wwPDB EM Validation Summary Report (i)

Sep 10, 2026 – 07:44 AM JST

PDB ID	:	8WQL / pdb_00008wql
EMDB ID	:	EMD-37749
Title	:	In situ PBS-PSII supercomplex from cyanobacterial Spirulina platensis
Authors	:	You, X.; Zhang, X.; Xiao, Y.N.; Sun, S.; Sui, S.F.
Deposited on	:	2023-10-11
Resolution	:	3.50 Å(reported)

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:

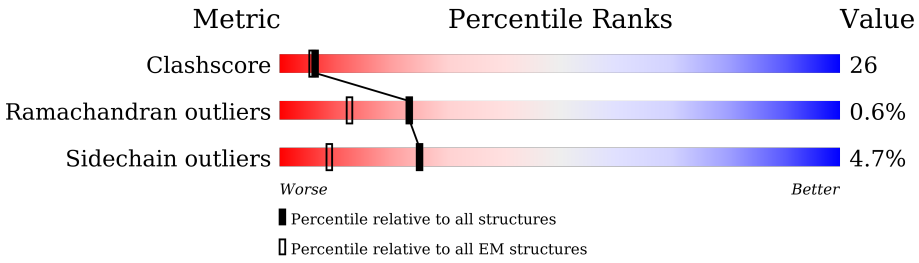
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

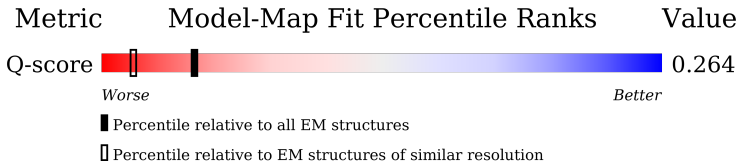
1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	B2	254	77% 65% 19% 8% • 6%
1	B3	254	79% 66% 19% 6% • 6%
1	B5	254	74% 68% 14% 8% • 6%
1	B6	254	83% 66% 20% 7% • 6%

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Mol	Chain	Length	Quality of chain
1	B7	254	79% 64% 19% 9% 6%
1	B8	254	70% 69% 14% 8% 6%
1	B9	254	78% 65% 21% 6% 6%
1	BA	254	77% 66% 19% 7% 6%
1	BC	254	79% 65% 17% 8% 6%
1	BH	254	72% 68% 15% 7% 6%
1	BI	254	80% 63% 19% 9% 6%
1	BJ	254	74% 68% 15% 8% 6%
2	B4	914	70% 25%
2	BB	914	70% 24%
2	C4	914	70% 23% 5%
2	CB	914	71% 23% 5%
3	4G	161	84% 15%
3	4L	161	84% 16%
3	6G	161	83% 14%
3	6L	161	83% 14%
3	9F	161	92% 7%
3	9K	161	91% 9%
3	AG	161	75% 24%
3	AL	161	77% 22%
3	GG	161	92% 7%
3	GL	161	92% 7%
3	IG	161	39% 55% 5%
3	IL	161	39% 53% 7%
3	JF	161	80% 19%

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Mol	Chain	Length	Quality of chain
3	JK	161	76% 22%
3	KG	161	83% 16%
3	KL	161	83% 17%
3	LF	161	92% 7%
3	LK	161	89% 11%
3	NG	161	86% 14%
3	NL	161	84% 15%
3	O4	161	10% 80% 20%
3	OB	161	9% 81% 18%
3	PG	161	85% 14%
3	PL	161	86% 13%
3	Q4	161	73% 27%
3	QB	161	71% 29%
3	RG	161	92% 7%
3	RL	161	91% 8%
3	S4	161	82% 17%
3	SB	161	81% 18%
3	TG	161	81% 18%
3	TL	161	81% 18%
3	V4	161	8% 76% 24%
3	VB	161	9% 82% 17%
3	X4	161	80% 19%
3	XB	161	78% 21%
3	XF	161	84% 14%
3	XK	161	83% 15%

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Mol	Chain	Length	Quality of chain
3	Z4	161	86% 14%
3	ZB	161	83% 16%
3	ZF	161	80% 19%
3	ZK	161	81% 19%
3	bF	161	86% 13%
3	bK	161	88% 12%
3	dF	161	78% 22%
3	dK	161	78% 22%
3	fF	161	83% 16%
3	fK	161	81% 18%
3	iF	161	90% 9%
3	iK	161	91% 9%
3	kF	161	83% 16%
3	kK	161	84% 15%
3	o4	161	76% 22%
3	oB	161	78% 20%
3	q4	161	78% 20%
3	qB	161	76% 22%
3	s4	161	86% 14%
3	sB	161	86% 14%
3	u4	161	6% 78% 21%
3	uB	161	79% 20%
3	w4	161	84% 15%
3	wB	161	83% 15%
3	y4	161	86% 14%

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Mol	Chain	Length	Quality of chain
3	yB	161	86% 13%
4	1G	161	87% 13%
4	1L	161	83% 16%
4	5G	161	83% 17%
4	5L	161	84% 16%
4	7G	161	81% 18%
4	7L	161	79% 20%
4	HG	161	89% 11%
4	HL	161	89% 11%
4	IF	161	81% 18%
4	IK	161	78% 20%
4	JG	161	76% 24%
4	JL	161	77% 23%
4	KF	161	82% 17%
4	KK	161	84% 15%
4	LG	161	87% 11%
4	LL	161	88% 11%
4	MF	161	87% 12%
4	MG	161	84% 16%
4	MK	161	86% 13%
4	ML	161	85% 15%
4	OG	161	81% 19%
4	OL	161	81% 19%
4	P4	161	81% 19%
4	PB	161	6% 81% 19%

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Mol	Chain	Length	Quality of chain
4	R4	161	79% 21%
4	RB	161	80% 20%
4	SG	161	80% 20%
4	SL	161	79% 21%
4	T4	161	75% 25%
4	TB	161	80% 20%
4	UG	161	88% 12%
4	UL	161	86% 14%
4	W4	161	83% 17%
4	WB	161	82% 17%
4	WG	161	88% 12%
4	WL	161	88% 12%
4	Y4	161	83% 17%
4	YB	161	82% 18%
4	YF	161	73% 25%
4	YK	161	73% 24%
4	a4	161	64% 27% 7%
4	aB	161	63% 29% 6%
4	aF	161	84% 16%
4	aK	161	87% 13%
4	cF	161	86% 14%
4	cK	161	85% 15%
4	eF	161	88% 12%
4	eK	161	90% 10%
4	hF	161	77% 22%

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Mol	Chain	Length	Quality of chain
4	hK	161	80% 19%
4	jF	161	88% 12%
4	jK	161	86% 14%
4	lF	161	83% 17%
4	lK	161	81% 19%
4	nF	161	84% 16%
4	nK	161	84% 16%
4	p4	161	86% 14%
4	pB	161	86% 14%
4	r4	161	84% 16%
4	rB	161	86% 14%
4	t4	161	87% 13%
4	tB	161	84% 14%
4	v4	161	82% 18%
4	vB	161	81% 19%
4	x4	161	83% 17%
4	xB	161	81% 19%
4	z4	161	85% 15%
4	zB	161	83% 17%
5	2G	67	79% 18%
5	2L	67	79% 18%
5	3F	67	91%
5	3K	67	88% 7%
5	8G	67	70% 25%
5	8L	67	70% 25%

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Mol	Chain	Length	Quality of chain
5	NF	67	82% 15%
5	NK	67	84% 13%
5	U4	67	64% 33%
5	UB	67	66% 31%
5	b4	67	6% 73% 24%
5	bB	67	73% 24%
6	A1	359	69% 23% 7%
6	AD	359	68% 25% 7%
6	AE	359	67% 25% 7%
6	a1	359	72% 20% 7%
6	aD	359	72% 20% 7%
6	aE	359	71% 21% 7%
7	B1	509	5% 65% 27% 6%
7	BD	509	64% 28% 6%
7	BE	509	5% 64% 28% 6%
7	b1	509	67% 25% 6%
7	bD	509	68% 24% 6%
7	bE	509	68% 24% 6%
8	C1	469	69% 22%
8	CD	469	70% 22%
8	CE	469	72% 21%
8	c1	469	68% 25%
8	cD	469	66% 26%
8	cE	469	5% 67% 26%
9	D1	352	61% 28% 6%

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Mol	Chain	Length	Quality of chain
9	DD	352	61% 28% 6%
9	DE	352	61% 28% 6%
9	d1	352	59% 29% 7%
9	dD	352	58% 31% 7%
9	dE	352	58% 31% 7%
10	E1	82	68% 22% 5% 5%
10	ED	82	67% 22% 6% 5%
10	EE	82	68% 21% 6% 5%
10	e1	82	68% 23% 5%
10	eD	82	5% 70% 22% 5%
10	eE	82	6% 70% 22% 5%
11	F1	44	52% 25% 20%
11	FD	44	48% 27% 5% 20%
11	FE	44	52% 25% 20%
11	f1	44	32% 39% 9% 20%
11	fD	44	34% 34% 16% 16%
11	fE	44	5% 34% 34% 11% 20%
12	H1	67	28% 82% 12%
12	HD	67	18% 76% 18%
12	HE	67	22% 70% 22%
12	h1	67	67% 27%
12	hD	67	9% 67% 27%
12	hE	67	67% 27%
13	I1	38	37% 37% 11% 11% 5%
13	ID	38	39% 32% 13% 11% 5%

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Mol	Chain	Length	Quality of chain
13	IE	38	37% 34% 13% 11% 5%
13	i1	38	26% 32% 29% 8% 5%
13	iD	38	26% 32% 29% 8% 5%
13	iE	38	26% 32% 29% 8% 5%
14	J1	39	10% 74% 13% 8% 5%
14	JD	39	10% 74% 13% 8% 5%
14	JE	39	13% 74% 13% 8% 5%
14	j1	39	21% 82% 18%
14	jD	39	18% 77% 23%
14	jE	39	23% 82% 18%
15	K1	45	7% 53% 24% 20%
15	KD	45	7% 56% 22% 20%
15	KE	45	56% 22% 20%
15	k1	45	33% 29% 11% 22%
15	kD	45	33% 27% 13% 22%
15	kE	45	33% 27% 13% 22%
16	L1	39	64% 28%
16	LD	39	59% 33%
16	LE	39	5% 59% 33%
16	l1	39	69% 21% 5%
16	lD	39	69% 21% 5%
16	lE	39	72% 18% 5%
17	M1	37	14% 46% 43% 8%
17	MD	37	16% 46% 43% 8%
17	ME	37	16% 46% 43% 8%

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Mol	Chain	Length	Quality of chain
17	m1	37	14% 41% 32% 22%
17	mD	37	16% 41% 32% 22%
17	mE	37	14% 41% 32% 22%
18	O1	278	8% 50% 29% 6% 13%
18	OD	278	6% 51% 28% 6% 13%
18	OE	278	6% 53% 28% 6% 13%
18	o1	278	7% 52% 28% 6% 13%
18	oD	278	7% 51% 27% 7% 13%
18	oE	278	7% 50% 29% 6% 13%
19	Q1	164	10% 44% 23% 5% 27%
19	QD	164	12% 44% 23% 5% 27%
19	QE	164	10% 44% 24% 5% 27%
19	q1	164	15% 43% 24% 5% 27%
19	qD	164	12% 43% 24% 5% 27%
19	qE	164	14% 43% 24% 5% 27%
20	R1	39	18% 62% 28% 10%
20	RD	39	18% 59% 31% 10%
20	RE	39	15% 59% 31% 10%
20	r1	39	62% 28% 10%
20	rD	39	10% 62% 28% 10%
20	rE	39	10% 62% 28% 10%
21	S1	47	15% 70% 30%
21	SD	47	19% 70% 30%
21	SE	47	21% 70% 30%
22	T1	31	81% 13% 6%

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Mol	Chain	Length	Quality of chain
22	TD	31	81% 13% 6%
22	TE	31	87% 6% 6%
22	t1	31	6% 74% 23%
22	tD	31	6% 74% 23%
22	tE	31	6% 74% 23%
23	U1	95	71% 26%
23	UD	95	68% 28%
23	UE	95	69% 27%
23	u1	95	72% 25%
23	uD	95	74% 23%
23	uE	95	74% 23%
24	V1	163	57% 20% 6% 17%
24	VD	163	56% 23% 17%
24	VE	163	55% 25% 17%
24	v1	163	61% 20% 17%
24	vD	163	58% 22% 17%
24	vE	163	60% 21% 17%
25	X1	48	10% 50% 31% 17%
25	XD	48	50% 31% 17%
25	XE	48	15% 50% 31% 17%
25	x1	48	8% 50% 31% 17%
25	xD	48	48% 33% 17%
25	xE	48	50% 31% 17%
26	Y1	43	12% 47% 28% 26%
26	YD	43	9% 47% 23% 5% 26%

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Mol	Chain	Length	Quality of chain
26	YE	43	7% 42% 28% 5% 26%
26	y1	43	14% 37% 26% 9% 26%
26	yD	43	14% 37% 26% 9% 26%
26	yE	43	14% 37% 26% 9% 26%
27	Z1	63	10% 52% 33% 10% 5%
27	ZD	63	16% 52% 33% 10% 5%
27	ZE	63	10% 52% 33% 10% 5%
27	z1	63	14% 43% 43% 10% 5%
27	zD	63	17% 41% 44% 10% 5%
27	zE	63	16% 41% 44% 10% 5%
28	BG	150	5% 7% 13% 7% 69%
28	BL	150	6% 6% 14% 7% 69%
28	EF	150	7% 6% 14% 69%
28	EK	150	7% 6% 14% 69%
29	QG	169	73% 21%
29	QL	169	75% 20%
29	gF	169	71% 23% 5%
29	gK	169	71% 23% 5%
30	VG	161	78% 19%
30	VL	161	78% 20%
30	mF	161	76% 23%
30	mK	161	76% 23%
31	b2	162	67% 64% 32%
31	b3	162	98% 65% 31%
31	b5	162	64% 64% 32%

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Mol	Chain	Length	Quality of chain
31	b6	162	88% 65% 31%
31	b7	162	93% 64% 32%
31	b8	162	77% 64% 32%
31	b9	162	77% 65% 31%
31	bA	162	99% 65% 31%
31	bC	162	91% 64% 32%
31	bH	162	62% 64% 32%
31	bI	162	82% 64% 32%
31	bJ	162	73% 64% 33%
31	d2	162	100% 67% 30%
31	d3	162	99% 68% 29%
31	d5	162	84% 68% 29%
31	d6	162	99% 68% 29%
31	d7	162	99% 68% 29%
31	d8	162	65% 67% 30%
31	d9	162	99% 69% 28%
31	dA	162	99% 68% 29%
31	dC	162	99% 69% 28%
31	dH	162	81% 68% 29%
31	dI	162	100% 67% 30%
31	dJ	162	60% 68% 29%
31	f2	162	95% 64% 33%
31	f3	162	92% 64% 33%
31	f5	162	94% 65% 31%
31	f6	162	98% 63% 34%

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Mol	Chain	Length	Quality of chain
31	f7	162	100% 64% 33%
31	f8	162	88% 65% 32%
31	f9	162	95% 64% 33%
31	fA	162	96% 64% 33%
31	fC	162	96% 64% 33%
31	fH	162	85% 65% 31%
31	fI	162	91% 64% 33%
31	fJ	162	86% 65% 32%
31	h2	162	87% 65% 31%
31	h3	162	100% 67% 29%
31	h5	162	78% 66% 30%
31	h6	162	91% 65% 31%
31	h7	162	100% 67% 30%
31	h8	162	85% 67% 30%
31	h9	162	93% 67% 29%
31	hA	162	100% 65% 31%
31	hC	162	99% 65% 31%
31	hH	162	74% 65% 31%
31	hI	162	98% 66% 30%
31	hJ	162	73% 66% 30%
31	j2	162	86% 71% 26%
31	j3	162	96% 71% 26%
31	j5	162	88% 71% 26%
31	j6	162	93% 71% 26%
31	j7	162	96% 71% 26%

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Mol	Chain	Length	Quality of chain
31	j8	162	81% 71% 26%
31	j9	162	84% 71% 26%
31	jA	162	94% 70% 27%
31	jC	162	94% 71% 26%
31	jH	162	75% 71% 26%
31	jI	162	83% 71% 26%
31	jJ	162	85% 70% 27%
31	l2	162	99% 67% 30%
31	l3	162	93% 69% 28%
31	l5	162	93% 67% 30%
31	l6	162	100% 67% 30%
31	l7	162	99% 69% 28%
31	l8	162	86% 68% 29%
31	l9	162	100% 69% 28%
31	lA	162	96% 69% 28%
31	lC	162	98% 69% 28%
31	lH	162	90% 69% 28%
31	lI	162	99% 67% 30%
31	lJ	162	80% 68% 29%
32	c2	172	94% 59% 36%
32	c3	172	99% 60% 35%
32	c5	172	81% 60% 35%
32	c6	172	95% 60% 35%
32	c7	172	99% 61% 34%
32	c8	172	85% 60% 35%

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Mol	Chain	Length	Quality of chain
32	c9	172	94% 59% 36%
32	cA	172	92% 60% 35%
32	cC	172	99% 60% 35%
32	cH	172	77% 60% 35%
32	cI	172	95% 60% 35%
32	cJ	172	80% 60% 35%
32	e2	172	99% 68% 28%
32	e3	172	98% 68% 28%
32	e5	172	97% 69% 27%
32	e6	172	100% 68% 28%
32	e7	172	99% 68% 28%
32	e8	172	94% 69% 27%
32	e9	172	99% 68% 28%
32	eA	172	99% 68% 28%
32	eC	172	100% 68% 28%
32	eH	172	96% 69% 27%
32	eI	172	100% 68% 28%
32	eJ	172	95% 69% 27%
32	g2	172	90% 60% 38%
32	g3	172	97% 59% 38%
32	g5	172	80% 60% 37%
32	g6	172	95% 60% 38%
32	g7	172	95% 59% 39%
32	g8	172	74% 60% 37%
32	g9	172	90% 59% 38%

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Mol	Chain	Length	Quality of chain
32	gA	172	95% 59% 38%
32	gC	172	89% 59% 38%
32	gH	172	70% 60% 37%
32	gI	172	95% 59% 38%
32	gJ	172	75% 60% 37%
32	i2	172	87% 55% 41%
32	i3	172	99% 55% 41%
32	i5	172	88% 56% 40%
32	i6	172	95% 55% 41%
32	i7	172	99% 55% 41%
32	i8	172	92% 56% 40%
32	i9	172	88% 55% 41%
32	iA	172	100% 55% 41%
32	iC	172	94% 56% 40%
32	iH	172	89% 58% 39%
32	iI	172	88% 55% 41%
32	iJ	172	92% 56% 40%
32	k2	172	97% 57% 40%
32	k3	172	98% 57% 40%
32	k5	172	98% 57% 40%
32	k6	172	99% 57% 40%
32	k7	172	100% 58% 38%
32	k8	172	98% 57% 40%
32	k9	172	92% 58% 39%
32	kA	172	98% 57% 40%

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Mol	Chain	Length	Quality of chain
32	kC	172	99% 57% 40%
32	kH	172	88% 57% 40%
32	kI	172	96% 57% 40%
32	kJ	172	94% 57% 40%
32	m2	172	97% 59% 38%
32	m3	172	93% 59% 38%
32	m5	172	81% 59% 38%
32	m6	172	100% 59% 38%
32	m7	172	99% 59% 38%
32	m8	172	81% 59% 38%
32	m9	172	98% 59% 38%
32	mA	172	97% 59% 38%
32	mC	172	98% 59% 38%
32	mH	172	81% 59% 38%
32	mI	172	99% 59% 38%
32	mJ	172	70% 59% 38%

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
33	CYC	IG	201	-	-	X	-
33	CYC	IL	201	-	-	X	-
33	CYC	JK	201	-	-	X	-
33	CYC	MF	201	-	-	X	-
33	CYC	MK	201	-	-	X	-
33	CYC	V4	201	-	-	X	-
33	CYC	VB	201	-	-	X	-
33	CYC	YF	201	-	-	X	-
33	CYC	YK	201	-	-	X	-
33	CYC	c2	202	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CYC	c3	202	-	-	X	-
33	CYC	c5	202	-	-	X	-
33	CYC	c6	202	-	-	X	-
33	CYC	c7	202	-	-	X	-
33	CYC	c8	202	-	-	X	-
33	CYC	c9	202	-	-	X	-
33	CYC	cA	202	-	-	X	-
33	CYC	cC	202	-	-	X	-
33	CYC	cH	202	-	-	X	-
33	CYC	cI	202	-	-	X	-
33	CYC	cJ	202	-	-	X	-
33	CYC	e2	202	-	-	X	-
33	CYC	e3	202	-	-	X	-
33	CYC	e5	202	-	-	X	-
33	CYC	e6	202	-	-	X	-
33	CYC	e7	202	-	-	X	-
33	CYC	e8	202	-	-	X	-
33	CYC	e9	202	-	-	X	-
33	CYC	eA	202	-	-	X	-
33	CYC	eC	202	-	-	X	-
33	CYC	eH	202	-	-	X	-
33	CYC	eI	202	-	-	X	-
33	CYC	eJ	202	-	-	X	-
33	CYC	g2	201	-	-	X	-
33	CYC	g3	201	-	-	X	-
33	CYC	g5	201	-	-	X	-
33	CYC	g6	201	-	-	X	-
33	CYC	g7	201	-	-	X	-
33	CYC	g8	201	-	-	X	-
33	CYC	g9	201	-	-	X	-
33	CYC	gA	302	-	-	X	-
33	CYC	gC	302	-	-	X	-
33	CYC	gH	201	-	-	X	-
33	CYC	gI	302	-	-	X	-
33	CYC	gJ	201	-	-	X	-
33	CYC	hF	201	-	-	X	-
33	CYC	hK	201	-	-	X	-
33	CYC	i2	201	-	-	X	-
33	CYC	i3	201	-	-	X	-
33	CYC	i5	201	-	-	X	-
33	CYC	i6	201	-	-	X	-
33	CYC	i7	201	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CYC	i8	201	-	-	X	-
33	CYC	i9	201	-	-	X	-
33	CYC	iA	201	-	-	X	-
33	CYC	iC	201	-	-	X	-
33	CYC	iH	201	-	-	X	-
33	CYC	iI	201	-	-	X	-
33	CYC	iJ	201	-	-	X	-
33	CYC	j2	202	-	-	X	-
33	CYC	j3	202	-	-	X	-
33	CYC	j5	202	-	-	X	-
33	CYC	j6	202	-	-	X	-
33	CYC	j7	202	-	-	X	-
33	CYC	j8	202	-	-	X	-
33	CYC	j9	202	-	-	X	-
33	CYC	jA	202	-	-	X	-
33	CYC	jC	202	-	-	X	-
33	CYC	jH	202	-	-	X	-
33	CYC	jI	202	-	-	X	-
33	CYC	jJ	202	-	-	X	-
33	CYC	m2	201	-	-	X	-
33	CYC	m3	201	-	-	X	-
33	CYC	m5	201	-	-	X	-
33	CYC	m6	201	-	-	X	-
33	CYC	m7	201	-	-	X	-
33	CYC	m8	201	-	-	X	-
33	CYC	m9	201	-	-	X	-
33	CYC	mA	201	-	-	X	-
33	CYC	mC	201	-	-	X	-
33	CYC	mH	201	-	-	X	-
33	CYC	mI	201	-	-	X	-
33	CYC	mJ	201	-	-	X	-
35	CL	A1	403	-	-	X	-
35	CL	AD	403	-	-	X	-
35	CL	AE	403	-	-	X	-
36	CLA	cD	510	-	-	X	-
40	LMT	B1	623	-	-	X	-
40	LMT	BD	623	-	-	X	-
40	LMT	BE	623	-	-	X	-
40	LMT	CD	521	-	-	X	-
40	LMT	cD	501	-	-	X	-
43	BCR	c1	515	-	-	X	-
43	BCR	cD	515	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	BCR	cE	515	-	-	X	-
45	PHO	DD	401	-	-	X	-

2 Entry composition (i)

There are 48 unique types of molecules in this entry. The entry contains 552008 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 LRC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	240	Total	C	N	O	S	0	0
			1948	1237	343	362	6		
1	BC	240	Total	C	N	O	S	0	0
			1942	1231	343	362	6		
1	BH	240	Total	C	N	O	S	0	0
			1850	1166	328	350	6		
1	BI	240	Total	C	N	O	S	0	0
			1925	1218	339	362	6		
1	BJ	240	Total	C	N	O	S	0	0
			1856	1172	328	350	6		
1	B2	240	Total	C	N	O	S	0	0
			1942	1233	342	361	6		
1	B3	240	Total	C	N	O	S	0	0
			1936	1228	340	362	6		
1	B5	240	Total	C	N	O	S	0	0
			1856	1172	328	350	6		
1	B6	240	Total	C	N	O	S	0	0
			1945	1234	343	362	6		
1	B7	240	Total	C	N	O	S	0	0
			1942	1234	340	362	6		
1	B8	240	Total	C	N	O	S	0	0
			1850	1166	328	350	6		
1	B9	240	Total	C	N	O	S	0	0
			1942	1234	340	362	6		

