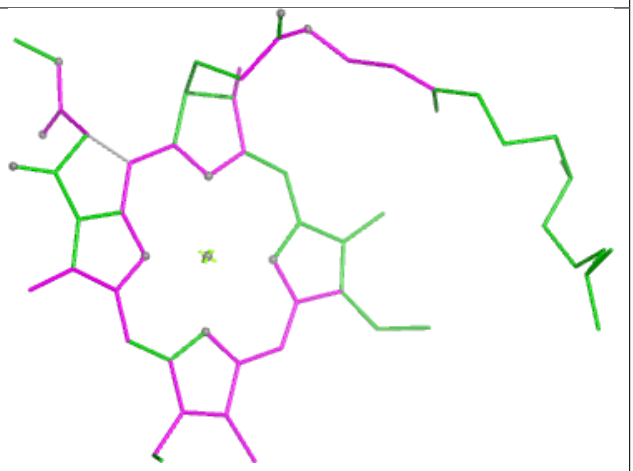


Rings

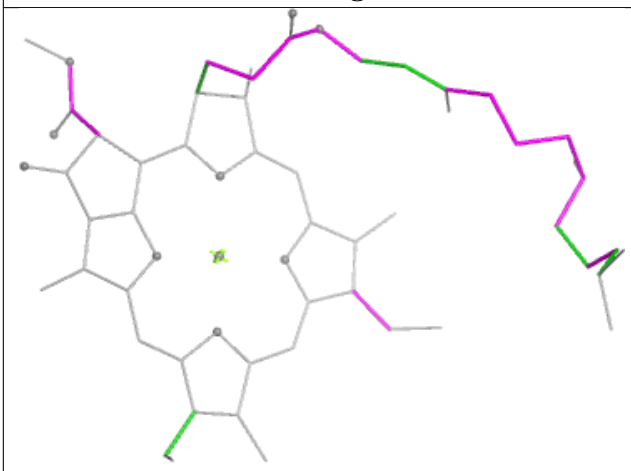
Ligand CLA r1 609



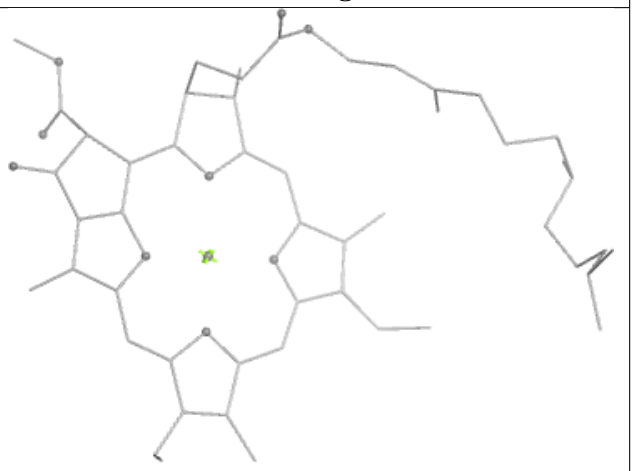
Bond lengths



Bond angles

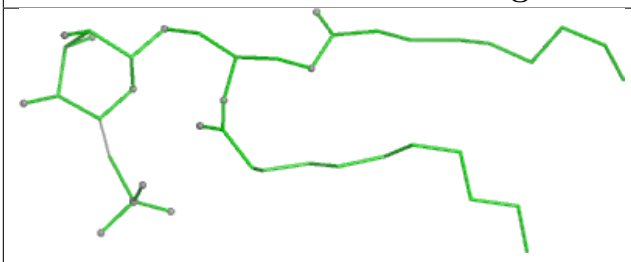


Torsions

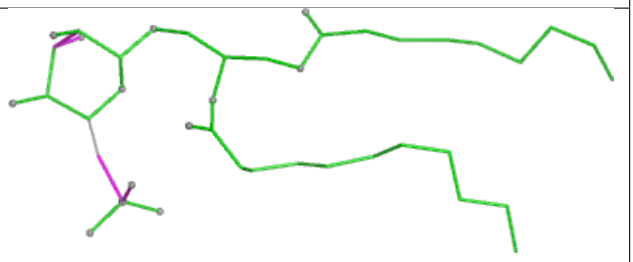


Rings

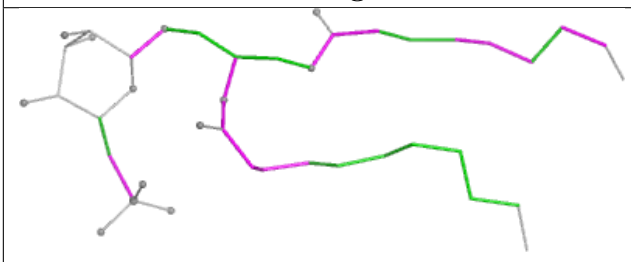
Ligand SQD M1 101



Bond lengths



Bond angles

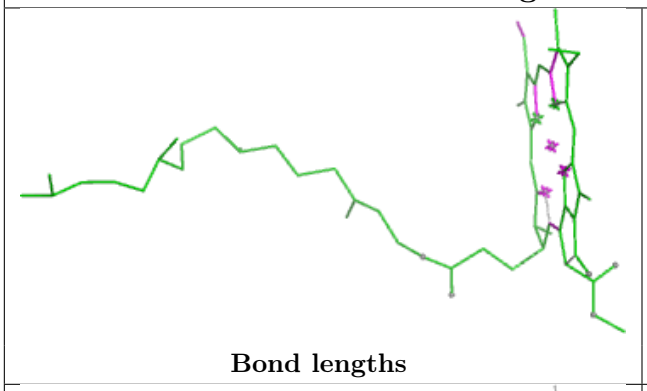


Torsions

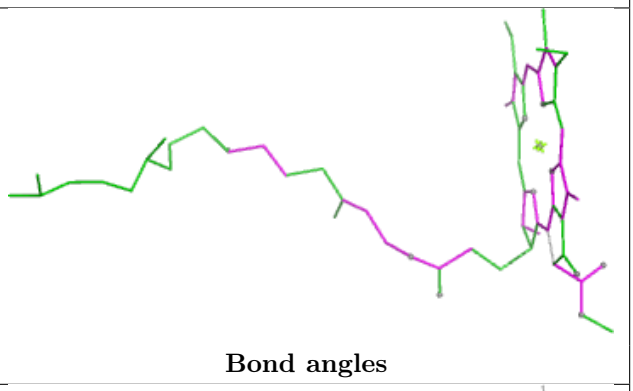


Rings

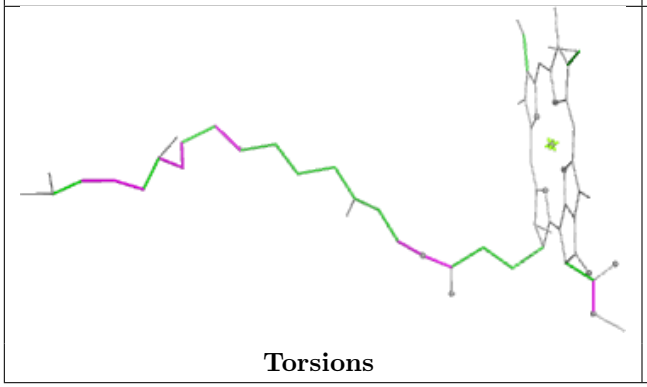
Ligand CLA d1 403



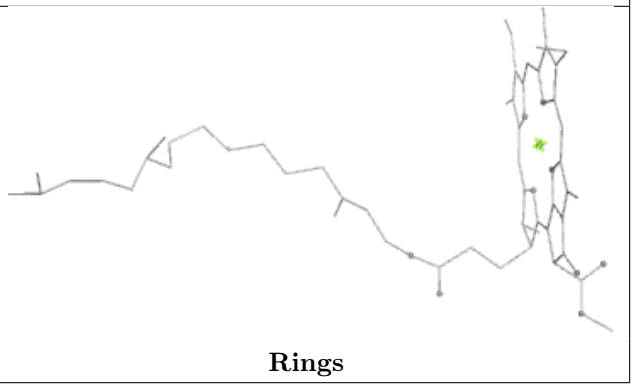
Bond lengths



Bond angles

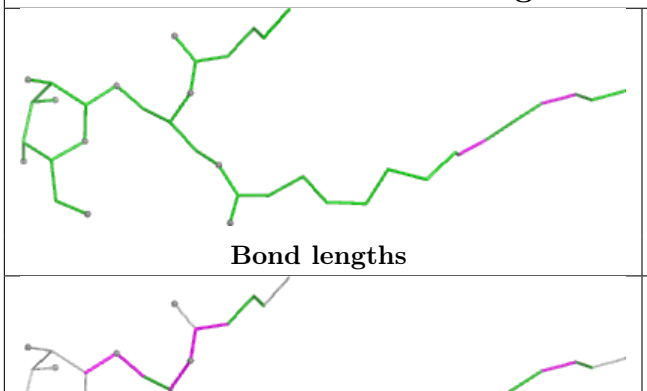


Torsions

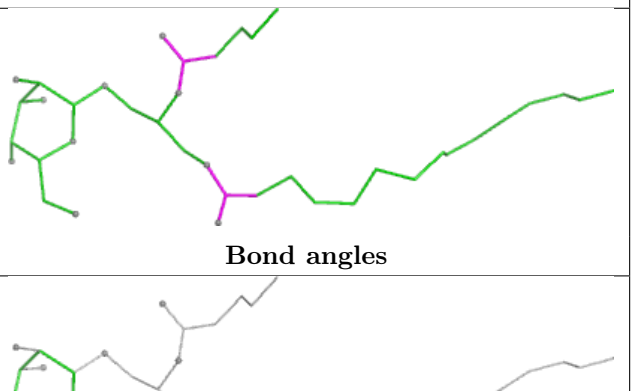


Rings

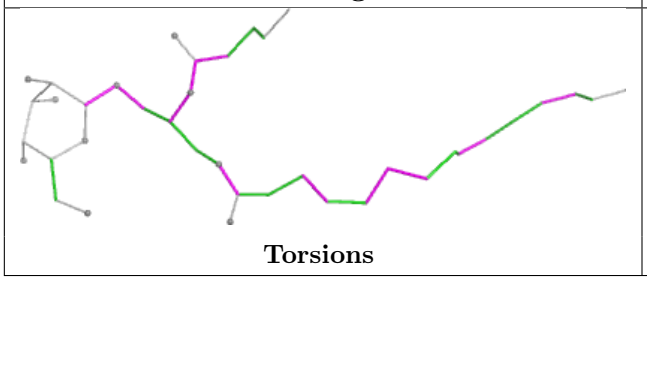
Ligand LMG W 201



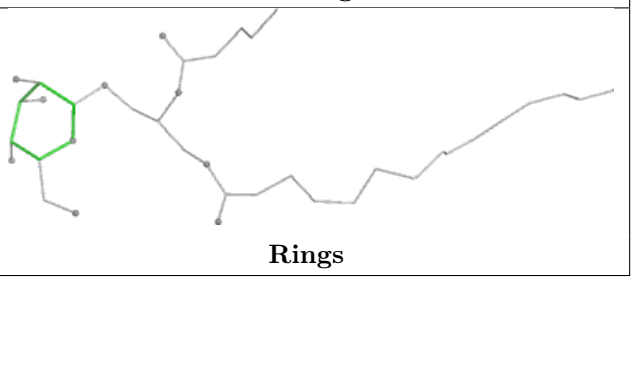
Bond lengths



Bond angles

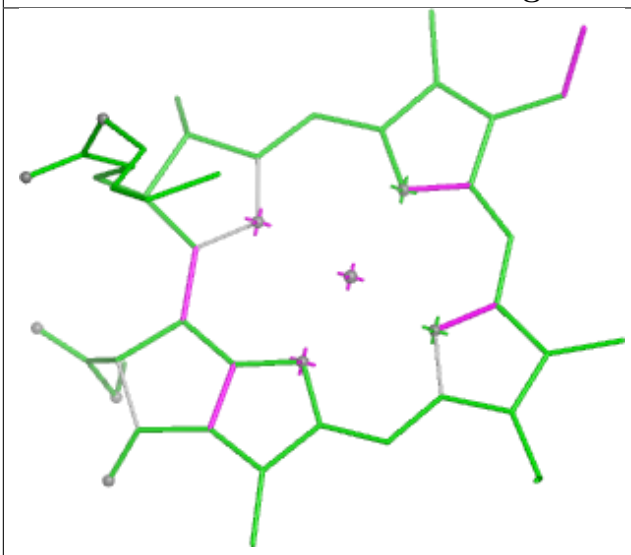


Torsions

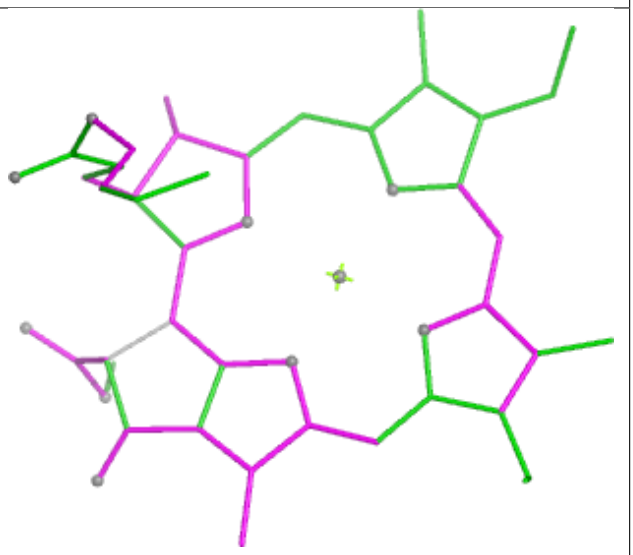


Rings

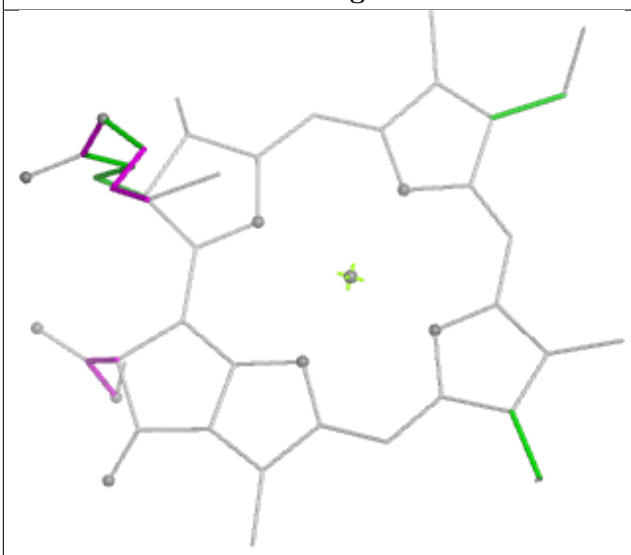
Ligand CLA G 604



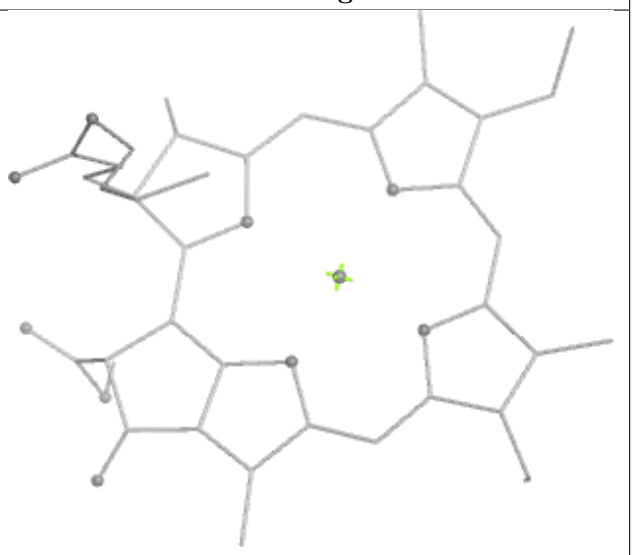
Bond lengths



Bond angles

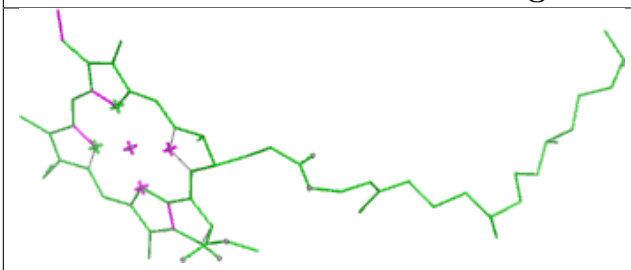


Torsions

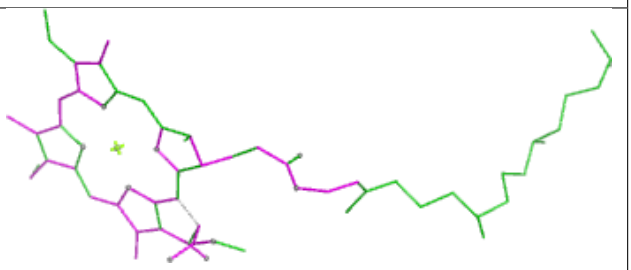


Rings

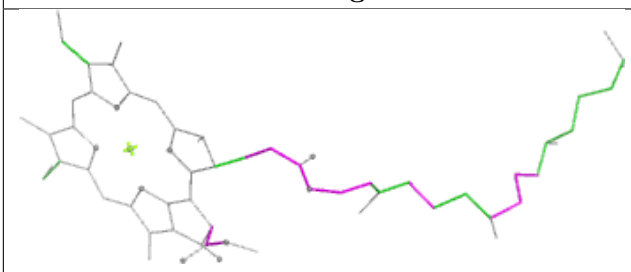
Ligand CLA a 405



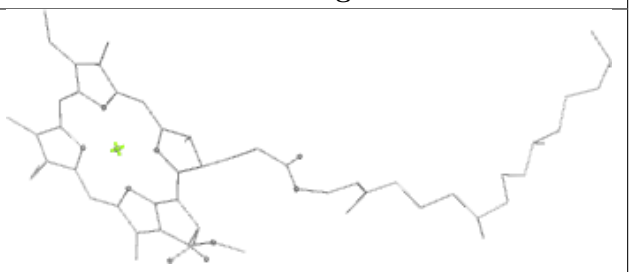
Bond lengths



Bond angles

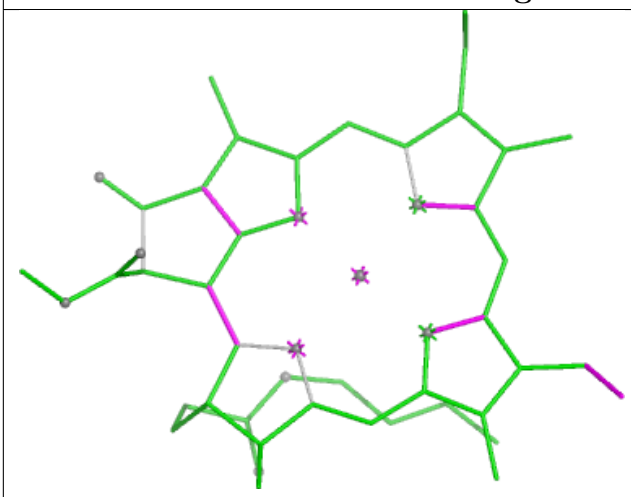


Torsions

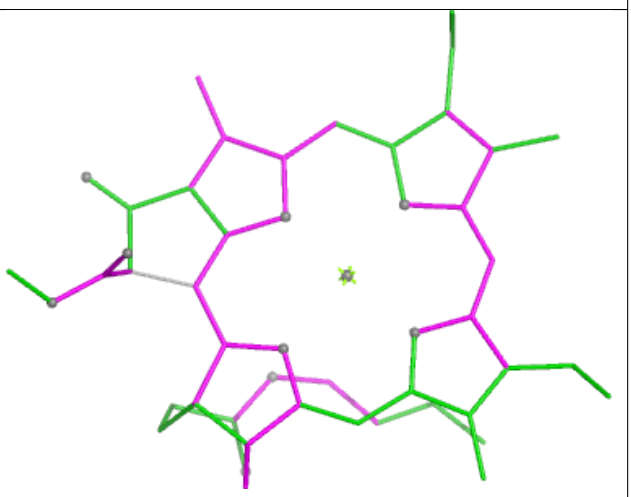


Rings

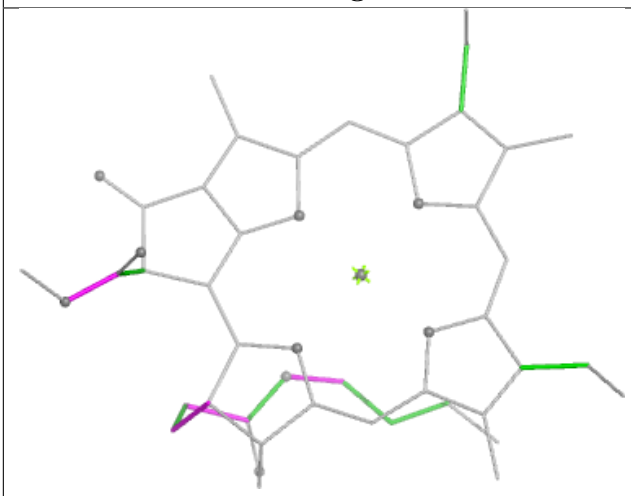
Ligand CLA N1 614



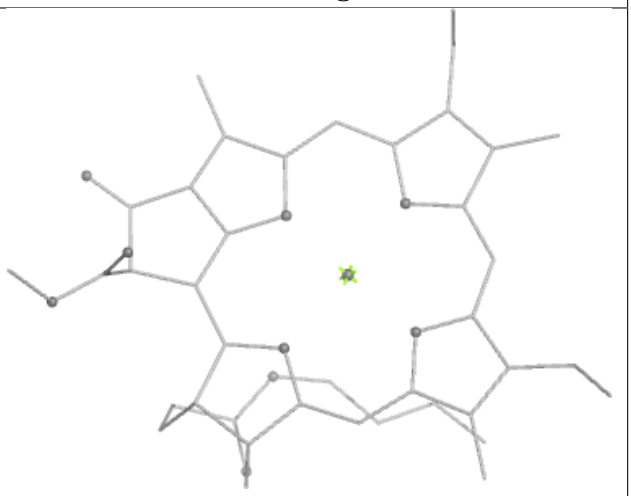
Bond lengths



Bond angles

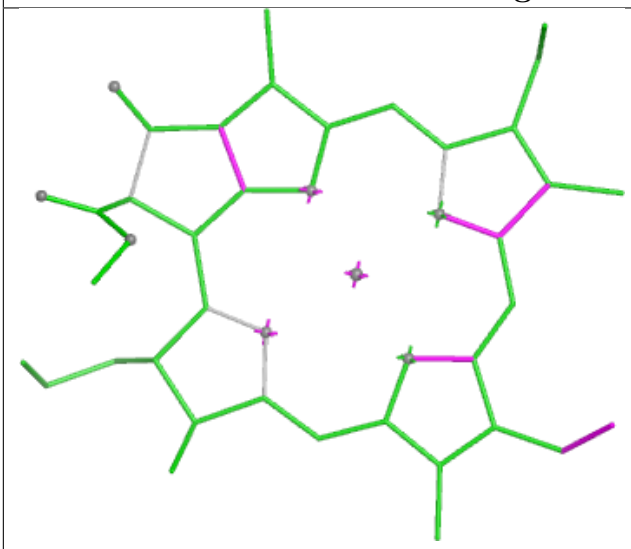


Torsions

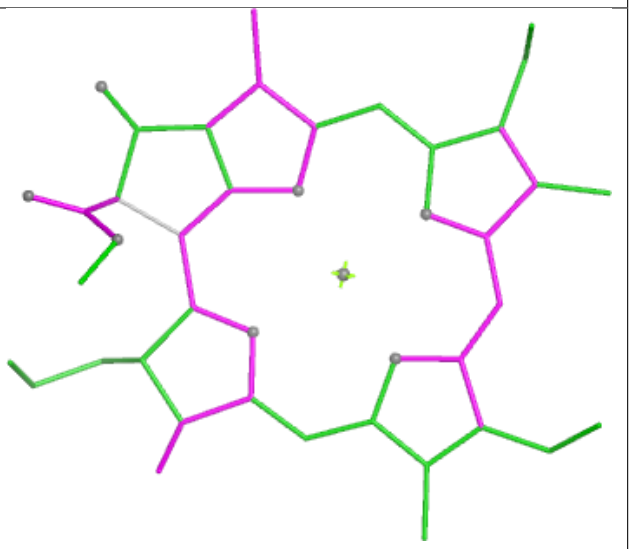


Rings

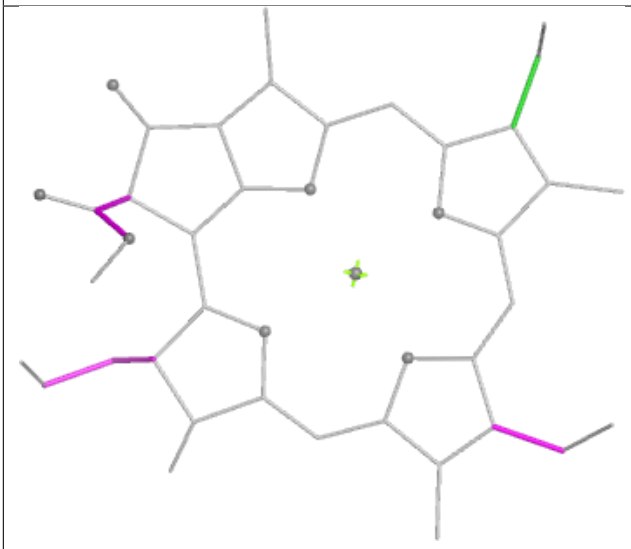
Ligand CLA G1 612



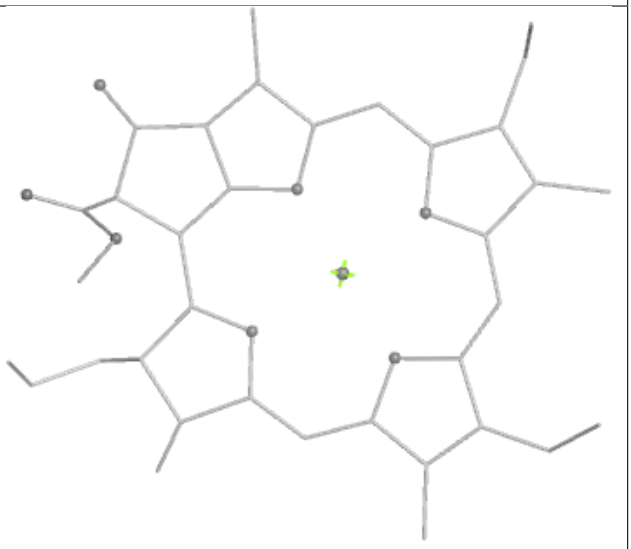
Bond lengths



Bond angles



Torsions

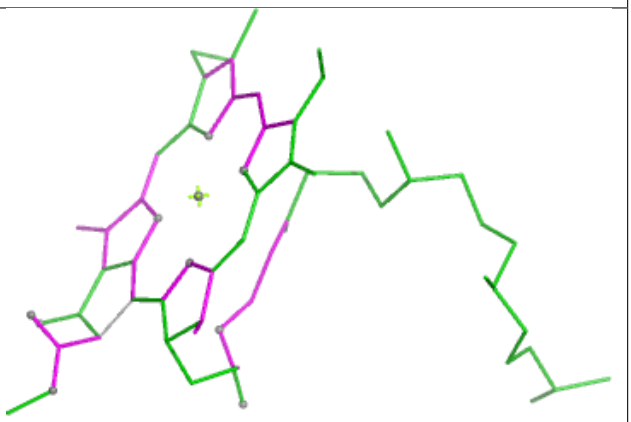


Rings

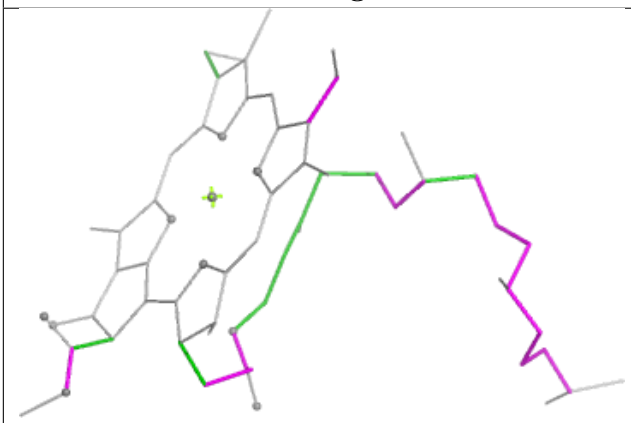
Ligand CLA Y1 613



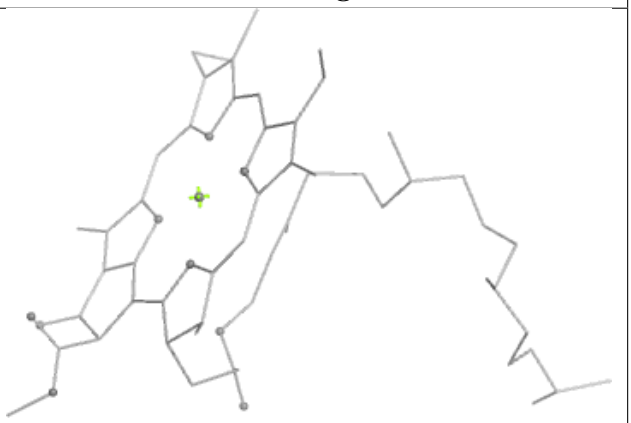
Bond lengths



Bond angles

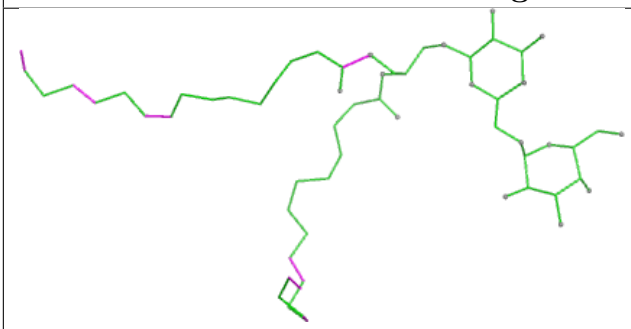


Torsions



Rings

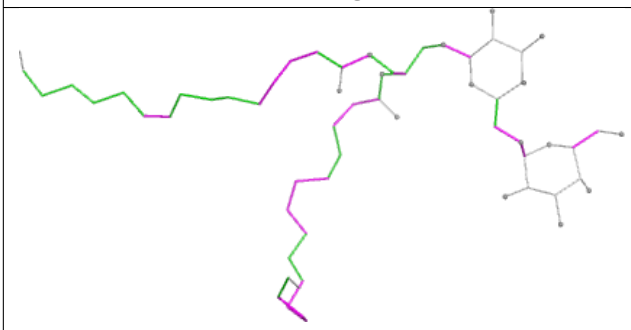
Ligand DGD C1 519



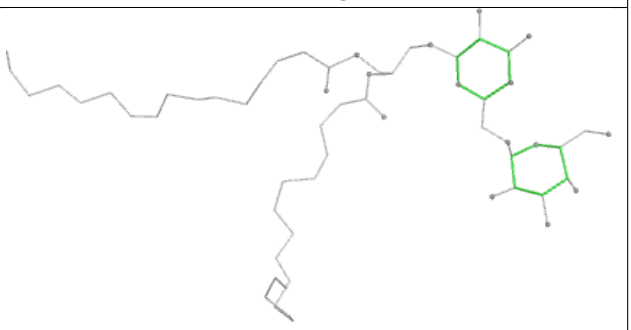
Bond lengths



Bond angles

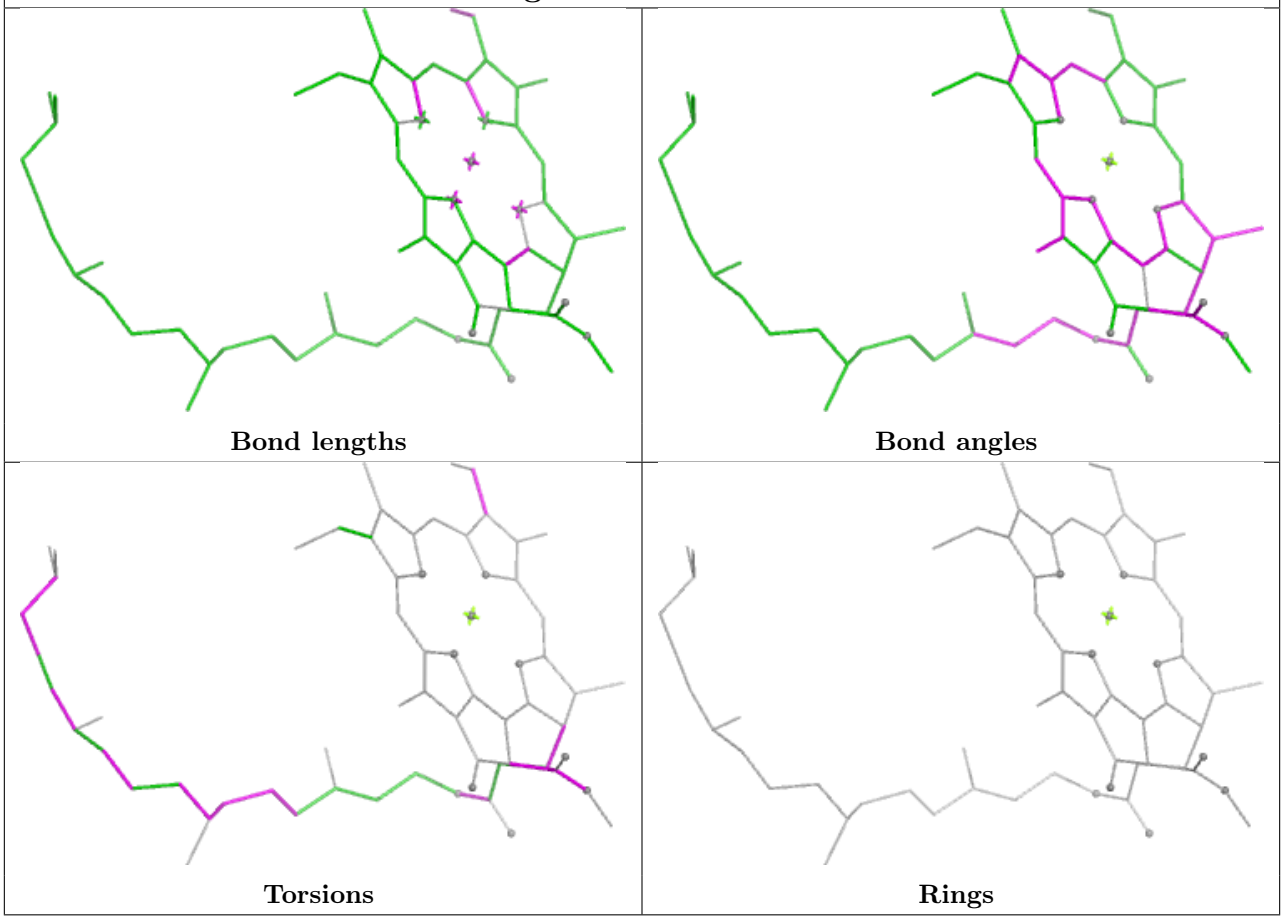


Torsions

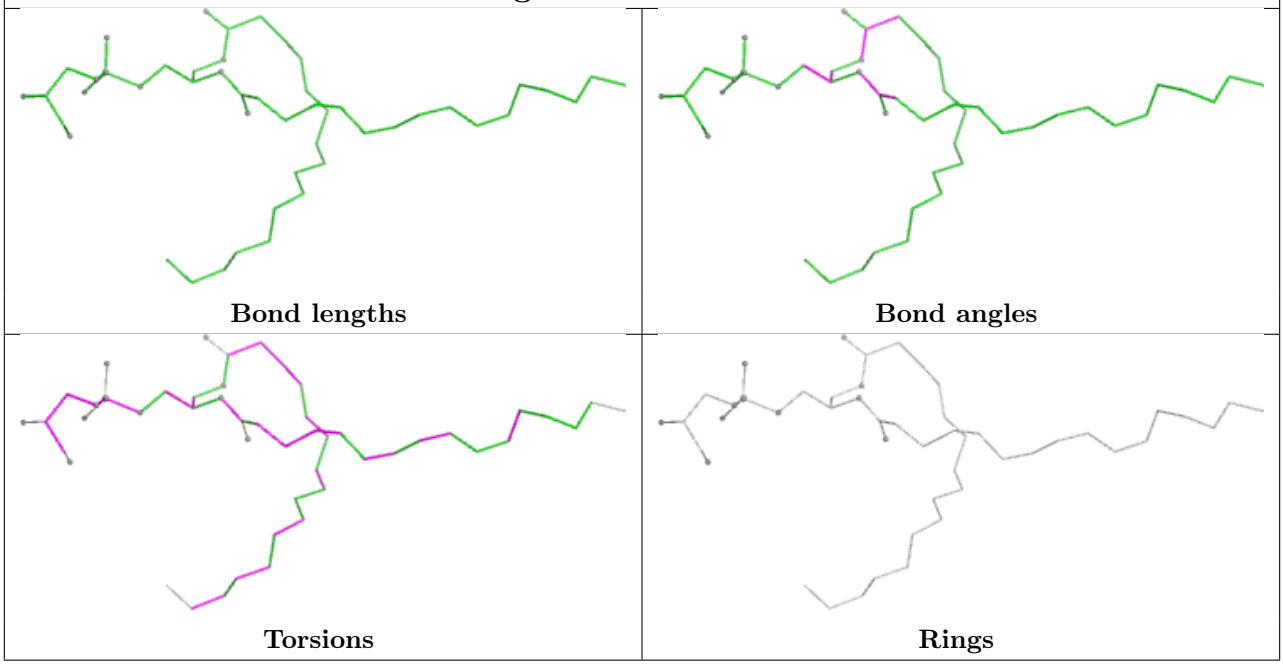


Rings

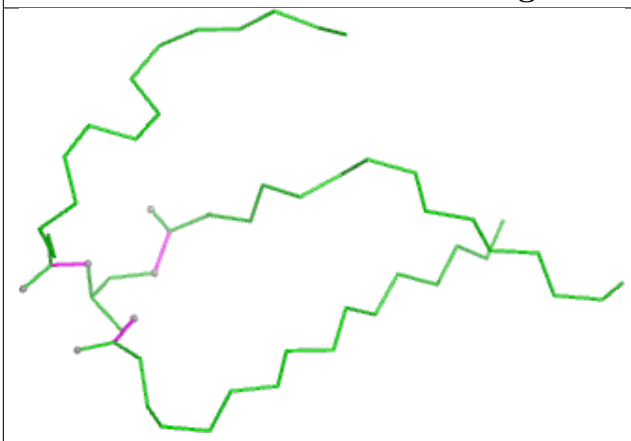
Ligand CLA G 611



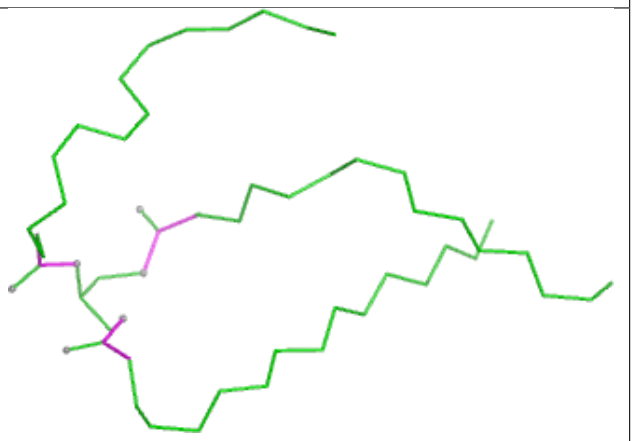
Ligand LHG G1 624



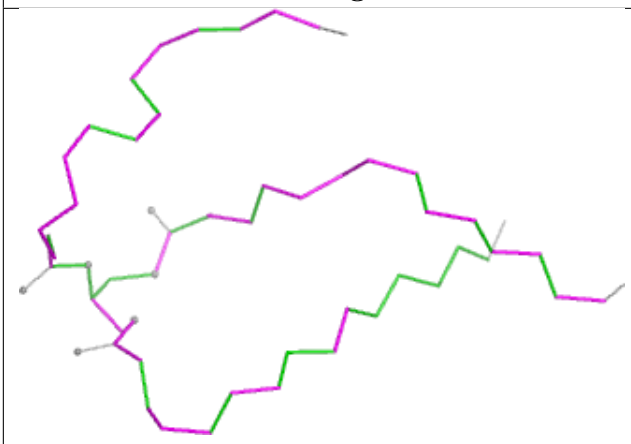
Ligand 4RF K1 101



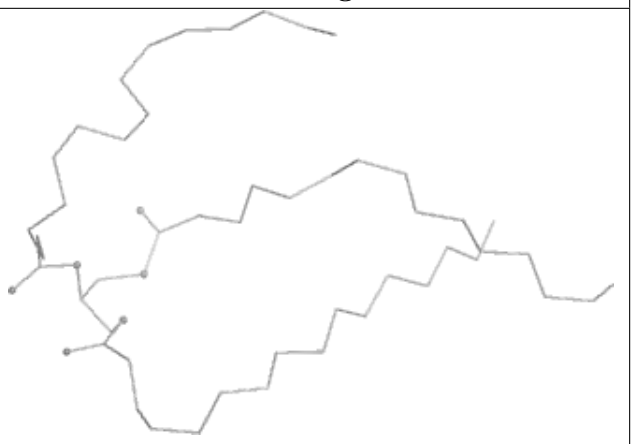
Bond lengths



Bond angles

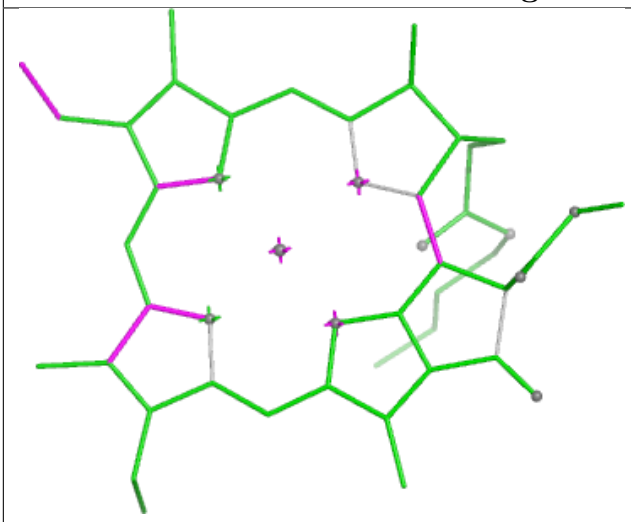


Torsions

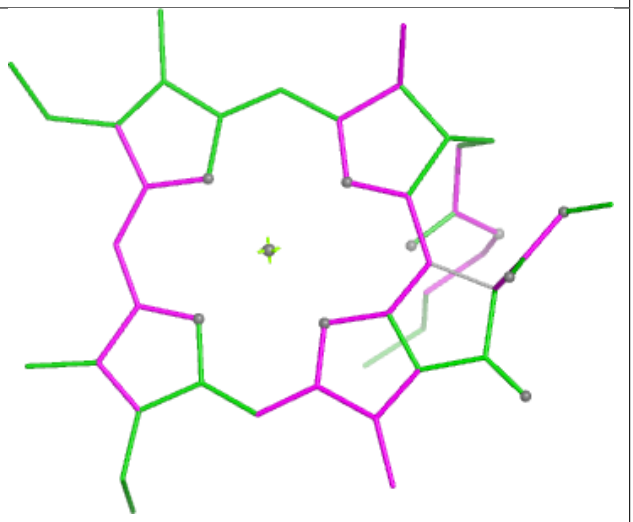


Rings

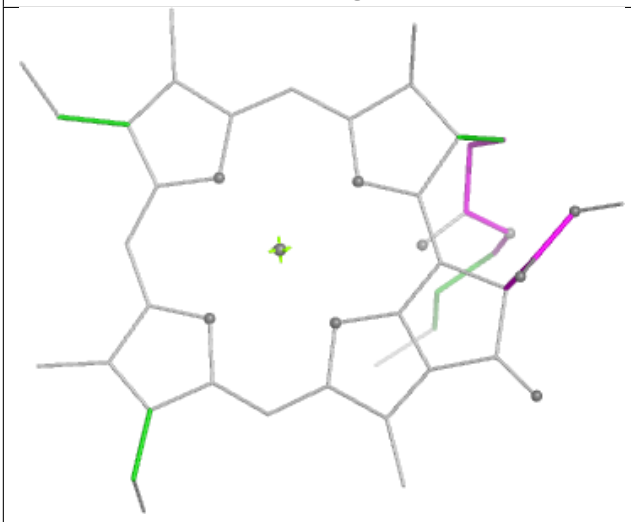
Ligand CLA r1 604



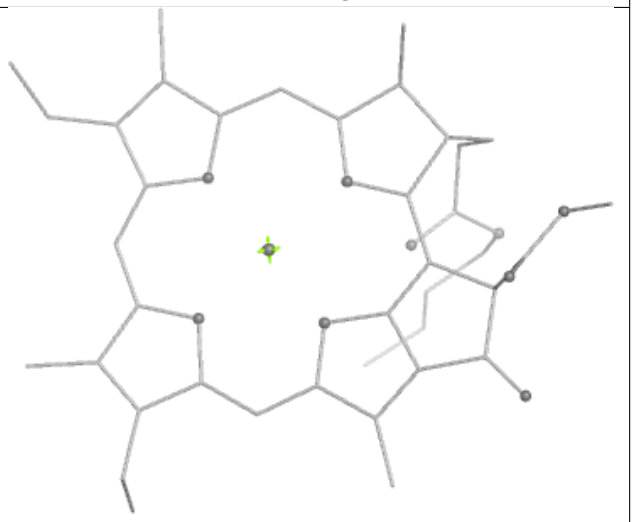
Bond lengths



Bond angles

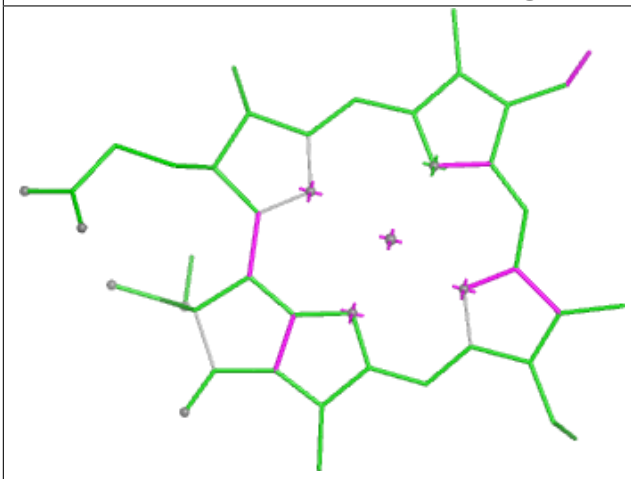


Torsions

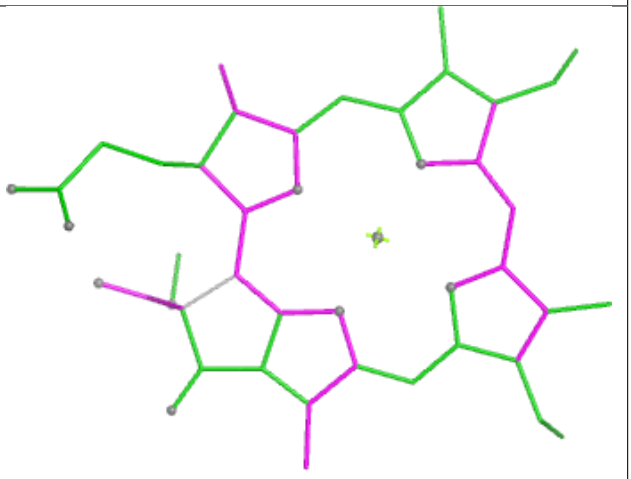


Rings

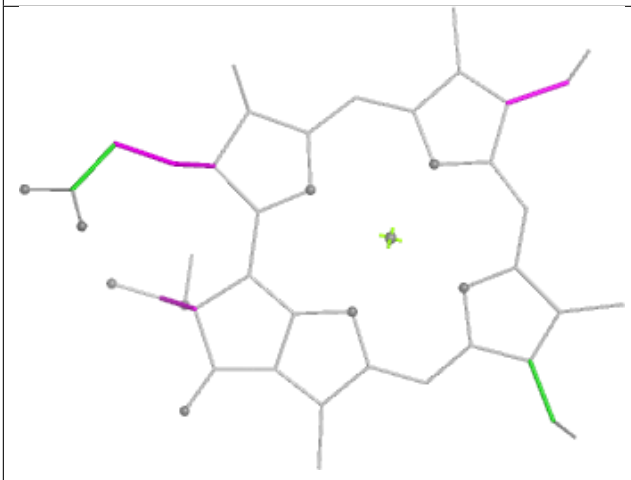
Ligand CLA s1 612



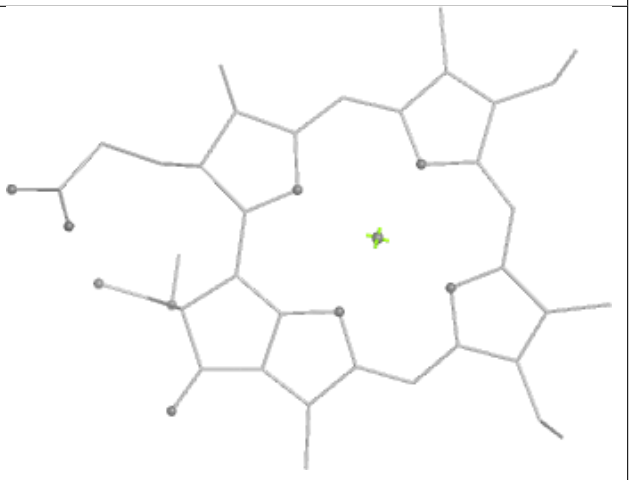
Bond lengths



Bond angles

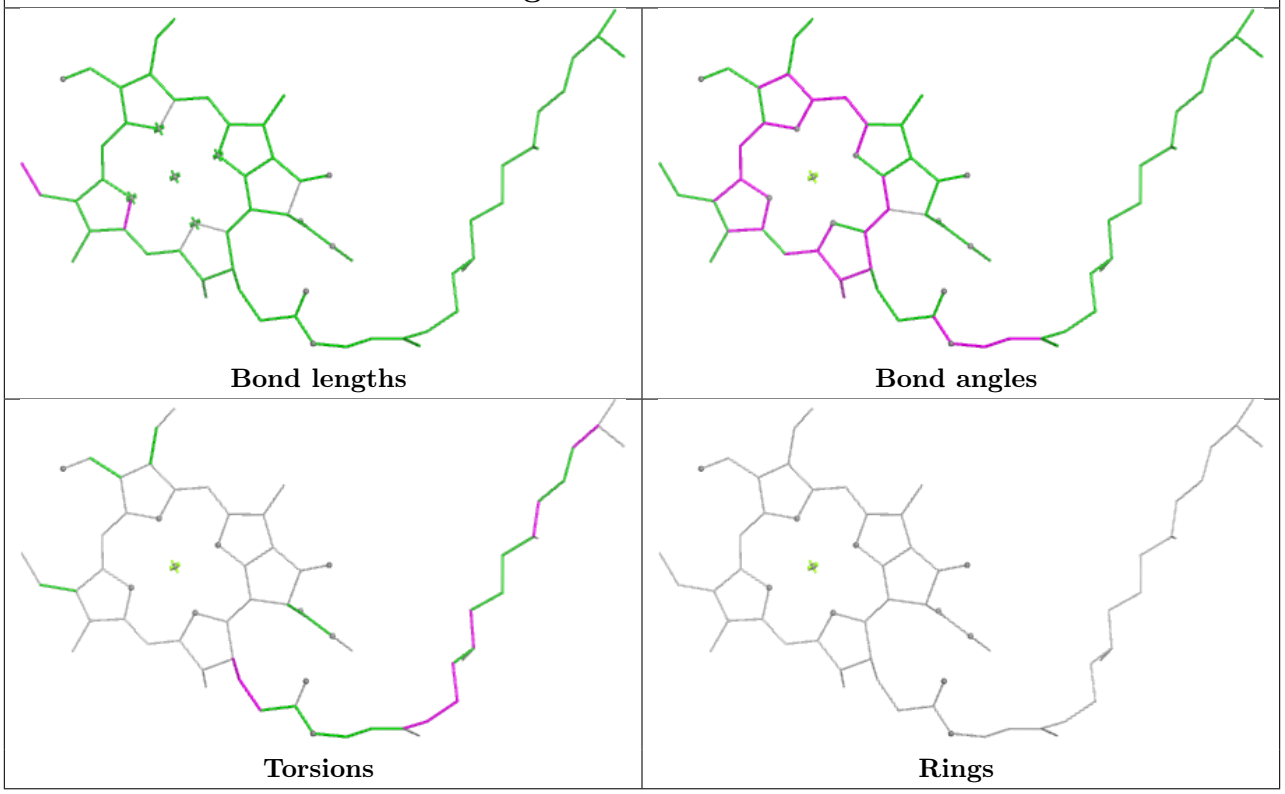


Torsions

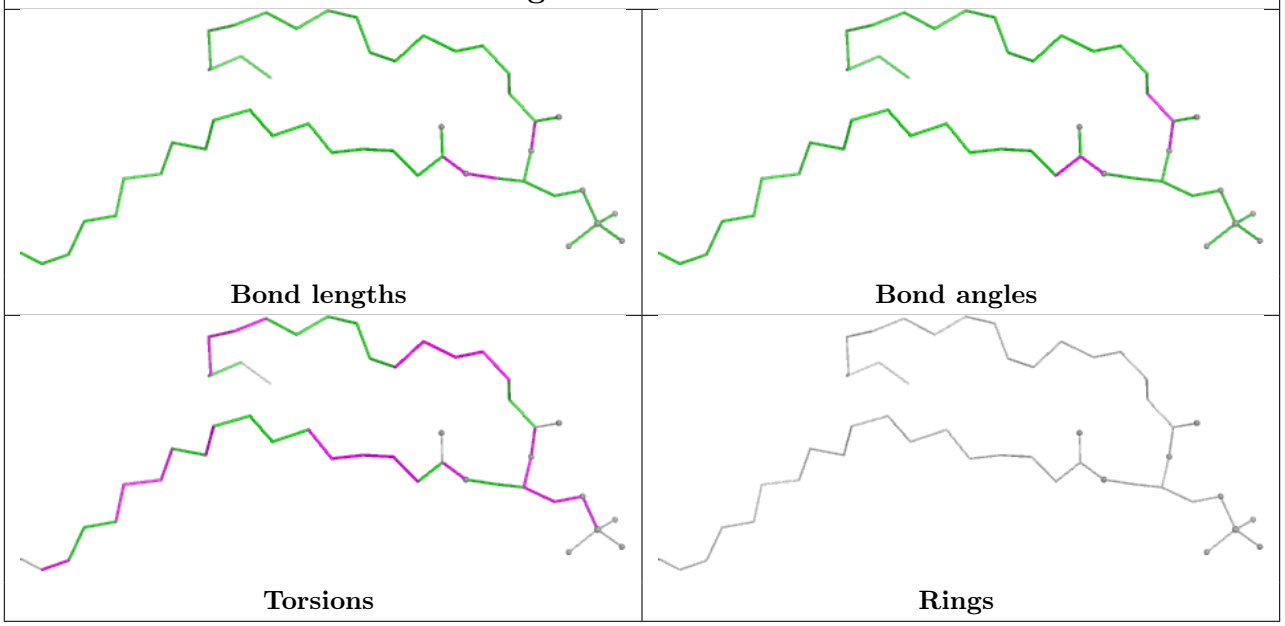


Rings

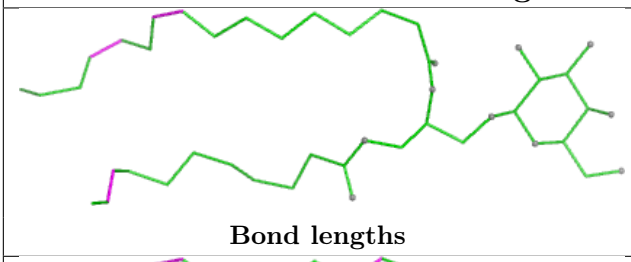
Ligand CHL N 606



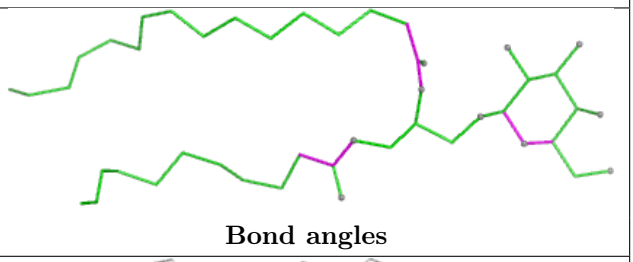
Ligand 3PH T 101



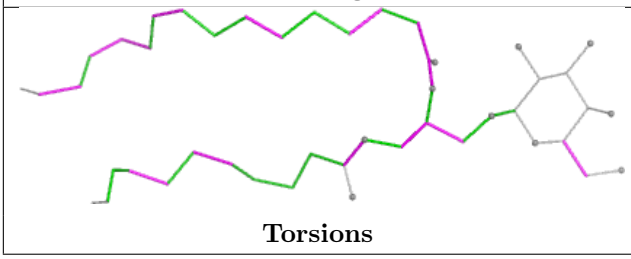
Ligand LMG d1 411



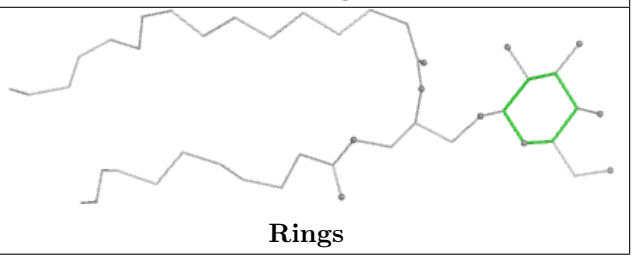
Bond lengths



Bond angles

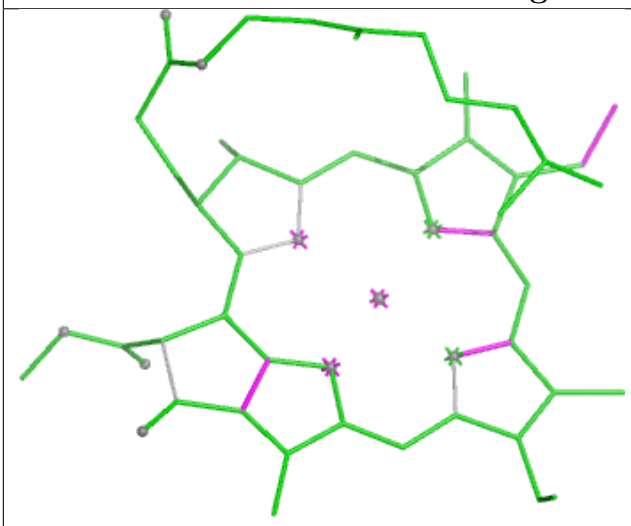


Torsions

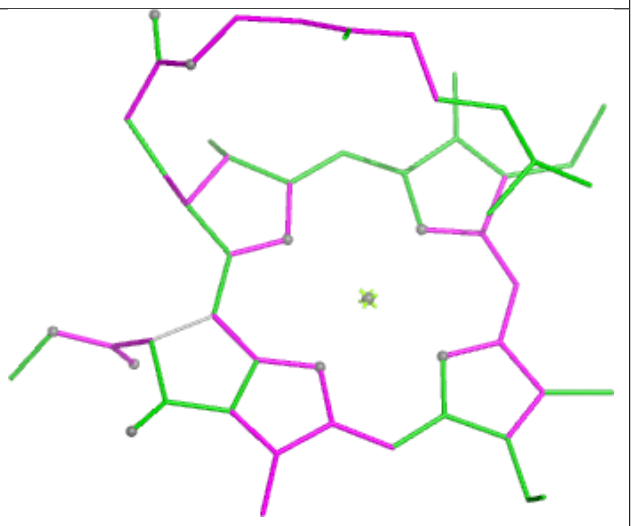


Rings

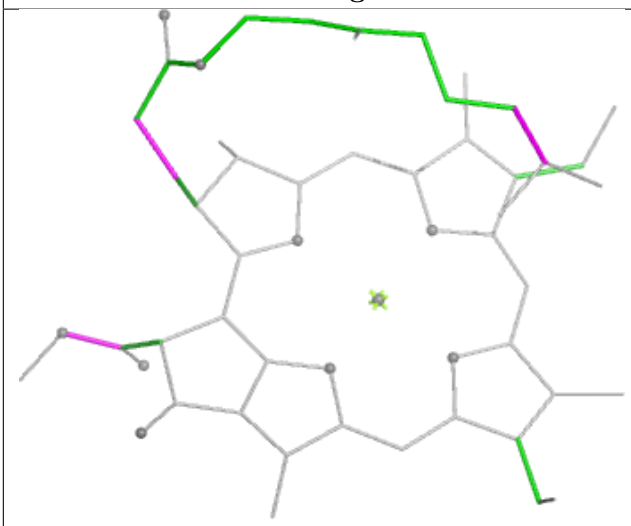
Ligand CLA s 614



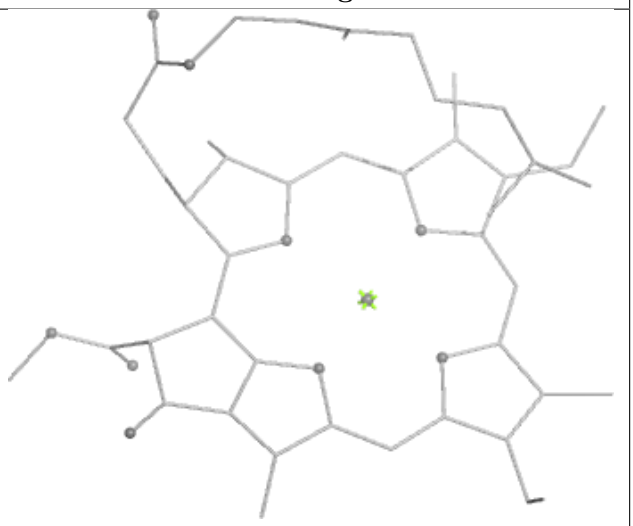
Bond lengths



Bond angles

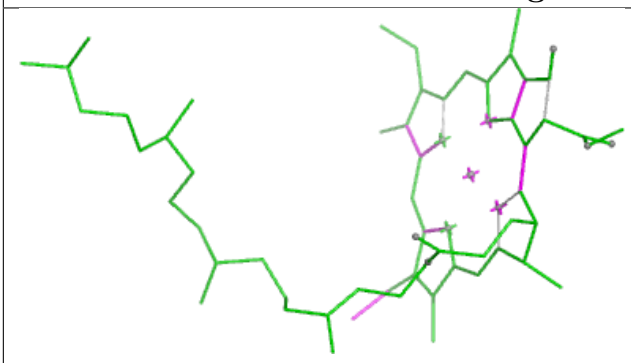


Torsions

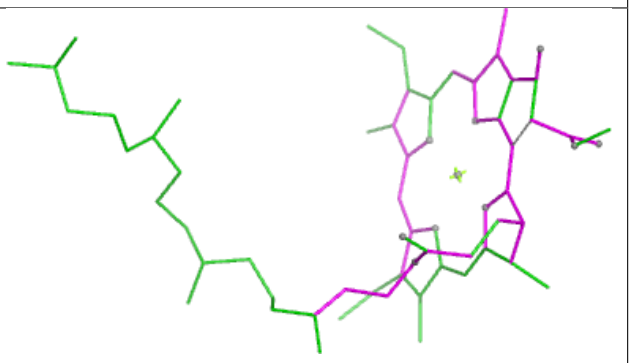


Rings

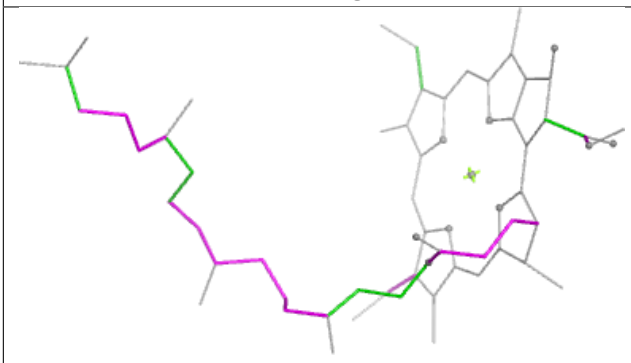
Ligand CLA S 610



Bond lengths



Bond angles

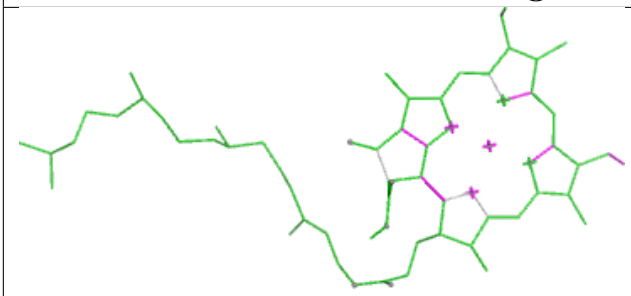


Torsions

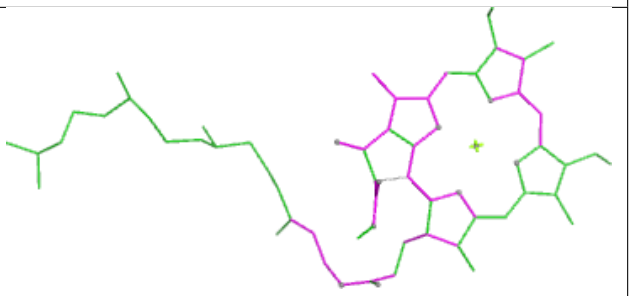


Rings

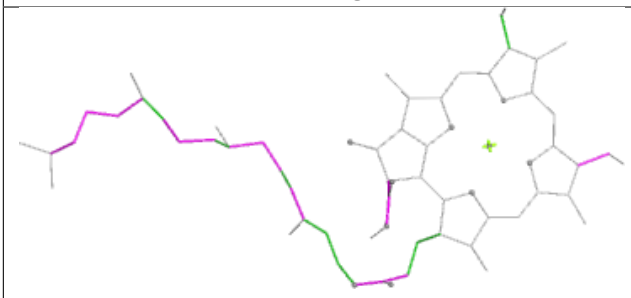
Ligand CLA b 603



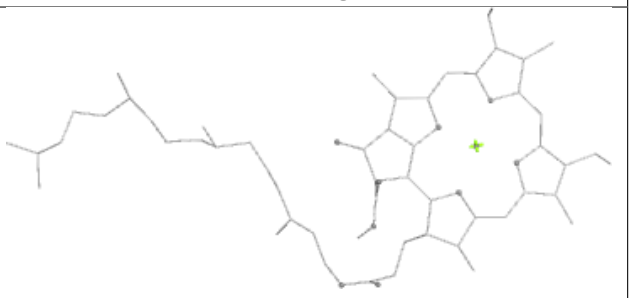
Bond lengths



Bond angles

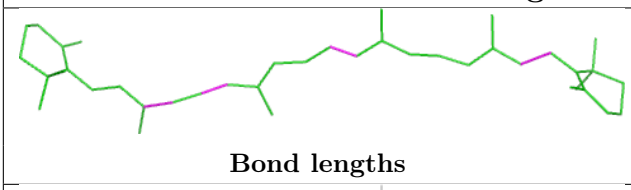


Torsions

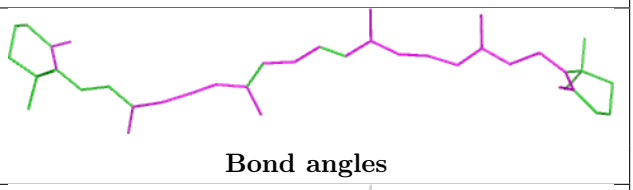


Rings

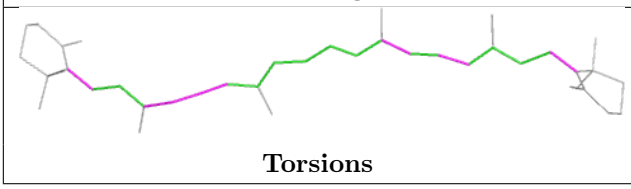
Ligand BCR a 411



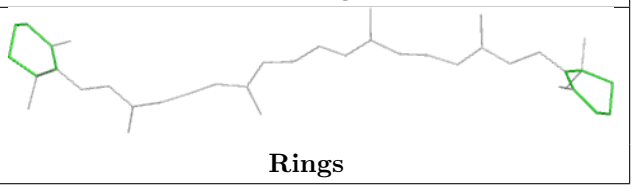
Bond lengths



Bond angles

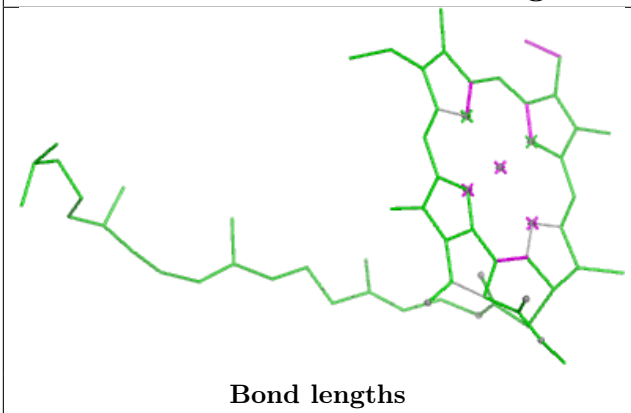


Torsions

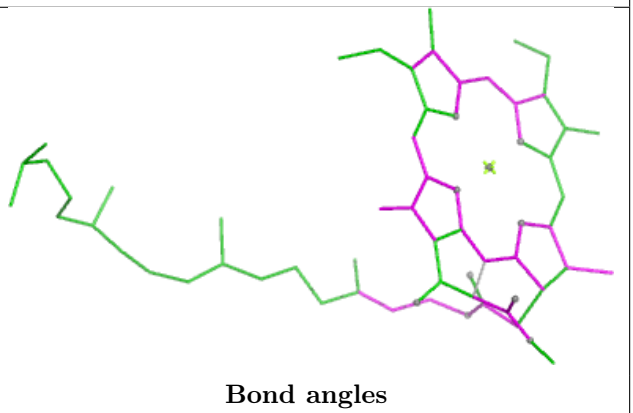


Rings

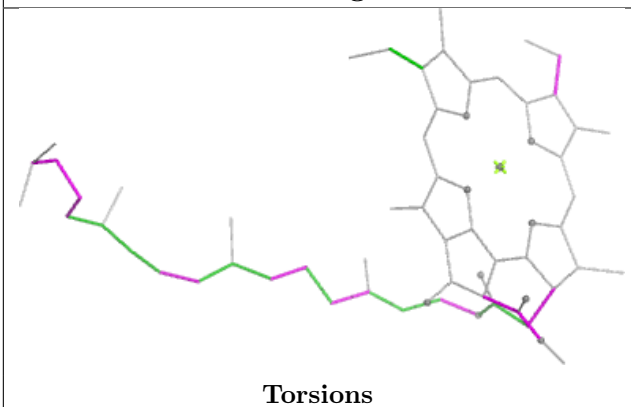
Ligand CLA S 611



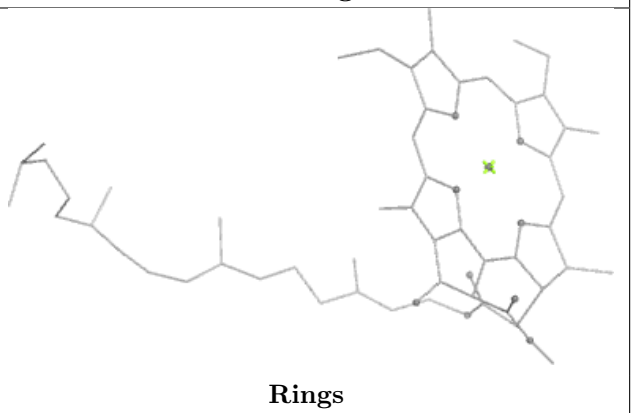
Bond lengths



Bond angles

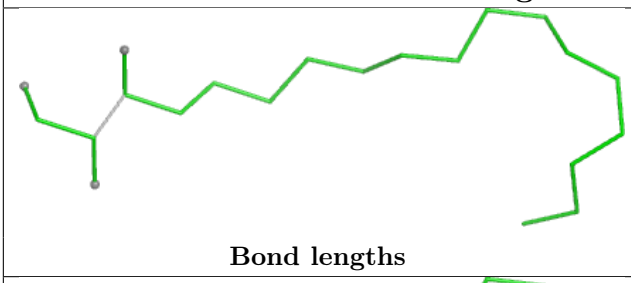


Torsions

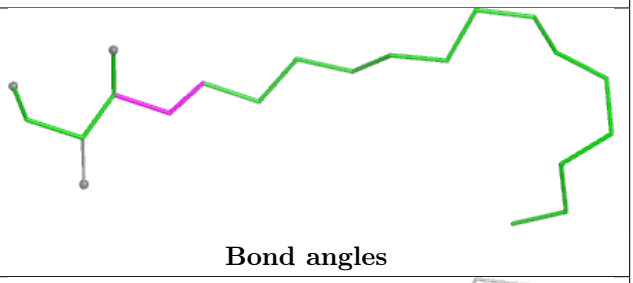


Rings

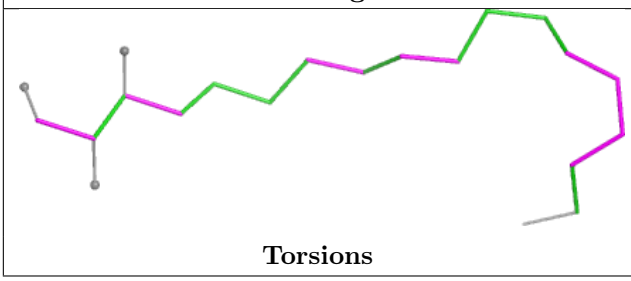
Ligand SPH Y1 625



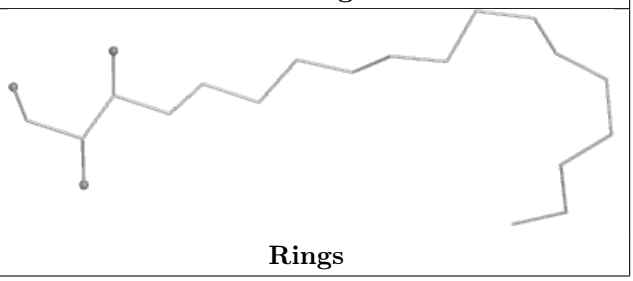
Bond lengths



Bond angles

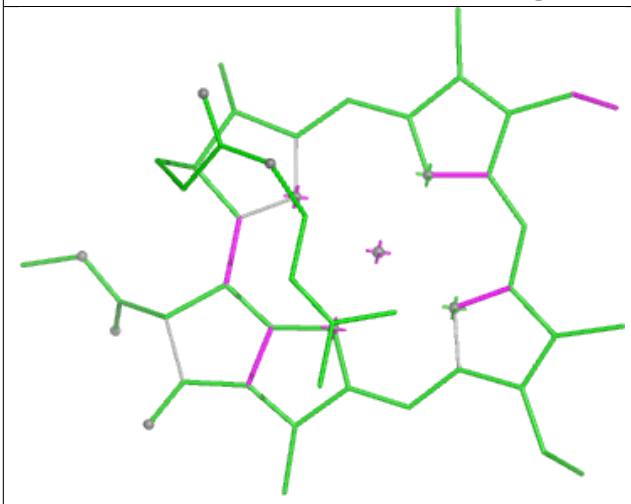


Torsions

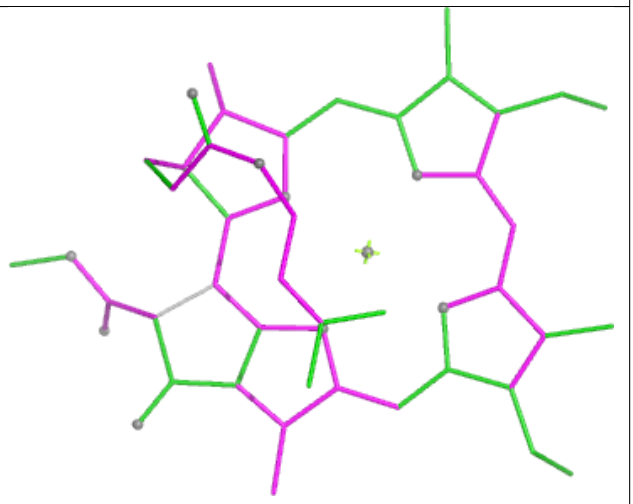


Rings

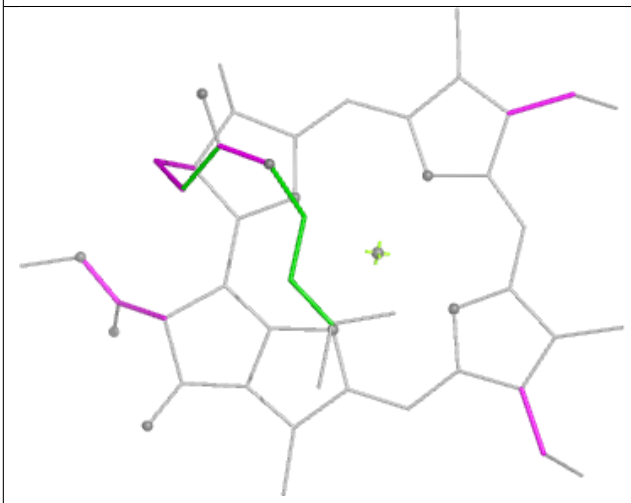
Ligand CLA s 605



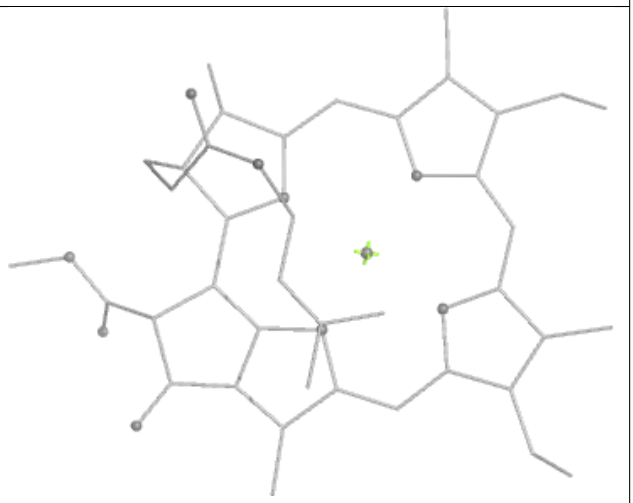
Bond lengths



Bond angles

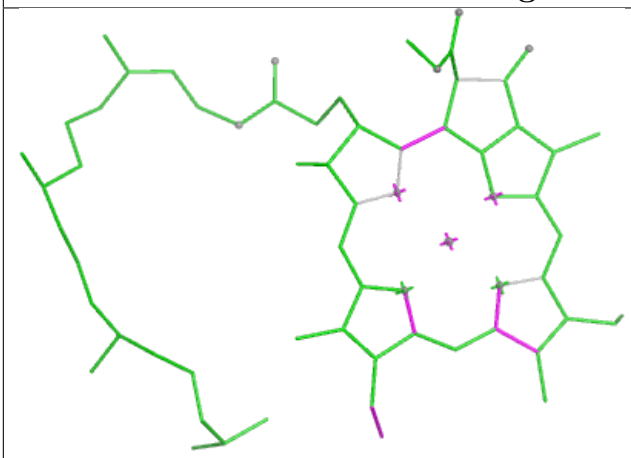


Torsions

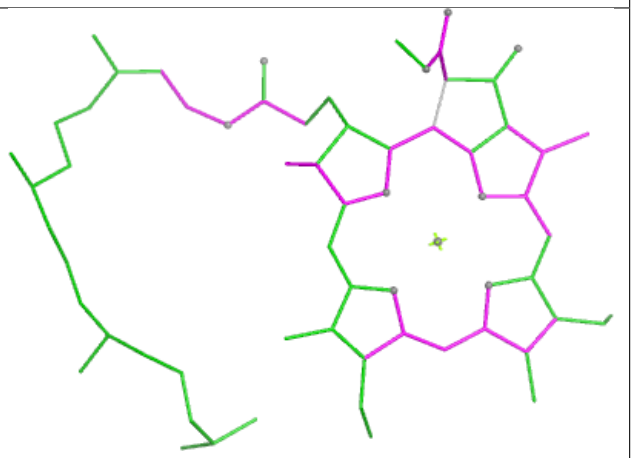


Rings

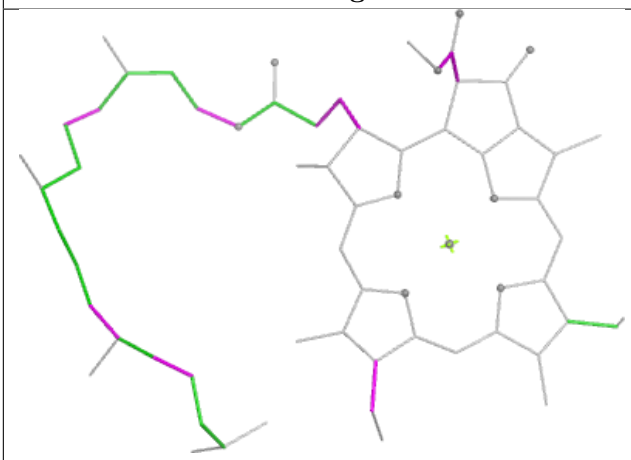
Ligand CLA S1 603



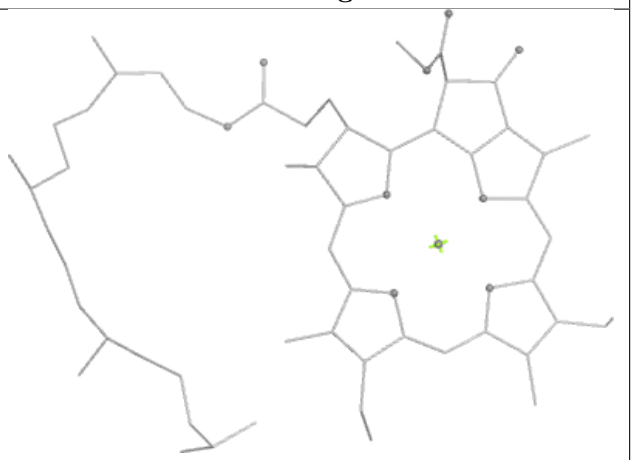
Bond lengths



Bond angles

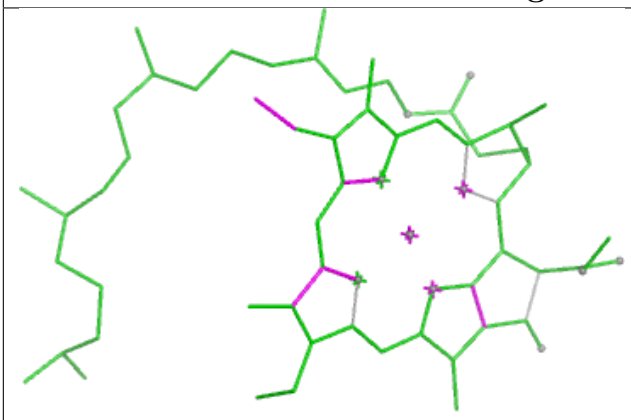


Torsions

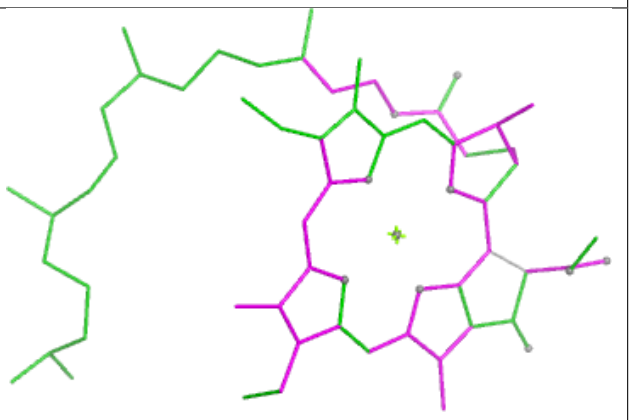


Rings

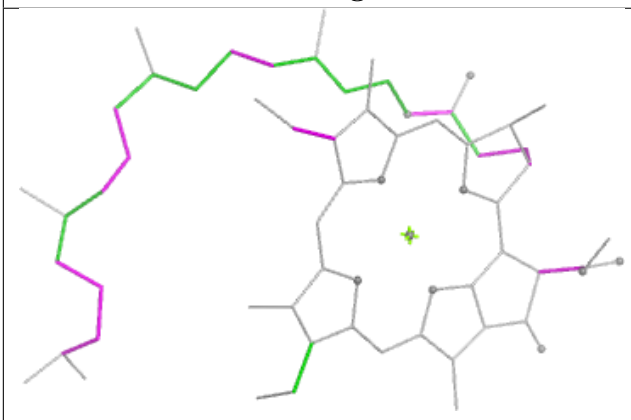
Ligand CLA n 602



Bond lengths



Bond angles

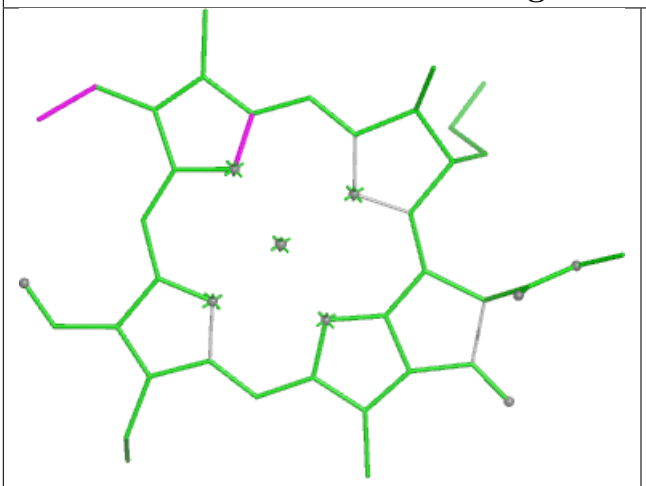


Torsions

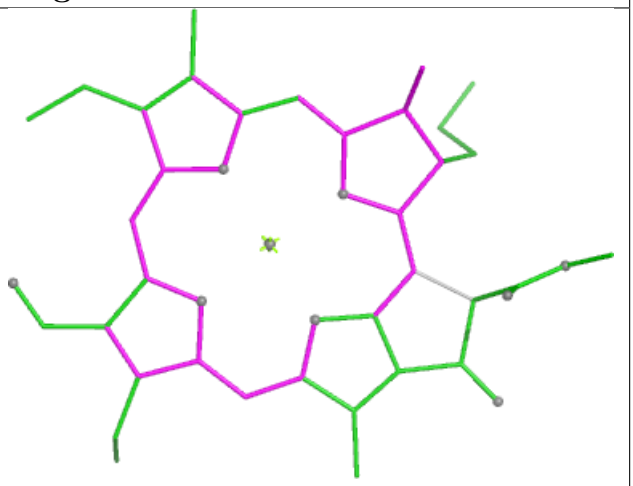


Rings

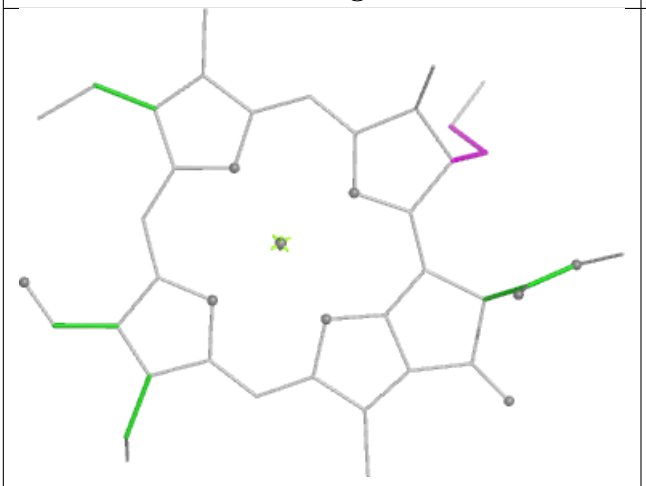