- Molecule 2 is a protein called LCM.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	888	Total	C	N	O	S	0	0
			7001	4444	1216	1324	17		
2	CB	866	Total	C	N	O	S	0	0
			6844	4349	1188	1290	17		
2	B4	888	Total	C	N	O	S	0	0
			7001	4444	1216	1324	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	C4	866	Total	C	N	O	S	0	0
			6844	4349	1188	1290	17		

- Molecule 3 is a protein called Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	OB	160	Total	C	N	O	S	0	0
			1199	750	203	240	6		
3	QB	160	Total	C	N	O	S	0	0
			1205	754	206	239	6		
3	SB	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	VB	160	Total	C	N	O	S	0	0
			1205	753	206	240	6		
3	XB	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	ZB	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	JF	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	LF	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	XF	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	ZF	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	AG	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	GG	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	IG	160	Total	C	N	O	S	0	0
			1206	755	207	238	6		
3	KG	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	NG	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	PG	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	RG	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	TG	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	JK	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	LK	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	XK	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	ZK	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	AL	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	GL	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	IL	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	KL	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	NL	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	PL	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	RL	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	TL	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	Z4	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	S4	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	V4	160	Total	C	N	O	S	0	0
			1205	753	206	240	6		
3	X4	160	Total	C	N	O	S	0	0
			1196	748	203	239	6		
3	s4	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	u4	160	Total	C	N	O	S	0	0
			1199	750	203	240	6		
3	w4	160	Total	C	N	O	S	0	0
			1196	749	204	238	5		
3	o4	160	Total	C	N	O	S	0	0
			1205	754	207	238	6		
3	q4	160	Total	C	N	O	S	0	0
			1198	748	207	237	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	y4	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	O4	160	Total	C	N	O	S	0	0
			1203	753	204	240	6		
3	Q4	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	sB	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	uB	160	Total	C	N	O	S	0	0
			1199	750	203	240	6		
3	wB	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	oB	160	Total	C	N	O	S	0	0
			1199	751	204	238	6		
3	qB	160	Total	C	N	O	S	0	0
			1198	748	207	237	6		
3	yB	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	bF	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	dF	160	Total	C	N	O	S	0	0
			1205	753	206	240	6		
3	fF	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	iF	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	kF	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	9F	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	4G	160	Total	C	N	O	S	0	0
			1205	753	206	240	6		
3	6G	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	bK	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	dK	160	Total	C	N	O	S	0	0
			1205	753	206	240	6		
3	fK	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	iK	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	kK	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	9K	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		
3	4L	160	Total	C	N	O	S	0	0
			1205	753	206	240	6		
3	6L	160	Total	C	N	O	S	0	0
			1209	756	207	240	6		

- Molecule 4 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	PB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	RB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	TB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	WB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	YB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	IF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	KF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	MF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	YF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	HG	161	Total	C	N	O	S	0	0
			1208	762	201	238	7		
4	JG	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	LG	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	MG	161	Total	C	N	O	S	0	0
			1210	763	204	236	7		
4	OG	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	SG	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	UG	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	WG	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	IK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	KK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	MK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	YK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	HL	161	Total	C	N	O	S	0	0
			1208	762	201	238	7		
4	JL	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	LL	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	ML	161	Total	C	N	O	S	0	0
			1210	763	204	236	7		
4	OL	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	SL	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	UL	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	WL	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	a4	160	Total	C	N	O	S	0	0
			1199	754	203	236	6		
4	T4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	W4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	Y4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	t4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	v4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	p4	161	Total	C	N	O	S	0	0
			1208	762	201	238	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	r4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	x4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	z4	161	Total	C	N	O	S	0	0
			1208	762	201	238	7		
4	P4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	R4	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	aB	160	Total	C	N	O	S	0	0
			1196	753	203	234	6		
4	tB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	vB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	pB	161	Total	C	N	O	S	0	0
			1208	762	201	238	7		
4	rB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	xB	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	zB	161	Total	C	N	O	S	0	0
			1208	762	201	238	7		
4	aF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	cF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	eF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	hF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	jF	161	Total	C	N	O	S	0	0
			1211	763	204	238	6		
4	lF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	nF	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	1G	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	5G	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	7G	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	aK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	cK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	eK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	hK	161	Total	C	N	O	S	0	0
			1208	762	201	238	7		
4	jK	161	Total	C	N	O	S	0	0
			1211	763	204	238	6		
4	lK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	nK	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	1L	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	5L	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		
4	7L	161	Total	C	N	O	S	0	0
			1214	765	204	238	7		

- Molecule 5 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UB	65	Total	C	N	O	S	0	0
			527	333	98	93	3		
5	NF	66	Total	C	N	O	S	0	0
			535	338	99	94	4		
5	NK	66	Total	C	N	O	S	0	0
			535	338	99	94	4		
5	b4	65	Total	C	N	O	S	0	0
			527	333	98	93	3		
5	U4	65	Total	C	N	O	S	0	0
			527	333	98	93	3		
5	bB	65	Total	C	N	O	S	0	0
			527	333	98	93	3		
5	3F	65	Total	C	N	O	S	0	0
			527	333	98	93	3		
5	2G	65	Total	C	N	O	S	0	0
			527	333	98	93	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	8G	65	Total	C	N	O	S	0	0
			527	333	98	93	3		
5	3K	65	Total	C	N	O	S	0	0
			527	333	98	93	3		
5	2L	65	Total	C	N	O	S	0	0
			527	333	98	93	3		
5	8L	65	Total	C	N	O	S	0	0
			527	333	98	93	3		

- Molecule 6 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AD	334	Total	C	N	O	S	0	0
			2606	1707	433	454	12		
6	AE	334	Total	C	N	O	S	0	0
			2606	1707	433	454	12		
6	A1	334	Total	C	N	O	S	0	0
			2613	1713	433	455	12		
6	a1	334	Total	C	N	O	S	0	0
			2611	1712	431	456	12		
6	aD	334	Total	C	N	O	S	0	0
			2617	1715	434	456	12		
6	aE	334	Total	C	N	O	S	0	0
			2617	1715	434	456	12		

- Molecule 7 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BD	502	Total	C	N	O	S	0	0
			3929	2563	662	691	13		
7	BE	502	Total	C	N	O	S	0	0
			3923	2560	659	691	13		
7	B1	502	Total	C	N	O	S	0	0
			3925	2561	662	689	13		
7	b1	504	Total	C	N	O	S	0	0
			3945	2572	667	693	13		
7	bD	504	Total	C	N	O	S	0	0
			3945	2572	667	693	13		
7	bE	504	Total	C	N	O	S	0	0
			3945	2572	667	693	13		

- Molecule 8 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CD	450	Total	C	N	O	S	0	0
			3485	2286	585	601	13		
8	CE	450	Total	C	N	O	S	0	0
			3485	2286	585	601	13		
8	C1	450	Total	C	N	O	S	0	0
			3485	2286	585	601	13		
8	c1	453	Total	C	N	O	S	0	0
			3484	2282	585	604	13		
8	cD	453	Total	C	N	O	S	0	0
			3480	2279	584	604	13		
8	cE	453	Total	C	N	O	S	0	0
			3482	2280	584	605	13		

- Molecule 9 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	DD	341	Total	C	N	O	S	0	0
			2713	1799	444	457	13		
9	DE	341	Total	C	N	O	S	0	0
			2713	1799	444	457	13		
9	D1	341	Total	C	N	O	S	0	0
			2713	1799	444	457	13		
9	d1	341	Total	C	N	O	S	0	0
			2709	1797	443	456	13		
9	dD	341	Total	C	N	O	S	0	0
			2709	1797	443	456	13		
9	dE	341	Total	C	N	O	S	0	0
			2709	1797	443	456	13		

- Molecule 10 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	ED	78	Total	C	N	O	0	0
			634	412	105	117		
10	EE	78	Total	C	N	O	0	0
			634	412	105	117		
10	E1	78	Total	C	N	O	0	0
			634	412	105	117		
10	e1	78	Total	C	N	O	0	0
			634	412	105	117		
10	eD	78	Total	C	N	O	0	0
			634	412	105	117		
10	eE	78	Total	C	N	O	0	0
			634	412	105	117		

- Molecule 11 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	FD	35	Total	C	N	O	S	0	0
			283	194	46	42	1		
11	FE	35	Total	C	N	O	S	0	0
			283	194	46	42	1		
11	F1	35	Total	C	N	O	S	0	0
			283	194	46	42	1		
11	f1	35	Total	C	N	O	S	0	0
			283	194	46	42	1		
11	fD	37	Total	C	N	O	S	0	0
			299	204	49	45	1		
11	fE	35	Total	C	N	O	S	0	0
			283	194	46	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	HD	64	Total	C	N	O	S	0	0
			504	335	82	85	2		
12	HE	64	Total	C	N	O	S	0	0
			504	335	82	85	2		
12	H1	64	Total	C	N	O	S	0	0
			512	340	83	87	2		
12	h1	64	Total	C	N	O	S	0	0
			512	340	83	87	2		
12	hD	64	Total	C	N	O	S	0	0
			512	340	83	87	2		
12	hE	64	Total	C	N	O	S	0	0
			512	340	83	87	2		

- Molecule 13 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	ID	36	Total	C	N	O	S	0	0
			294	197	50	46	1		
13	IE	36	Total	C	N	O	S	0	0
			294	197	50	46	1		
13	I1	36	Total	C	N	O	S	0	0
			294	197	50	46	1		
13	i1	36	Total	C	N	O	S	0	0
			290	194	49	46	1		
13	iD	36	Total	C	N	O	S	0	0
			290	194	49	46	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	iE	36	Total	C	N	O	S	0	0
			290	194	49	46	1		

- Molecule 14 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	JD	37	Total	C	N	O		0	0
			262	179	39	44			
14	JE	37	Total	C	N	O		0	0
			262	179	39	44			
14	J1	37	Total	C	N	O		0	0
			262	179	39	44			
14	j1	39	Total	C	N	O	S	0	0
			276	187	41	47	1		
14	jD	39	Total	C	N	O	S	0	0
			276	187	41	47	1		
14	jE	39	Total	C	N	O	S	0	0
			276	187	41	47	1		

- Molecule 15 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	KD	36	Total	C	N	O	0	0
			286	203	39	44		
15	KE	36	Total	C	N	O	0	0
			286	203	39	44		
15	K1	36	Total	C	N	O	0	0
			286	203	39	44		
15	k1	35	Total	C	N	O	0	0
			277	197	37	43		
15	kD	35	Total	C	N	O	0	0
			277	197	37	43		
15	kE	35	Total	C	N	O	0	0
			277	197	37	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LD	38	Total	C	N	O	S	0	0
			315	209	52	53	1		
16	LE	38	Total	C	N	O	S	0	0
			315	209	52	53	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	L1	38	Total	C	N	O	S	0	0
			315	209	52	53	1		
16	l1	38	Total	C	N	O	S	0	0
			315	209	52	53	1		
16	lD	38	Total	C	N	O	S	0	0
			315	209	52	53	1		
16	lE	38	Total	C	N	O	S	0	0
			315	209	52	53	1		

- Molecule 17 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	MD	36	Total	C	N	O	S	0	0
			286	190	43	52	1		
17	ME	36	Total	C	N	O	S	0	0
			286	190	43	52	1		
17	M1	36	Total	C	N	O	S	0	0
			286	190	43	52	1		
17	m1	36	Total	C	N	O	S	0	0
			286	190	43	52	1		
17	mD	36	Total	C	N	O	S	0	0
			286	190	43	52	1		
17	mE	36	Total	C	N	O	S	0	0
			286	190	43	52	1		

- Molecule 18 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	OD	243	Total	C	N	O	S	0	0
			1856	1174	308	372	2		
18	OE	243	Total	C	N	O	S	0	0
			1856	1174	308	372	2		
18	O1	243	Total	C	N	O	S	0	0
			1856	1174	308	372	2		
18	o1	243	Total	C	N	O	S	0	0
			1856	1174	308	372	2		
18	oD	243	Total	C	N	O	S	0	0
			1856	1174	308	372	2		
18	oE	243	Total	C	N	O	S	0	0
			1856	1174	308	372	2		

- Molecule 19 is a protein called PsbQ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	QD	119	Total	C	N	O	S	0	0
			966	610	165	189	2		
19	QE	119	Total	C	N	O	S	0	0
			966	610	165	189	2		
19	Q1	119	Total	C	N	O	S	0	0
			966	610	165	189	2		
19	q1	119	Total	C	N	O	S	0	0
			966	610	165	189	2		
19	qD	119	Total	C	N	O	S	0	0
			966	610	165	189	2		
19	qE	119	Total	C	N	O	S	0	0
			966	610	165	189	2		

- Molecule 20 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	RD	35	Total	C	N	O	S	0	0
			260	175	43	41	1		
20	RE	35	Total	C	N	O	S	0	0
			260	175	43	41	1		
20	R1	35	Total	C	N	O	S	0	0
			260	175	43	41	1		
20	r1	35	Total	C	N	O	S	0	0
			260	175	43	41	1		
20	rD	35	Total	C	N	O	S	0	0
			260	175	43	41	1		
20	rE	35	Total	C	N	O	S	0	0
			260	175	43	41	1		

- Molecule 21 is a protein called LPP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	SD	47	Total	C	N	O	0	0
			235	141	47	47		
21	SE	47	Total	C	N	O	0	0
			235	141	47	47		
21	S1	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 22 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	TD	29	Total	C	N	O		0	0
			225	154	35	36			
22	TE	29	Total	C	N	O		0	0
			225	154	35	36			
22	T1	29	Total	C	N	O		0	0
			225	154	35	36			
22	t1	30	Total	C	N	O	S	0	0
			233	159	36	37	1		
22	tD	30	Total	C	N	O	S	0	0
			233	159	36	37	1		
22	tE	30	Total	C	N	O	S	0	0
			233	159	36	37	1		

- Molecule 23 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	UD	95	Total	C	N	O	S	0	0
			755	484	121	148	2		
23	UE	95	Total	C	N	O	S	0	0
			755	484	121	148	2		
23	U1	95	Total	C	N	O	S	0	0
			755	484	121	148	2		
23	u1	95	Total	C	N	O	S	0	0
			755	484	121	148	2		
23	uD	95	Total	C	N	O	S	0	0
			755	484	121	148	2		
23	uE	95	Total	C	N	O	S	0	0
			755	484	121	148	2		

- Molecule 24 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	VD	135	Total	C	N	O	S	0	0
			1043	662	175	203	3		
24	VE	135	Total	C	N	O	S	0	0
			1043	662	175	203	3		
24	V1	135	Total	C	N	O	S	0	0
			1043	662	175	203	3		
24	v1	135	Total	C	N	O	S	0	0
			1043	662	175	203	3		
24	vD	135	Total	C	N	O	S	0	0
			1043	662	175	203	3		
24	vE	135	Total	C	N	O	S	0	0
			1043	662	175	203	3		

- Molecule 25 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	XD	40	Total	C	N	O	S	0	0
			313	210	50	51	2		
25	XE	40	Total	C	N	O	S	0	0
			313	210	50	51	2		
25	X1	40	Total	C	N	O	S	0	0
			313	210	50	51	2		
25	x1	40	Total	C	N	O	S	0	0
			313	210	50	51	2		
25	xD	40	Total	C	N	O	S	0	0
			313	210	50	51	2		
25	xE	40	Total	C	N	O	S	0	0
			313	210	50	51	2		

- Molecule 26 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	YD	32	Total	C	N	O	S	0	0
			239	162	37	39	1		
26	YE	32	Total	C	N	O	S	0	0
			239	162	37	39	1		
26	Y1	32	Total	C	N	O	S	0	0
			239	162	37	39	1		
26	y1	32	Total	C	N	O	S	0	0
			239	162	37	39	1		
26	yD	32	Total	C	N	O	S	0	0
			239	162	37	39	1		
26	yE	32	Total	C	N	O	S	0	0
			239	162	37	39	1		

- Molecule 27 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	ZD	60	Total	C	N	O	S	0	0
			461	319	68	73	1		
27	ZE	60	Total	C	N	O	S	0	0
			461	319	68	73	1		
27	Z1	60	Total	C	N	O	S	0	0
			461	319	68	73	1		
27	z1	60	Total	C	N	O	S	0	0
			461	319	68	73	1		
27	zD	60	Total	C	N	O	S	0	0
			461	319	68	73	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	zE	60	Total	C	N	O	S	0	0
			461	319	68	73	1		

- Molecule 28 is a protein called LPP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	EF	46	Total	C	N	O	S	0	0
			354	214	69	66	5		
28	BG	46	Total	C	N	O	S	0	0
			357	216	69	66	6		
28	EK	46	Total	C	N	O	S	0	0
			354	214	69	66	5		
28	BL	46	Total	C	N	O	S	0	0
			357	216	69	66	6		

- Molecule 29 is a protein called Allophycocyanin beta-18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	QG	169	Total	C	N	O	S	0	0
			1297	818	219	257	3		
29	QL	169	Total	C	N	O	S	0	0
			1297	818	219	257	3		
29	gF	169	Total	C	N	O	S	0	0
			1297	818	219	257	3		
29	gK	169	Total	C	N	O	S	0	0
			1297	818	219	257	3		

- Molecule 30 is a protein called Allophycocyanin-B alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	VG	160	Total	C	N	O	S	0	0
			1254	795	212	241	6		
30	VL	160	Total	C	N	O	S	0	0
			1254	795	212	241	6		
30	mF	160	Total	C	N	O	S	0	0
			1254	795	212	241	6		
30	mK	160	Total	C	N	O	S	0	0
			1254	795	212	241	6		

- Molecule 31 is a protein called C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b2	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	d2	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	f2	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	h2	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	j2	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	l2	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	b3	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	d3	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	f3	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	h3	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	j3	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	l3	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	b5	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	d5	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	f5	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	h5	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	j5	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	l5	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	b6	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	d6	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	f6	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	h6	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	j6	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	l6	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	b7	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	d7	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	f7	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	h7	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	j7	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	l7	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	b8	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	d8	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	f8	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	h8	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	j8	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	l8	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	b9	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	d9	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	f9	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	h9	162	Total	C	N	O	S	0	0
			1036	634	186	214	2		
31	j9	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	l9	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	bA	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	dA	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	fA	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	hA	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	jA	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	lA	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	bC	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	dC	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	fC	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	hC	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	jC	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	lC	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	bH	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	dH	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	fH	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	hH	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	jH	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	lH	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	bI	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	dI	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	fI	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	hI	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	jI	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	lI	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		
31	bJ	162	Total	C	N	O	S	0	0
			1052	645	186	218	3		
31	dJ	162	Total	C	N	O	S	0	0
			1013	619	181	212	1		
31	fJ	162	Total	C	N	O	S	0	0
			1030	634	179	215	2		
31	hJ	162	Total	C	N	O	S	0	0
			1042	637	189	214	2		
31	jJ	162	Total	C	N	O	S	0	0
			1029	633	182	212	2		
31	lJ	162	Total	C	N	O	S	0	0
			1059	650	186	222	1		

- Molecule 32 is a protein called Phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c2	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	e2	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	g2	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	i2	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	k2	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	m2	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	c3	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	e3	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	g3	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	i3	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	k3	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
32	m3	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	c5	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	e5	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	g5	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	i5	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	k5	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	m5	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	c6	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	e6	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	g6	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	i6	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	k6	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	m6	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	c7	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	e7	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	g7	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	i7	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	k7	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	m7	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	c8	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	e8	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		

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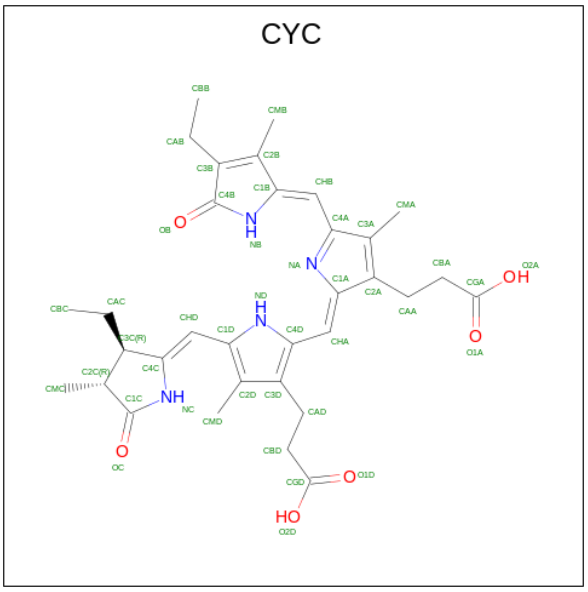
Mol	Chain	Residues	Atoms					AltConf	Trace
32	g8	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	i8	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	k8	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	m8	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	c9	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	e9	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	g9	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	i9	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	k9	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	m9	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	cA	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	eA	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	gA	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	iA	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	kA	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	mA	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	cC	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	eC	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	gC	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	iC	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	kC	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
32	mC	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	cH	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	eH	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	gH	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	iH	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	kH	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	mH	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	cI	172	Total	C	N	O	S	0	0
			1073	650	190	227	6		
32	eI	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	gI	172	Total	C	N	O	S	0	0
			1085	654	197	227	7		
32	iI	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	kI	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	mI	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		
32	cJ	172	Total	C	N	O	S	0	0
			1076	651	191	228	6		
32	eJ	172	Total	C	N	O	S	0	0
			1063	642	188	228	5		
32	gJ	172	Total	C	N	O	S	0	0
			1088	655	198	228	7		
32	iJ	172	Total	C	N	O	S	0	0
			1086	654	195	231	6		
32	kJ	172	Total	C	N	O	S	0	0
			1103	665	195	238	5		
32	mJ	172	Total	C	N	O	S	0	0
			1098	662	195	235	6		