Ligand CHL g 608



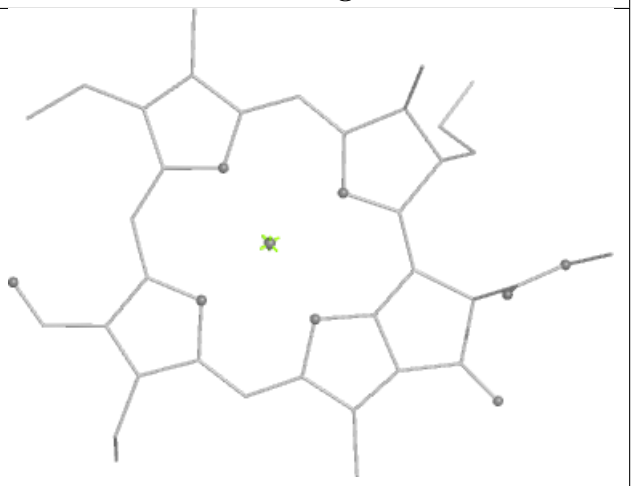
Bond lengths



Bond angles

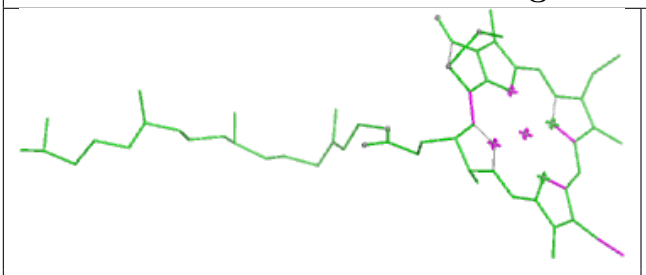


Torsions

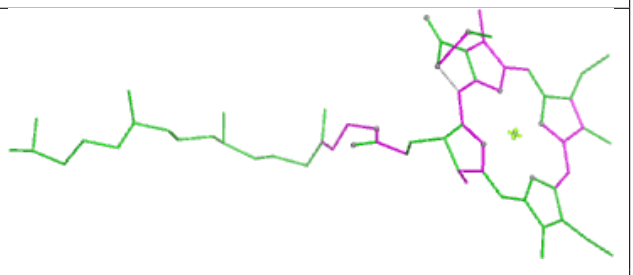


Rings

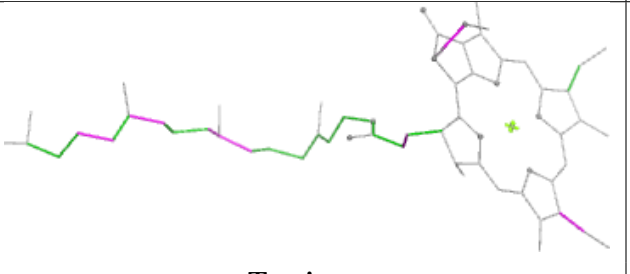
Ligand CLA c 502



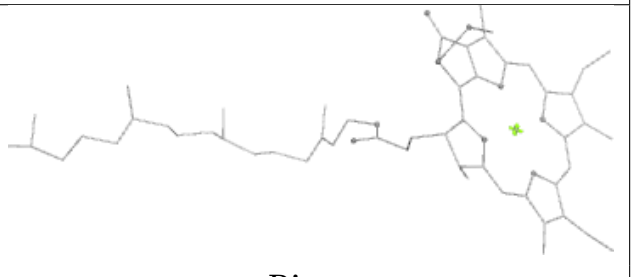
Bond lengths



Bond angles

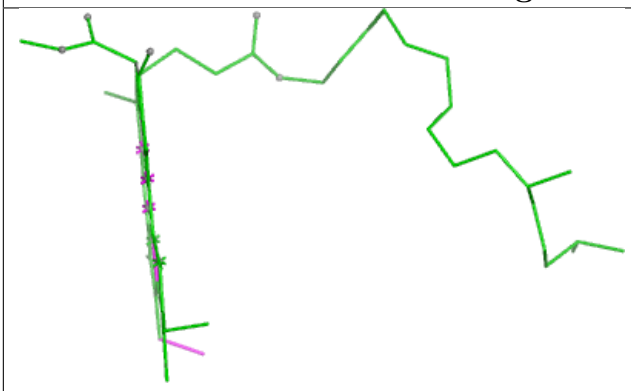


Torsions

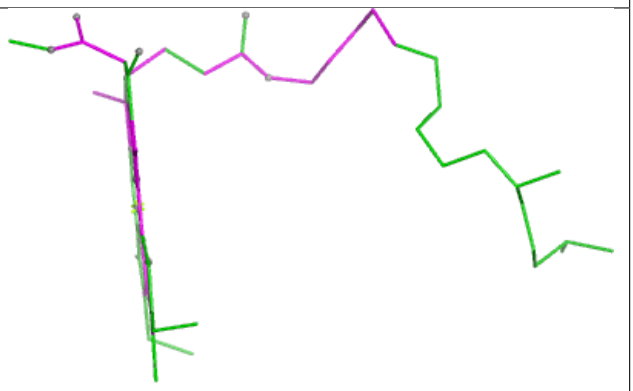


Rings

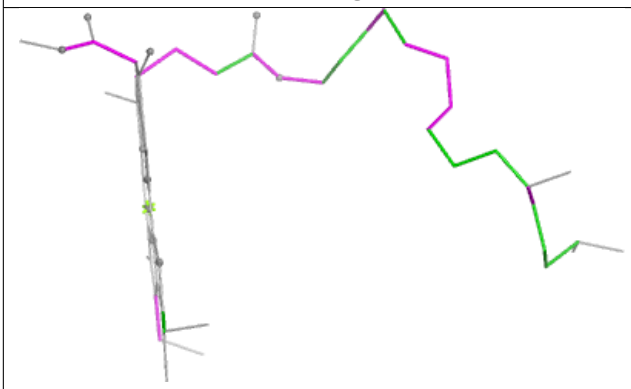
Ligand CLA C1 506



Bond lengths



Bond angles

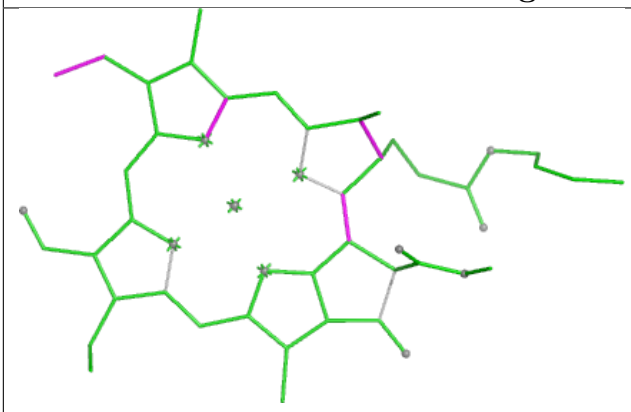


Torsions

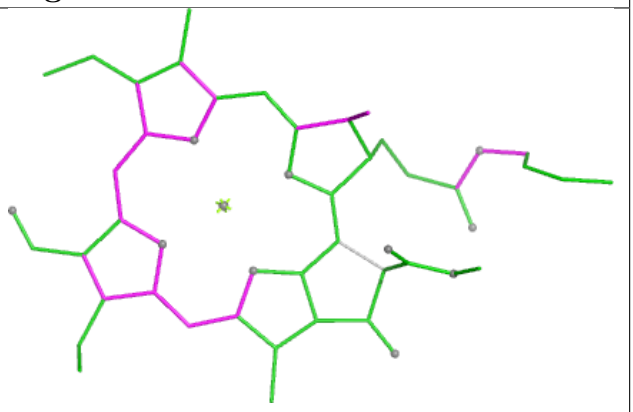


Rings

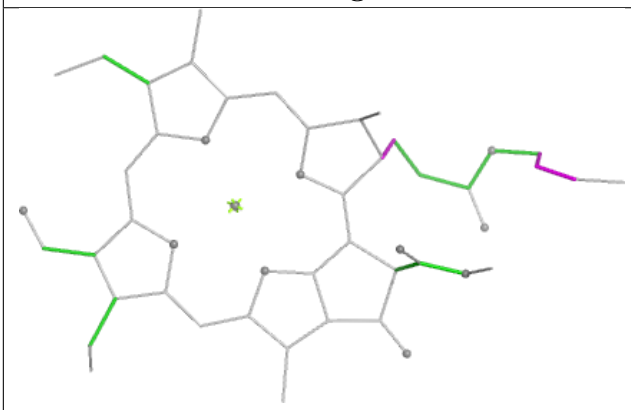
Ligand CHL g1 606



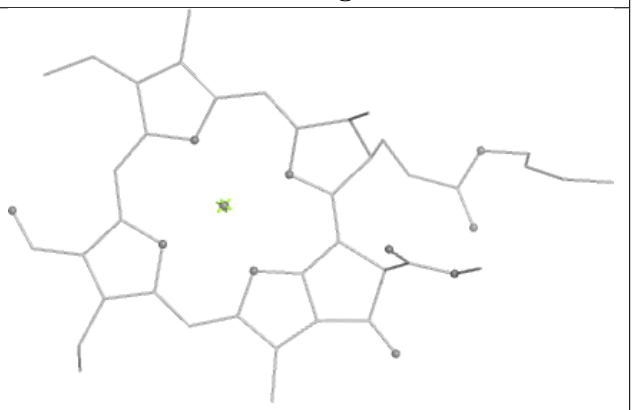
Bond lengths



Bond angles

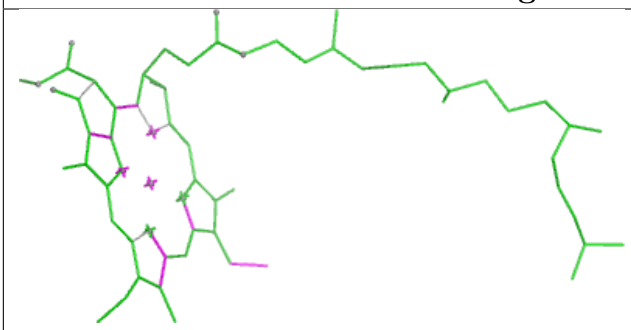


Torsions

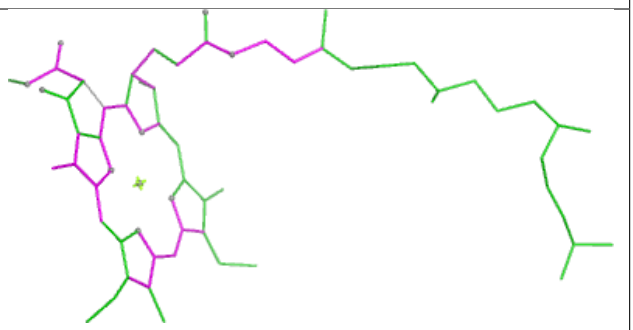


Rings

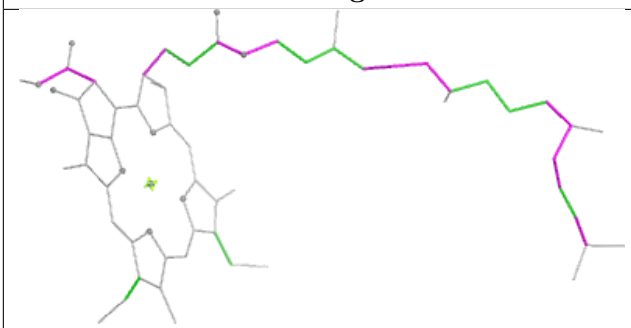
Ligand CLA b1 610



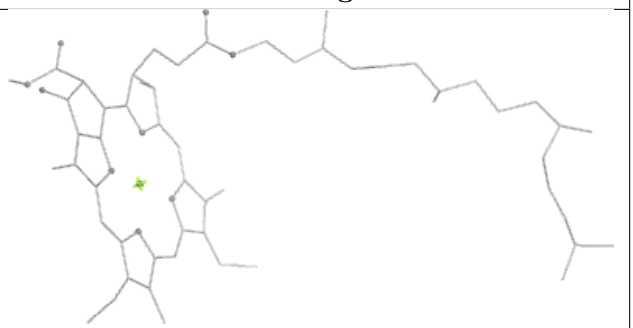
Bond lengths



Bond angles



Torsions

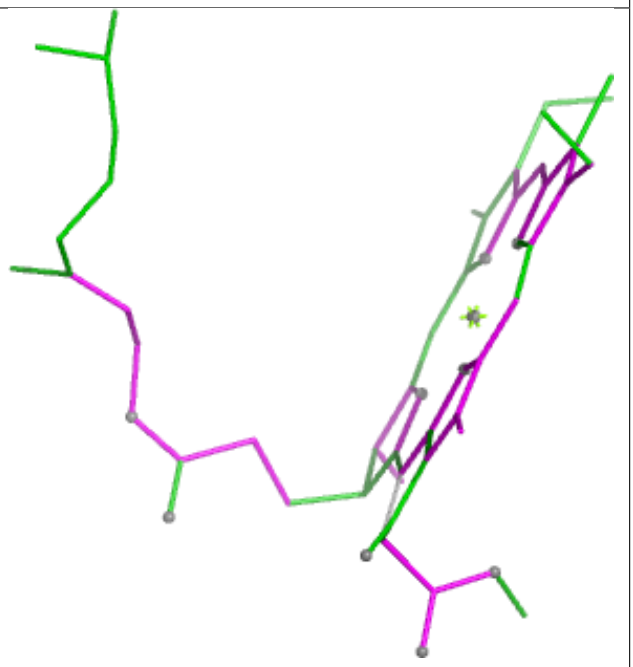


Rings

Ligand CLA S1 604



Bond lengths



Bond angles

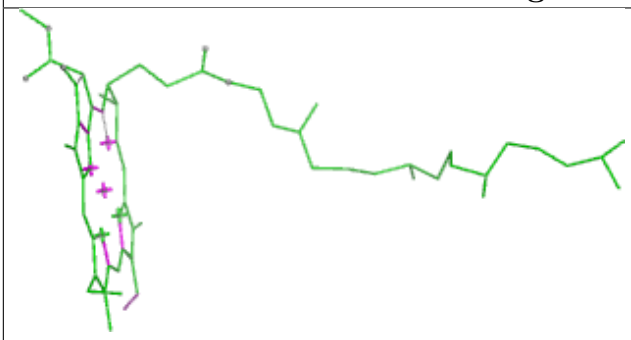


Torsions

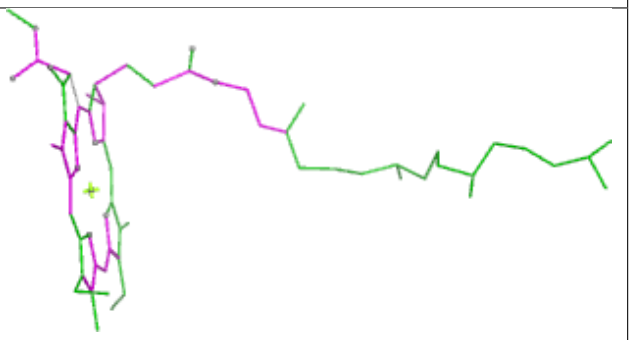


Rings

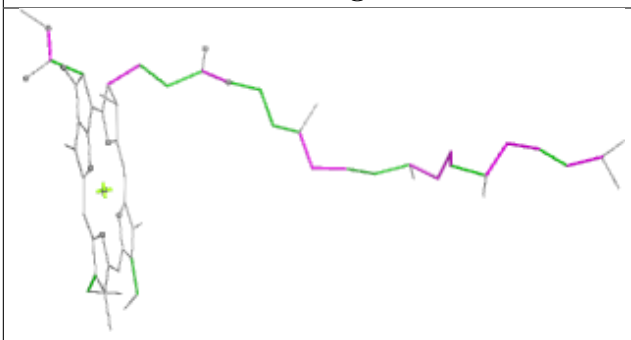
Ligand CLA d 403



Bond lengths



Bond angles

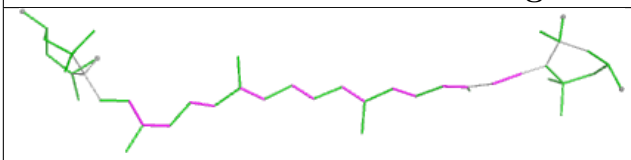


Torsions

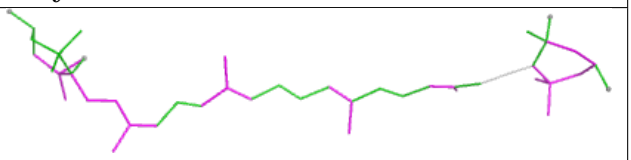


Rings

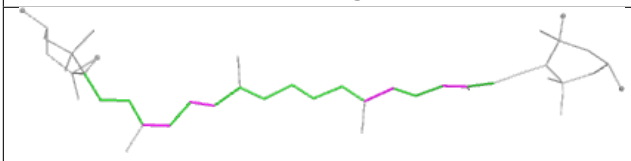
Ligand NEX y 623



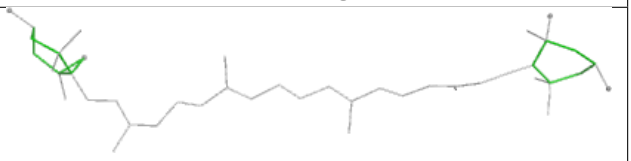
Bond lengths



Bond angles

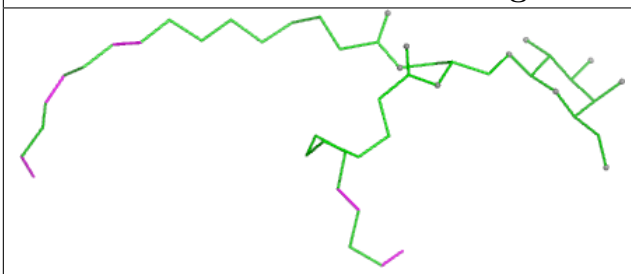


Torsions

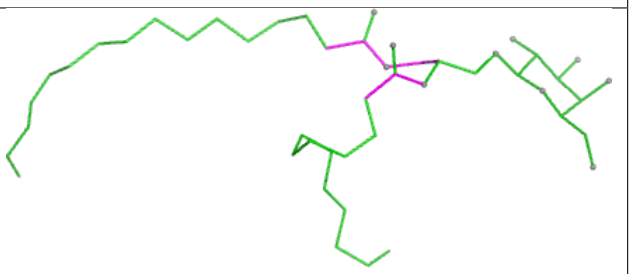


Rings

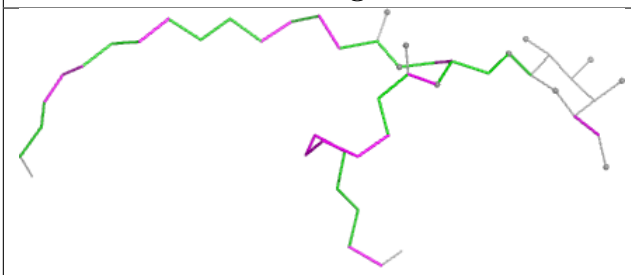
Ligand LMG H1 102



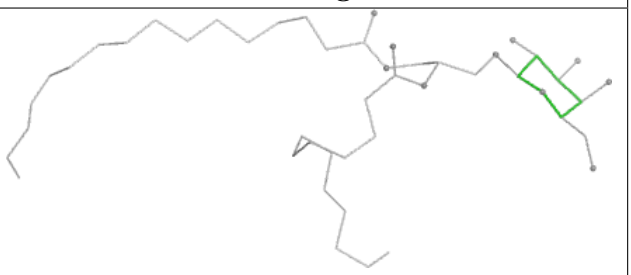
Bond lengths



Bond angles

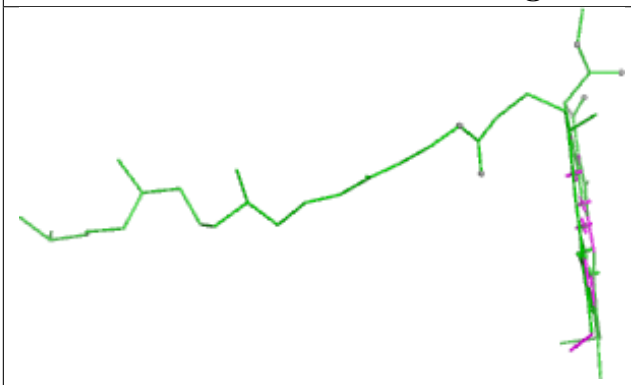


Torsions

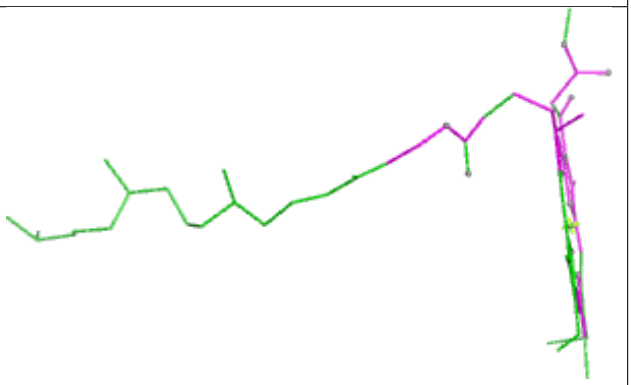


Rings

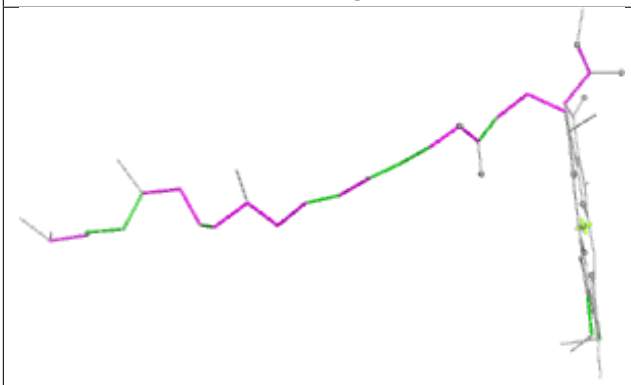
Ligand CLA B 607



Bond lengths



Bond angles

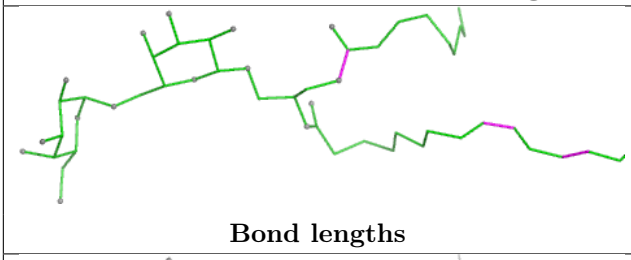


Torsions

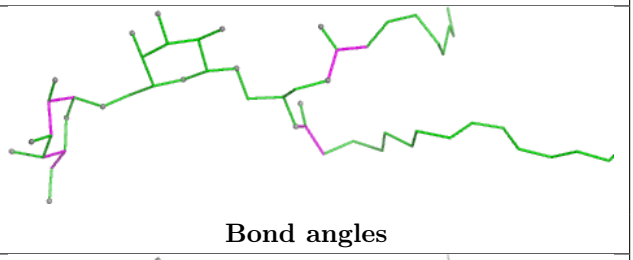


Rings

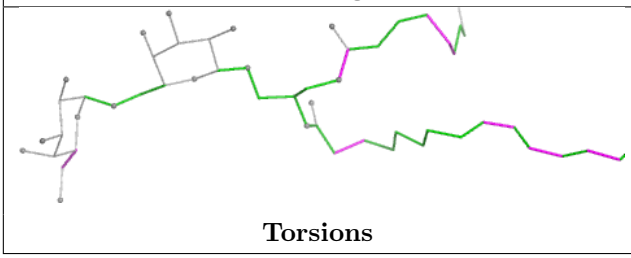
Ligand DGD c 518



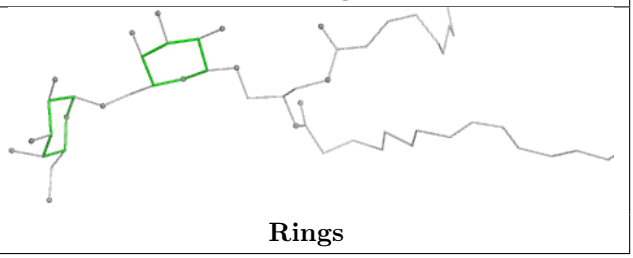
Bond lengths



Bond angles

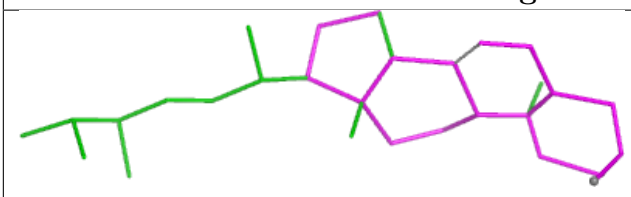


Torsions

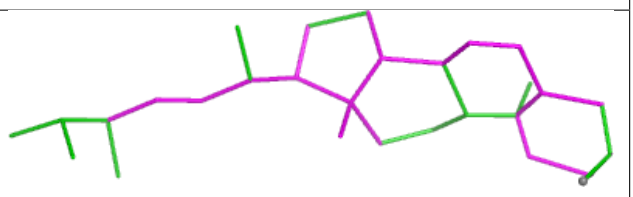


Rings

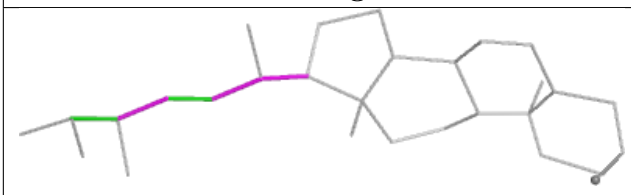
Ligand ERG r1 626



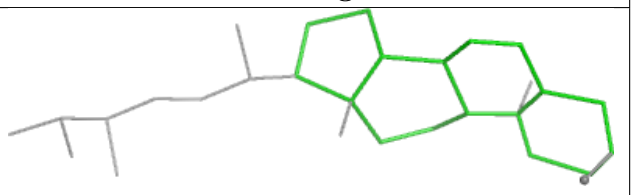
Bond lengths



Bond angles

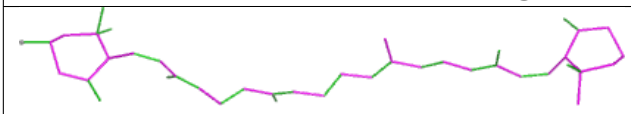


Torsions

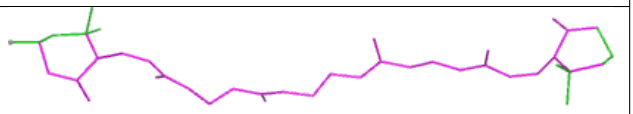


Rings

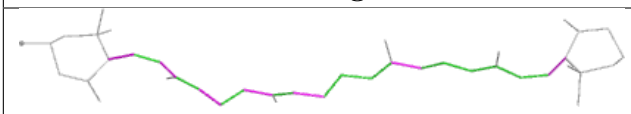
Ligand RRX h1 101



Bond lengths



Bond angles

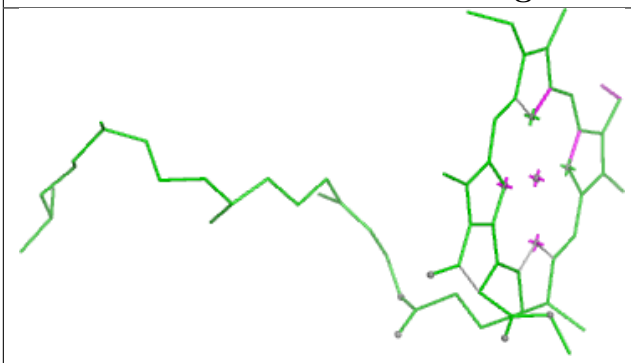


Torsions

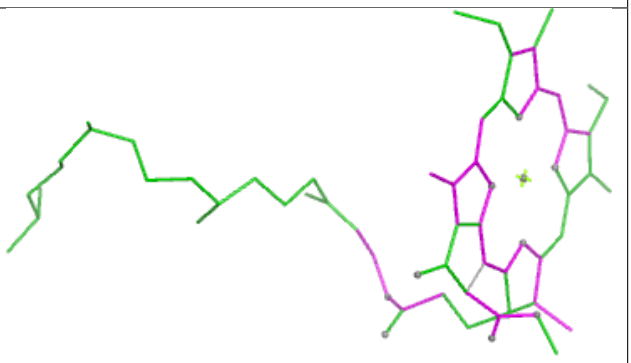


Rings

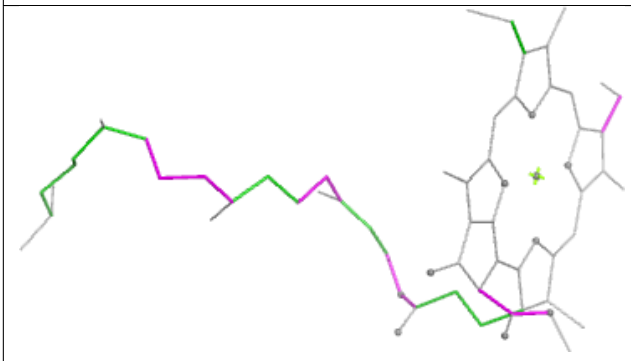
Ligand CLA Y1 604



Bond lengths



Bond angles

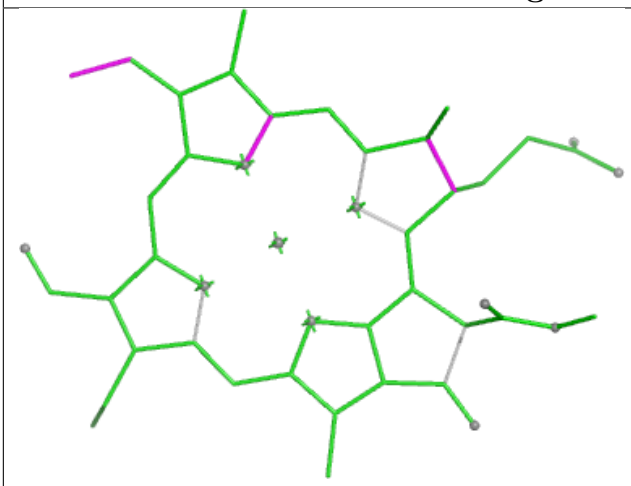


Torsions

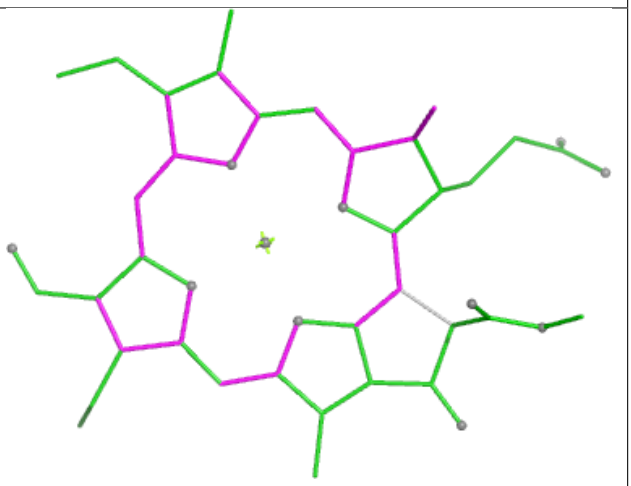


Rings

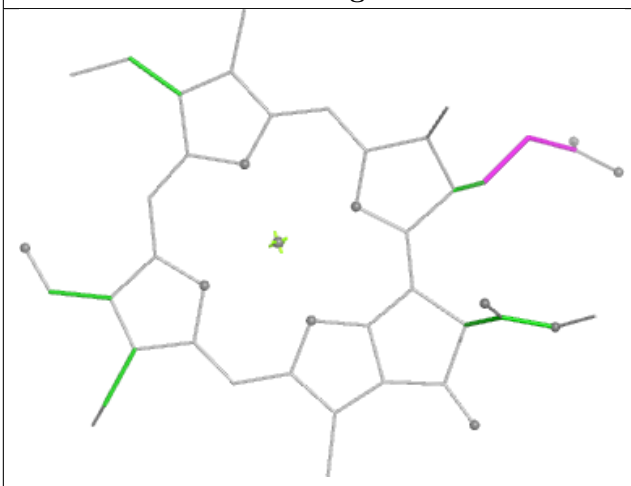
Ligand CHL S 601



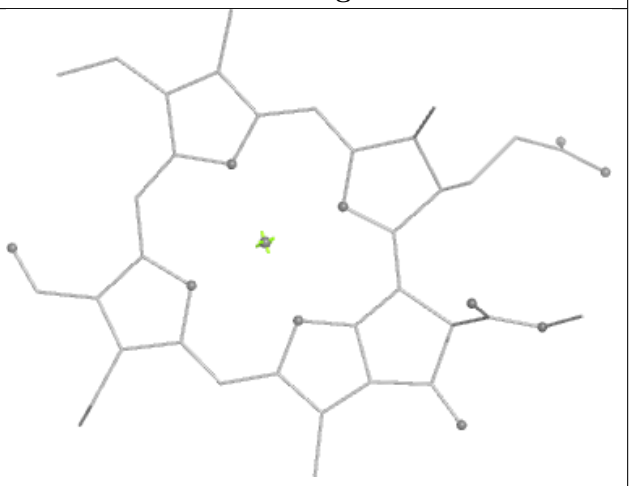
Bond lengths



Bond angles

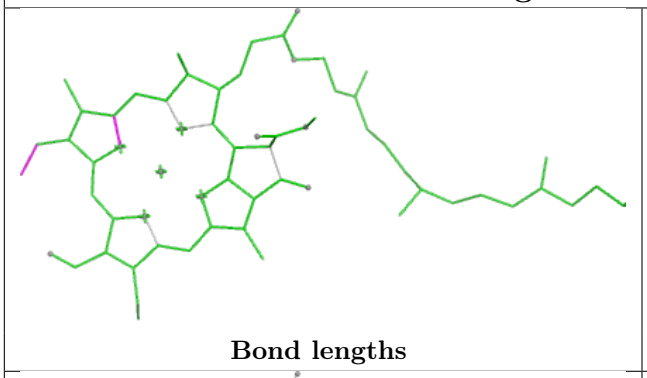


Torsions

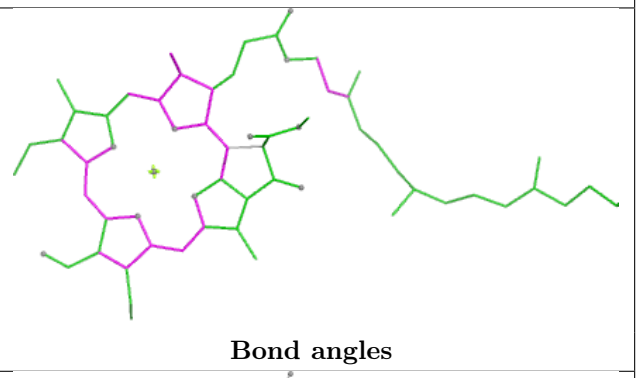


Rings

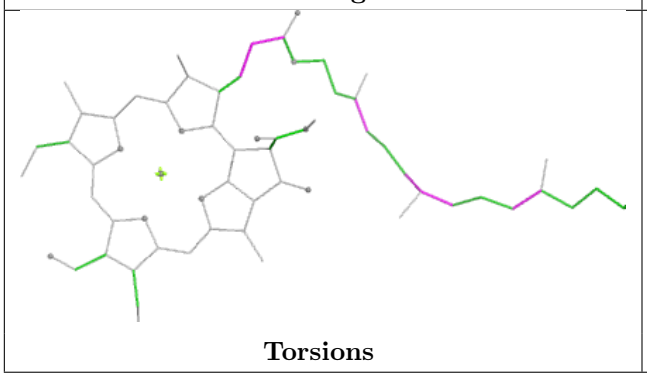
Ligand CHL N1 605



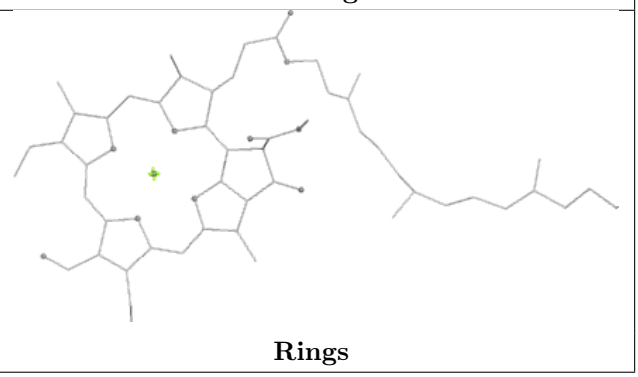
Bond lengths



Bond angles

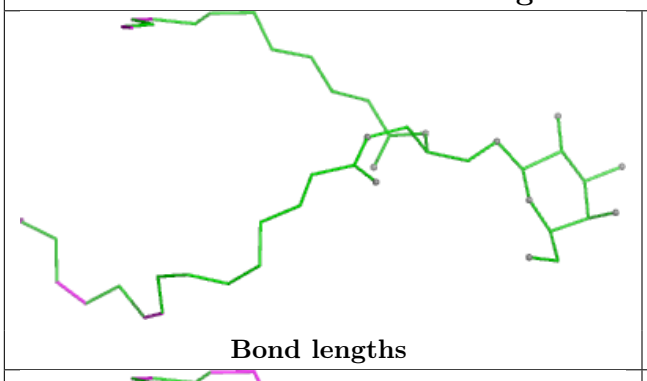


Torsions

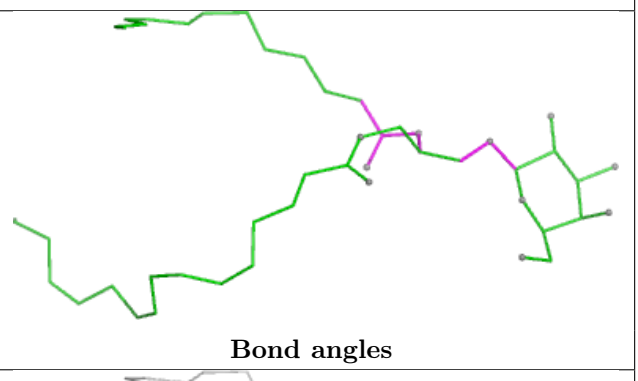


Rings

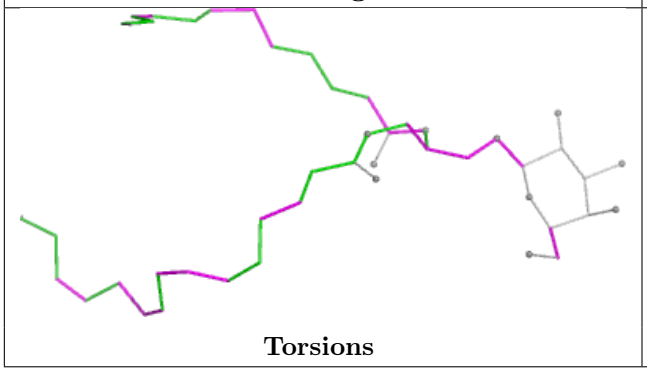
Ligand LMG a1 413



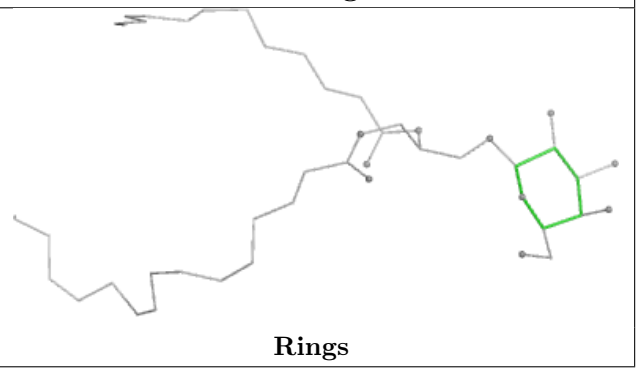
Bond lengths



Bond angles

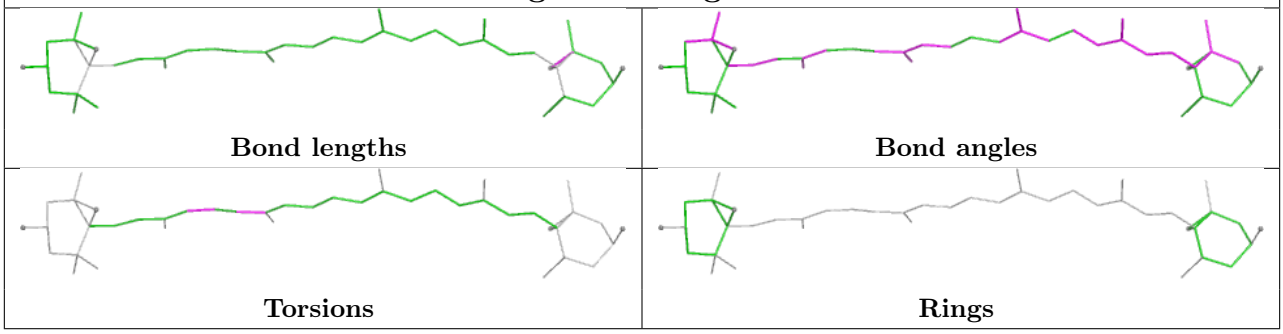


Torsions

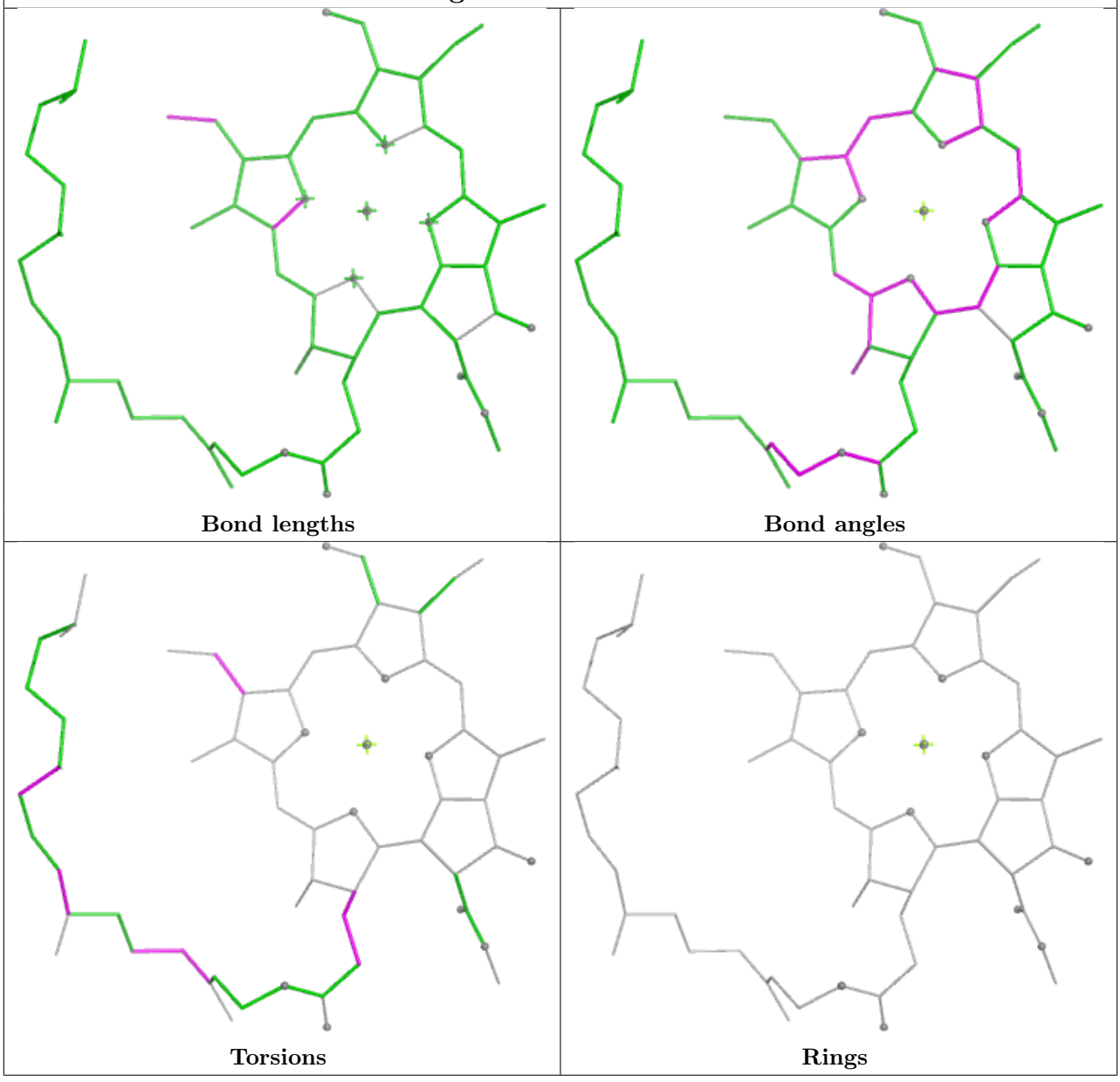


Rings

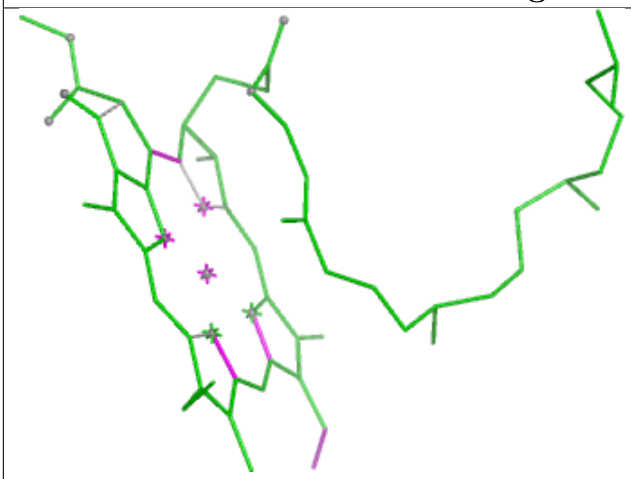
Ligand XAT g 622



Ligand CHL N1 607



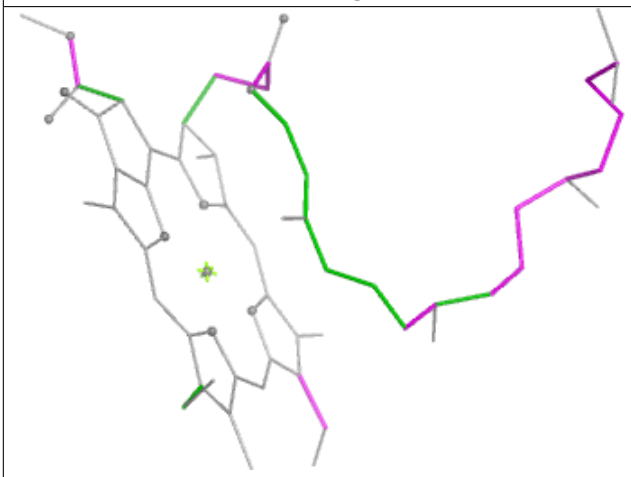
Ligand CLA g 613



Bond lengths



Bond angles



Torsions



Rings

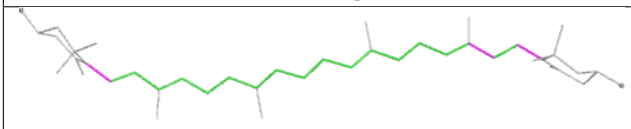
Ligand LUT y 620



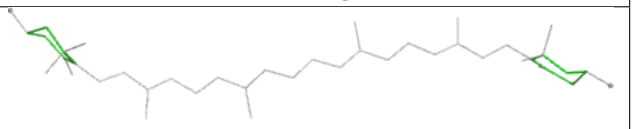
Bond lengths



Bond angles

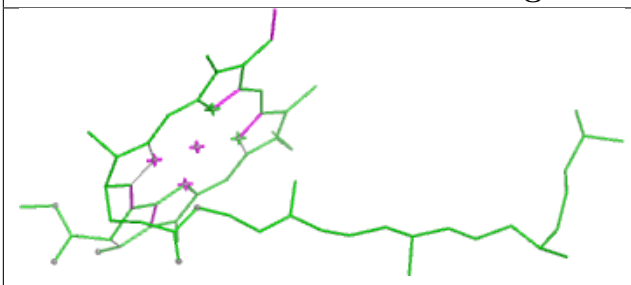


Torsions

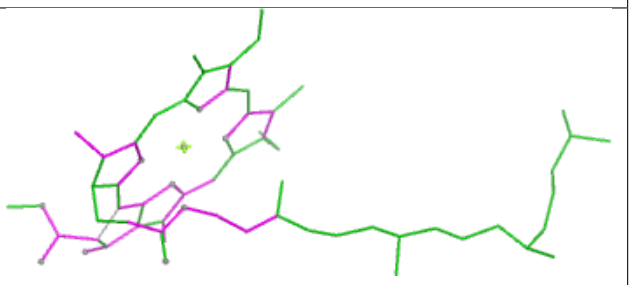


Rings

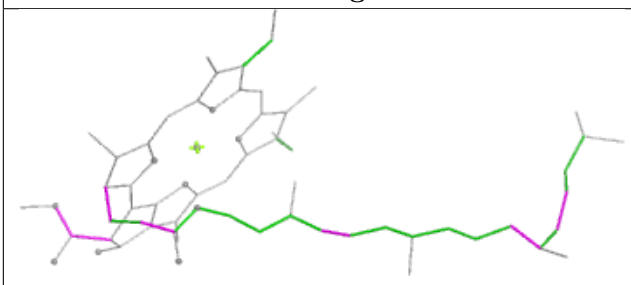
Ligand CLA B 609



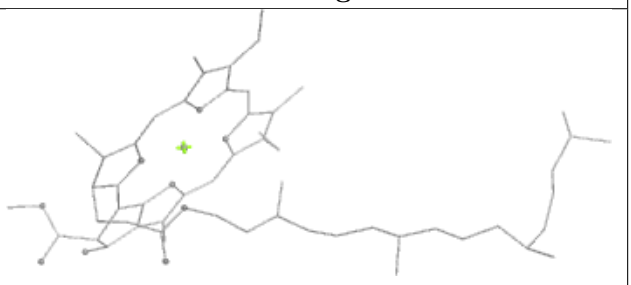
Bond lengths



Bond angles

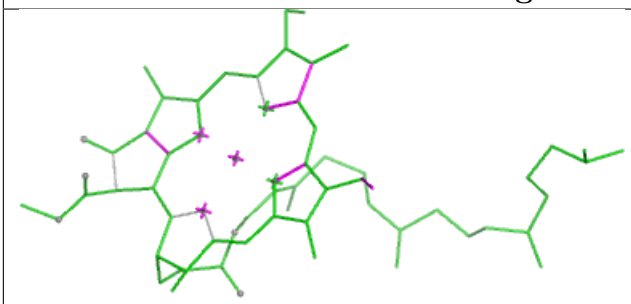


Torsions

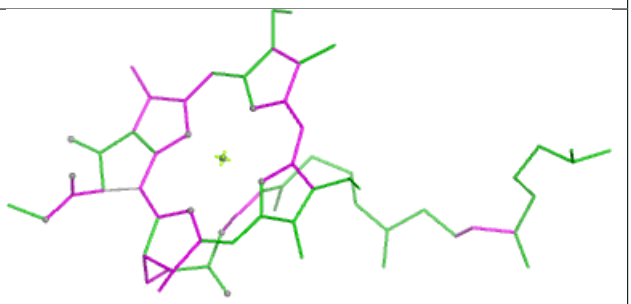


Rings

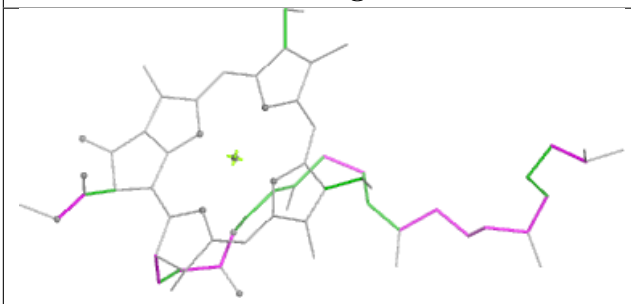
Ligand CLA C1 513



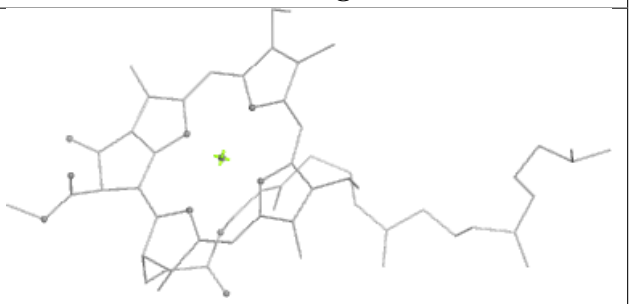
Bond lengths



Bond angles

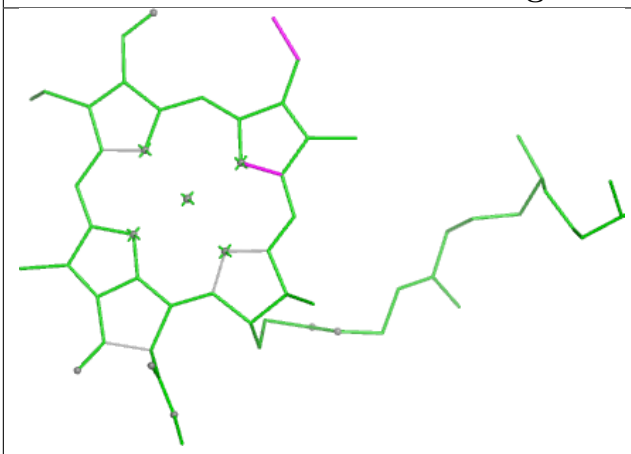


Torsions

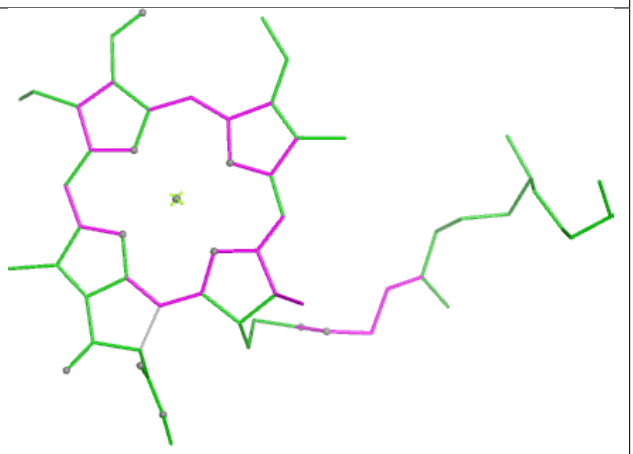


Rings

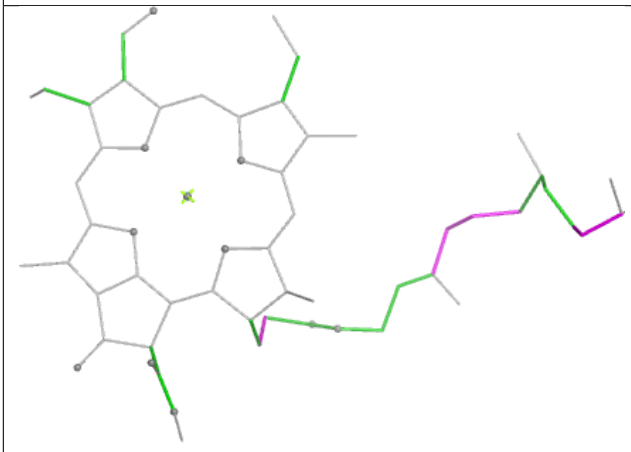
Ligand CHL S 608



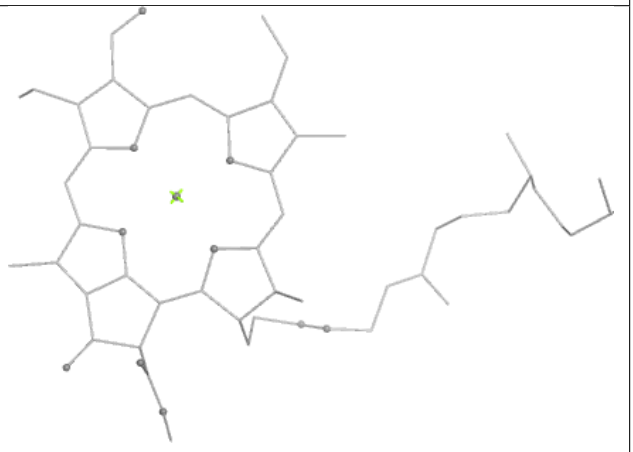
Bond lengths



Bond angles

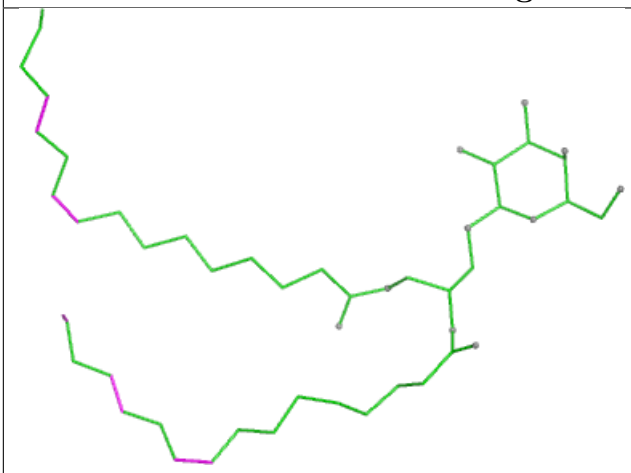


Torsions

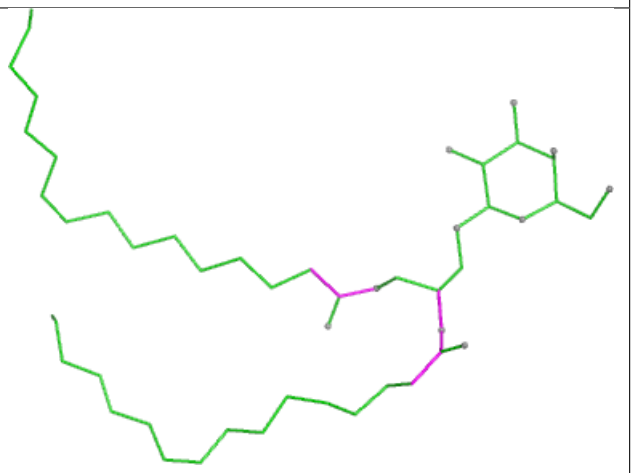


Rings

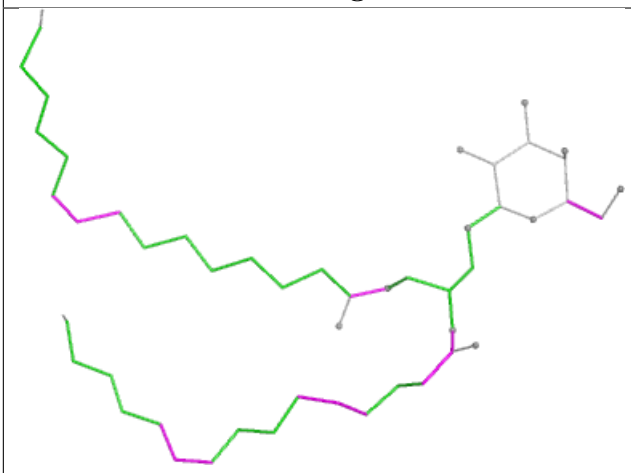
Ligand LMG c1 521



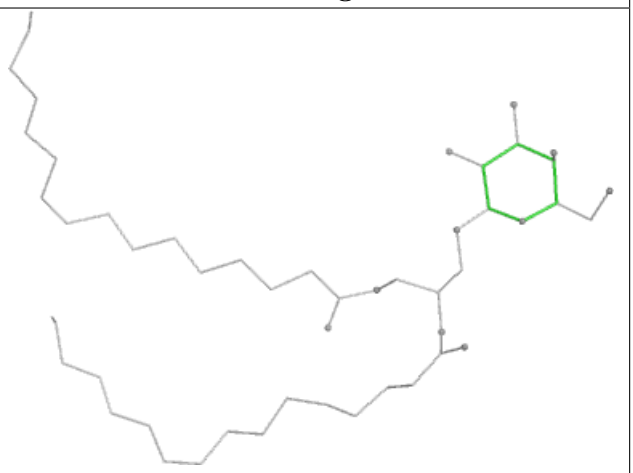
Bond lengths



Bond angles

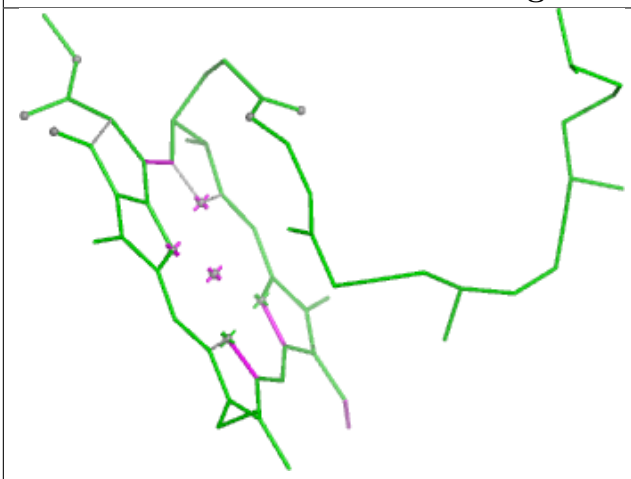


Torsions

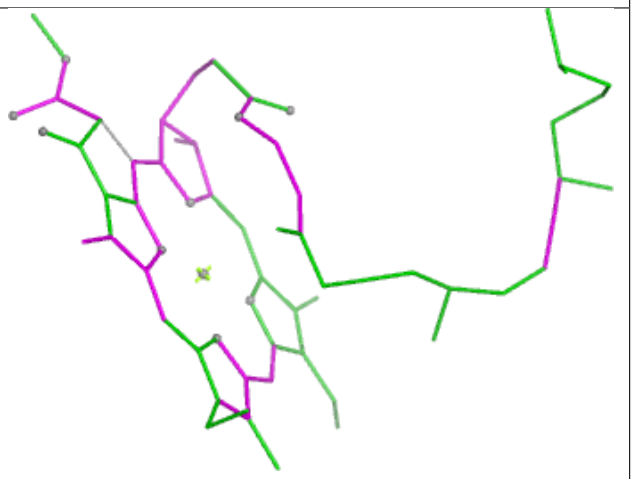


Rings

Ligand CLA n 613



Bond lengths



Bond angles

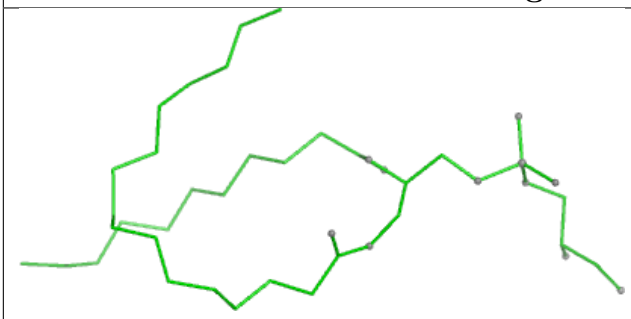


Torsions

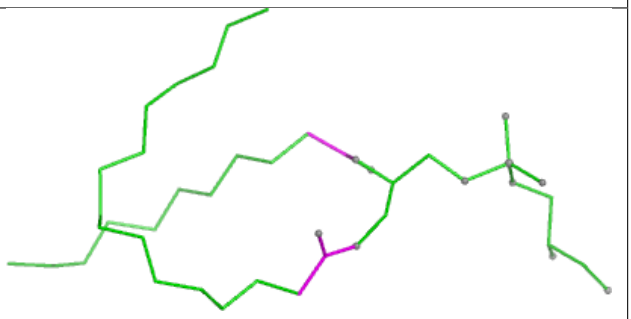


Rings

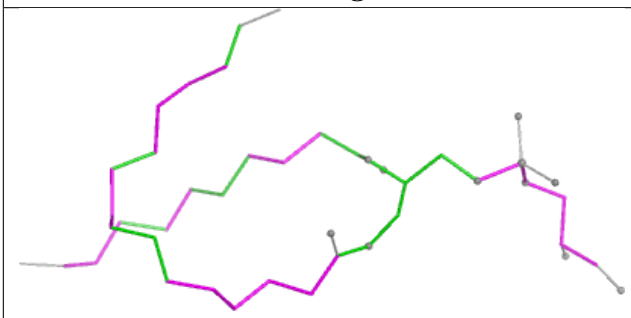
Ligand LHG d 408



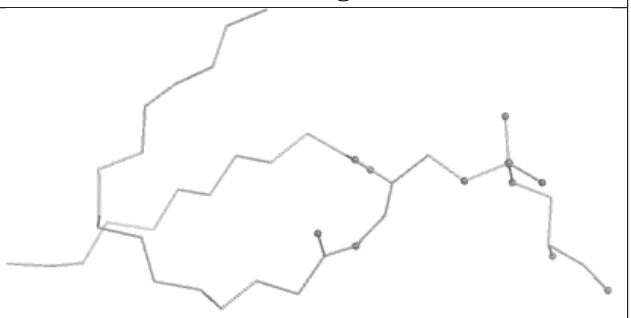
Bond lengths



Bond angles

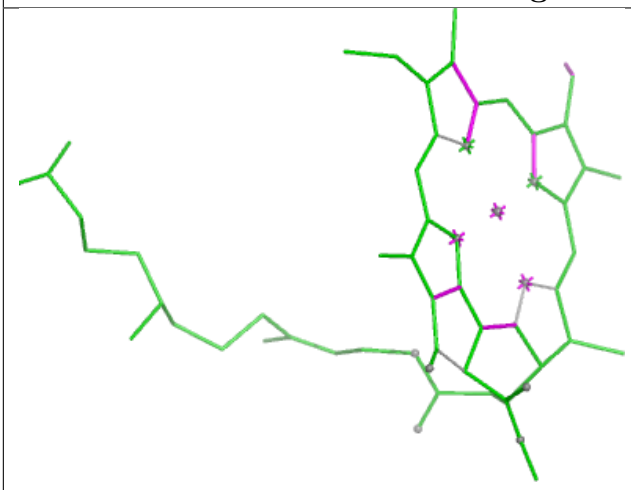


Torsions

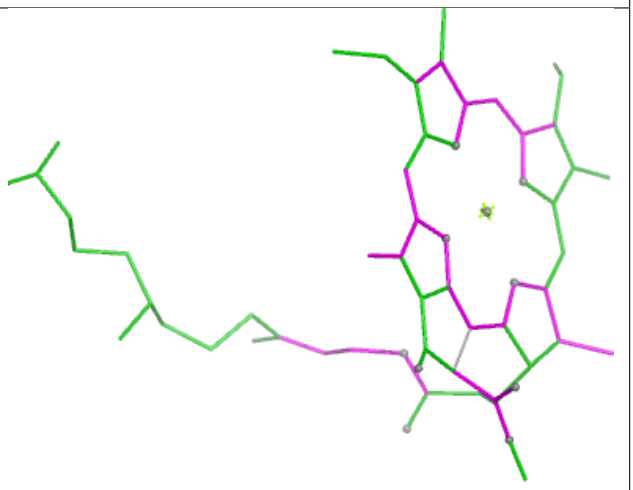


Rings

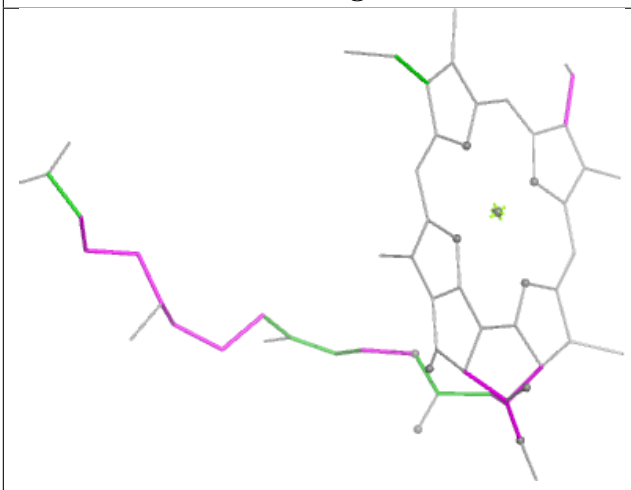
Ligand CLA s 609



Bond lengths



Bond angles

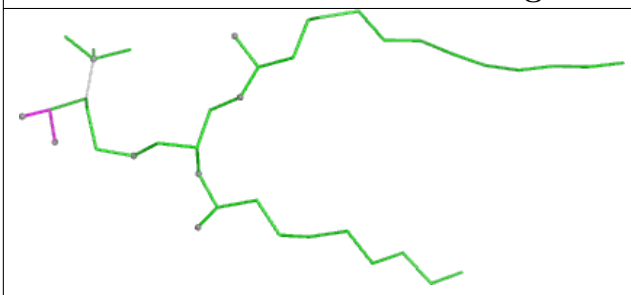


Torsions