- Molecule 33 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
33	BB	1	Total	C	N	O	0
			43	33	4	6	
33	BB	1	Total	C	N	O	0
			43	33	4	6	
33	CB	1	Total	C	N	O	0
			43	33	4	6	
33	OB	1	Total	C	N	O	0
			43	33	4	6	
33	PB	1	Total	C	N	O	0
			43	33	4	6	
33	QB	1	Total	C	N	O	0
			43	33	4	6	
33	RB	1	Total	C	N	O	0
			43	33	4	6	
33	SB	1	Total	C	N	O	0
			43	33	4	6	
33	TB	1	Total	C	N	O	0
			43	33	4	6	
33	VB	1	Total	C	N	O	0
			43	33	4	6	
33	WB	1	Total	C	N	O	0
			43	33	4	6	
33	XB	1	Total	C	N	O	0
			43	33	4	6	
33	YB	1	Total	C	N	O	0
			43	33	4	6	
33	ZB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	IF	1	Total	C	N	O	0
			43	33	4	6	
33	JF	1	Total	C	N	O	0
			43	33	4	6	
33	KF	1	Total	C	N	O	0
			43	33	4	6	
33	LF	1	Total	C	N	O	0
			43	33	4	6	
33	MF	1	Total	C	N	O	0
			43	33	4	6	
33	XF	1	Total	C	N	O	0
			43	33	4	6	
33	YF	1	Total	C	N	O	0
			43	33	4	6	
33	ZF	1	Total	C	N	O	0
			43	33	4	6	
33	AG	1	Total	C	N	O	0
			43	33	4	6	
33	GG	1	Total	C	N	O	0
			43	33	4	6	
33	HG	1	Total	C	N	O	0
			43	33	4	6	
33	IG	1	Total	C	N	O	0
			43	33	4	6	
33	JG	1	Total	C	N	O	0
			43	33	4	6	
33	KG	1	Total	C	N	O	0
			43	33	4	6	
33	LG	1	Total	C	N	O	0
			43	33	4	6	
33	MG	1	Total	C	N	O	0
			43	33	4	6	
33	NG	1	Total	C	N	O	0
			43	33	4	6	
33	OG	1	Total	C	N	O	0
			43	33	4	6	
33	PG	1	Total	C	N	O	0
			43	33	4	6	
33	QG	1	Total	C	N	O	0
			43	33	4	6	
33	RG	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	SG	1	Total	C	N	O	0
			43	33	4	6	
33	TG	1	Total	C	N	O	0
			43	33	4	6	
33	VG	1	Total	C	N	O	0
			43	33	4	6	
33	WG	1	Total	C	N	O	0
			43	33	4	6	
33	IK	1	Total	C	N	O	0
			43	33	4	6	
33	JK	1	Total	C	N	O	0
			43	33	4	6	
33	KK	1	Total	C	N	O	0
			43	33	4	6	
33	LK	1	Total	C	N	O	0
			43	33	4	6	
33	MK	1	Total	C	N	O	0
			43	33	4	6	
33	XK	1	Total	C	N	O	0
			43	33	4	6	
33	YK	1	Total	C	N	O	0
			43	33	4	6	
33	ZK	1	Total	C	N	O	0
			43	33	4	6	
33	AL	1	Total	C	N	O	0
			43	33	4	6	
33	GL	1	Total	C	N	O	0
			43	33	4	6	
33	HL	1	Total	C	N	O	0
			43	33	4	6	
33	IL	1	Total	C	N	O	0
			43	33	4	6	
33	JL	1	Total	C	N	O	0
			43	33	4	6	
33	KL	1	Total	C	N	O	0
			43	33	4	6	
33	LL	1	Total	C	N	O	0
			43	33	4	6	
33	ML	1	Total	C	N	O	0
			43	33	4	6	
33	NL	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	OL	1	Total	C	N	O	0
			43	33	4	6	
33	PL	1	Total	C	N	O	0
			43	33	4	6	
33	QL	1	Total	C	N	O	0
			43	33	4	6	
33	RL	1	Total	C	N	O	0
			43	33	4	6	
33	SL	1	Total	C	N	O	0
			43	33	4	6	
33	TL	1	Total	C	N	O	0
			43	33	4	6	
33	VL	1	Total	C	N	O	0
			43	33	4	6	
33	WL	1	Total	C	N	O	0
			43	33	4	6	
33	b2	1	Total	C	N	O	0
			43	33	4	6	
33	c2	1	Total	C	N	O	0
			43	33	4	6	
33	c2	1	Total	C	N	O	0
			43	33	4	6	
33	d2	1	Total	C	N	O	0
			43	33	4	6	
33	e2	1	Total	C	N	O	0
			43	33	4	6	
33	e2	1	Total	C	N	O	0
			43	33	4	6	
33	f2	1	Total	C	N	O	0
			43	33	4	6	
33	g2	1	Total	C	N	O	0
			43	33	4	6	
33	g2	1	Total	C	N	O	0
			43	33	4	6	
33	h2	1	Total	C	N	O	0
			43	33	4	6	
33	i2	1	Total	C	N	O	0
			43	33	4	6	
33	i2	1	Total	C	N	O	0
			43	33	4	6	
33	j2	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	j2	1	Total	C	N	O	0
			43	33	4	6	
33	k2	1	Total	C	N	O	0
			43	33	4	6	
33	l2	1	Total	C	N	O	0
			43	33	4	6	
33	m2	1	Total	C	N	O	0
			43	33	4	6	
33	b3	1	Total	C	N	O	0
			43	33	4	6	
33	c3	1	Total	C	N	O	0
			43	33	4	6	
33	c3	1	Total	C	N	O	0
			43	33	4	6	
33	d3	1	Total	C	N	O	0
			43	33	4	6	
33	e3	1	Total	C	N	O	0
			43	33	4	6	
33	e3	1	Total	C	N	O	0
			43	33	4	6	
33	f3	1	Total	C	N	O	0
			43	33	4	6	
33	g3	1	Total	C	N	O	0
			43	33	4	6	
33	g3	1	Total	C	N	O	0
			43	33	4	6	
33	h3	1	Total	C	N	O	0
			43	33	4	6	
33	i3	1	Total	C	N	O	0
			43	33	4	6	
33	i3	1	Total	C	N	O	0
			43	33	4	6	
33	j3	1	Total	C	N	O	0
			43	33	4	6	
33	j3	1	Total	C	N	O	0
			43	33	4	6	
33	k3	1	Total	C	N	O	0
			43	33	4	6	
33	l3	1	Total	C	N	O	0
			43	33	4	6	
33	m3	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	Z4	1	Total	C	N	O	0
			43	33	4	6	
33	a4	1	Total	C	N	O	0
			43	33	4	6	
33	S4	1	Total	C	N	O	0
			43	33	4	6	
33	T4	1	Total	C	N	O	0
			43	33	4	6	
33	V4	1	Total	C	N	O	0
			43	33	4	6	
33	W4	1	Total	C	N	O	0
			43	33	4	6	
33	X4	1	Total	C	N	O	0
			43	33	4	6	
33	Y4	1	Total	C	N	O	0
			43	33	4	6	
33	s4	1	Total	C	N	O	0
			43	33	4	6	
33	t4	1	Total	C	N	O	0
			43	33	4	6	
33	u4	1	Total	C	N	O	0
			43	33	4	6	
33	v4	1	Total	C	N	O	0
			43	33	4	6	
33	w4	1	Total	C	N	O	0
			43	33	4	6	
33	o4	1	Total	C	N	O	0
			43	33	4	6	
33	p4	1	Total	C	N	O	0
			43	33	4	6	
33	q4	1	Total	C	N	O	0
			43	33	4	6	
33	r4	1	Total	C	N	O	0
			43	33	4	6	
33	y4	1	Total	C	N	O	0
			43	33	4	6	
33	z4	1	Total	C	N	O	0
			43	33	4	6	
33	B4	1	Total	C	N	O	0
			43	33	4	6	
33	B4	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	C4	1	Total	C	N	O	0
			43	33	4	6	
33	O4	1	Total	C	N	O	0
			43	33	4	6	
33	P4	1	Total	C	N	O	0
			43	33	4	6	
33	Q4	1	Total	C	N	O	0
			43	33	4	6	
33	R4	1	Total	C	N	O	0
			43	33	4	6	
33	b5	1	Total	C	N	O	0
			43	33	4	6	
33	c5	1	Total	C	N	O	0
			43	33	4	6	
33	c5	1	Total	C	N	O	0
			43	33	4	6	
33	d5	1	Total	C	N	O	0
			43	33	4	6	
33	e5	1	Total	C	N	O	0
			43	33	4	6	
33	e5	1	Total	C	N	O	0
			43	33	4	6	
33	f5	1	Total	C	N	O	0
			43	33	4	6	
33	g5	1	Total	C	N	O	0
			43	33	4	6	
33	g5	1	Total	C	N	O	0
			43	33	4	6	
33	h5	1	Total	C	N	O	0
			43	33	4	6	
33	i5	1	Total	C	N	O	0
			43	33	4	6	
33	i5	1	Total	C	N	O	0
			43	33	4	6	
33	j5	1	Total	C	N	O	0
			43	33	4	6	
33	j5	1	Total	C	N	O	0
			43	33	4	6	
33	k5	1	Total	C	N	O	0
			43	33	4	6	
33	l5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	m5	1	Total	C	N	O	0
			43	33	4	6	
33	b6	1	Total	C	N	O	0
			43	33	4	6	
33	c6	1	Total	C	N	O	0
			43	33	4	6	
33	c6	1	Total	C	N	O	0
			43	33	4	6	
33	d6	1	Total	C	N	O	0
			43	33	4	6	
33	e6	1	Total	C	N	O	0
			43	33	4	6	
33	e6	1	Total	C	N	O	0
			43	33	4	6	
33	f6	1	Total	C	N	O	0
			43	33	4	6	
33	g6	1	Total	C	N	O	0
			43	33	4	6	
33	g6	1	Total	C	N	O	0
			43	33	4	6	
33	h6	1	Total	C	N	O	0
			43	33	4	6	
33	i6	1	Total	C	N	O	0
			43	33	4	6	
33	i6	1	Total	C	N	O	0
			43	33	4	6	
33	j6	1	Total	C	N	O	0
			43	33	4	6	
33	j6	1	Total	C	N	O	0
			43	33	4	6	
33	k6	1	Total	C	N	O	0
			43	33	4	6	
33	l6	1	Total	C	N	O	0
			43	33	4	6	
33	m6	1	Total	C	N	O	0
			43	33	4	6	
33	b7	1	Total	C	N	O	0
			43	33	4	6	
33	c7	1	Total	C	N	O	0
			43	33	4	6	
33	c7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	d7	1	Total	C	N	O	0
			43	33	4	6	
33	e7	1	Total	C	N	O	0
			43	33	4	6	
33	e7	1	Total	C	N	O	0
			43	33	4	6	
33	f7	1	Total	C	N	O	0
			43	33	4	6	
33	g7	1	Total	C	N	O	0
			43	33	4	6	
33	g7	1	Total	C	N	O	0
			43	33	4	6	
33	h7	1	Total	C	N	O	0
			43	33	4	6	
33	i7	1	Total	C	N	O	0
			43	33	4	6	
33	i7	1	Total	C	N	O	0
			43	33	4	6	
33	j7	1	Total	C	N	O	0
			43	33	4	6	
33	j7	1	Total	C	N	O	0
			43	33	4	6	
33	k7	1	Total	C	N	O	0
			43	33	4	6	
33	l7	1	Total	C	N	O	0
			43	33	4	6	
33	m7	1	Total	C	N	O	0
			43	33	4	6	
33	b8	1	Total	C	N	O	0
			43	33	4	6	
33	c8	1	Total	C	N	O	0
			43	33	4	6	
33	c8	1	Total	C	N	O	0
			43	33	4	6	
33	d8	1	Total	C	N	O	0
			43	33	4	6	
33	e8	1	Total	C	N	O	0
			43	33	4	6	
33	e8	1	Total	C	N	O	0
			43	33	4	6	
33	f8	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	g8	1	Total	C	N	O	0
			43	33	4	6	
33	g8	1	Total	C	N	O	0
			43	33	4	6	
33	h8	1	Total	C	N	O	0
			43	33	4	6	
33	i8	1	Total	C	N	O	0
			43	33	4	6	
33	i8	1	Total	C	N	O	0
			43	33	4	6	
33	j8	1	Total	C	N	O	0
			43	33	4	6	
33	j8	1	Total	C	N	O	0
			43	33	4	6	
33	k8	1	Total	C	N	O	0
			43	33	4	6	
33	l8	1	Total	C	N	O	0
			43	33	4	6	
33	m8	1	Total	C	N	O	0
			43	33	4	6	
33	b9	1	Total	C	N	O	0
			43	33	4	6	
33	c9	1	Total	C	N	O	0
			43	33	4	6	
33	c9	1	Total	C	N	O	0
			43	33	4	6	
33	d9	1	Total	C	N	O	0
			43	33	4	6	
33	e9	1	Total	C	N	O	0
			43	33	4	6	
33	e9	1	Total	C	N	O	0
			43	33	4	6	
33	f9	1	Total	C	N	O	0
			43	33	4	6	
33	g9	1	Total	C	N	O	0
			43	33	4	6	
33	g9	1	Total	C	N	O	0
			43	33	4	6	
33	h9	1	Total	C	N	O	0
			43	33	4	6	
33	i9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	i9	1	Total	C	N	O	0
			43	33	4	6	
33	j9	1	Total	C	N	O	0
			43	33	4	6	
33	j9	1	Total	C	N	O	0
			43	33	4	6	
33	k9	1	Total	C	N	O	0
			43	33	4	6	
33	l9	1	Total	C	N	O	0
			43	33	4	6	
33	m9	1	Total	C	N	O	0
			43	33	4	6	
33	bA	1	Total	C	N	O	0
			43	33	4	6	
33	cA	1	Total	C	N	O	0
			43	33	4	6	
33	cA	1	Total	C	N	O	0
			43	33	4	6	
33	dA	1	Total	C	N	O	0
			43	33	4	6	
33	eA	1	Total	C	N	O	0
			43	33	4	6	
33	eA	1	Total	C	N	O	0
			43	33	4	6	
33	fA	1	Total	C	N	O	0
			43	33	4	6	
33	gA	1	Total	C	N	O	0
			43	33	4	6	
33	gA	1	Total	C	N	O	0
			43	33	4	6	
33	hA	1	Total	C	N	O	0
			43	33	4	6	
33	iA	1	Total	C	N	O	0
			43	33	4	6	
33	iA	1	Total	C	N	O	0
			43	33	4	6	
33	jA	1	Total	C	N	O	0
			43	33	4	6	
33	jA	1	Total	C	N	O	0
			43	33	4	6	
33	kA	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	lA	1	Total	C	N	O	0
			43	33	4	6	
33	mA	1	Total	C	N	O	0
			43	33	4	6	
33	aB	1	Total	C	N	O	0
			43	33	4	6	
33	sB	1	Total	C	N	O	0
			43	33	4	6	
33	tB	1	Total	C	N	O	0
			43	33	4	6	
33	uB	1	Total	C	N	O	0
			43	33	4	6	
33	vB	1	Total	C	N	O	0
			43	33	4	6	
33	wB	1	Total	C	N	O	0
			43	33	4	6	
33	oB	1	Total	C	N	O	0
			43	33	4	6	
33	pB	1	Total	C	N	O	0
			43	33	4	6	
33	qB	1	Total	C	N	O	0
			43	33	4	6	
33	rB	1	Total	C	N	O	0
			43	33	4	6	
33	yB	1	Total	C	N	O	0
			43	33	4	6	
33	zB	1	Total	C	N	O	0
			43	33	4	6	
33	bC	1	Total	C	N	O	0
			43	33	4	6	
33	cC	1	Total	C	N	O	0
			43	33	4	6	
33	cC	1	Total	C	N	O	0
			43	33	4	6	
33	dC	1	Total	C	N	O	0
			43	33	4	6	
33	eC	1	Total	C	N	O	0
			43	33	4	6	
33	eC	1	Total	C	N	O	0
			43	33	4	6	
33	fC	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	gC	1	Total	C	N	O	0
			43	33	4	6	
33	gC	1	Total	C	N	O	0
			43	33	4	6	
33	hC	1	Total	C	N	O	0
			43	33	4	6	
33	iC	1	Total	C	N	O	0
			43	33	4	6	
33	iC	1	Total	C	N	O	0
			43	33	4	6	
33	jC	1	Total	C	N	O	0
			43	33	4	6	
33	jC	1	Total	C	N	O	0
			43	33	4	6	
33	kC	1	Total	C	N	O	0
			43	33	4	6	
33	lC	1	Total	C	N	O	0
			43	33	4	6	
33	mC	1	Total	C	N	O	0
			43	33	4	6	
33	aF	1	Total	C	N	O	0
			43	33	4	6	
33	bF	1	Total	C	N	O	0
			43	33	4	6	
33	cF	1	Total	C	N	O	0
			43	33	4	6	
33	dF	1	Total	C	N	O	0
			43	33	4	6	
33	eF	1	Total	C	N	O	0
			43	33	4	6	
33	3F	1	Total	C	N	O	0
			43	33	4	6	
33	fF	1	Total	C	N	O	0
			43	33	4	6	
33	gF	1	Total	C	N	O	0
			43	33	4	6	
33	hF	1	Total	C	N	O	0
			43	33	4	6	
33	jF	1	Total	C	N	O	0
			43	33	4	6	
33	kF	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	mF	1	Total	C	N	O	0
			43	33	4	6	
33	nF	1	Total	C	N	O	0
			43	33	4	6	
33	nF	1	Total	C	N	O	0
			43	33	4	6	
33	9F	1	Total	C	N	O	0
			43	33	4	6	
33	2G	1	Total	C	N	O	0
			43	33	4	6	
33	1G	1	Total	C	N	O	0
			43	33	4	6	
33	4G	1	Total	C	N	O	0
			43	33	4	6	
33	5G	1	Total	C	N	O	0
			43	33	4	6	
33	6G	1	Total	C	N	O	0
			43	33	4	6	
33	7G	1	Total	C	N	O	0
			43	33	4	6	
33	bH	1	Total	C	N	O	0
			43	33	4	6	
33	cH	1	Total	C	N	O	0
			43	33	4	6	
33	cH	1	Total	C	N	O	0
			43	33	4	6	
33	dH	1	Total	C	N	O	0
			43	33	4	6	
33	eH	1	Total	C	N	O	0
			43	33	4	6	
33	eH	1	Total	C	N	O	0
			43	33	4	6	
33	fH	1	Total	C	N	O	0
			43	33	4	6	
33	gH	1	Total	C	N	O	0
			43	33	4	6	
33	gH	1	Total	C	N	O	0
			43	33	4	6	
33	hH	1	Total	C	N	O	0
			43	33	4	6	
33	iH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	iH	1	Total	C	N	O	0
			43	33	4	6	
33	jH	1	Total	C	N	O	0
			43	33	4	6	
33	jH	1	Total	C	N	O	0
			43	33	4	6	
33	kH	1	Total	C	N	O	0
			43	33	4	6	
33	lH	1	Total	C	N	O	0
			43	33	4	6	
33	mH	1	Total	C	N	O	0
			43	33	4	6	
33	bI	1	Total	C	N	O	0
			43	33	4	6	
33	cI	1	Total	C	N	O	0
			43	33	4	6	
33	cI	1	Total	C	N	O	0
			43	33	4	6	
33	dI	1	Total	C	N	O	0
			43	33	4	6	
33	eI	1	Total	C	N	O	0
			43	33	4	6	
33	eI	1	Total	C	N	O	0
			43	33	4	6	
33	fI	1	Total	C	N	O	0
			43	33	4	6	
33	gI	1	Total	C	N	O	0
			43	33	4	6	
33	gI	1	Total	C	N	O	0
			43	33	4	6	
33	hI	1	Total	C	N	O	0
			43	33	4	6	
33	iI	1	Total	C	N	O	0
			43	33	4	6	
33	iI	1	Total	C	N	O	0
			43	33	4	6	
33	jI	1	Total	C	N	O	0
			43	33	4	6	
33	jI	1	Total	C	N	O	0
			43	33	4	6	
33	kI	1	Total	C	N	O	0
			43	33	4	6	

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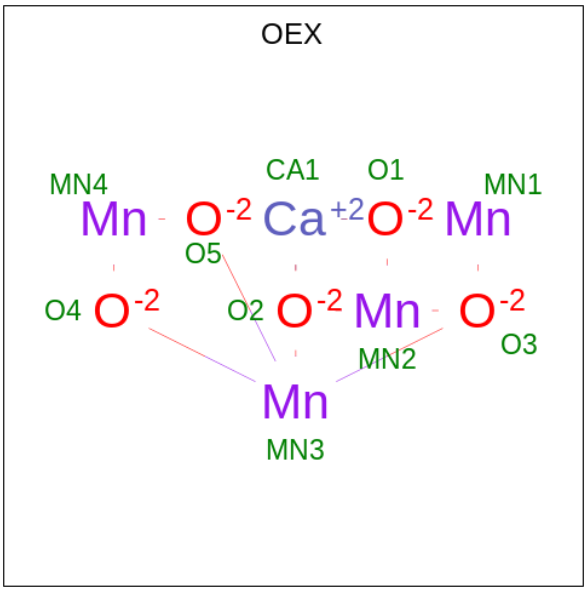
Mol	Chain	Residues	Atoms				AltConf
33	lI	1	Total	C	N	O	0
			43	33	4	6	
33	mI	1	Total	C	N	O	0
			43	33	4	6	
33	bJ	1	Total	C	N	O	0
			43	33	4	6	
33	cJ	1	Total	C	N	O	0
			43	33	4	6	
33	cJ	1	Total	C	N	O	0
			43	33	4	6	
33	dJ	1	Total	C	N	O	0
			43	33	4	6	
33	eJ	1	Total	C	N	O	0
			43	33	4	6	
33	eJ	1	Total	C	N	O	0
			43	33	4	6	
33	fJ	1	Total	C	N	O	0
			43	33	4	6	
33	gJ	1	Total	C	N	O	0
			43	33	4	6	
33	gJ	1	Total	C	N	O	0
			43	33	4	6	
33	hJ	1	Total	C	N	O	0
			43	33	4	6	
33	iJ	1	Total	C	N	O	0
			43	33	4	6	
33	iJ	1	Total	C	N	O	0
			43	33	4	6	
33	jJ	1	Total	C	N	O	0
			43	33	4	6	
33	jJ	1	Total	C	N	O	0
			43	33	4	6	
33	kJ	1	Total	C	N	O	0
			43	33	4	6	
33	lJ	1	Total	C	N	O	0
			43	33	4	6	
33	mJ	1	Total	C	N	O	0
			43	33	4	6	
33	aK	1	Total	C	N	O	0
			43	33	4	6	
33	bK	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
33	cK	1	Total	C	N	O	0
			43	33	4	6	
33	dK	1	Total	C	N	O	0
			43	33	4	6	
33	eK	1	Total	C	N	O	0
			43	33	4	6	
33	3K	1	Total	C	N	O	0
			43	33	4	6	
33	fK	1	Total	C	N	O	0
			43	33	4	6	
33	gK	1	Total	C	N	O	0
			43	33	4	6	
33	hK	1	Total	C	N	O	0
			43	33	4	6	
33	jK	1	Total	C	N	O	0
			43	33	4	6	
33	kK	1	Total	C	N	O	0
			43	33	4	6	
33	mK	1	Total	C	N	O	0
			43	33	4	6	
33	nK	1	Total	C	N	O	0
			43	33	4	6	
33	nK	1	Total	C	N	O	0
			43	33	4	6	
33	9K	1	Total	C	N	O	0
			43	33	4	6	
33	2L	1	Total	C	N	O	0
			43	33	4	6	
33	1L	1	Total	C	N	O	0
			43	33	4	6	
33	4L	1	Total	C	N	O	0
			43	33	4	6	
33	5L	1	Total	C	N	O	0
			43	33	4	6	
33	6L	1	Total	C	N	O	0
			43	33	4	6	
33	7L	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 34 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

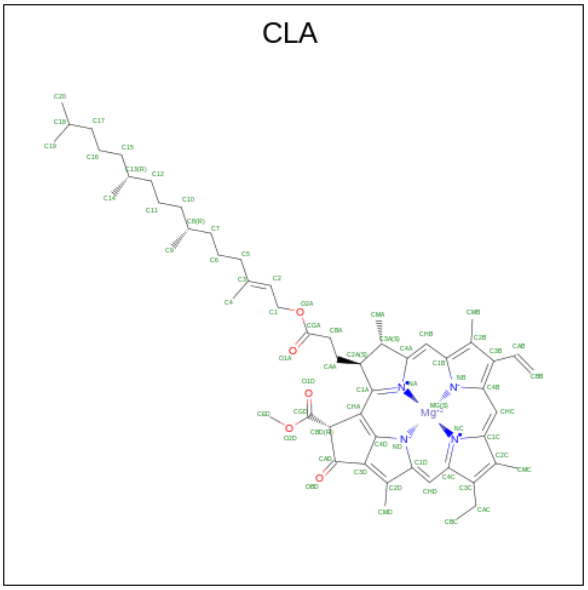


Mol	Chain	Residues	Atoms				AltConf
34	AD	1	Total 10	Ca 1	Mn 4	O 5	0
34	AE	1	Total 10	Ca 1	Mn 4	O 5	0
34	A1	1	Total 10	Ca 1	Mn 4	O 5	0
34	a1	1	Total 10	Ca 1	Mn 4	O 5	0
34	aD	1	Total 10	Ca 1	Mn 4	O 5	0
34	aE	1	Total 10	Ca 1	Mn 4	O 5	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
35	AD	2	Total 2	Cl 2	0
35	AE	2	Total 2	Cl 2	0
35	A1	2	Total 2	Cl 2	0
35	a1	2	Total 2	Cl 2	0
35	aD	2	Total 2	Cl 2	0
35	aE	2	Total 2	Cl 2	0

- Molecule 36 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
36	AD	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	AD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	CD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	DD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	DD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	HD	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	HD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	ID	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	XD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	AE	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	AE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	BE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	CE	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	CE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	DE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	DE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	HE	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	HE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	IE	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	XE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	A1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	C1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	D1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	D1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	H1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	H1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	I1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	X1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	a1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	h1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	h1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	x1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	aD	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	aD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	aD	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
36	cD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	dD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	dD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	dD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	hD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	hD	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	iD	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	xD	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	aE	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
36	aE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	aE	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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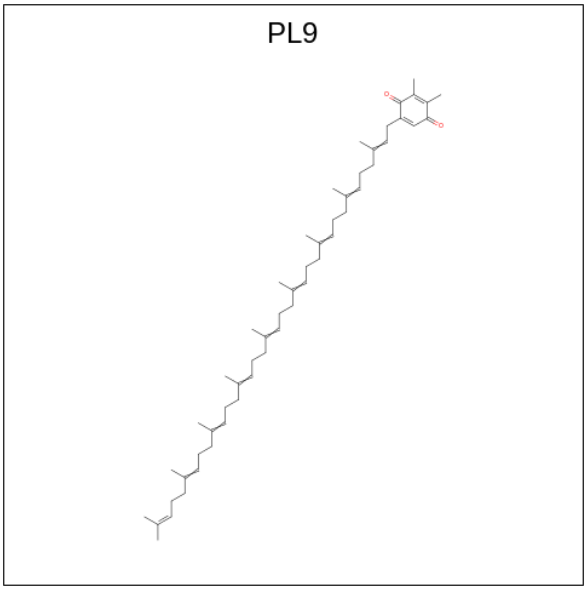
Mol	Chain	Residues	Atoms					AltConf
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	bE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	cE	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
36	cE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	dE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	dE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	dE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	hE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	hE	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	iE	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
36	xE	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 37 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: $C_{53}H_{80}O_2$).