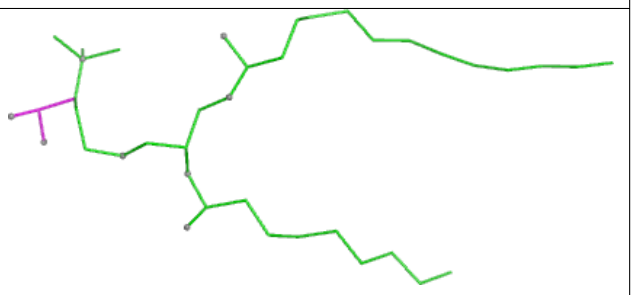


Rings

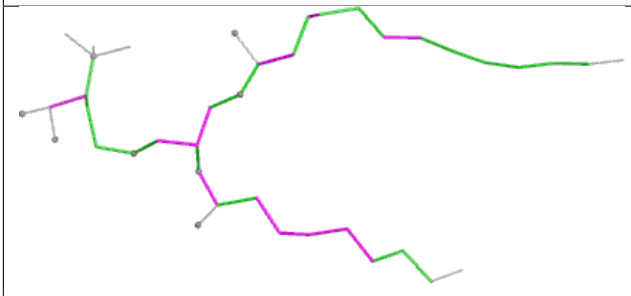
Ligand LMK c 527



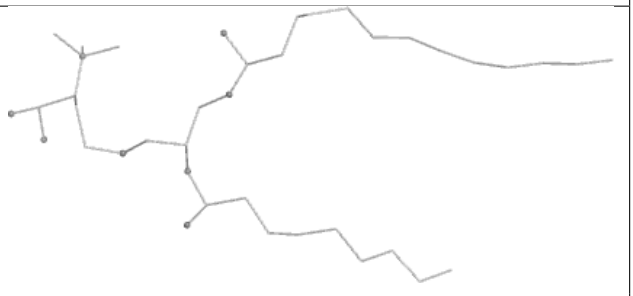
Bond lengths



Bond angles

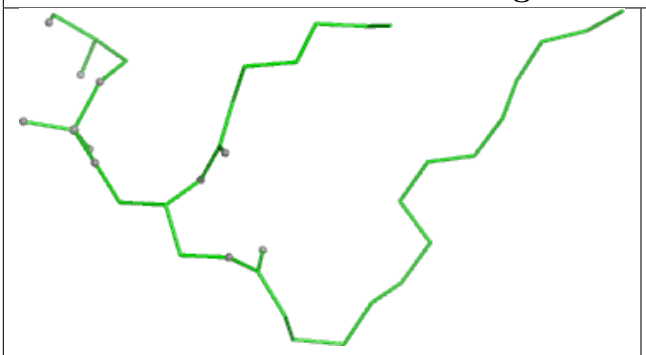


Torsions



Rings

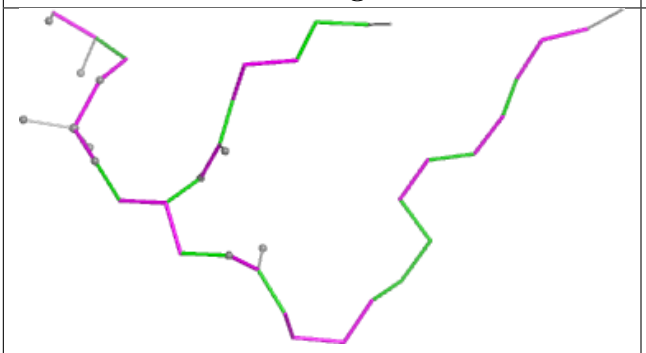
Ligand LHG D1 410



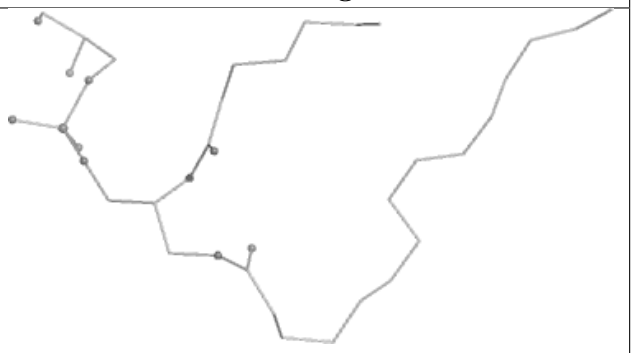
Bond lengths



Bond angles

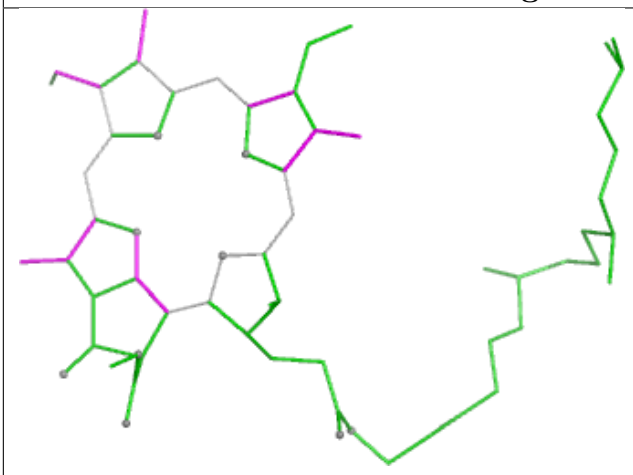


Torsions

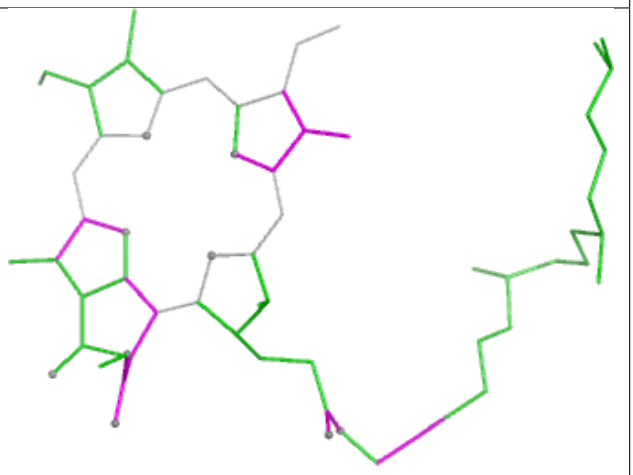


Rings

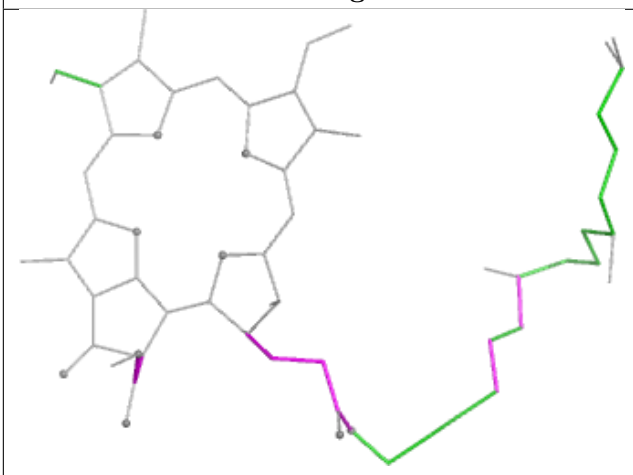
Ligand PHO A 409



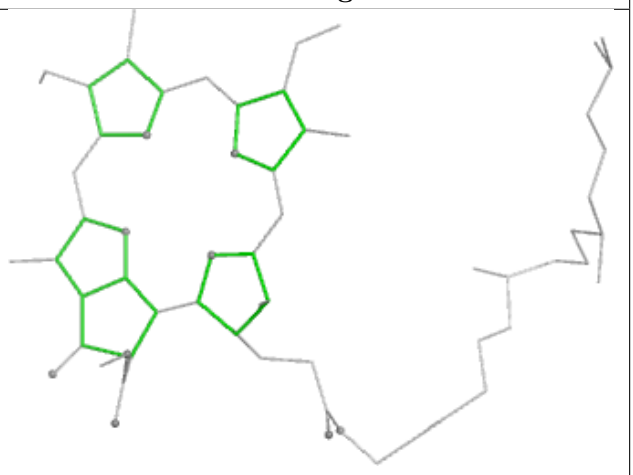
Bond lengths



Bond angles

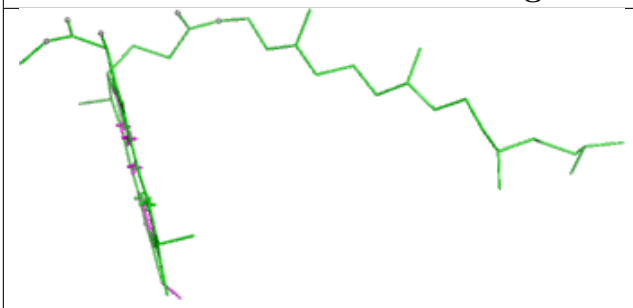


Torsions

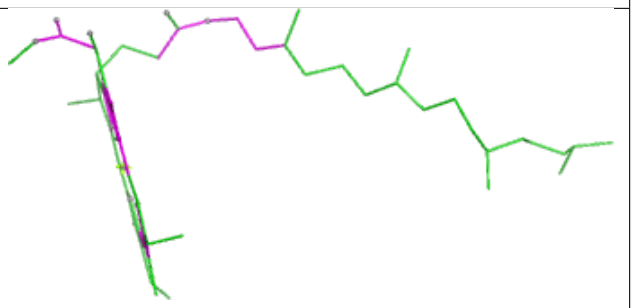


Rings

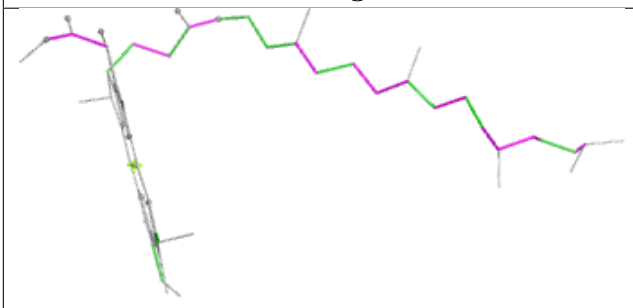
Ligand CLA B 606



Bond lengths



Bond angles



Torsions

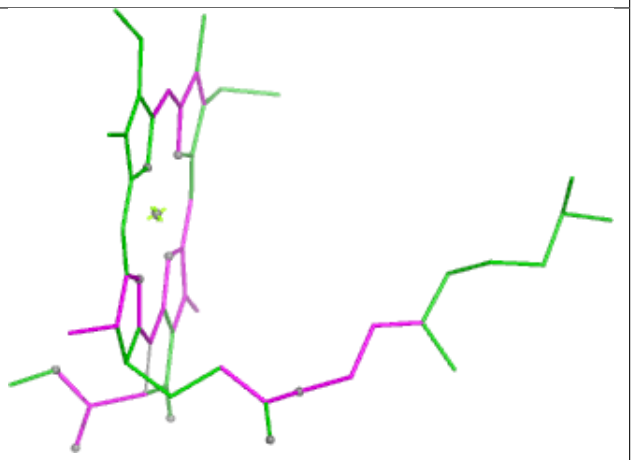


Rings

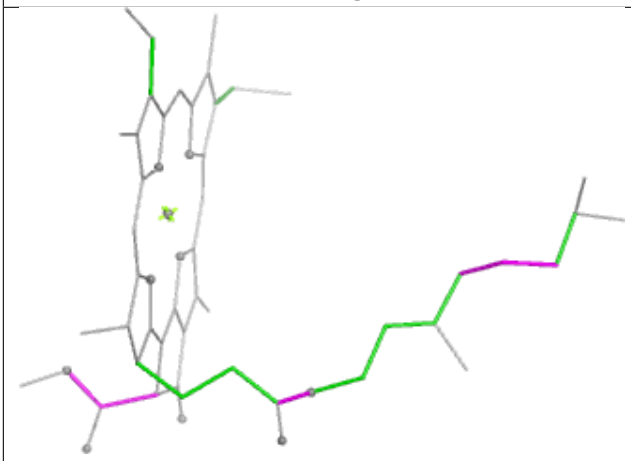
Ligand CLA s1 604



Bond lengths



Bond angles

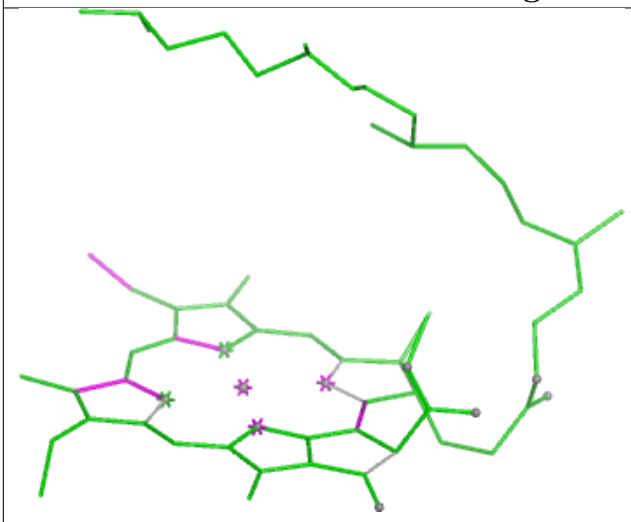


Torsions

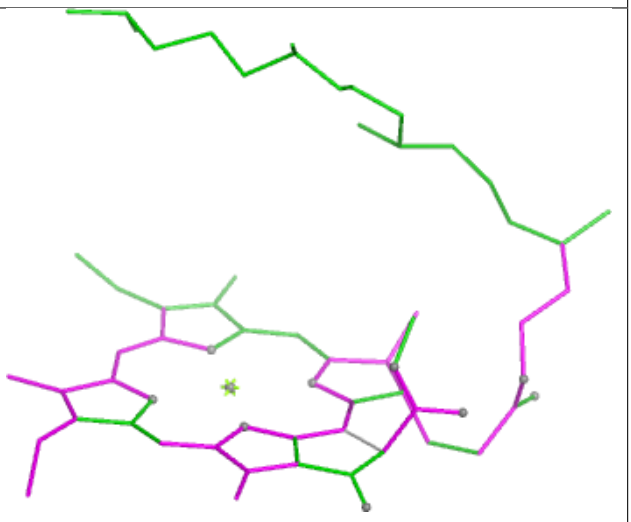


Rings

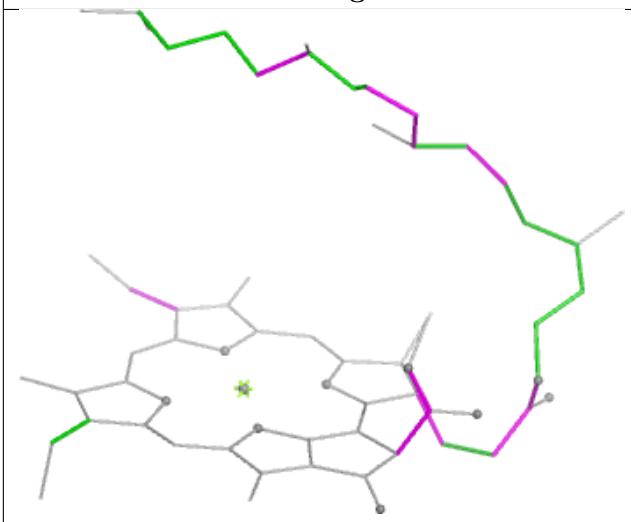
Ligand CLA G 603



Bond lengths



Bond angles

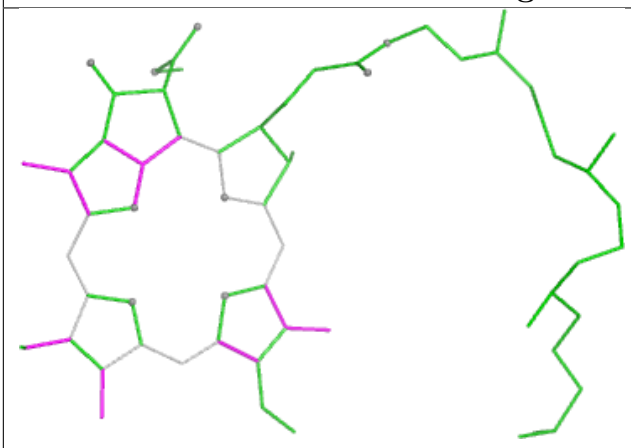


Torsions

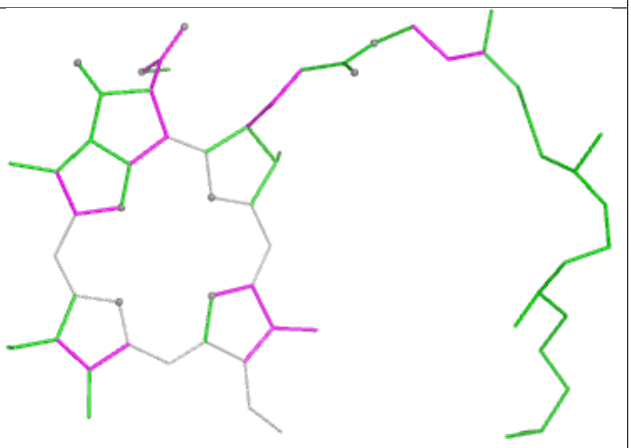


Rings

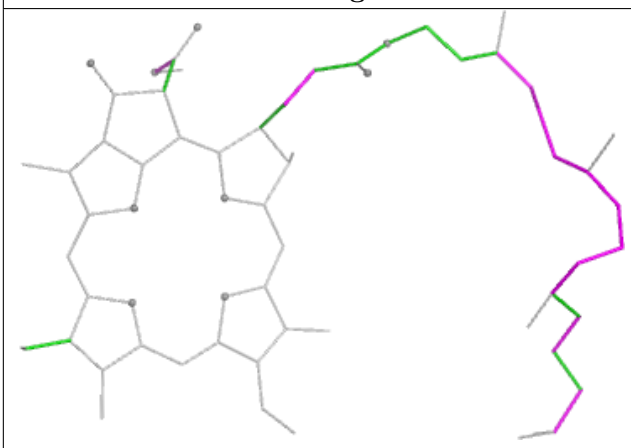
Ligand PHO a1 408



Bond lengths



Bond angles

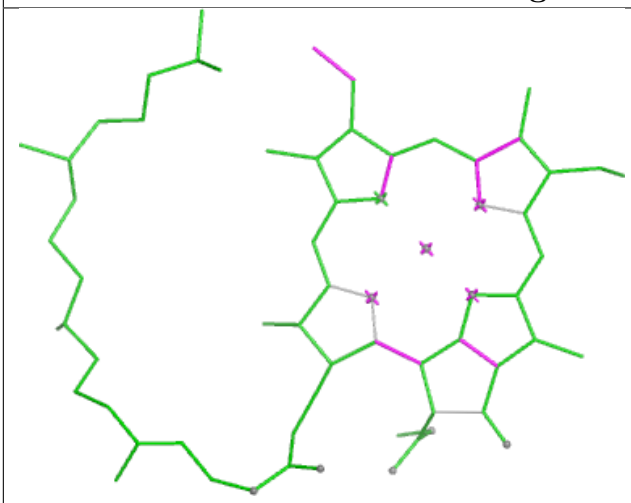


Torsions

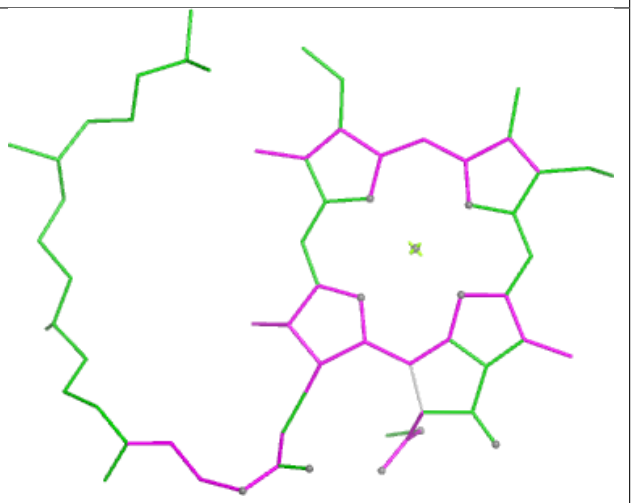


Rings

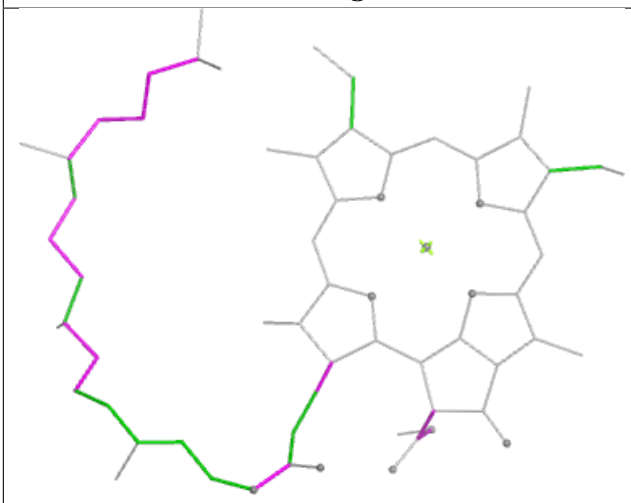
Ligand CLA c 512



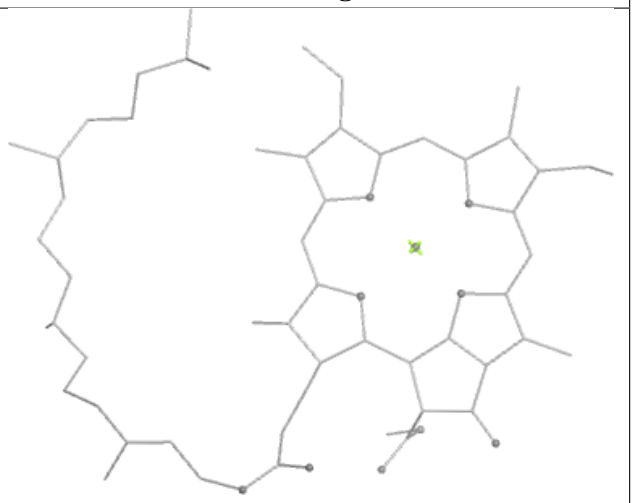
Bond lengths



Bond angles

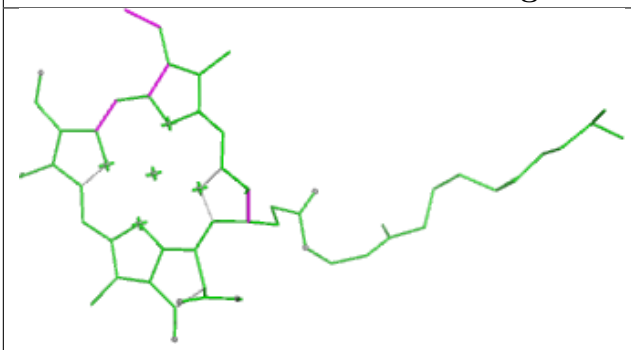


Torsions

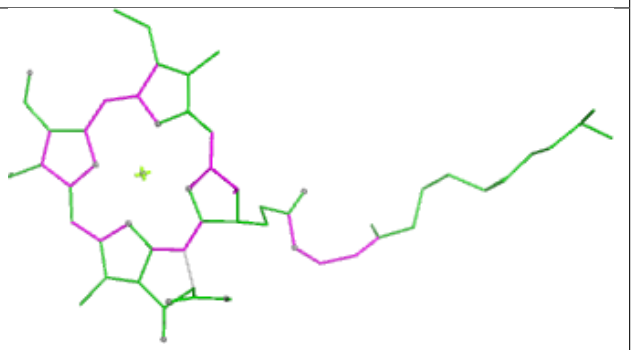


Rings

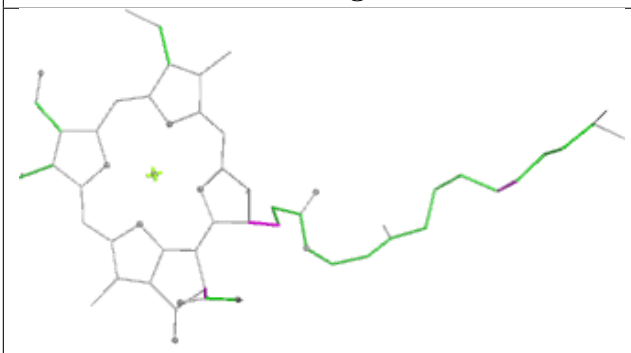
Ligand CHL s1 608



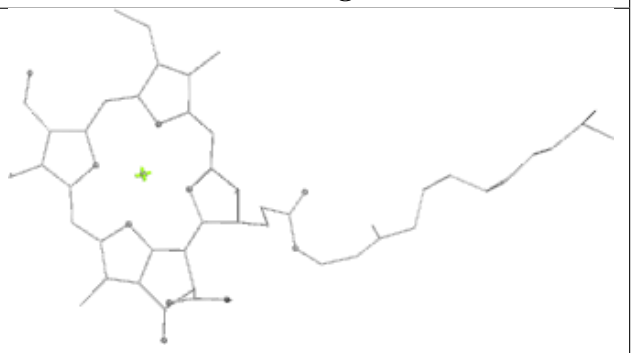
Bond lengths



Bond angles

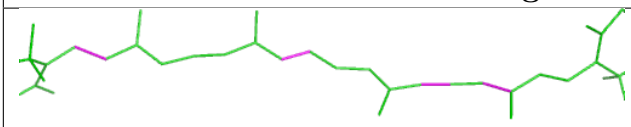


Torsions

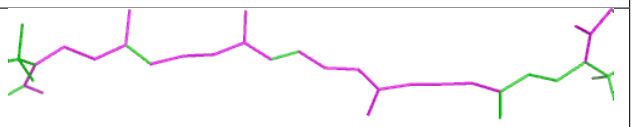


Rings

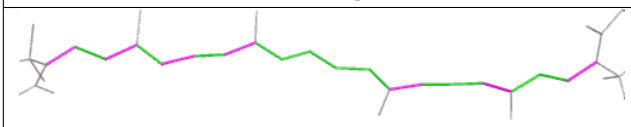
Ligand BCR A 411



Bond lengths



Bond angles

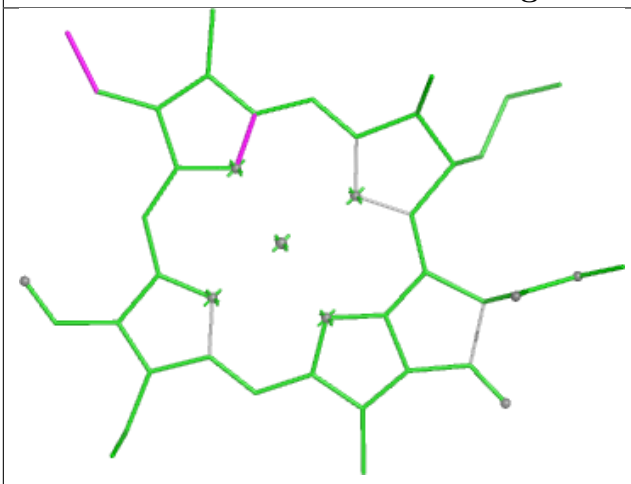


Torsions

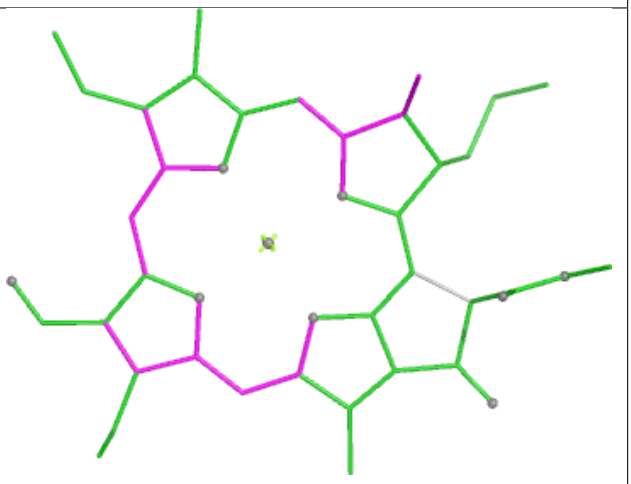


Rings

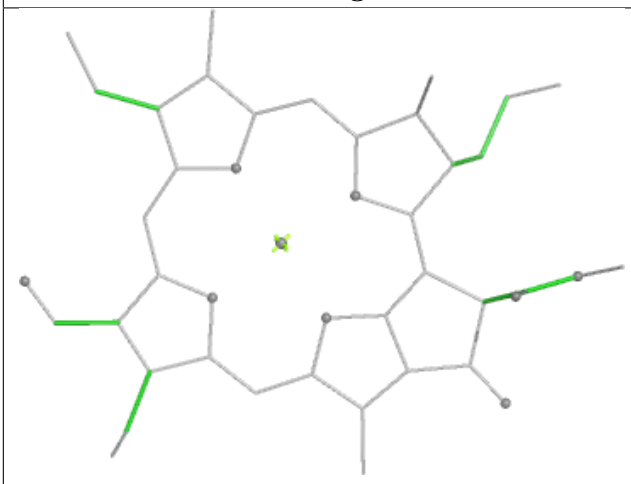
Ligand CHL s1 606



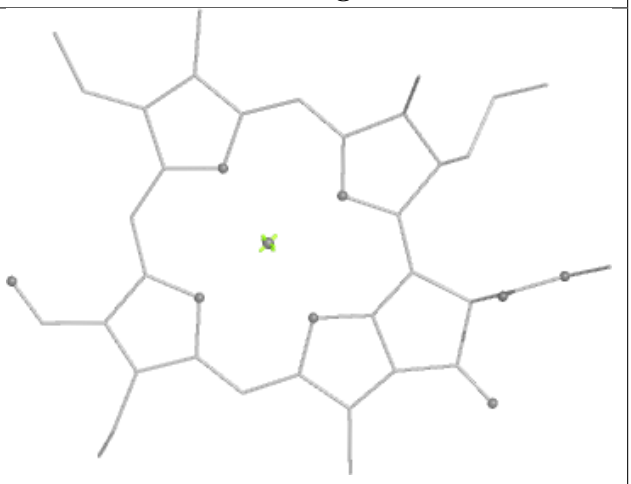
Bond lengths



Bond angles

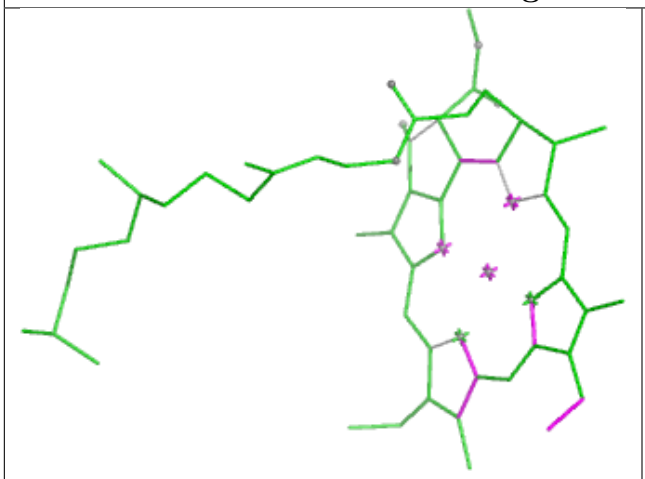


Torsions

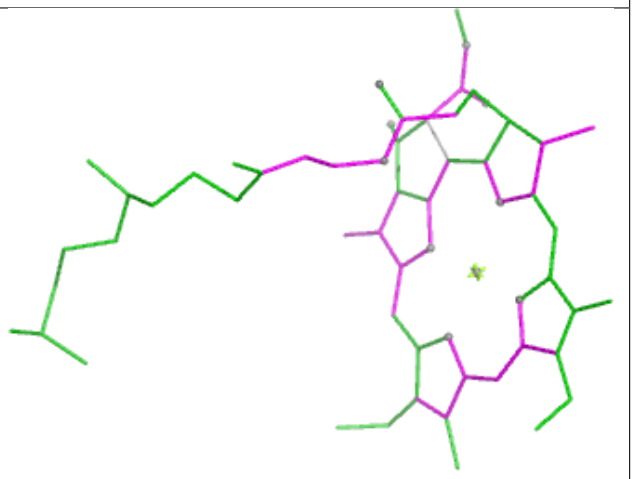


Rings

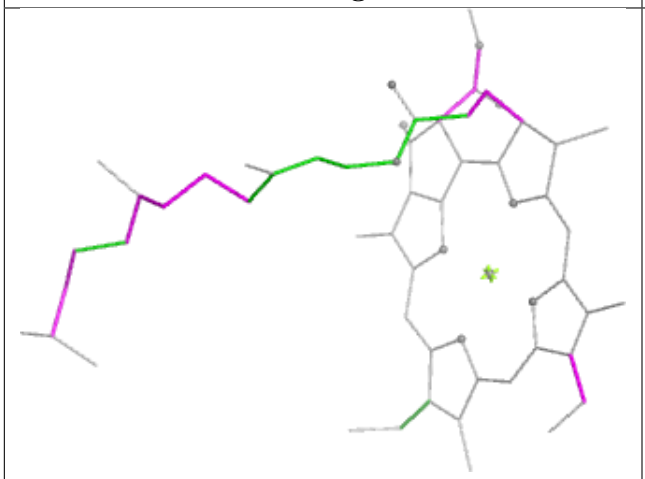
Ligand CLA s1 609



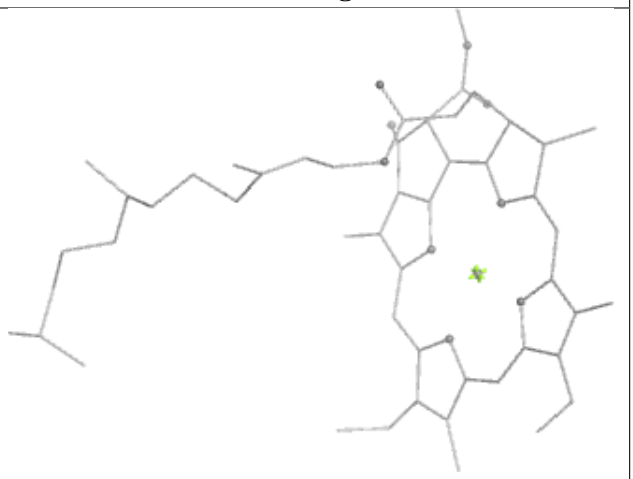
Bond lengths



Bond angles

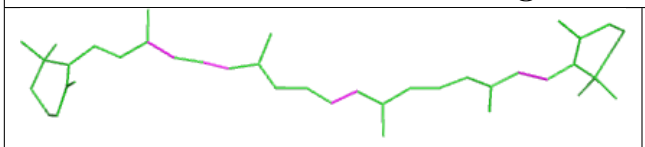


Torsions

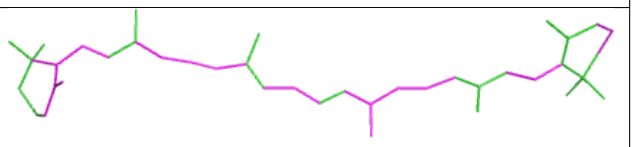


Rings

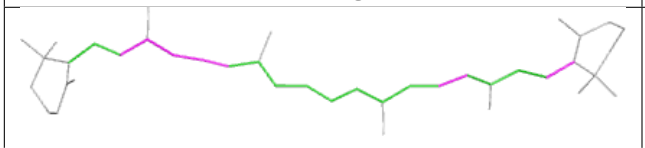
Ligand BCR b1 619



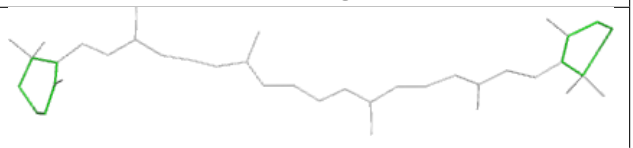
Bond lengths



Bond angles

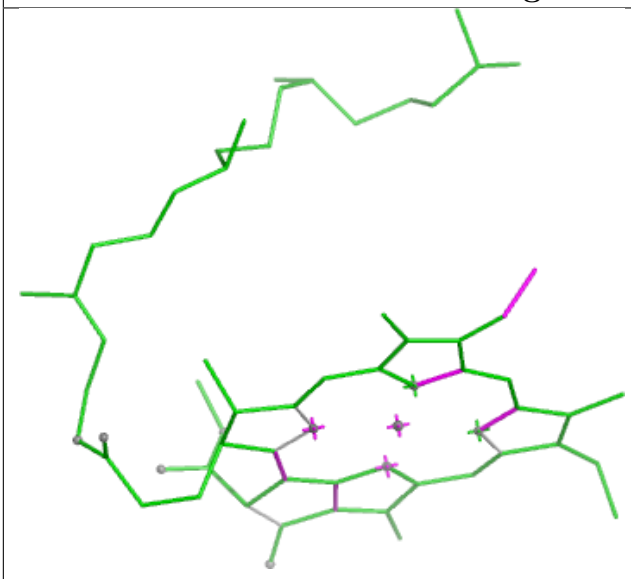


Torsions

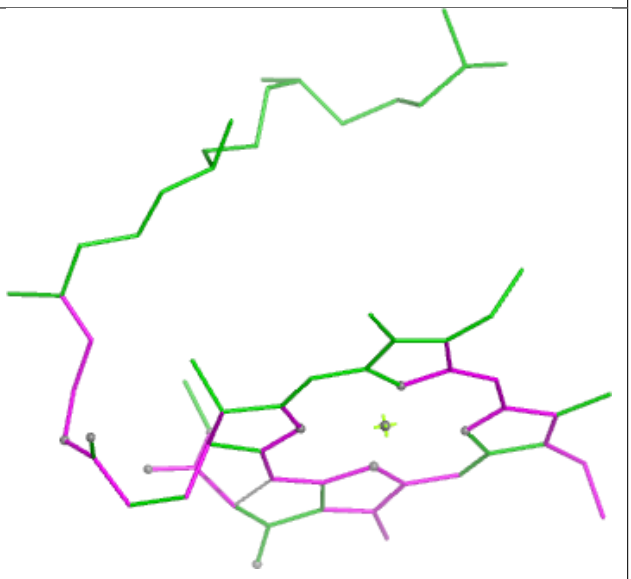


Rings

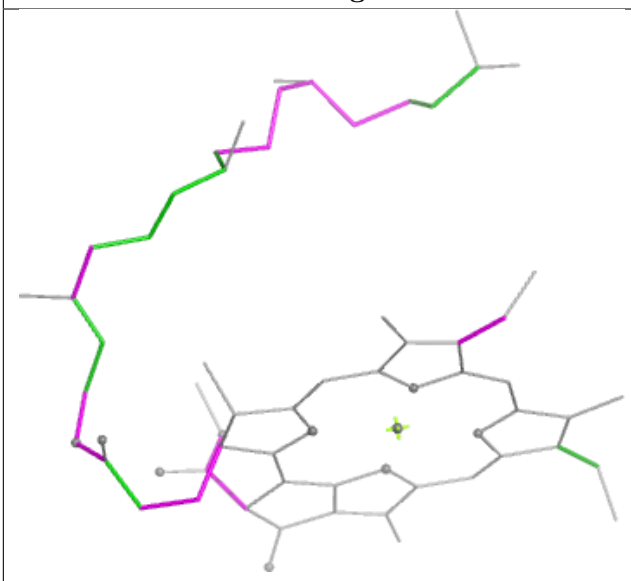
Ligand CLA N 603



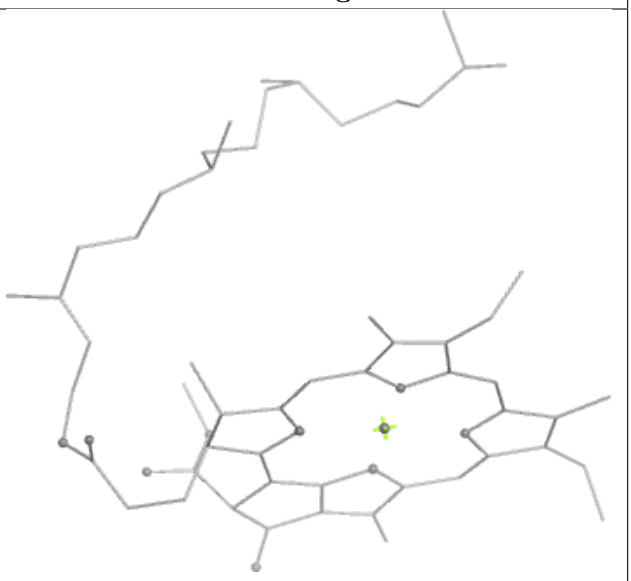
Bond lengths



Bond angles

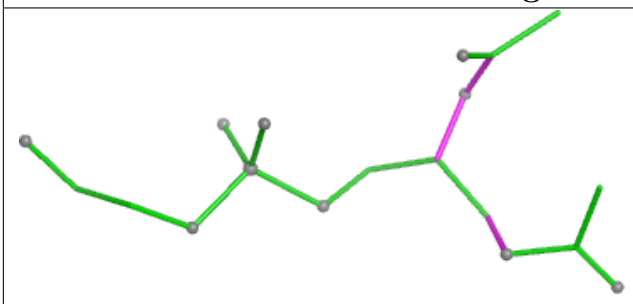


Torsions

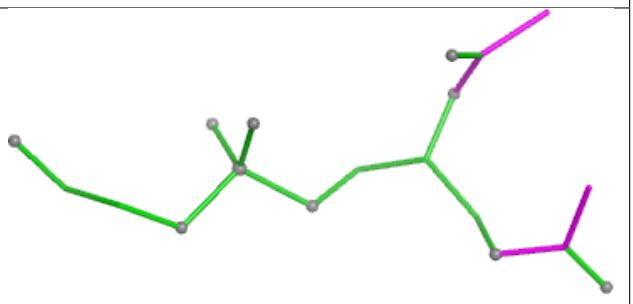


Rings

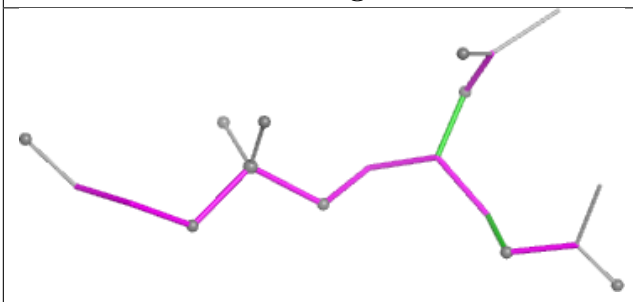
Ligand PTY Y 627



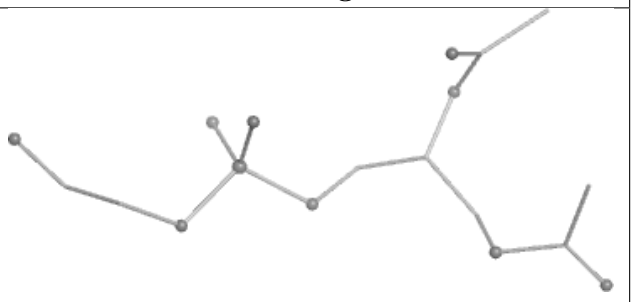
Bond lengths



Bond angles

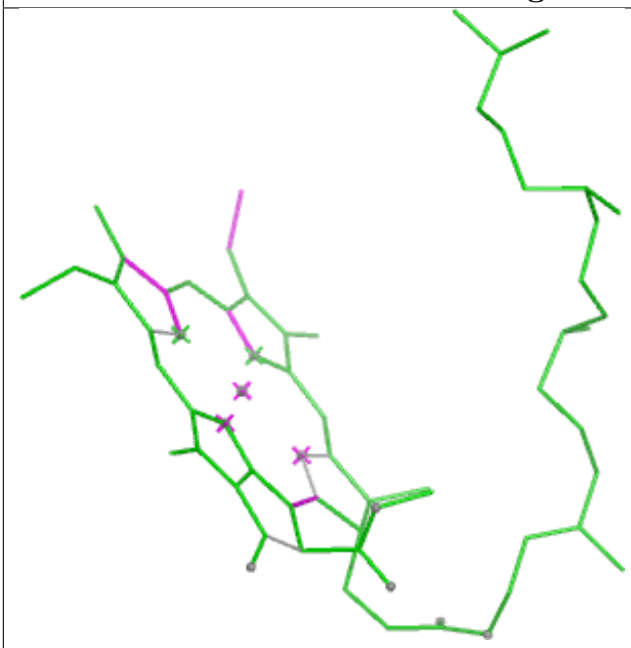


Torsions

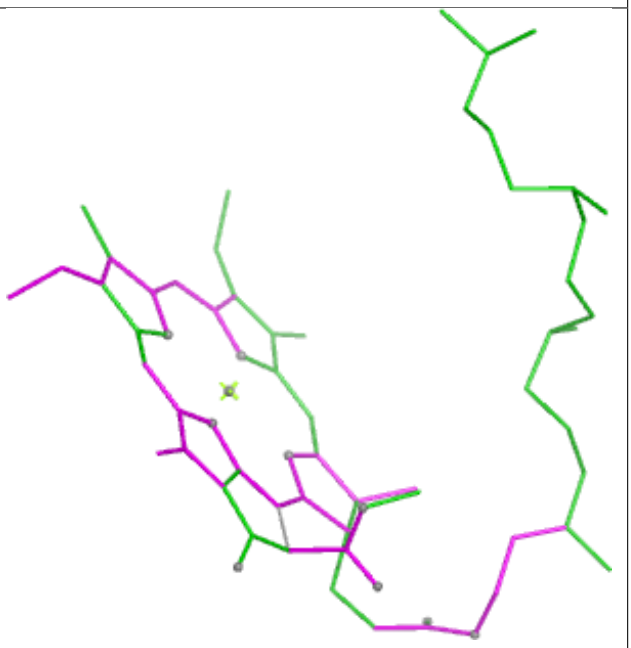


Rings

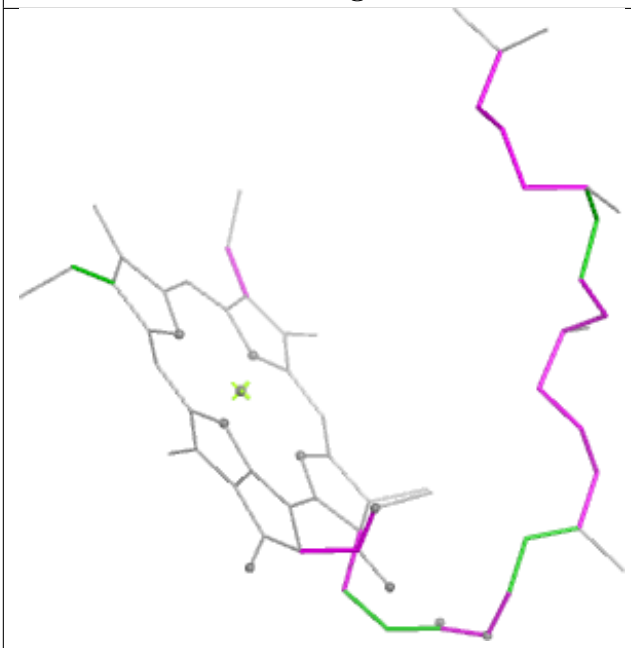
Ligand CLA n 603



Bond lengths



Bond angles

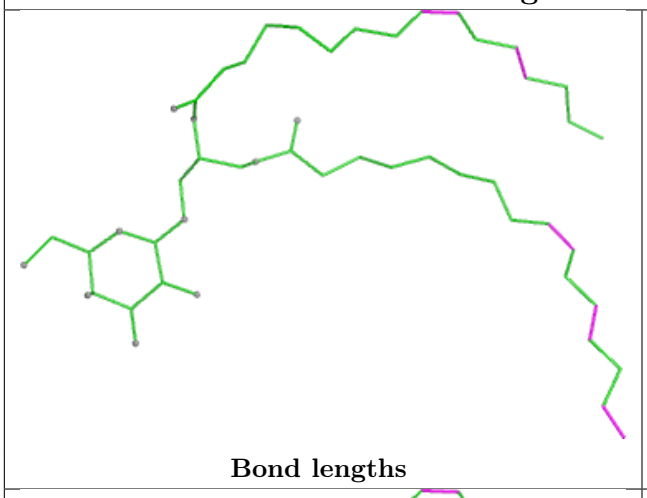


Torsions

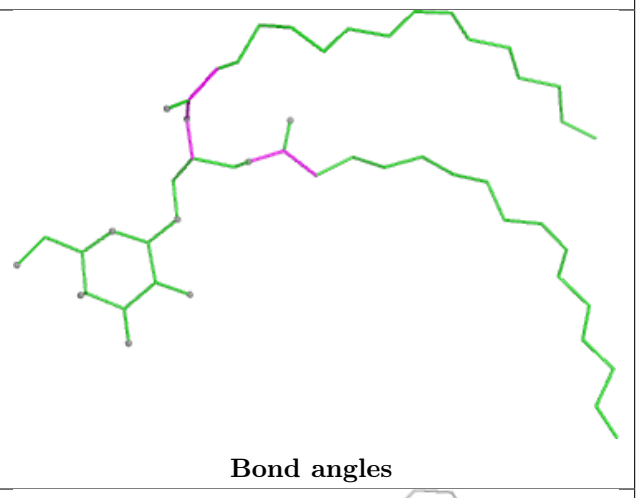


Rings

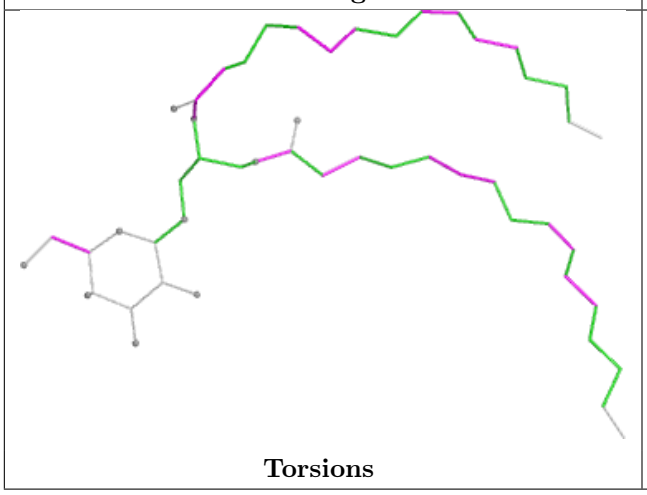
Ligand LMG C 521



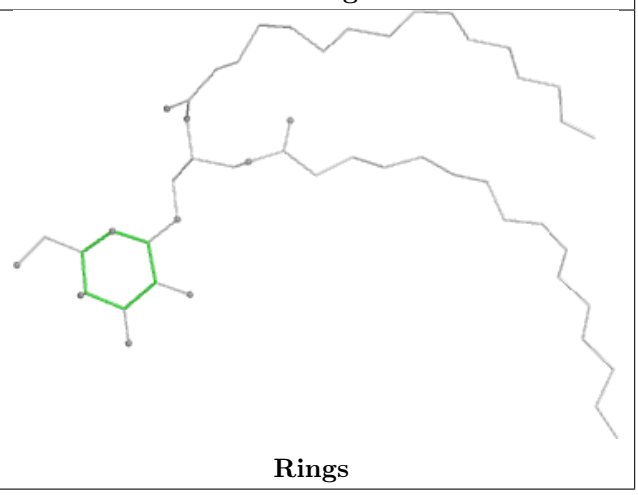
Bond lengths



Bond angles

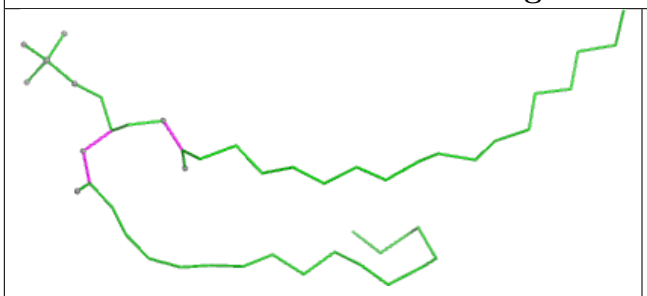


Torsions

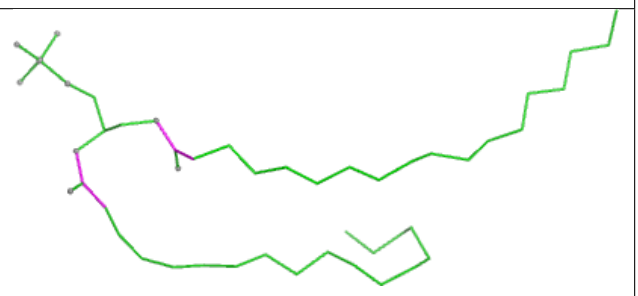


Rings

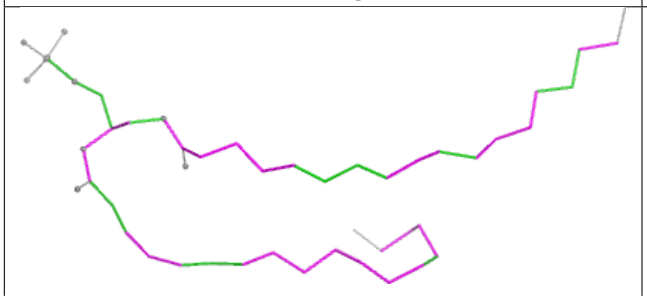
Ligand 3PH t1 101



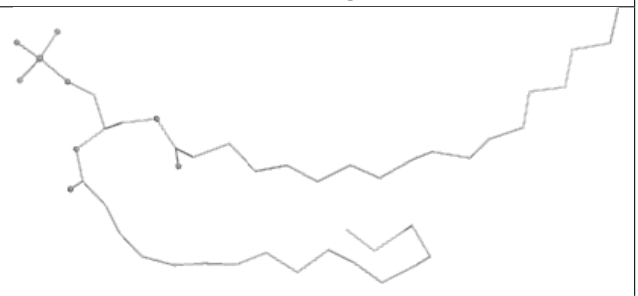
Bond lengths



Bond angles

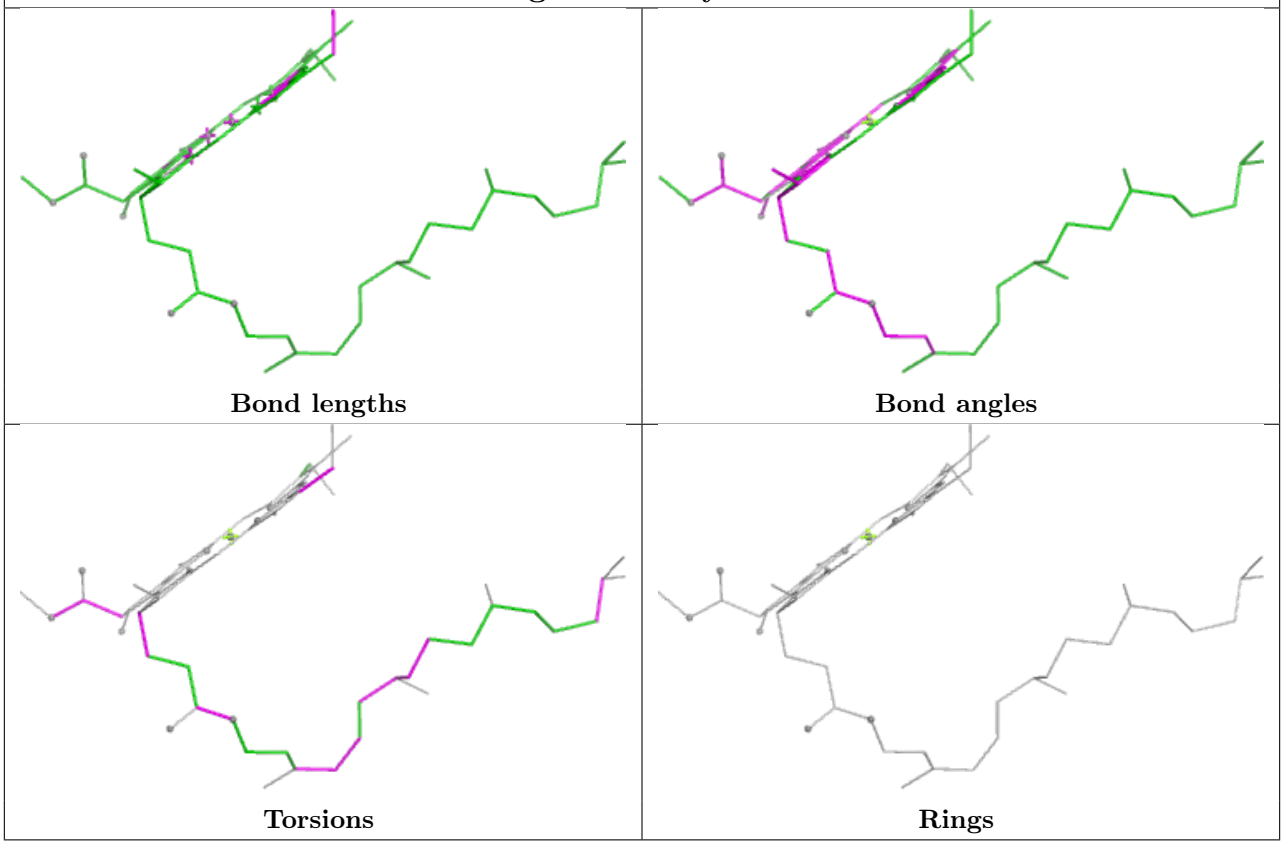


Torsions

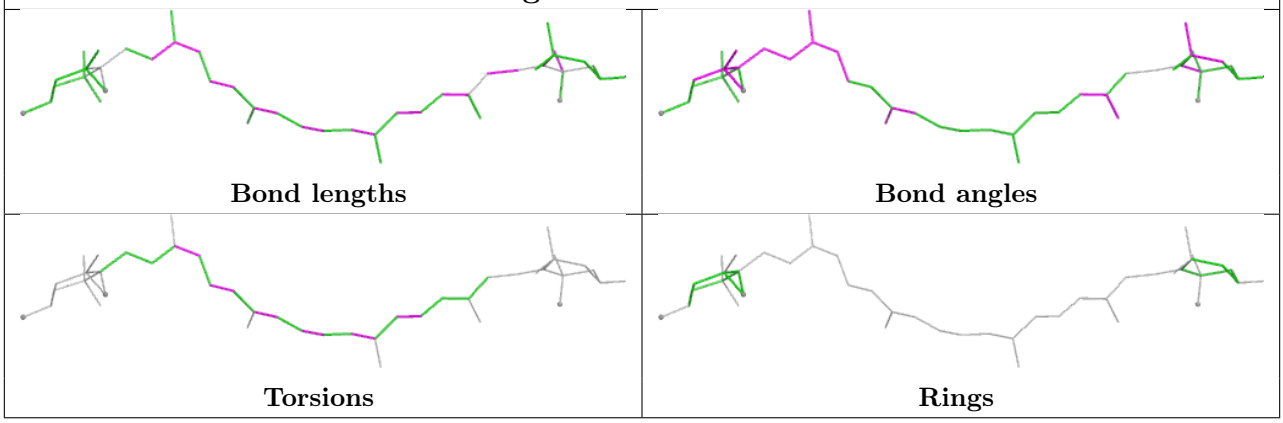


Rings

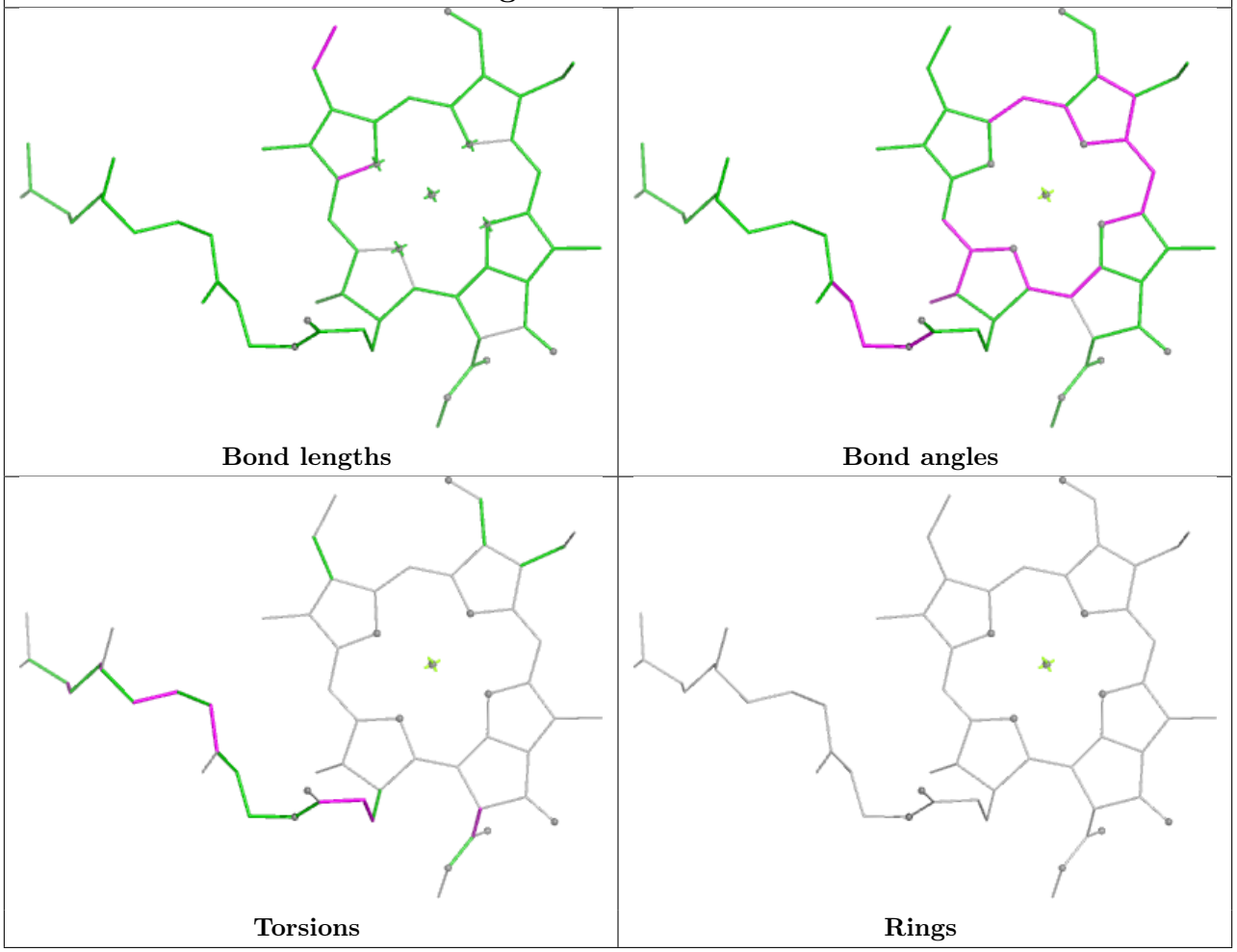
Ligand CLA y 614



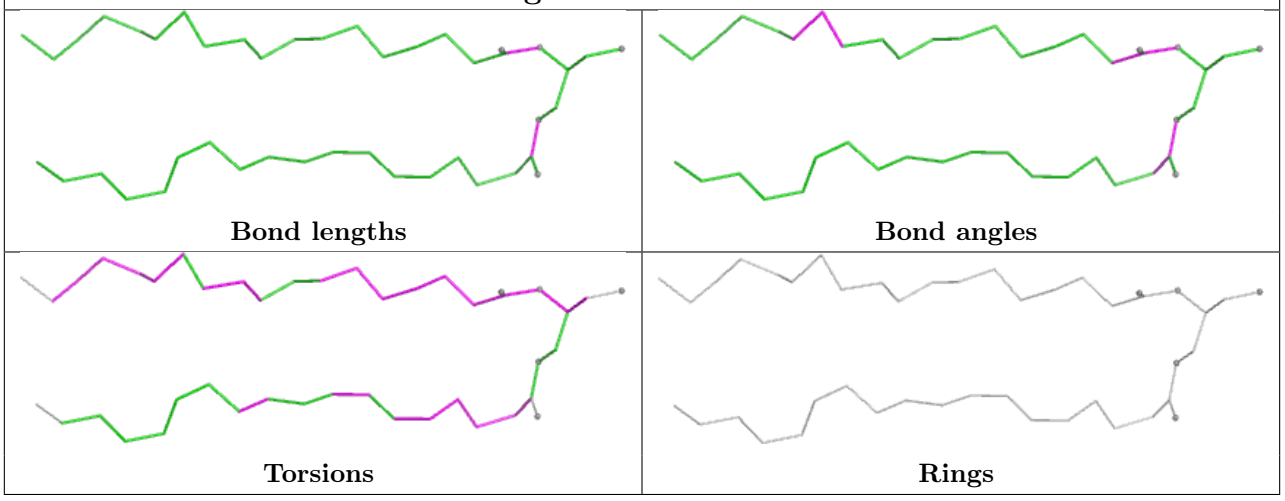
Ligand NEX R 622



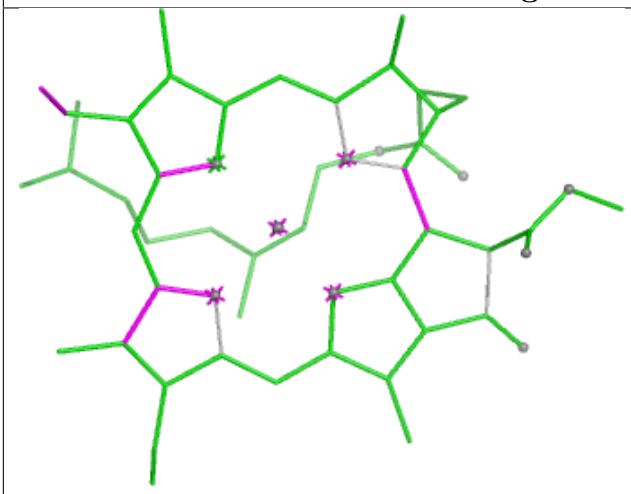
Ligand CHL S1 608



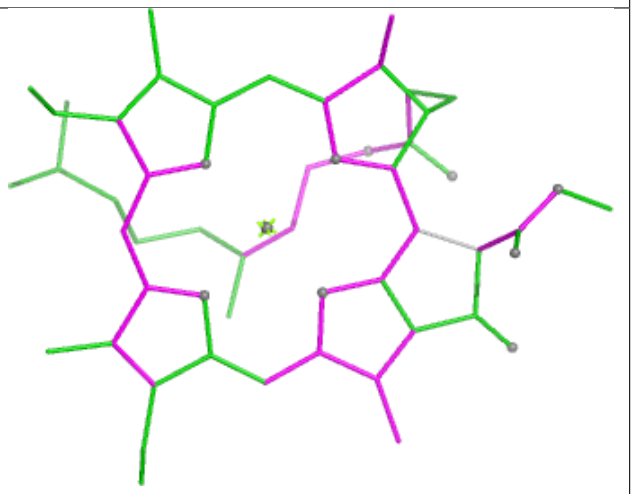
Ligand DGA b 625



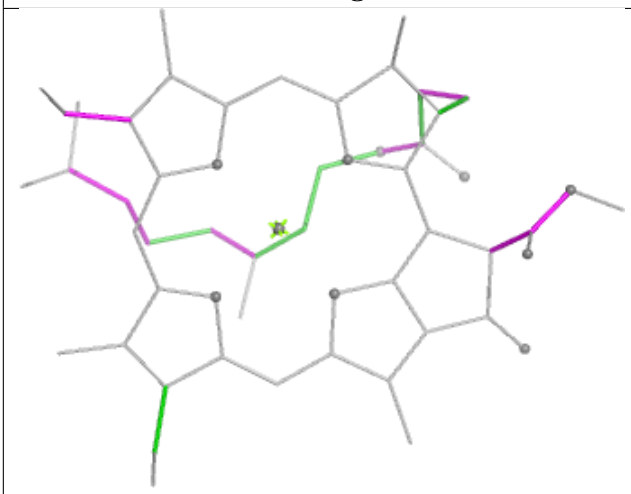
Ligand CLA s1 613



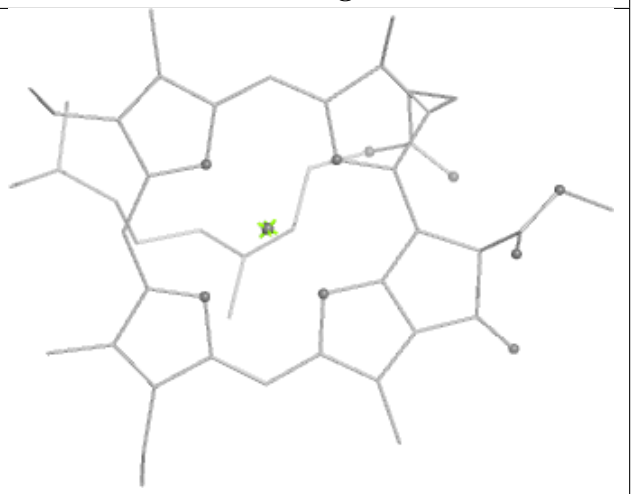
Bond lengths



Bond angles

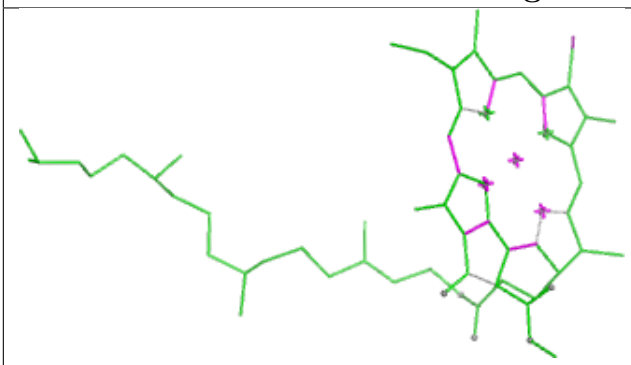


Torsions

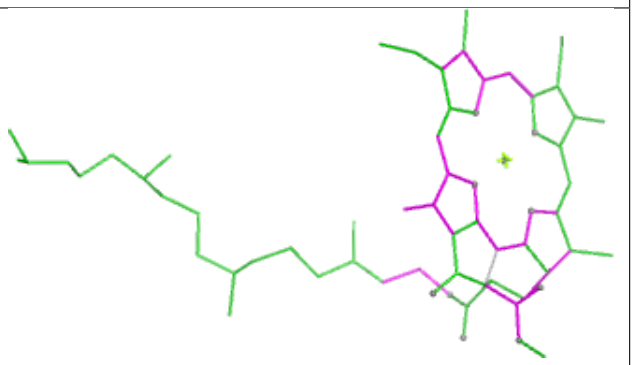


Rings

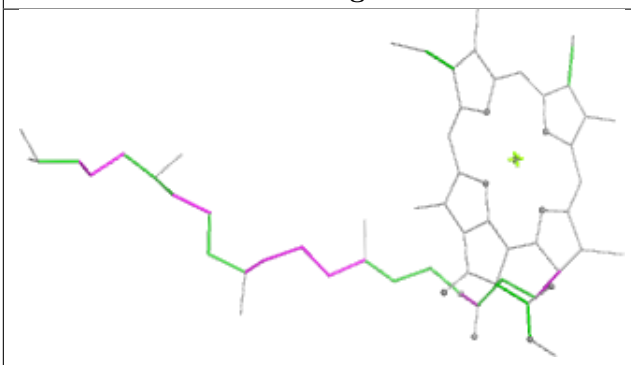
Ligand CLA Y 611



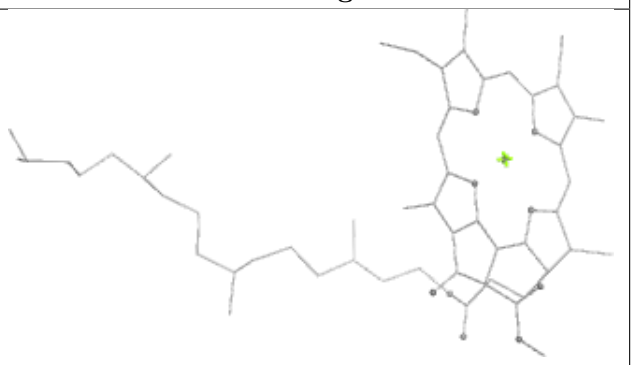
Bond lengths



Bond angles

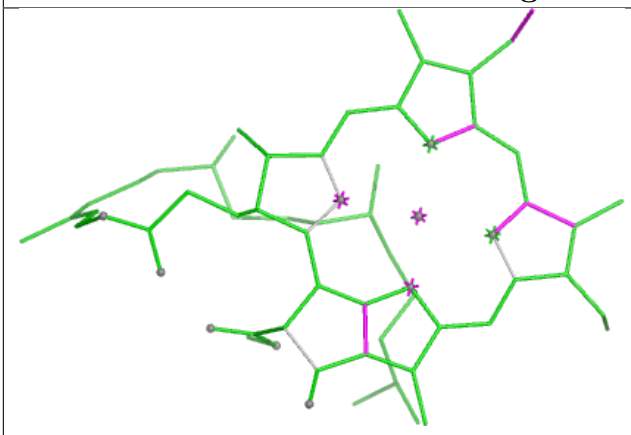


Torsions

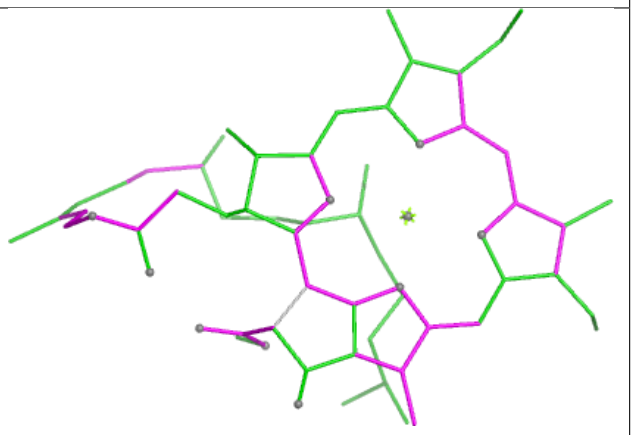


Rings

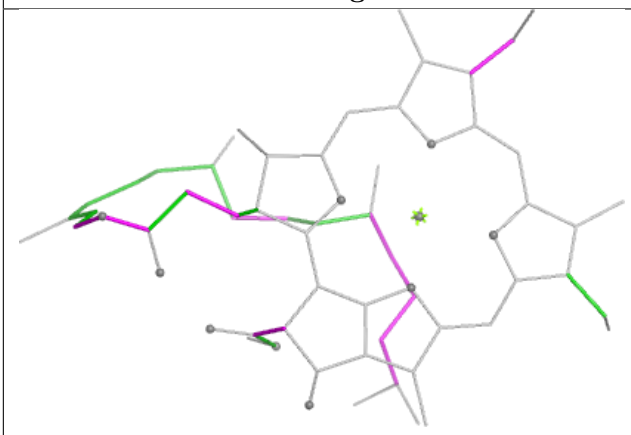
Ligand CLA c1 510



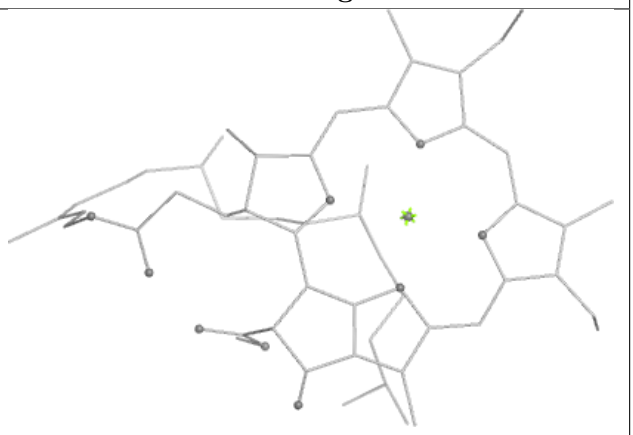
Bond lengths



Bond angles

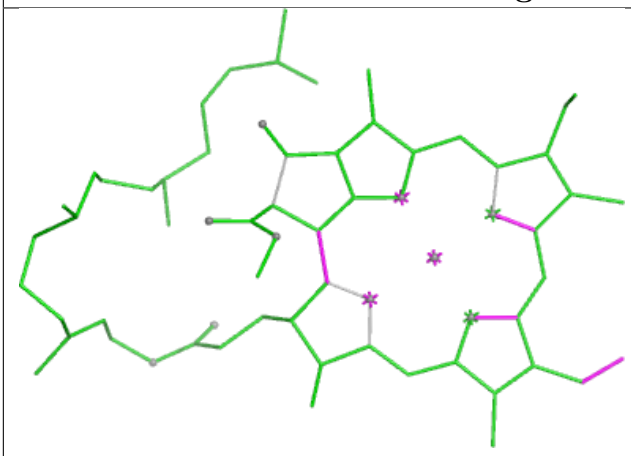


Torsions

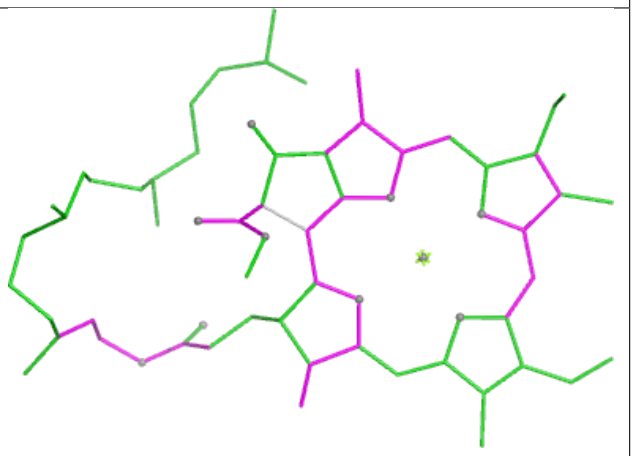


Rings

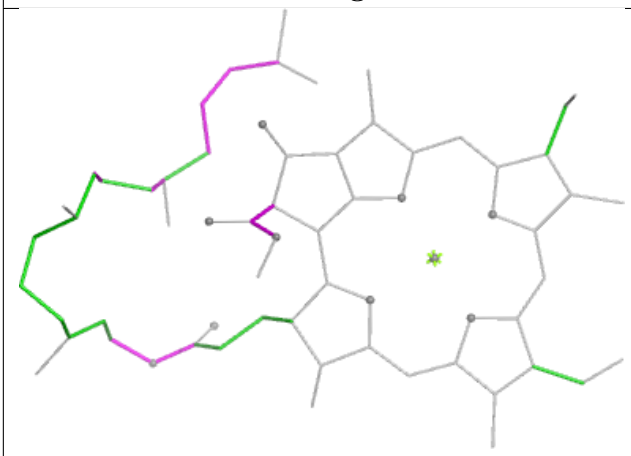
Ligand CLA B1 611



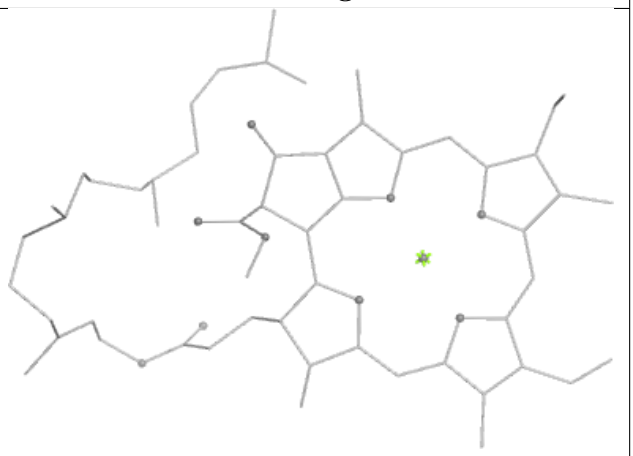
Bond lengths



Bond angles

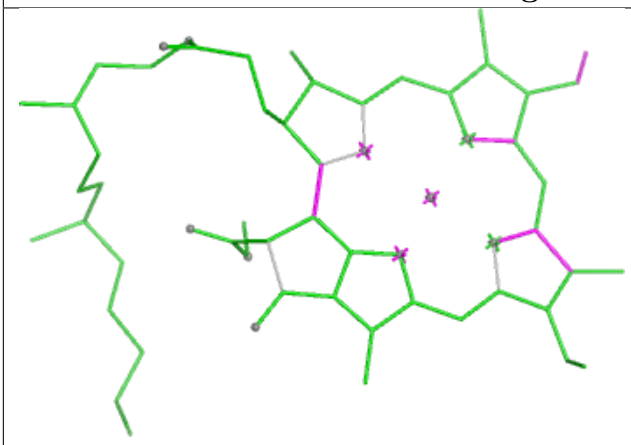


Torsions

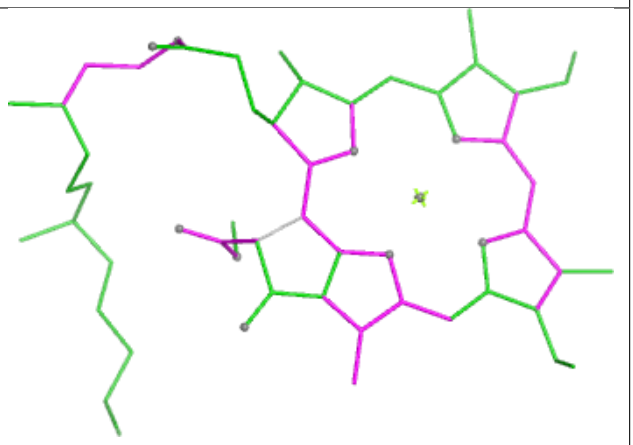


Rings

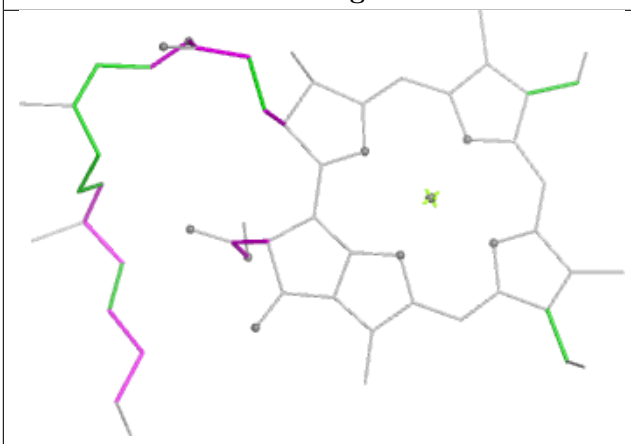
Ligand CLA r1 612



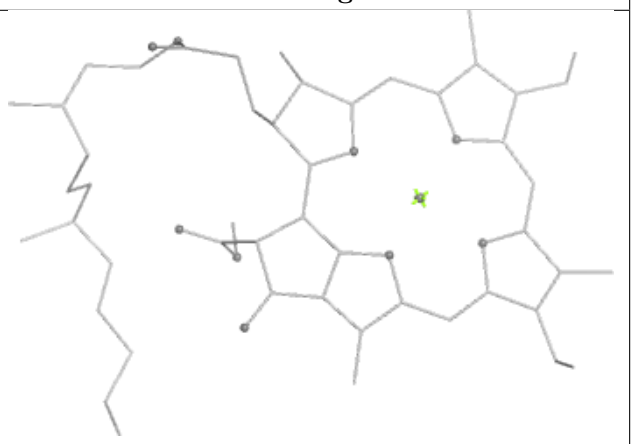
Bond lengths



Bond angles

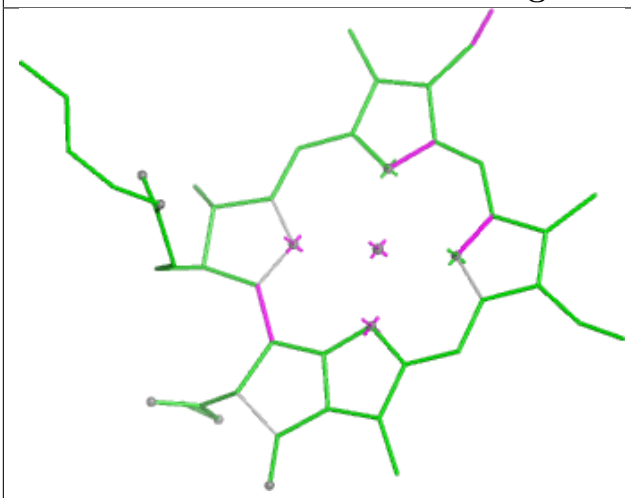


Torsions

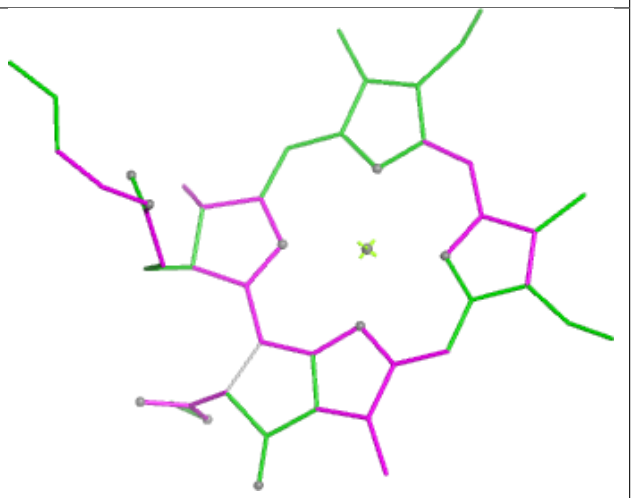


Rings

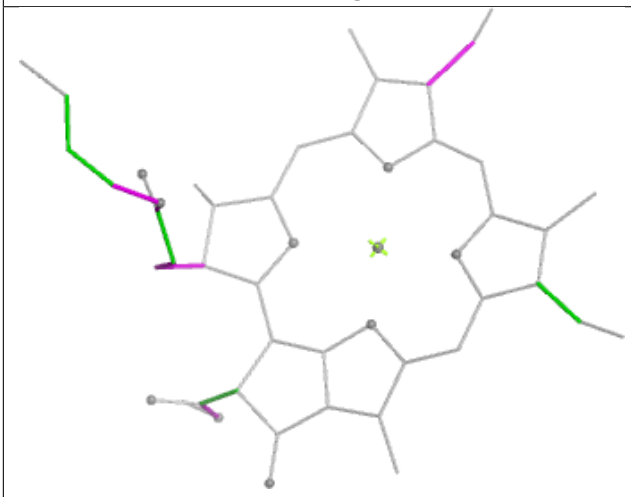
Ligand CLA a 407



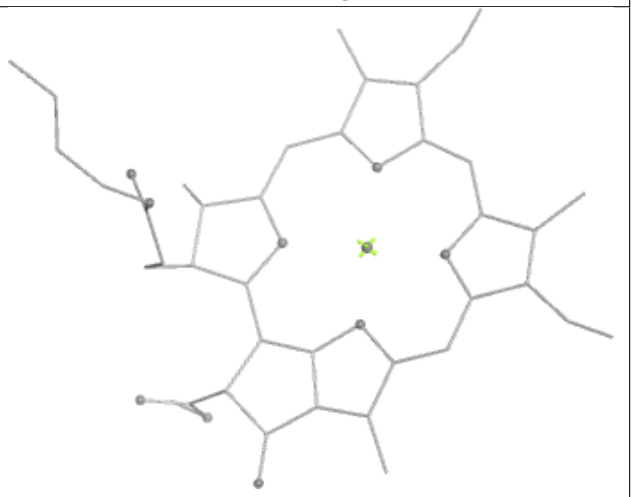
Bond lengths



Bond angles

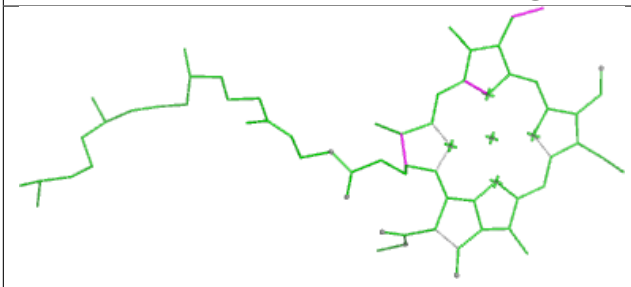


Torsions

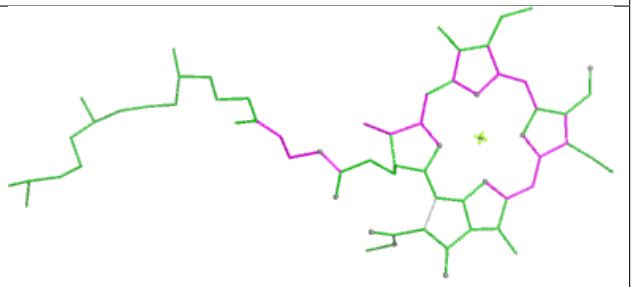


Rings

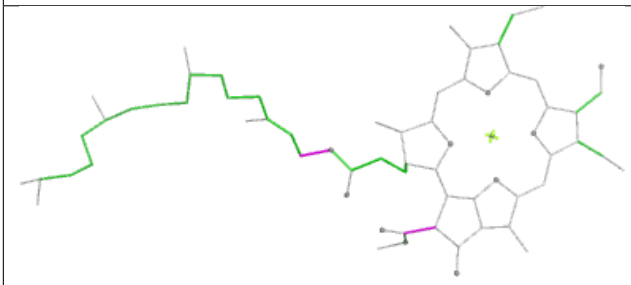
Ligand CHL n 601



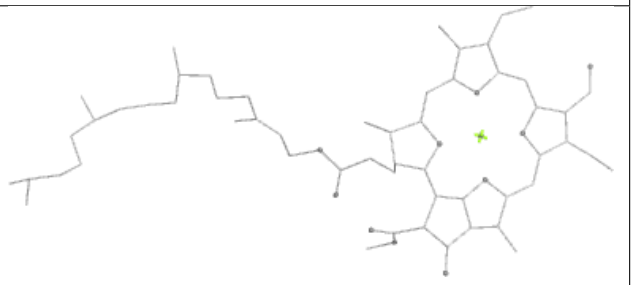
Bond lengths



Bond angles

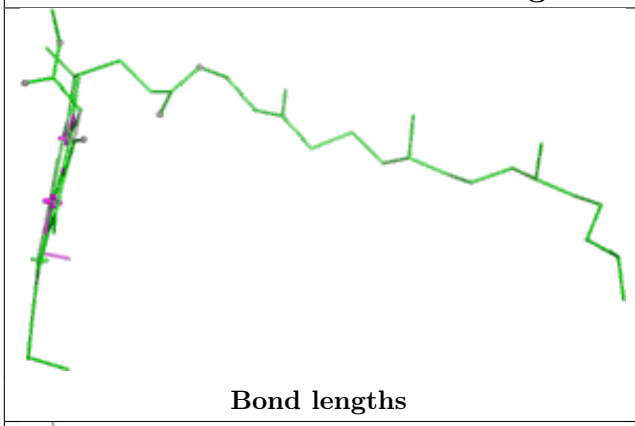


Torsions

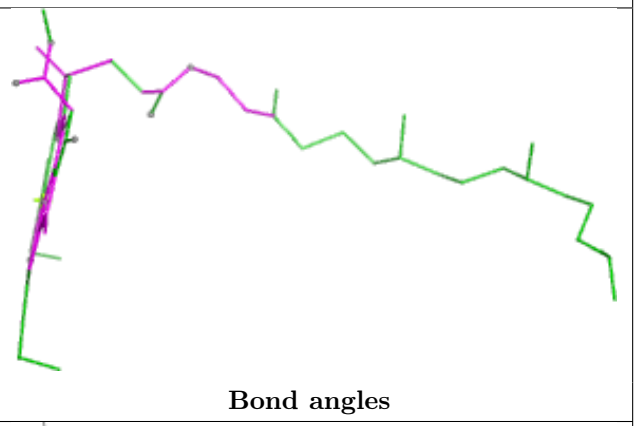


Rings

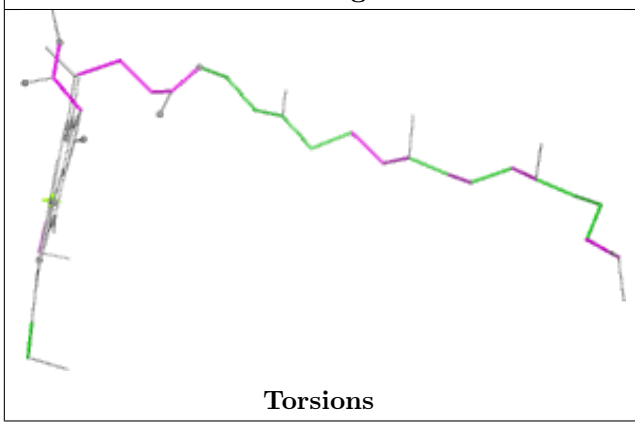
Ligand CLA b 607



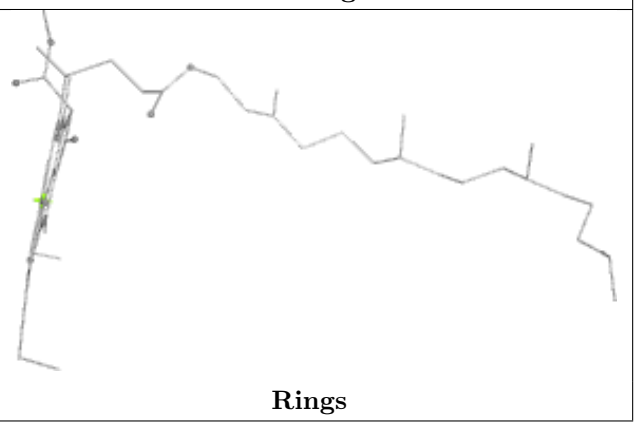
Bond lengths



Bond angles

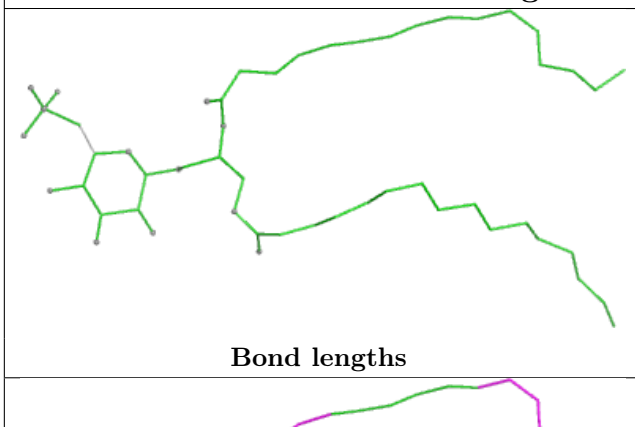


Torsions

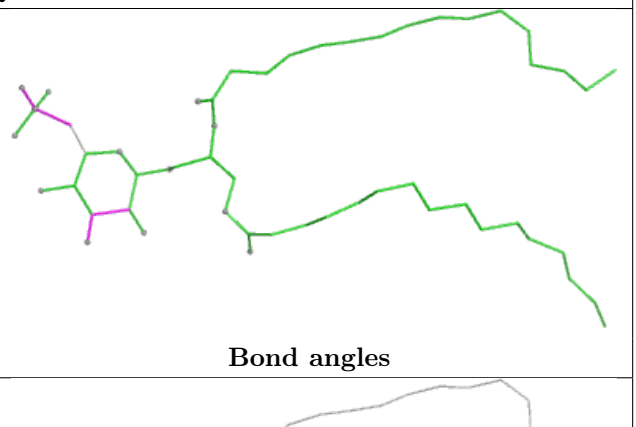


Rings

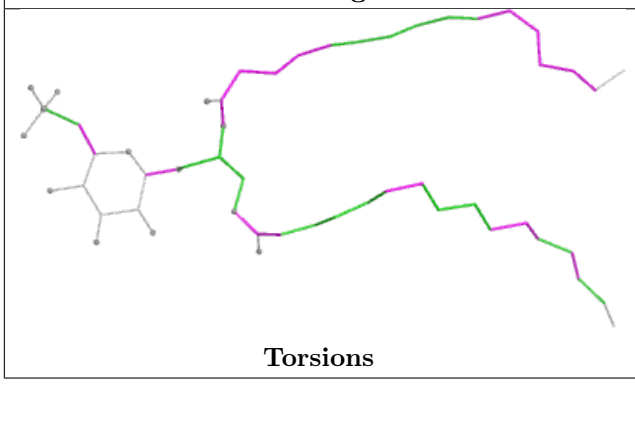
Ligand SQD c1 526



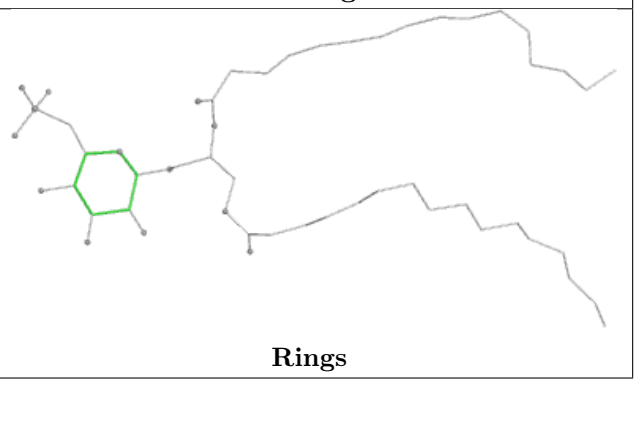
Bond lengths



Bond angles

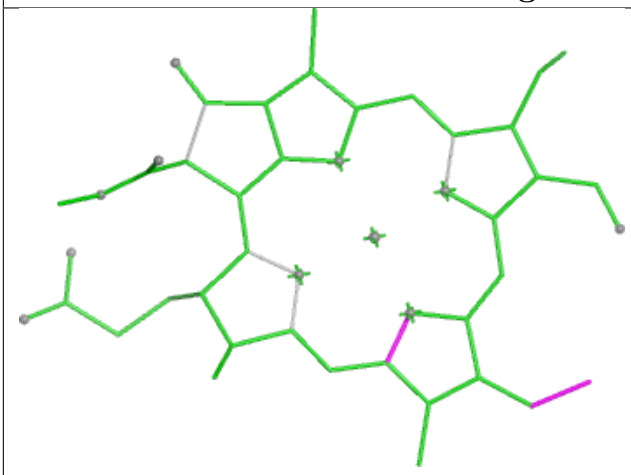


Torsions

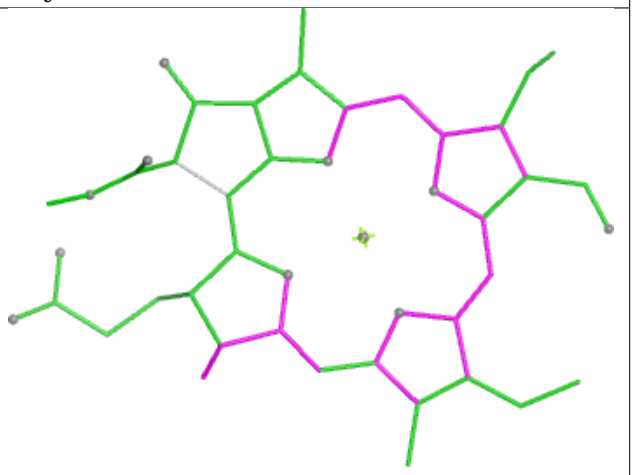


Rings

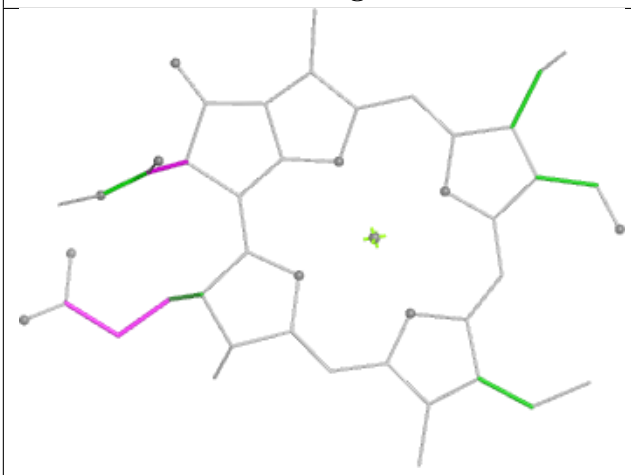
Ligand CHL y1 605



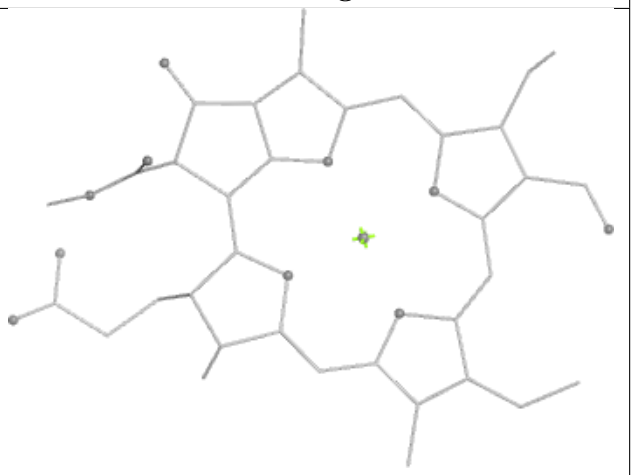
Bond lengths



Bond angles

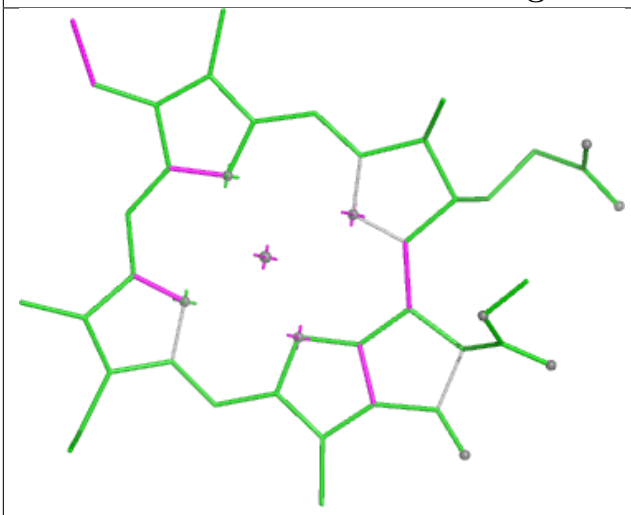


Torsions

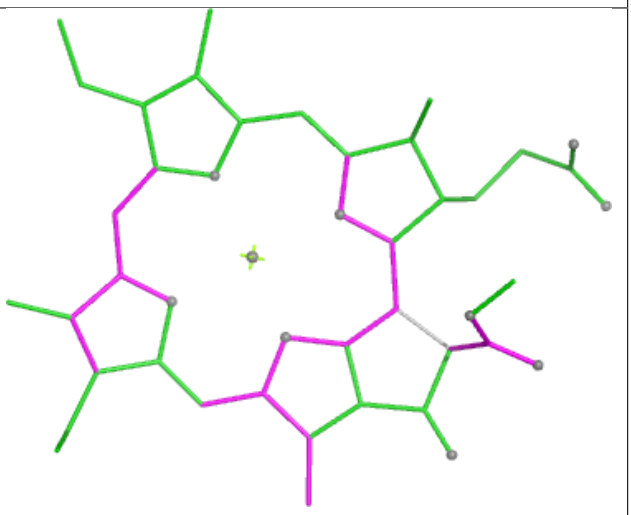


Rings

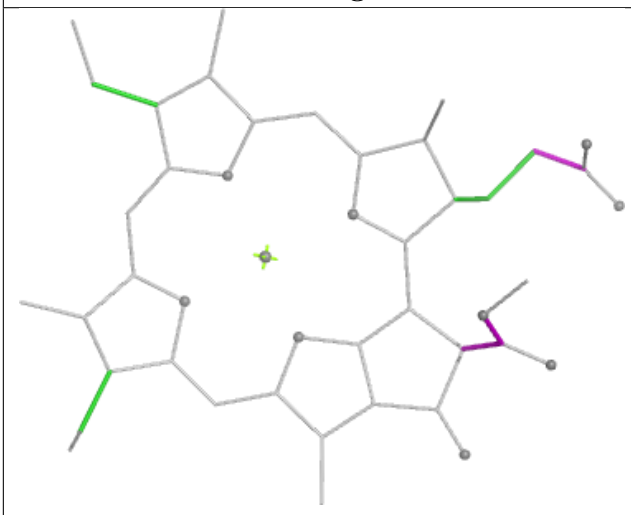
Ligand CLA S 612



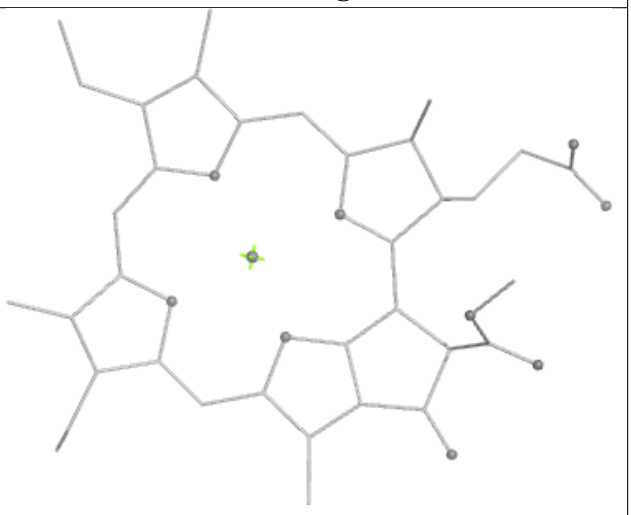
Bond lengths



Bond angles



Torsions

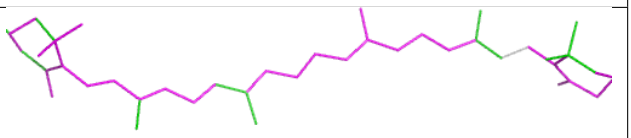


Rings

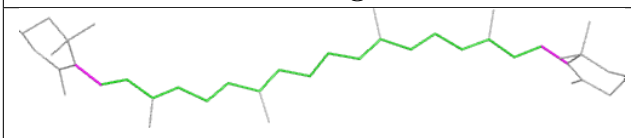
Ligand LUT S 620



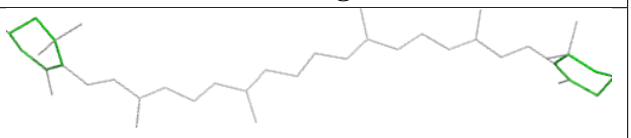
Bond lengths



Bond angles

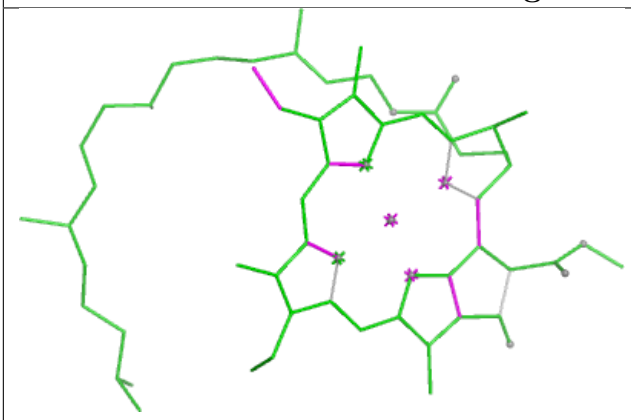


Torsions

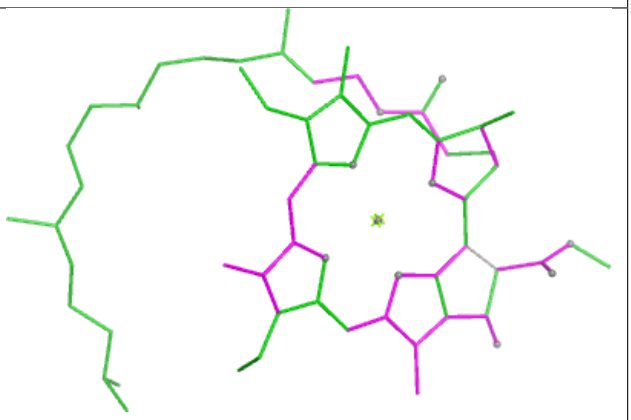


Rings

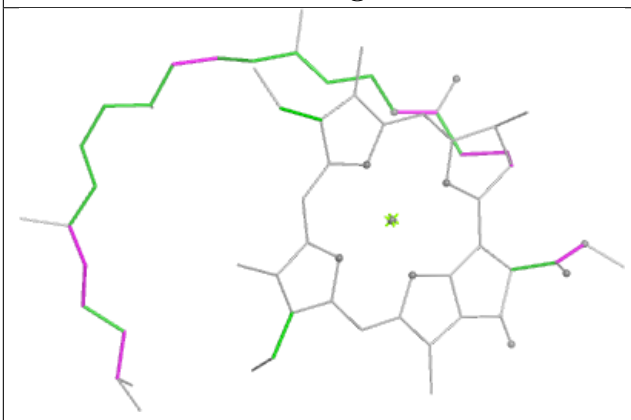
Ligand CLA Y 610



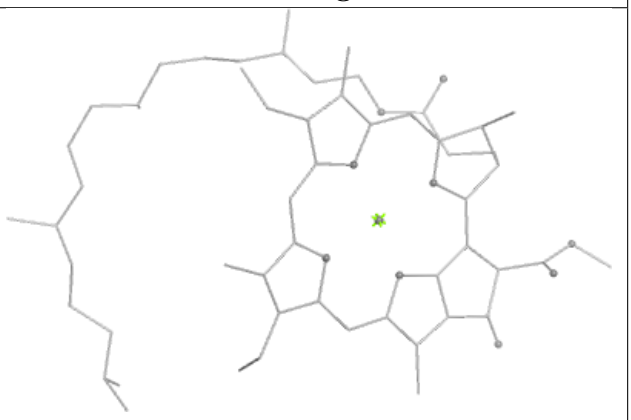
Bond lengths



Bond angles

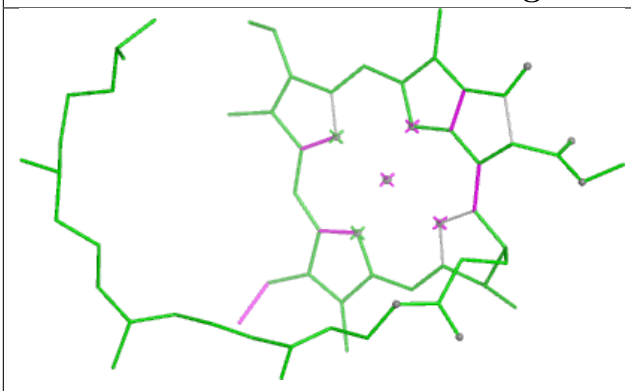


Torsions

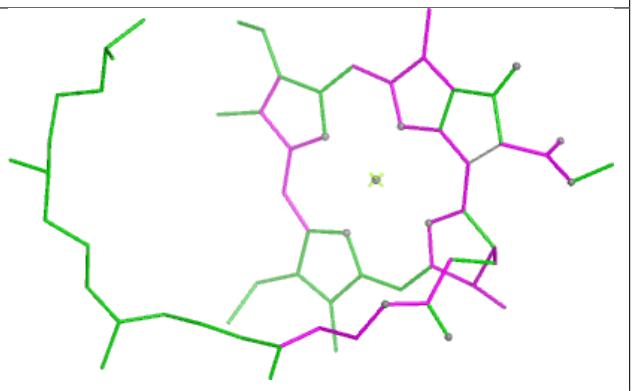


Rings

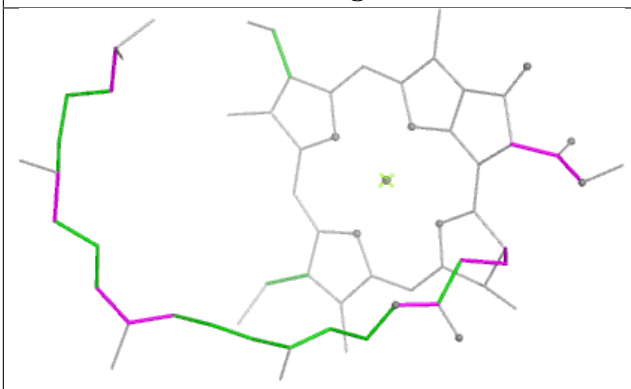
Ligand CLA G 610



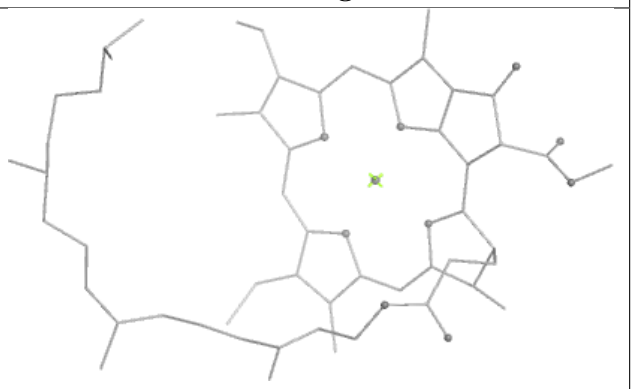
Bond lengths



Bond angles

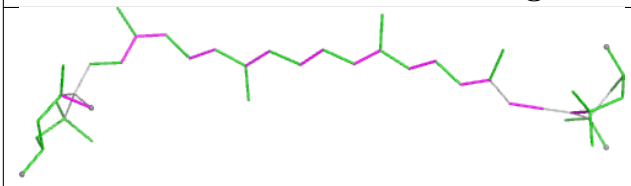


Torsions

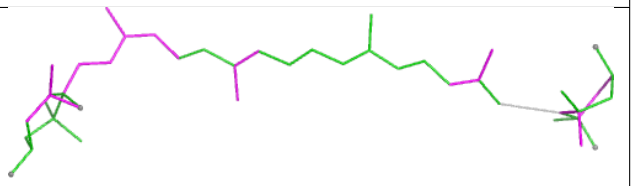


Rings

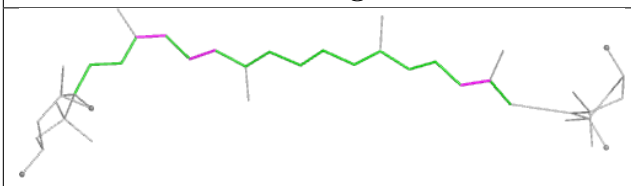
Ligand NEX n 623



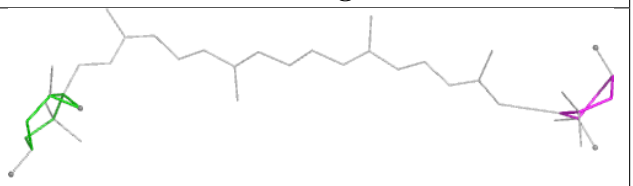
Bond lengths



Bond angles

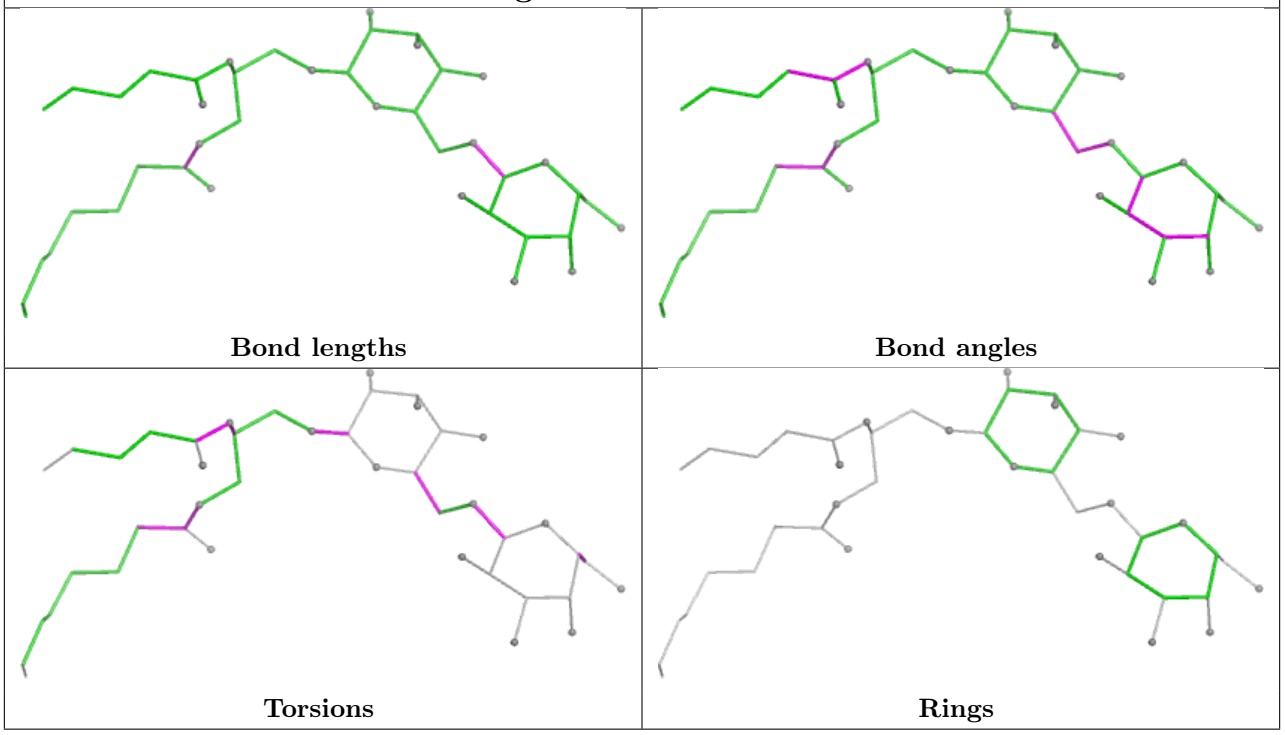


Torsions

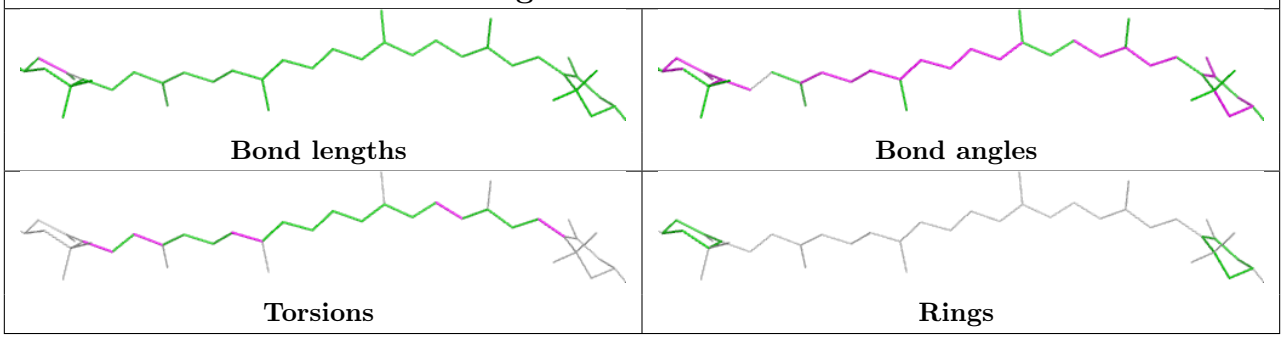


Rings

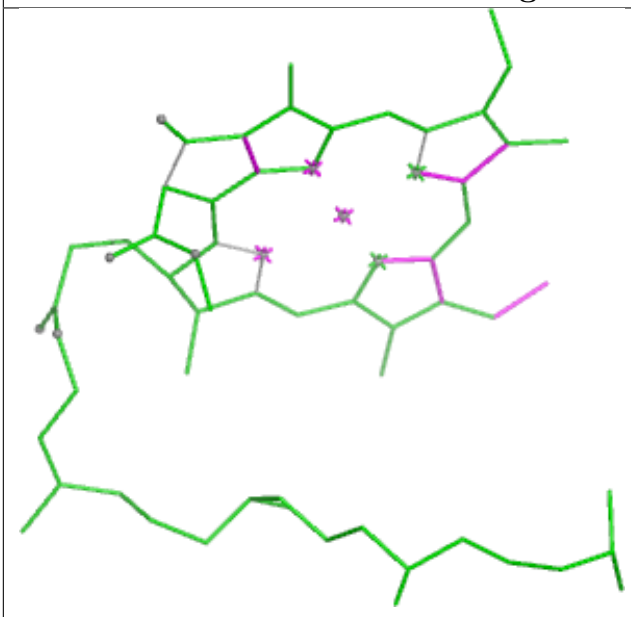
Ligand DGD b1 623



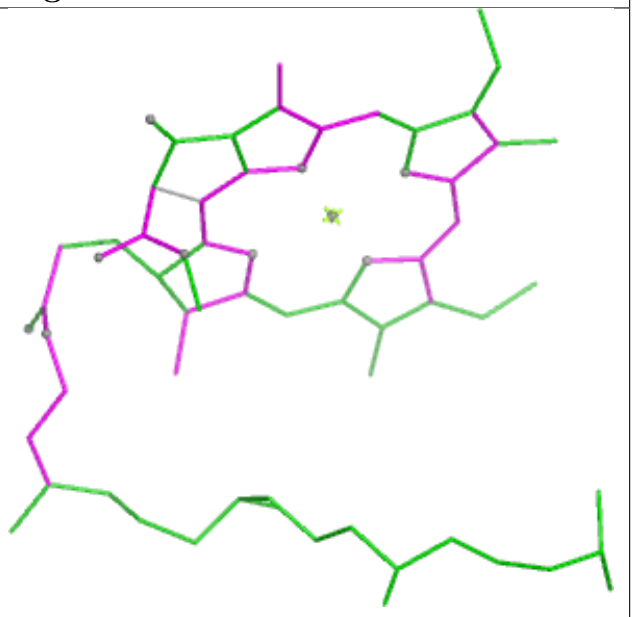
Ligand LUT Y1 620



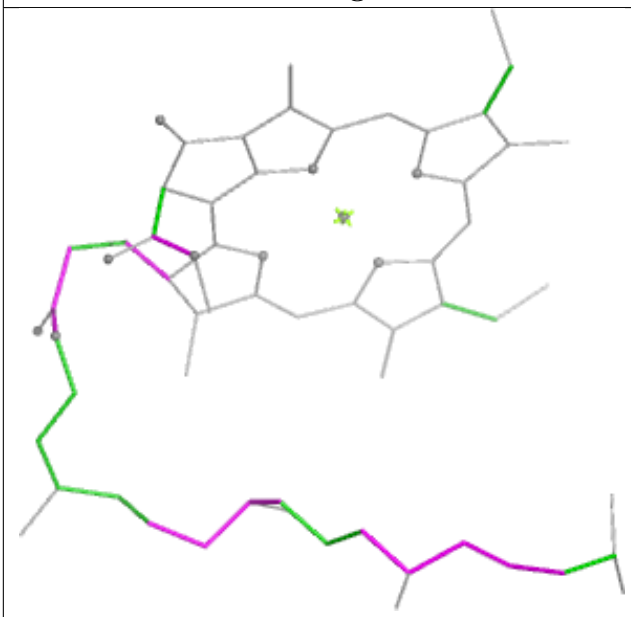
Ligand CLA g1 603



Bond lengths



Bond angles

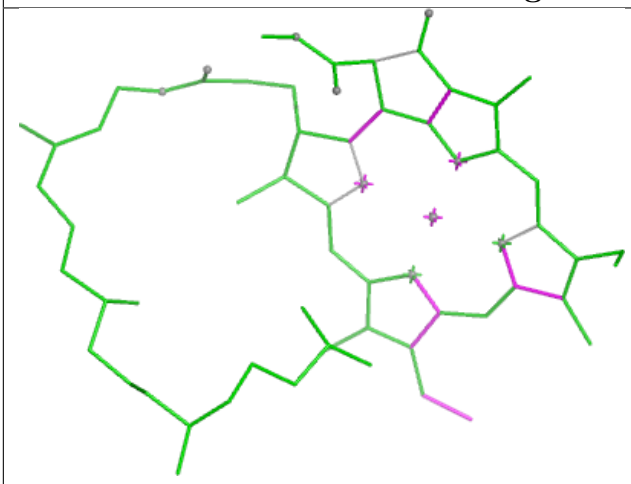


Torsions

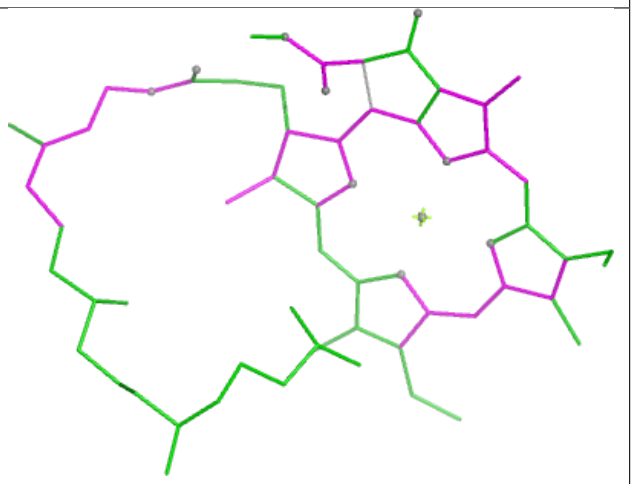


Rings

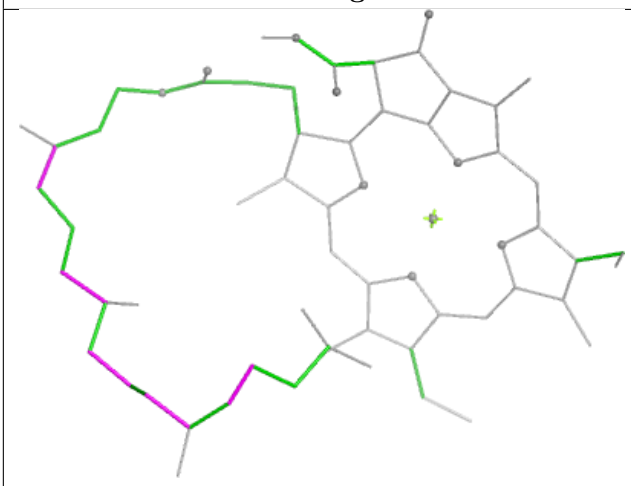
Ligand CLA B 616



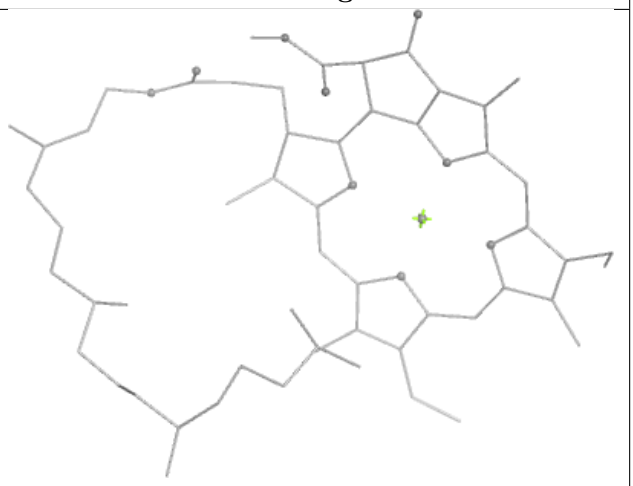
Bond lengths



Bond angles

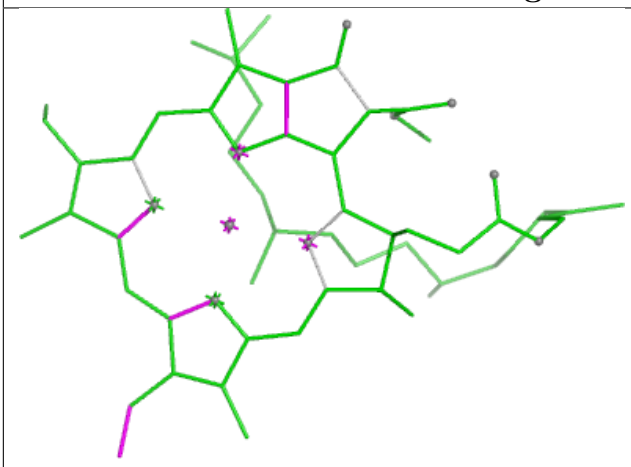


Torsions

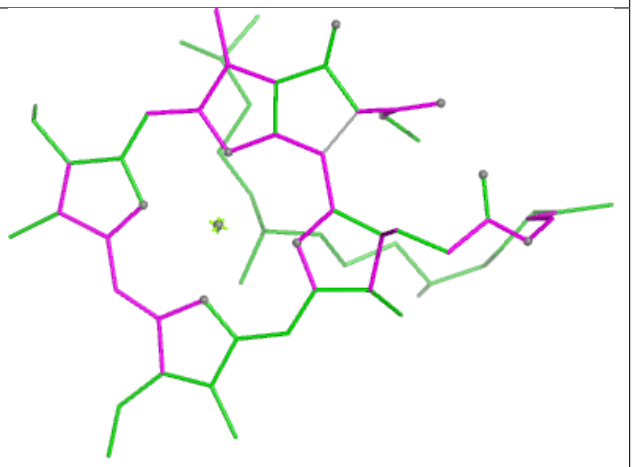


Rings

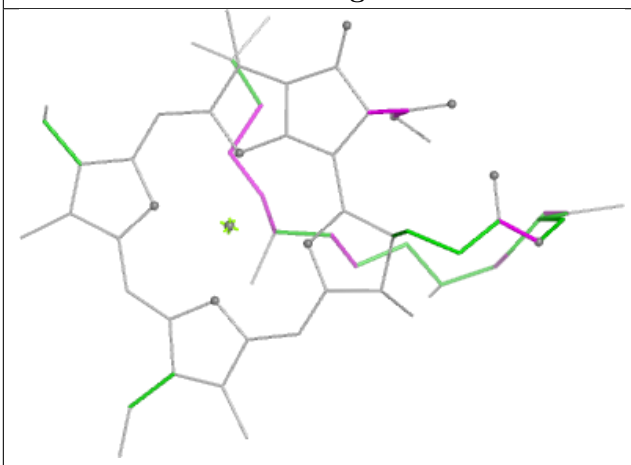
Ligand CLA C 510



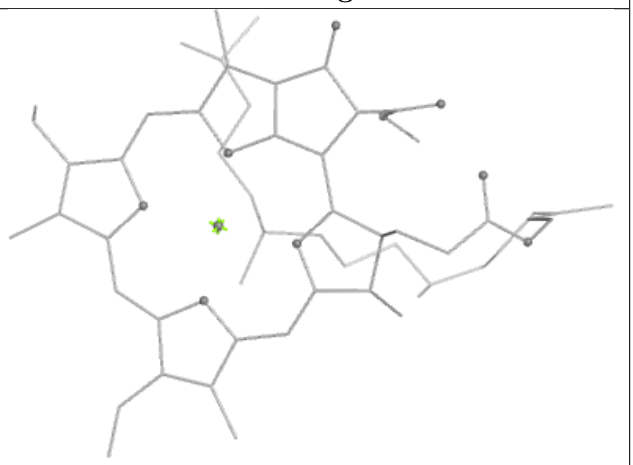
Bond lengths



Bond angles

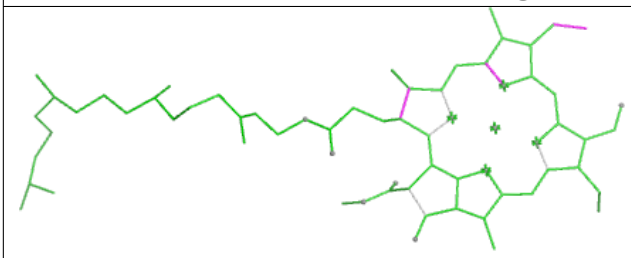


Torsions

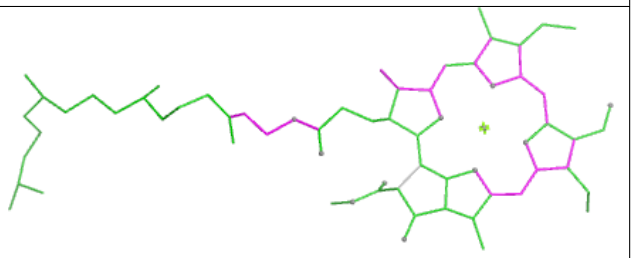


Rings

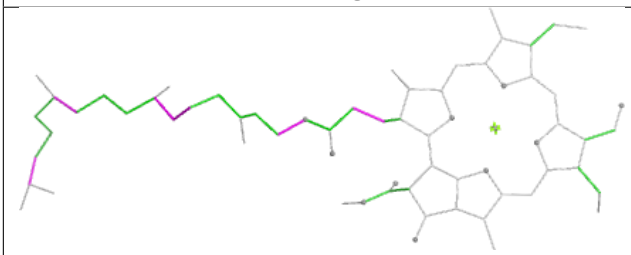
Ligand CHL Y1 606



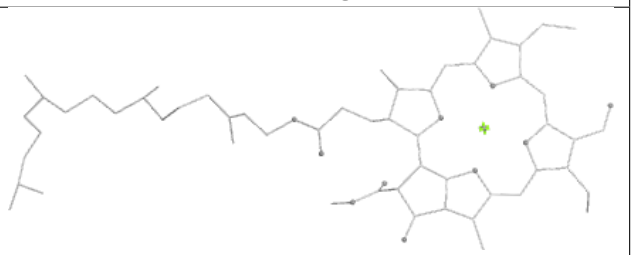
Bond lengths



Bond angles

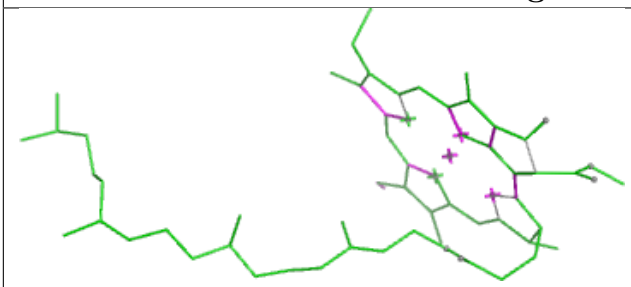


Torsions

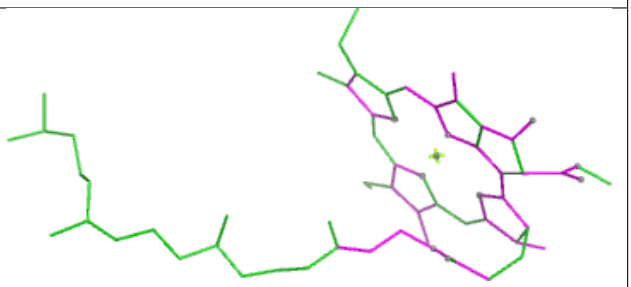


Rings

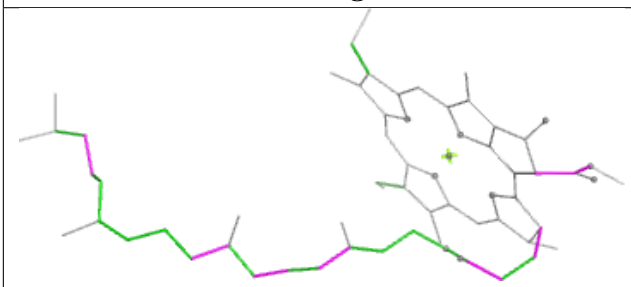
Ligand CLA b 609



Bond lengths



Bond angles

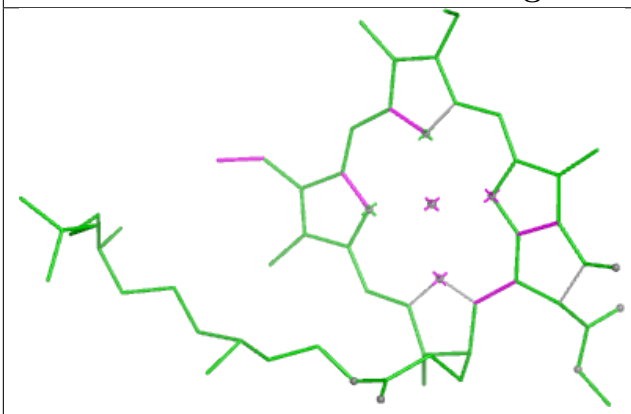


Torsions

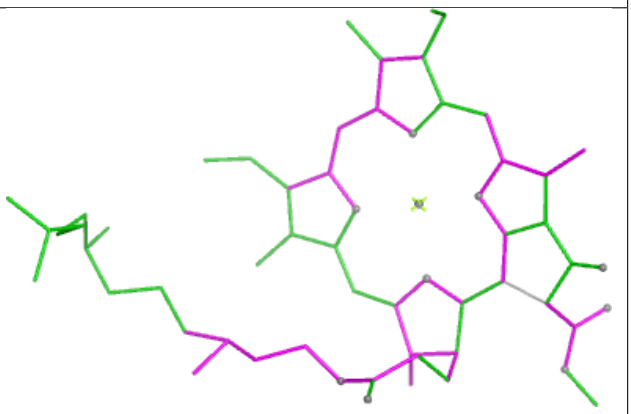


Rings

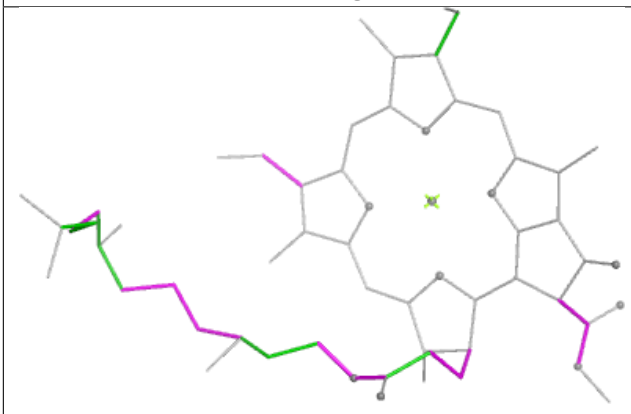
Ligand CLA R 609



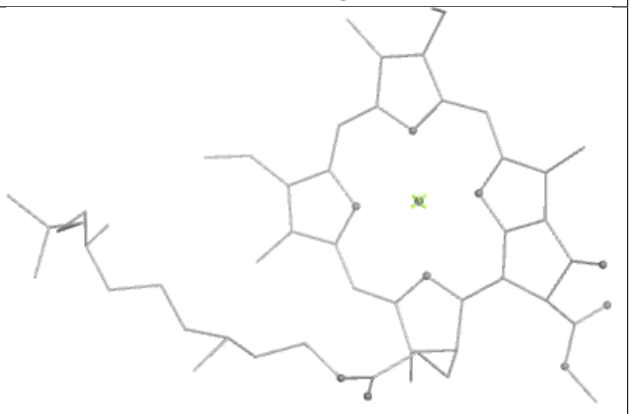
Bond lengths



Bond angles

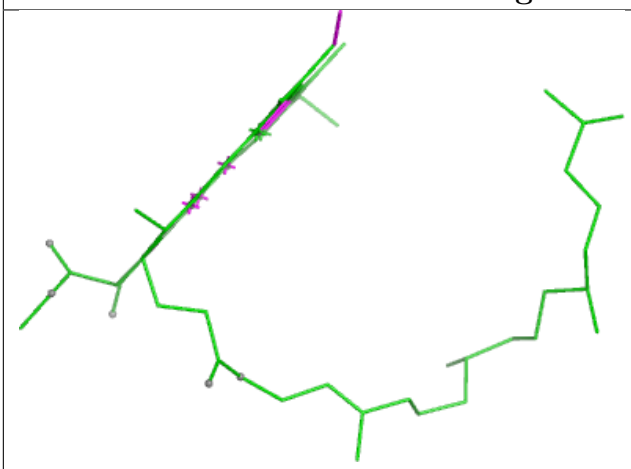


Torsions

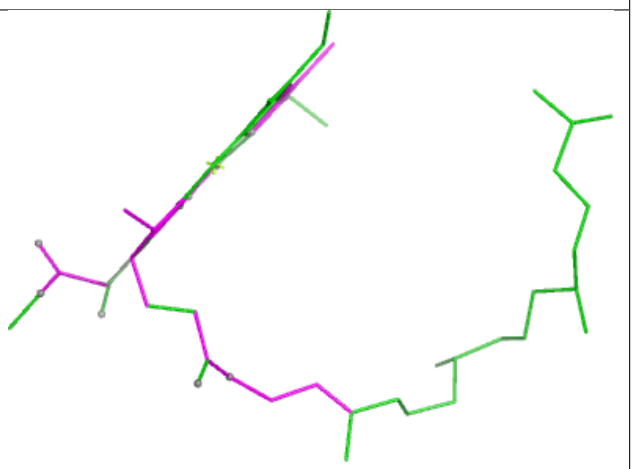


Rings

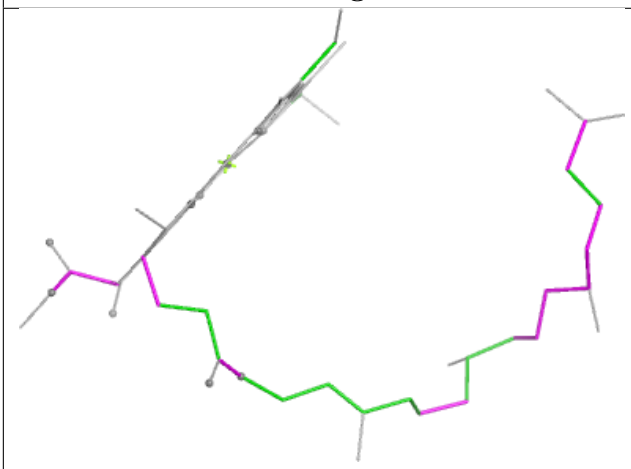
Ligand CLA B1 612



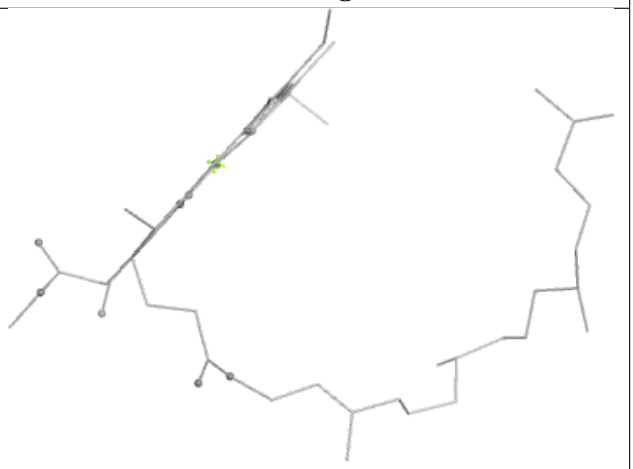
Bond lengths



Bond angles

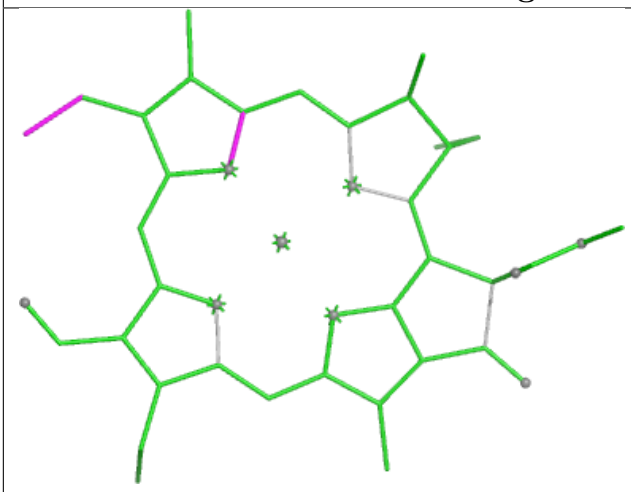


Torsions

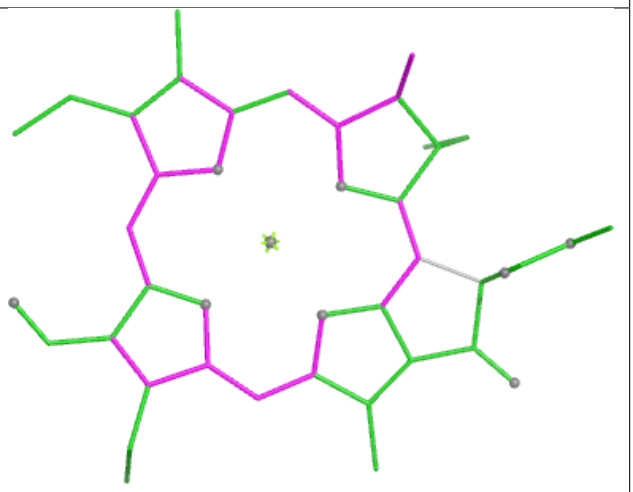


Rings

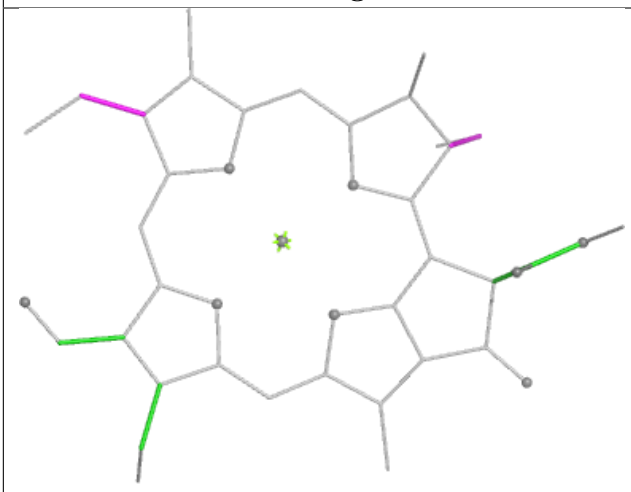
Ligand CHL S1 607



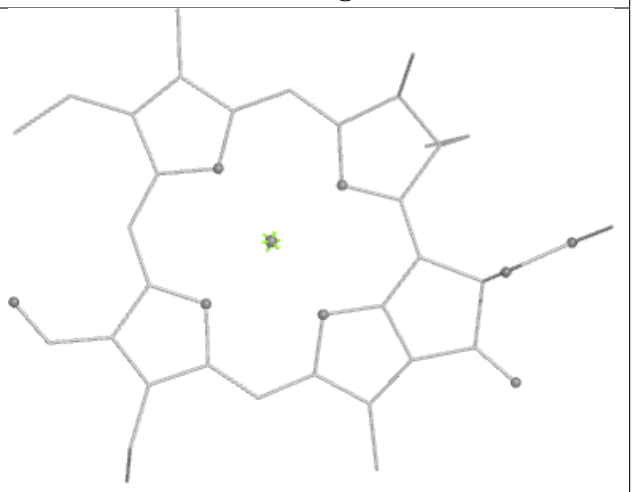
Bond lengths



Bond angles



Torsions

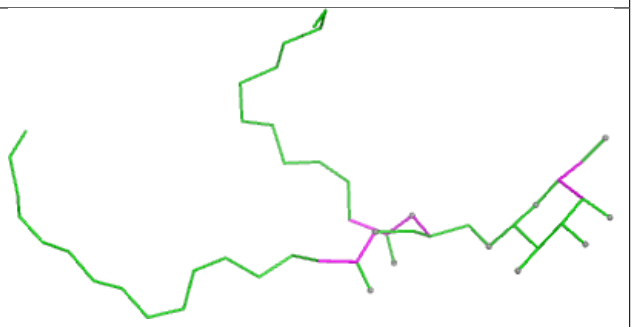


Rings

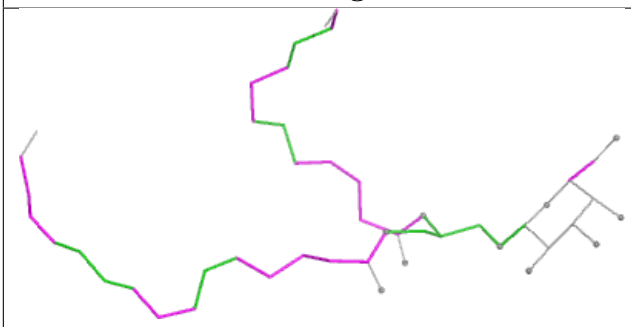
Ligand LMG h1 102



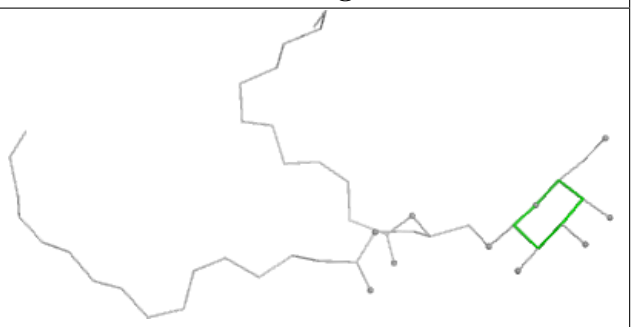
Bond lengths



Bond angles

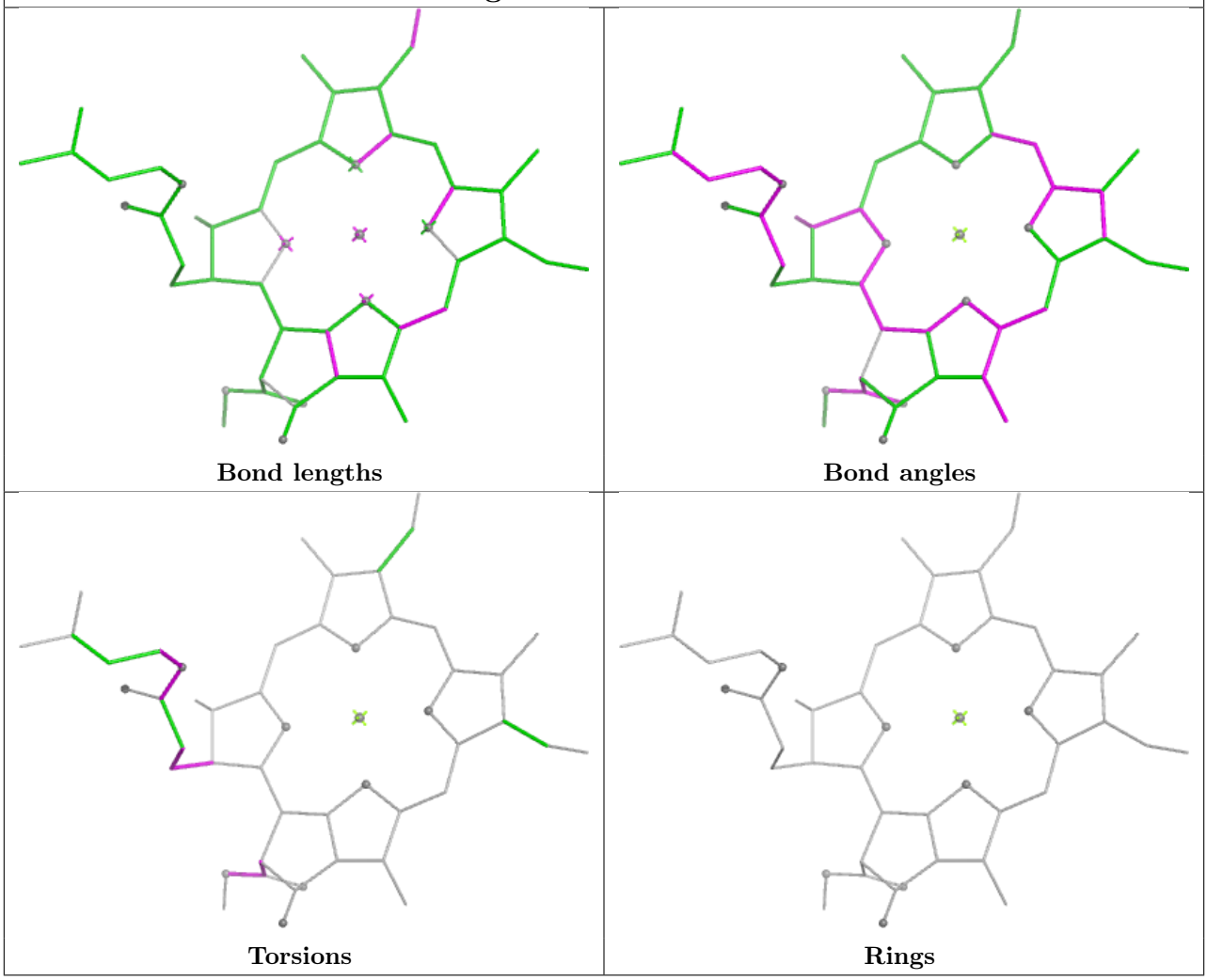


Torsions



Rings

Ligand CLA A1 407



Ligand BCR c 514



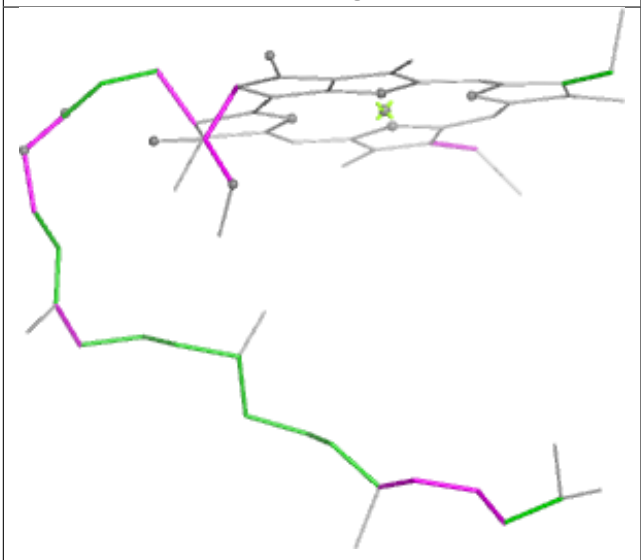
Ligand CLA Y1 603



Bond lengths



Bond angles

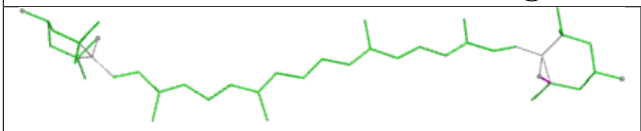


Torsions

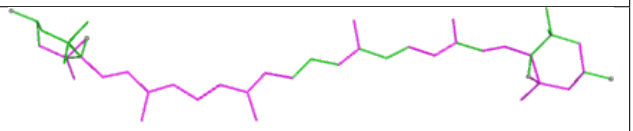


Rings

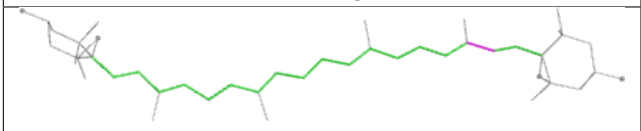
Ligand XAT R 621



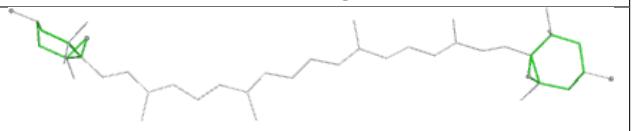
Bond lengths



Bond angles

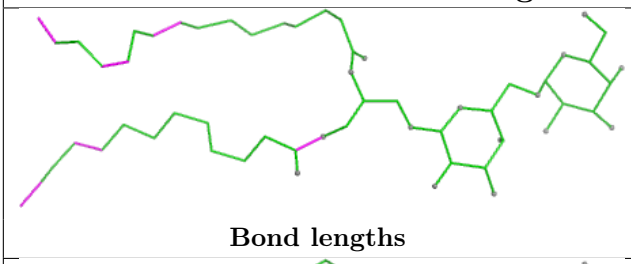


Torsions

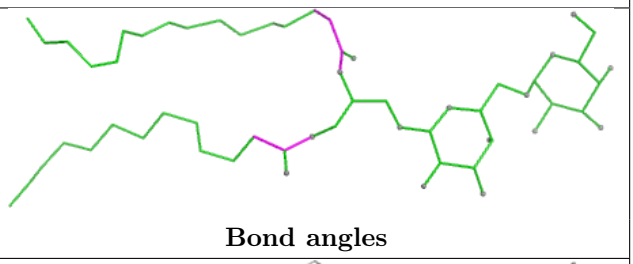


Rings

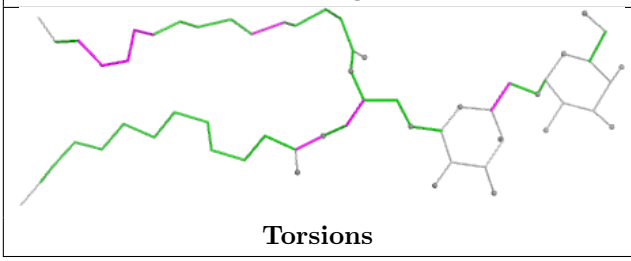
Ligand DGD c1 520



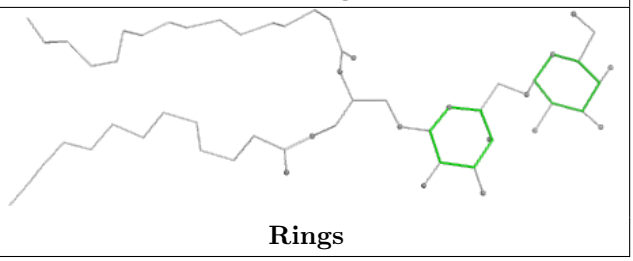
Bond lengths



Bond angles

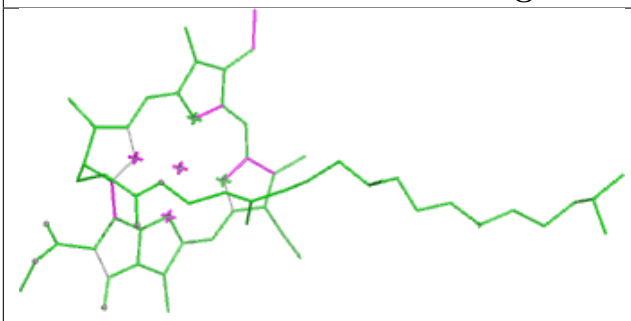


Torsions

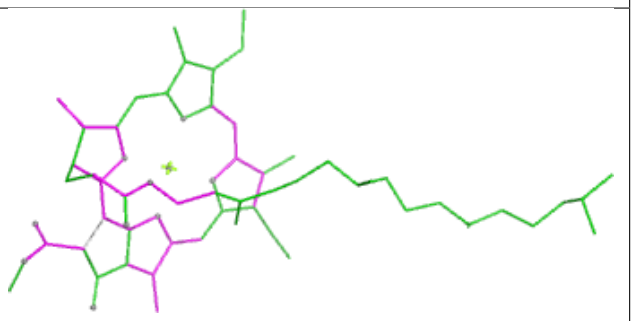


Rings

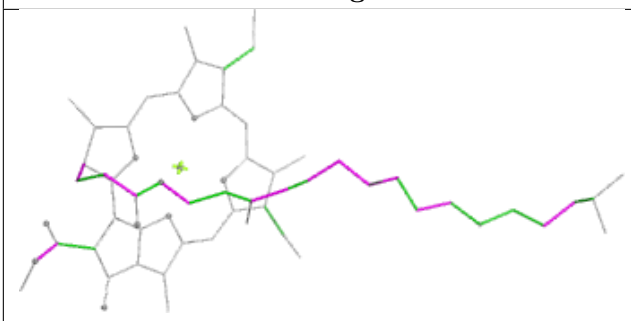
Ligand CLA B1 615



Bond lengths



Bond angles

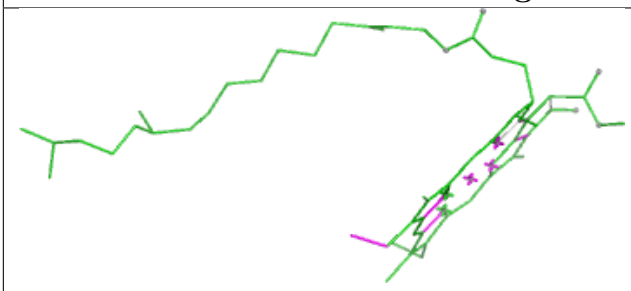


Torsions

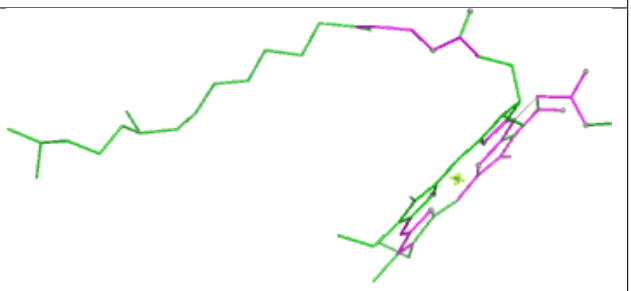


Rings

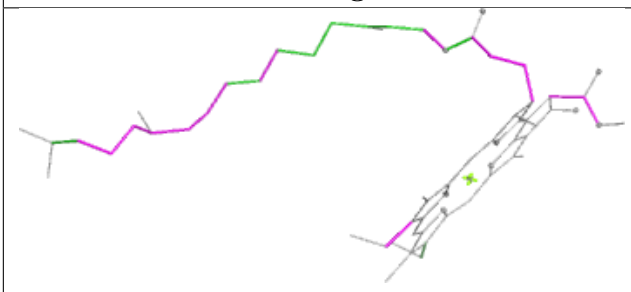
Ligand CLA N1 604



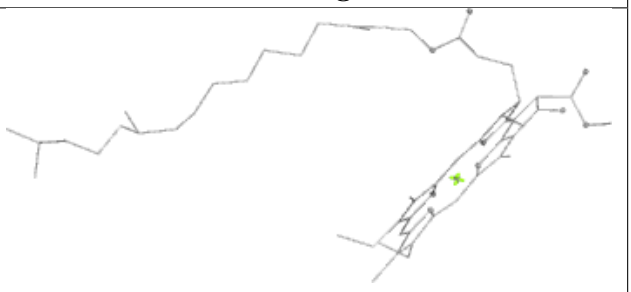
Bond lengths



Bond angles

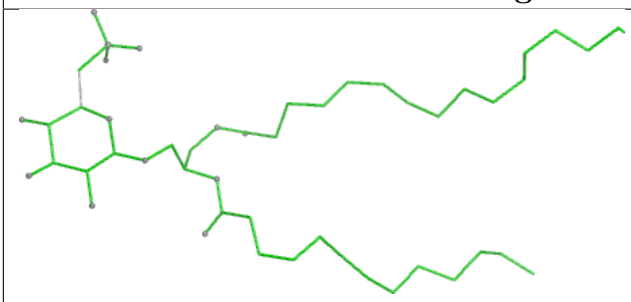


Torsions

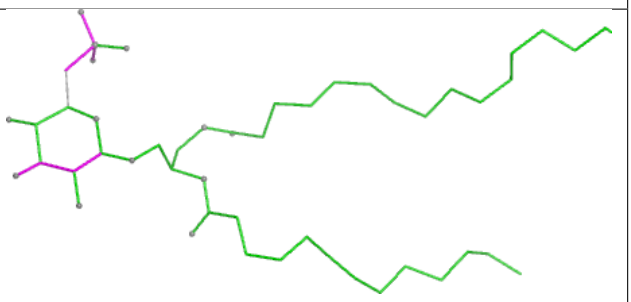


Rings

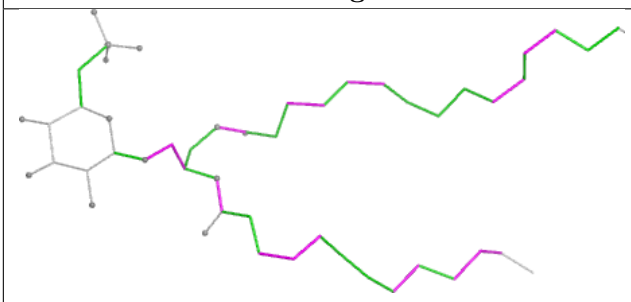
Ligand SQD A1 412



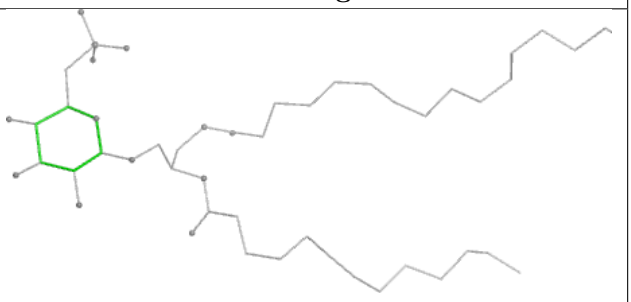
Bond lengths



Bond angles

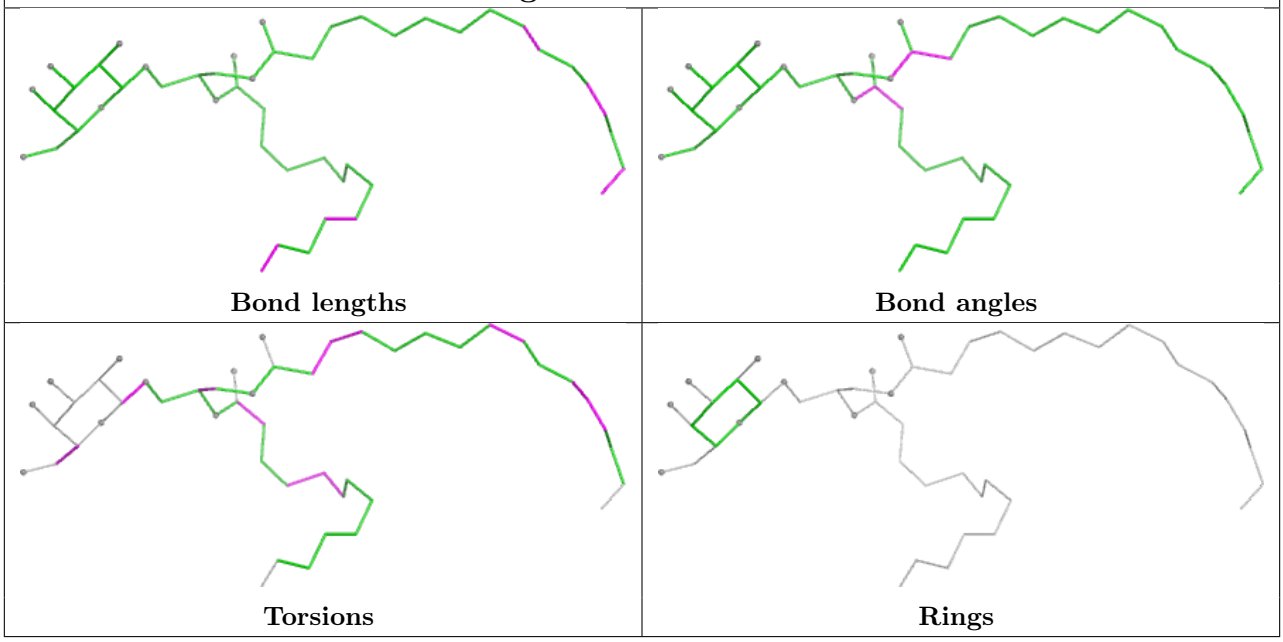


Torsions