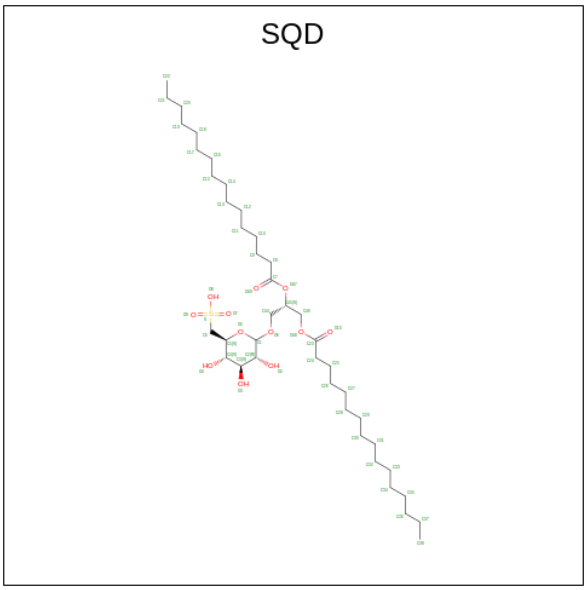
Mol	Chain	Residues	Atoms			AltConf
37	AD	1	Total	C	O	0
			55	53	2	
37	DD	1	Total	C	O	0
			55	53	2	

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Mol	Chain	Residues	Atoms	AltConf
37	AE	1	Total C O 55 53 2	0
37	DE	1	Total C O 55 53 2	0
37	A1	1	Total C O 55 53 2	0
37	D1	1	Total C O 55 53 2	0
37	a1	1	Total C O 55 53 2	0
37	d1	1	Total C O 55 53 2	0
37	aD	1	Total C O 55 53 2	0
37	dD	1	Total C O 55 53 2	0
37	aE	1	Total C O 55 53 2	0
37	dE	1	Total C O 55 53 2	0

- Molecule 38 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
38	AD	1	Total C O S 46 33 12 1	0

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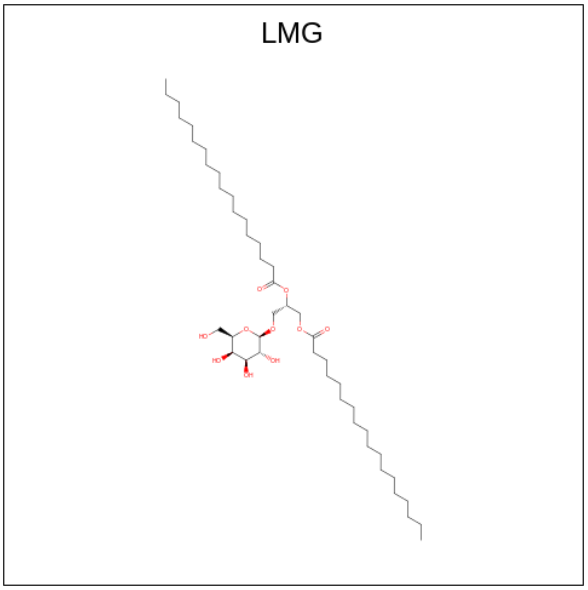
Mol	Chain	Residues	Atoms				AltConf
38	BD	1	Total	C	O	S	0
			38	25	12	1	
38	CD	1	Total	C	O	S	0
			54	41	12	1	
38	DD	1	Total	C	O	S	0
			34	21	12	1	
38	LD	1	Total	C	O	S	0
			43	30	12	1	
38	LD	1	Total	C	O	S	0
			43	30	12	1	
38	AE	1	Total	C	O	S	0
			46	33	12	1	
38	BE	1	Total	C	O	S	0
			38	25	12	1	
38	CE	1	Total	C	O	S	0
			54	41	12	1	
38	DE	1	Total	C	O	S	0
			34	21	12	1	
38	LE	1	Total	C	O	S	0
			43	30	12	1	
38	LE	1	Total	C	O	S	0
			43	30	12	1	
38	A1	1	Total	C	O	S	0
			46	33	12	1	
38	B1	1	Total	C	O	S	0
			38	25	12	1	
38	C1	1	Total	C	O	S	0
			54	41	12	1	
38	D1	1	Total	C	O	S	0
			34	21	12	1	
38	L1	1	Total	C	O	S	0
			43	30	12	1	
38	L1	1	Total	C	O	S	0
			43	30	12	1	
38	c1	1	Total	C	O	S	0
			54	41	12	1	
38	d1	1	Total	C	O	S	0
			34	21	12	1	
38	h1	1	Total	C	O	S	0
			35	22	12	1	
38	cD	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
38	dD	1	Total	C	O	S	0
			34	21	12	1	
38	hD	1	Total	C	O	S	0
			35	22	12	1	
38	cE	1	Total	C	O	S	0
			54	41	12	1	
38	dE	1	Total	C	O	S	0
			34	21	12	1	
38	hE	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 39 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
39	AD	1	Total	C	O	0
			36	26	10	
39	BD	1	Total	C	O	0
			51	41	10	
39	CD	1	Total	C	O	0
			51	41	10	
39	CD	1	Total	C	O	0
			51	41	10	
39	DD	1	Total	C	O	0
			51	41	10	
39	JD	1	Total	C	O	0
			27	17	10	

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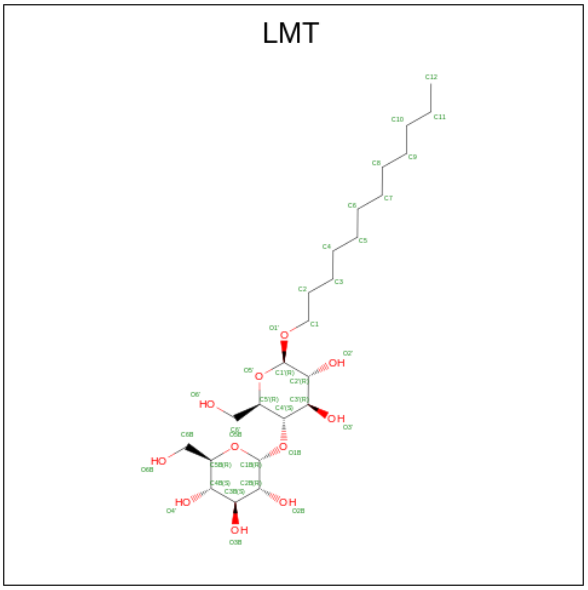
Mol	Chain	Residues	Atoms	AltConf
39	MD	1	Total C O 36 26 10	0
39	TD	1	Total C O 36 26 10	0
39	AE	1	Total C O 36 26 10	0
39	BE	1	Total C O 51 41 10	0
39	CE	1	Total C O 51 41 10	0
39	CE	1	Total C O 51 41 10	0
39	DE	1	Total C O 51 41 10	0
39	JE	1	Total C O 27 17 10	0
39	ME	1	Total C O 36 26 10	0
39	TE	1	Total C O 36 26 10	0
39	A1	1	Total C O 36 26 10	0
39	B1	1	Total C O 51 41 10	0
39	C1	1	Total C O 51 41 10	0
39	C1	1	Total C O 51 41 10	0
39	D1	1	Total C O 51 41 10	0
39	J1	1	Total C O 27 17 10	0
39	M1	1	Total C O 36 26 10	0
39	T1	1	Total C O 36 26 10	0
39	a1	1	Total C O 51 41 10	0
39	a1	1	Total C O 36 26 10	0
39	b1	1	Total C O 51 41 10	0

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Mol	Chain	Residues	Atoms	AltConf
39	d1	1	Total C O 51 41 10	0
39	j1	1	Total C O 27 17 10	0
39	m1	1	Total C O 36 26 10	0
39	t1	1	Total C O 36 26 10	0
39	y1	1	Total C O 51 41 10	0
39	aD	1	Total C O 51 41 10	0
39	aD	1	Total C O 36 26 10	0
39	bD	1	Total C O 51 41 10	0
39	dD	1	Total C O 51 41 10	0
39	jD	1	Total C O 27 17 10	0
39	mD	1	Total C O 36 26 10	0
39	tD	1	Total C O 36 26 10	0
39	yD	1	Total C O 51 41 10	0
39	aE	1	Total C O 51 41 10	0
39	aE	1	Total C O 36 26 10	0
39	bE	1	Total C O 51 41 10	0
39	dE	1	Total C O 51 41 10	0
39	jE	1	Total C O 27 17 10	0
39	mE	1	Total C O 36 26 10	0
39	tE	1	Total C O 36 26 10	0
39	yE	1	Total C O 51 41 10	0

- Molecule 40 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
40	AD	1	Total C O 24 18 6	0
40	AD	1	Total C O 35 24 11	0
40	BD	1	Total C O 24 18 6	0
40	BD	1	Total C O 35 24 11	0
40	BD	1	Total C O 24 18 6	0
40	CD	1	Total C O 24 18 6	0
40	DD	1	Total C O 24 18 6	0
40	DD	1	Total C O 25 19 6	0
40	DD	1	Total C O 22 16 6	0
40	AE	1	Total C O 24 18 6	0
40	AE	1	Total C O 35 24 11	0
40	BE	1	Total C O 24 18 6	0
40	BE	1	Total C O 35 24 11	0

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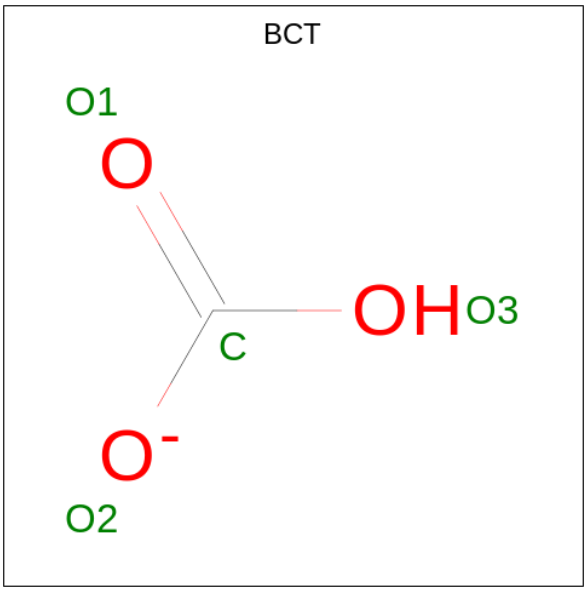
Mol	Chain	Residues	Atoms	AltConf
40	BE	1	Total C O 24 18 6	0
40	DE	1	Total C O 24 18 6	0
40	DE	1	Total C O 25 19 6	0
40	DE	1	Total C O 22 16 6	0
40	A1	1	Total C O 24 18 6	0
40	A1	1	Total C O 35 24 11	0
40	B1	1	Total C O 24 18 6	0
40	B1	1	Total C O 24 18 6	0
40	B1	1	Total C O 24 18 6	0
40	C1	1	Total C O 24 18 6	0
40	D1	1	Total C O 24 18 6	0
40	D1	1	Total C O 25 19 6	0
40	D1	1	Total C O 22 16 6	0
40	a1	1	Total C O 35 24 11	0
40	b1	1	Total C O 35 24 11	0
40	b1	1	Total C O 24 18 6	0
40	b1	1	Total C O 24 18 6	0
40	d1	1	Total C O 24 18 6	0
40	d1	1	Total C O 25 19 6	0
40	d1	1	Total C O 22 16 6	0
40	i1	1	Total C O 24 18 6	0

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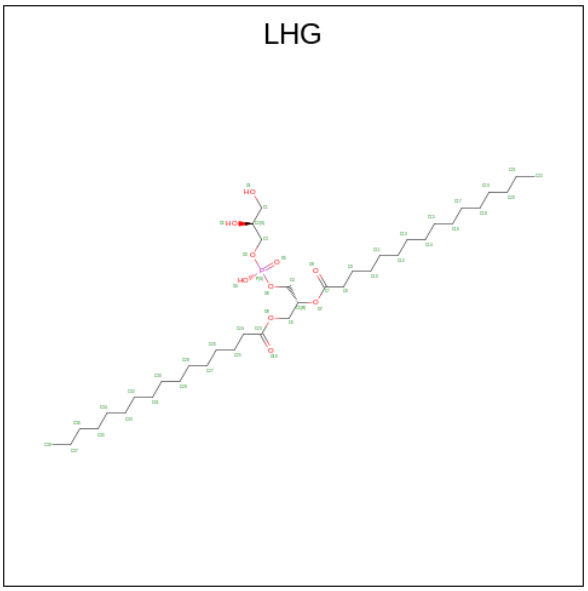
Mol	Chain	Residues	Atoms	AltConf
40	j1	1	Total C O 35 24 11	0
40	bD	1	Total C O 35 24 11	0
40	bD	1	Total C O 24 18 6	0
40	bD	1	Total C O 24 18 6	0
40	cD	1	Total C O 24 18 6	0
40	dD	1	Total C O 24 18 6	0
40	dD	1	Total C O 25 19 6	0
40	dD	1	Total C O 22 16 6	0
40	iD	1	Total C O 24 18 6	0
40	jD	1	Total C O 35 24 11	0
40	bE	1	Total C O 35 24 11	0
40	bE	1	Total C O 24 18 6	0
40	bE	1	Total C O 24 18 6	0
40	bE	1	Total C O 24 18 6	0
40	cE	1	Total C O 24 18 6	0
40	dE	1	Total C O 24 18 6	0
40	dE	1	Total C O 25 19 6	0
40	dE	1	Total C O 22 16 6	0
40	iE	1	Total C O 24 18 6	0
40	jE	1	Total C O 35 24 11	0

- Molecule 41 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
41	AD	1	Total	C	O	0
			4	1	3	
41	AE	1	Total	C	O	0
			4	1	3	
41	A1	1	Total	C	O	0
			4	1	3	
41	a1	1	Total	C	O	0
			4	1	3	
41	aD	1	Total	C	O	0
			4	1	3	
41	aE	1	Total	C	O	0
			4	1	3	

- Molecule 42 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



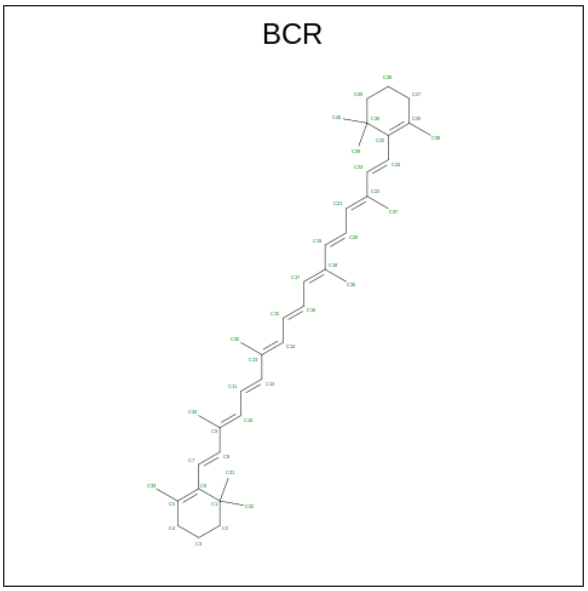
Mol	Chain	Residues	Atoms				AltConf
42	AD	1	Total	C	O	P	0
			38	27	10	1	
42	BD	1	Total	C	O	P	0
			49	38	10	1	
42	DD	1	Total	C	O	P	0
			49	38	10	1	
42	DD	1	Total	C	O	P	0
			49	38	10	1	
42	AE	1	Total	C	O	P	0
			38	27	10	1	
42	BE	1	Total	C	O	P	0
			49	38	10	1	
42	DE	1	Total	C	O	P	0
			49	38	10	1	
42	DE	1	Total	C	O	P	0
			49	38	10	1	
42	A1	1	Total	C	O	P	0
			38	27	10	1	
42	B1	1	Total	C	O	P	0
			49	38	10	1	
42	D1	1	Total	C	O	P	0
			49	38	10	1	
42	D1	1	Total	C	O	P	0
			49	38	10	1	
42	a1	1	Total	C	O	P	0
			38	27	10	1	
42	d1	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
42	d1	1	Total	C	O	P	0
			49	38	10	1	
42	e1	1	Total	C	O	P	0
			40	29	10	1	
42	l1	1	Total	C	O	P	0
			49	38	10	1	
42	aD	1	Total	C	O	P	0
			38	27	10	1	
42	dD	1	Total	C	O	P	0
			49	38	10	1	
42	dD	1	Total	C	O	P	0
			49	38	10	1	
42	eD	1	Total	C	O	P	0
			40	29	10	1	
42	lD	1	Total	C	O	P	0
			49	38	10	1	
42	aE	1	Total	C	O	P	0
			38	27	10	1	
42	dE	1	Total	C	O	P	0
			49	38	10	1	
42	dE	1	Total	C	O	P	0
			49	38	10	1	
42	eE	1	Total	C	O	P	0
			40	29	10	1	
42	lE	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 43 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
43	BD	1	Total C 40 40	0
43	BD	1	Total C 40 40	0
43	BD	1	Total C 40 40	0
43	CD	1	Total C 40 40	0
43	CD	1	Total C 40 40	0
43	CD	1	Total C 40 40	0
43	DD	1	Total C 40 40	0
43	ID	1	Total C 40 40	0
43	XD	1	Total C 40 40	0
43	ZD	1	Total C 40 40	0
43	BE	1	Total C 40 40	0
43	BE	1	Total C 40 40	0
43	BE	1	Total C 40 40	0
43	CE	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
43	CE	1	Total C 40 40	0
43	DE	1	Total C 40 40	0
43	IE	1	Total C 40 40	0
43	XE	1	Total C 40 40	0
43	ZE	1	Total C 40 40	0
43	ZE	1	Total C 40 40	0
43	B1	1	Total C 40 40	0
43	B1	1	Total C 40 40	0
43	B1	1	Total C 40 40	0
43	C1	1	Total C 40 40	0
43	C1	1	Total C 40 40	0
43	D1	1	Total C 40 40	0
43	I1	1	Total C 40 40	0
43	X1	1	Total C 40 40	0
43	Z1	1	Total C 40 40	0
43	Z1	1	Total C 40 40	0
43	b1	1	Total C 40 40	0
43	b1	1	Total C 40 40	0
43	b1	1	Total C 40 40	0
43	c1	1	Total C 40 40	0
43	c1	1	Total C 40 40	0

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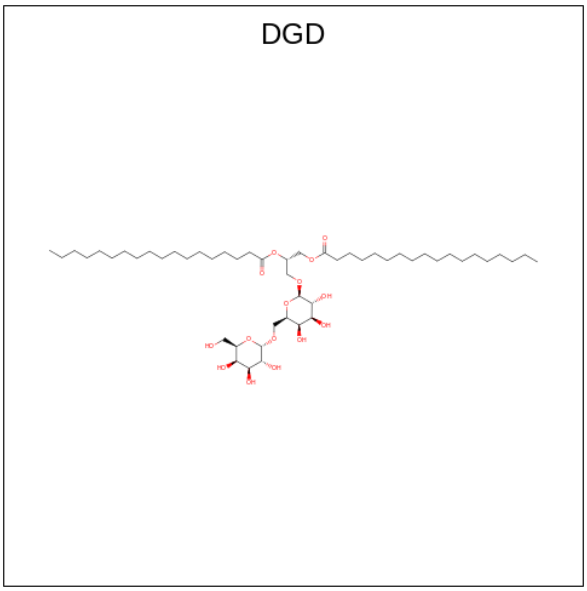
Mol	Chain	Residues	Atoms	AltConf
43	d1	1	Total C 40 40	0
43	h1	1	Total C 40 40	0
43	i1	1	Total C 40 40	0
43	k1	1	Total C 40 40	0
43	z1	1	Total C 40 40	0
43	bD	1	Total C 40 40	0
43	bD	1	Total C 40 40	0
43	bD	1	Total C 40 40	0
43	cD	1	Total C 40 40	0
43	cD	1	Total C 40 40	0
43	dD	1	Total C 40 40	0
43	hD	1	Total C 40 40	0
43	iD	1	Total C 40 40	0
43	kD	1	Total C 40 40	0
43	zD	1	Total C 40 40	0
43	bE	1	Total C 40 40	0
43	bE	1	Total C 40 40	0
43	bE	1	Total C 40 40	0
43	cE	1	Total C 40 40	0
43	cE	1	Total C 40 40	0
43	dE	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
43	hE	1	Total C 40 40	0
43	iE	1	Total C 40 40	0
43	kE	1	Total C 40 40	0
43	zE	1	Total C 40 40	0

- Molecule 44 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



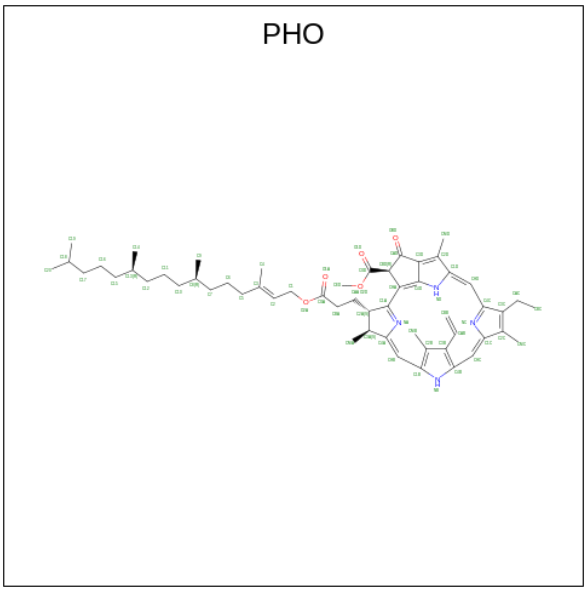
Mol	Chain	Residues	Atoms	AltConf
44	CD	1	Total C O 47 32 15	0
44	CD	1	Total C O 62 47 15	0
44	HD	1	Total C O 62 47 15	0
44	JD	1	Total C O 62 47 15	0
44	CE	1	Total C O 47 32 15	0
44	CE	1	Total C O 62 47 15	0
44	HE	1	Total C O 62 47 15	0

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Mol	Chain	Residues	Atoms	AltConf
44	JE	1	Total C O 62 47 15	0
44	C1	1	Total C O 47 32 15	0
44	C1	1	Total C O 62 47 15	0
44	H1	1	Total C O 62 47 15	0
44	J1	1	Total C O 62 47 15	0
44	c1	1	Total C O 47 32 15	0
44	c1	1	Total C O 62 47 15	0
44	c1	1	Total C O 62 47 15	0
44	h1	1	Total C O 62 47 15	0
44	cD	1	Total C O 47 32 15	0
44	cD	1	Total C O 62 47 15	0
44	cD	1	Total C O 62 47 15	0
44	hD	1	Total C O 62 47 15	0
44	cE	1	Total C O 47 32 15	0
44	cE	1	Total C O 62 47 15	0
44	cE	1	Total C O 62 47 15	0
44	hE	1	Total C O 62 47 15	0

- Molecule 45 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).