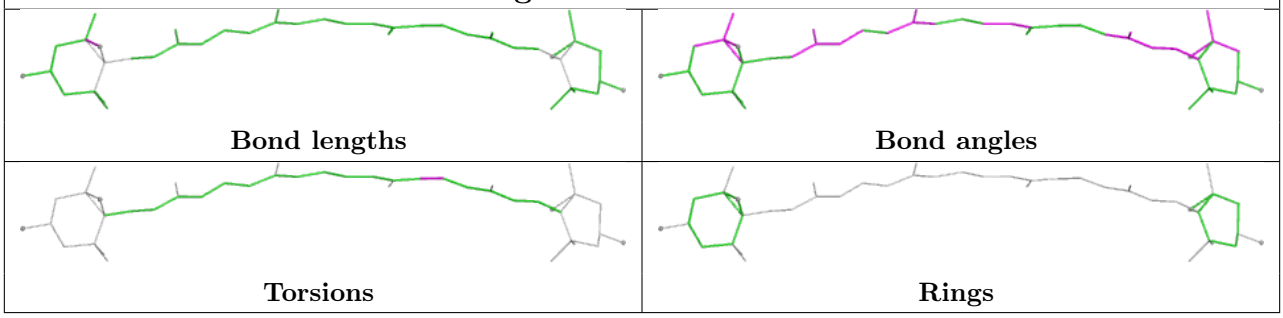


Rings

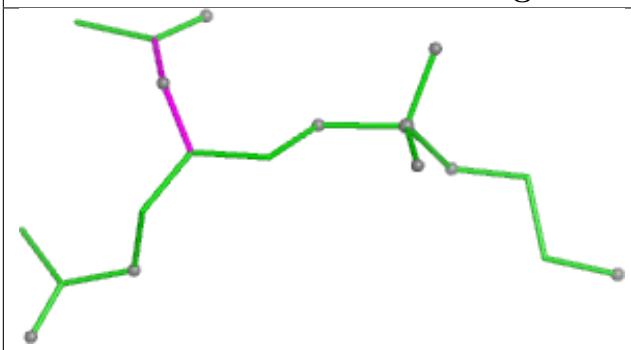
Ligand LMG H 102



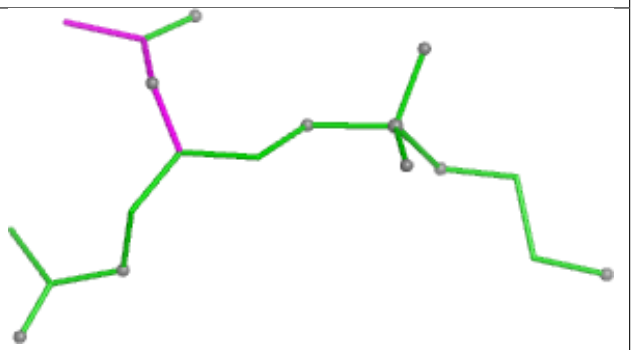
Ligand XAT N1 622



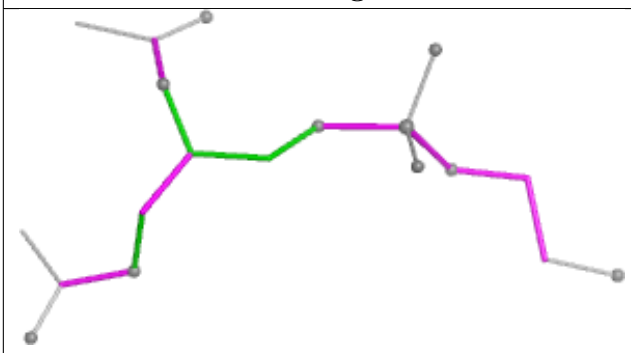
Ligand PTY Y1 627



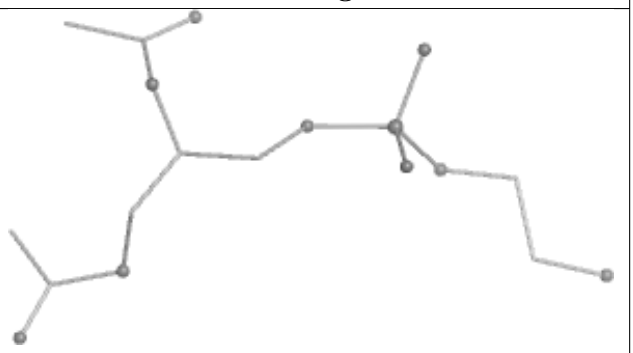
Bond lengths



Bond angles

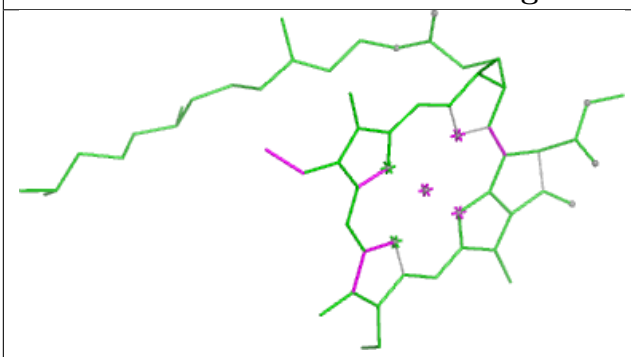


Torsions

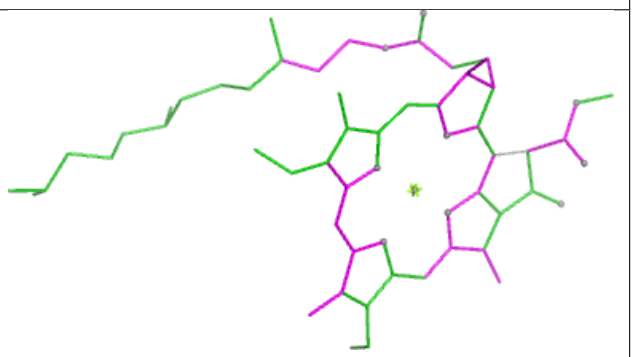


Rings

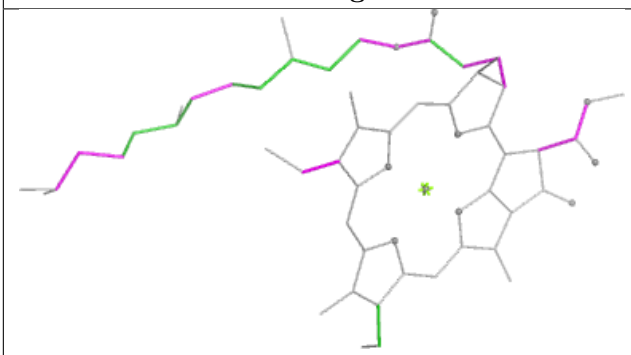
Ligand CLA r1 610



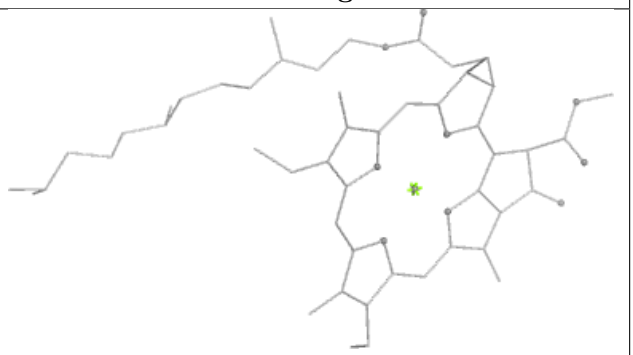
Bond lengths



Bond angles

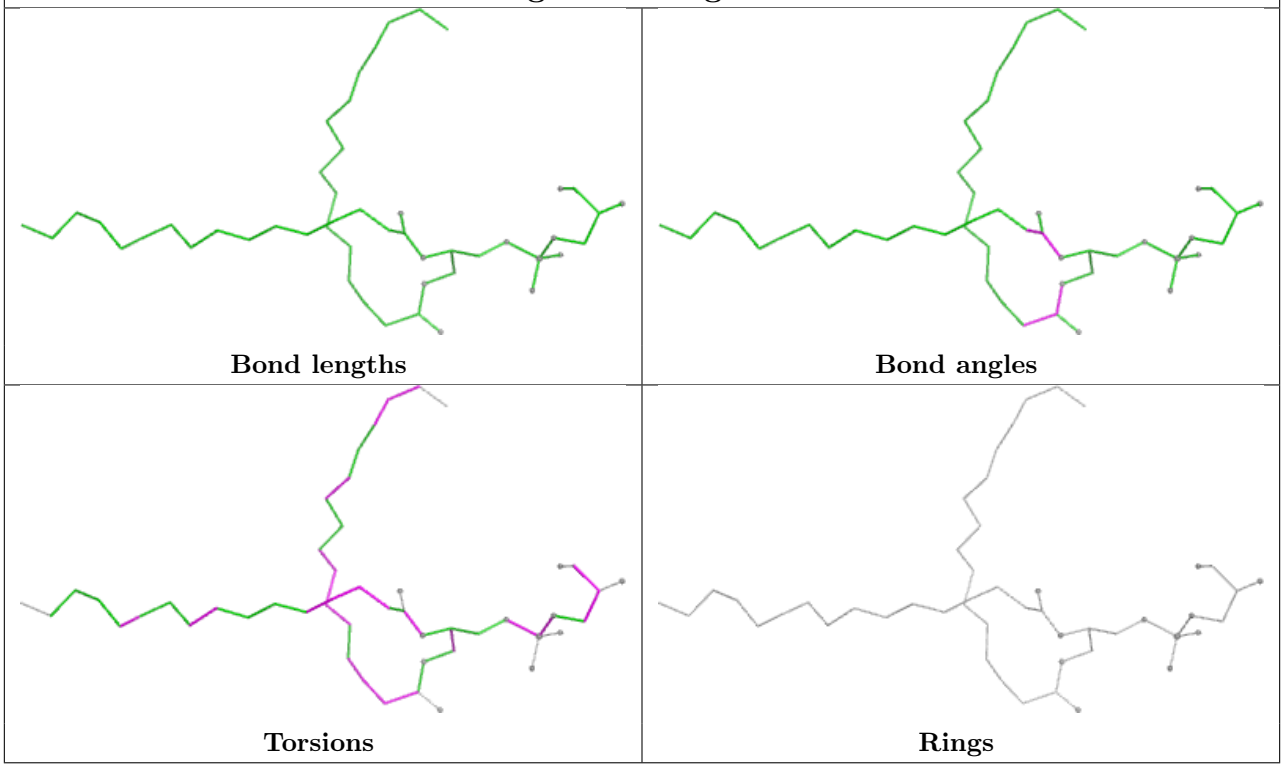


Torsions

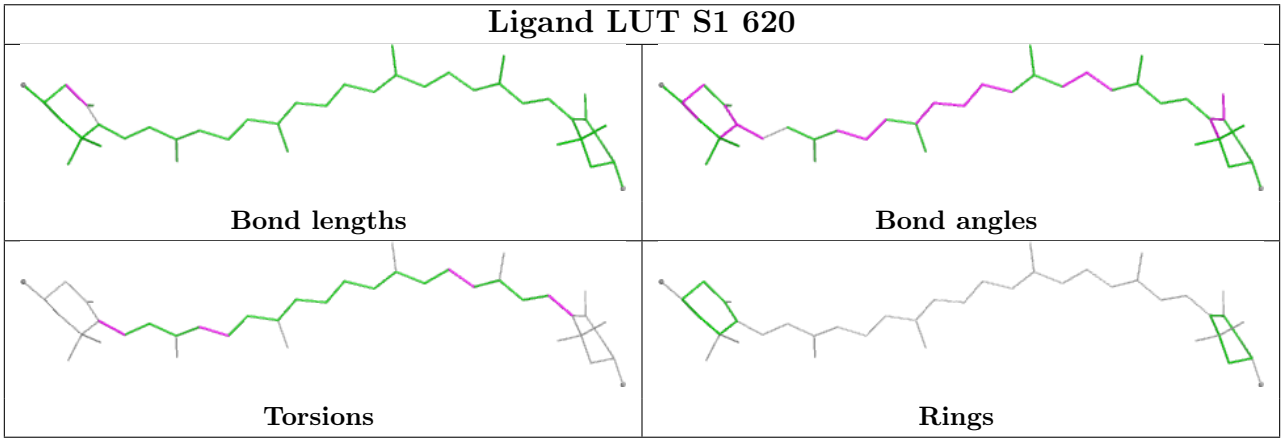


Rings

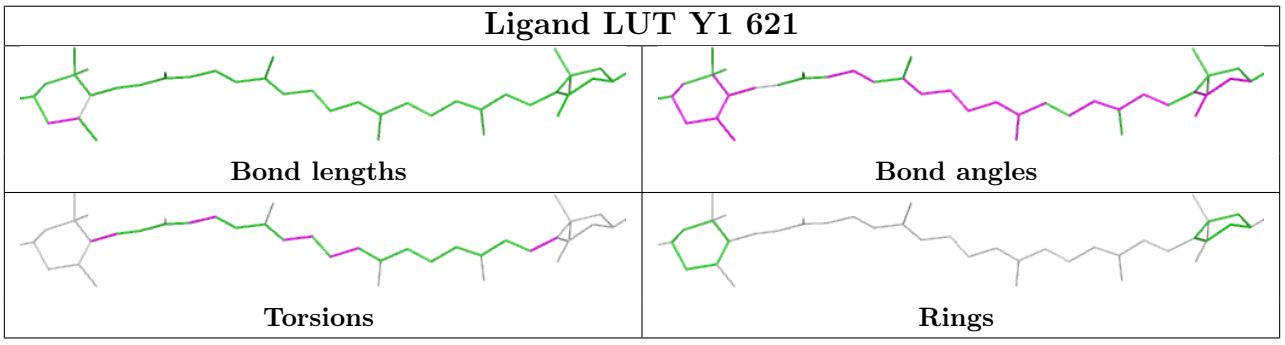
Ligand LHG g 624



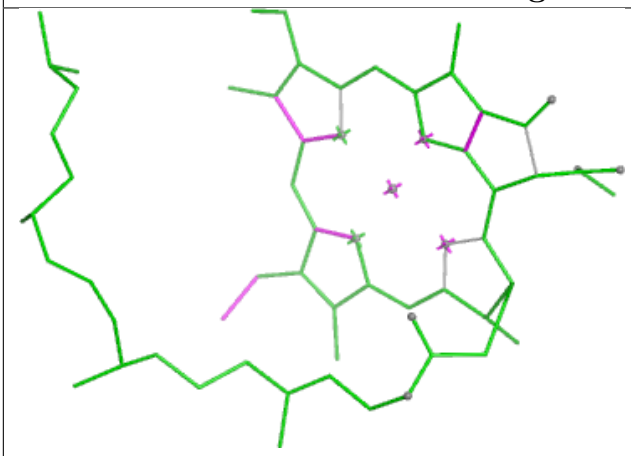
Ligand LUT S1 620



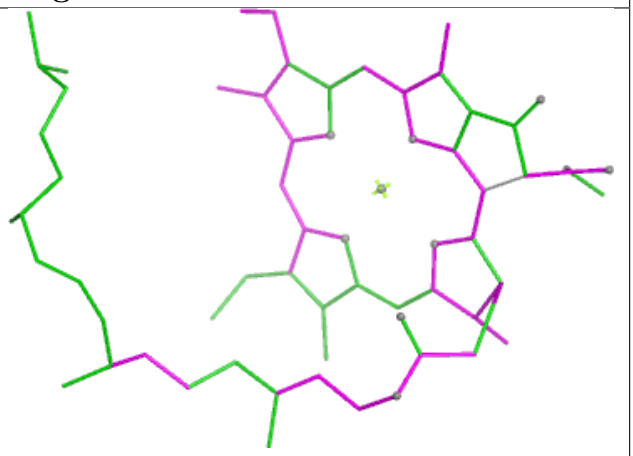
Ligand LUT Y1 621



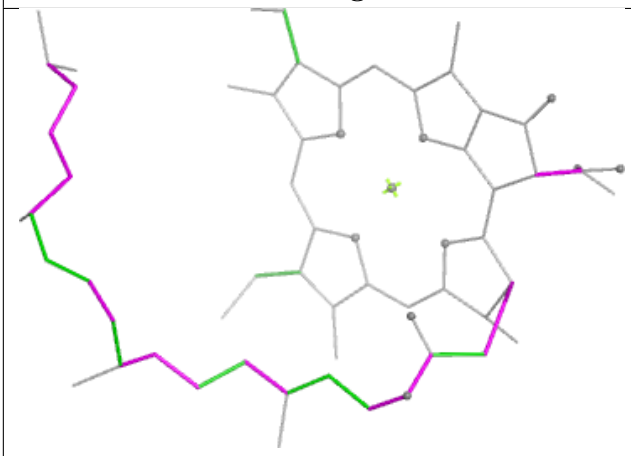
Ligand CLA g 602



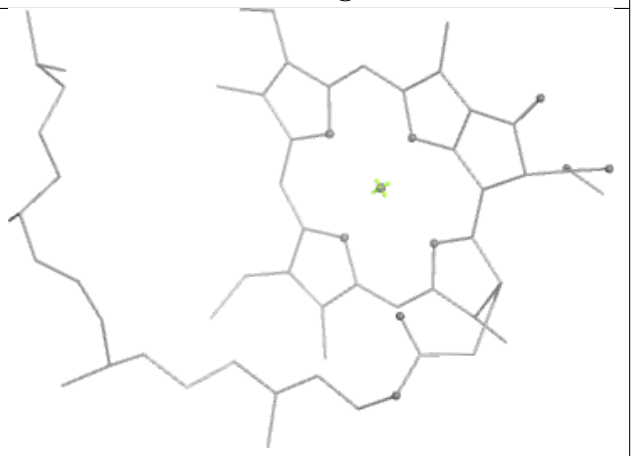
Bond lengths



Bond angles

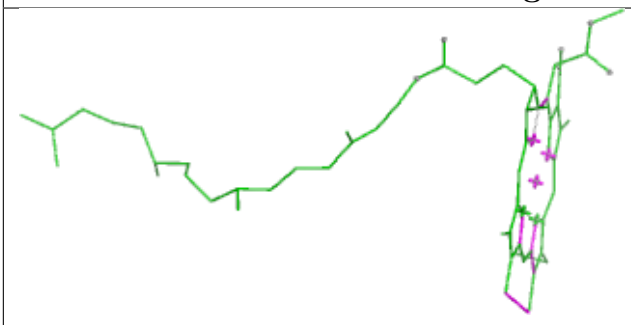


Torsions

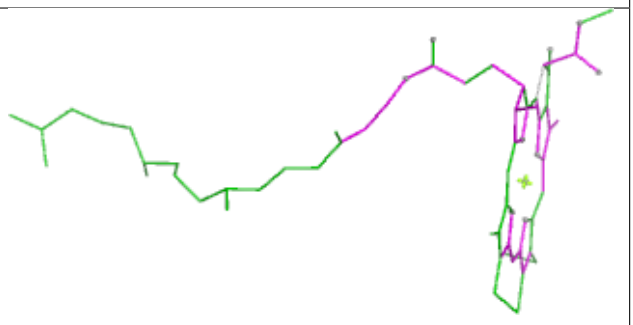


Rings

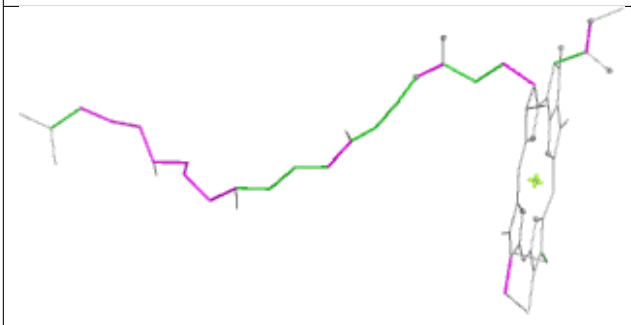
Ligand CLA D 403



Bond lengths



Bond angles

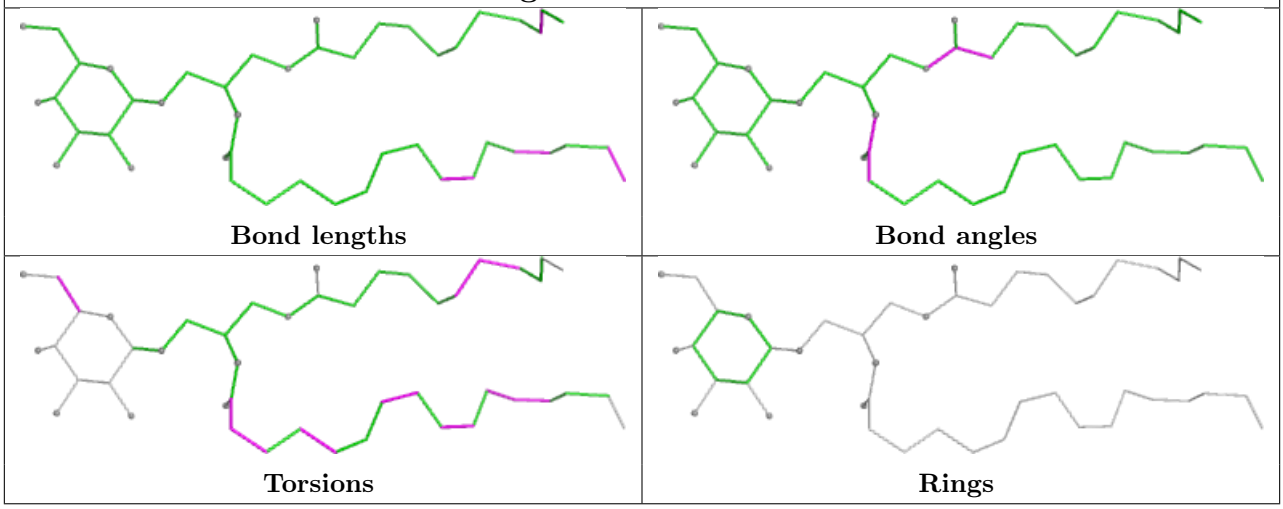


Torsions

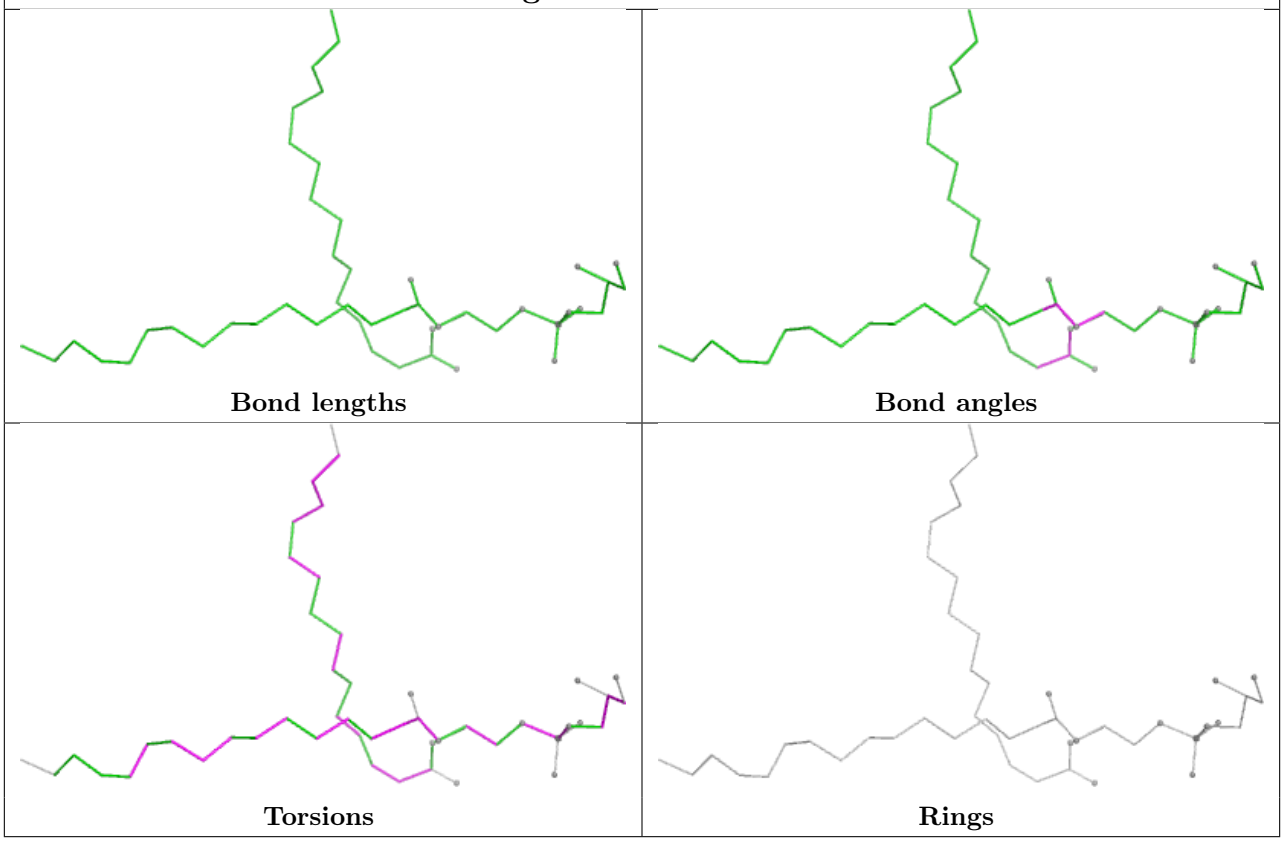


Rings

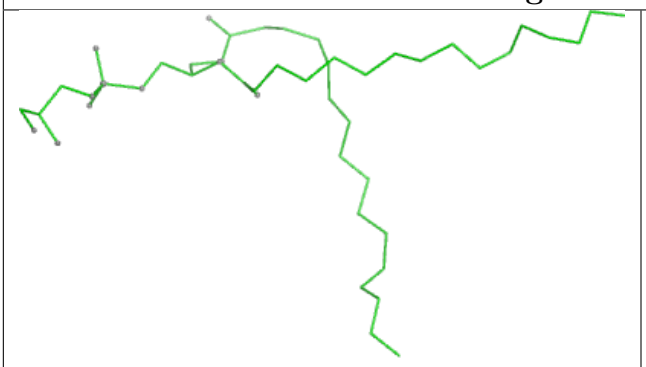
Ligand LMG D 411



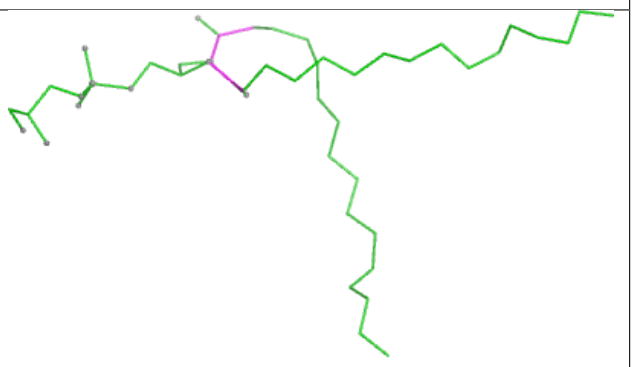
Ligand LHG N 624



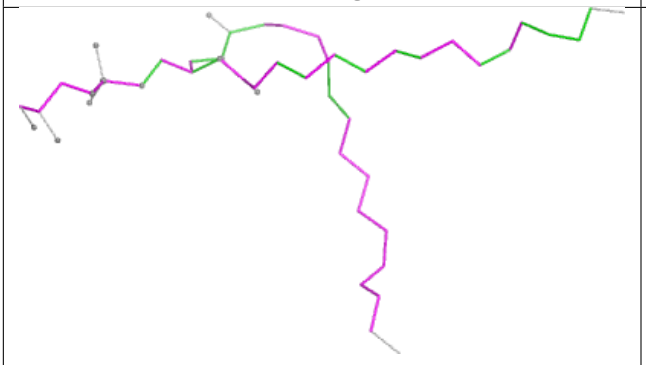
Ligand LHG n 624



Bond lengths



Bond angles

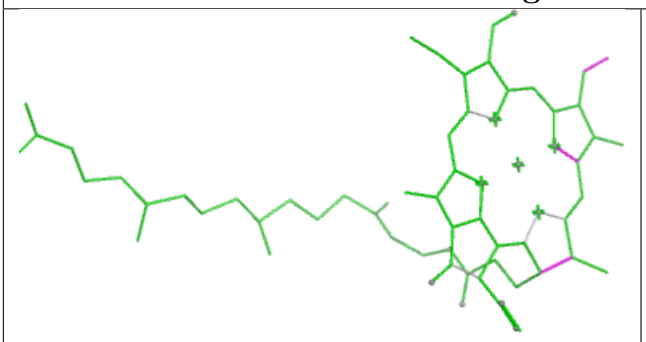


Torsions

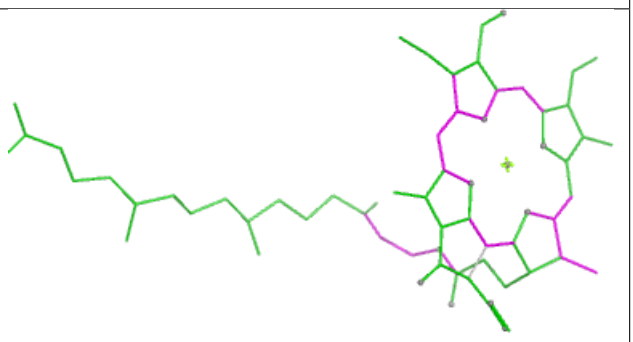


Rings

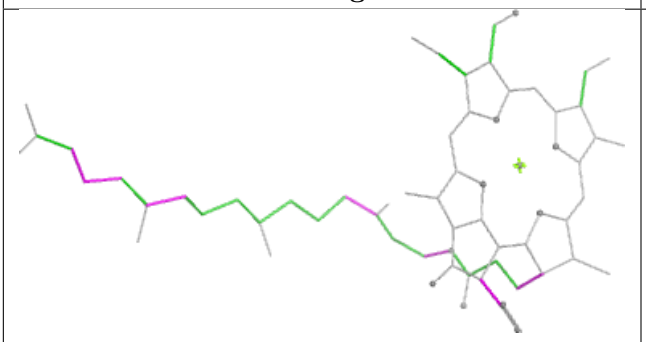
Ligand CHL N 609



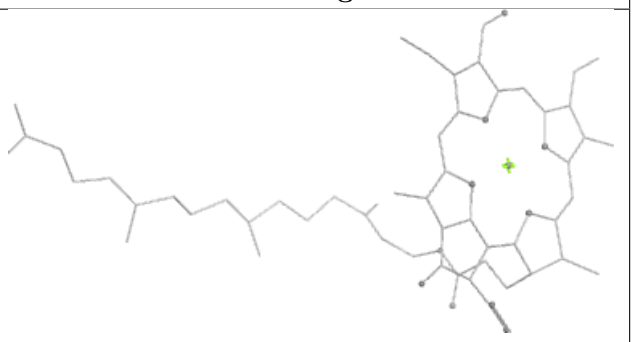
Bond lengths



Bond angles

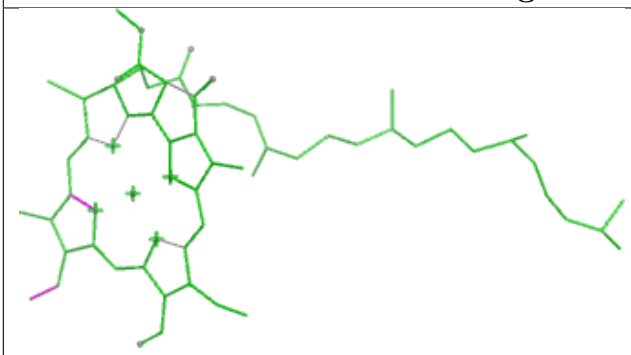


Torsions

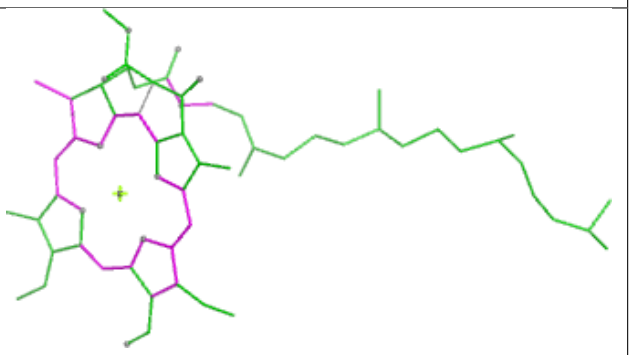


Rings

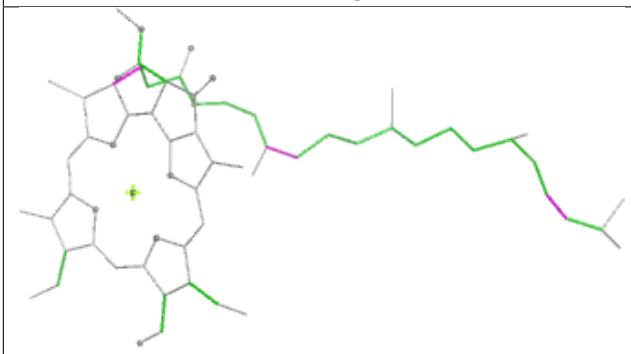
Ligand CHL n1 609



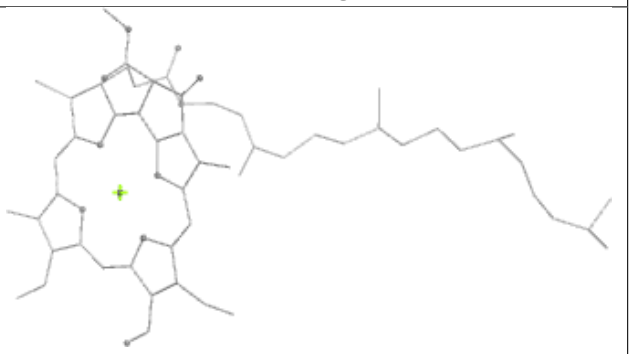
Bond lengths



Bond angles

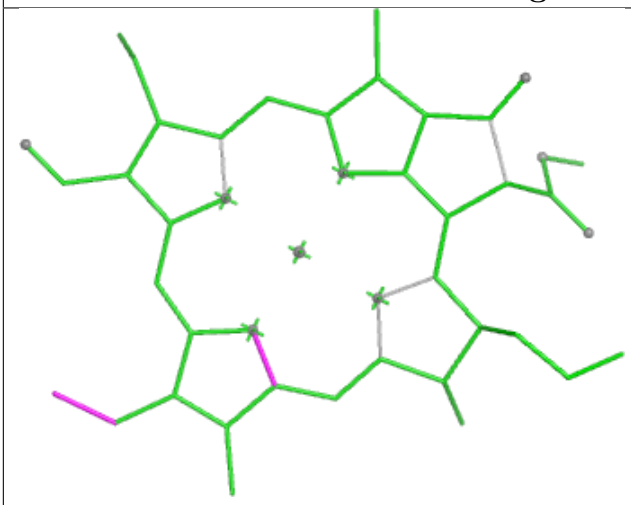


Torsions

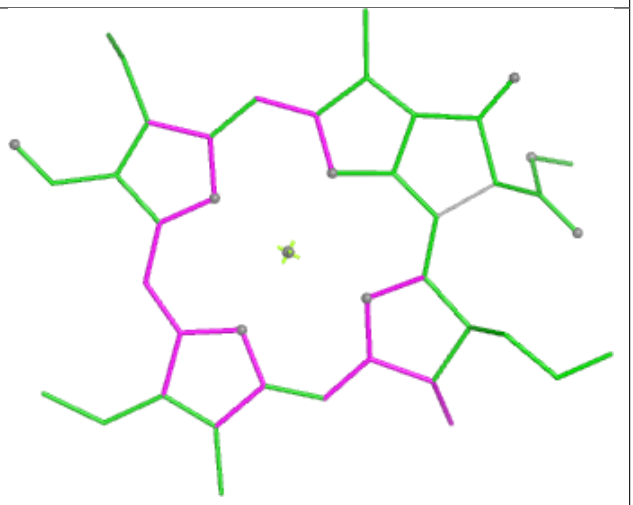


Rings

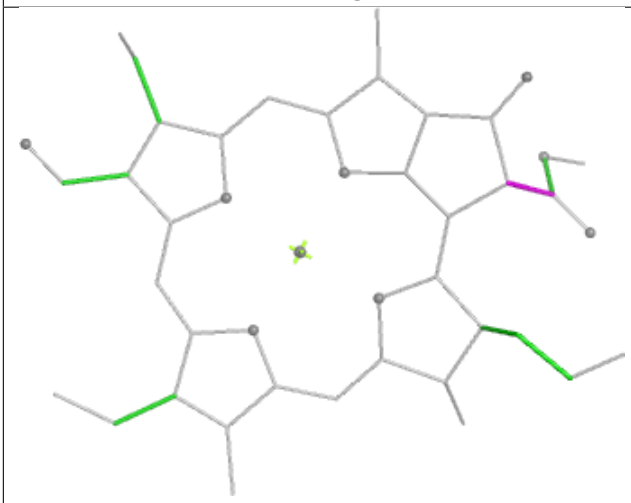
Ligand CHL r 606



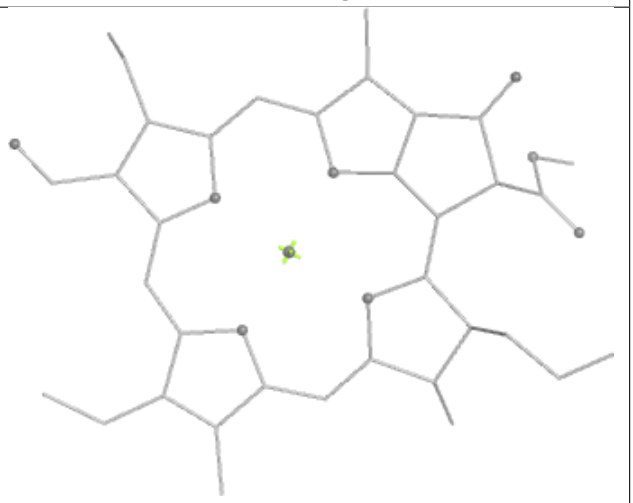
Bond lengths



Bond angles

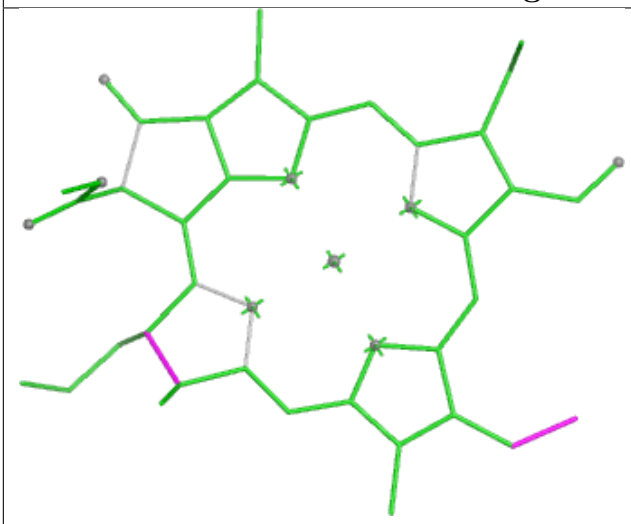


Torsions

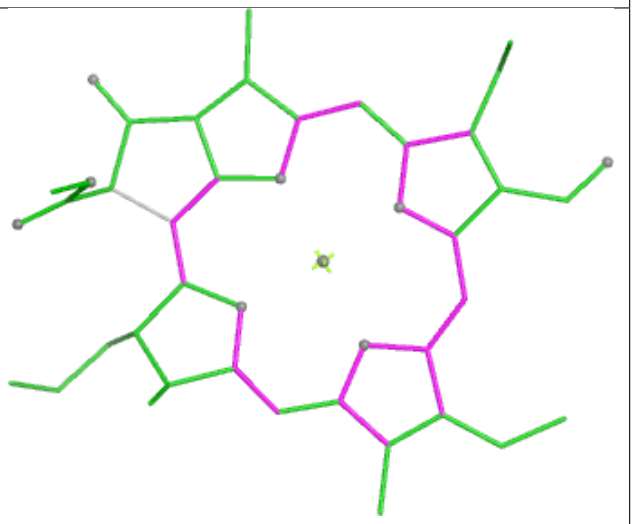


Rings

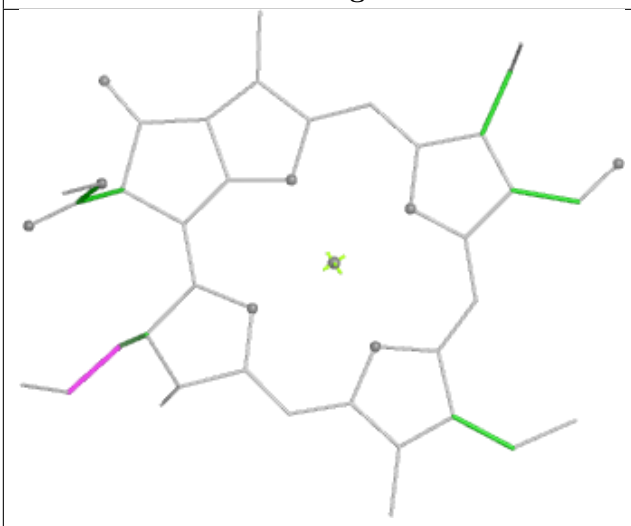
Ligand CHL R 606



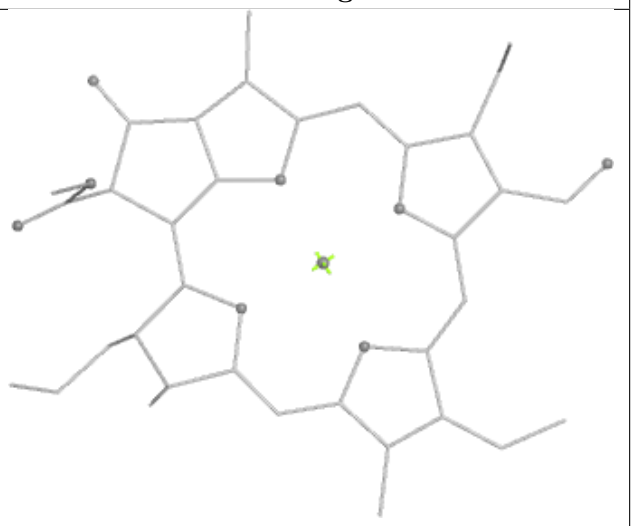
Bond lengths



Bond angles

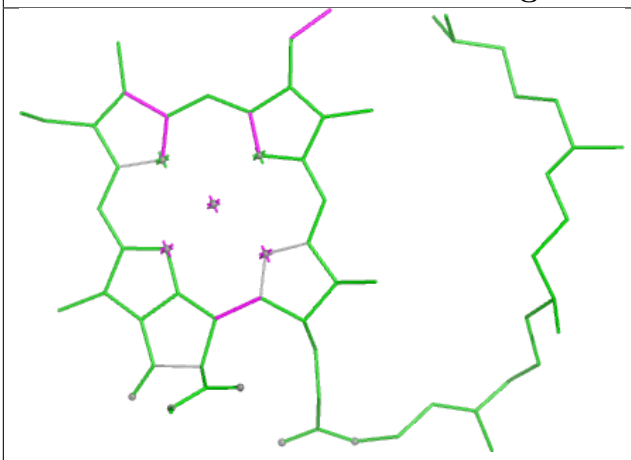


Torsions

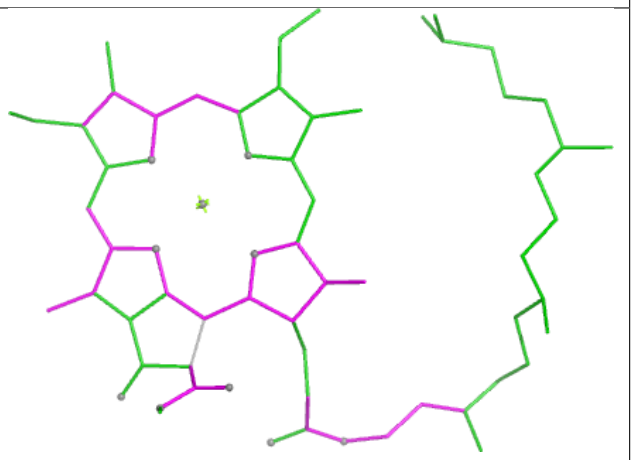


Rings

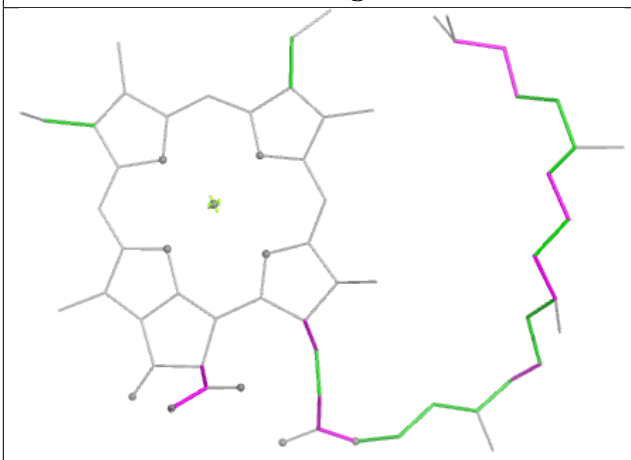
Ligand CLA c1 512



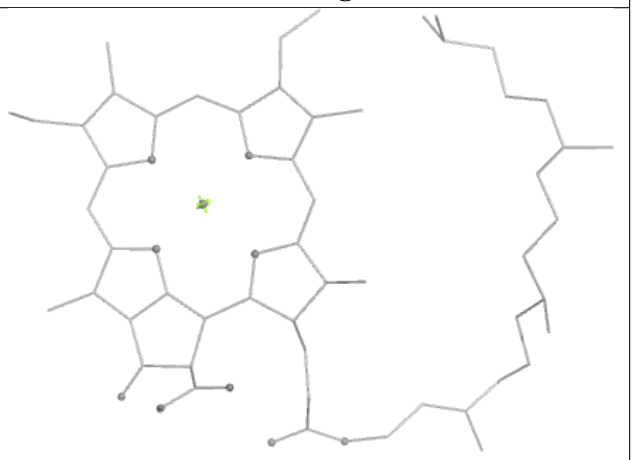
Bond lengths



Bond angles

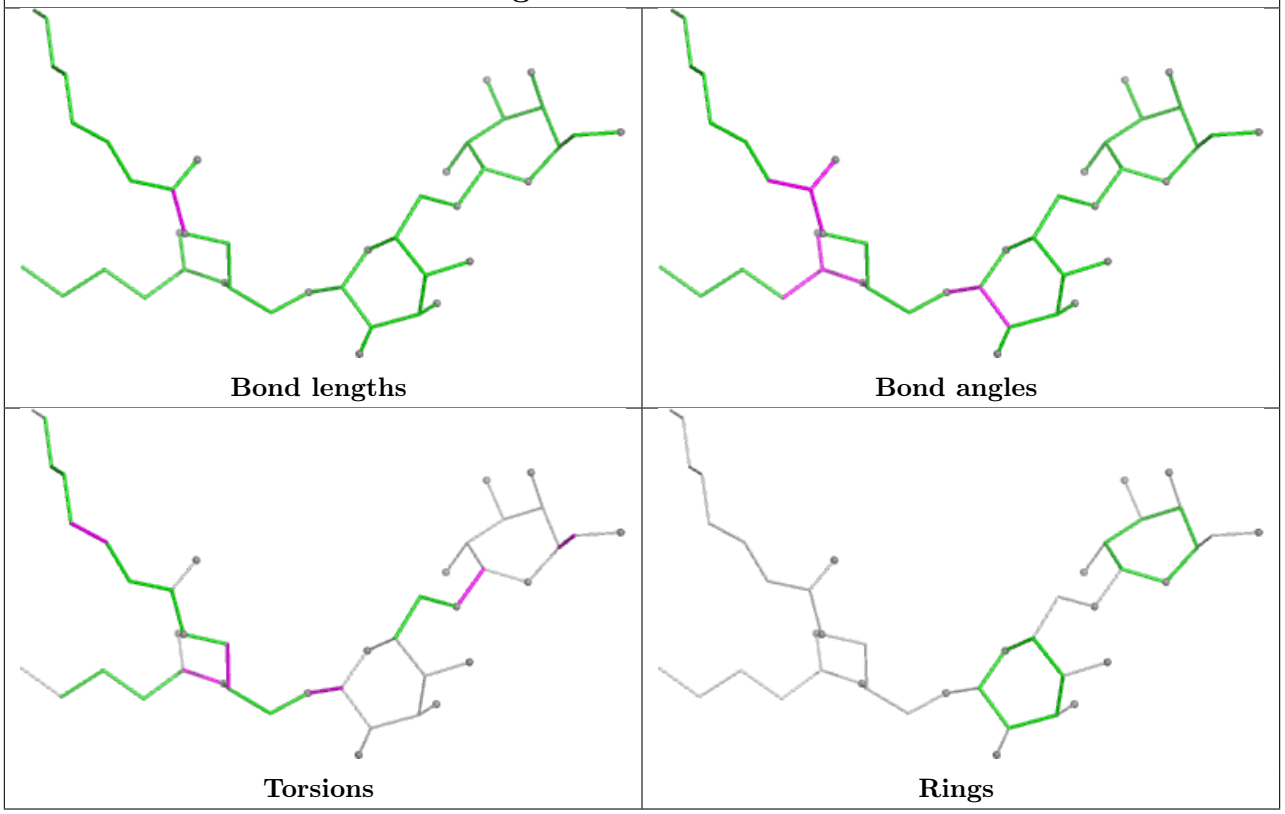


Torsions

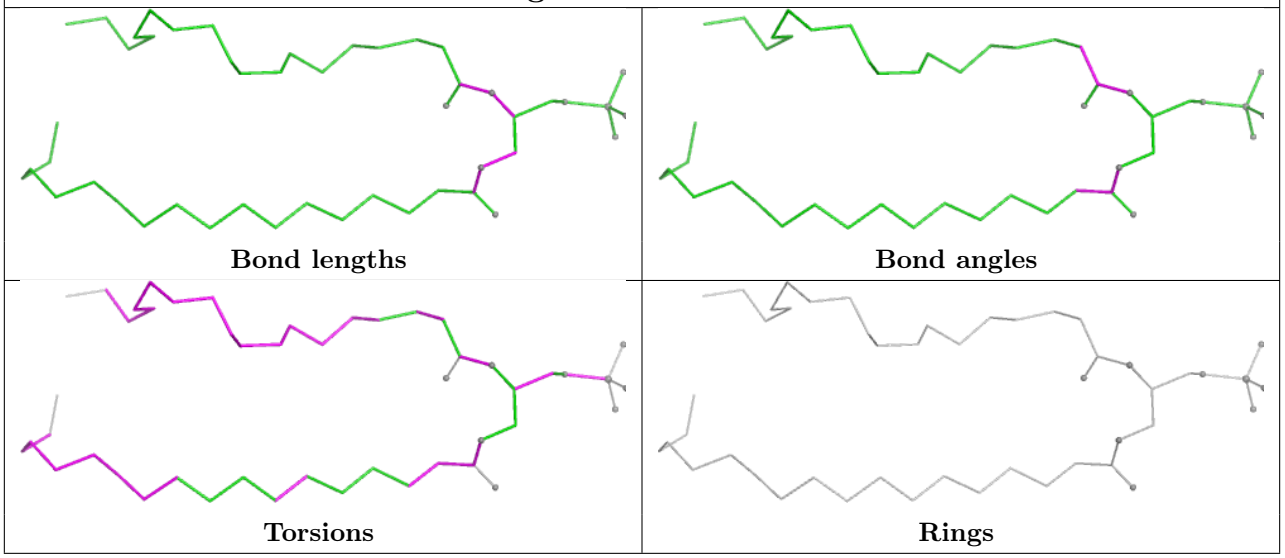


Rings

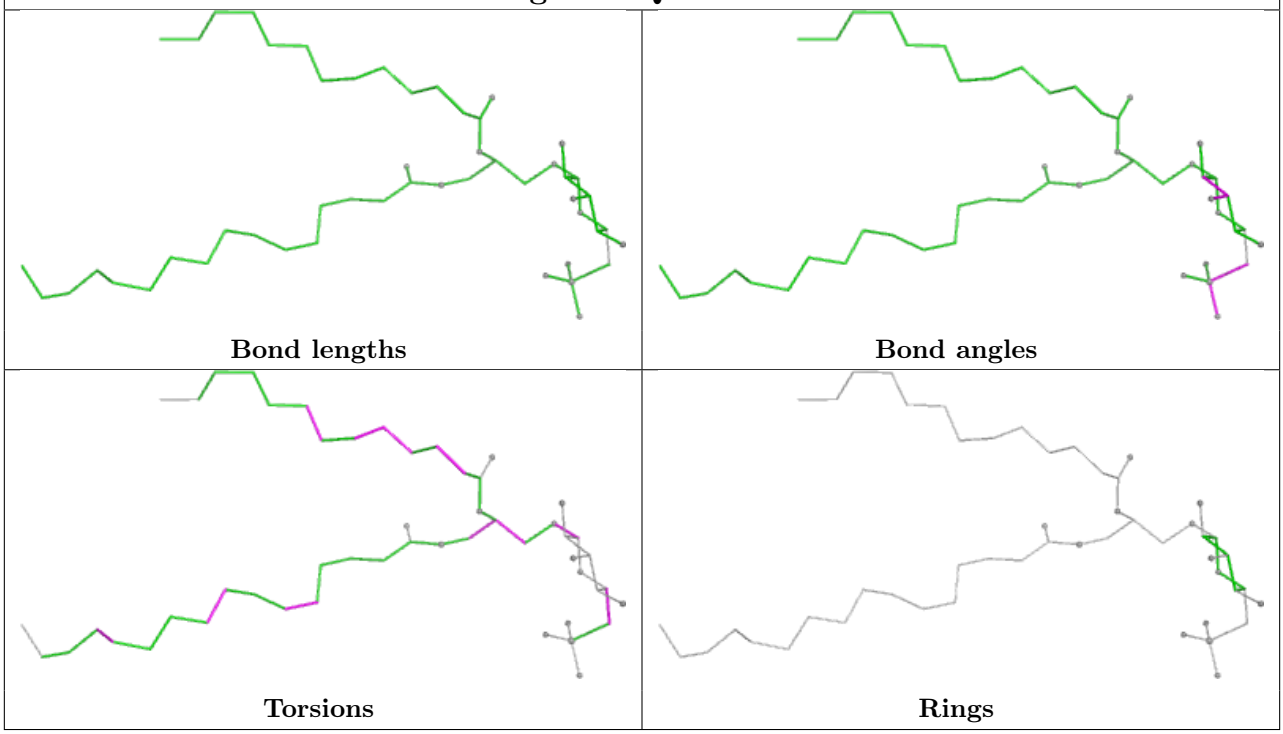
Ligand DGD B1 623



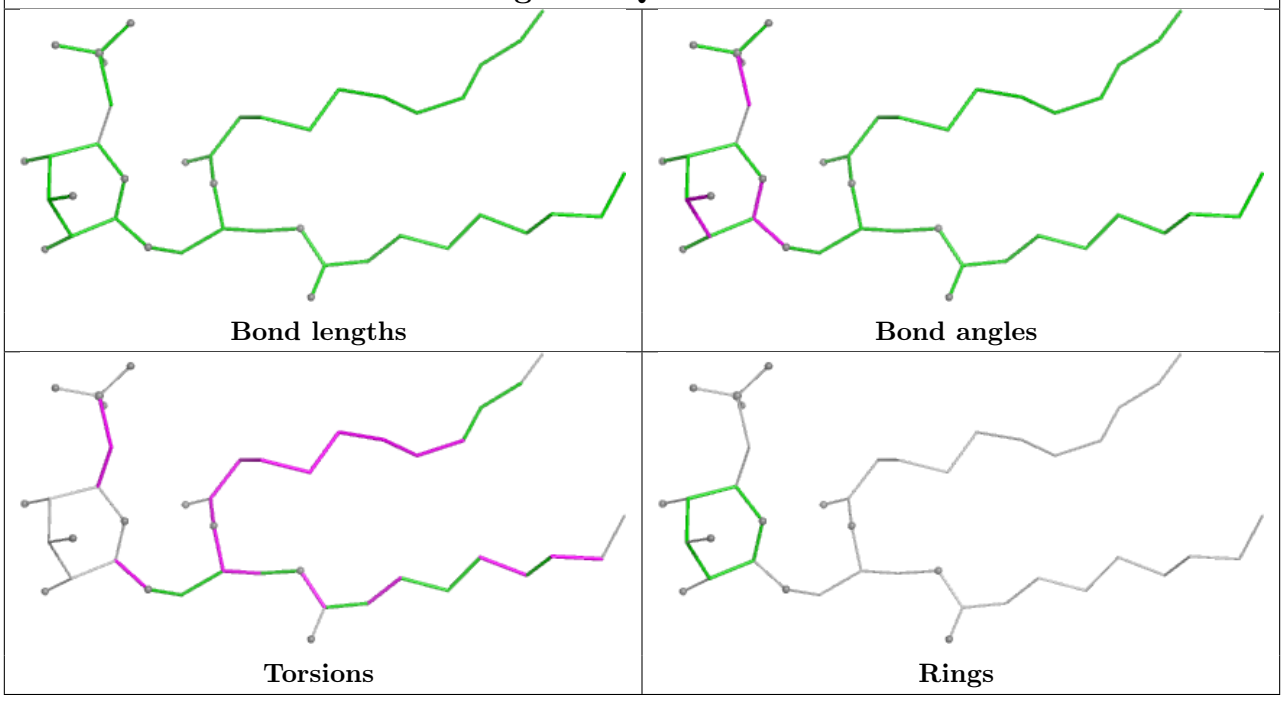
Ligand 3PH B 624



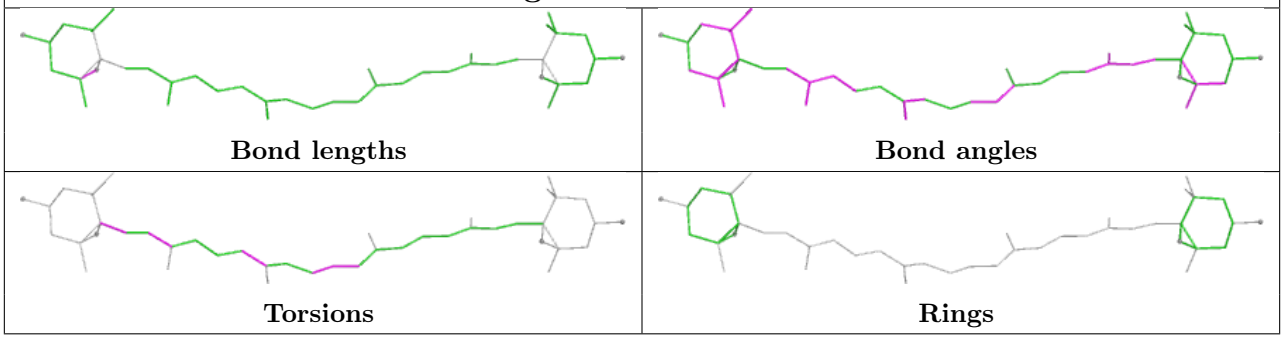
Ligand SQD a 412



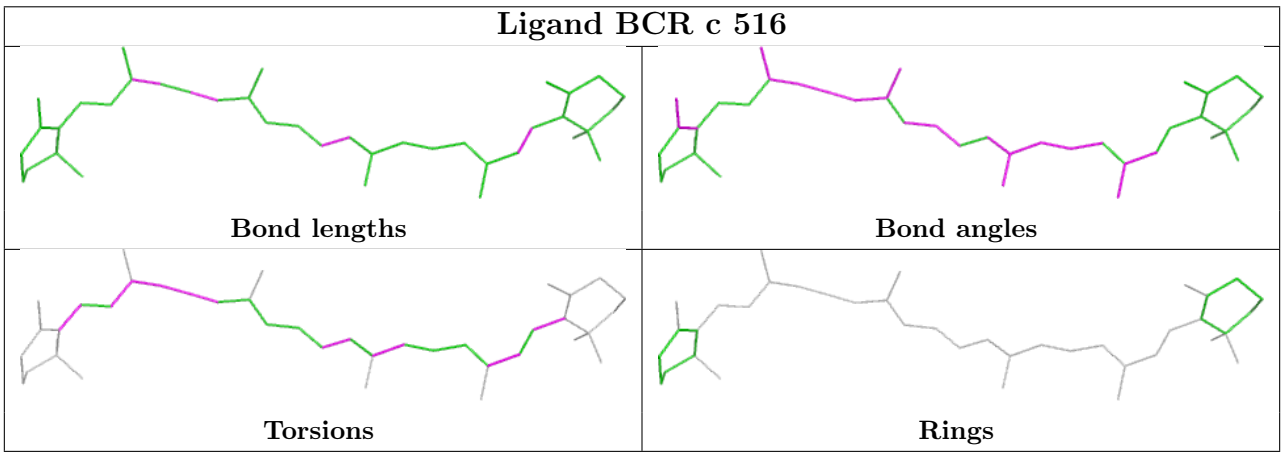
Ligand SQD m1 101



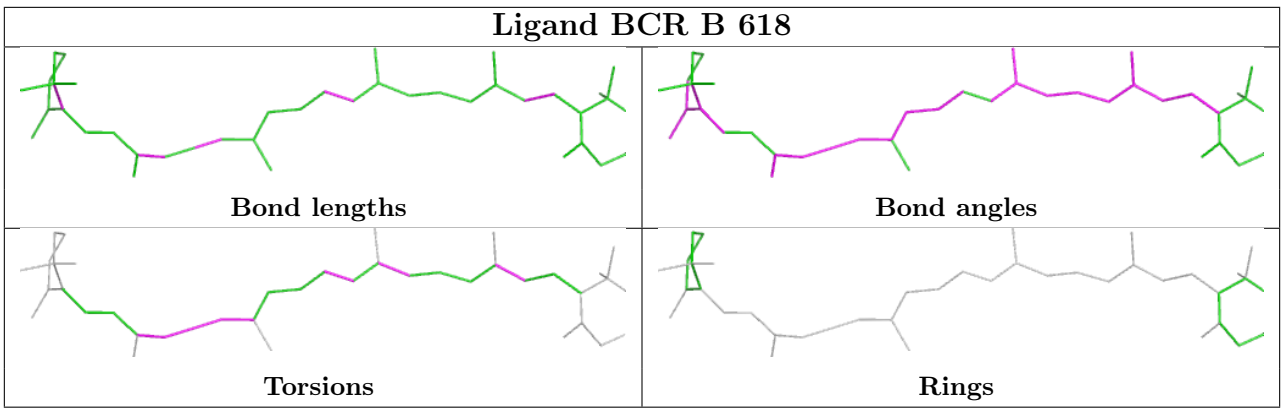
Ligand XAT Y 622



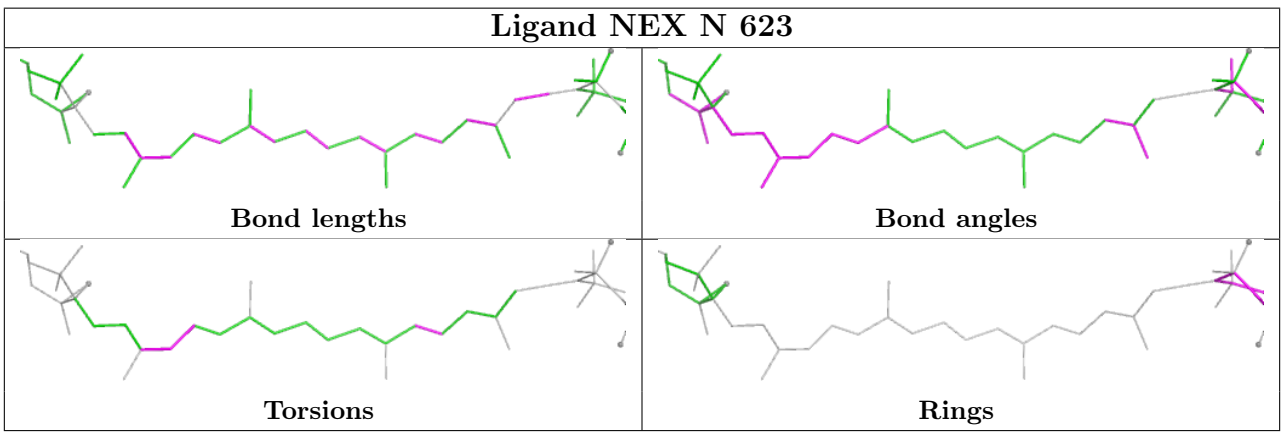
Ligand BCR c 516



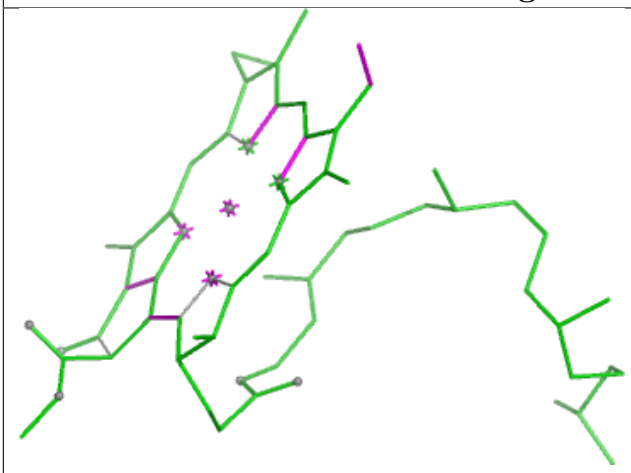
Ligand BCR B 618



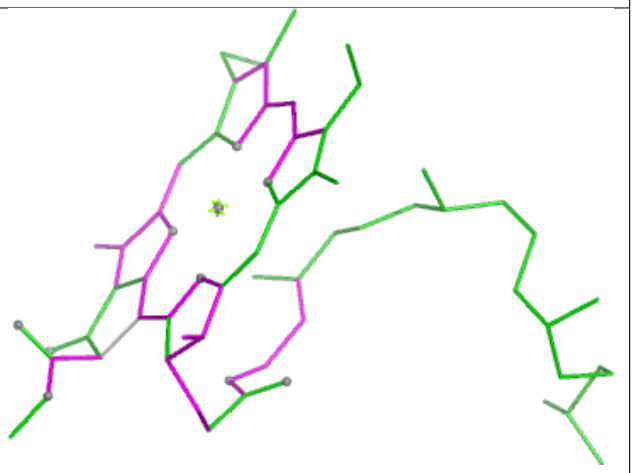
Ligand NEX N 623



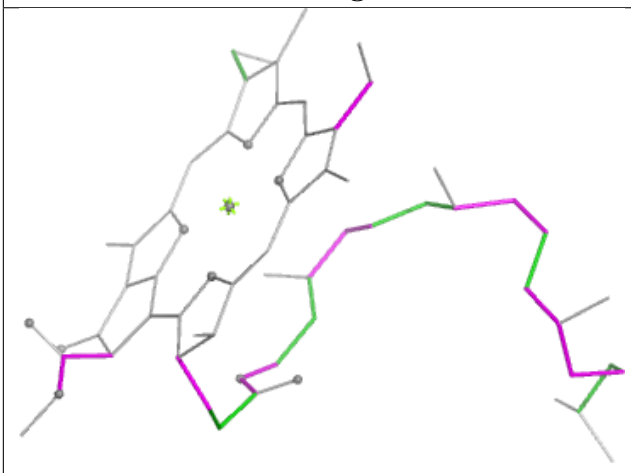
Ligand CLA n1 613



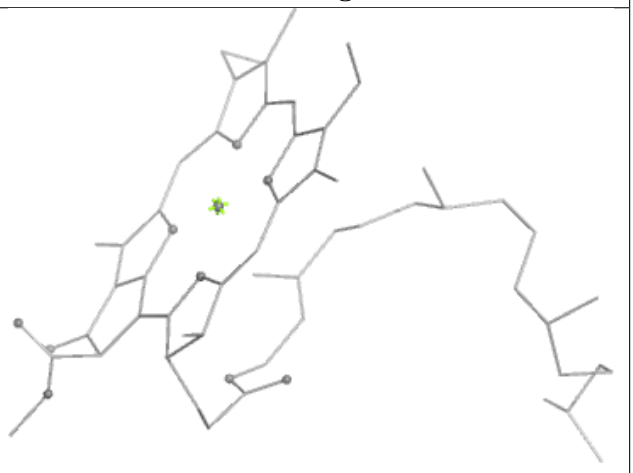
Bond lengths



Bond angles

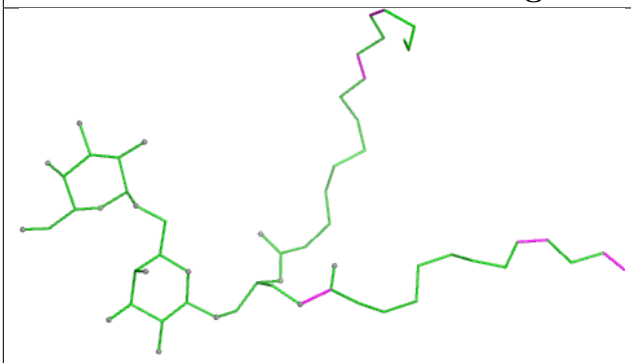


Torsions

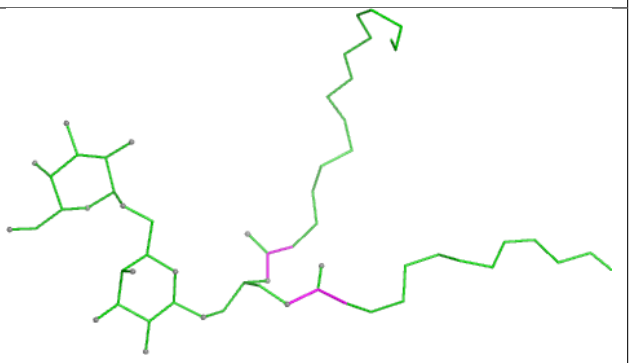


Rings

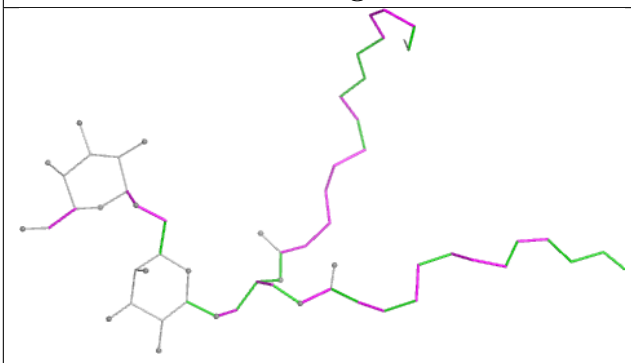
Ligand DGD c 519



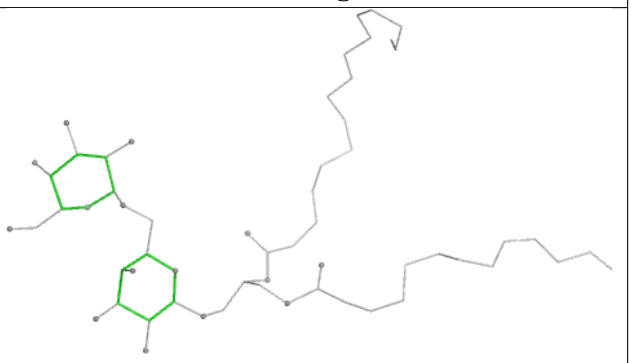
Bond lengths



Bond angles

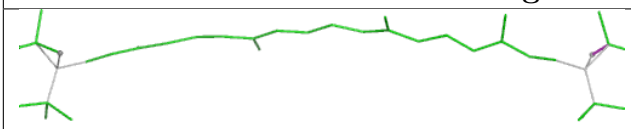


Torsions

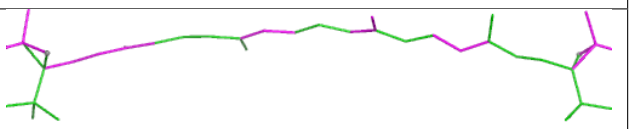


Rings

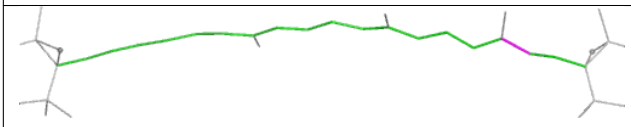
Ligand XAT N 622



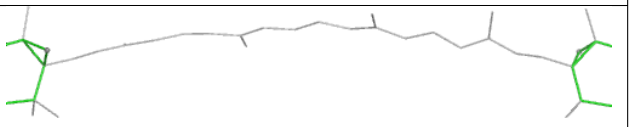
Bond lengths



Bond angles

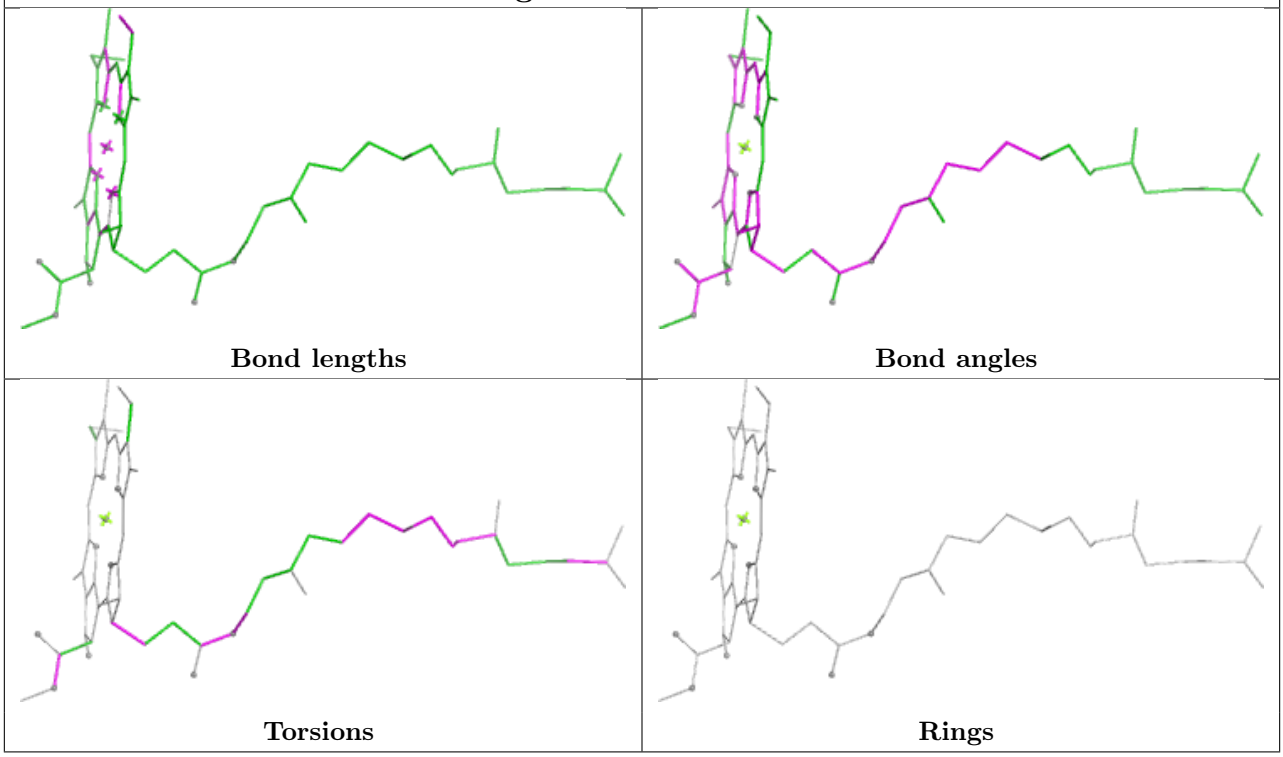


Torsions



Rings

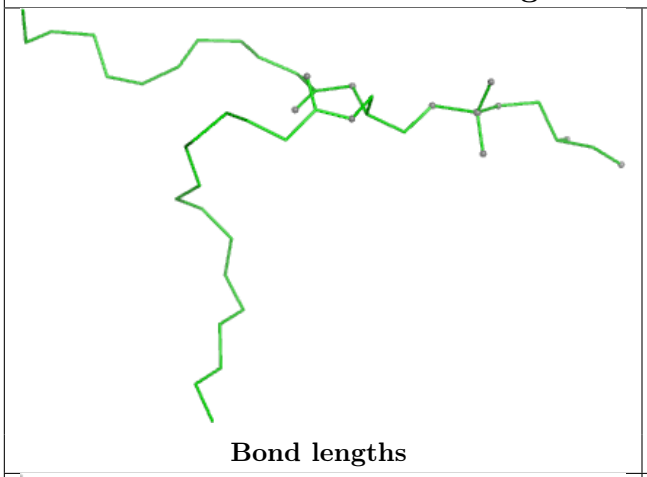
Ligand CLA D1 403



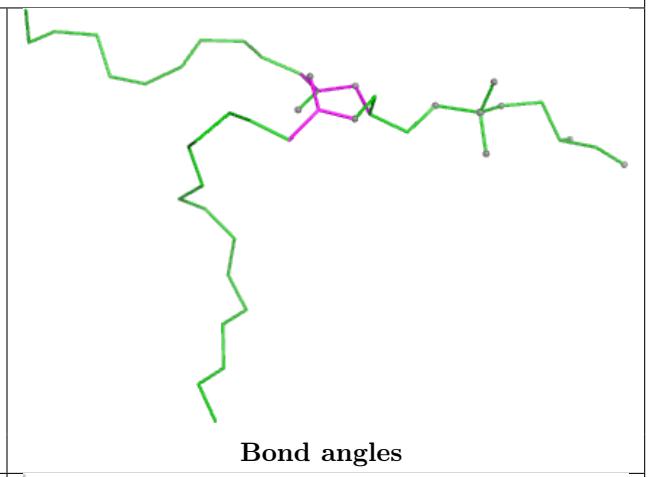
Ligand C7Z b1 620



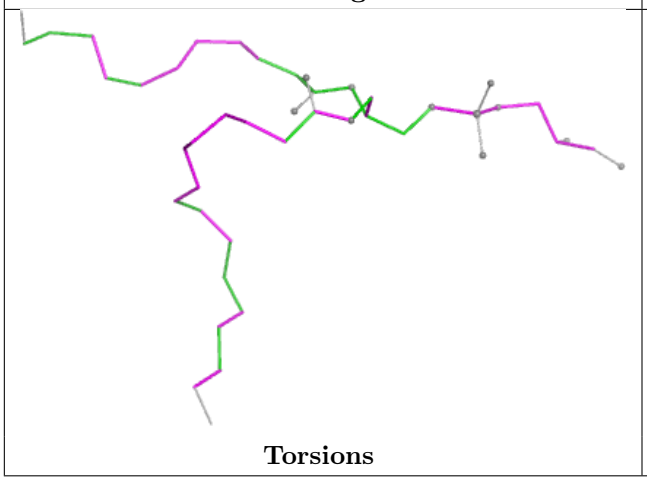
Ligand LHG s1 624



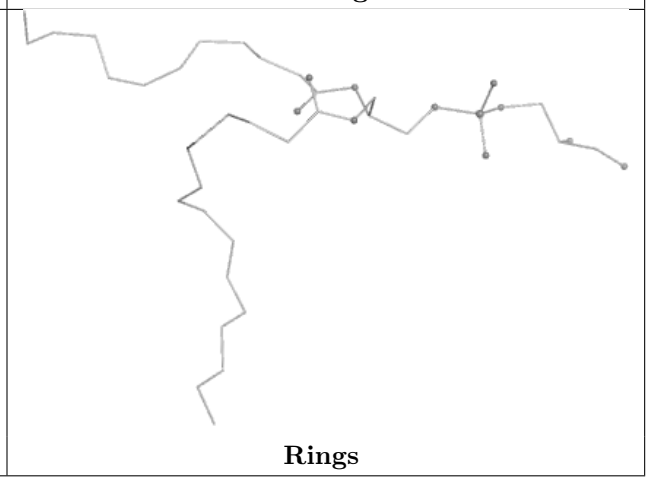
Bond lengths



Bond angles

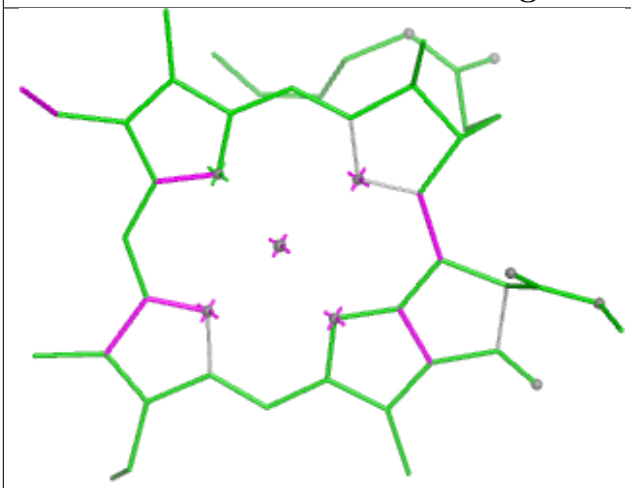


Torsions

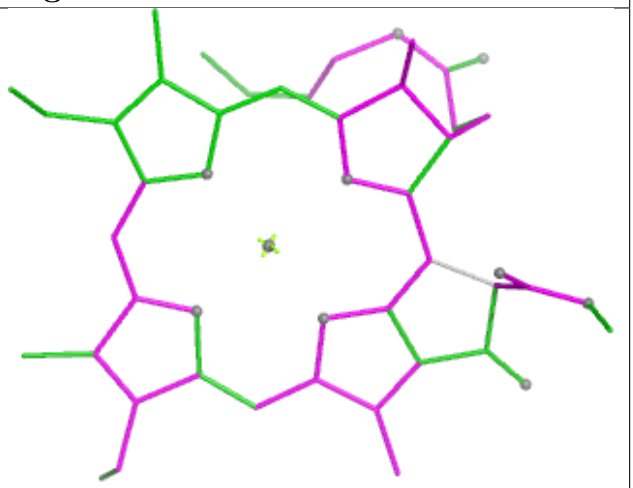


Rings

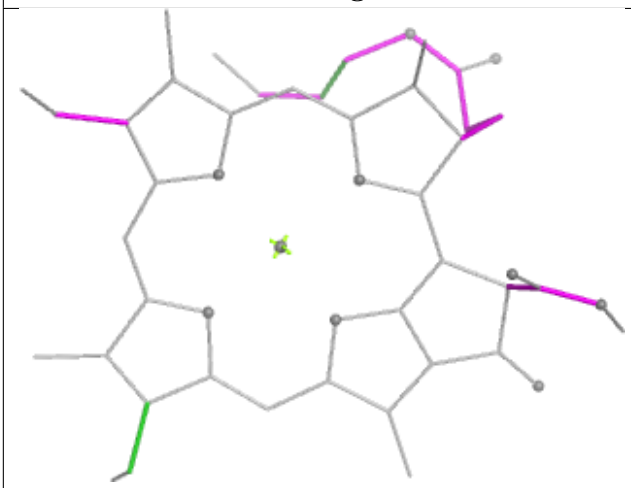
Ligand CLA g1 614



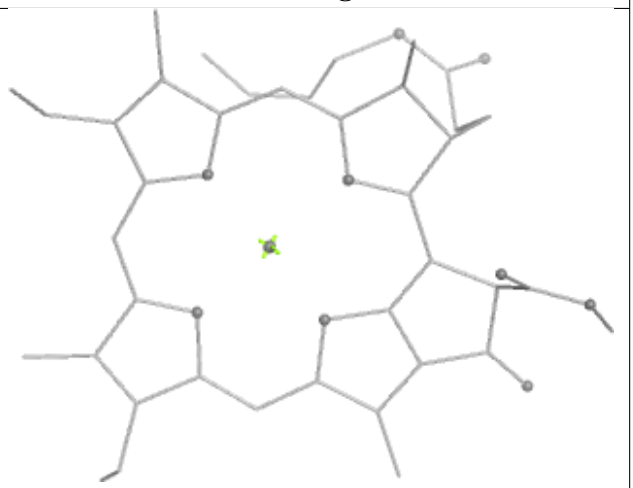
Bond lengths



Bond angles

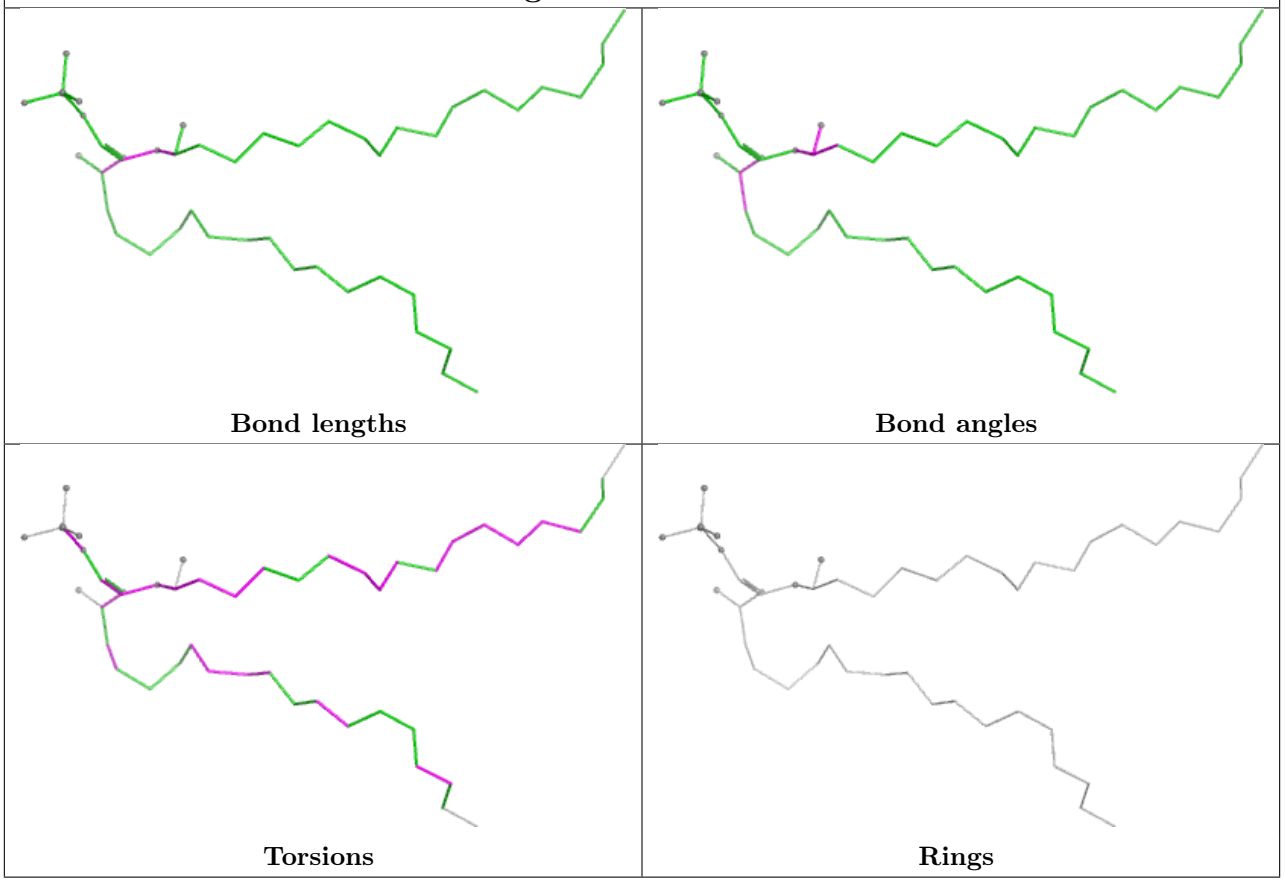


Torsions

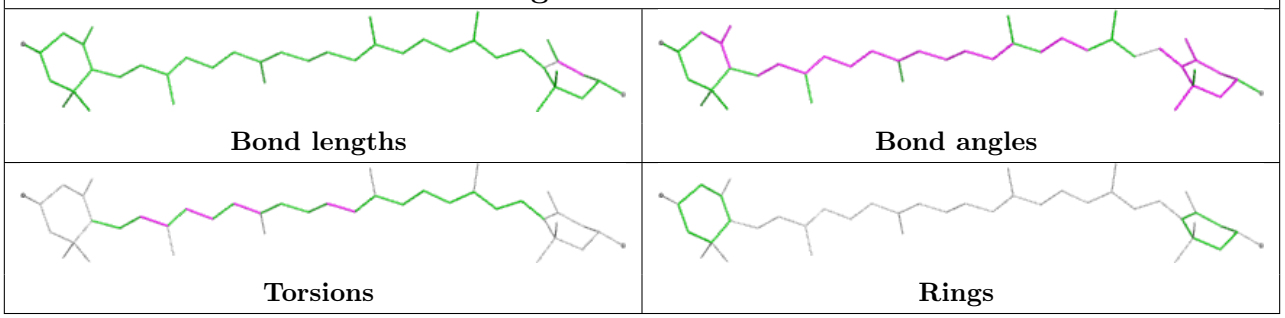


Rings

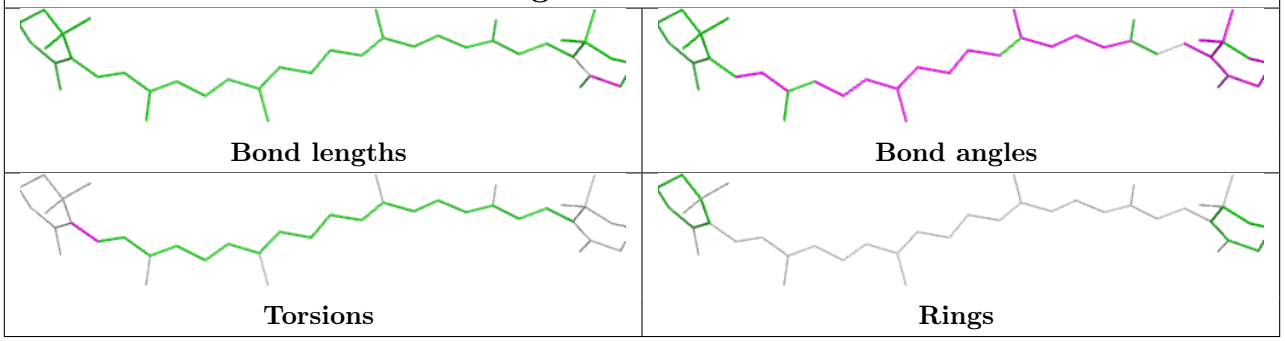
Ligand 3PH s1 626



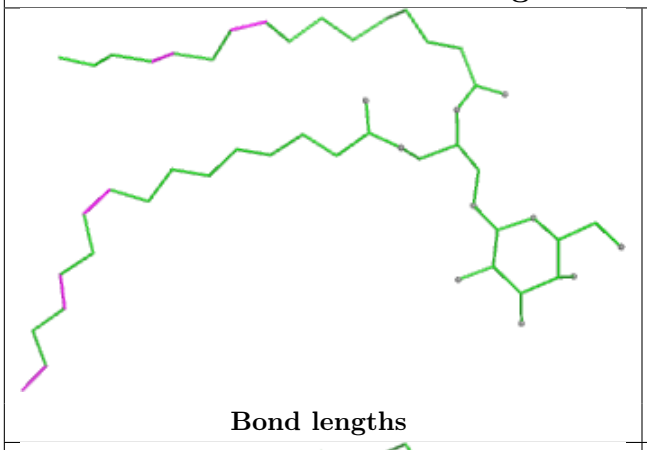
Ligand LUT r 620



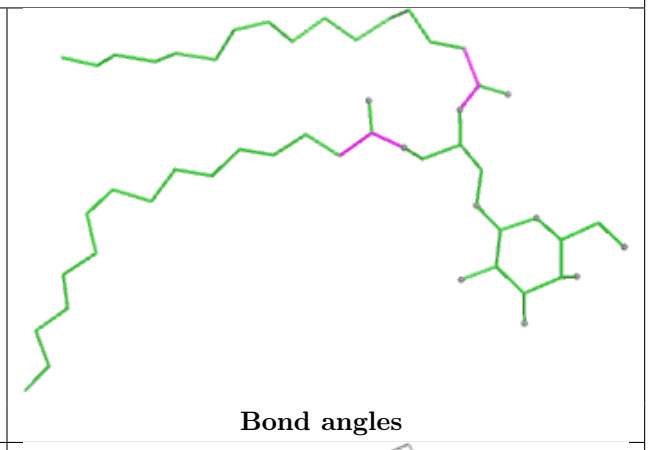
Ligand LUT s 620



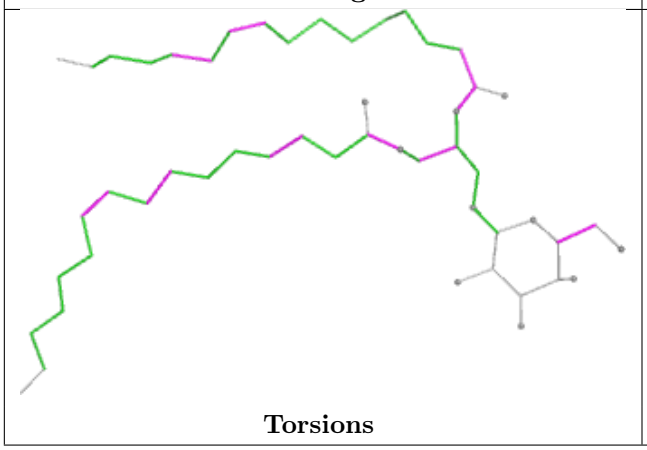
Ligand LMG C1 521



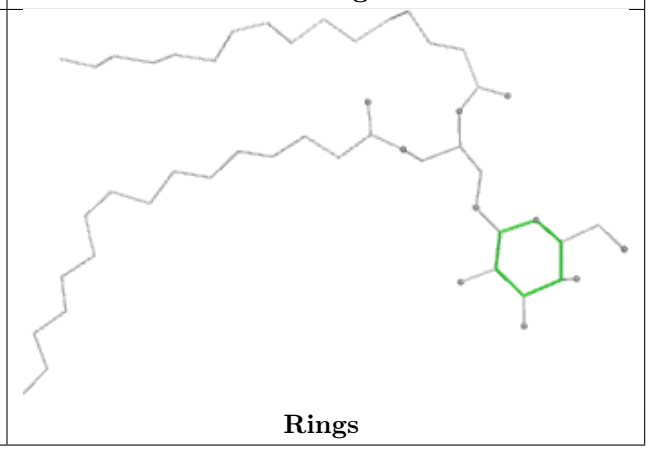
Bond lengths



Bond angles

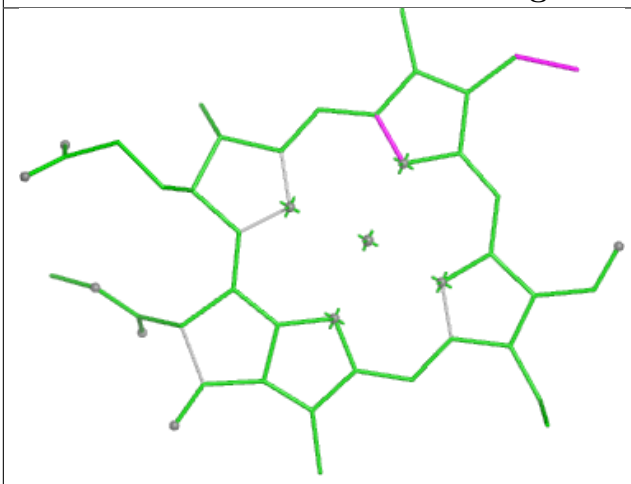


Torsions

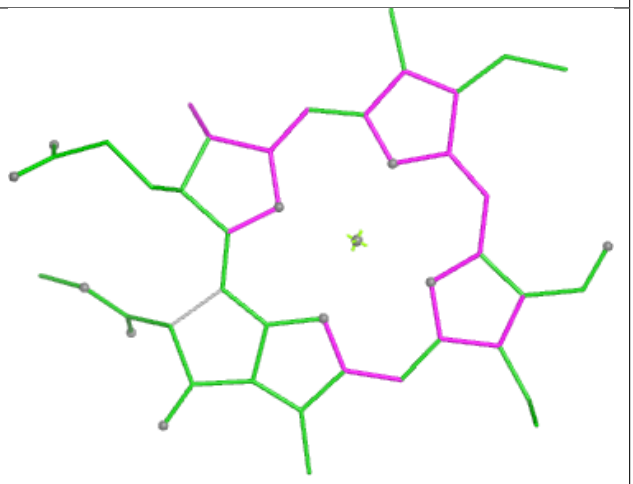


Rings

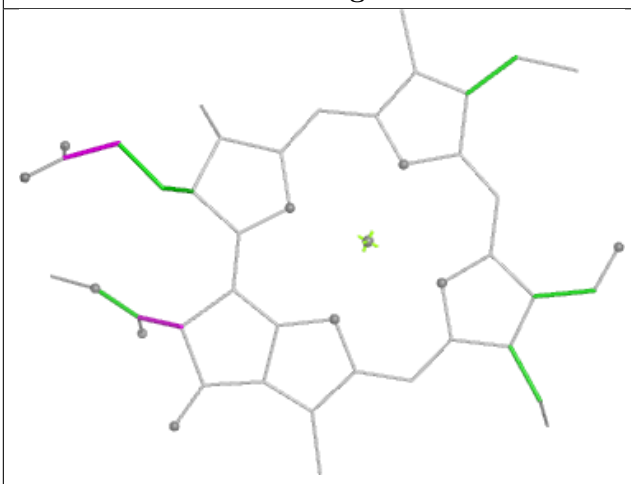
Ligand CHL s 601



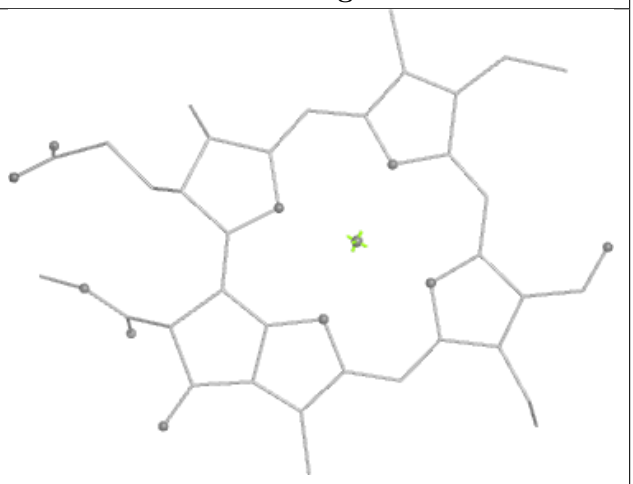
Bond lengths



Bond angles

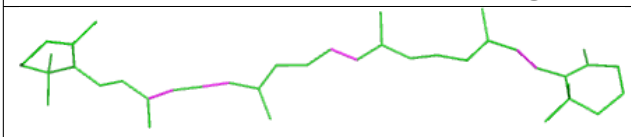


Torsions

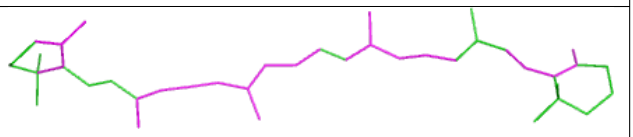


Rings

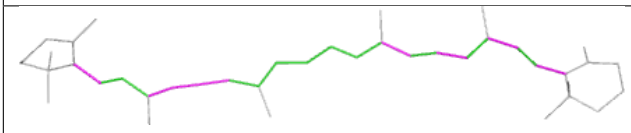
Ligand BCR d 404



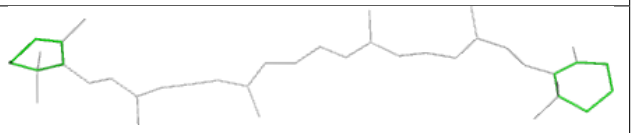
Bond lengths



Bond angles

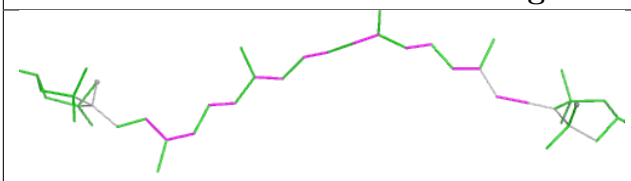


Torsions

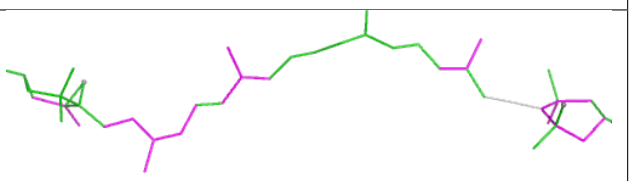


Rings

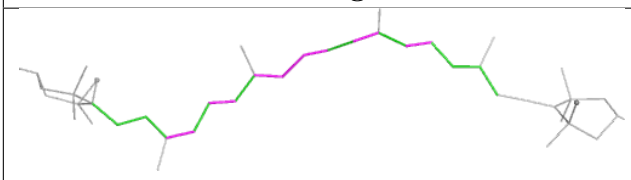
Ligand NEX r 622



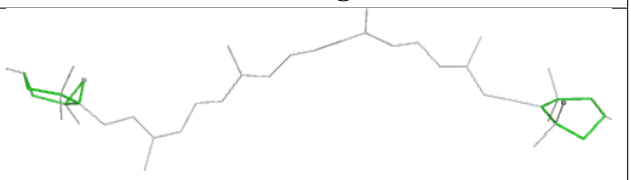
Bond lengths



Bond angles

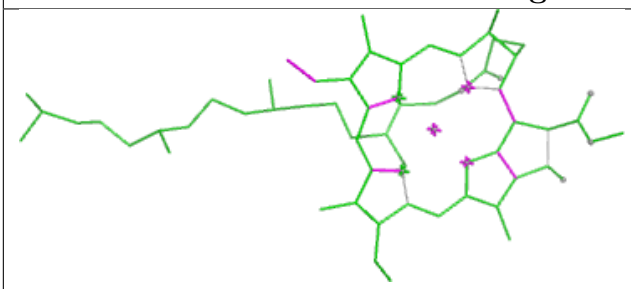