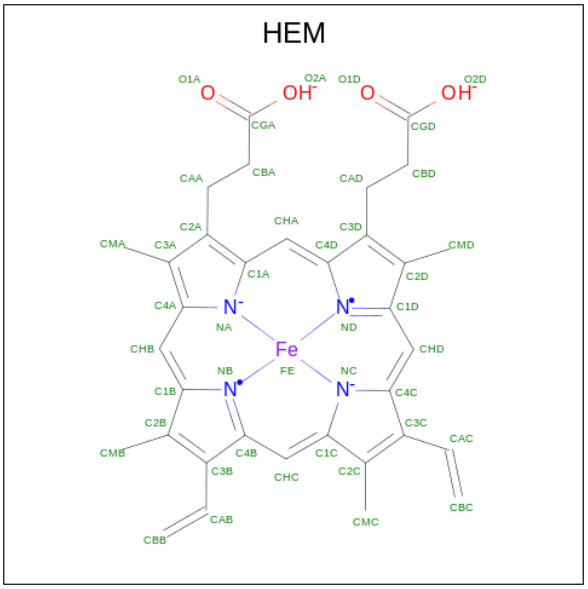


Mol	Chain	Residues	Atoms				AltConf
45	DD	1	Total	C	N	O	0
			64	55	4	5	
45	DD	1	Total	C	N	O	0
			58	49	4	5	
45	DE	1	Total	C	N	O	0
			64	55	4	5	
45	DE	1	Total	C	N	O	0
			64	55	4	5	
45	A1	1	Total	C	N	O	0
			64	55	4	5	
45	D1	1	Total	C	N	O	0
			64	55	4	5	
45	a1	1	Total	C	N	O	0
			52	43	4	5	
45	d1	1	Total	C	N	O	0
			64	55	4	5	
45	aD	1	Total	C	N	O	0
			64	55	4	5	
45	dD	1	Total	C	N	O	0
			52	43	4	5	
45	aE	1	Total	C	N	O	0
			56	47	4	5	
45	dE	1	Total	C	N	O	0
			56	47	4	5	

- Molecule 46 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
46	DD	1	Total Fe 1 1	0
46	DE	1	Total Fe 1 1	0
46	D1	1	Total Fe 1 1	0
46	d1	1	Total Fe 1 1	0
46	dD	1	Total Fe 1 1	0
46	dE	1	Total Fe 1 1	0

- Molecule 47 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	AltConf
47	ED	1	Total C Fe N O 43 34 1 4 4	0
47	VD	1	Total C Fe N O 43 34 1 4 4	0
47	EE	1	Total C Fe N O 43 34 1 4 4	0
47	VE	1	Total C Fe N O 43 34 1 4 4	0
47	E1	1	Total C Fe N O 43 34 1 4 4	0

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Mol	Chain	Residues	Atoms					AltConf
47	V1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	f1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	v1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	fD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	vD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	fE	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	vE	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 48 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
48	KD	1	Total	Ca	0
			1	1	
48	UD	1	Total	Ca	0
			1	1	
48	VD	1	Total	Ca	0
			1	1	
48	KE	1	Total	Ca	0
			1	1	
48	UE	1	Total	Ca	0
			1	1	
48	VE	1	Total	Ca	0
			1	1	
48	K1	1	Total	Ca	0
			1	1	
48	U1	1	Total	Ca	0
			1	1	
48	V1	1	Total	Ca	0
			1	1	
48	k1	1	Total	Ca	0
			1	1	
48	u1	1	Total	Ca	0
			1	1	
48	v1	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
48	kD	1	Total Ca 1 1	0
48	uD	1	Total Ca 1 1	0
48	vD	1	Total Ca 1 1	0
48	kE	1	Total Ca 1 1	0
48	uE	1	Total Ca 1 1	0
48	vE	1	Total Ca 1 1	0

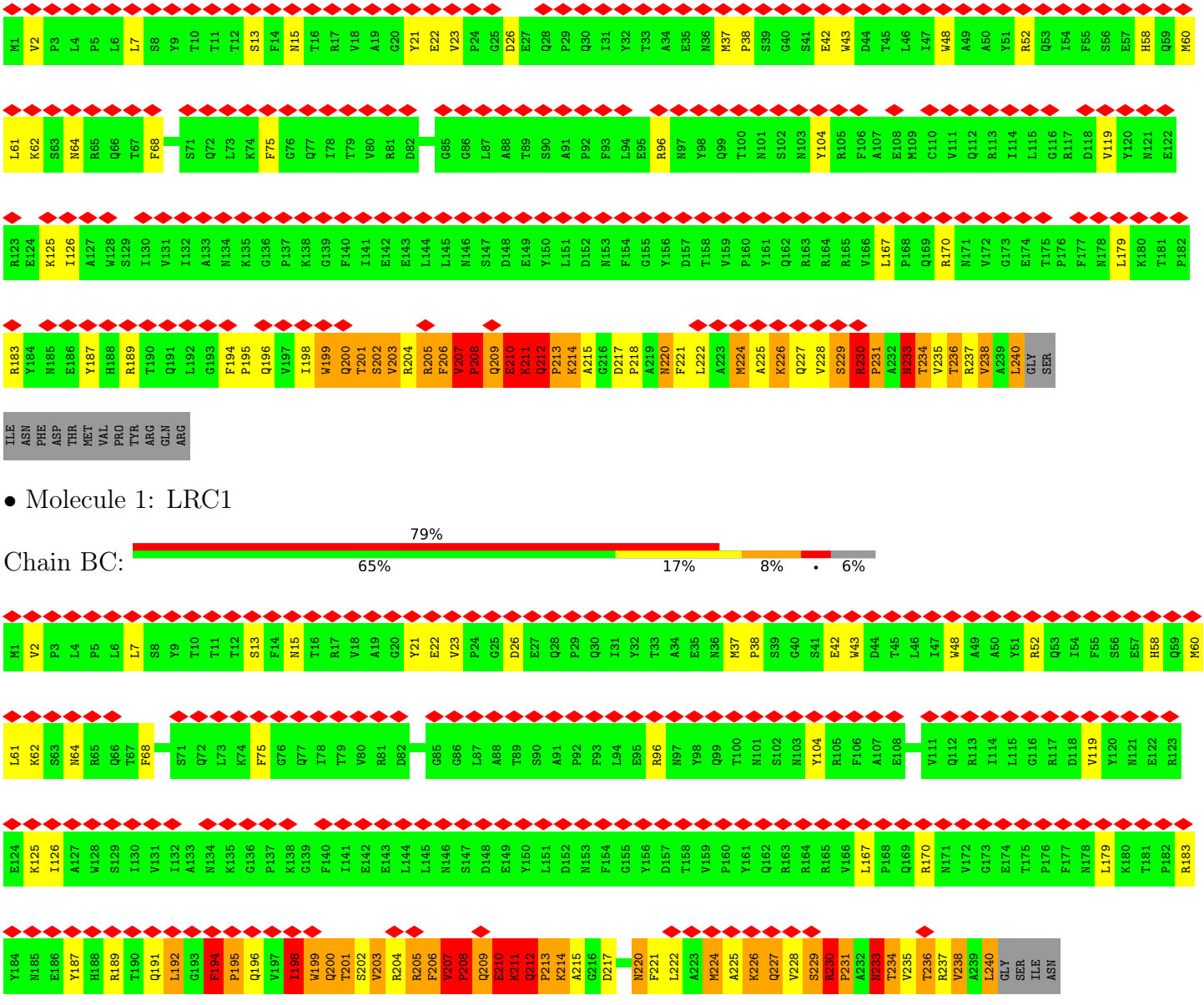
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: LRC1

Chain BA:





- Molecule 1: LRC1

Chain BC:

PHE ASP THR MET VAL PRO TYR ARG GLN ARG

• Molecule 1: LRC1

Chain BH:



M1 V2 P3 L4 P5 L6 L7 S8 Y9 T10 T11 T12 S13 F14 N15 T16 R17 V18 A19 G20 Y21 E22 V23 P24 G25 D26 E27 Q28 P29 Q30 I31 Y32 T33 A34 E35 N36 M37 P38 S39 G40 S41 E42 W43 D44 T45 L46 I47 W48 A49 A50 Y51 R52 Q53 I54 F55 S56 E57 H58 Q59 M60

L61 K62 S63 N64 R65 Q66 T67 F68 L69 E70 S71 Q72 L73 K74 F75 G76 Q77 I78 T79 V80 R81 D82 F83 I84 G85 G86 L87 A88 T89 S90 A91 P92 F93 L94 E95 R96 N97 Y98 Q99 T100 N101 S102 N103 Y104 R105 F106 A107 E108 M109 C110 V111 I114 L115 G116 R117 D118 V119 Y120 N121

E122 R123 E124 K125 I126 A127 W128 S129 I130 V131 I132 A133 N134 K135 G136 P137 K138 G139 F140 I141 E142 E143 L144 L145 N146 S147 D148 E149 Y150 L151 D152 N153 F154 G155 Y156 D157 T158 V159 P160 Y161 Q162 R163 R164 R165 V166 L167 P168 Q169 R170 N171 V172 G173 E174 T175 P176 F177 N178 L179 K180 T181

P182 R183 Y184 N185 E186 Y187 H188 R189 T190 Q191 L192 G193 F194 P195 Q196 V197 I198 W199 Q200 T201 S202 V203 R204 R205 F206 V207 P208 Q209 E210 K211 Q212 P213 K214 A215 G216 D217 P218 A219 N220 F221 L222 A223 M224 A225 K226 Q227 V228 S229 R230 P231 A232 N233 T234 V235 T236 R237 V238 A239 L240 GLY

SER ILE ASN PHE ASP THR MET VAL PRO TYR ARG GLN ARG

• Molecule 1: LRC1

Chain BI:



M1 V2 P3 L4 P5 L6 L7 S8 Y9 T10 T11 T12 S13 F14 N15 T16 R17 V18 A19 G20 Y21 E22 V23 P24 G25 D26 E27 Q28 P29 Q30 I31 Y32 T33 A34 E35 N36 M37 P38 S39 G40 S41 E42 W43 D44 T45 L46 I47 W48 A49 A50 Y51 R52 Q53 I54 F55 S56 E57 H58 Q59 M60

L61 K62 S63 N64 R65 Q66 T67 F68 L69 E70 S71 Q72 L73 K74 F75 G76 Q77 I78 T79 V80 R81 D82 F83 I84 G85 G86 L87 A88 T89 S90 A91 P92 F93 L94 E95 R96 N97 Y98 Q99 T100 N101 S102 N103 Y104 R105 F106 A107 E108 M109 C110 V111 Q112 R113 I114 L115 G116 R117 D118 V119 Y120

N121 E122 R123 E124 K125 I126 A127 W128 S129 I130 V131 I132 A133 N134 K135 G136 P137 K138 G139 F140 I141 E142 E143 L144 L145 N146 S147 D148 E149 Y150 L151 D152 N153 F154 G155 Y156 D157 T158 V159 P160 Y161 Q162 R163 R164 R165 V166 L167 P168 Q169 R170 N171 V172 G173 E174 T175 P176 F177 N178 L179 K180

T181 P182 R183 Y184 N185 E186 Y187 H188 R189 T190 Q191 L192 G193 F194 P195 Q196 V197 I198 W199 Q200 T201 S202 V203 R204 R205 F206 V207 P208 Q209 E210 K211 Q212 P213 K214 A215 P218 A219 N220 F221 L222 A223 M224 A225 K226 Q227 V228 S229 R230 P231 A232 N233 T234 V235 T236 R237 V238 A239 L240 GLY

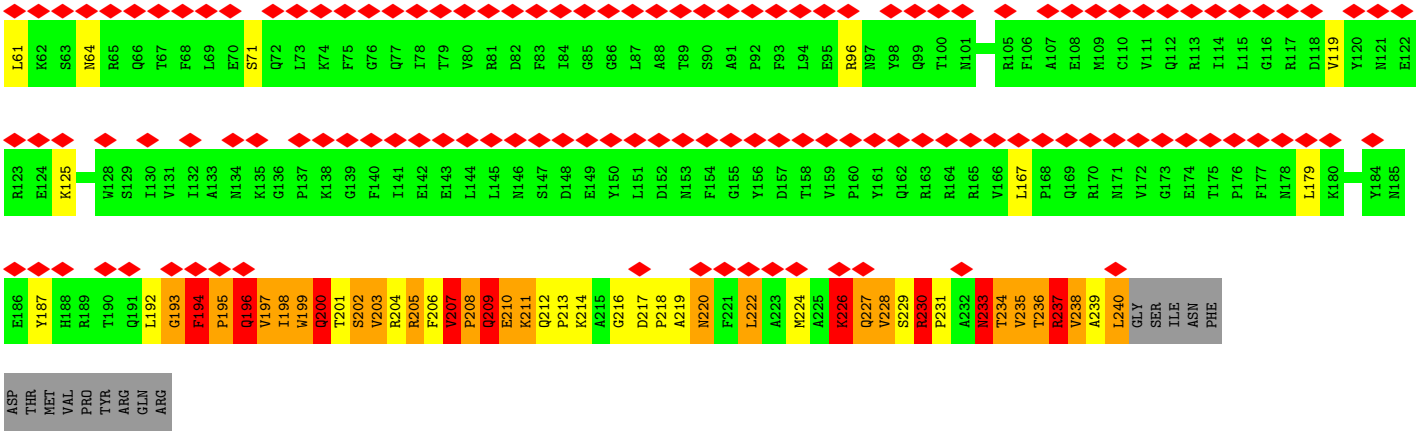
SER ILE ASN PHE ASP THR MET VAL PRO TYR ARG GLN ARG

• Molecule 1: LRC1

Chain BJ:



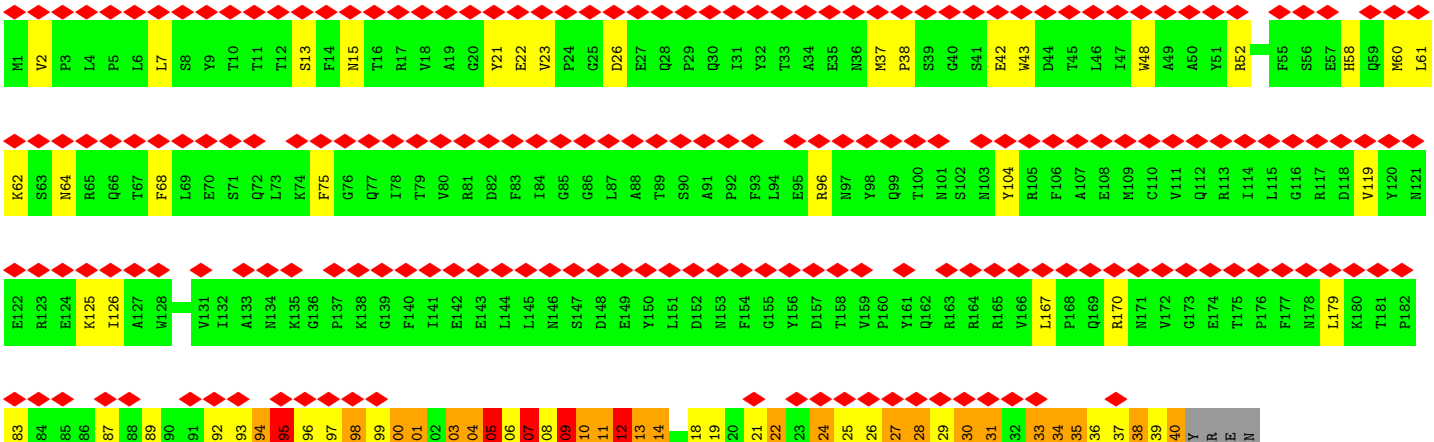
M1 V2 P3 L4 P5 L6 L7 S8 Y9 T10 T11 T12 S13 F14 N15 T16 R17 V18 A19 G20 Y21 E22 V23 P24 G25 D26 E27 Q28 P29 Q30 I31 Y32 T33 A34 E35 N36 M37 P38 S39 G40 S41 E42 W43 D44 T45 L46 I47 W48 A49 A50 Y51 R52 Q53 I54 F55 S56 E57 H58 Q59 M60



• Molecule 1: LRC1

Chain B2:

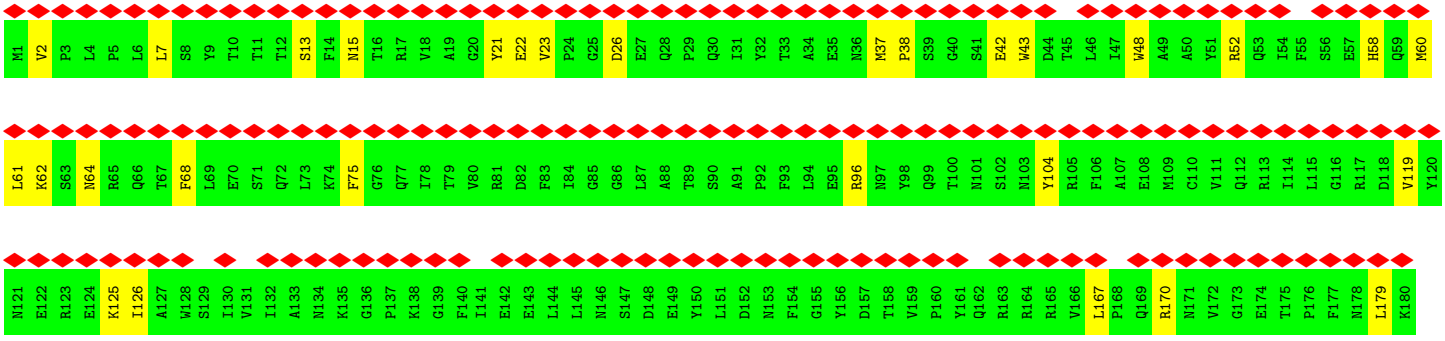


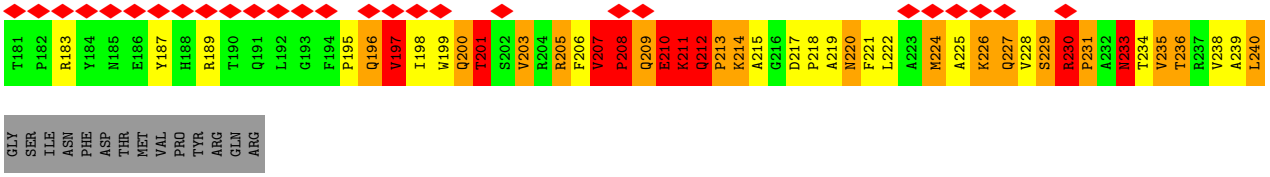


• Molecule 1: LRC1

Chain B3:



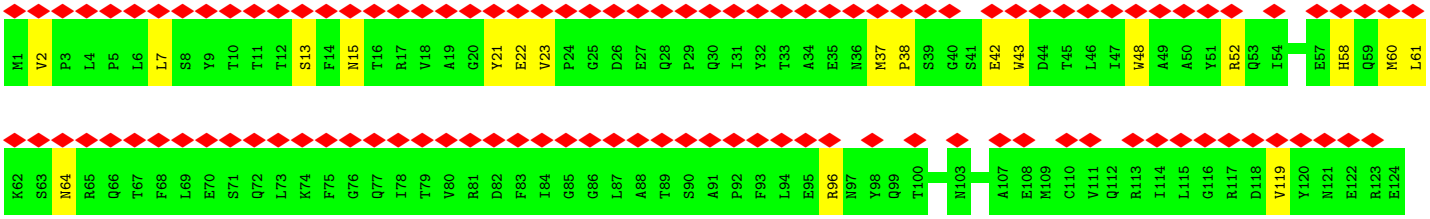




• Molecule 1: LRC1

Chain B5:

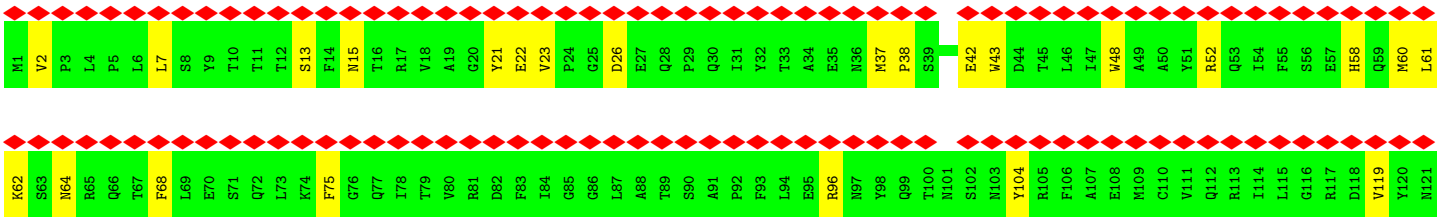




• Molecule 1: LRC1

Chain B6:

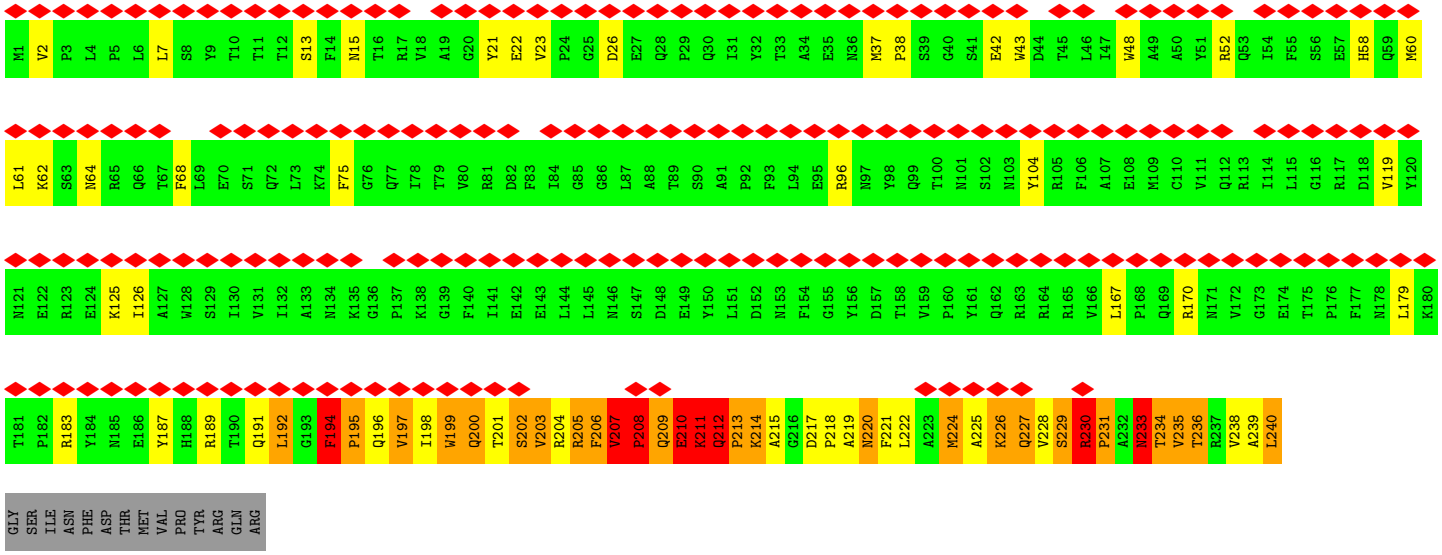




• Molecule 1: LRC1

Chain B7:

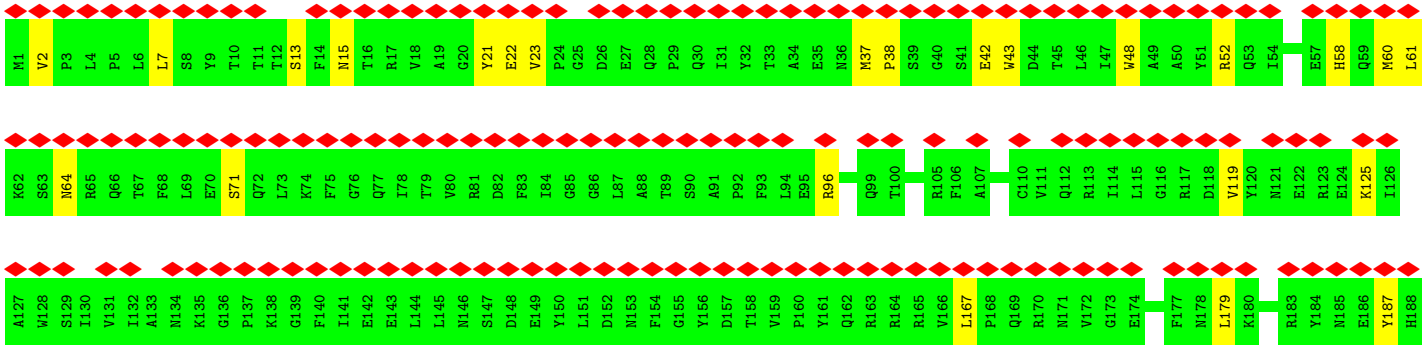




• Molecule 1: LRC1

Chain B8:

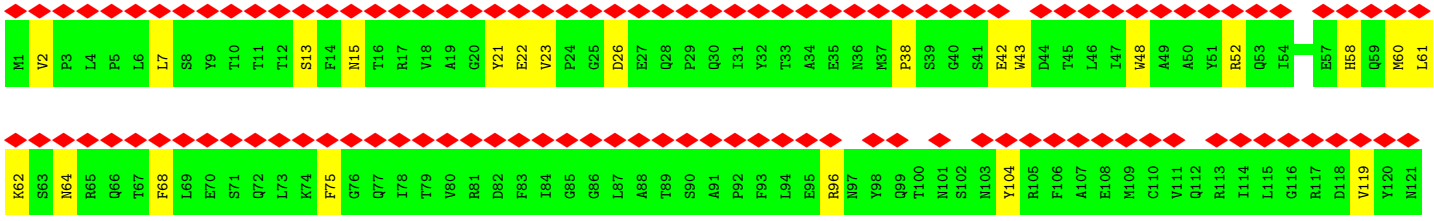


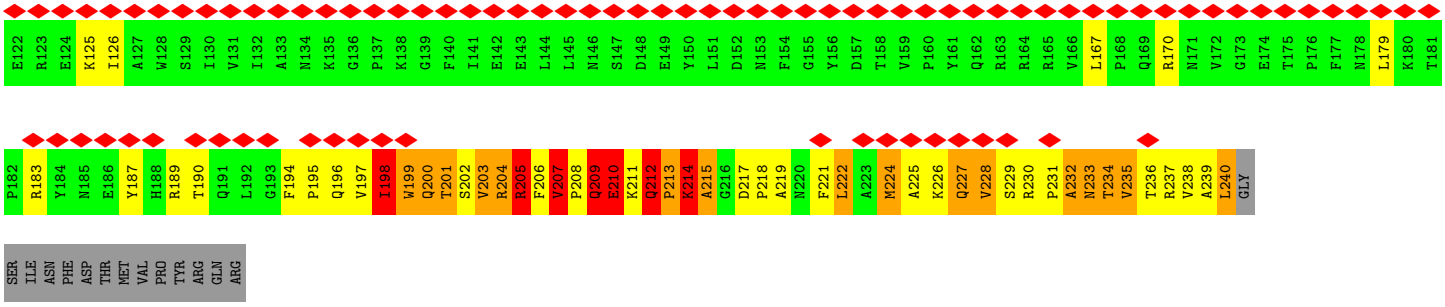


• Molecule 1: LRC1

Chain B9:



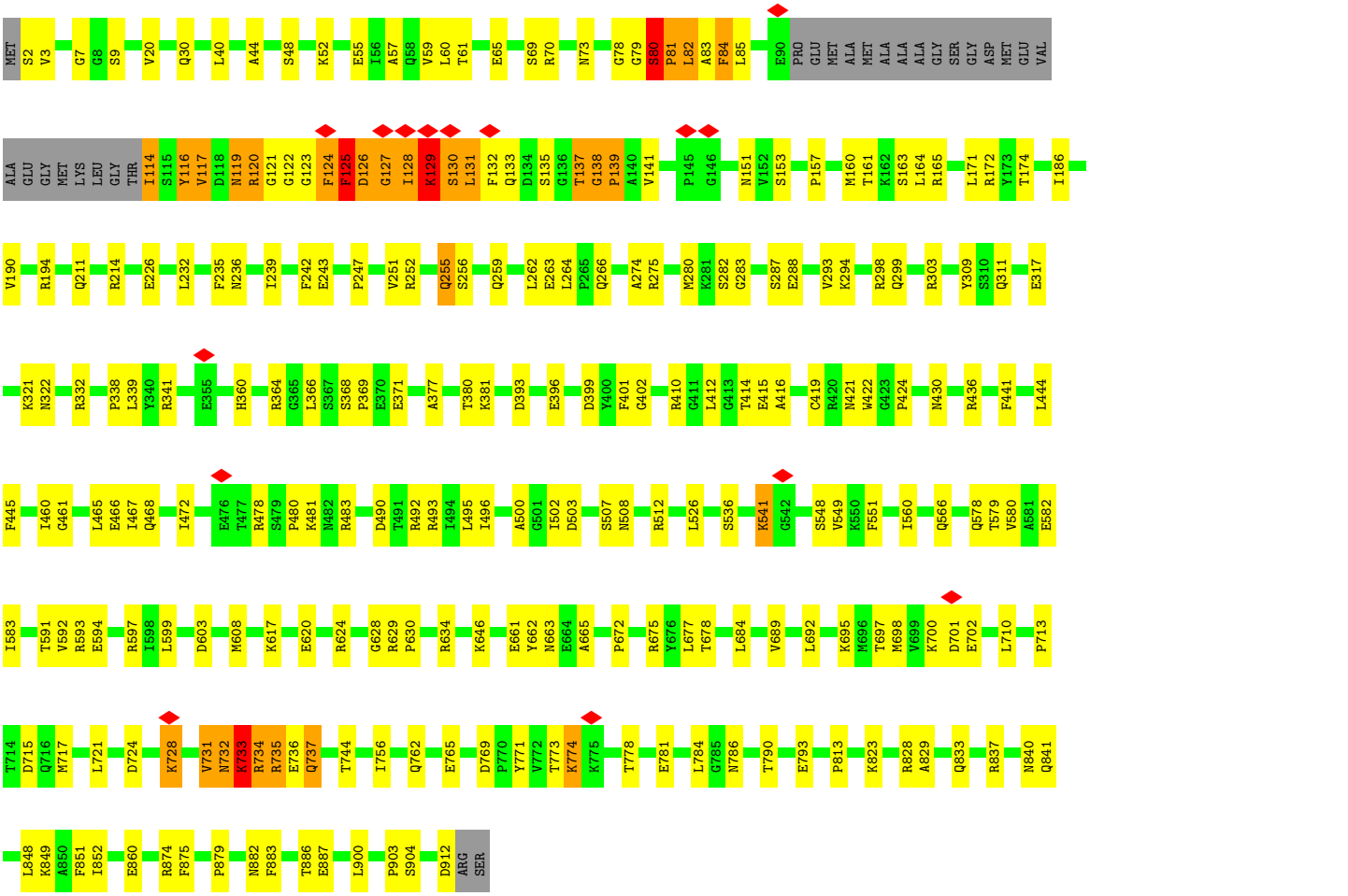




• Molecule 2: LCM

Chain BB:

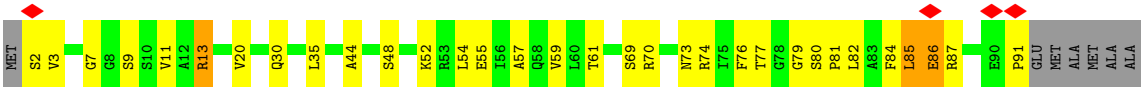


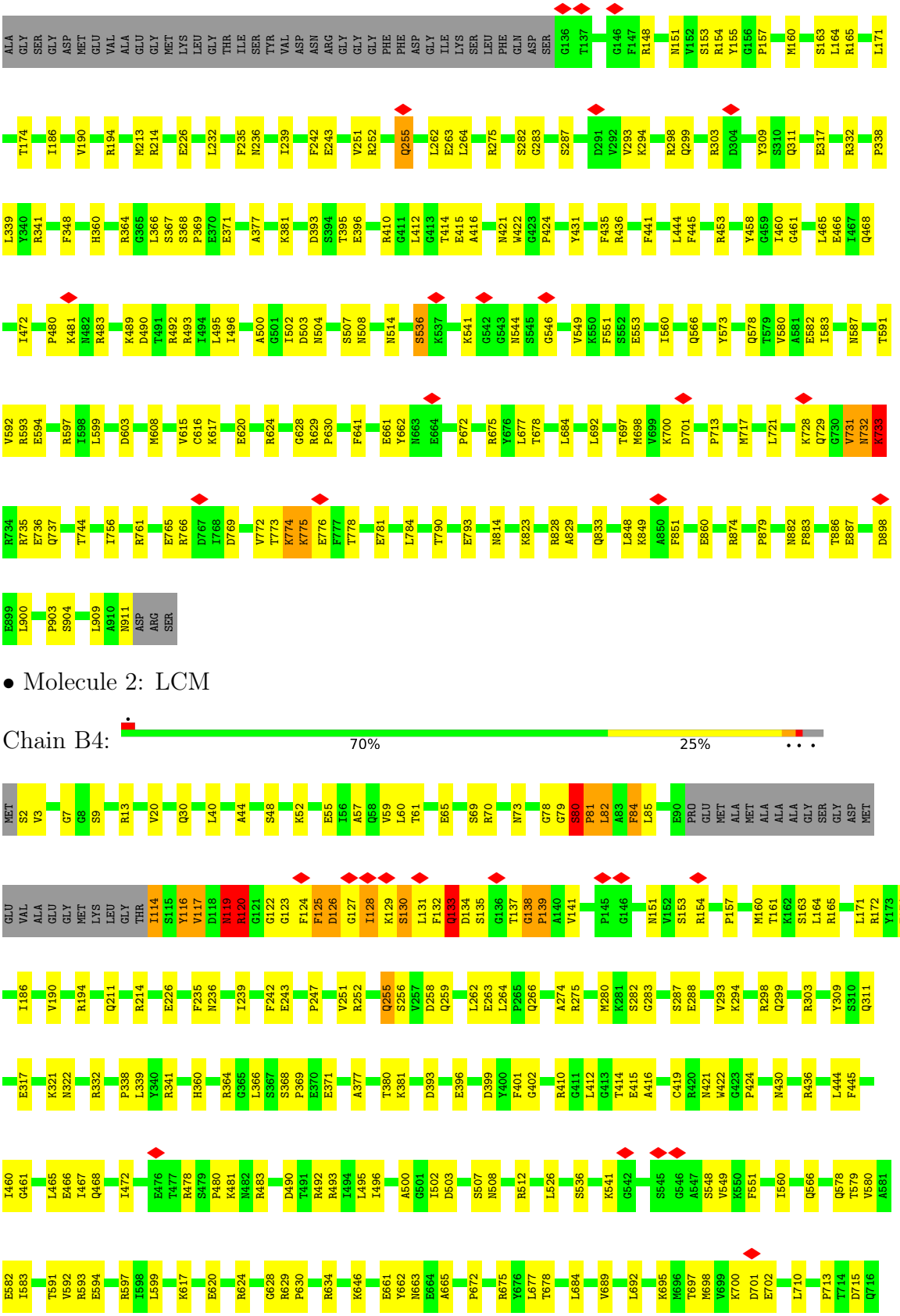


• Molecule 2: LCM

Chain CB:

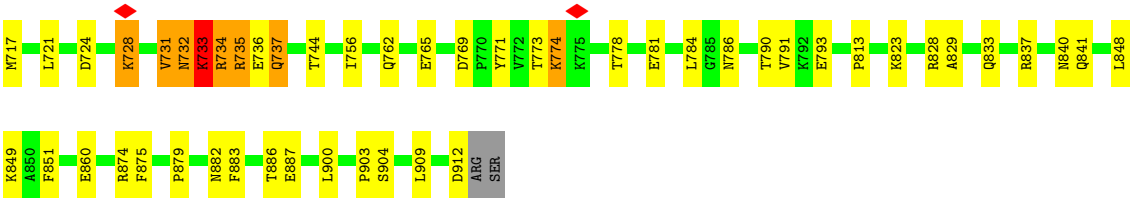






• Molecule 2: LCM

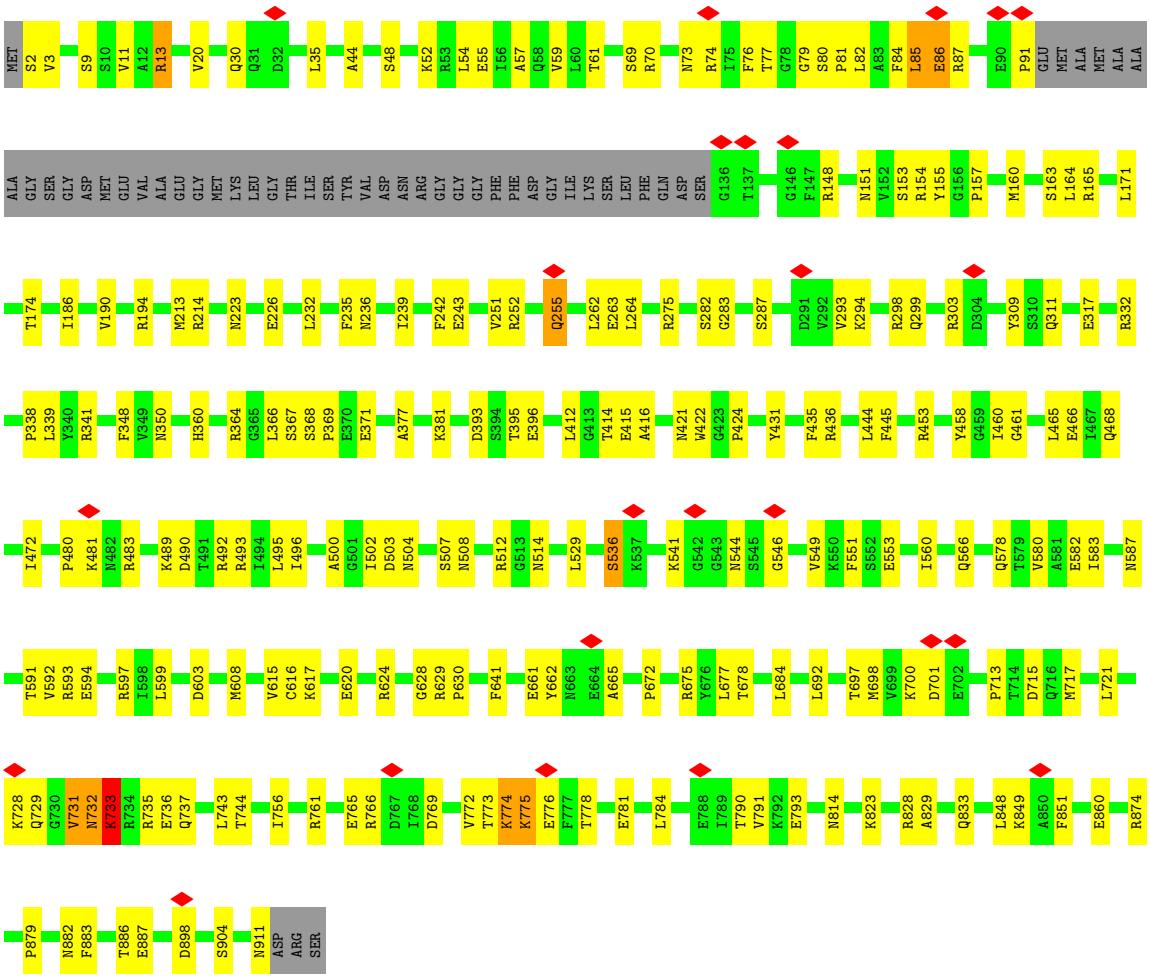
Chain B4:



• Molecule 2: LCM

Chain C4:

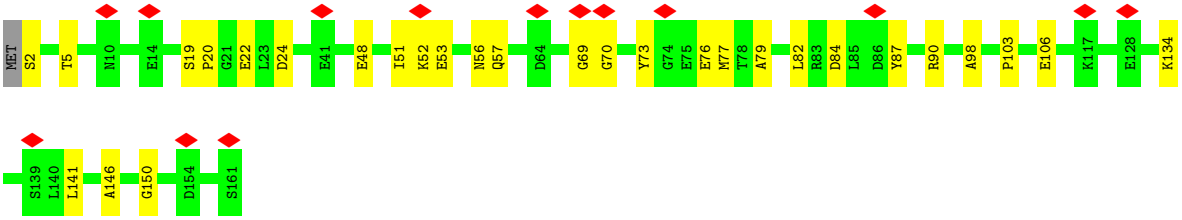




• Molecule 3: Allophycocyanin alpha chain

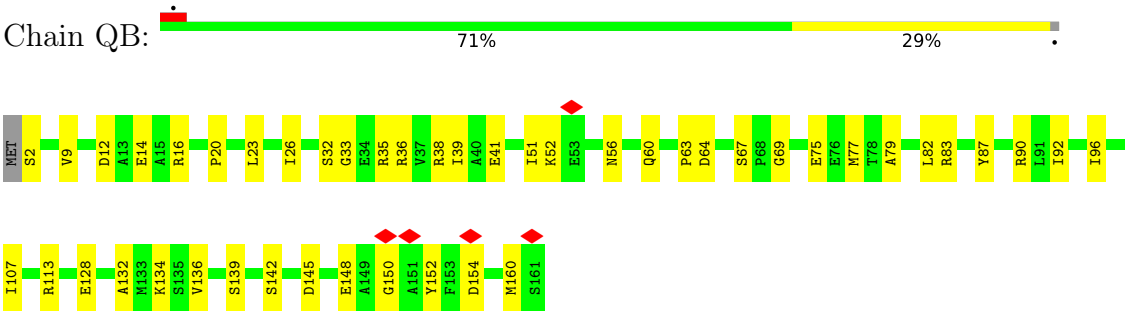
Chain OB:





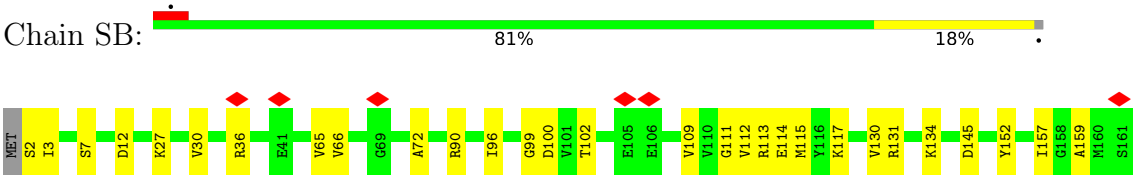
• Molecule 3: Allophycocyanin alpha chain

Chain QB:



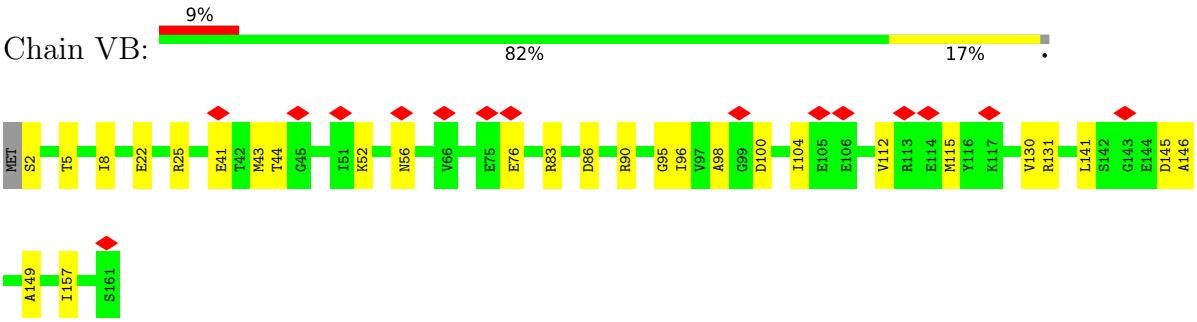
• Molecule 3: Allophycocyanin alpha chain

Chain SB:



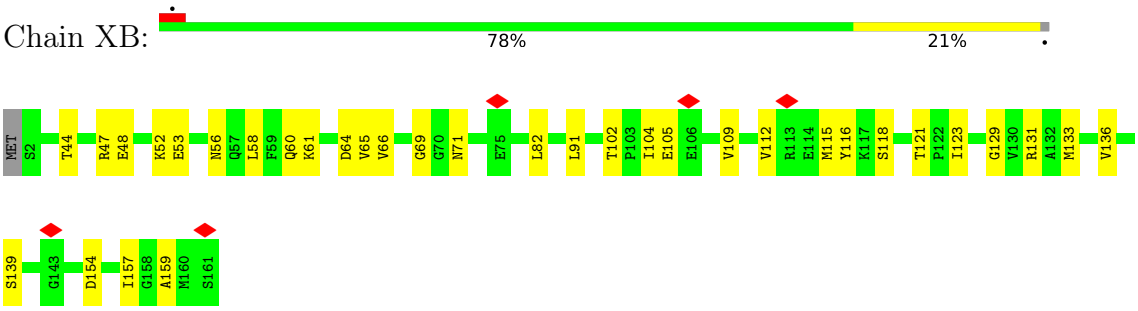
• Molecule 3: Allophycocyanin alpha chain

Chain VB:



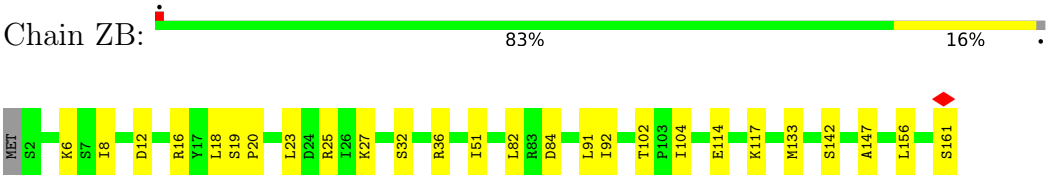
• Molecule 3: Allophycocyanin alpha chain

Chain XB:



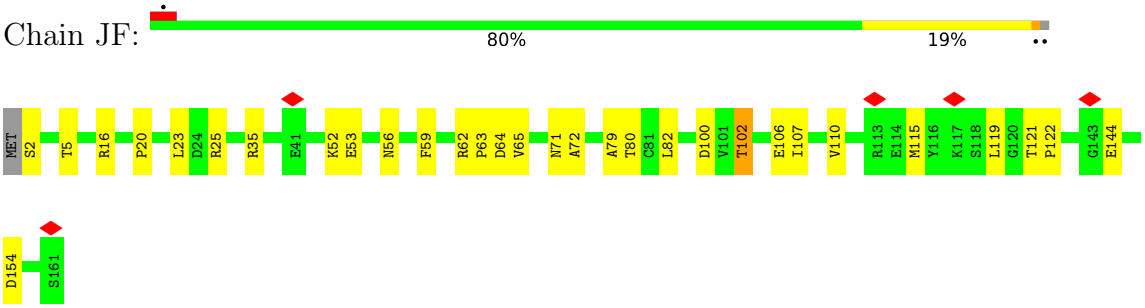
• Molecule 3: Allophycocyanin alpha chain

Chain ZB:



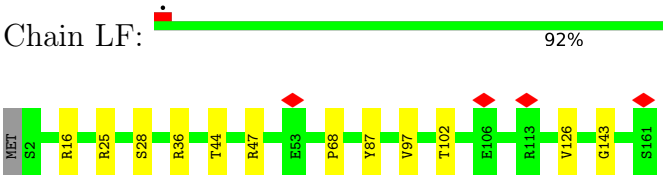
• Molecule 3: Allophycocyanin alpha chain

Chain JF:



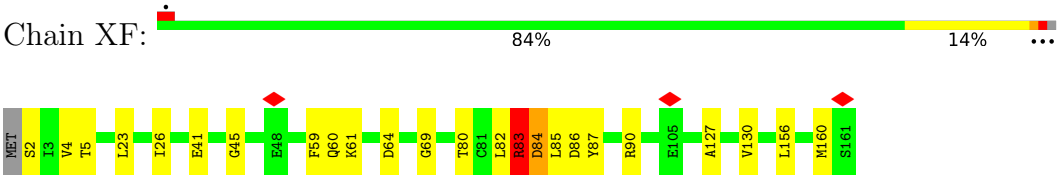
• Molecule 3: Allophycocyanin alpha chain

Chain LF:



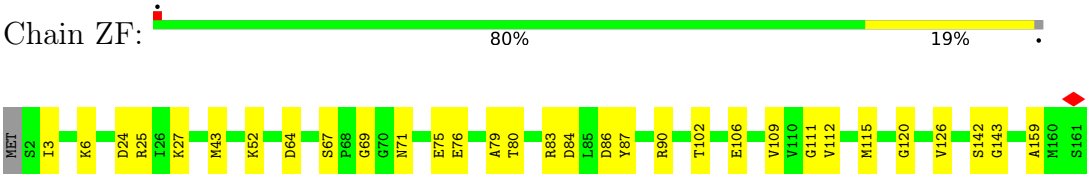
• Molecule 3: Allophycocyanin alpha chain

Chain XF:



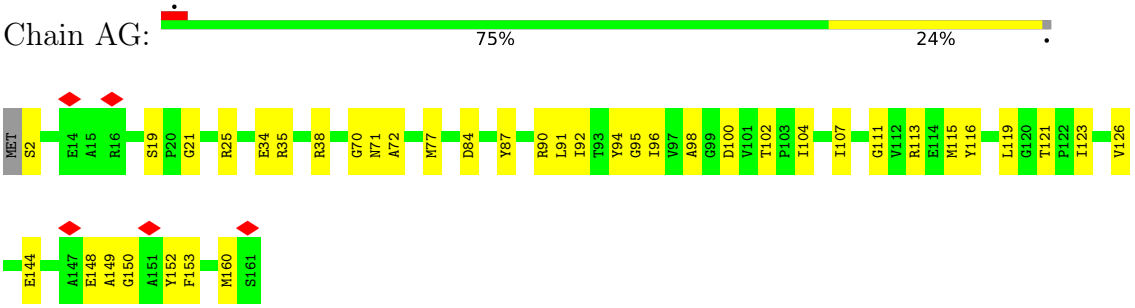
• Molecule 3: Allophycocyanin alpha chain

Chain ZF:



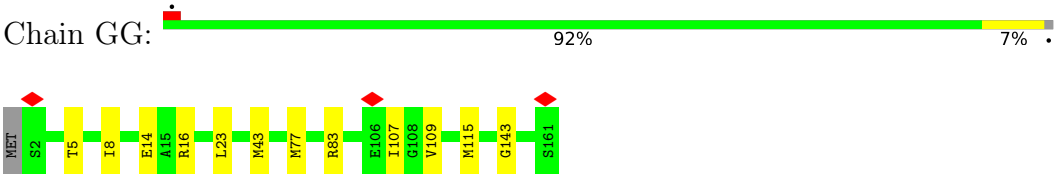
• Molecule 3: Allophycocyanin alpha chain

Chain AG:



• Molecule 3: Allophycocyanin alpha chain

Chain GG:



• Molecule 3: Allophycocyanin alpha chain

Chain IG:





• Molecule 3: Allophycocyanin alpha chain

Chain KG:

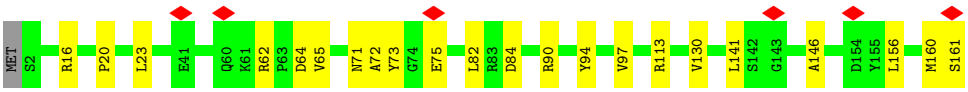




• Molecule 3: Allophycocyanin alpha chain

Chain NG:

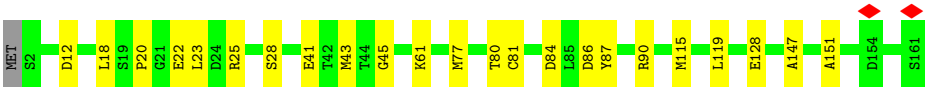




• Molecule 3: Allophycocyanin alpha chain

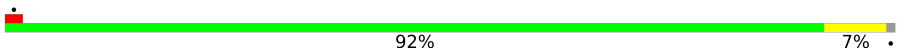
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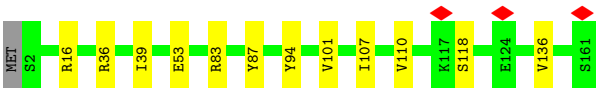




• Molecule 3: Allophycocyanin alpha chain

Chain RG:

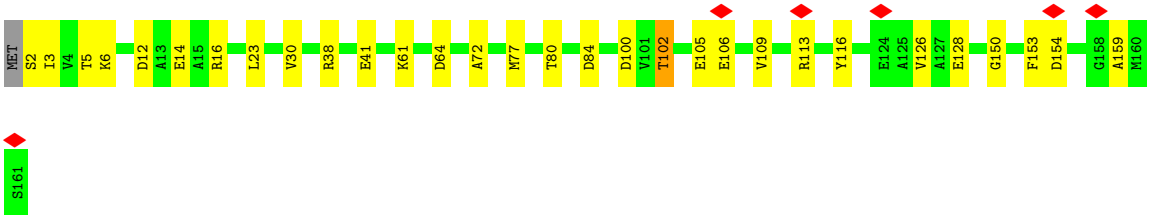




• Molecule 3: Allophycocyanin alpha chain

Chain TG:

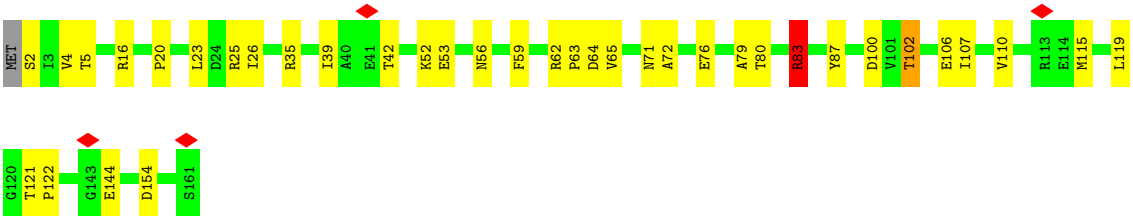




• Molecule 3: Allophycocyanin alpha chain

Chain JK:

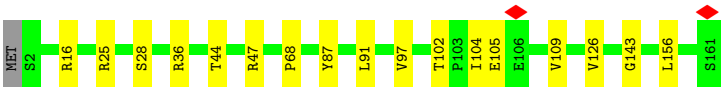




• Molecule 3: Allophycocyanin alpha chain

Chain LK:

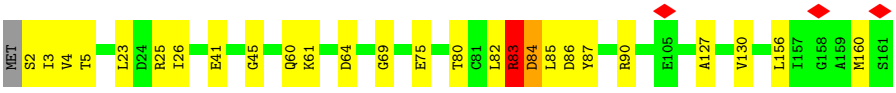




• Molecule 3: Allophycocyanin alpha chain

Chain XK:

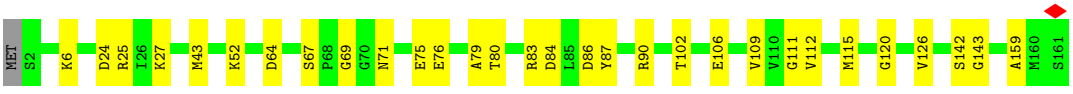




• Molecule 3: Allophycocyanin alpha chain

Chain ZK:



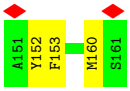


• Molecule 3: Allophycocyanin alpha chain

Chain AL:

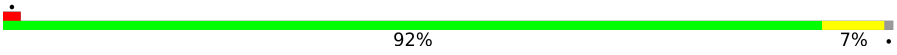


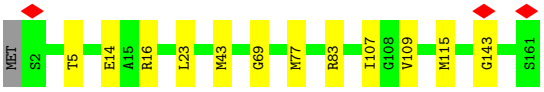




• Molecule 3: Allophycocyanin alpha chain

Chain GL:

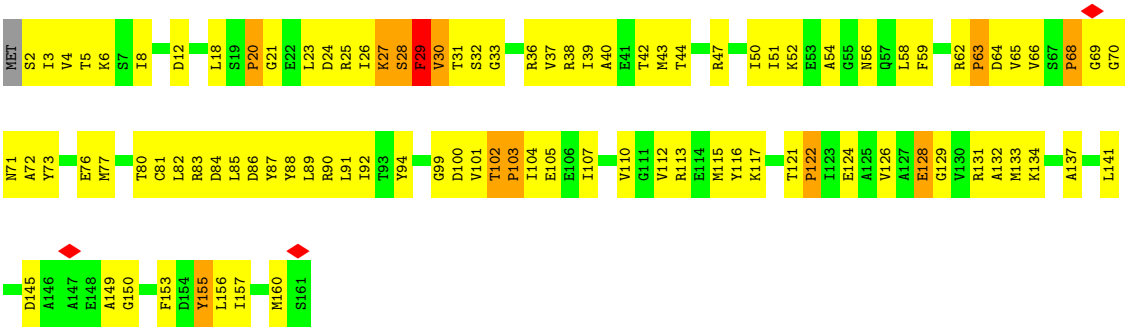




• Molecule 3: Allophycocyanin alpha chain

Chain IL:

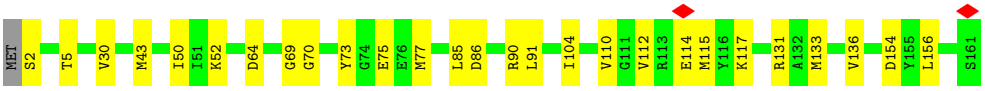




• Molecule 3: Allophycocyanin alpha chain

Chain KL:

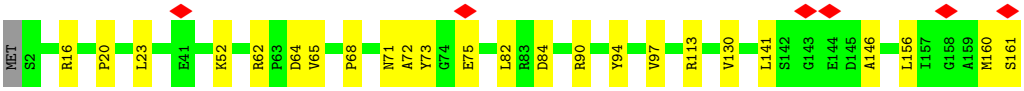




• Molecule 3: Allophycocyanin alpha chain

Chain NL:

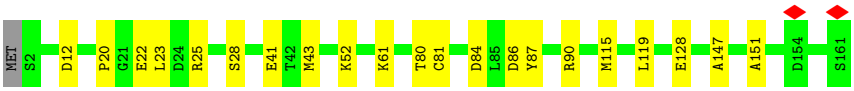




• Molecule 3: Allophycocyanin alpha chain

Chain PL:

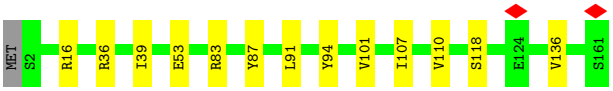




• Molecule 3: Allophycocyanin alpha chain

Chain RL:

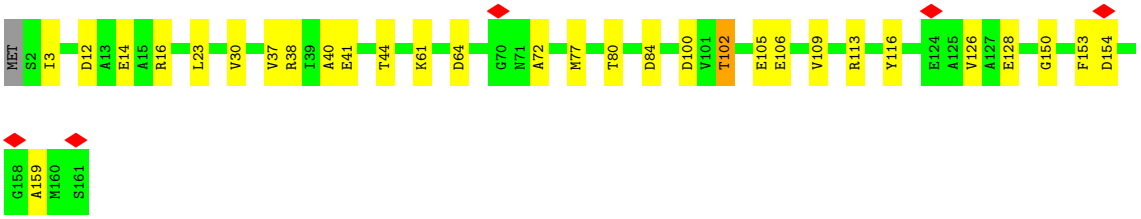




• Molecule 3: Allophycocyanin alpha chain

Chain TL:

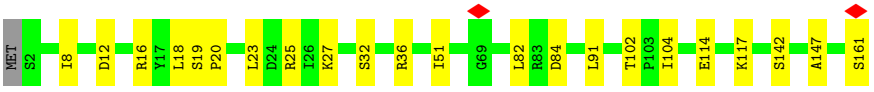




• Molecule 3: Allophycocyanin alpha chain

Chain Z4:

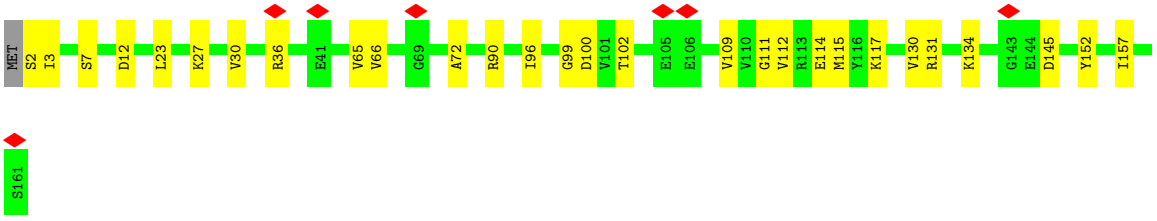




• Molecule 3: Allophycocyanin alpha chain

Chain S4:

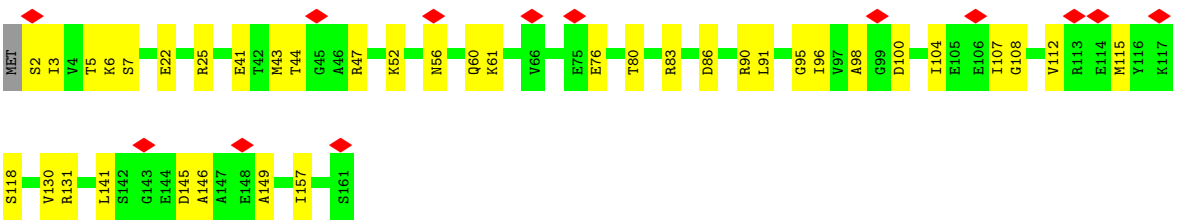




• Molecule 3: Allophycocyanin alpha chain

Chain V4:

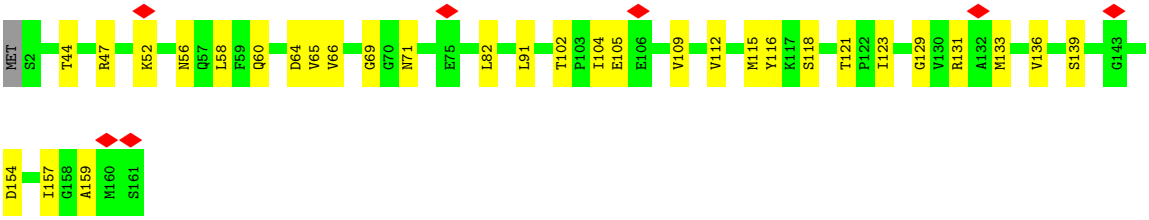




• Molecule 3: Allophycocyanin alpha chain

Chain X4:

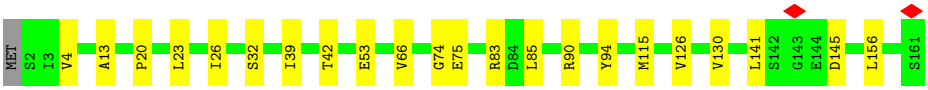




• Molecule 3: Allophycocyanin alpha chain

Chain s4:

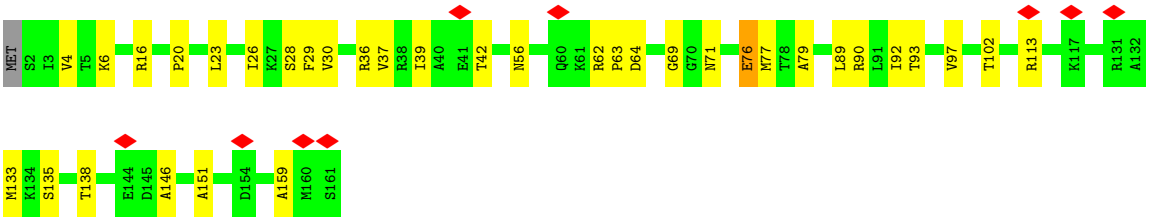




• Molecule 3: Allophycocyanin alpha chain

Chain u4:

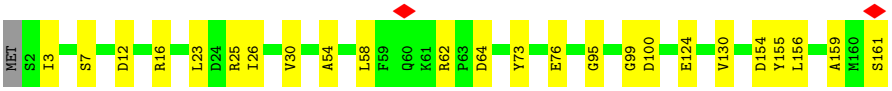




• Molecule 3: Allophycocyanin alpha chain

Chain w4:

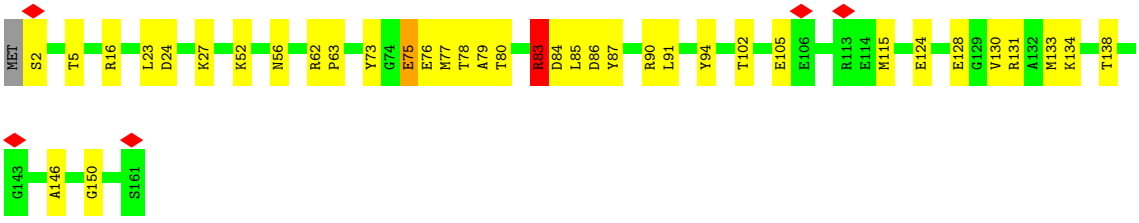




• Molecule 3: Allophycocyanin alpha chain

Chain o4:

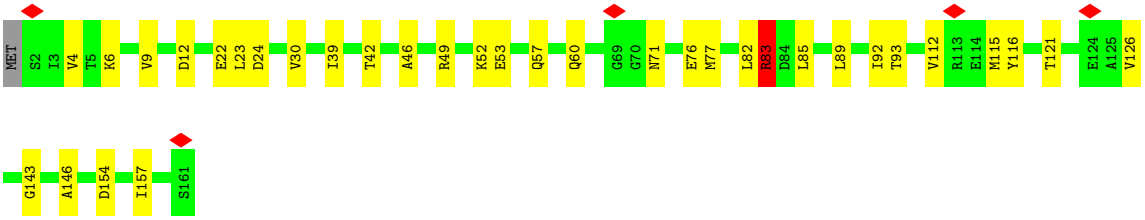




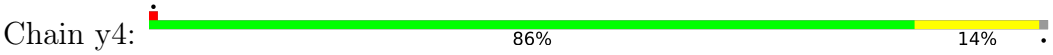
• Molecule 3: Allophycocyanin alpha chain

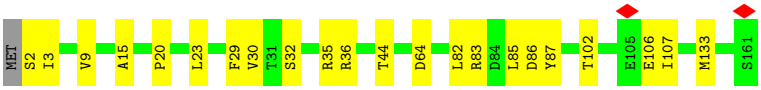
Chain q4:



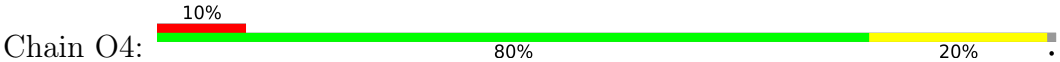


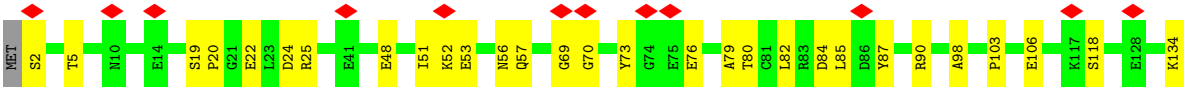
• Molecule 3: Allophycocyanin alpha chain

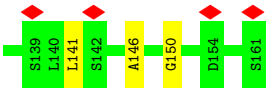




• Molecule 3: Allophycocyanin alpha chain

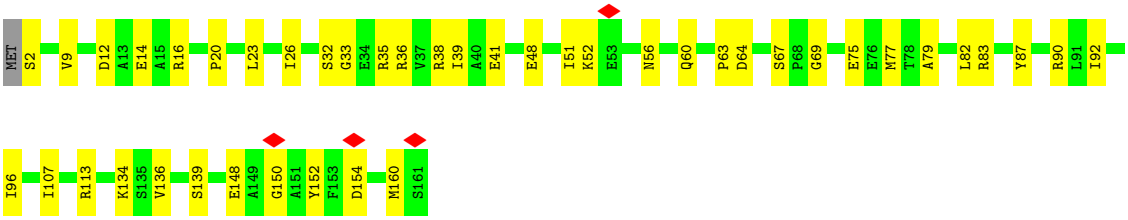




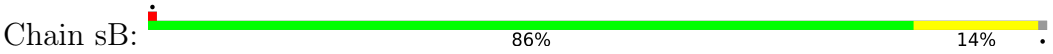


• Molecule 3: Allophycocyanin alpha chain



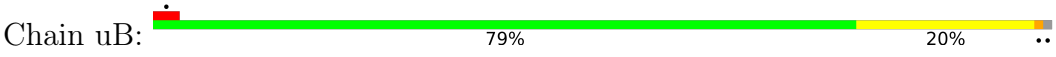


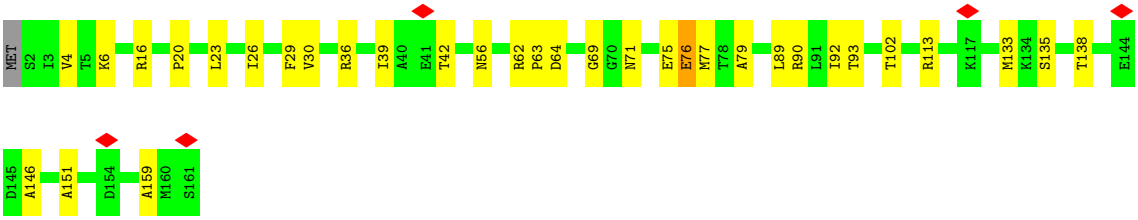
• Molecule 3: Allophycocyanin alpha chain





• Molecule 3: Allophycocyanin alpha chain





• Molecule 3: Allophycocyanin alpha chain

Chain wB:

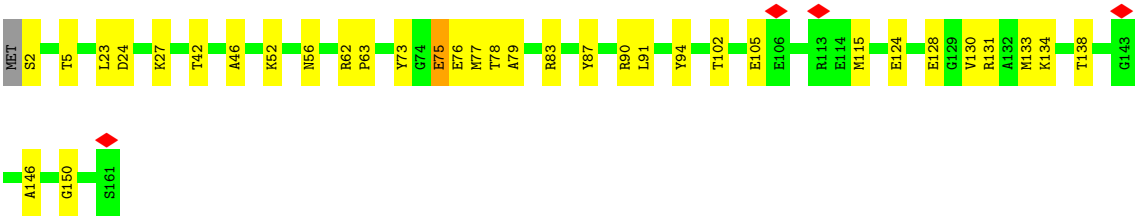




• Molecule 3: Allophycocyanin alpha chain

Chain oB:

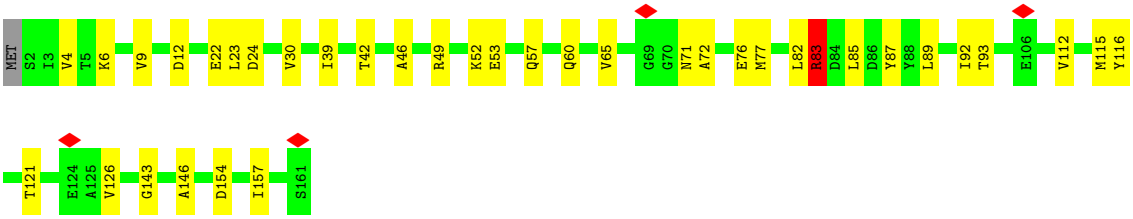




• Molecule 3: Allophycocyanin alpha chain

Chain qB:





• Molecule 3: Allophycocyanin alpha chain

Chain yB:

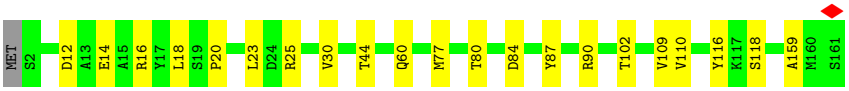




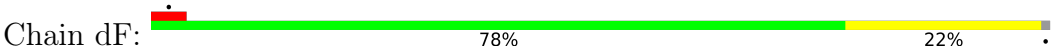
• Molecule 3: Allophycocyanin alpha chain

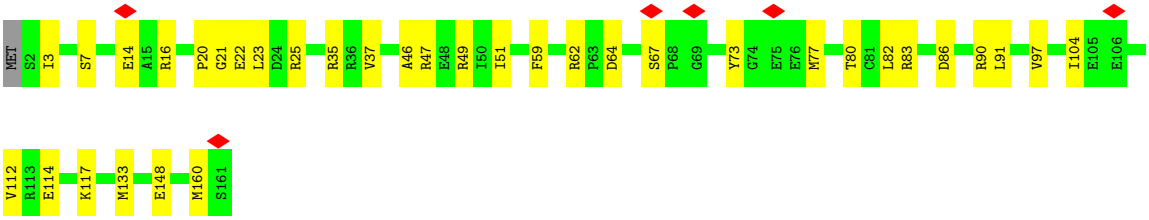
Chain bF:



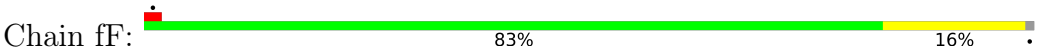


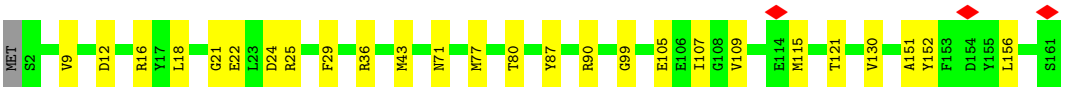
• Molecule 3: Allophycocyanin alpha chain



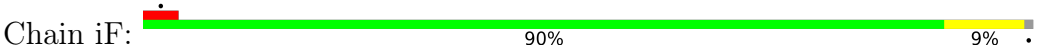


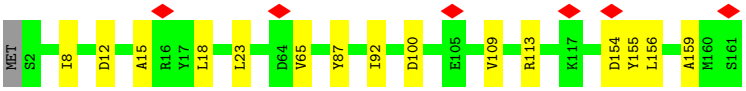
• Molecule 3: Allophycocyanin alpha chain



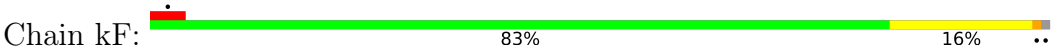


• Molecule 3: Allophycocyanin alpha chain



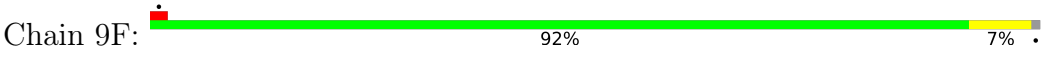


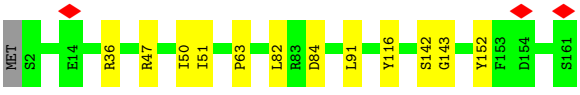
• Molecule 3: Allophycocyanin alpha chain