Torsions

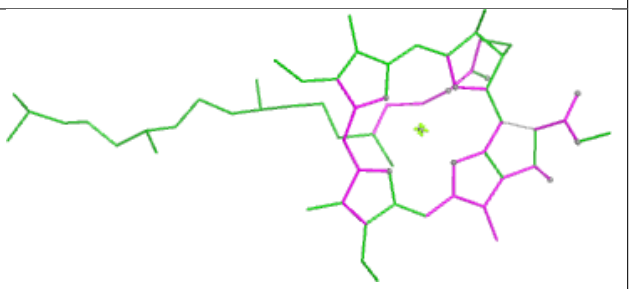


Rings

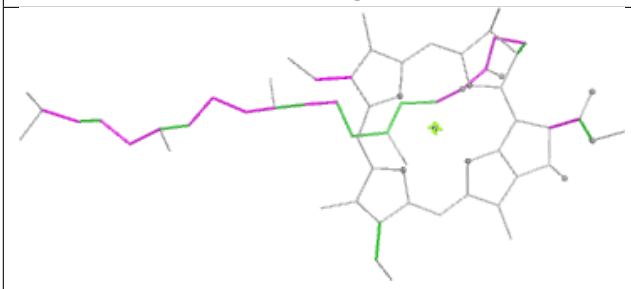
Ligand CLA c 505



Bond lengths



Bond angles

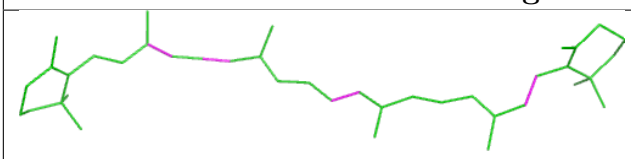


Torsions

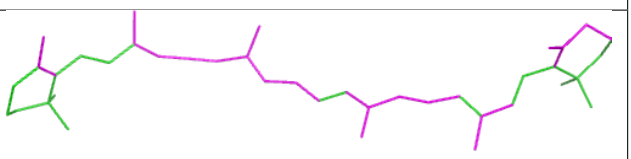


Rings

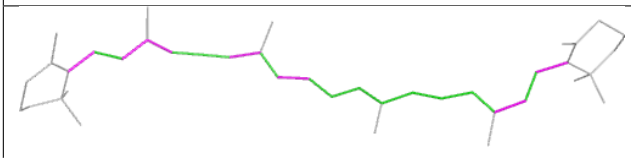
Ligand BCR C 516



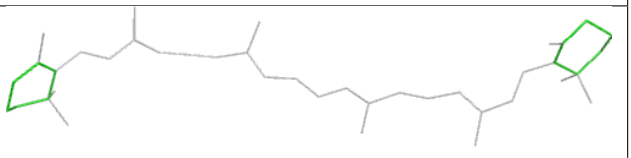
Bond lengths



Bond angles

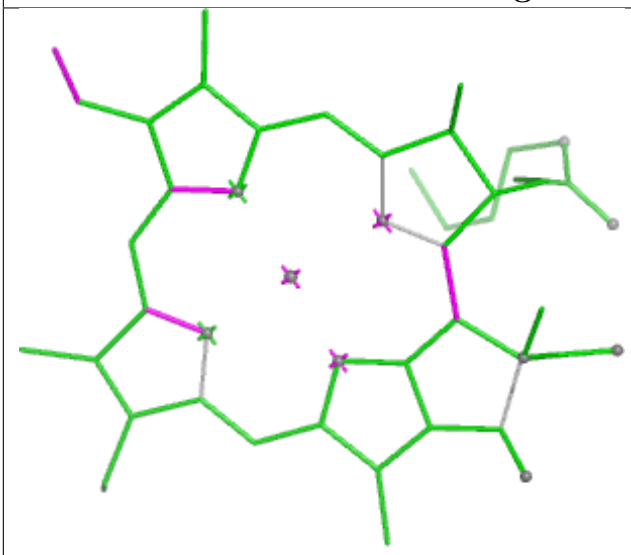


Torsions

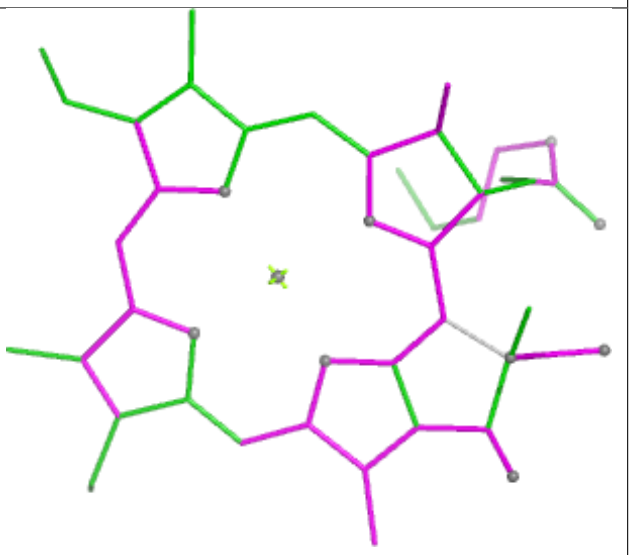


Rings

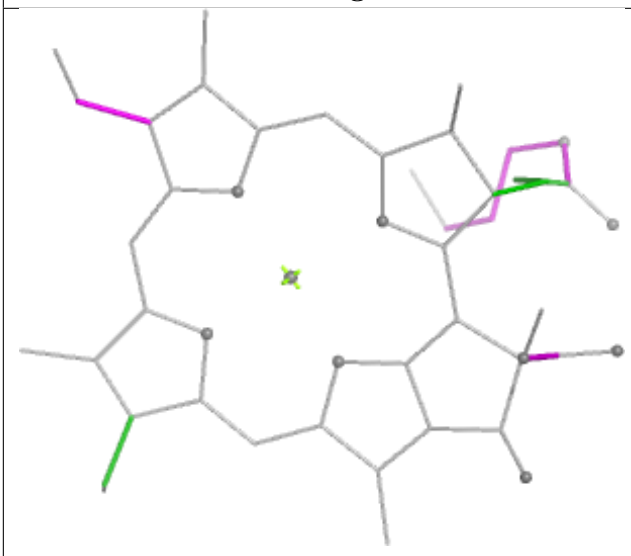
Ligand CLA G1 604



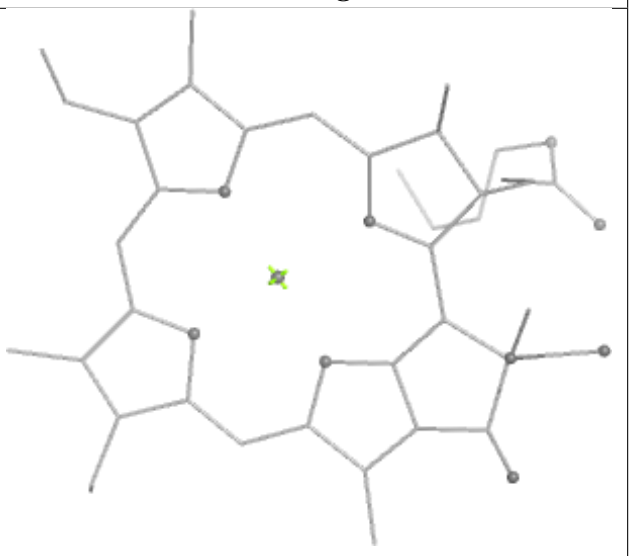
Bond lengths



Bond angles

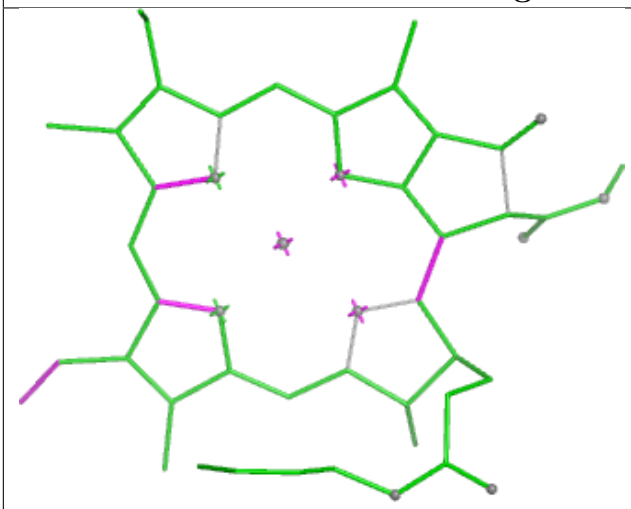


Torsions

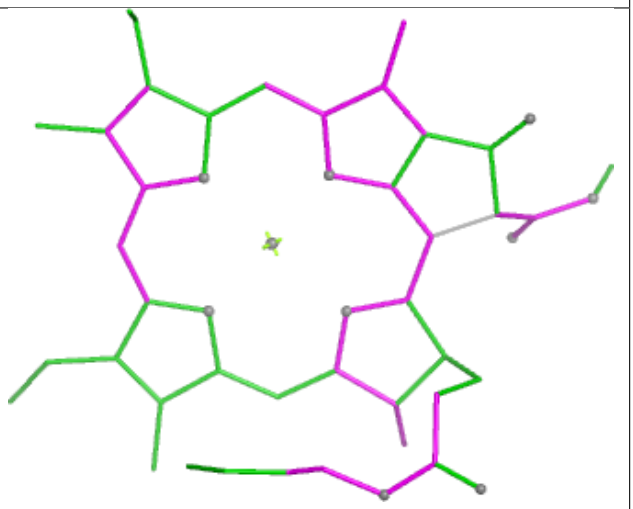


Rings

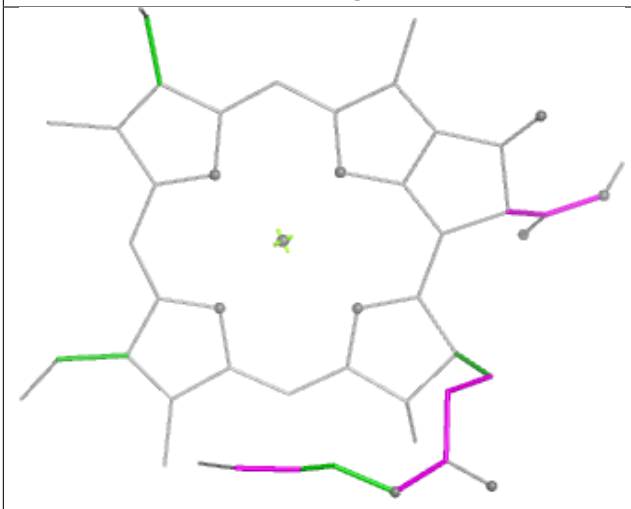
Ligand CLA G1 614



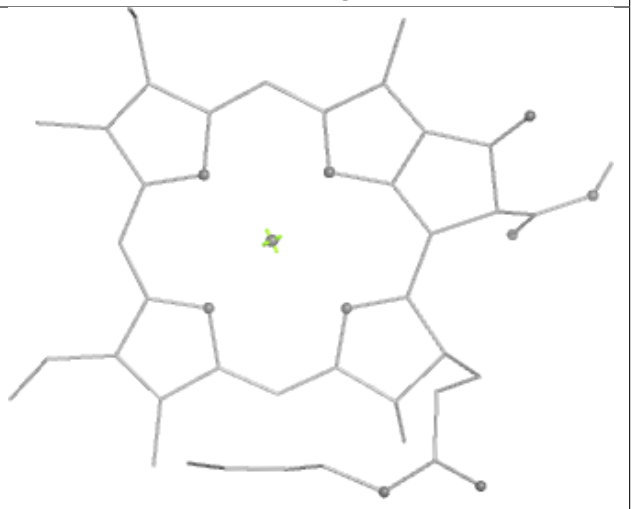
Bond lengths



Bond angles

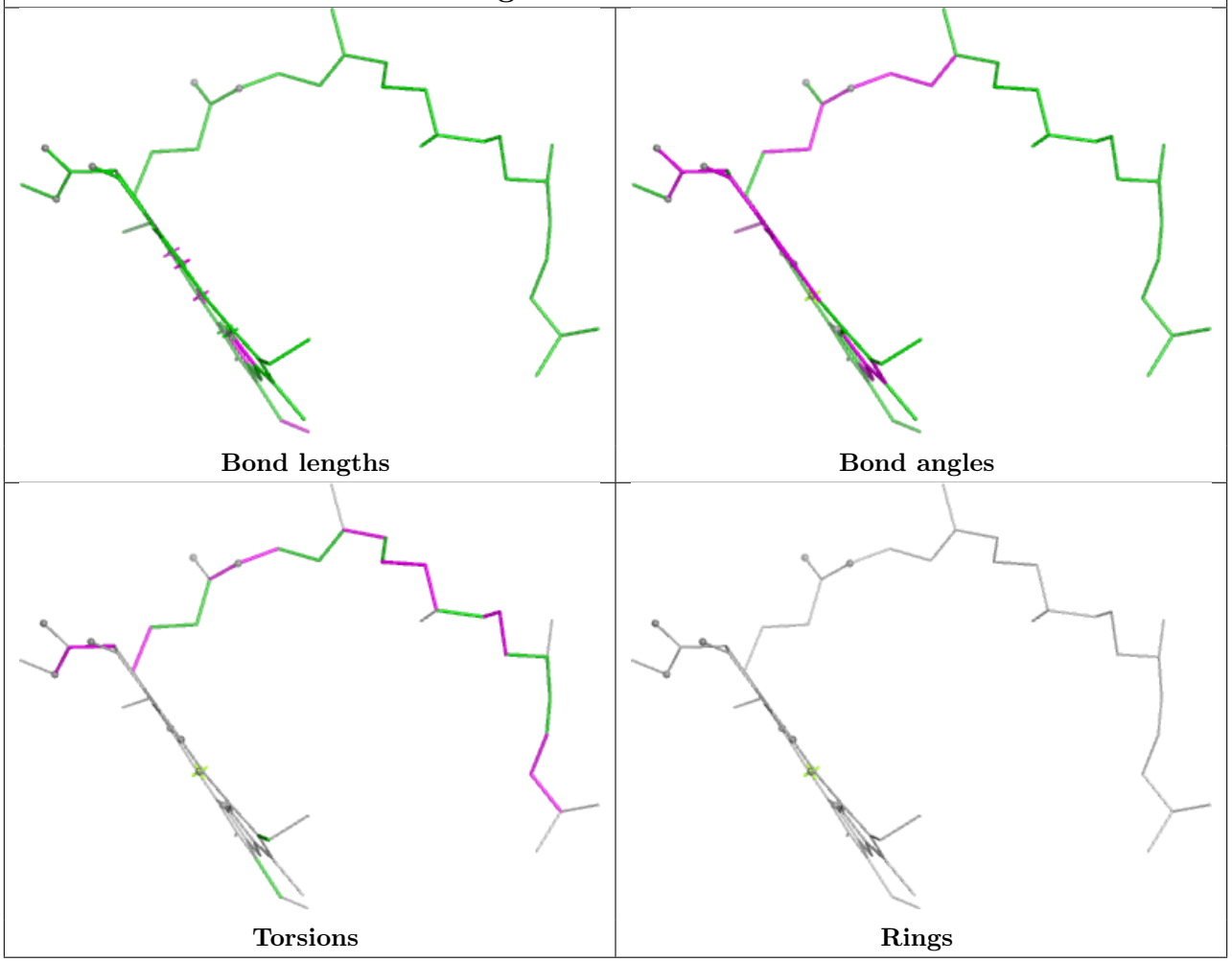


Torsions

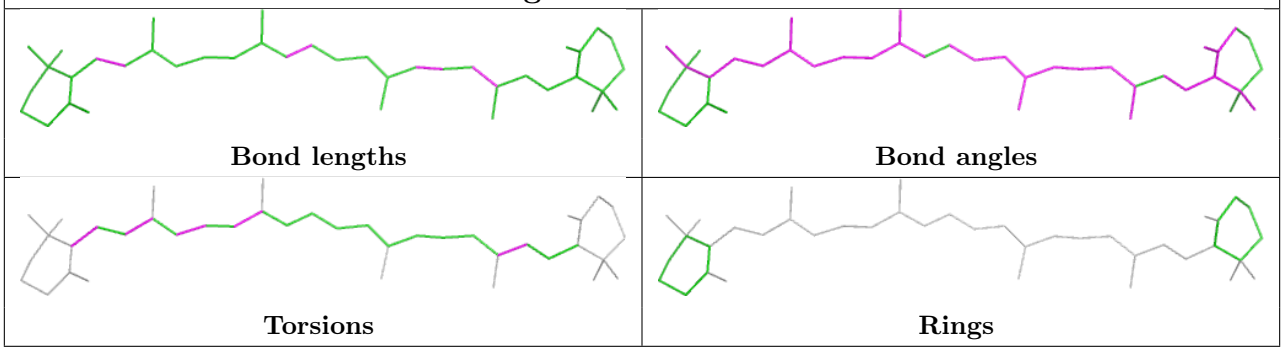


Rings

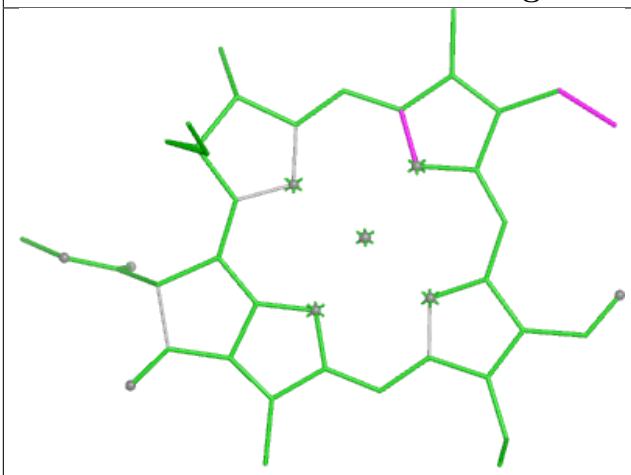
Ligand CLA b1 612



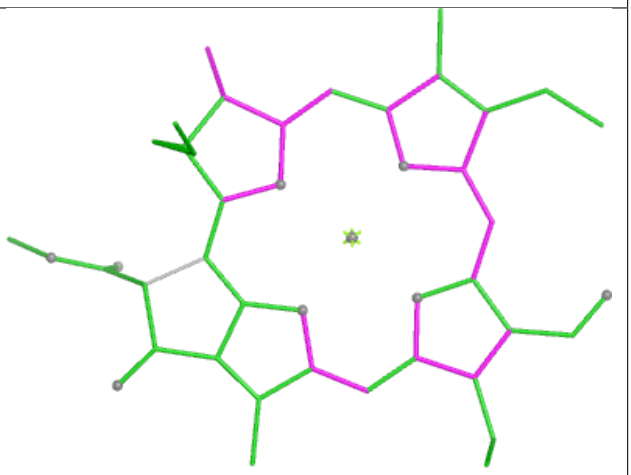
Ligand BCR B 619



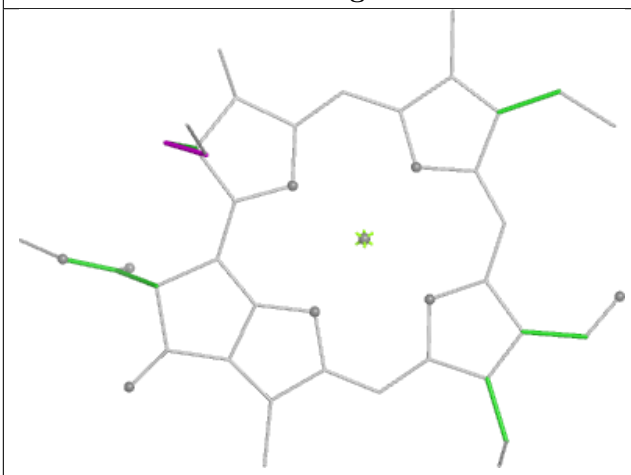
Ligand CHL G 608



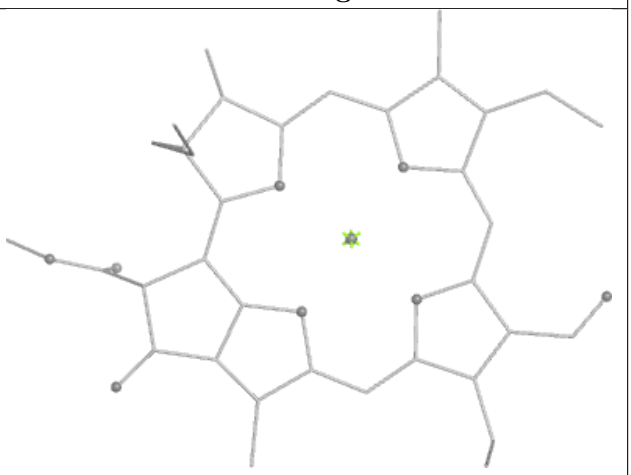
Bond lengths



Bond angles

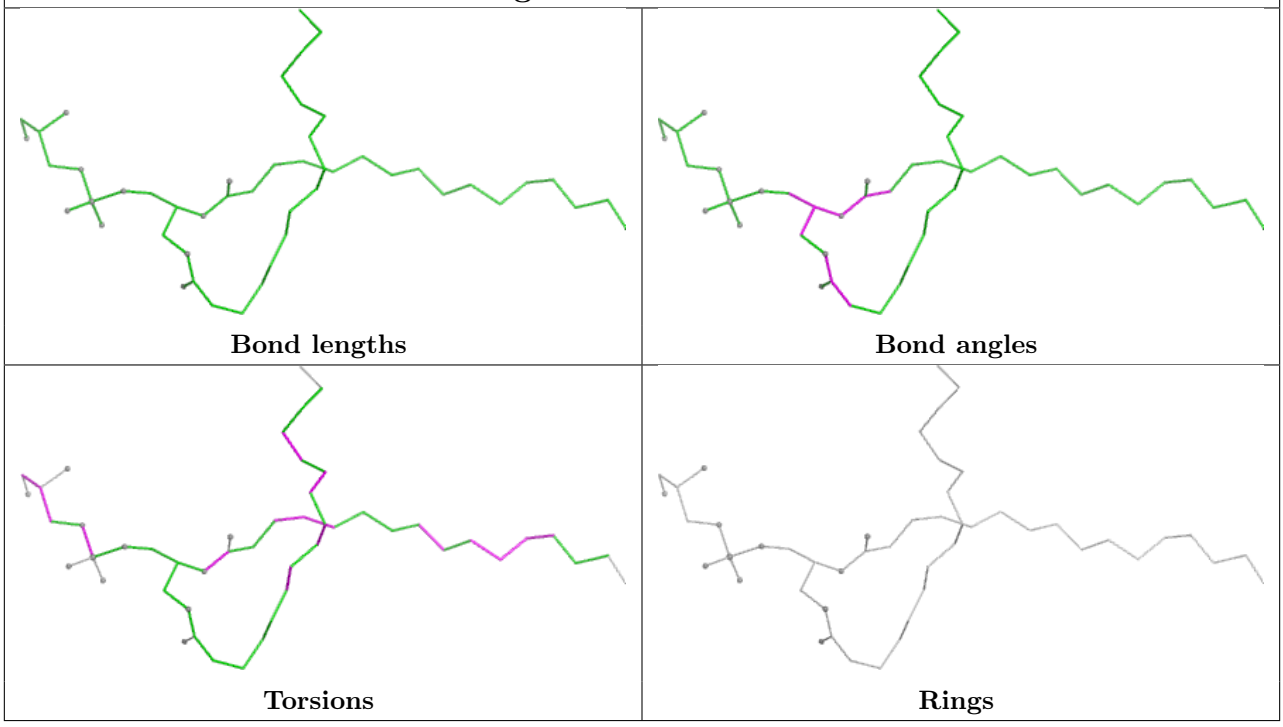


Torsions

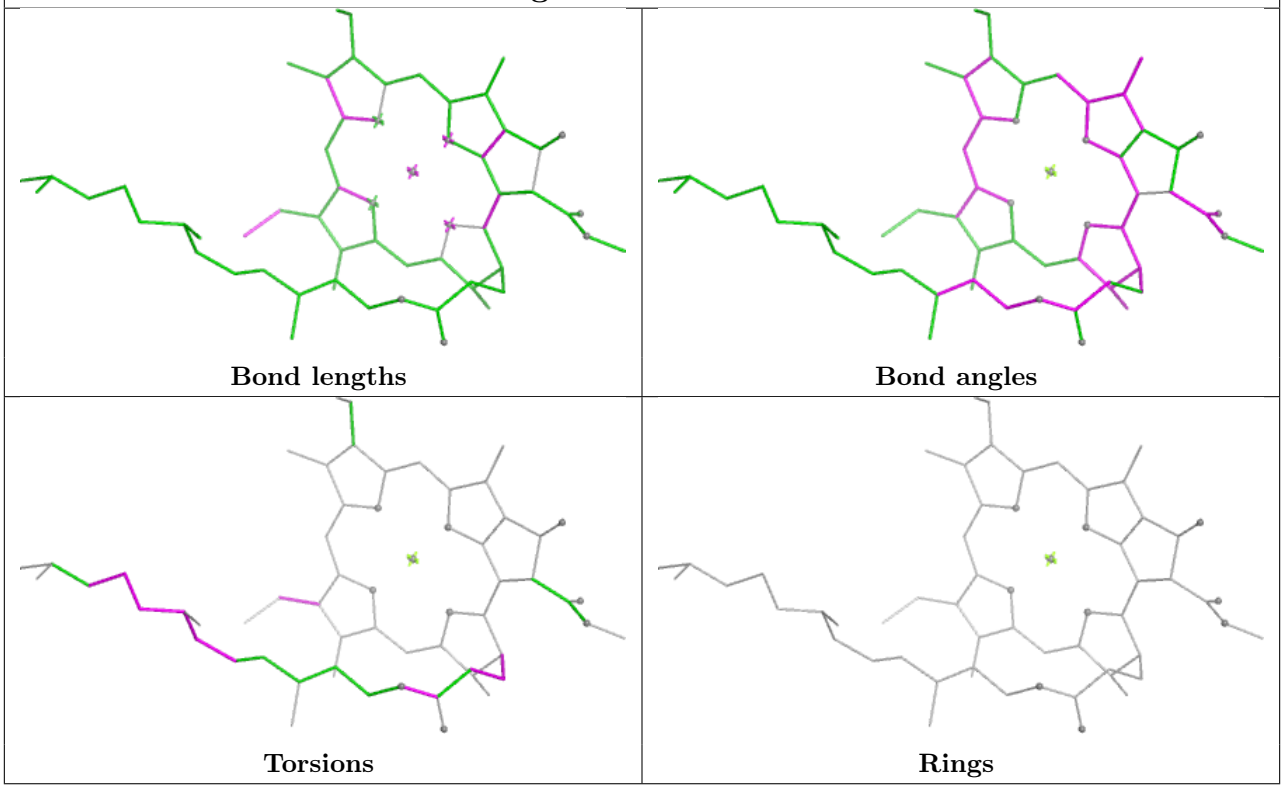


Rings

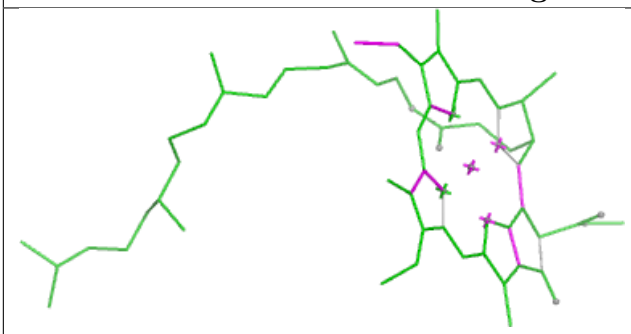
Ligand LHG Y1 624



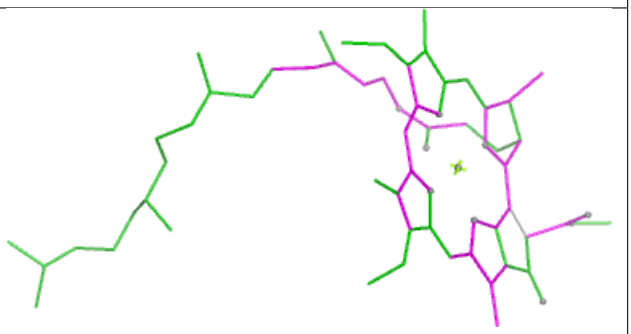
Ligand CLA r 610



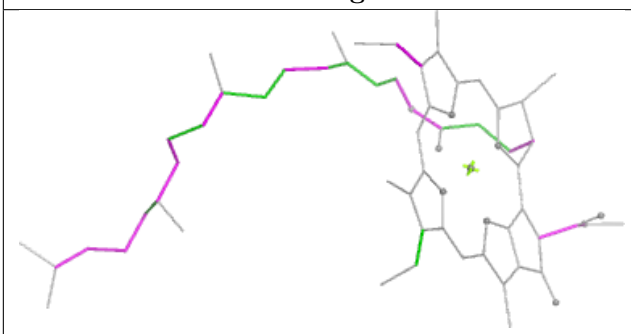
Ligand CLA s 610



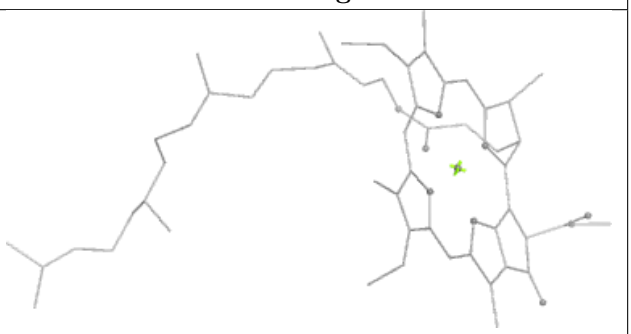
Bond lengths



Bond angles

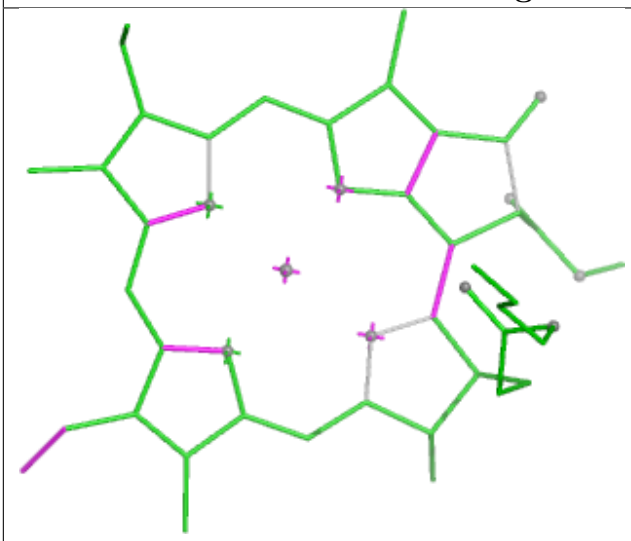


Torsions

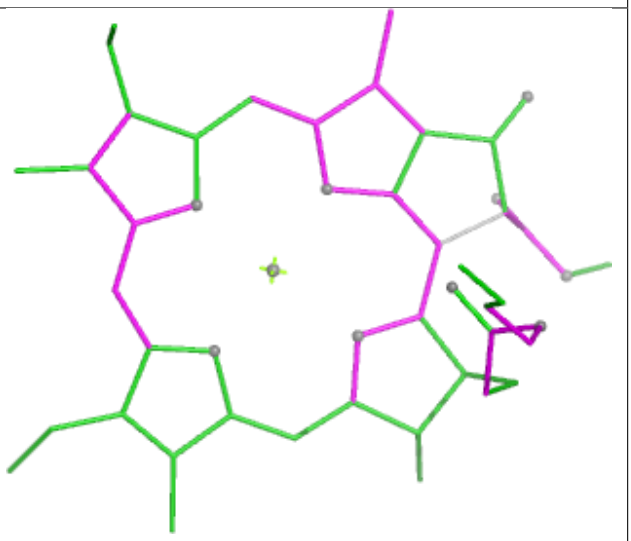


Rings

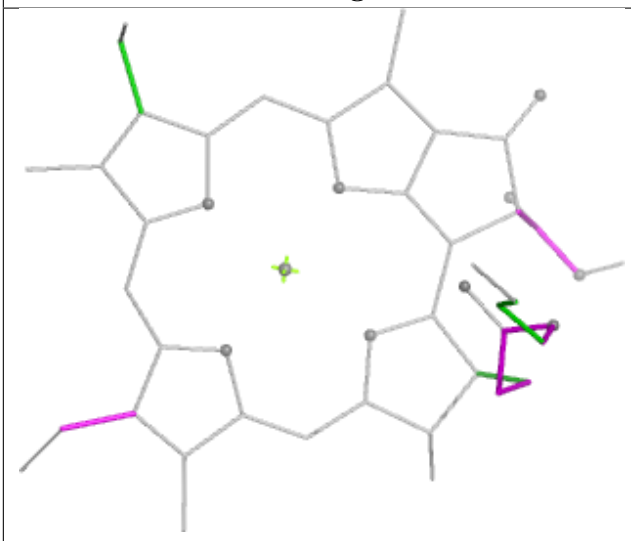
Ligand CLA R1 604



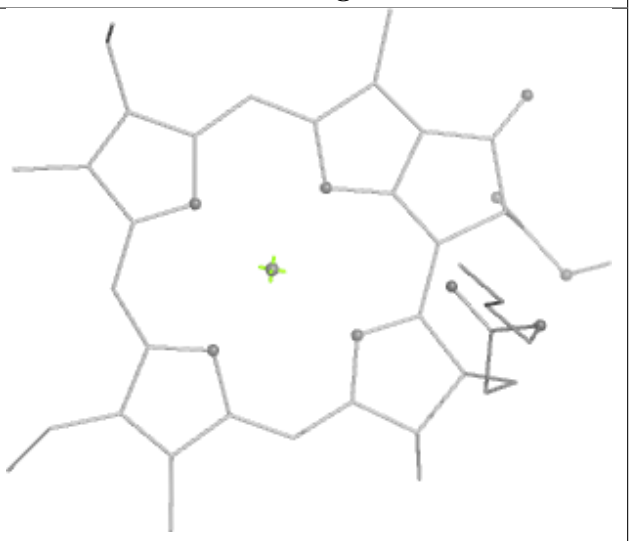
Bond lengths



Bond angles

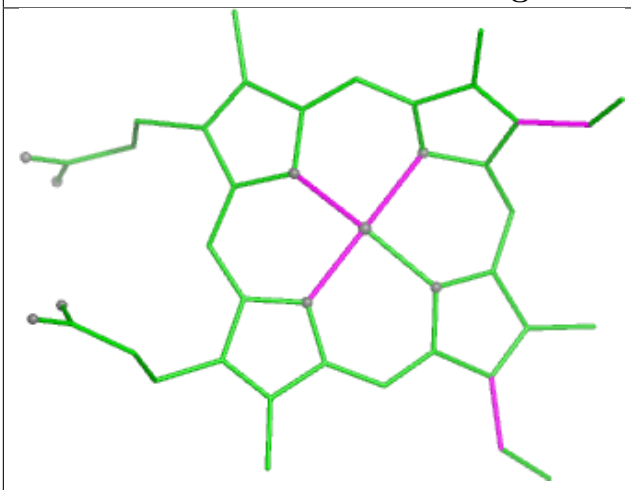


Torsions

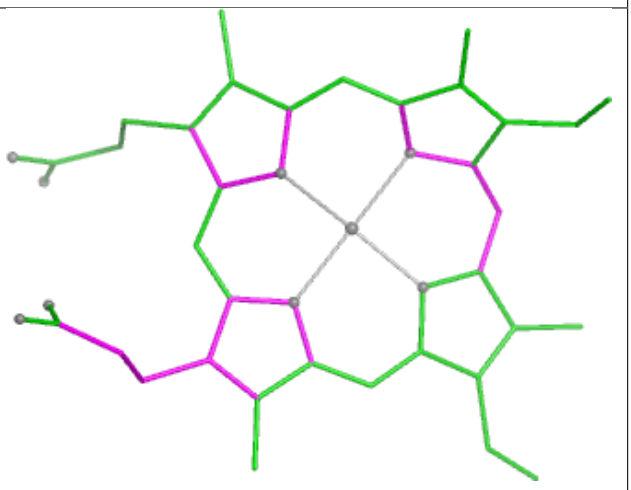


Rings

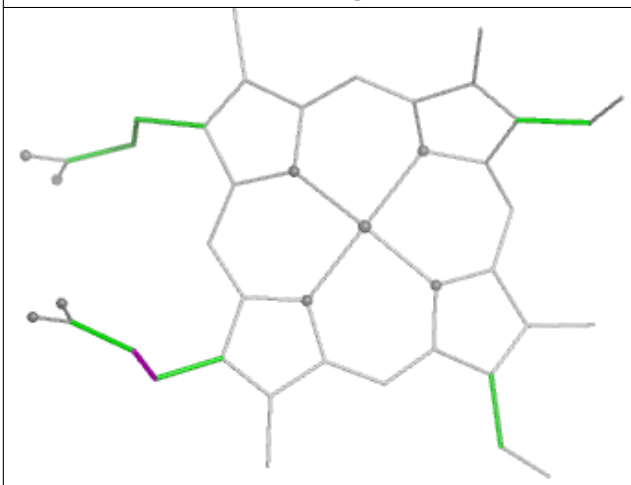
Ligand HEM F1 101



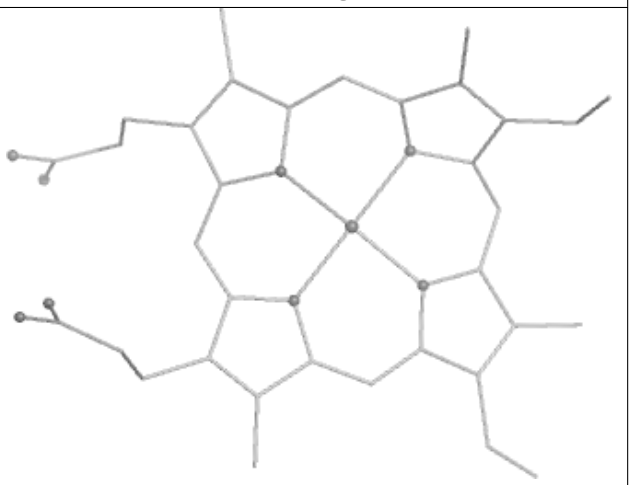
Bond lengths



Bond angles

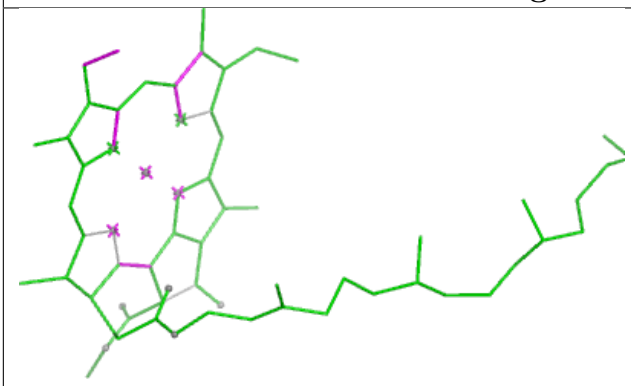


Torsions

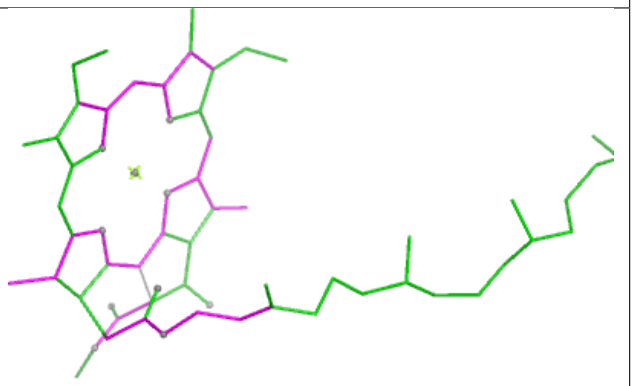


Rings

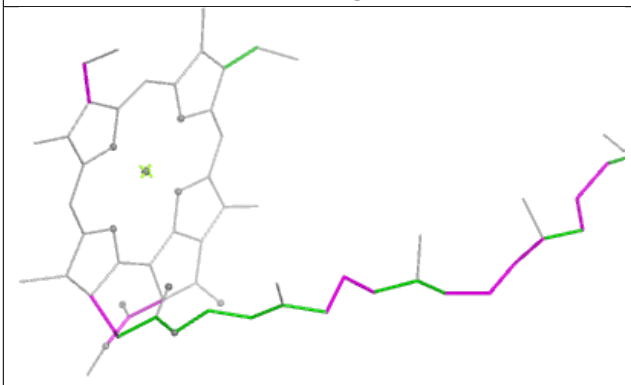
Ligand CLA s 611



Bond lengths



Bond angles

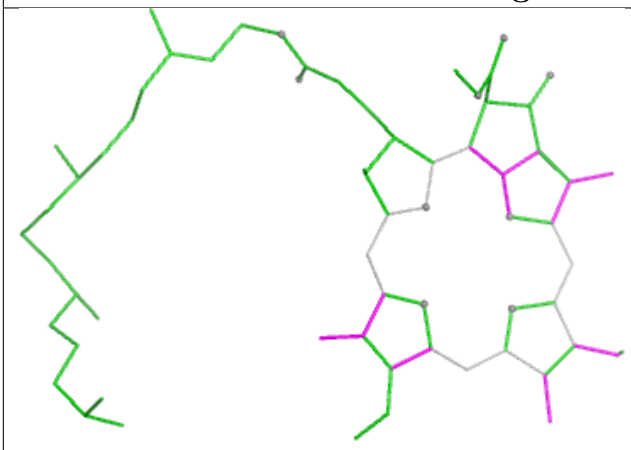


Torsions

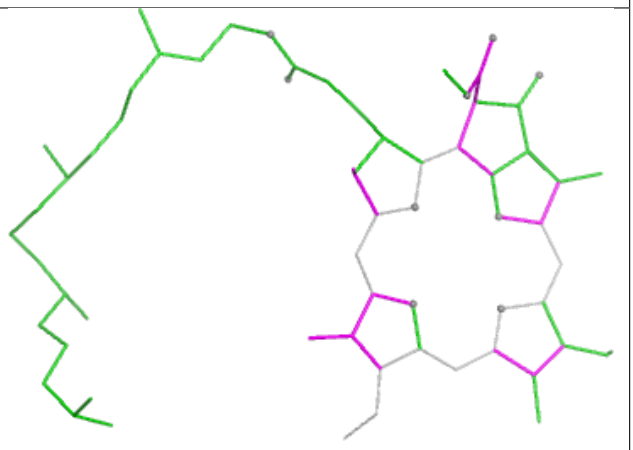


Rings

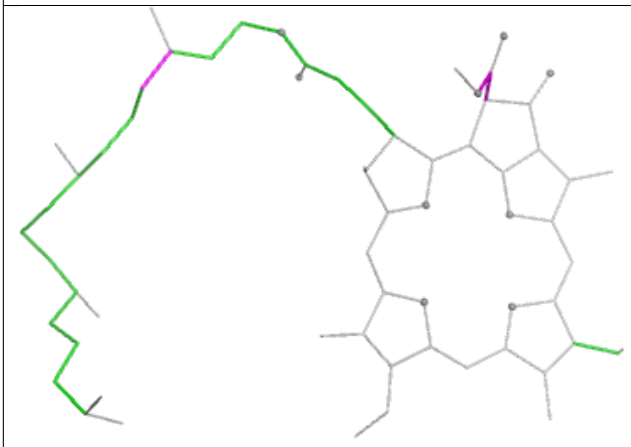
Ligand PHO A1 408



Bond lengths



Bond angles

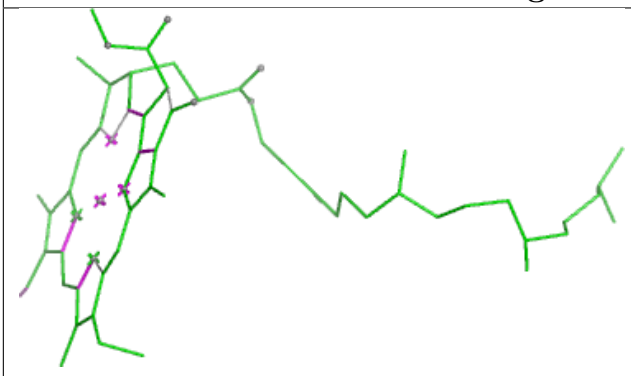


Torsions

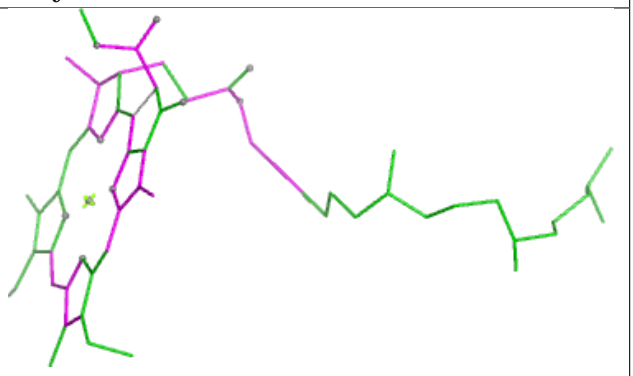


Rings

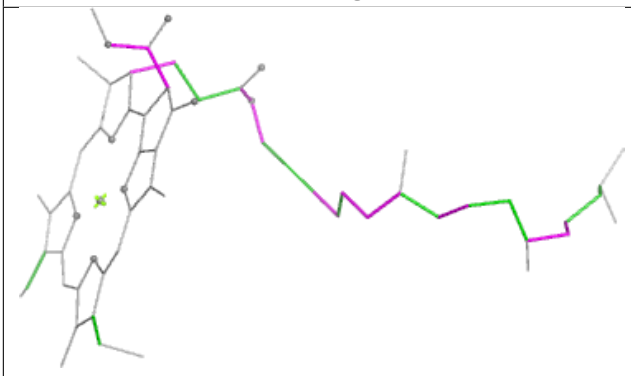
Ligand CLA y 604



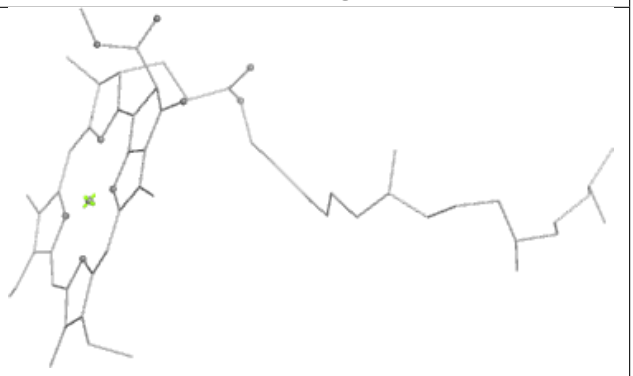
Bond lengths



Bond angles

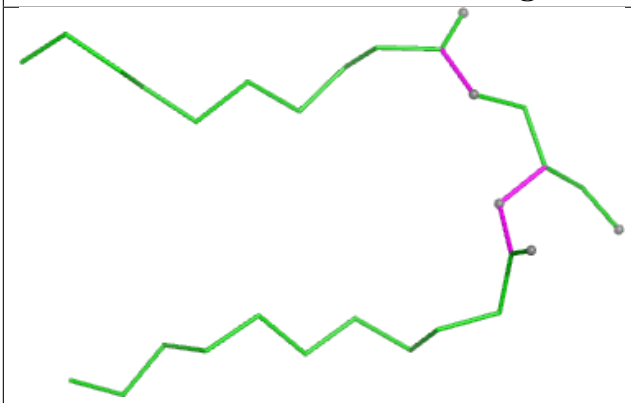


Torsions

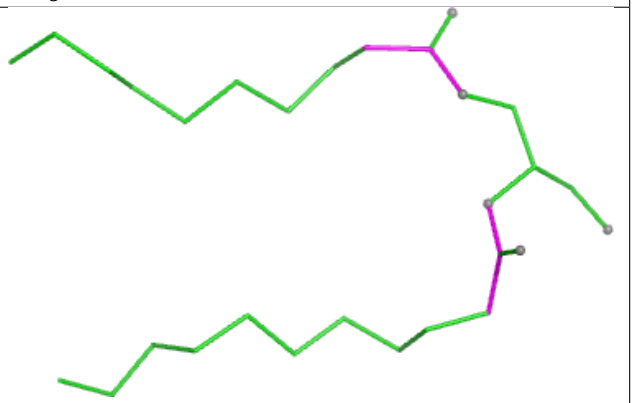


Rings

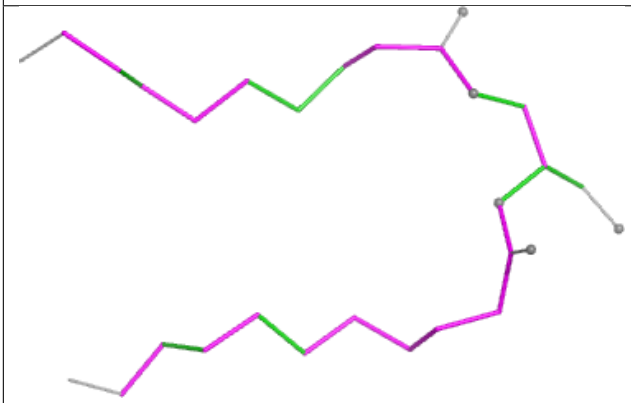
Ligand DGA j1 101



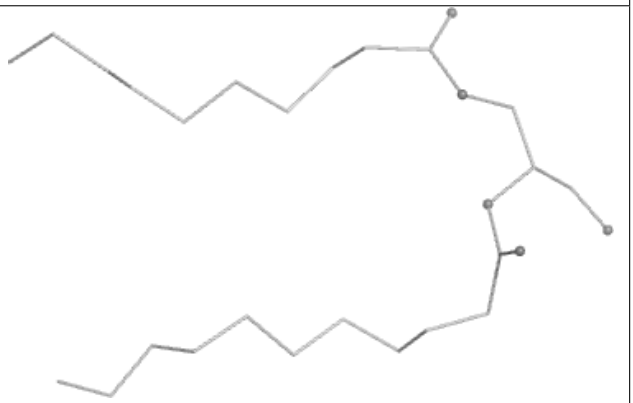
Bond lengths



Bond angles

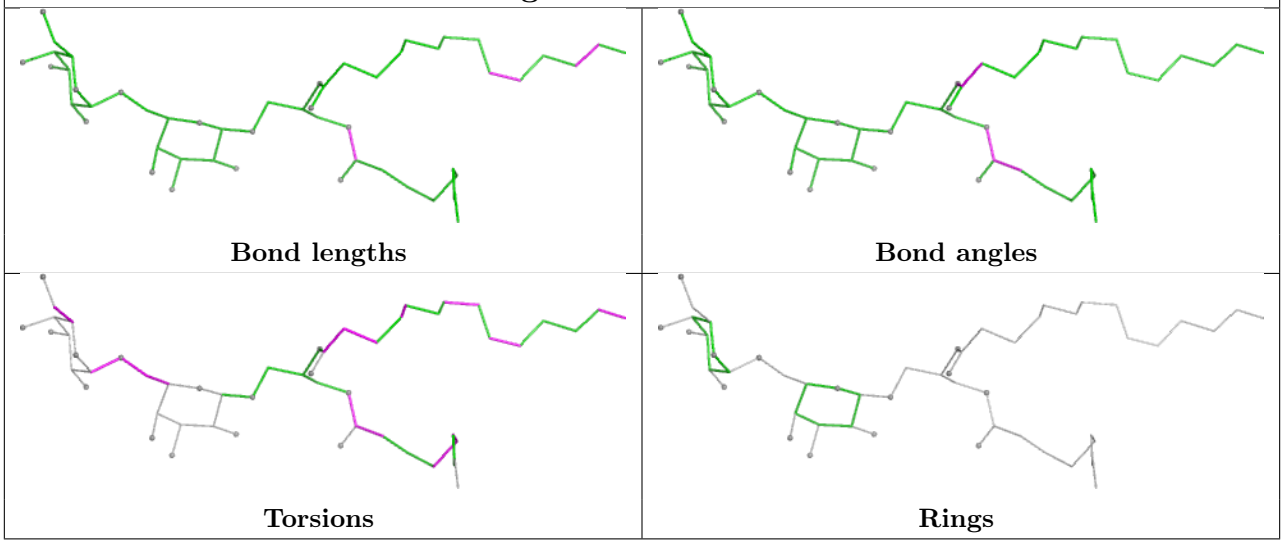


Torsions

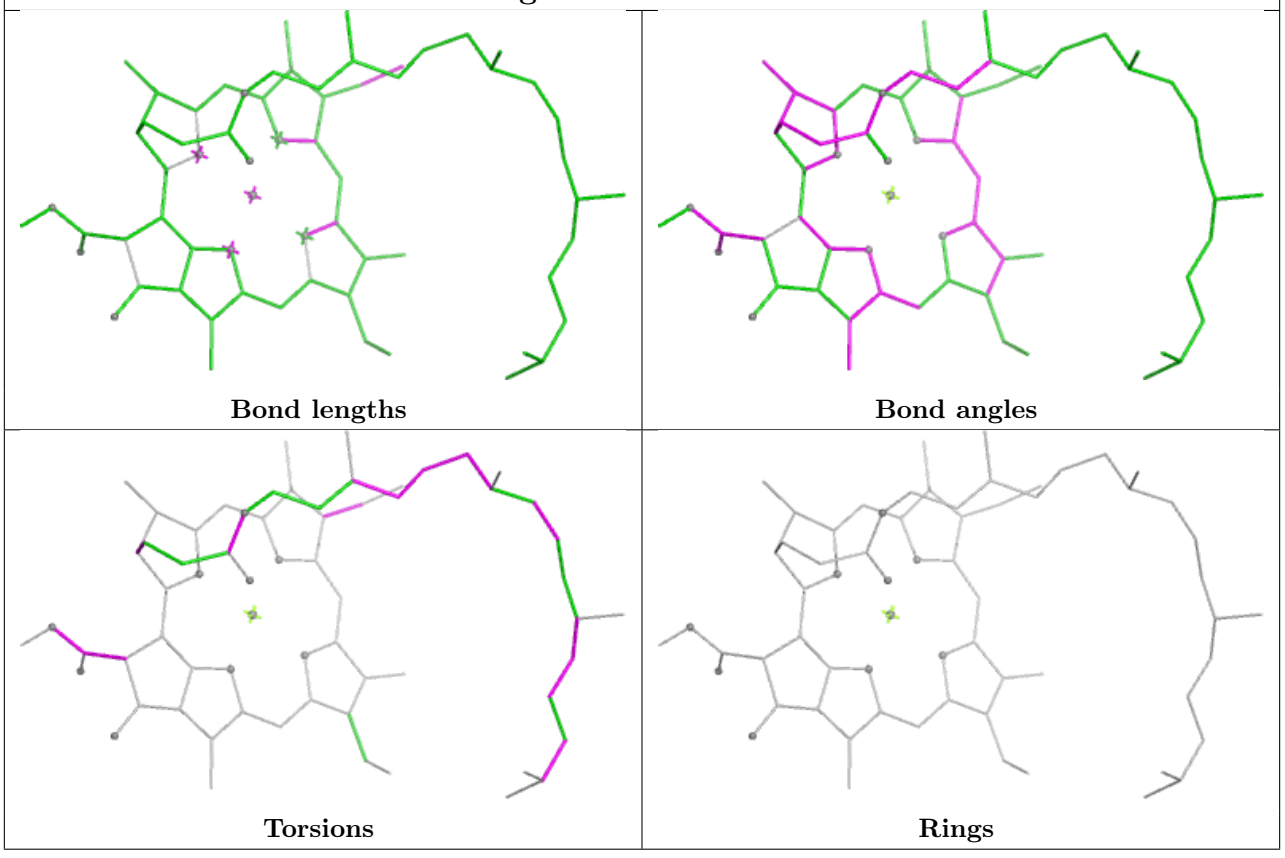


Rings

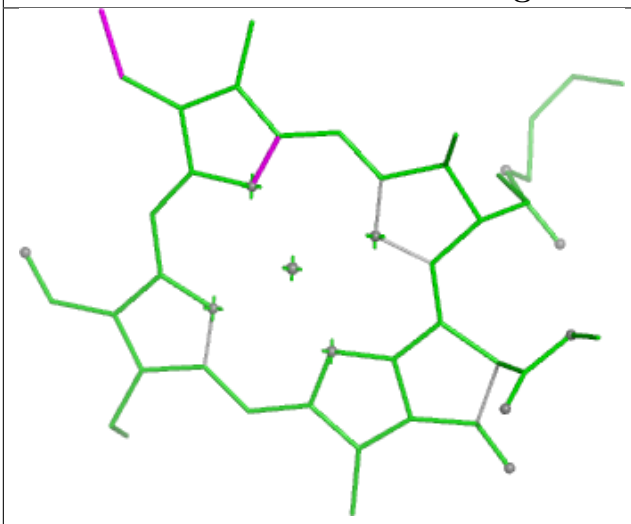
Ligand DGD C 518



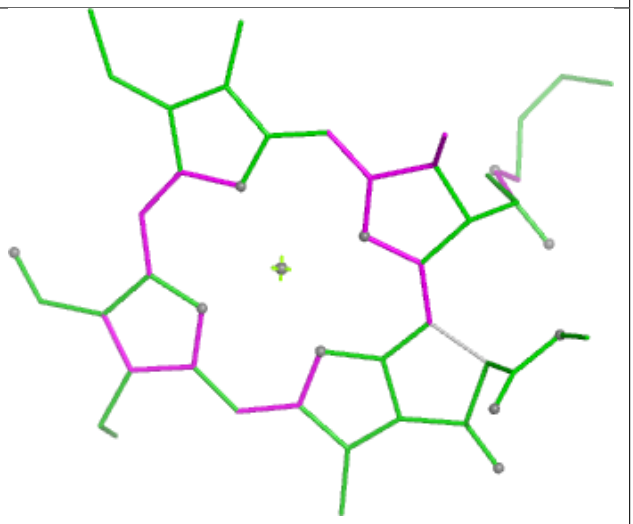
Ligand CLA n1 610



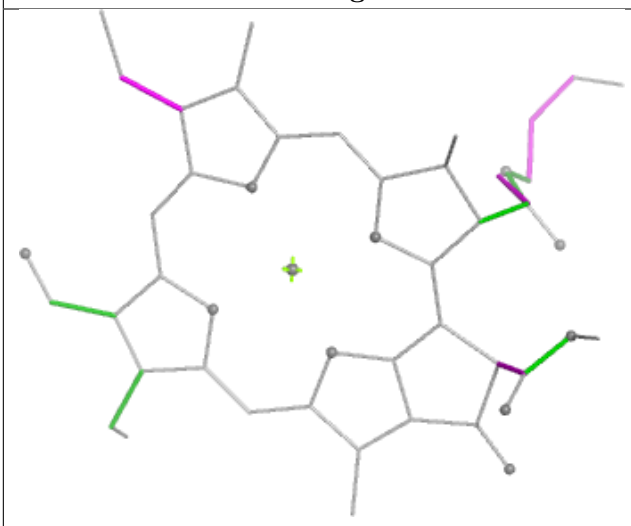
Ligand CHL N1 608



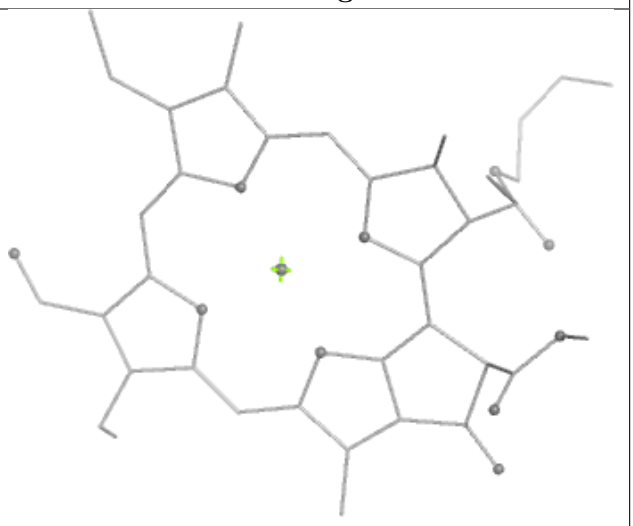
Bond lengths



Bond angles

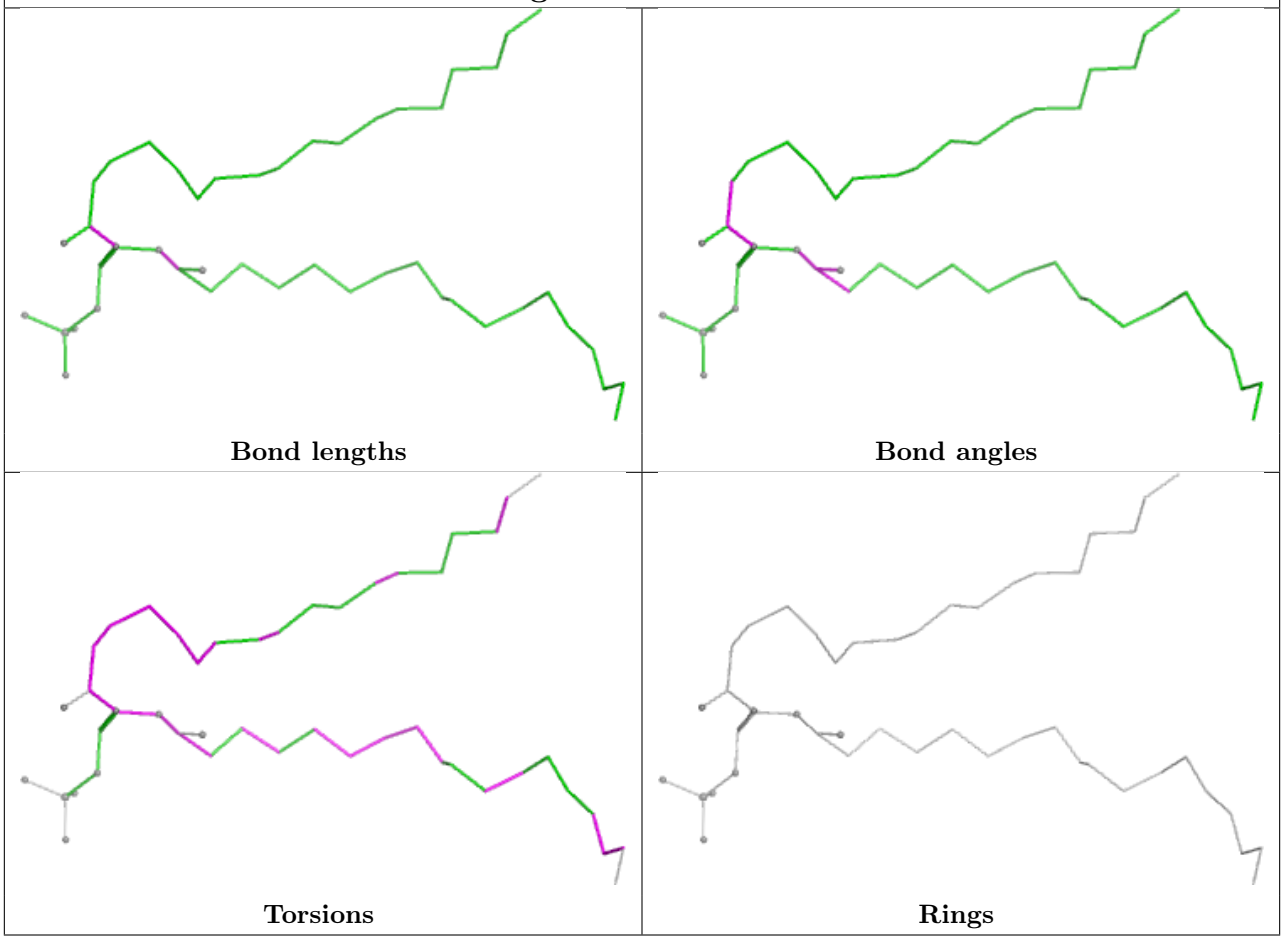


Torsions

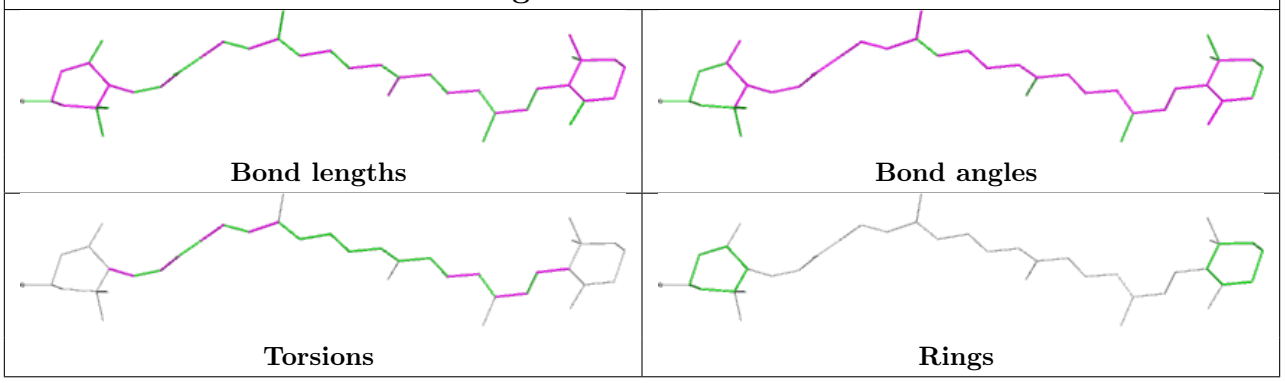


Rings

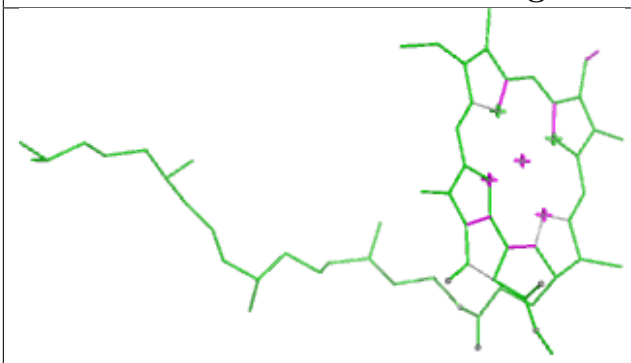
Ligand 3PH S 626



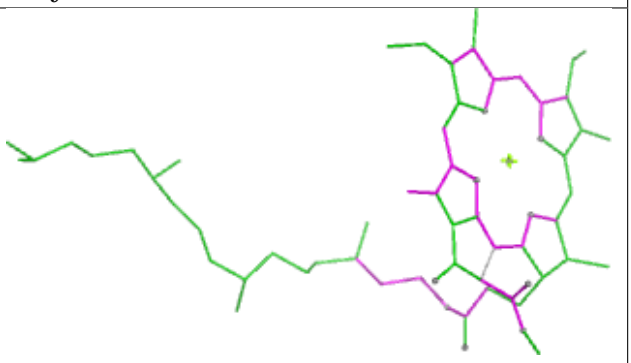
Ligand RRX H1 101



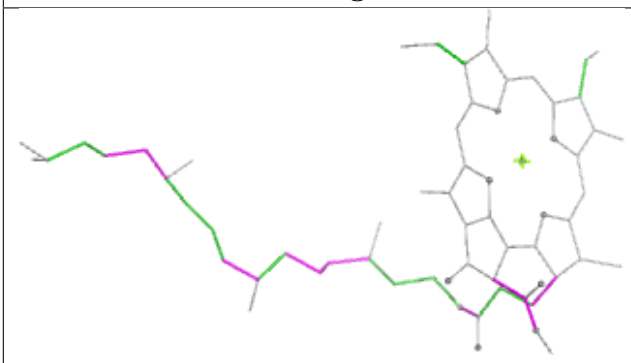
Ligand CLA y 611



Bond lengths



Bond angles

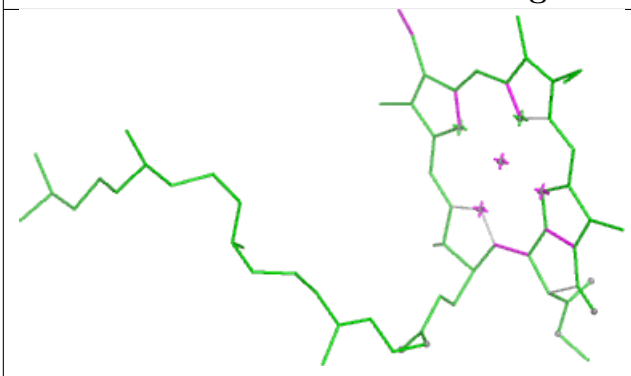


Torsions

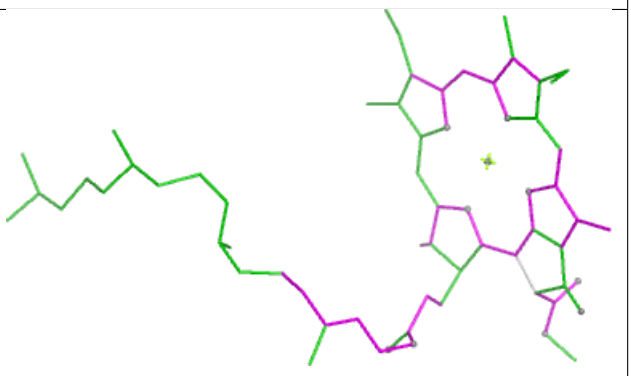


Rings

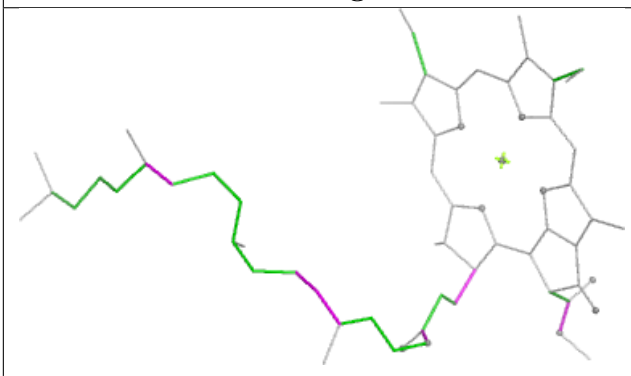
Ligand CLA c 511



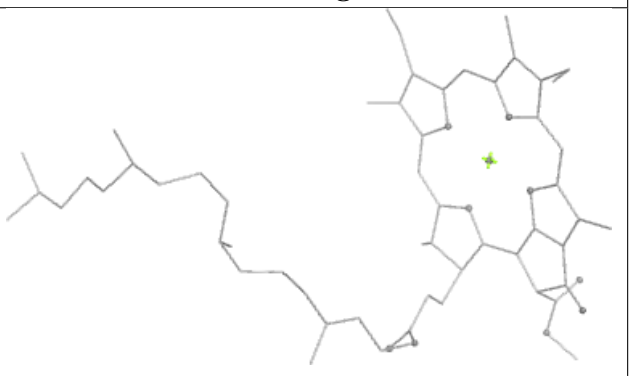
Bond lengths



Bond angles

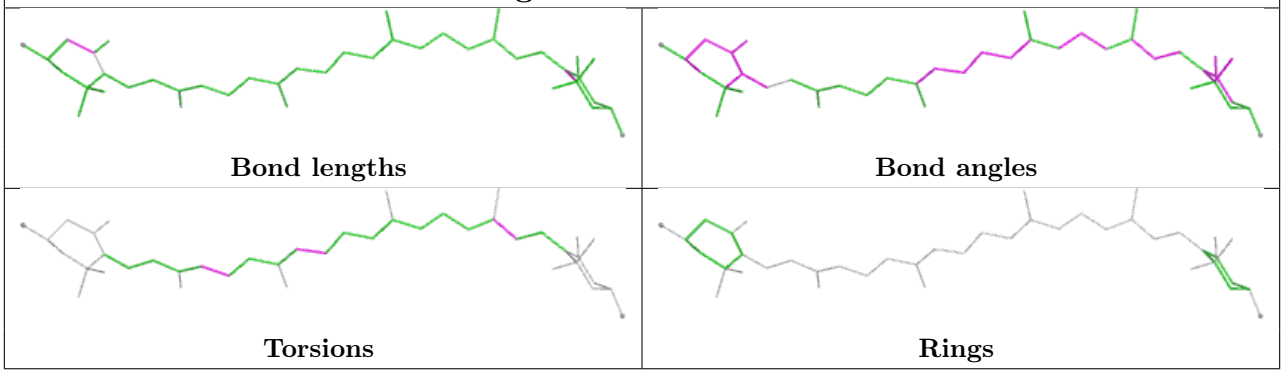


Torsions

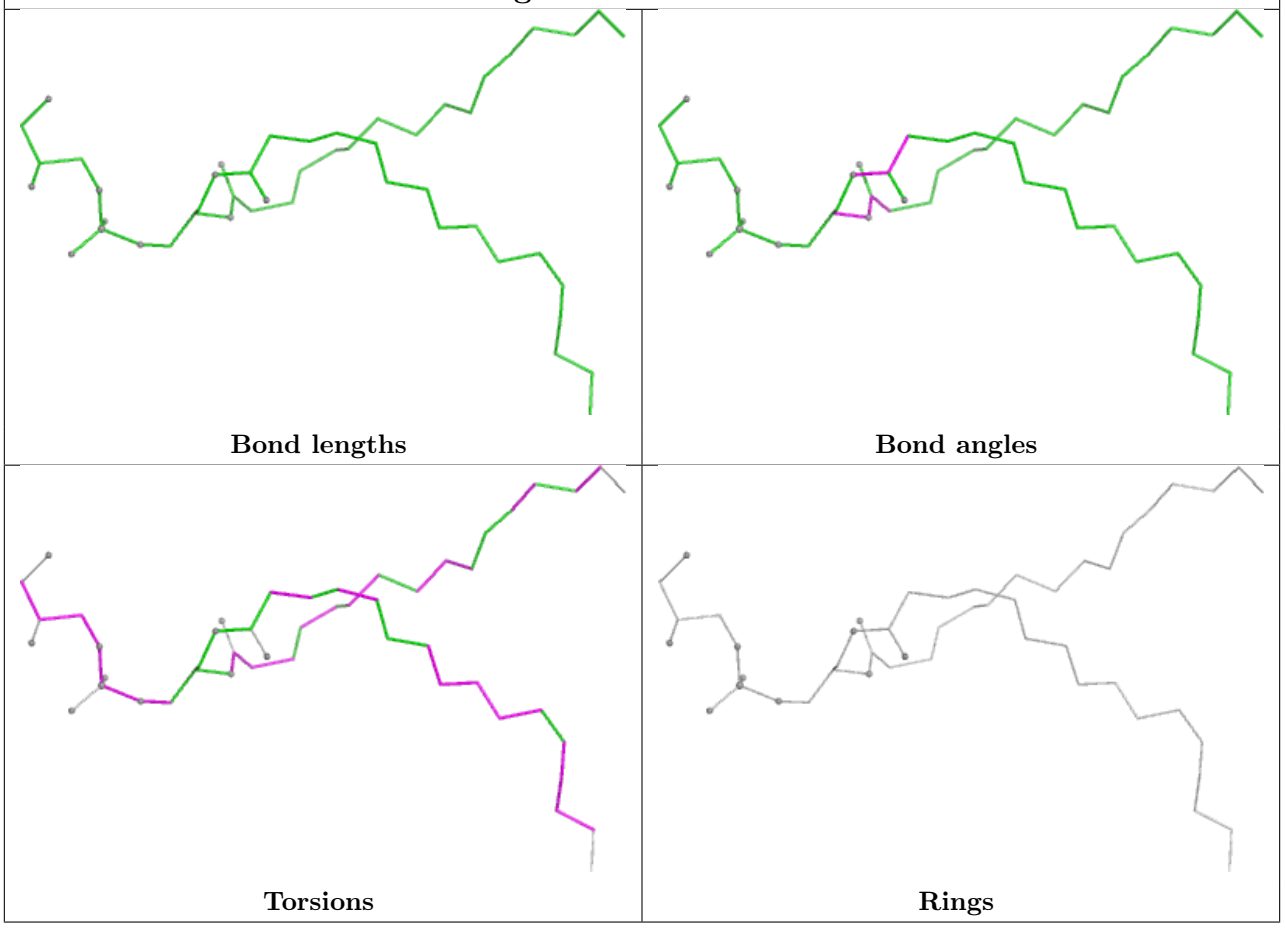


Rings

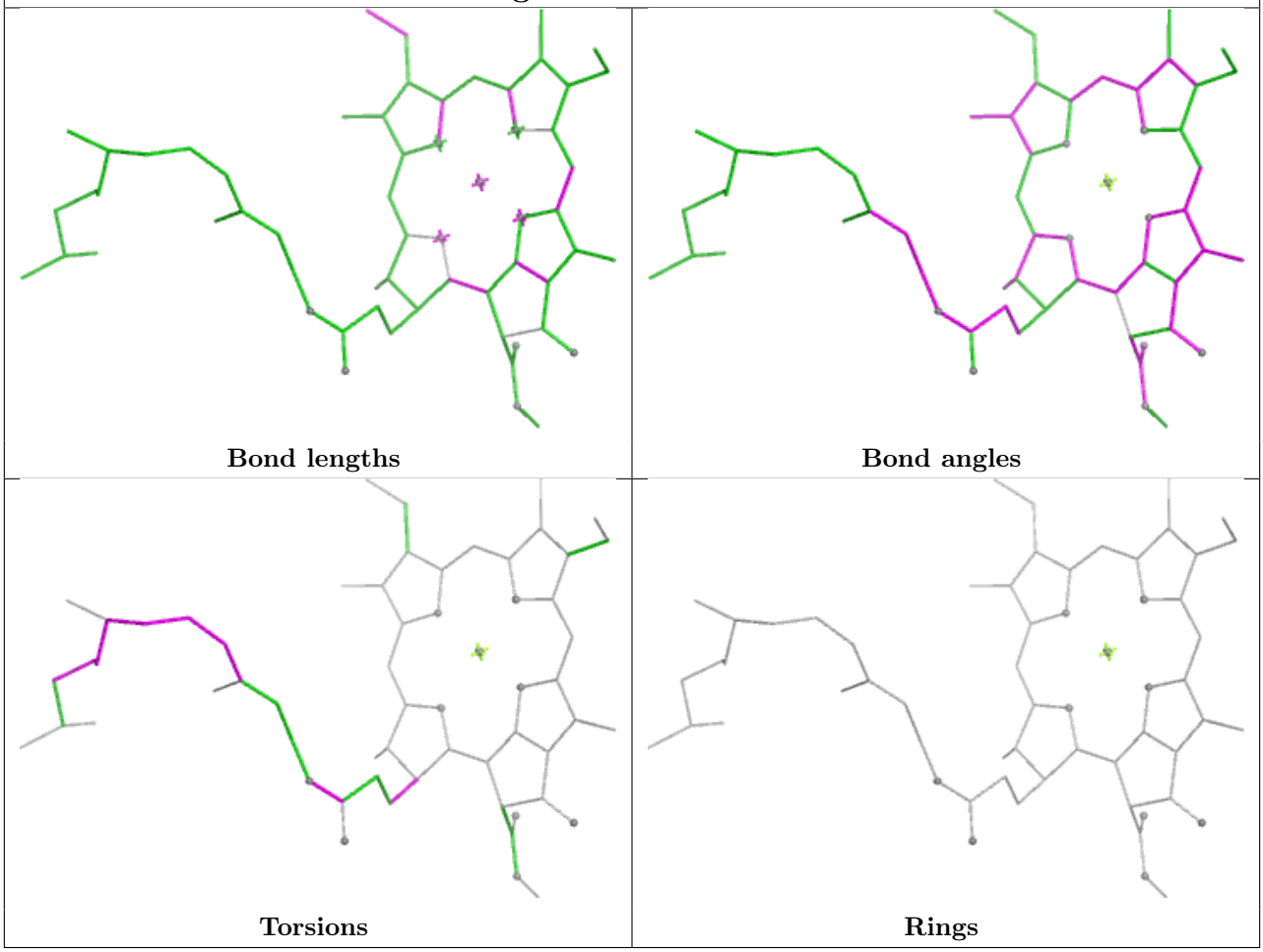
Ligand LUT N1 621



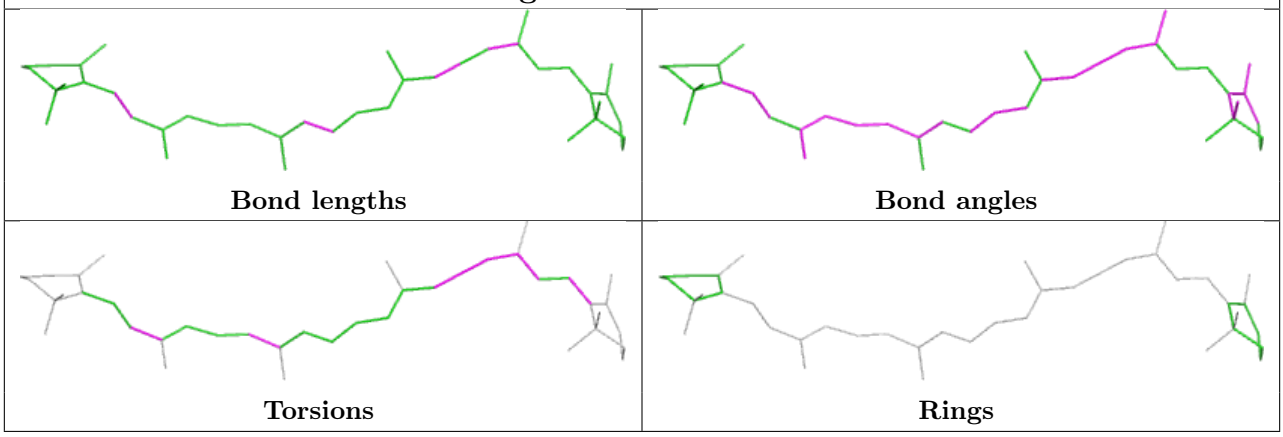
Ligand LHG D1 409



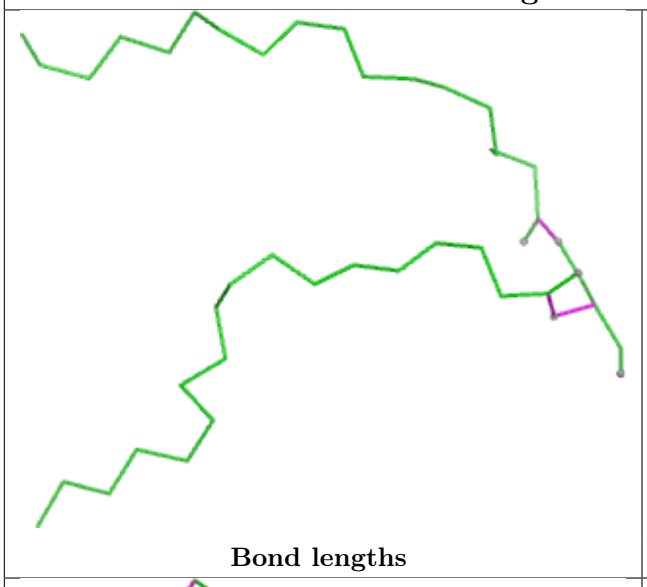
Ligand CLA a1 410



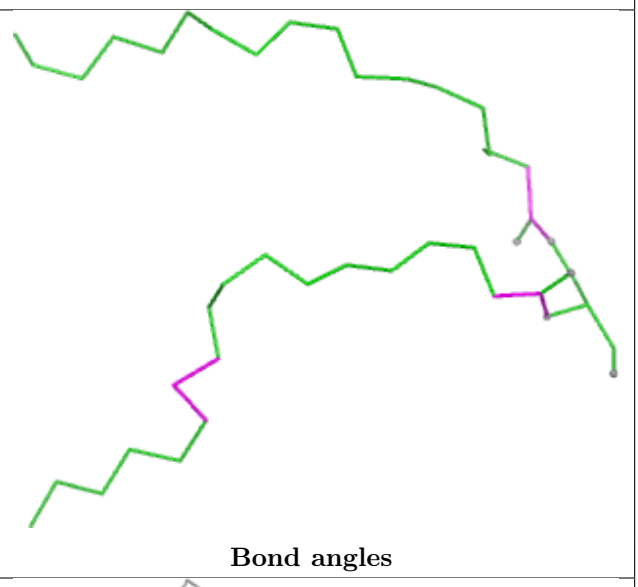
Ligand BCR c1 516



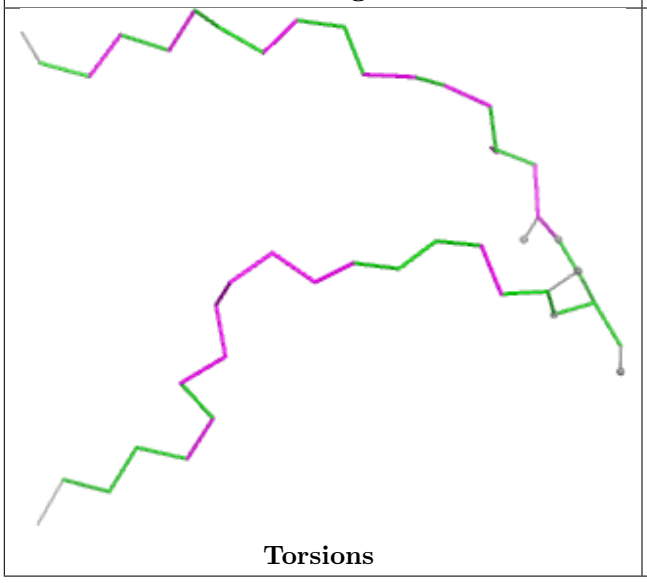
Ligand DGA C 524



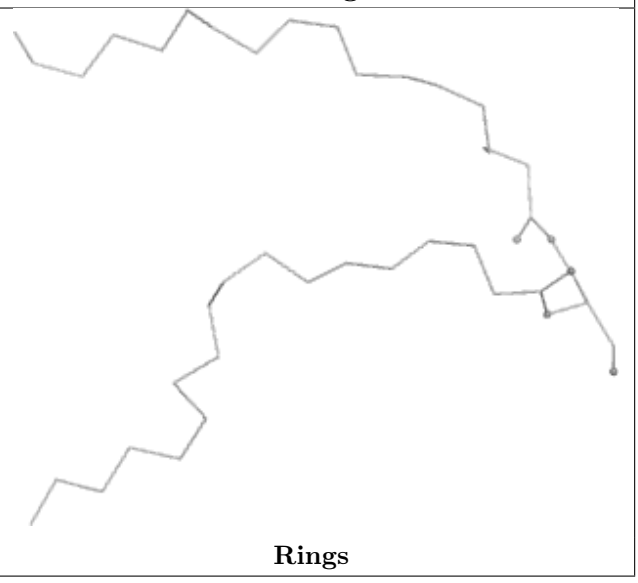
Bond lengths



Bond angles

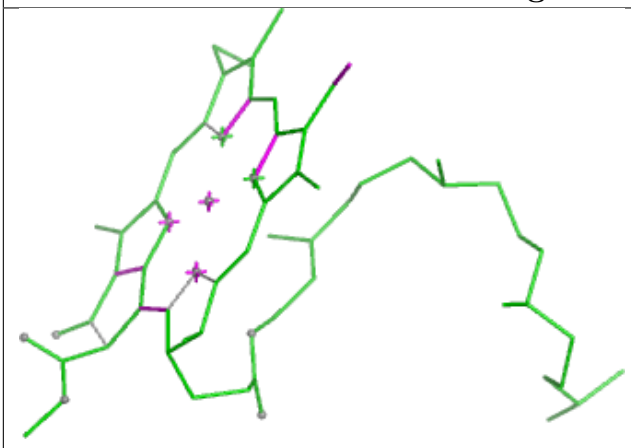


Torsions

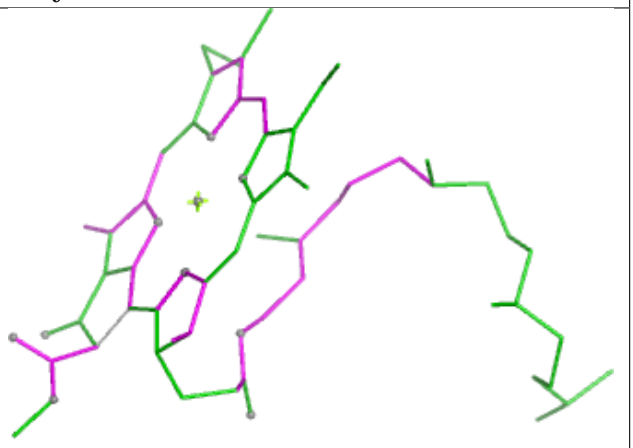


Rings

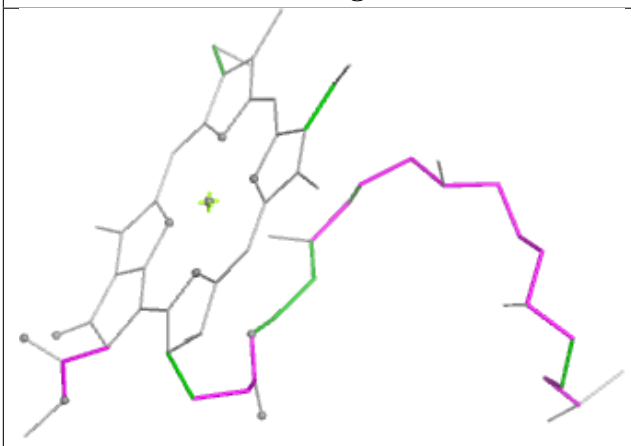
Ligand CLA y 613



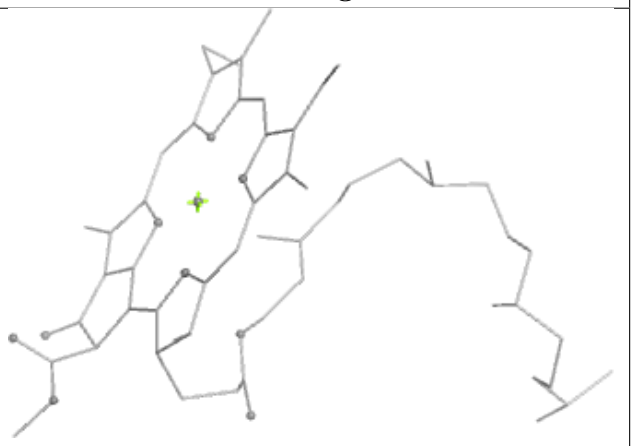
Bond lengths



Bond angles

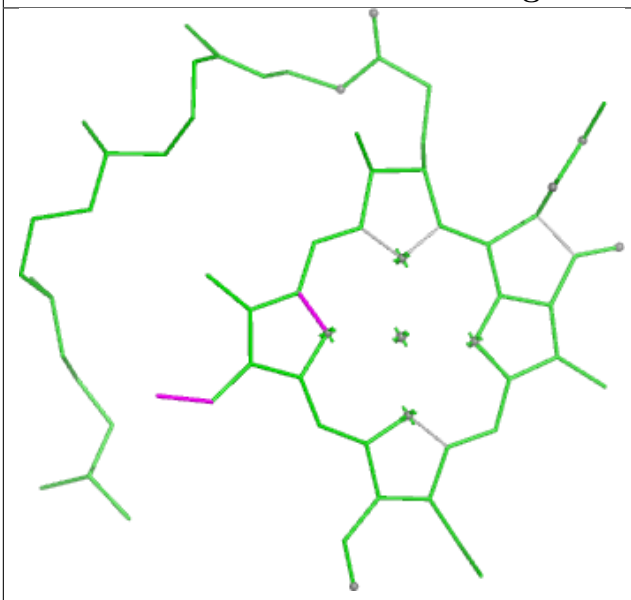


Torsions

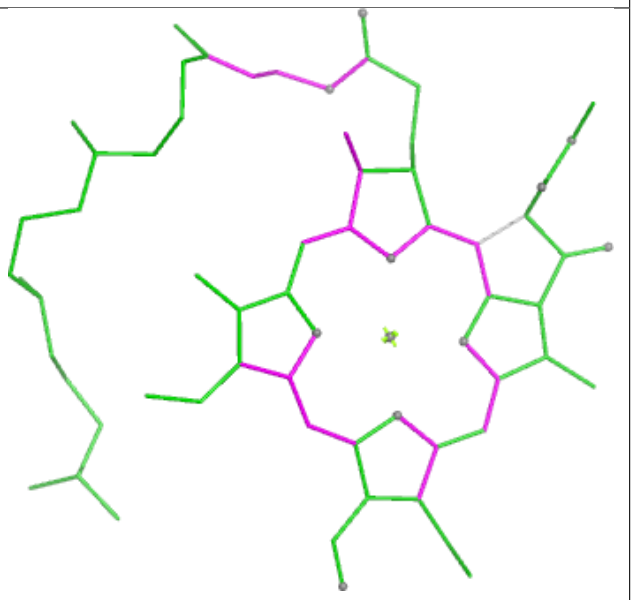


Rings

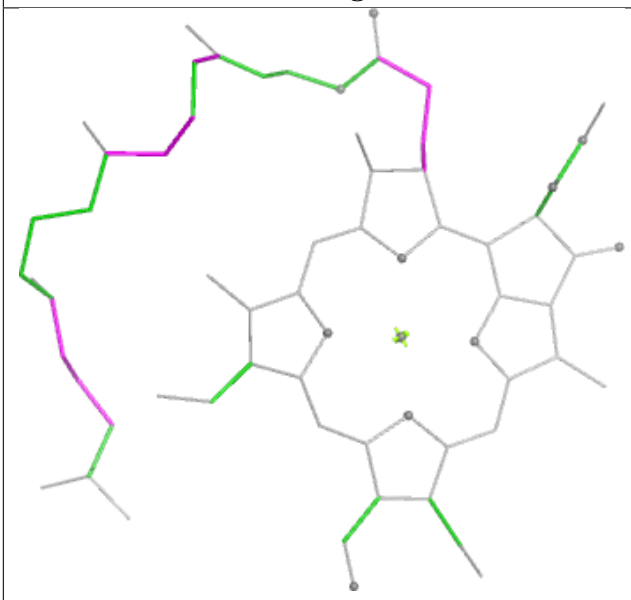
Ligand CHL G 607



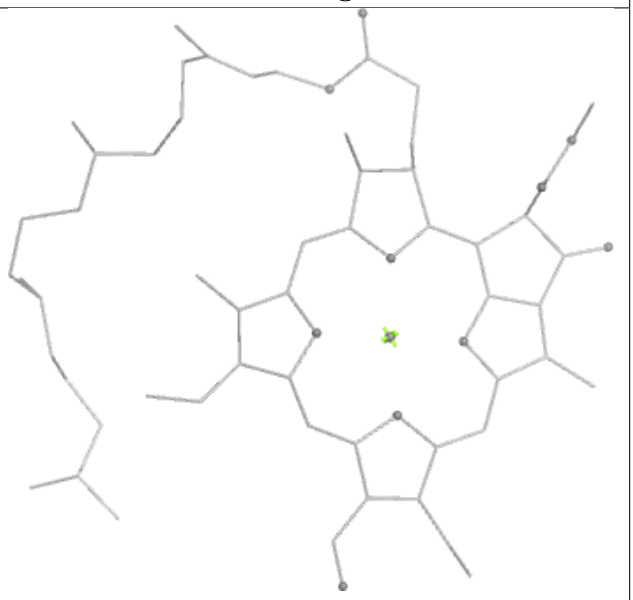
Bond lengths



Bond angles

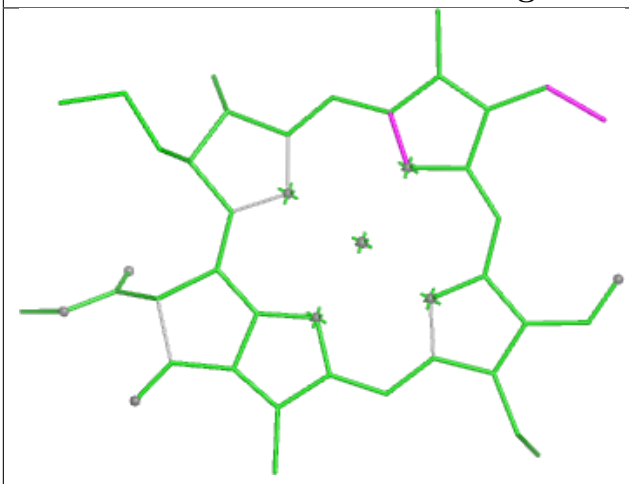


Torsions

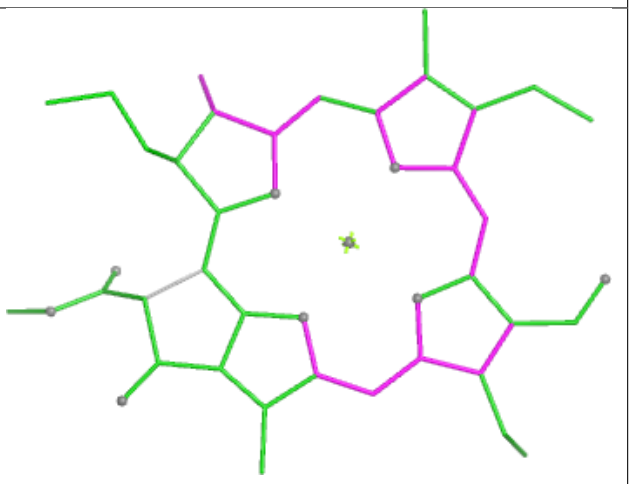


Rings

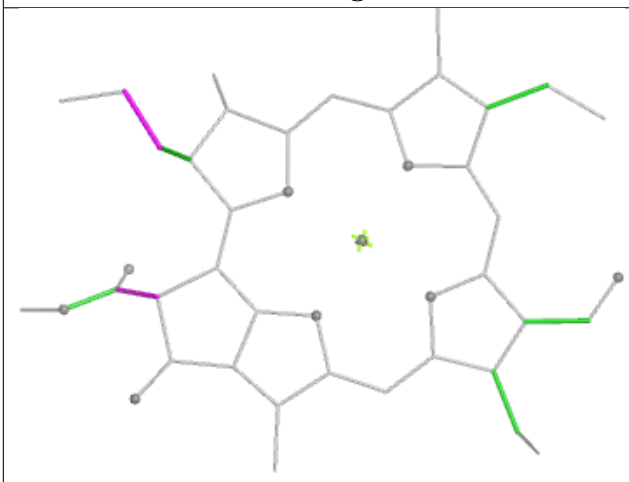
Ligand CHL S1 606



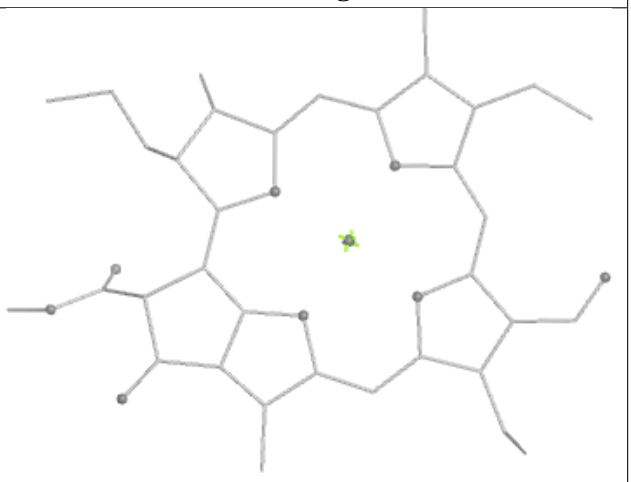
Bond lengths



Bond angles

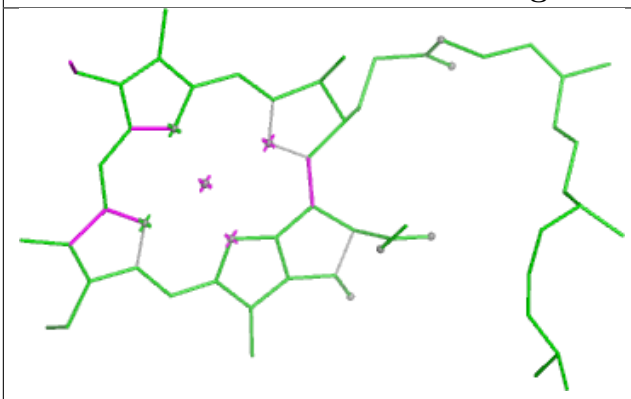


Torsions

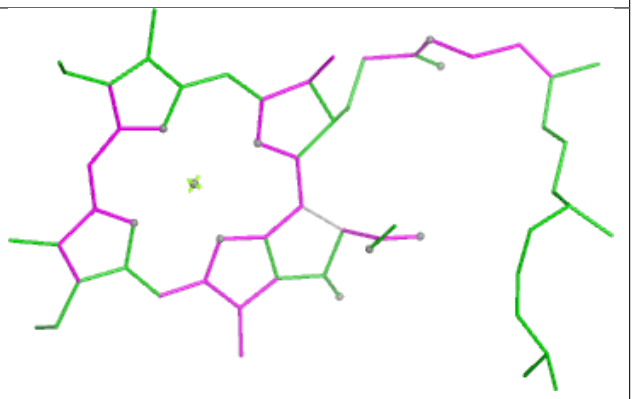


Rings

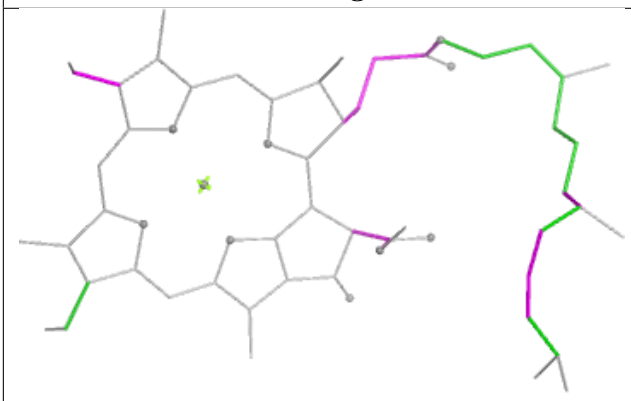
Ligand CLA r 612



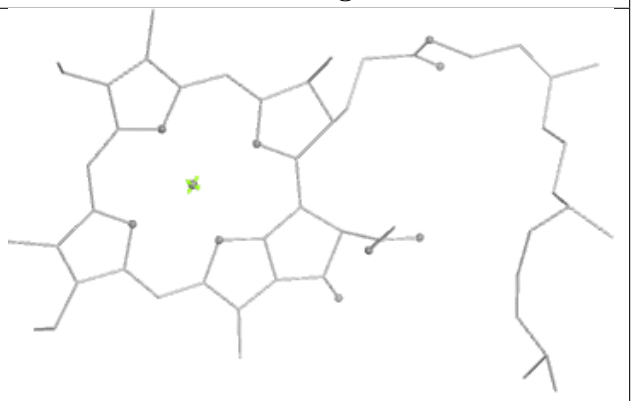
Bond lengths



Bond angles

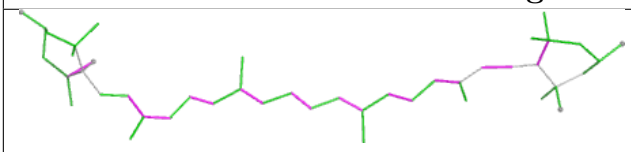


Torsions

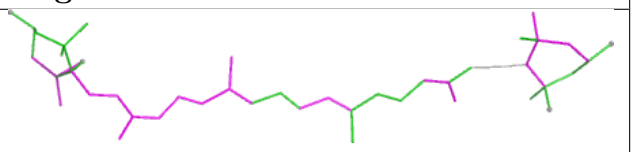


Rings

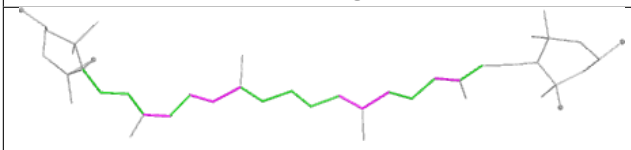
Ligand NEX g 623



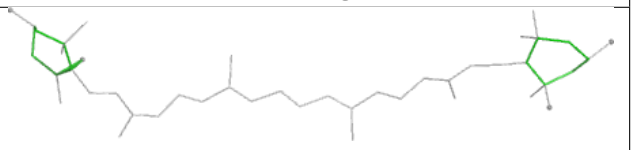
Bond lengths



Bond angles

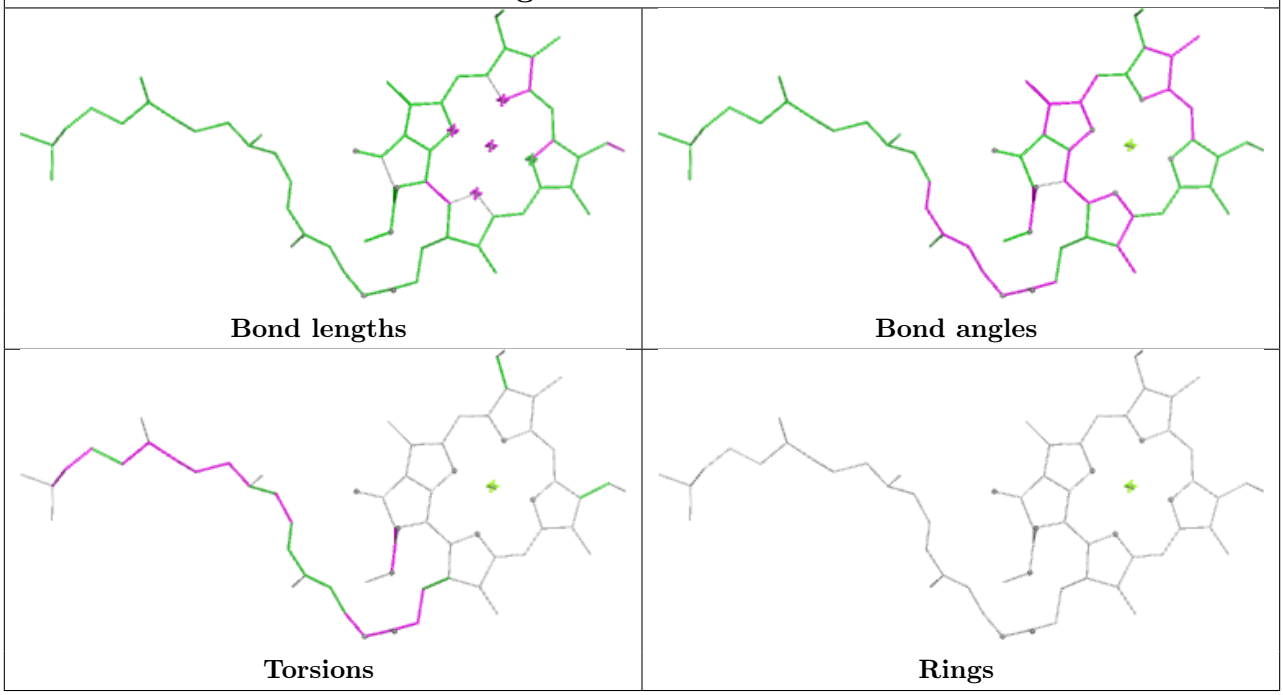


Torsions



Rings

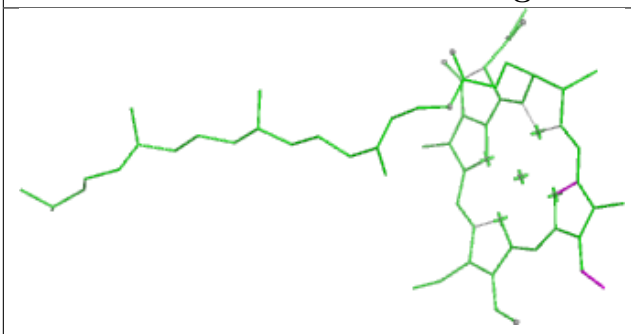
Ligand CLA B1 603



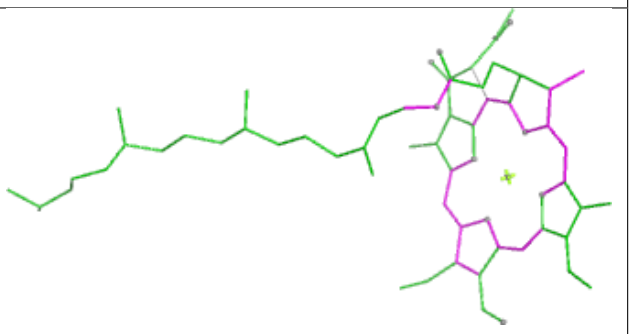
Ligand LUT s 621



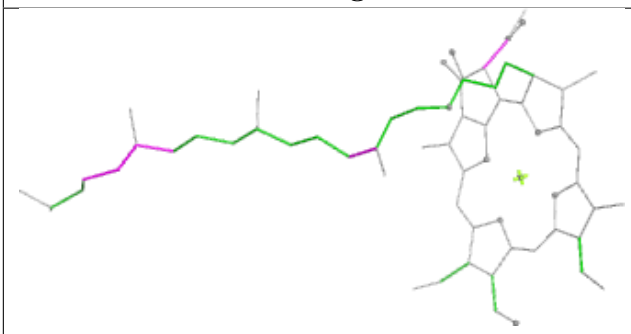
Ligand CHL N1 609



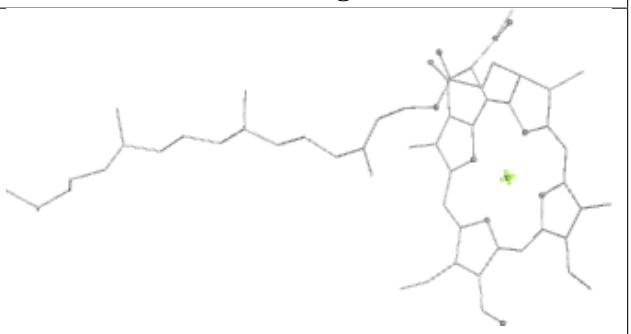
Bond lengths



Bond angles

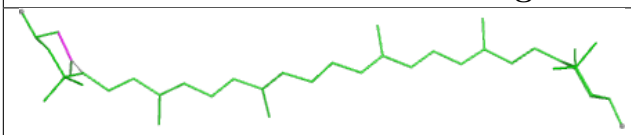


Torsions

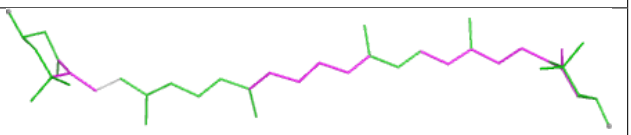


Rings

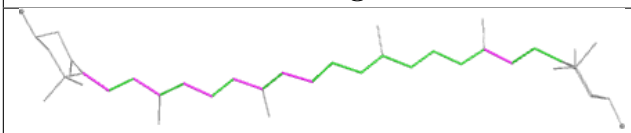
Ligand LUT R1 620



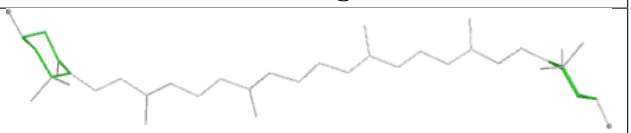
Bond lengths



Bond angles

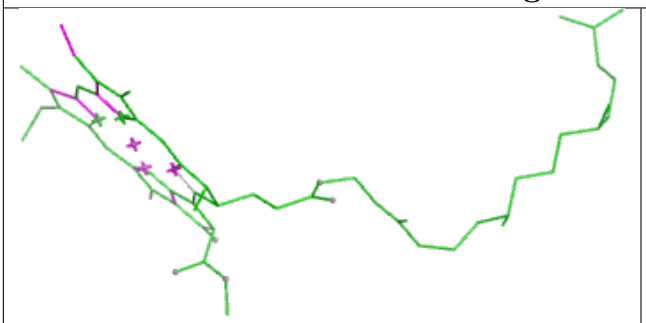


Torsions

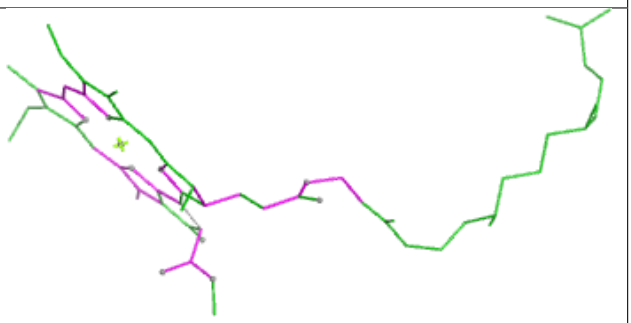


Rings

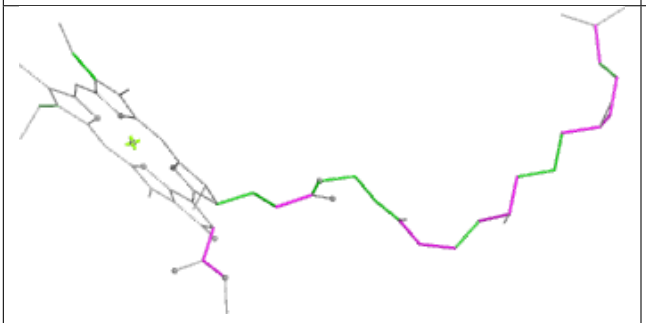
Ligand CLA D 402



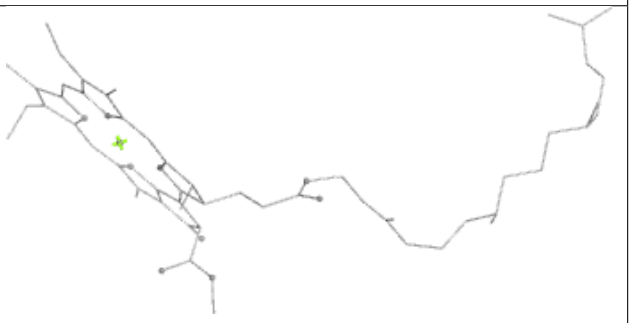
Bond lengths



Bond angles

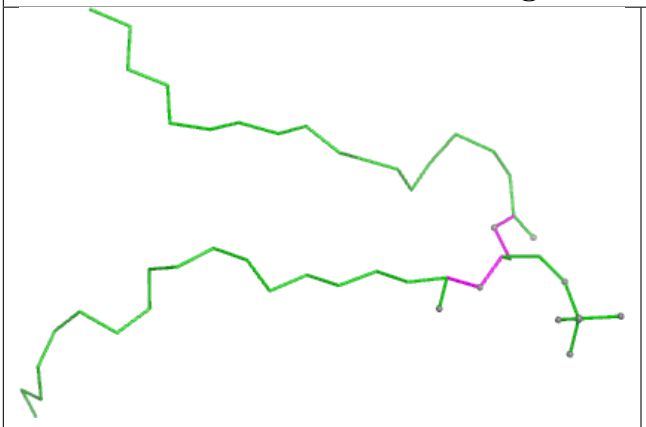


Torsions

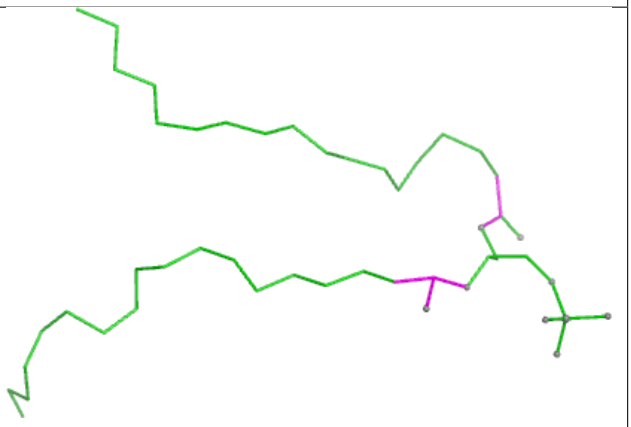


Rings

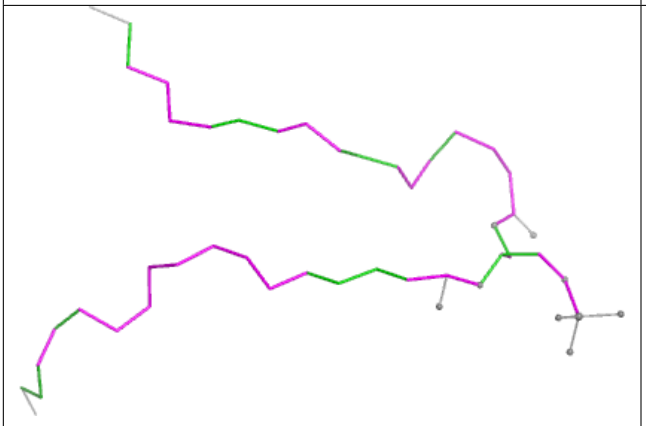
Ligand 3PH S1 626



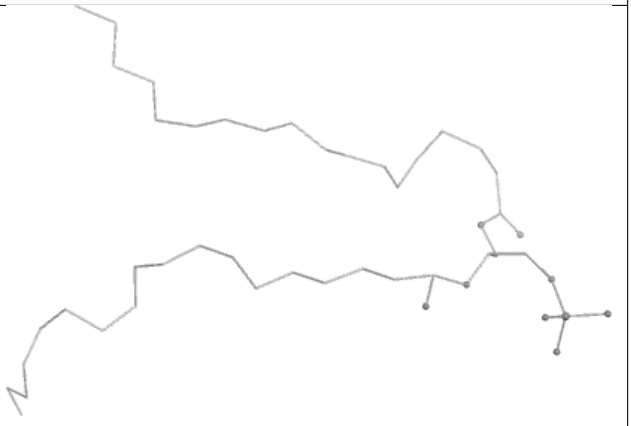
Bond lengths



Bond angles

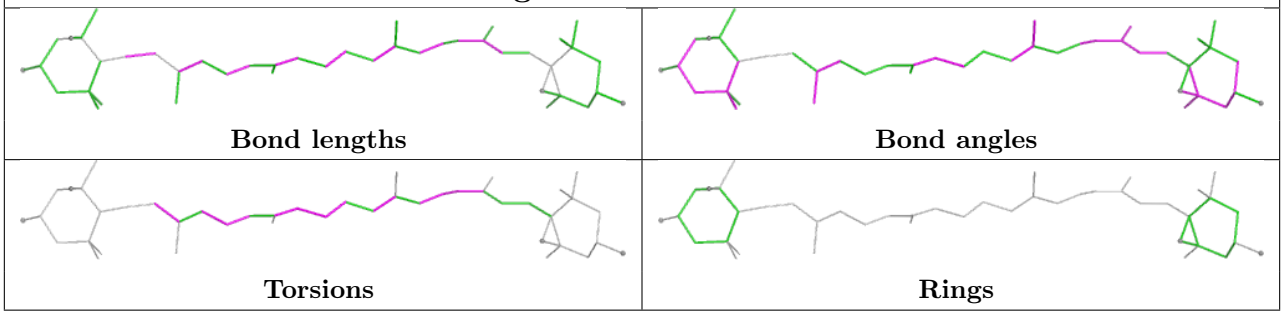


Torsions

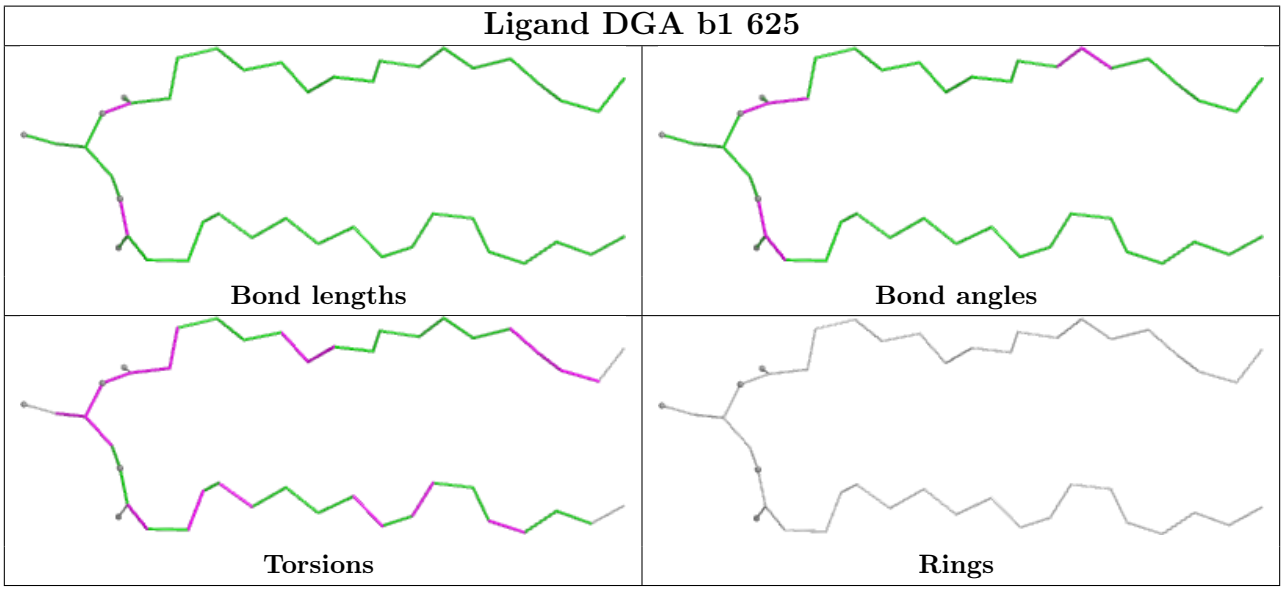


Rings

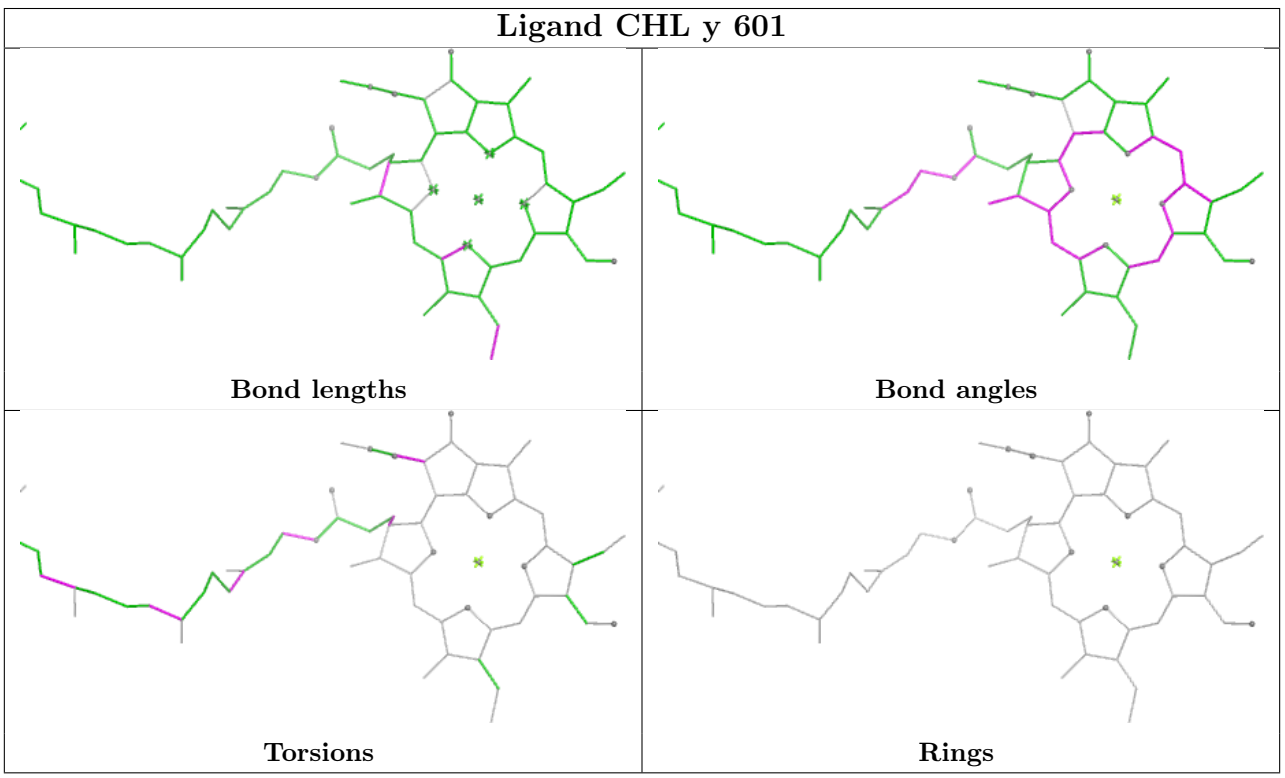
Ligand NEX R1 622



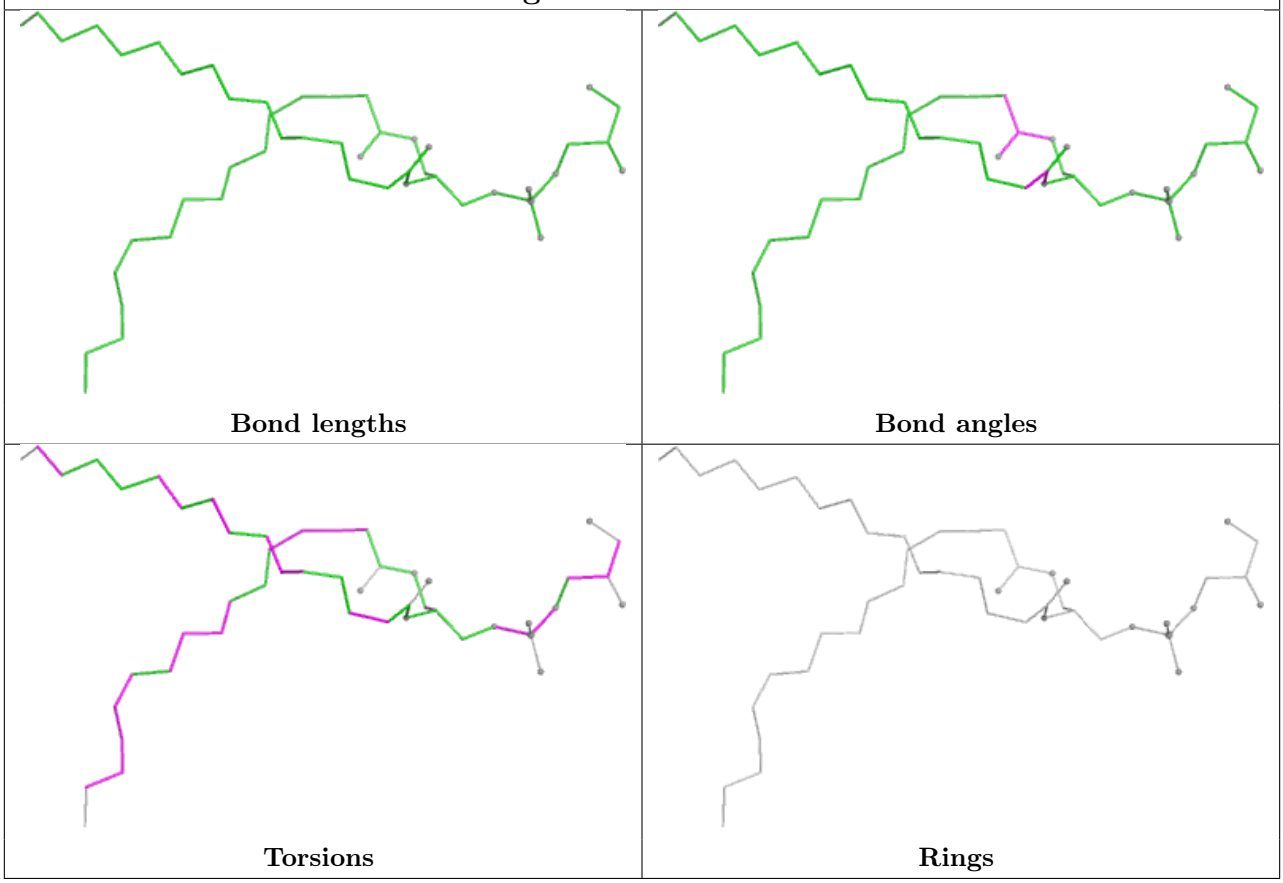
Ligand DGA b1 625



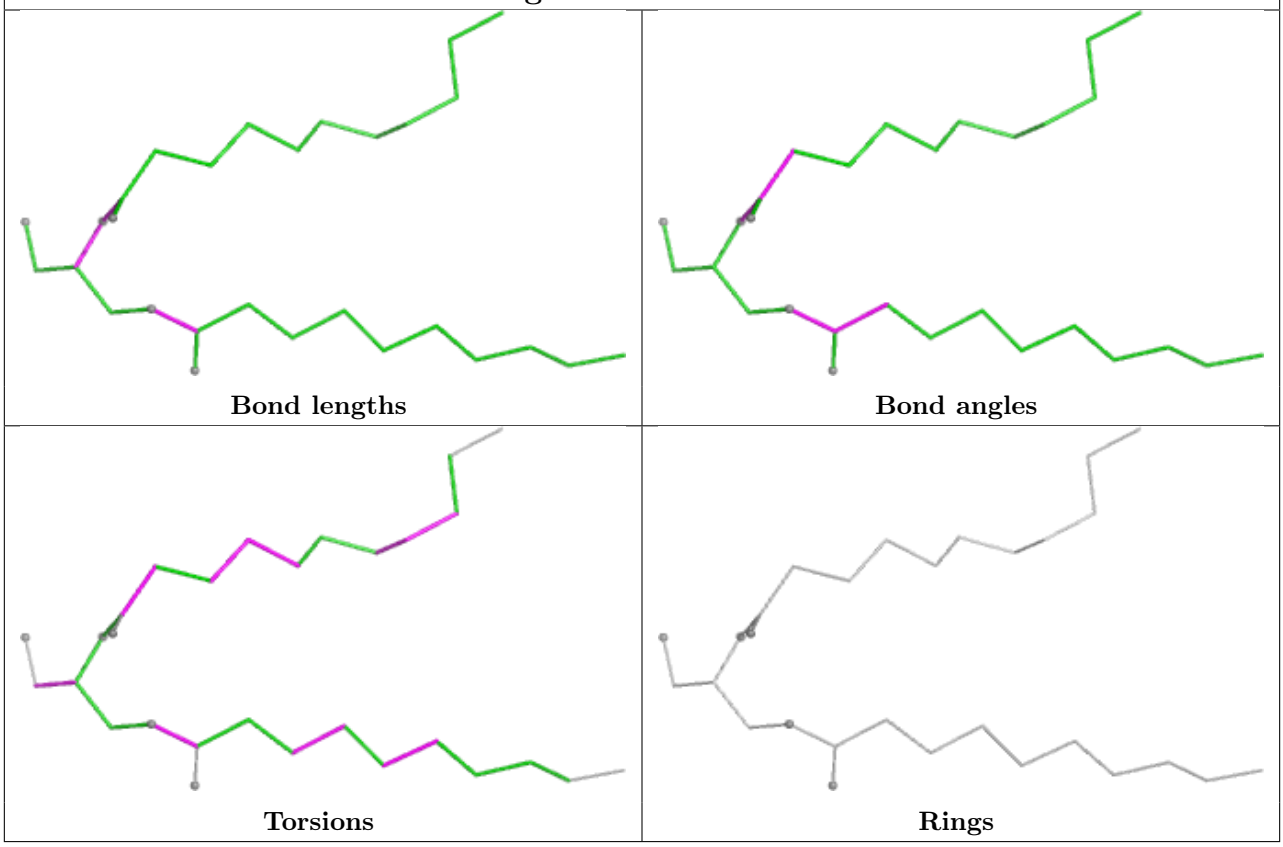
Ligand CHL y 601



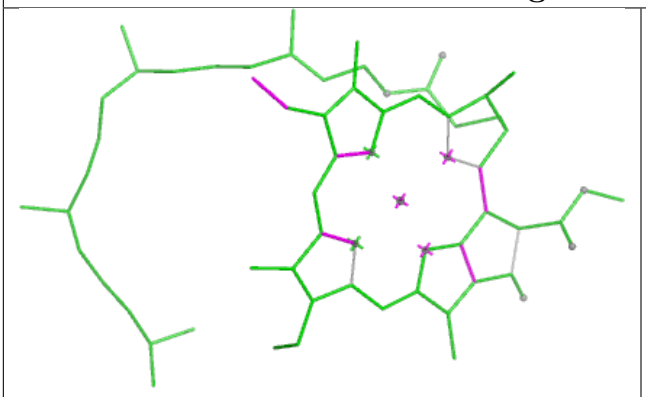
Ligand LHG D 409



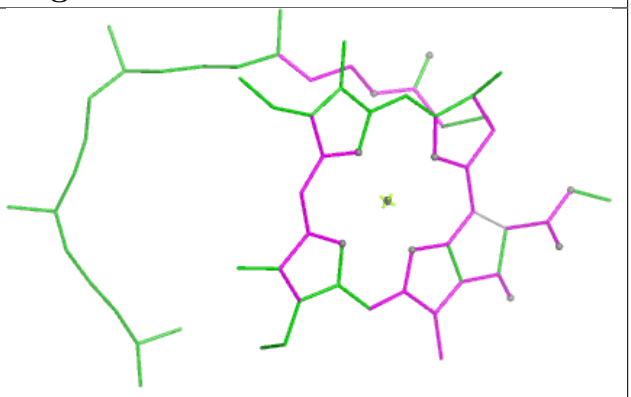
Ligand DGA J 101



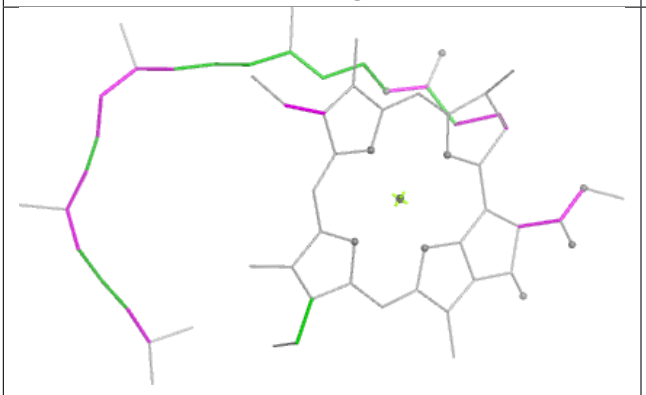
Ligand CLA g 610



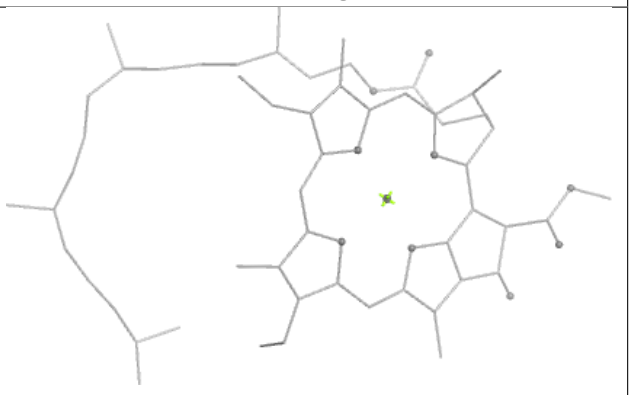
Bond lengths



Bond angles

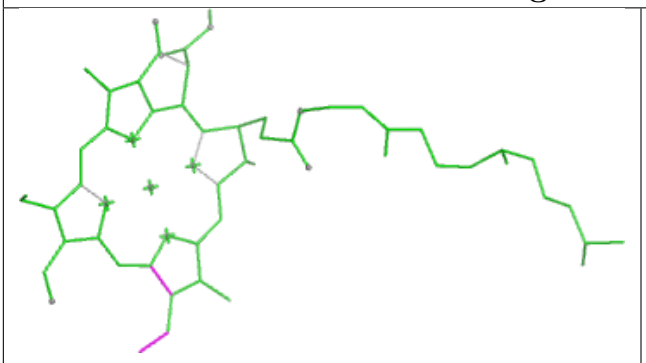


Torsions

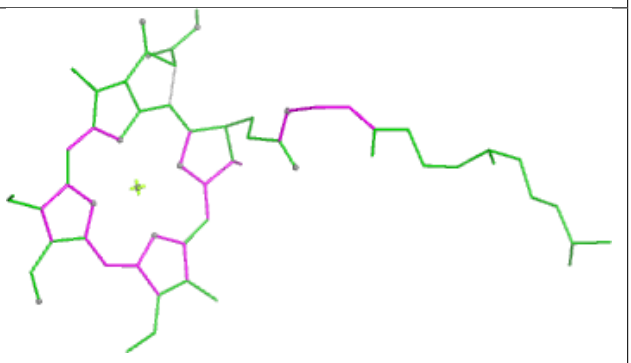


Rings

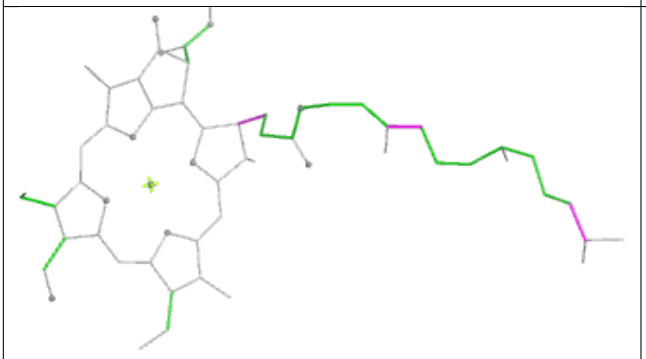
Ligand CHL s 608



Bond lengths



Bond angles

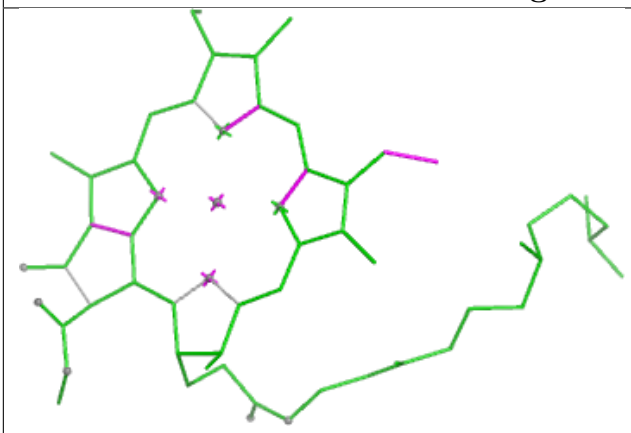


Torsions

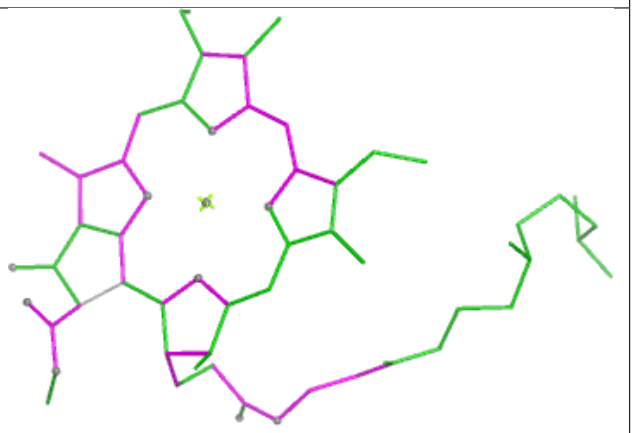


Rings

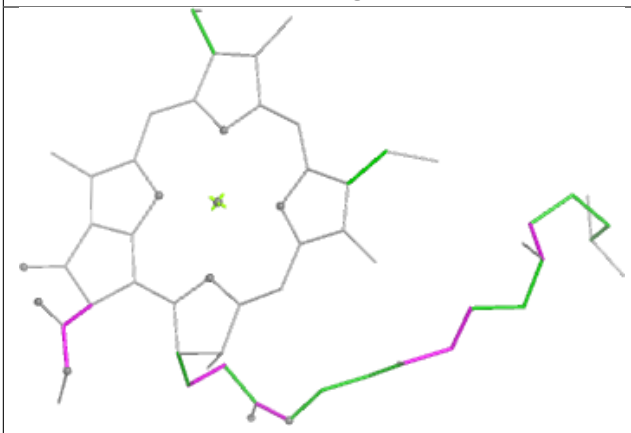
Ligand CLA r 609



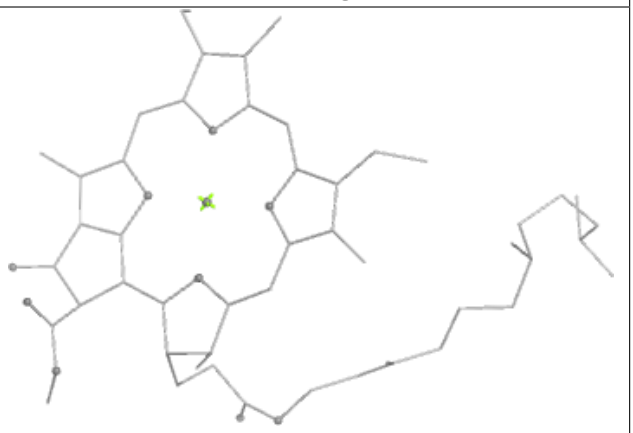
Bond lengths



Bond angles

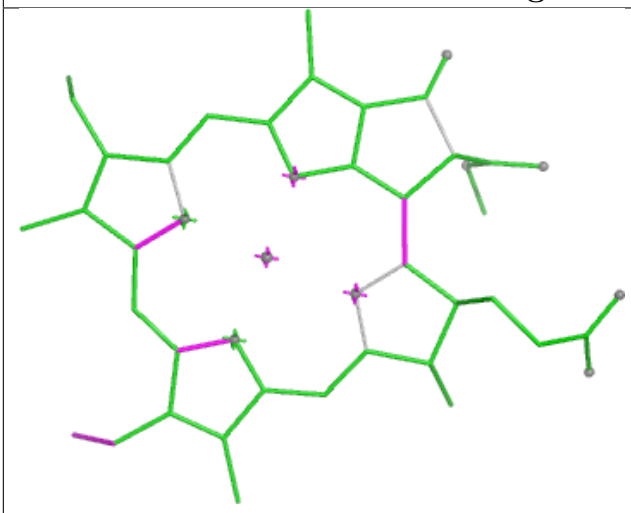


Torsions

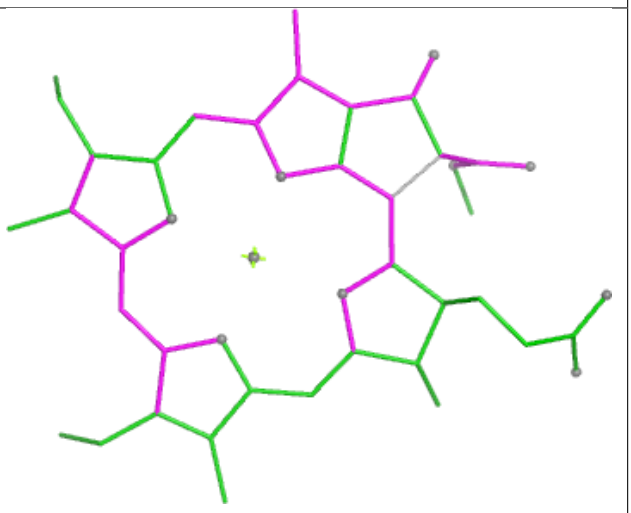


Rings

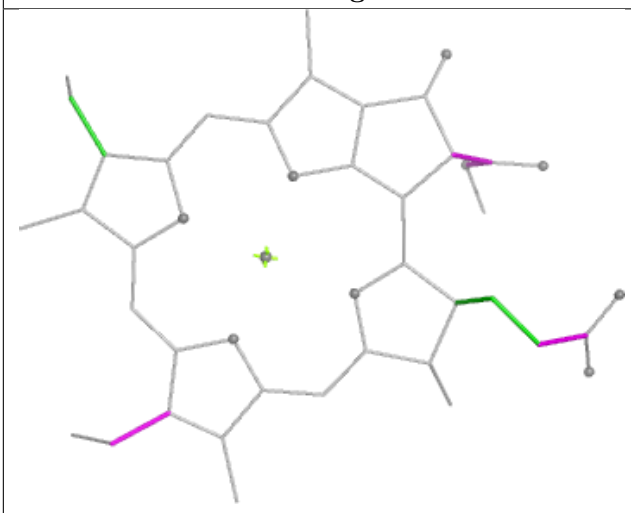
Ligand CLA n 612



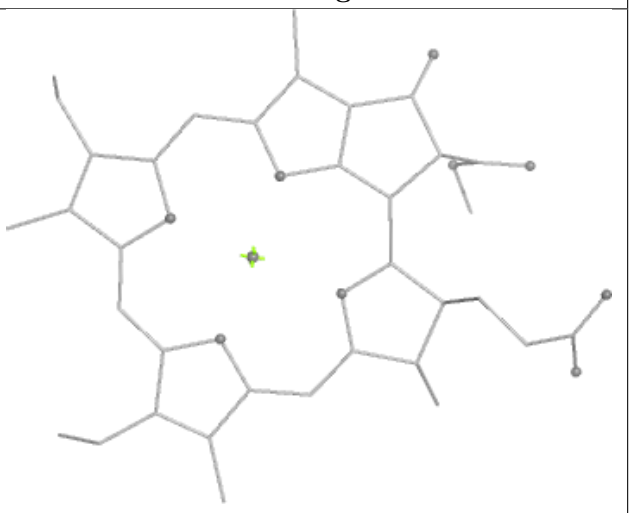
Bond lengths



Bond angles

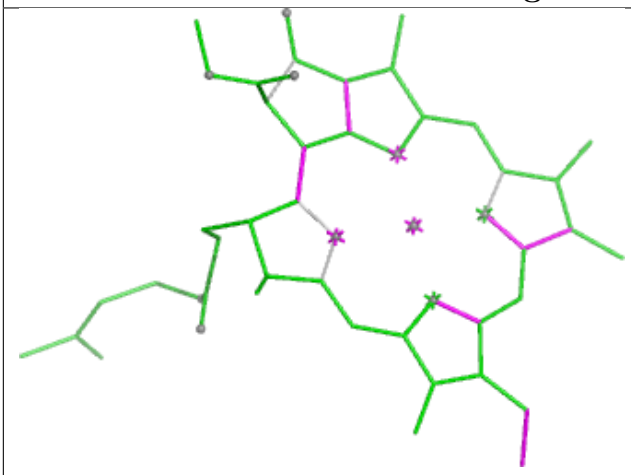


Torsions

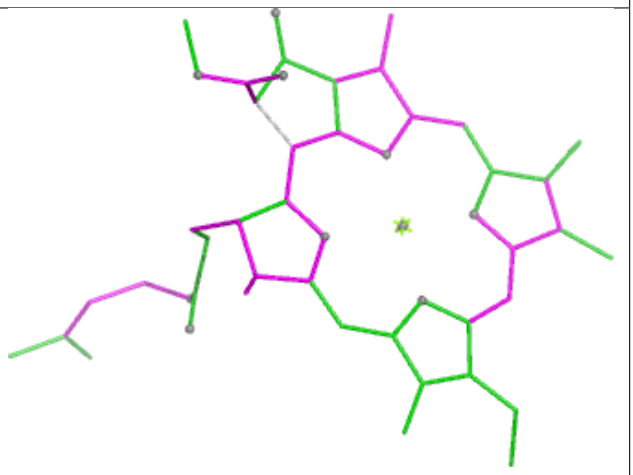


Rings

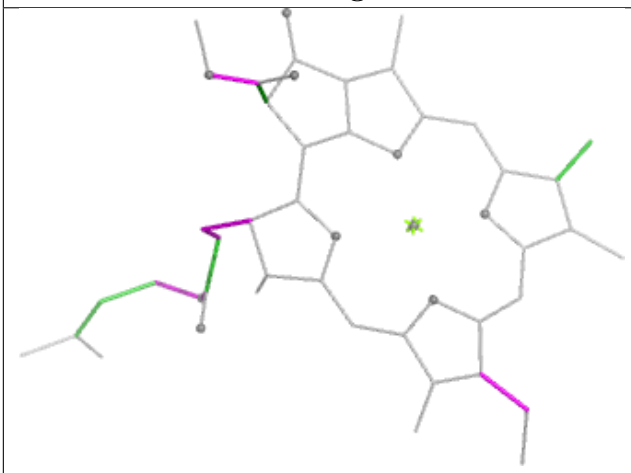
Ligand CLA Y 608



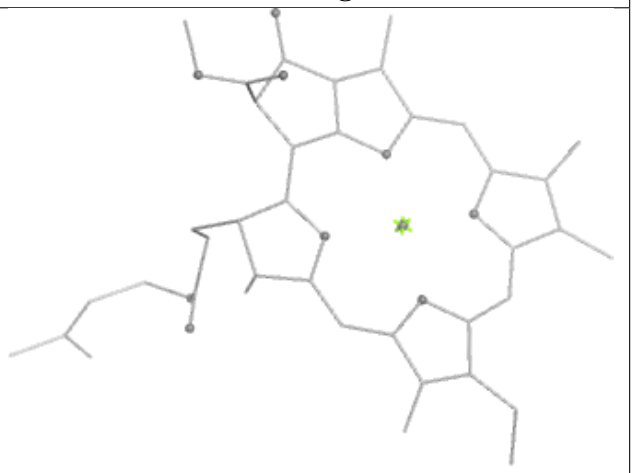
Bond lengths



Bond angles

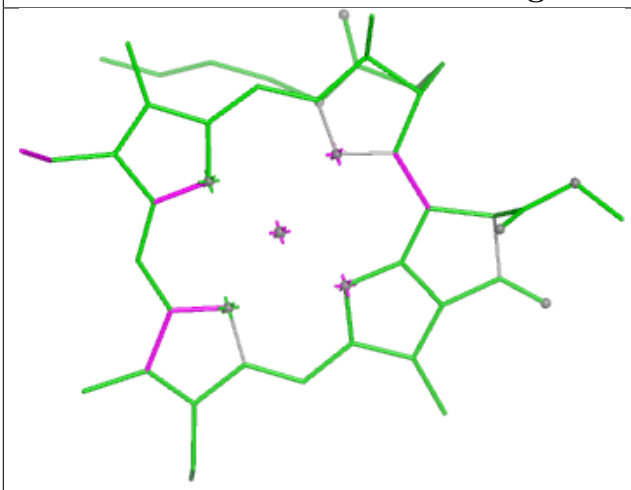


Torsions

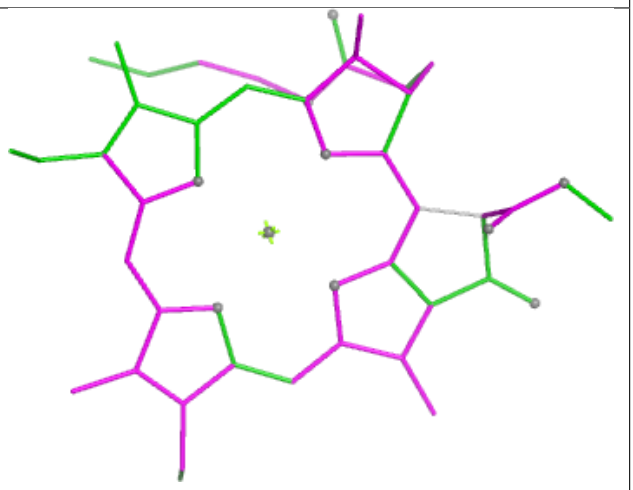


Rings

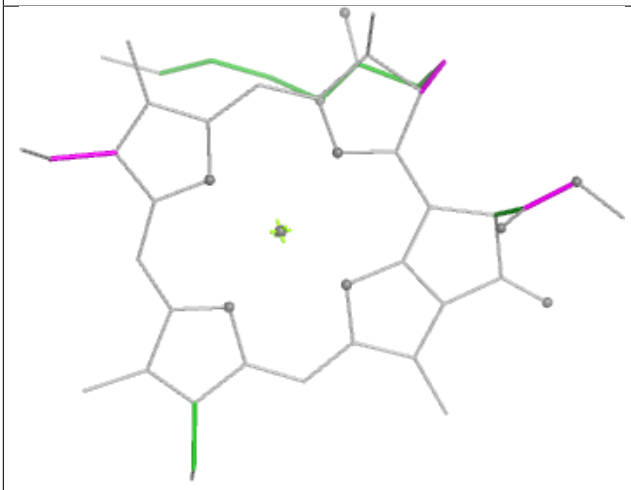
Ligand CLA n 614



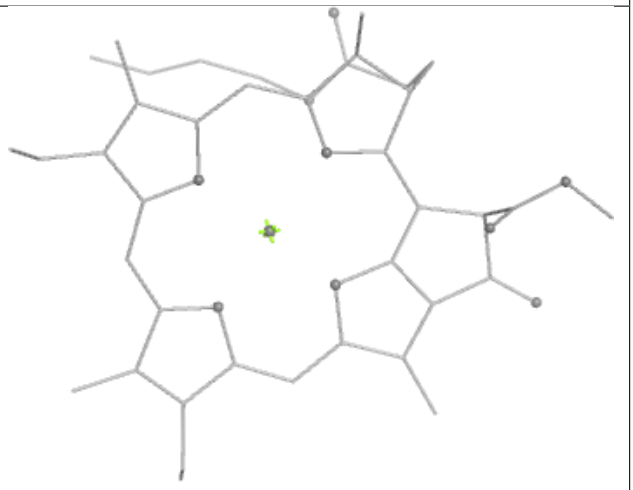
Bond lengths



Bond angles

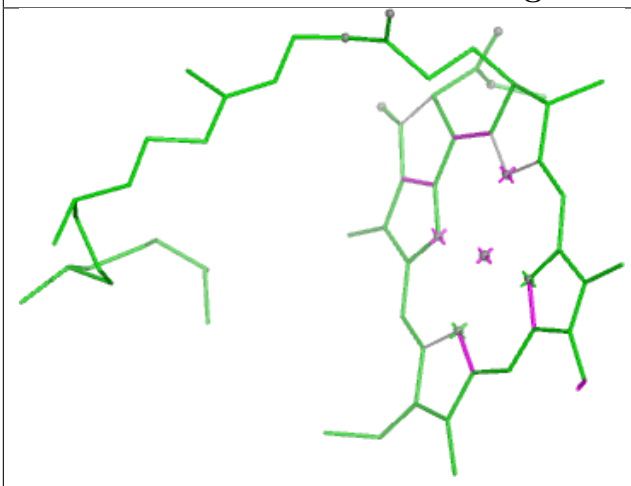


Torsions

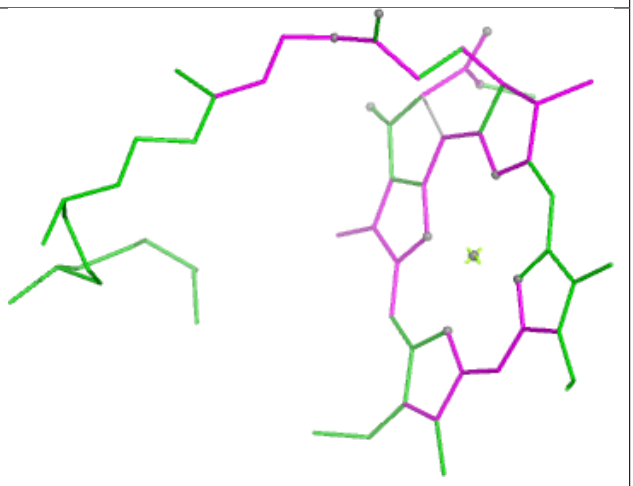


Rings

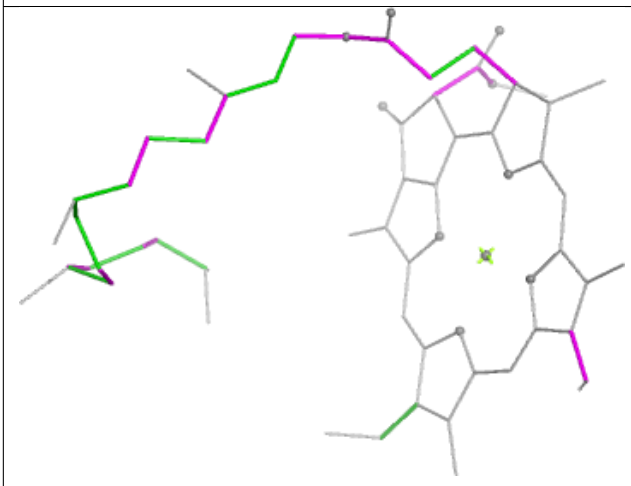
Ligand CLA C 503



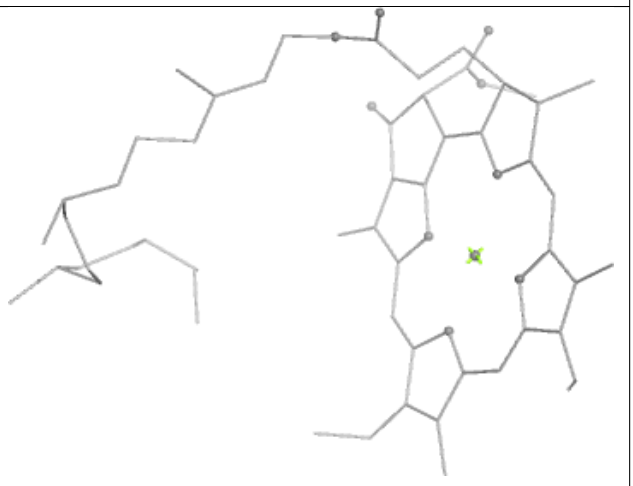
Bond lengths



Bond angles

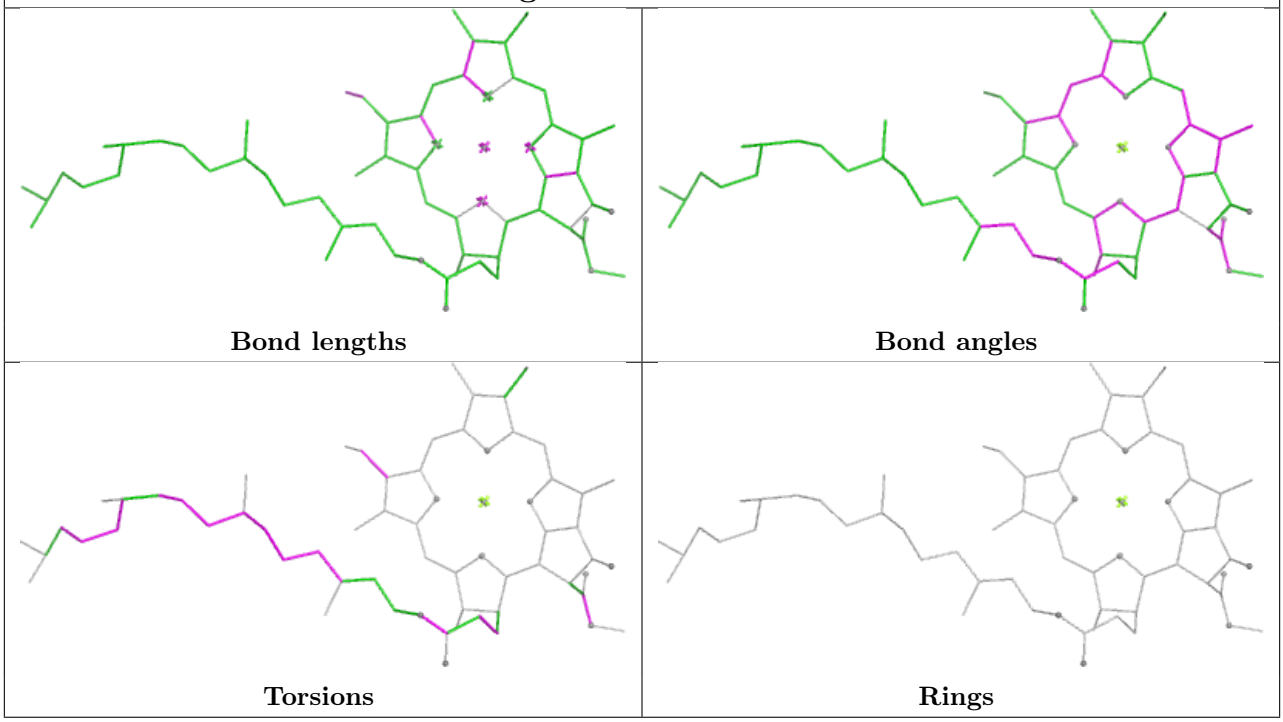


Torsions

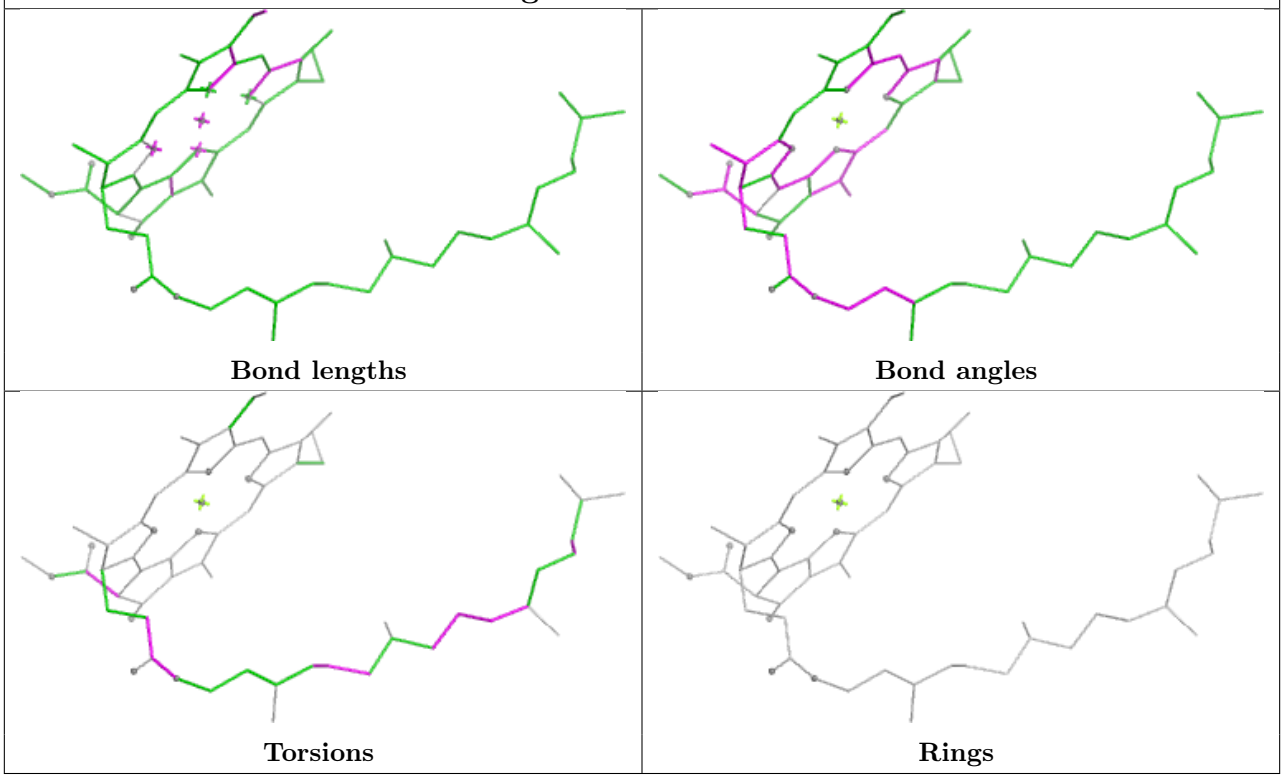


Rings

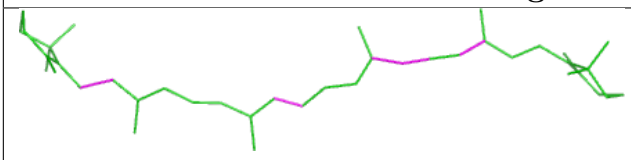
Ligand CLA b1 604



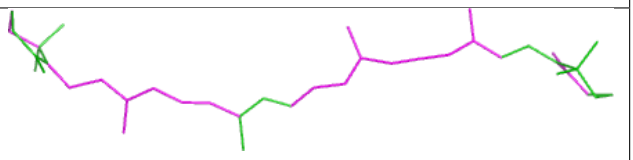
Ligand CLA c1 508



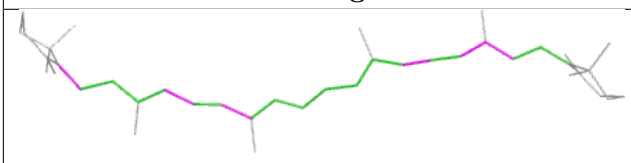
Ligand BCR c 515



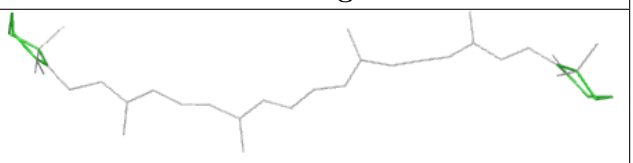
Bond lengths



Bond angles

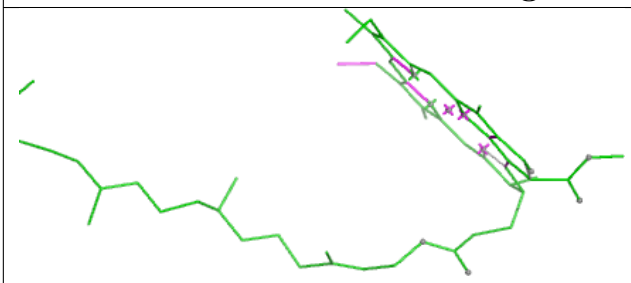


Torsions

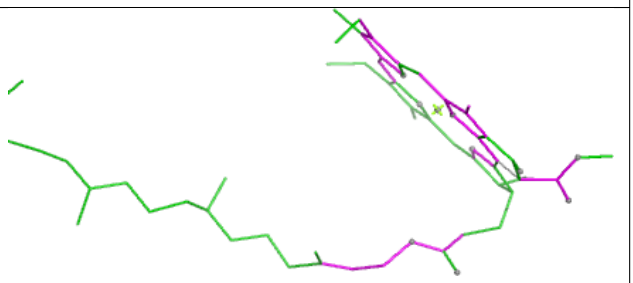


Rings

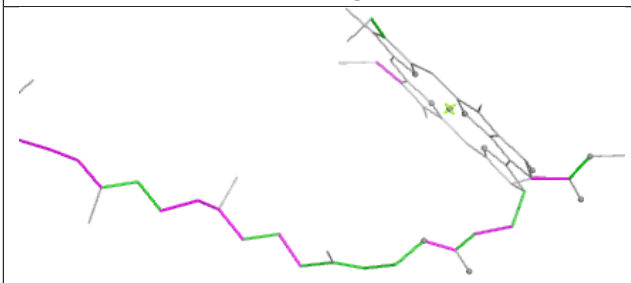
Ligand CLA c1 504



Bond lengths



Bond angles

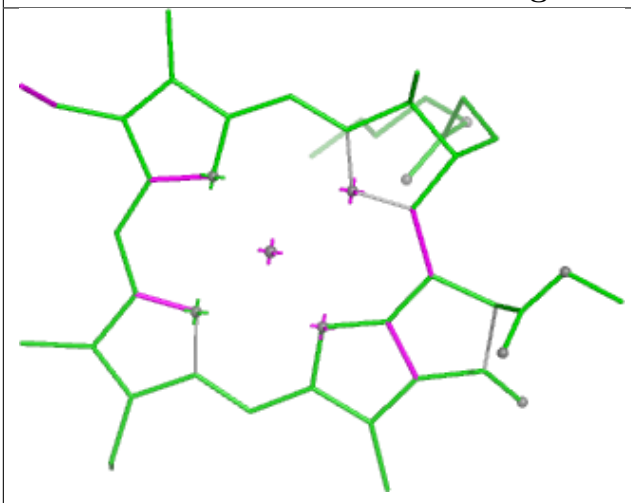


Torsions

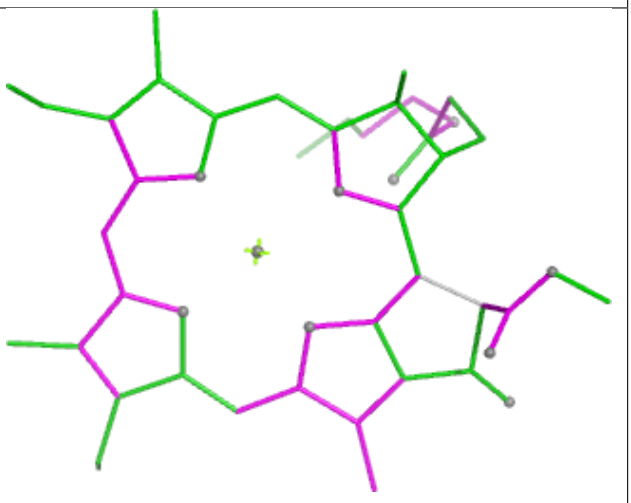


Rings

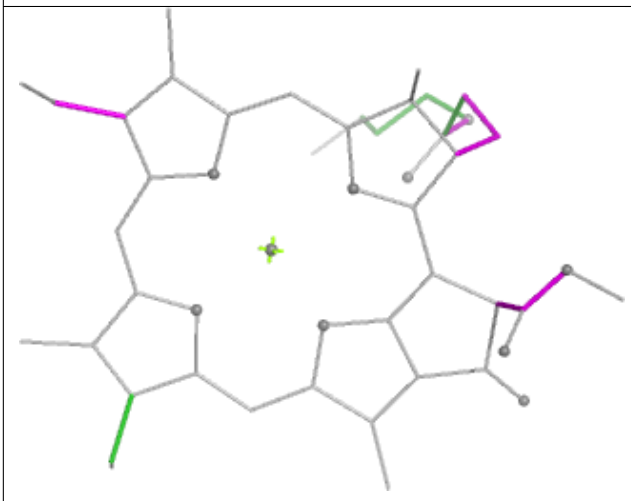
Ligand CLA r 604



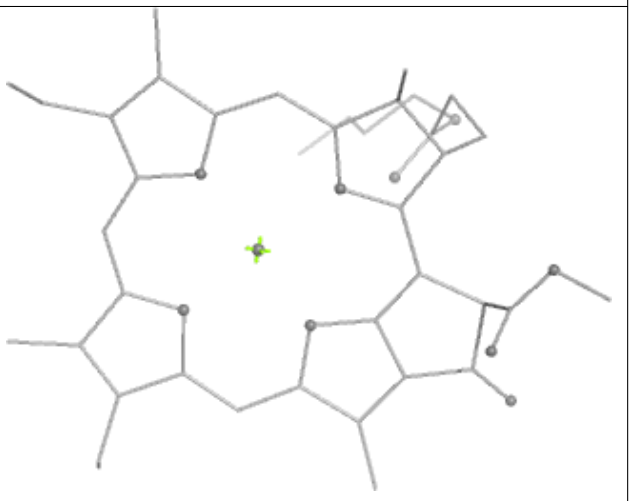
Bond lengths



Bond angles

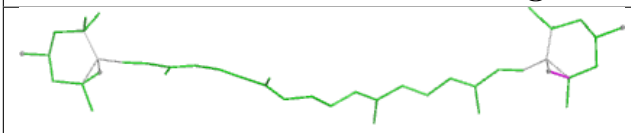


Torsions

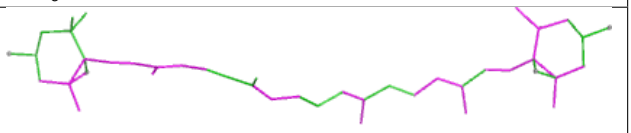


Rings

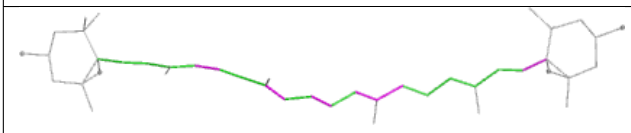
Ligand XAT y 622



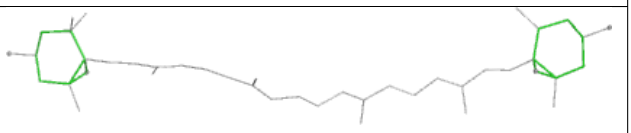
Bond lengths



Bond angles

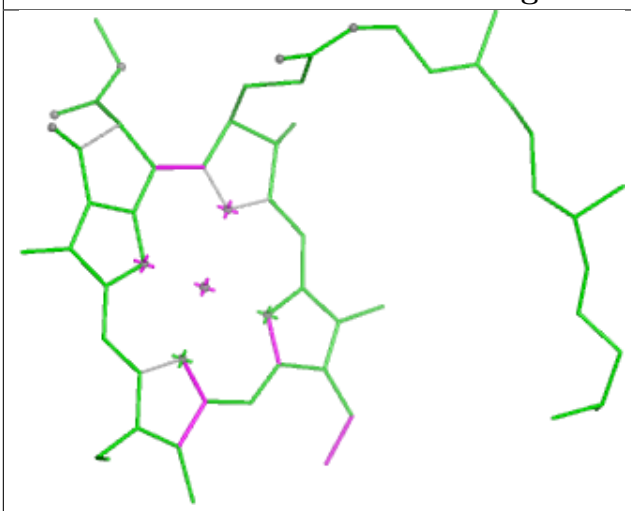


Torsions

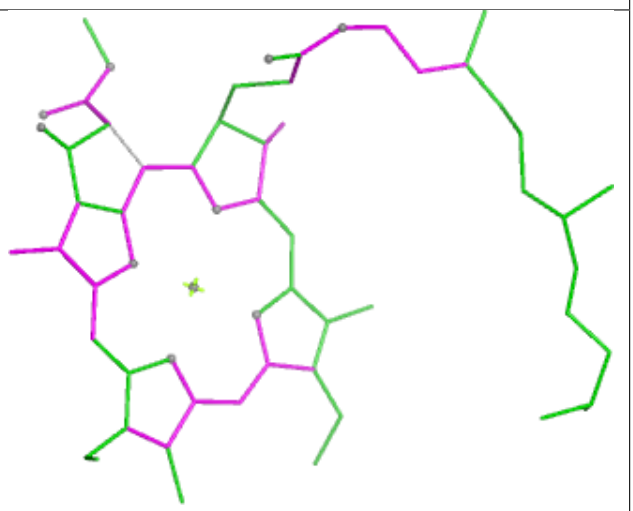


Rings

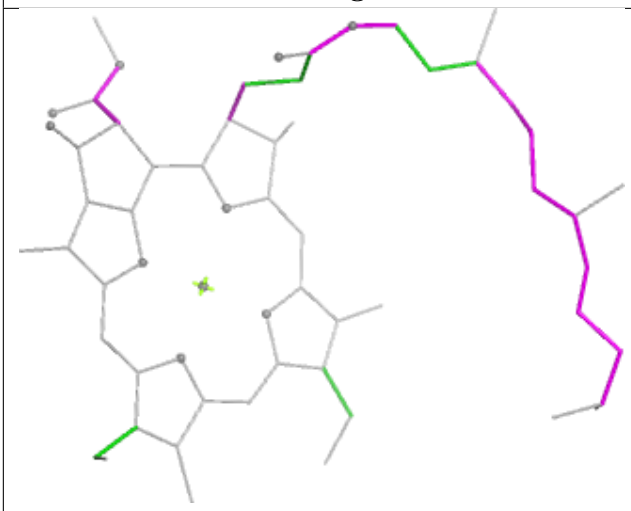
Ligand CLA r1 603



Bond lengths



Bond angles

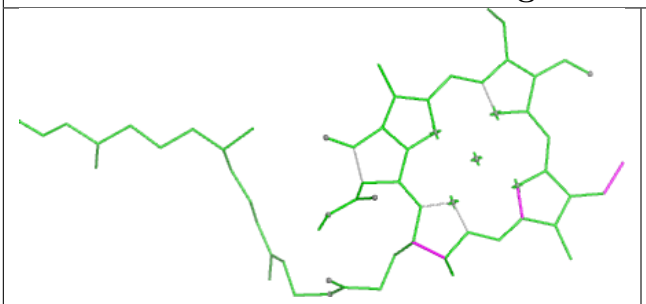


Torsions

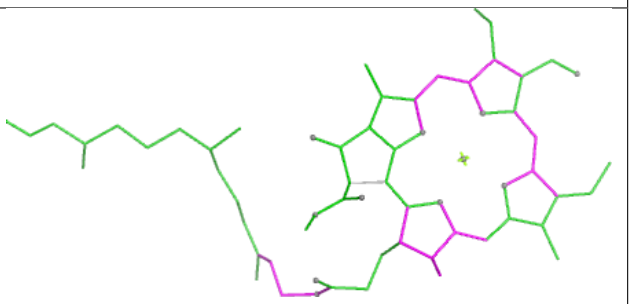


Rings

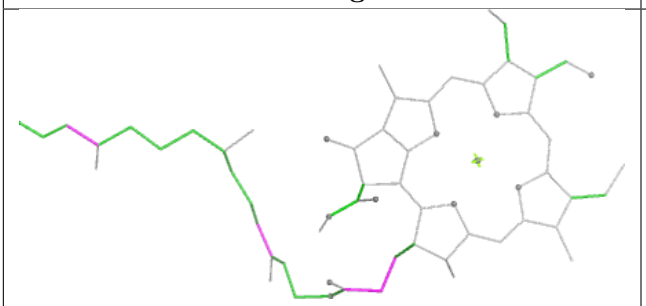
Ligand CHL n1 605



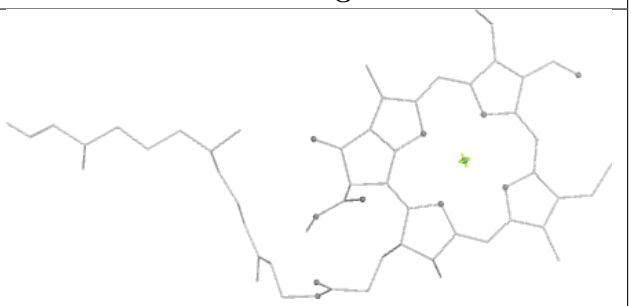
Bond lengths



Bond angles

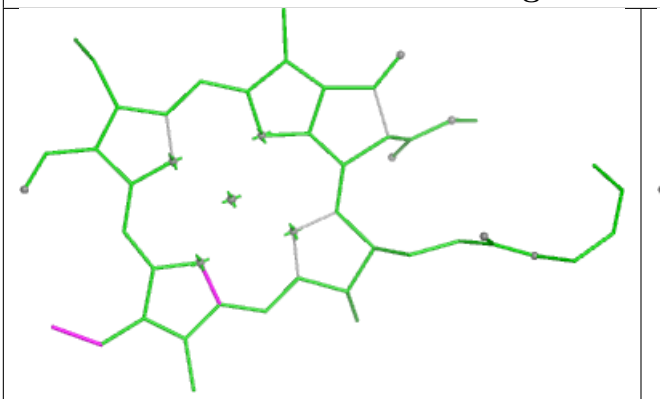


Torsions

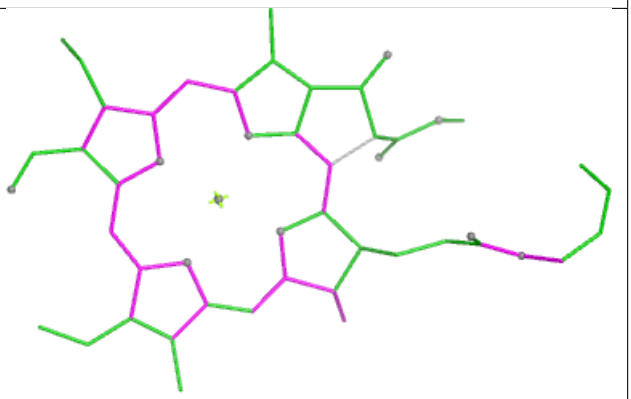


Rings

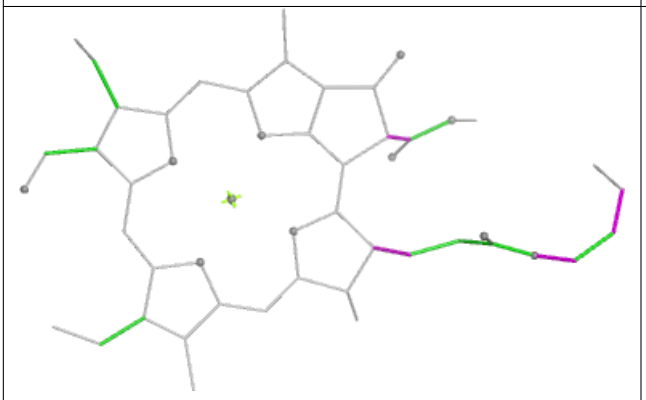
Ligand CHL G 606



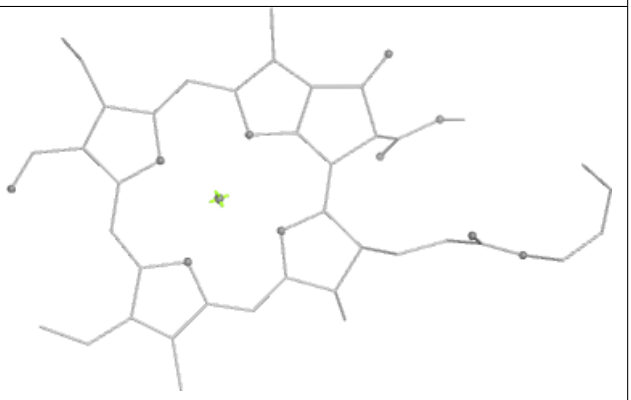
Bond lengths



Bond angles

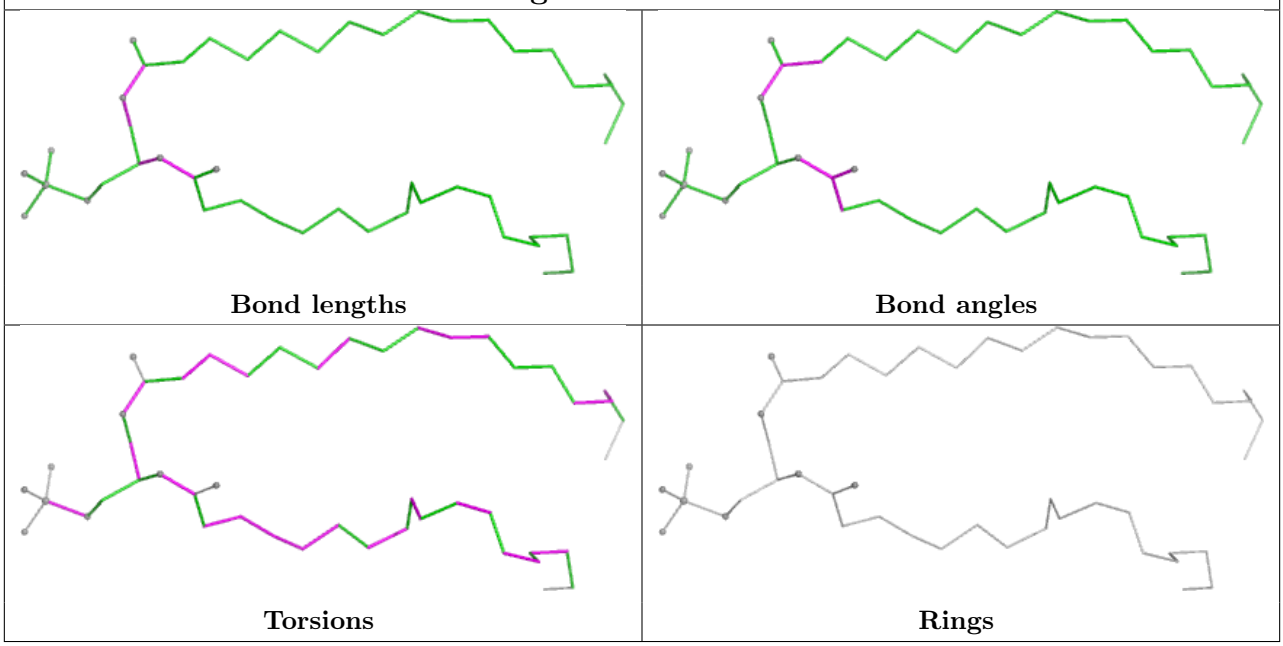


Torsions

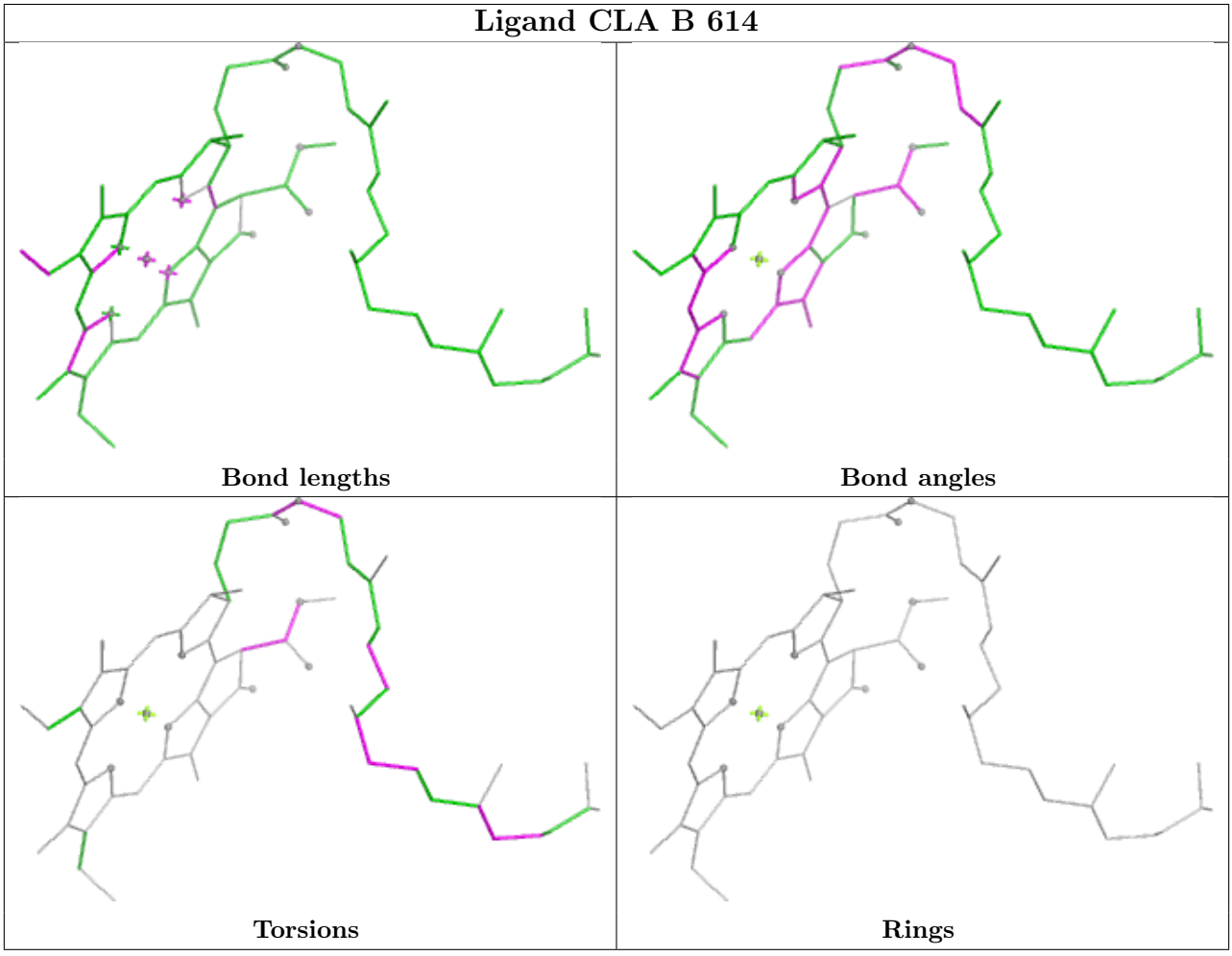


Rings

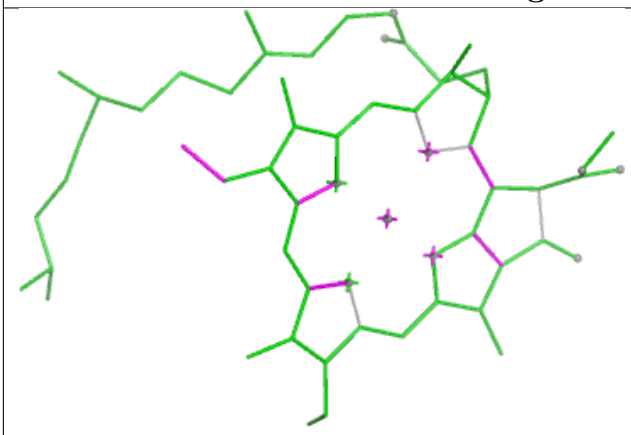
Ligand 3PH b 624



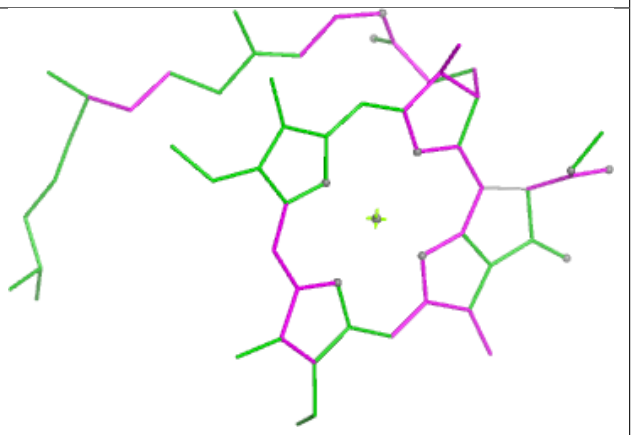
Ligand CLA B 614



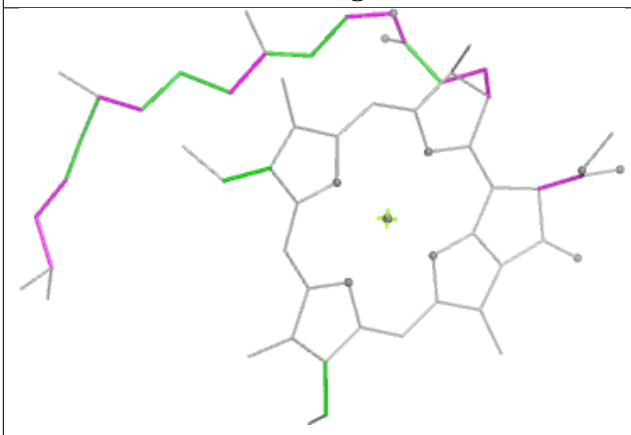
Ligand CLA S 602



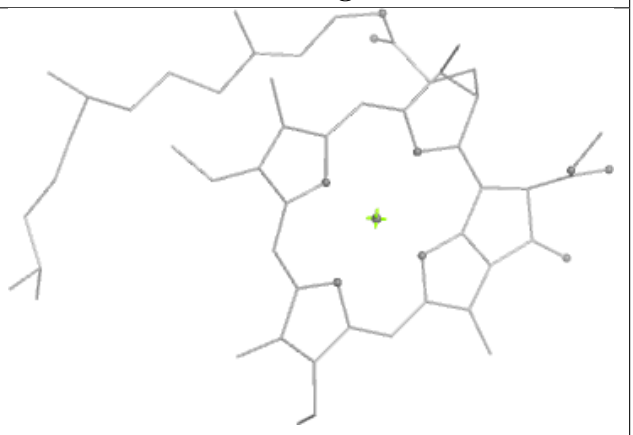
Bond lengths



Bond angles

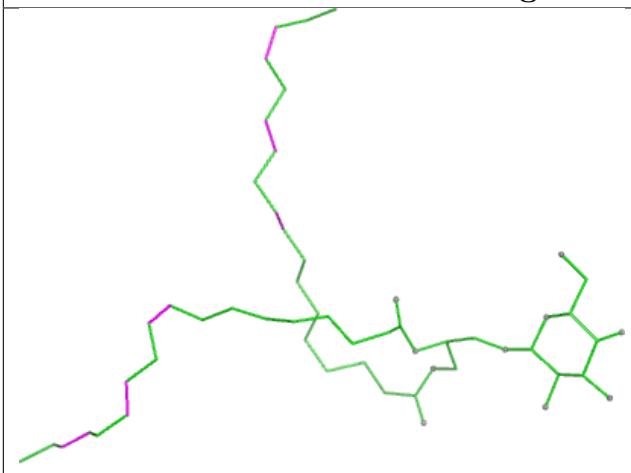


Torsions

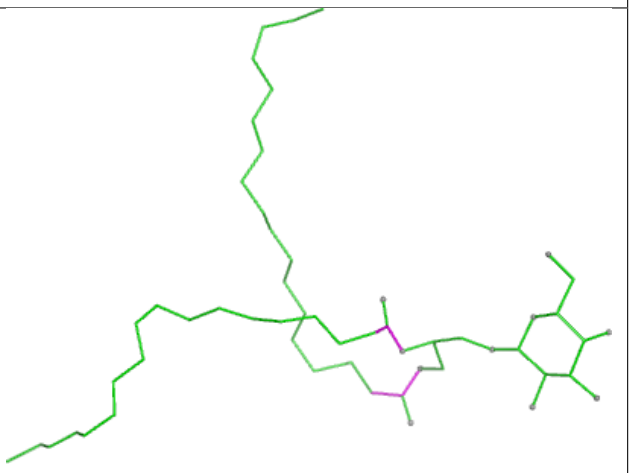


Rings

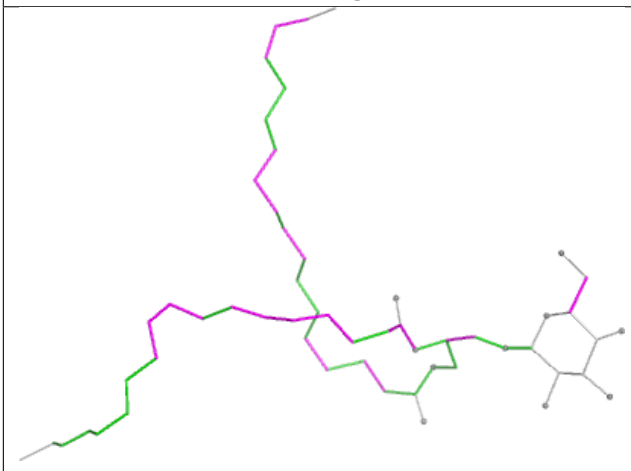
Ligand LMG C 523



Bond lengths



Bond angles

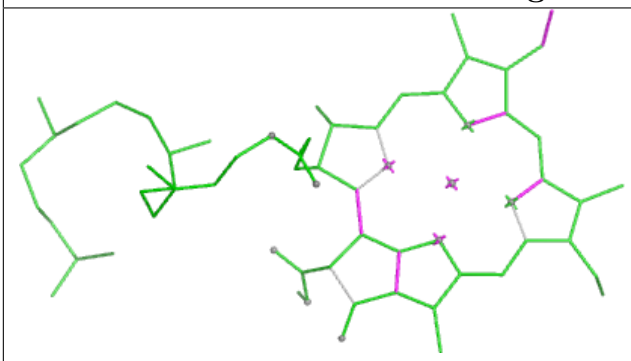


Torsions

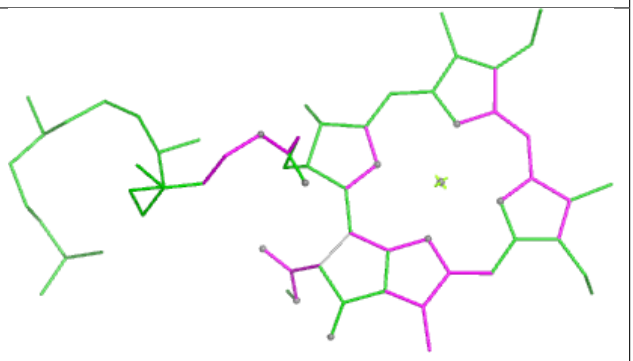


Rings

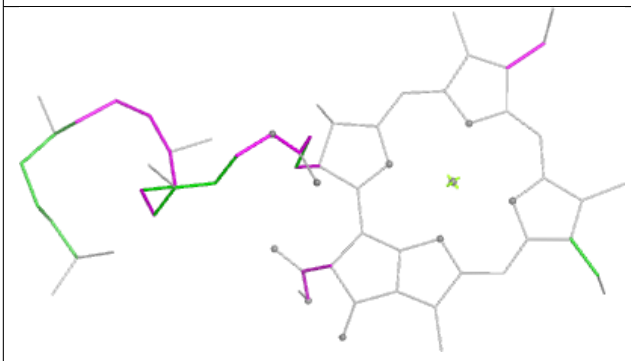
Ligand CLA b 613



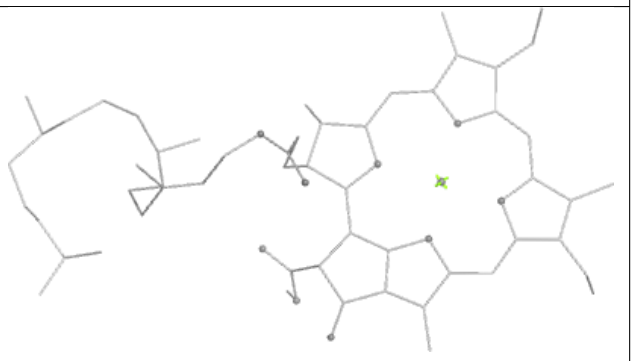
Bond lengths



Bond angles

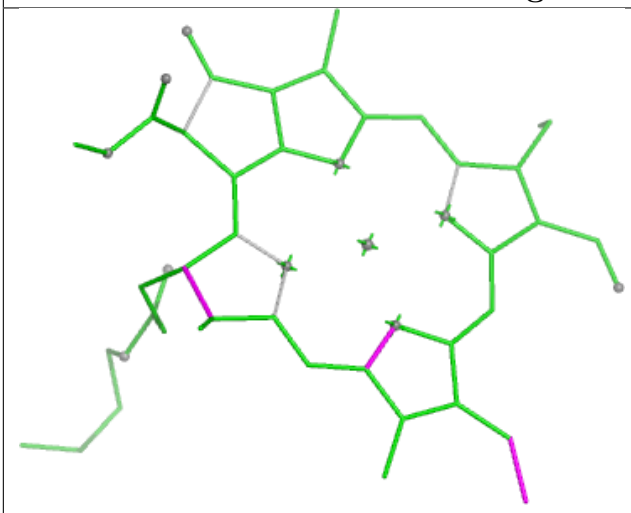


Torsions

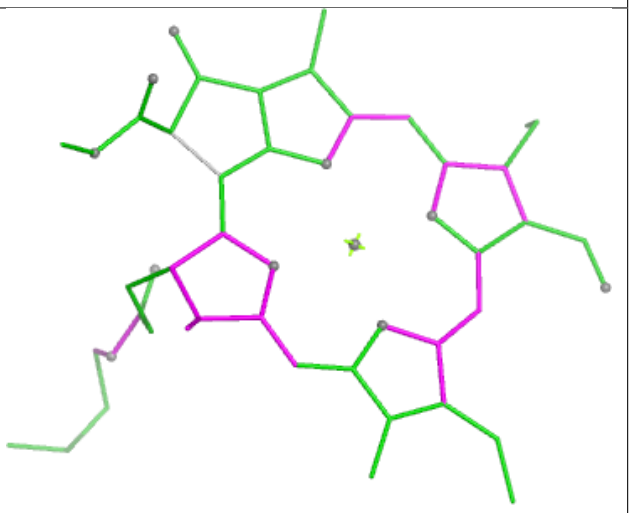


Rings

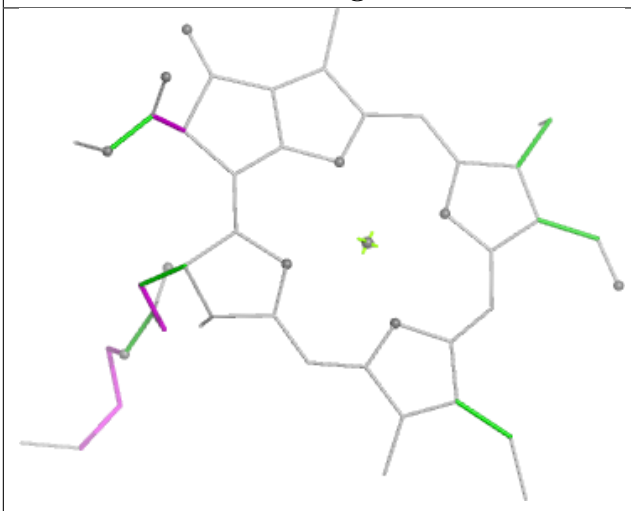
Ligand CHL n 608



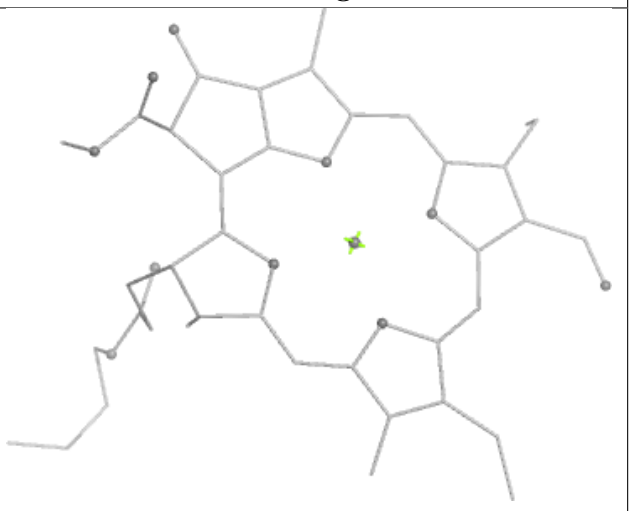
Bond lengths



Bond angles

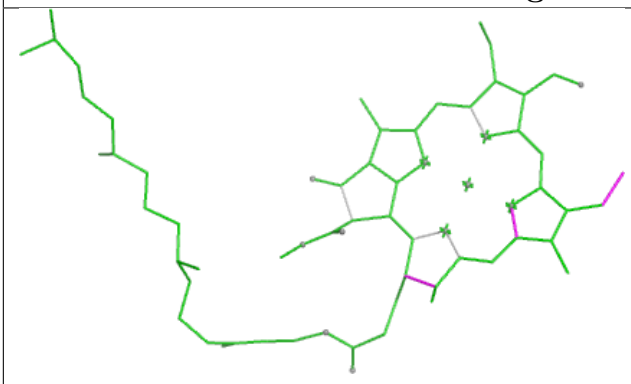


Torsions

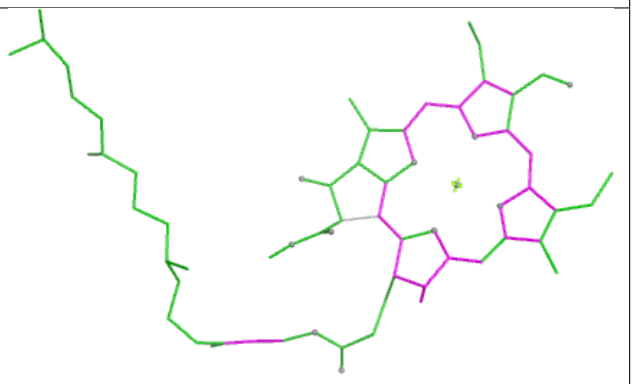


Rings

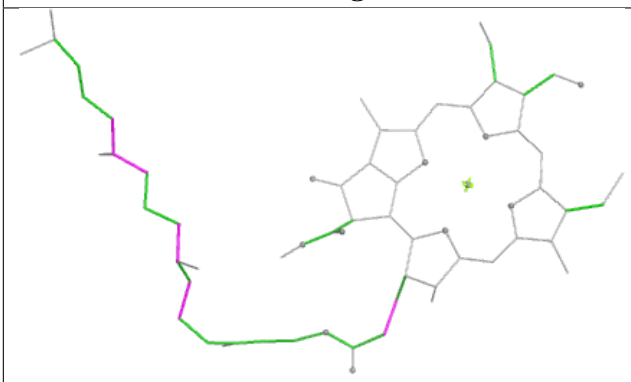
Ligand CHL n 606



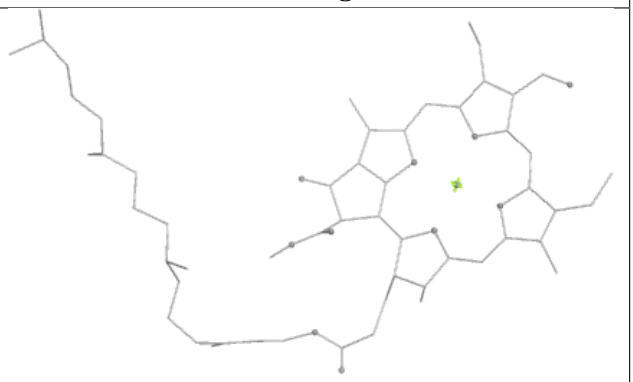
Bond lengths



Bond angles

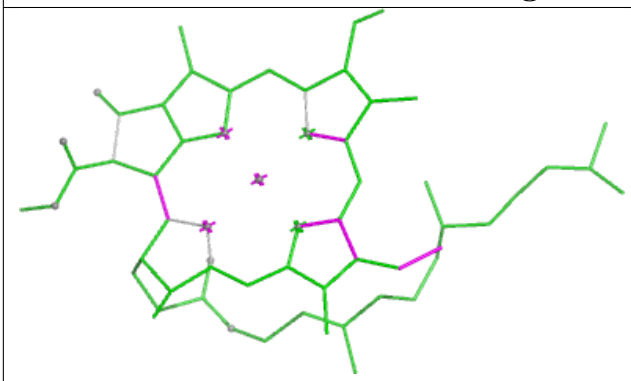


Torsions

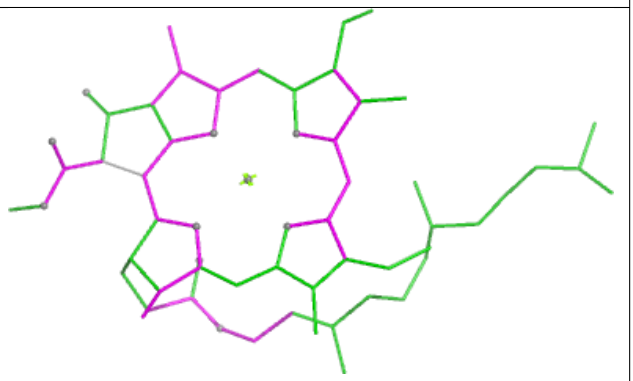


Rings

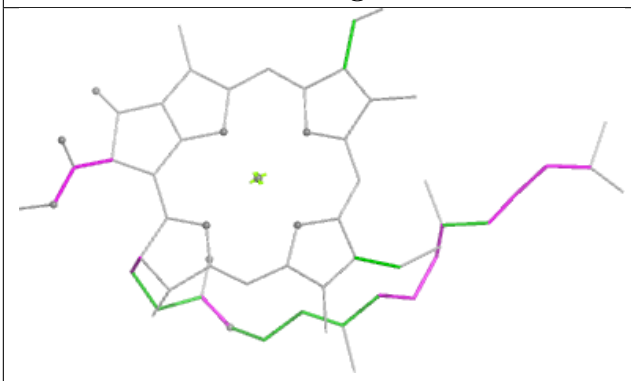
Ligand CLA r1 608



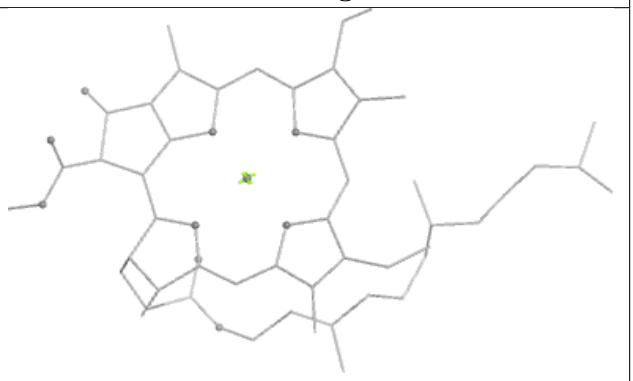
Bond lengths



Bond angles

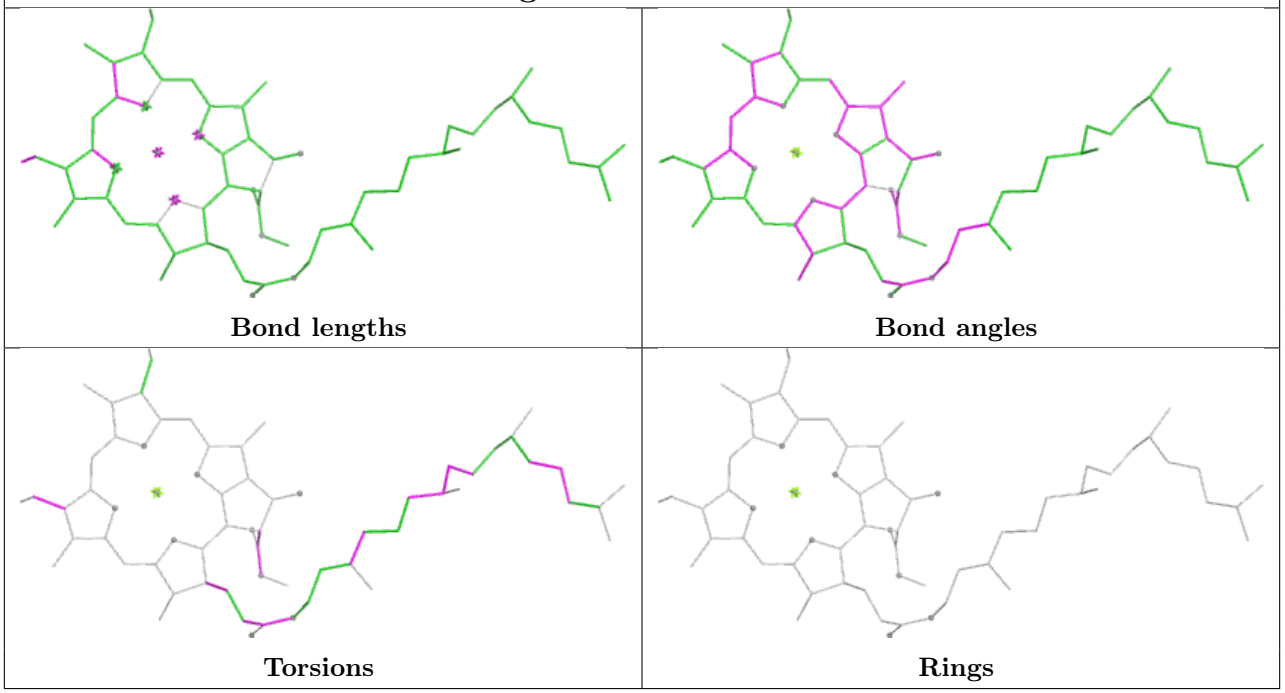


Torsions



Rings

Ligand CLA b1 603



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	r1	1
22	R1	1
22	R	1
20	n1	1
20	n	1
21	G1	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.15
1	r1	110:PRO	C	126:GLU	N	13.08
1	R1	110:PRO	C	126:GLU	N	12.94
1	R	110:PRO	C	126:GLU	N	12.16

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	n1	57:PRO	C	58:PRO	N	3.54

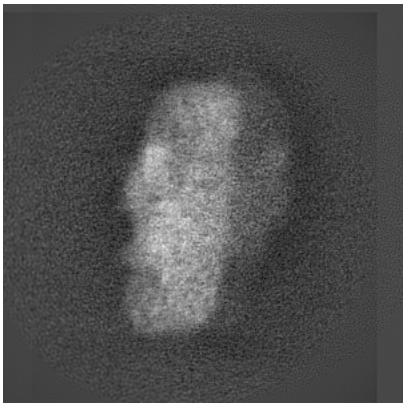
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13444. These allow visual inspection of the internal detail of the map and identification of artifacts.

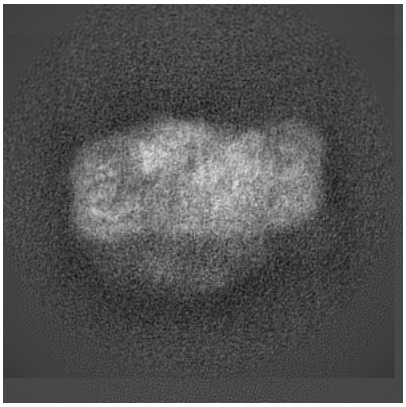
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

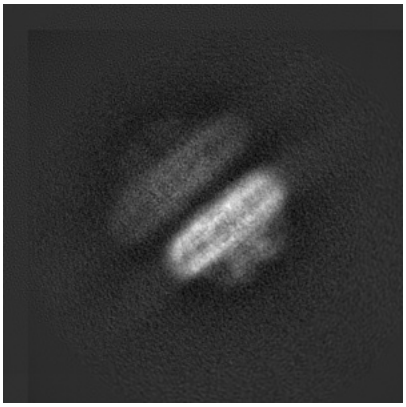
6.1.1 Primary map



X



Y

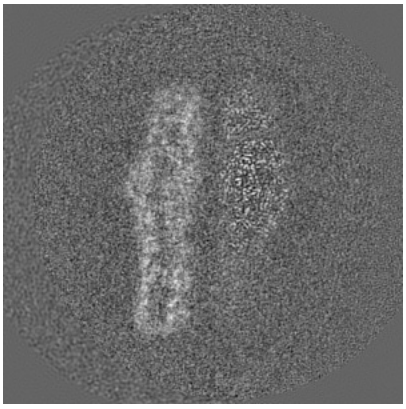


Z

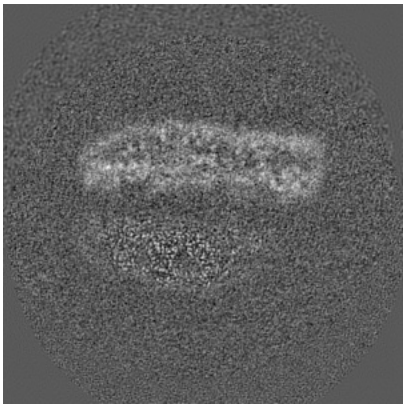
The images above show the map projected in three orthogonal directions.

6.2 Central slices

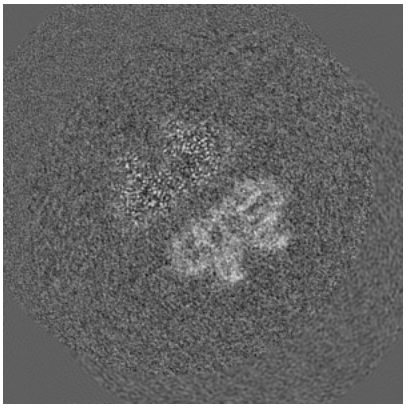
6.2.1 Primary map



X Index: 240



Y Index: 240

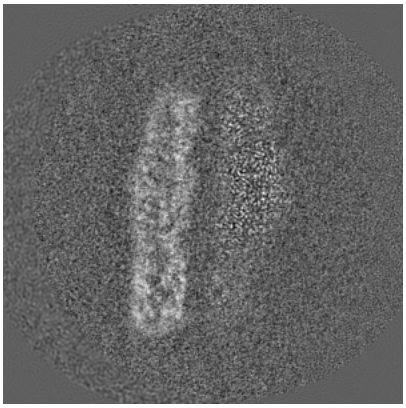


Z Index: 240

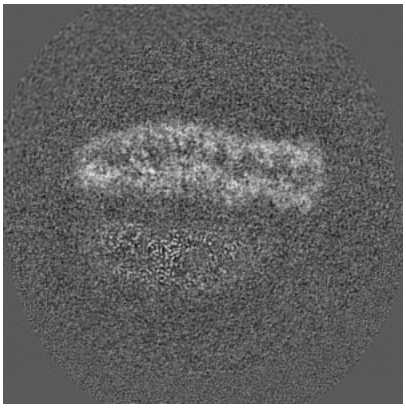
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

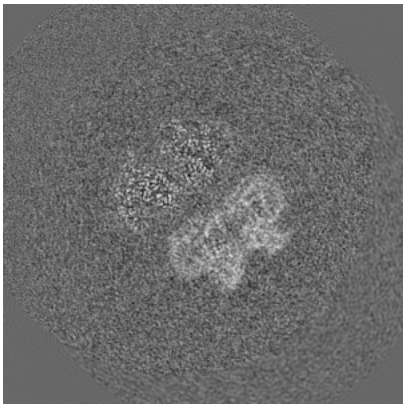
6.3.1 Primary map



X Index: 232



Y Index: 233

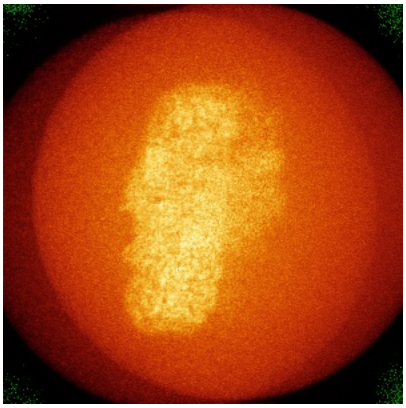


Z Index: 236

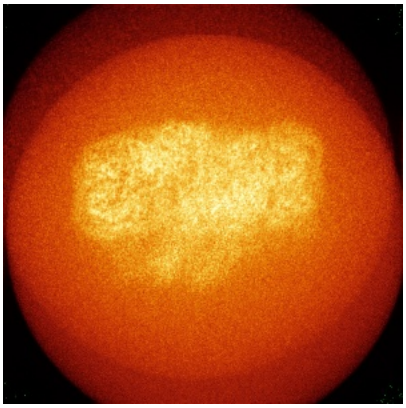
The images above show the largest variance slices of the map in three orthogonal directions.

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

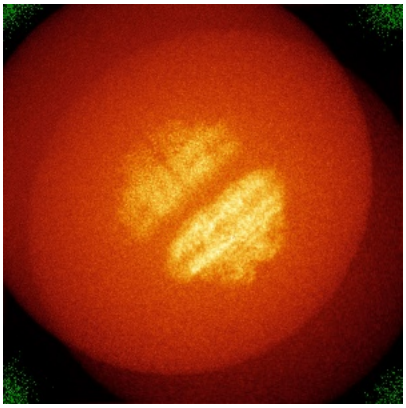
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

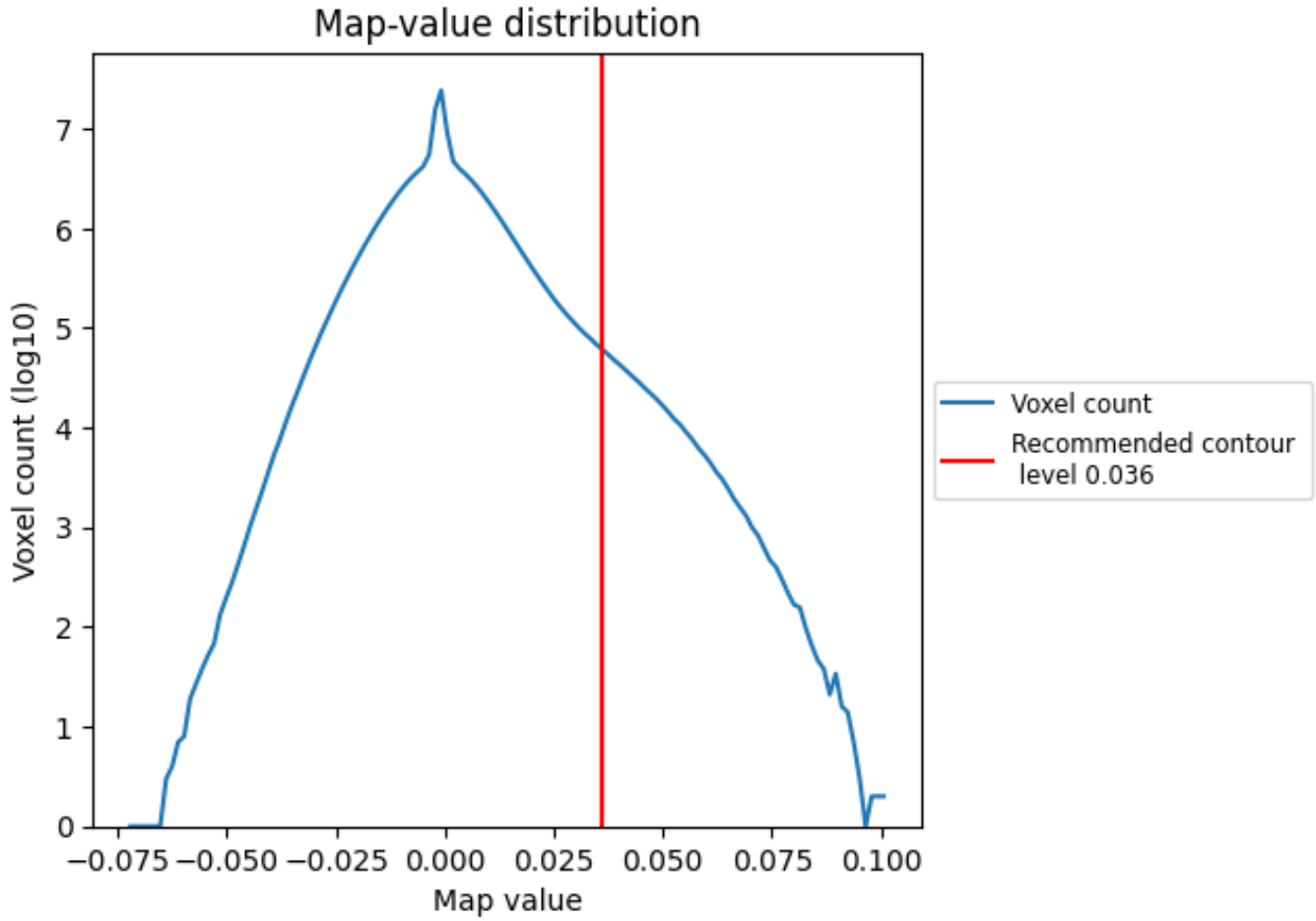
6.6 Mask visualisation (i)

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

7 Map analysis

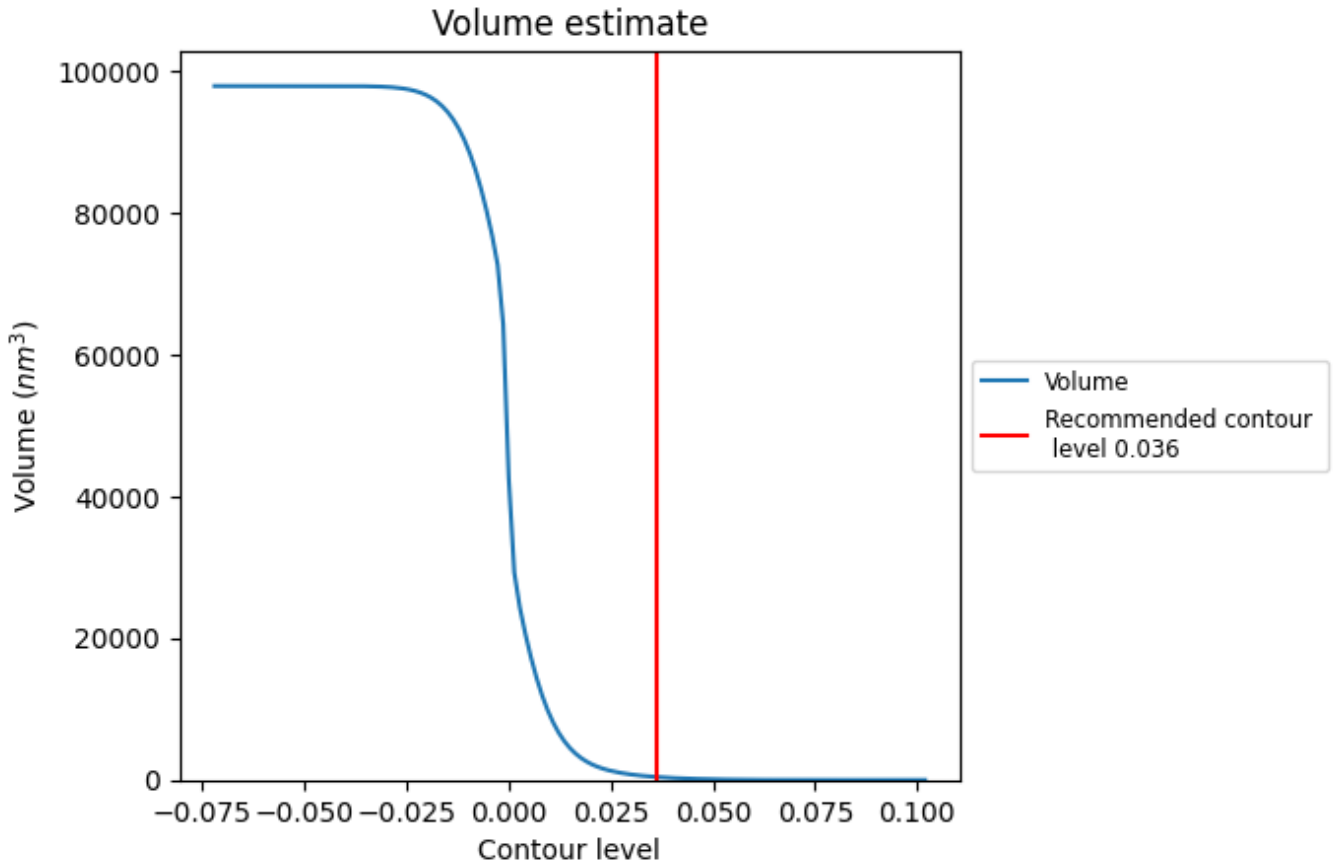
This section contains the results of statistical analysis of the map.

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.

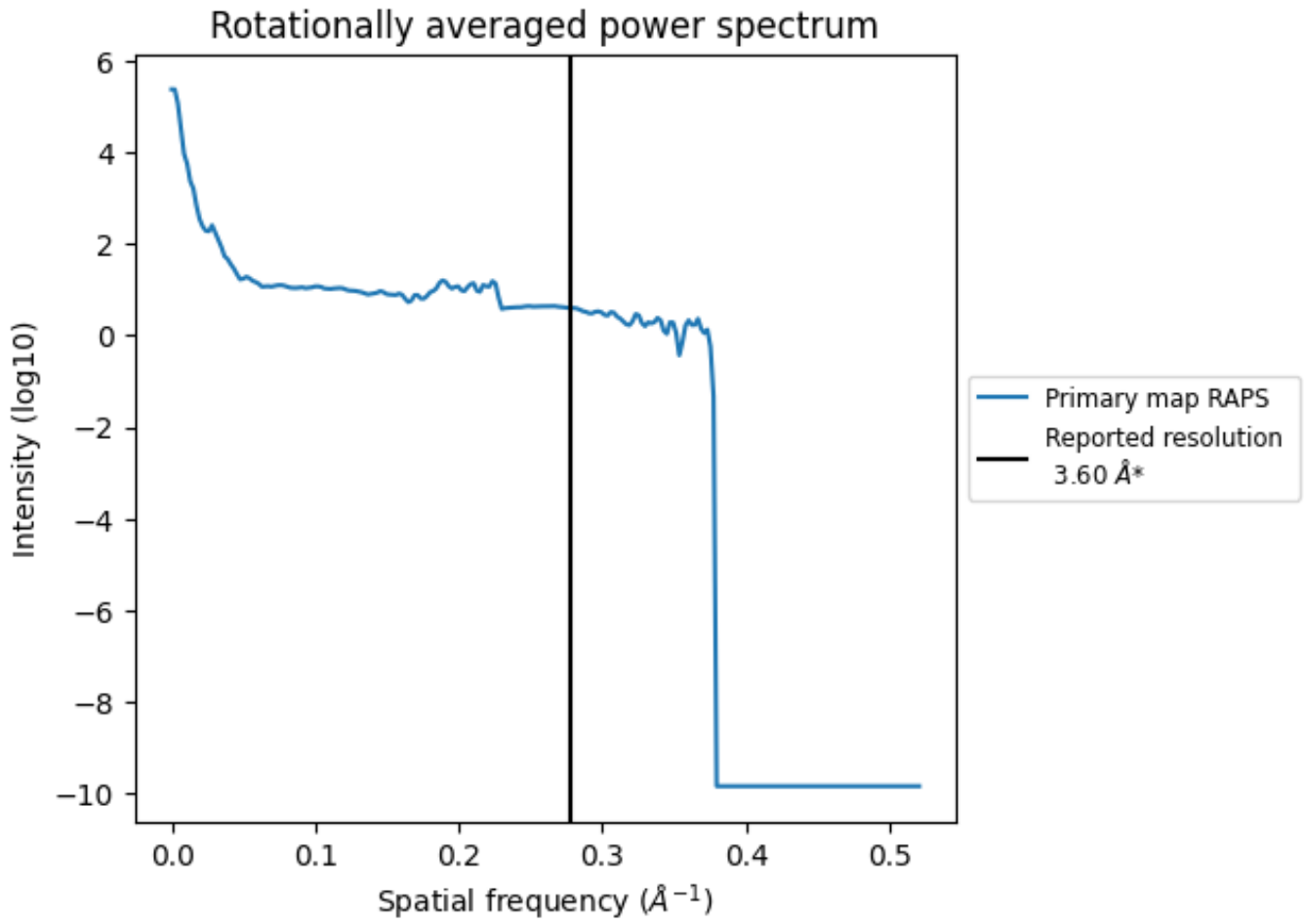
7.2 Volume estimate (i)



The volume at the recommended contour level is 429 nm^3; this corresponds to an approximate mass of 387 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)

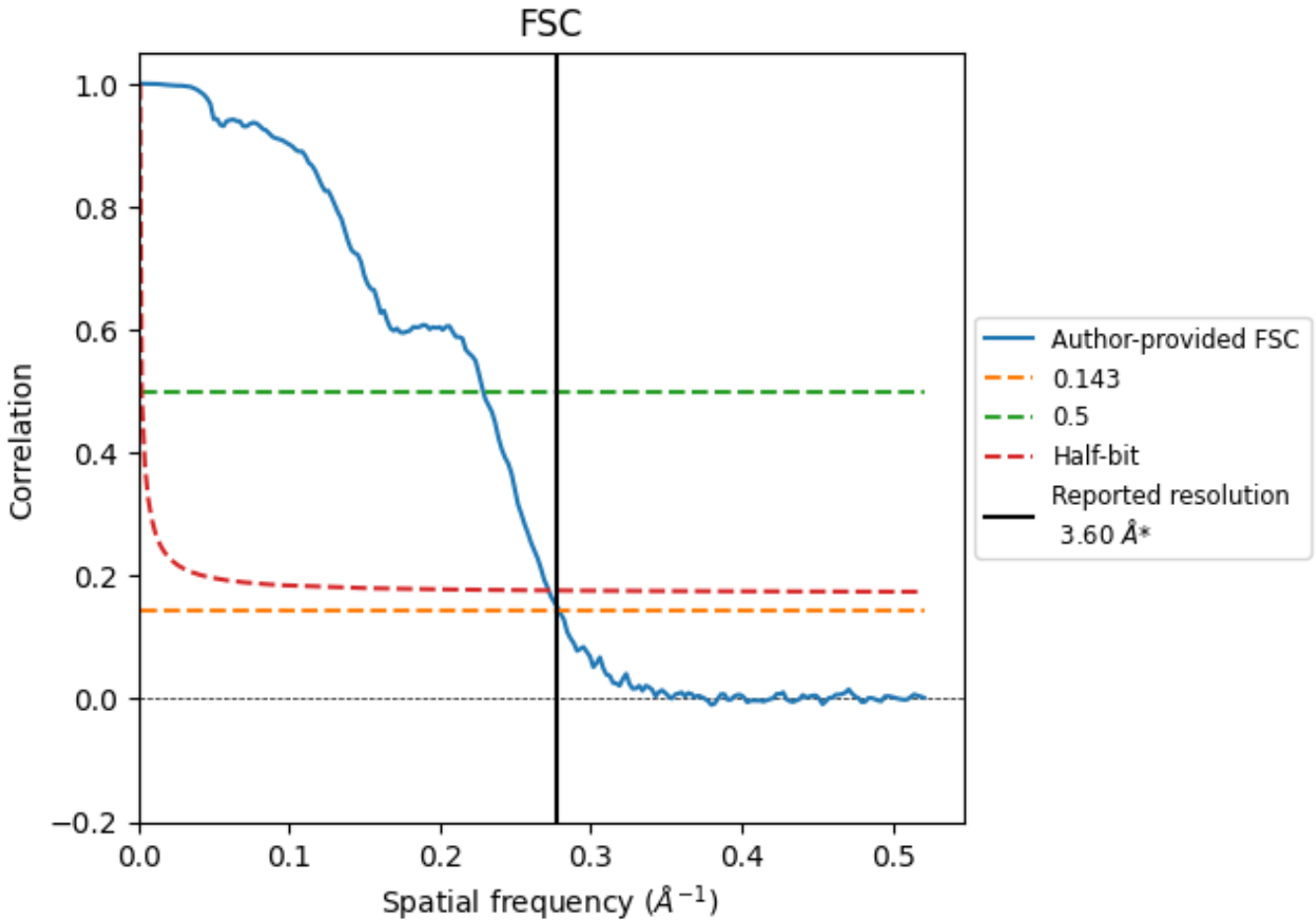


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

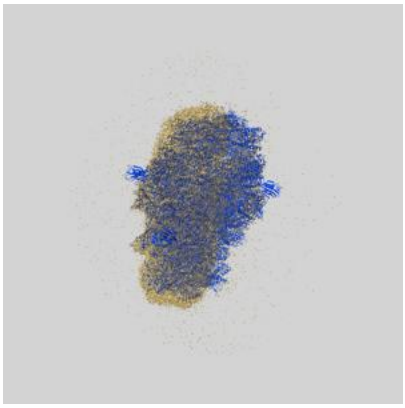
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.37	3.68
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

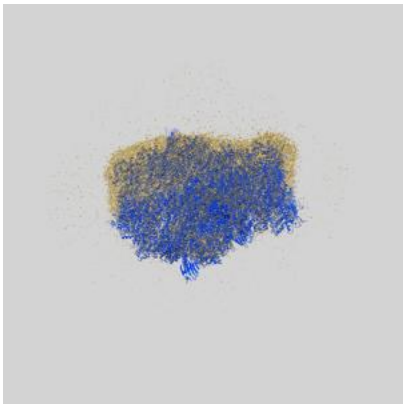
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13444 and PDB model 7PIN. Per-residue inclusion information can be found in section 3 on page 64.

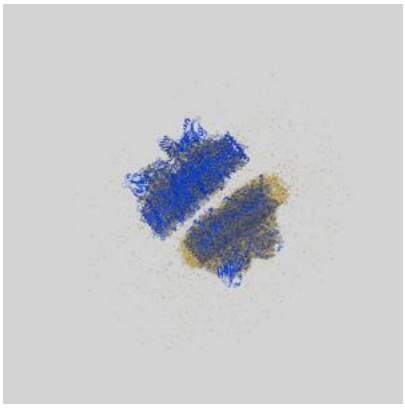
9.1 Map-model overlay



X



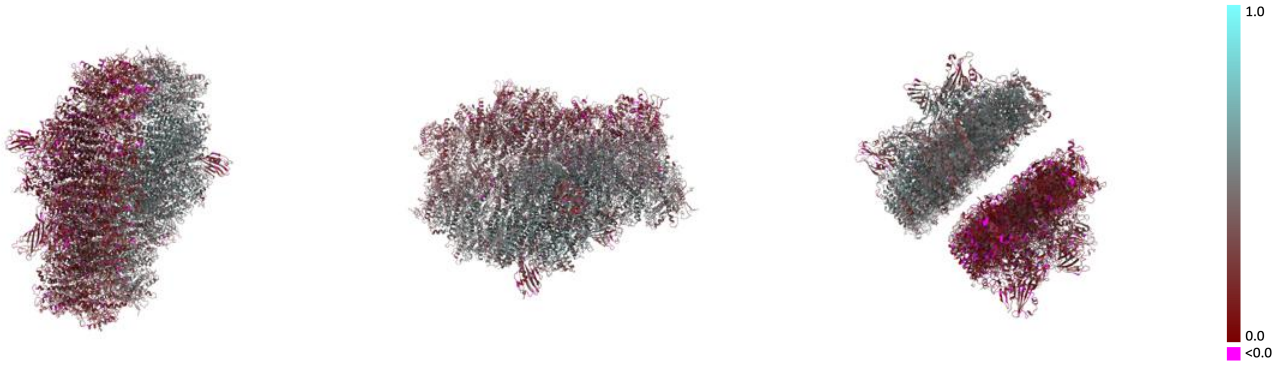
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036 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.

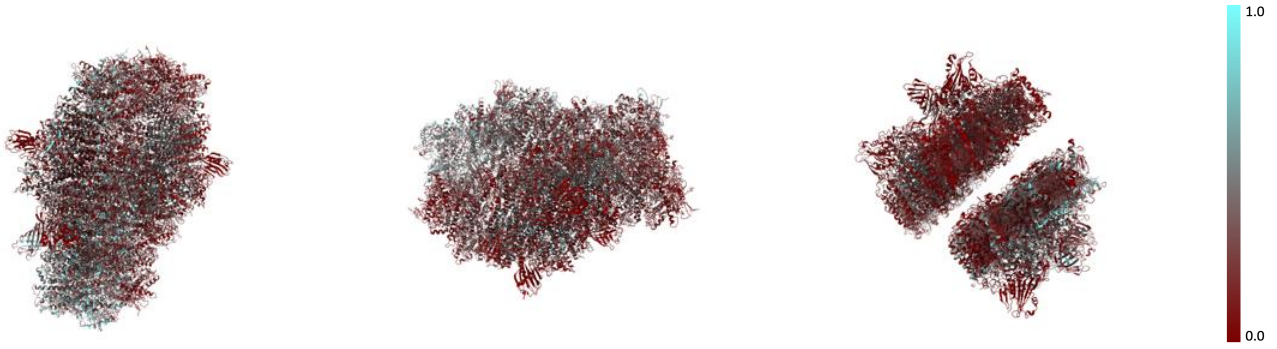
9.2 Q-score mapped to coordinate model



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.

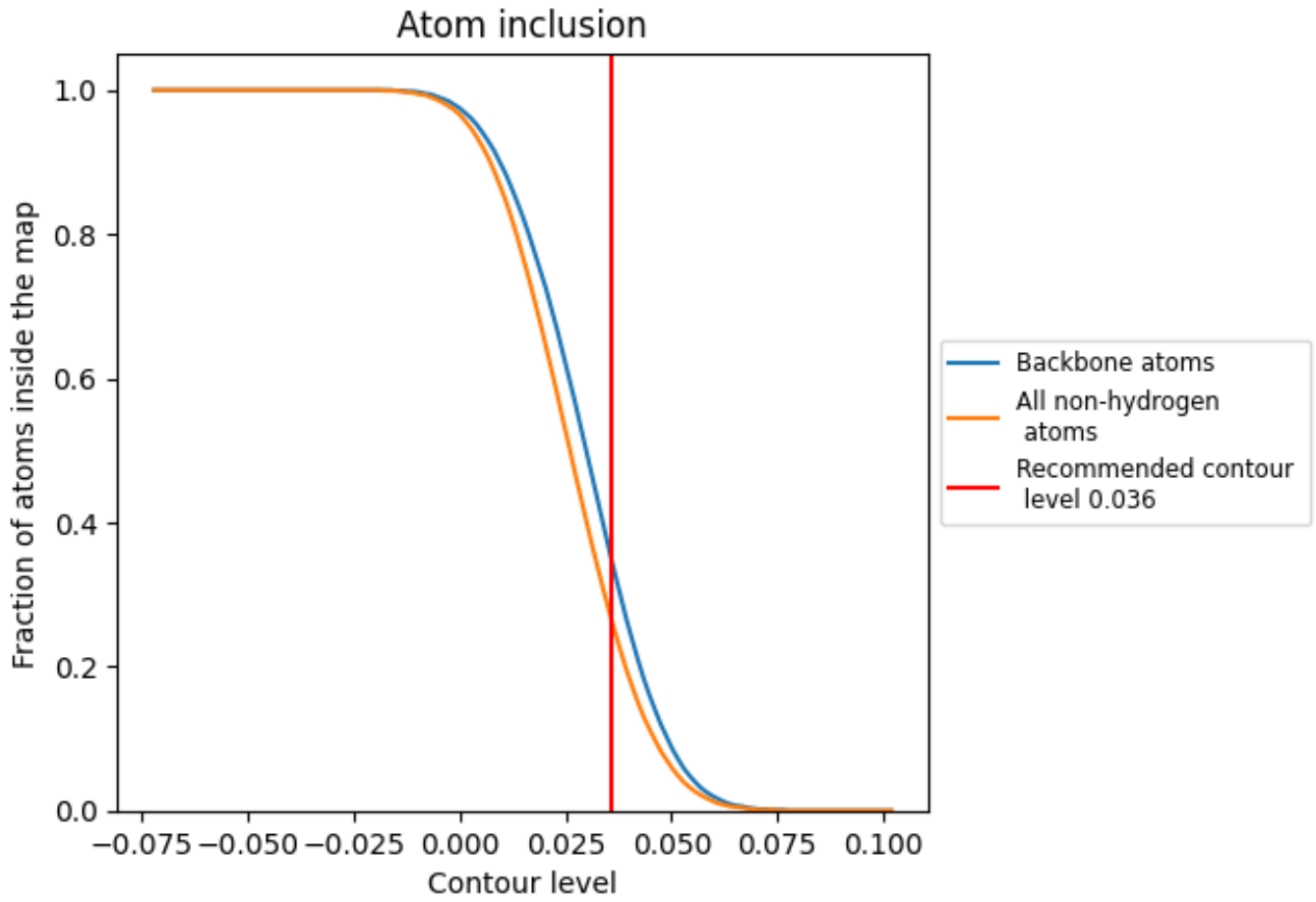
9.3 Atom inclusion mapped to coordinate model



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 (0.036).

9.4 Atom inclusion (i)



At the recommended contour level, 34% of all backbone atoms, 26% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2620	0.3280
A	0.3530	0.5260
A1	0.3490	0.2350
B	0.2800	0.5100
B1	0.2940	0.2060
C	0.3490	0.5370
C1	0.4040	0.2440
D	0.3190	0.5320
D1	0.3360	0.2300
E	0.1680	0.4510
E1	0.3960	0.2140
F	0.2270	0.4540
F1	0.3850	0.1930
G	0.1010	0.4070
G1	0.4160	0.1980
H	0.2160	0.4790
H1	0.2710	0.1950
I	0.2710	0.4970
I1	0.2800	0.2390
J	0.1660	0.4880
J1	0.2520	0.1960
K	0.2340	0.4820
K1	0.3910	0.2320
L	0.2820	0.5100
L1	0.2230	0.2170
M	0.1850	0.4500
M1	0.1740	0.2160
N	0.1410	0.4480
N1	0.4420	0.2080
O	0.1150	0.4130
O1	0.3020	0.2040
P	0.0010	0.2320
P1	0.0250	0.1680
R	0.0980	0.3800
R1	0.2380	0.1720



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S	0.1780	0.4500
S1	0.4390	0.2170
T	0.1700	0.4490
T1	0.1940	0.2630
U	0.0830	0.3800
U1	0.2200	0.2430
V	0.1470	0.4630
V1	0.2800	0.2330
W	0.1420	0.4380
W1	0.2650	0.2450
X	0.1290	0.3870
X1	0.3880	0.2580
Y	0.2290	0.4840
Y1	0.4010	0.2140
Z	0.1710	0.4810
Z1	0.3890	0.2370
a	0.3670	0.5310
a1	0.2620	0.1770
b	0.2920	0.5100
b1	0.2540	0.1730
c	0.3480	0.5280
c1	0.2840	0.1760
d	0.3360	0.5210
d1	0.2310	0.1470
e	0.1580	0.4380
e1	0.2260	0.1560
f	0.1640	0.4470
f1	0.2730	0.1240
g	0.0990	0.3840
g1	0.3060	0.1490
h	0.2150	0.4800
h1	0.1890	0.1490
i	0.2940	0.4960
i1	0.2430	0.2320
j	0.2100	0.4710
j1	0.2070	0.1650
k	0.2460	0.4880
k1	0.2370	0.1790
l	0.2790	0.5200
m	0.1820	0.4480
m1	0.2000	0.2000
n	0.1580	0.4320

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n1	0.3230	0.1490
o	0.1070	0.4000
o1	0.2650	0.2040
p	0.0010	0.2150
p1	0.0250	0.1470
r	0.0910	0.3850
r1	0.2370	0.1650
s	0.1790	0.4480
s1	0.2430	0.1250
t	0.2150	0.4900
t1	0.1700	0.2200
u	0.0370	0.3030
u1	0.1280	0.1660
v	0.1690	0.4370
v1	0.1470	0.1550
w	0.1640	0.4320
w1	0.2460	0.2170
x	0.0850	0.3690
x1	0.2090	0.1910
y	0.2250	0.4760
y1	0.2950	0.1590
z	0.1690	0.4790
z1	0.1960	0.1480