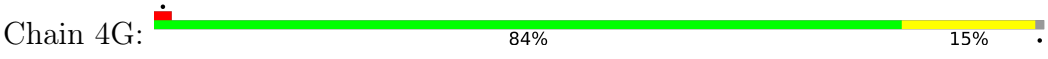


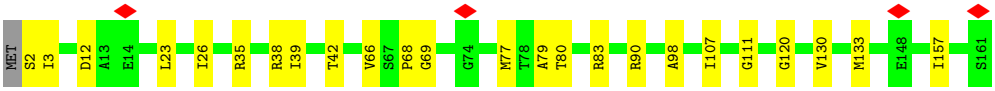
• Molecule 3: Allophycocyanin alpha chain





• Molecule 3: Allophycocyanin alpha chain

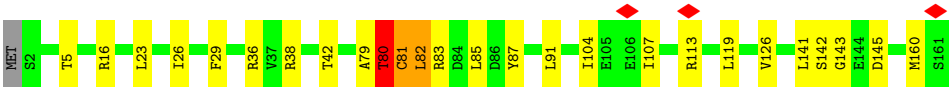




• Molecule 3: Allophycocyanin alpha chain

Chain 6G:

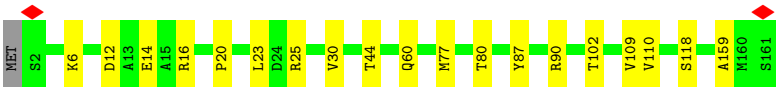




• Molecule 3: Allophycocyanin alpha chain

Chain bK:

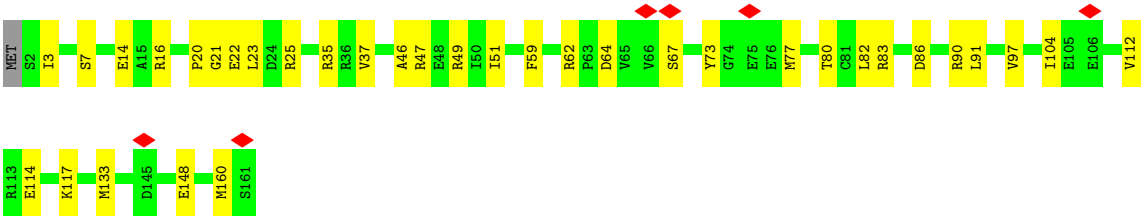




• Molecule 3: Allophycocyanin alpha chain

Chain dK:

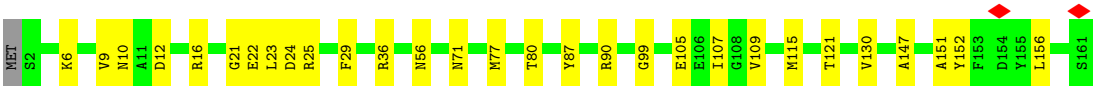




• Molecule 3: Allophycocyanin alpha chain

Chain fK:

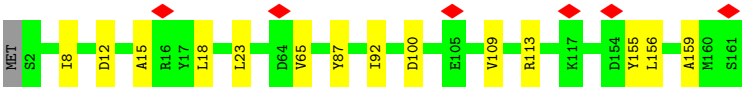




• Molecule 3: Allophycocyanin alpha chain

Chain iK:

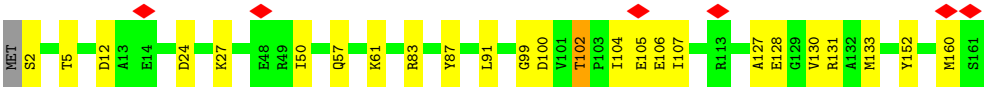




• Molecule 3: Allophycocyanin alpha chain

Chain kK:

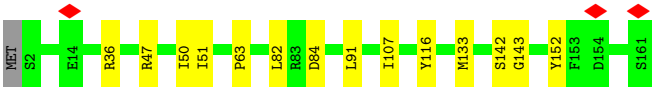




• Molecule 3: Allophycocyanin alpha chain

Chain 9K:

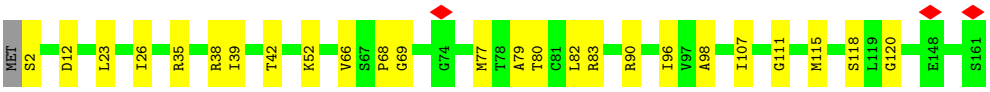




• Molecule 3: Allophycocyanin alpha chain

Chain 4L:

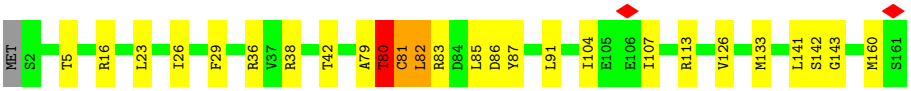




• Molecule 3: Allophycocyanin alpha chain

Chain 6L:

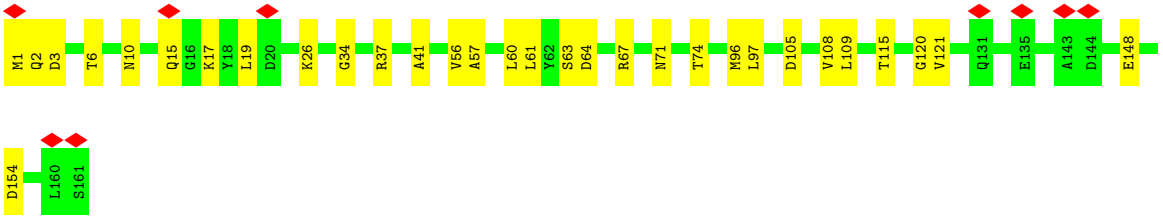




• Molecule 4: Allophycocyanin beta chain

Chain PB:

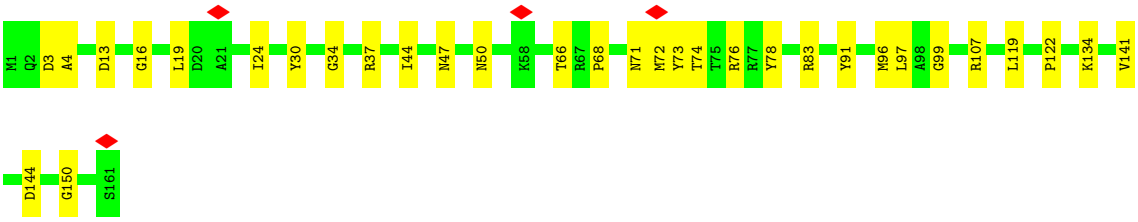




• Molecule 4: Allophycocyanin beta chain

Chain RB:

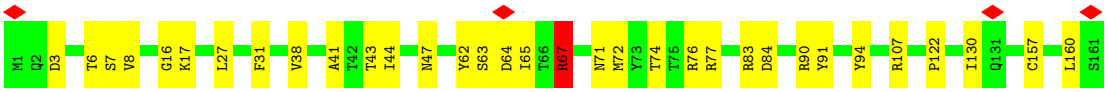




• Molecule 4: Allophycocyanin beta chain

Chain TB:

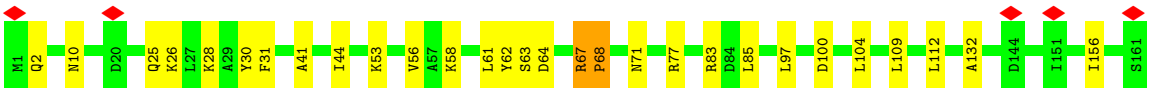




• Molecule 4: Allophycocyanin beta chain

Chain WB:

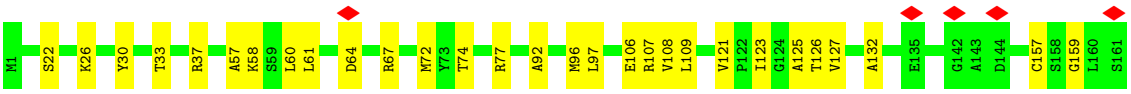




• Molecule 4: Allophycocyanin beta chain

Chain YB:

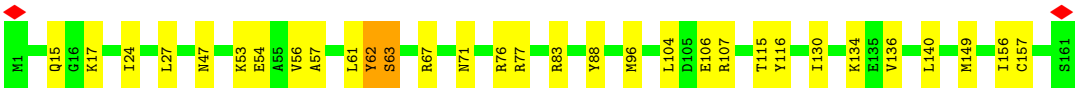




• Molecule 4: Allophycocyanin beta chain

Chain IF:

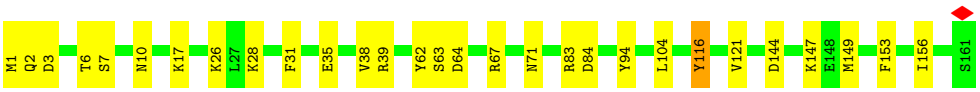




• Molecule 4: Allophycocyanin beta chain

Chain KF:

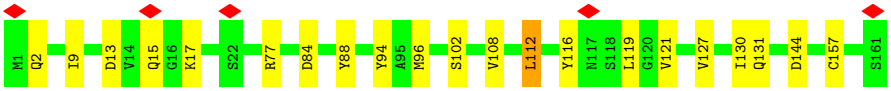




• Molecule 4: Allophycocyanin beta chain

Chain MF:

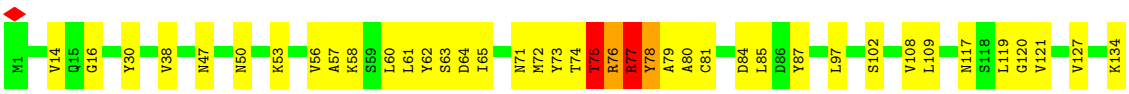


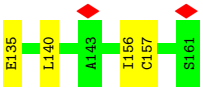


• Molecule 4: Allophycocyanin beta chain

Chain YF:



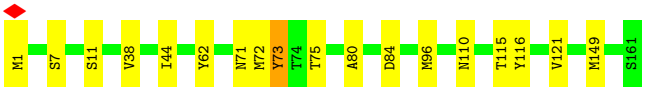




• Molecule 4: Allophycocyanin beta chain

Chain HG:



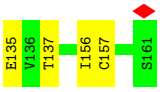


• Molecule 4: Allophycocyanin beta chain

Chain JG:



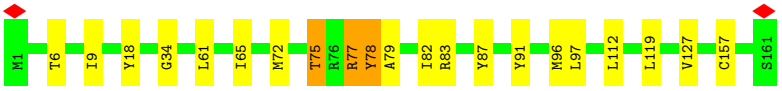




• Molecule 4: Allophycocyanin beta chain

Chain LG:





• Molecule 4: Allophycocyanin beta chain

Chain MG:

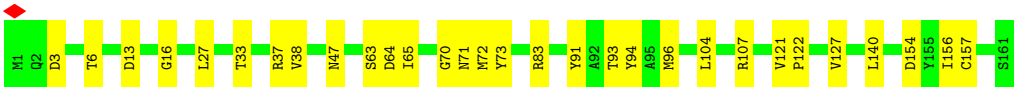




• Molecule 4: Allophycocyanin beta chain

Chain OG:

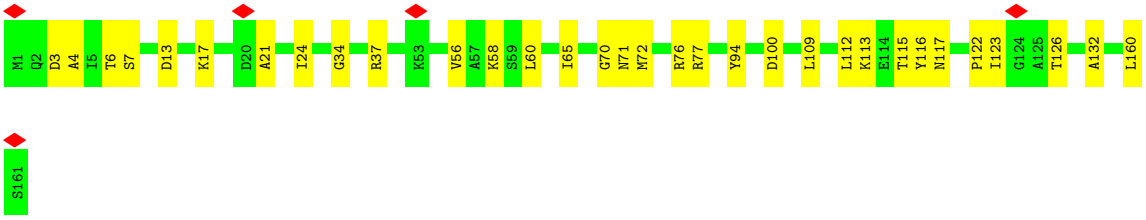




• Molecule 4: Allophycocyanin beta chain

Chain SG:

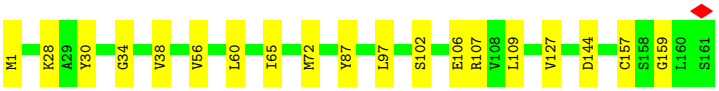




• Molecule 4: Allophycocyanin beta chain

Chain UG:

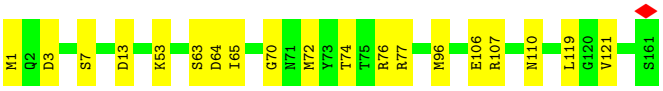




• Molecule 4: Allophycocyanin beta chain

Chain WG:

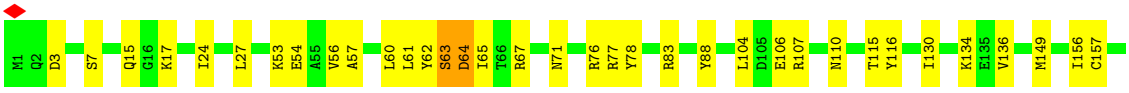




• Molecule 4: Allophycocyanin beta chain

Chain IK:

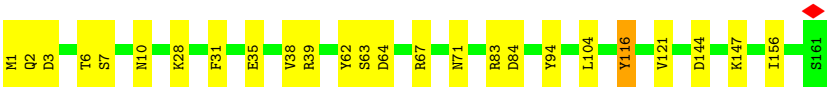




• Molecule 4: Allophycocyanin beta chain

Chain KK:

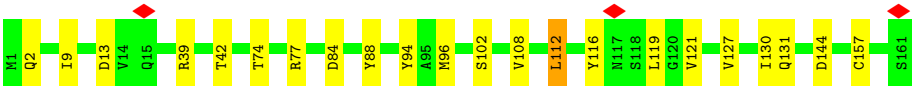




• Molecule 4: Allophycocyanin beta chain

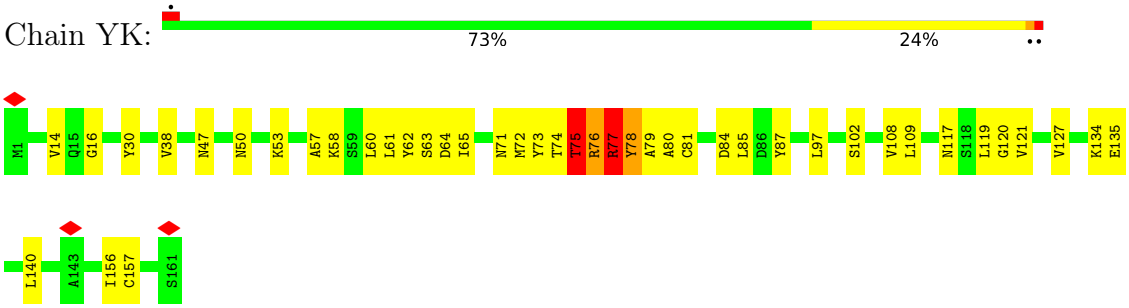
Chain MK:





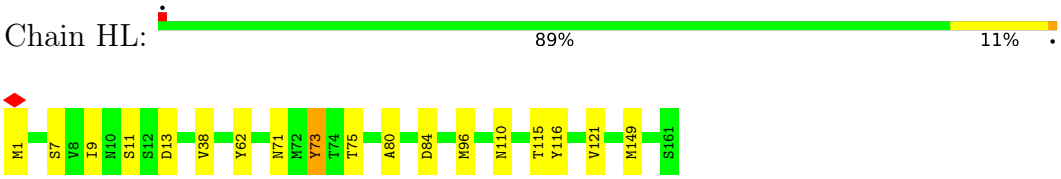
• Molecule 4: Allophycocyanin beta chain

Chain YK:



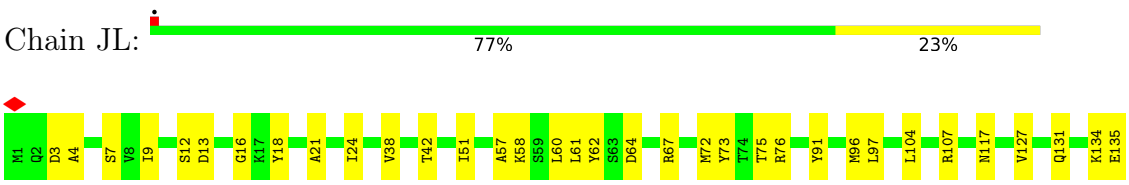
• Molecule 4: Allophycocyanin beta chain

Chain HL:



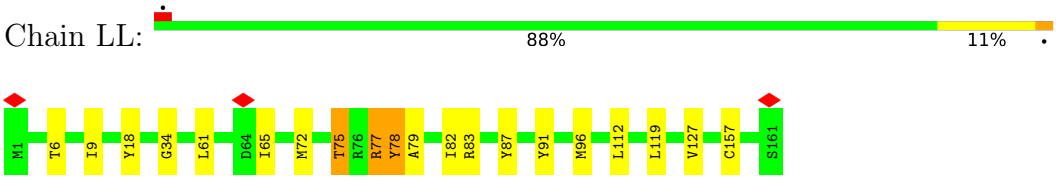
• Molecule 4: Allophycocyanin beta chain

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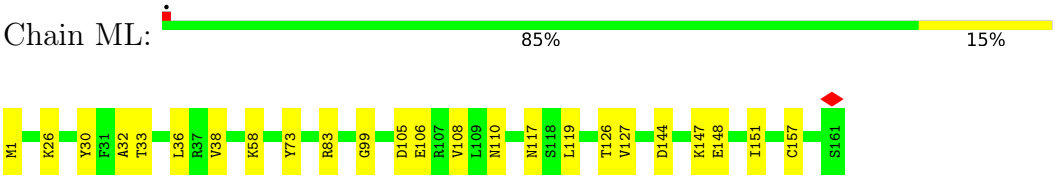
• Molecule 4: Allophycocyanin beta chain

Chain LL:



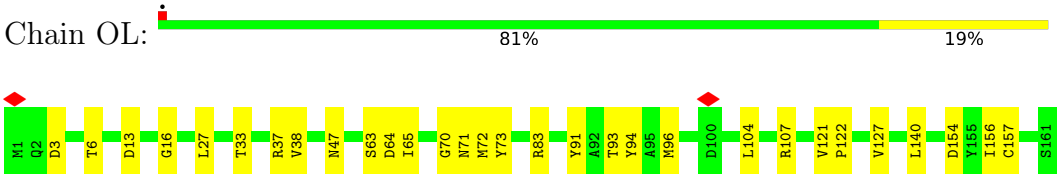
• Molecule 4: Allophycocyanin beta chain

Chain ML:



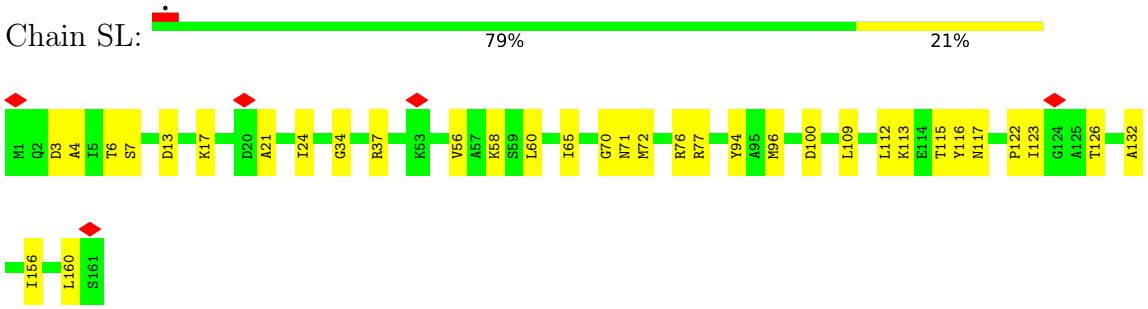
• Molecule 4: Allophycocyanin beta chain

Chain OL:



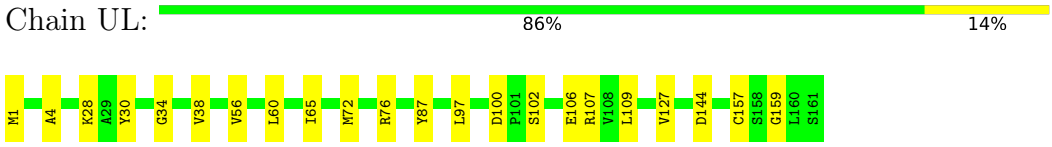
• Molecule 4: Allophycocyanin beta chain

Chain SL:



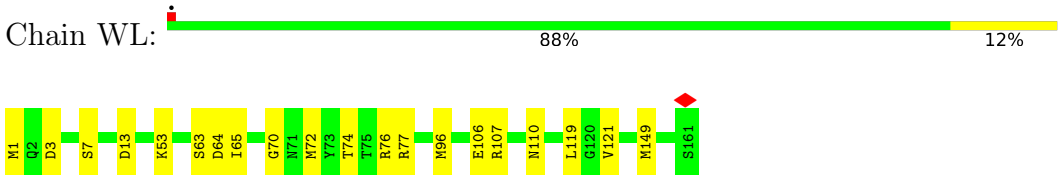
• Molecule 4: Allophycocyanin beta chain

Chain UL:



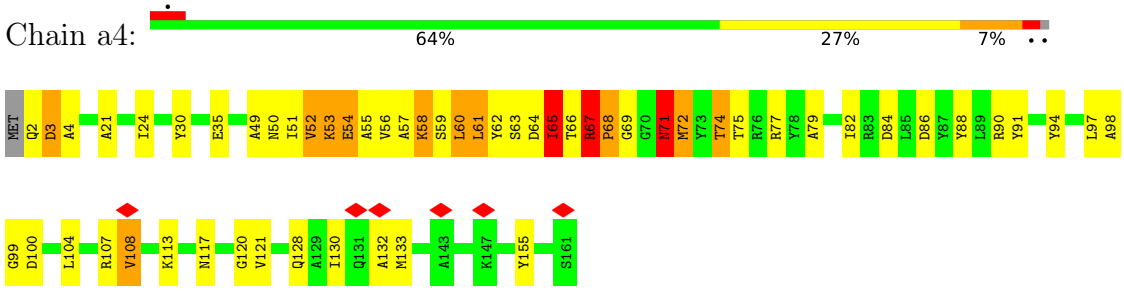
• Molecule 4: Allophycocyanin beta chain

Chain WL:



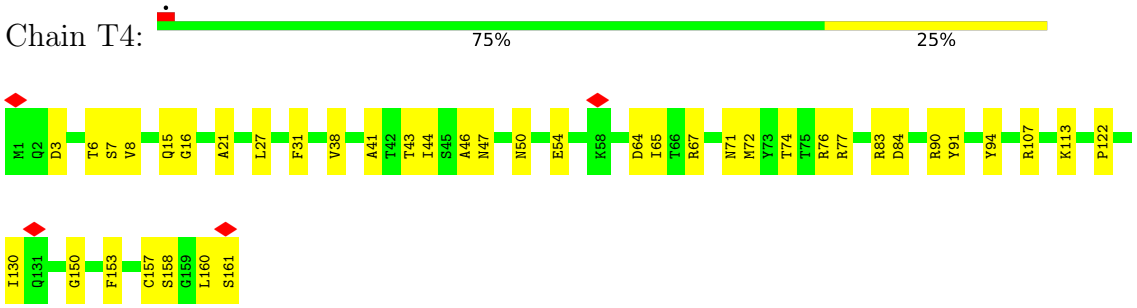
• Molecule 4: Allophycocyanin beta chain

Chain a4:



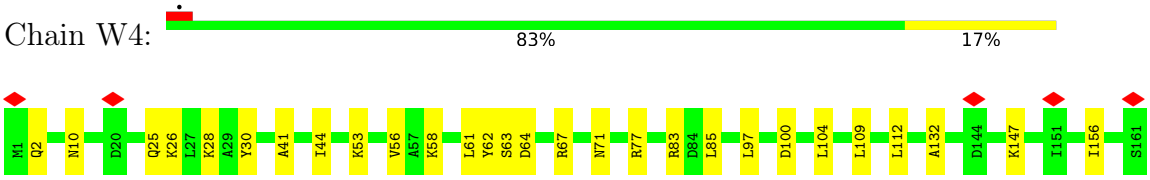
• Molecule 4: Allophycocyanin beta chain

Chain T4:



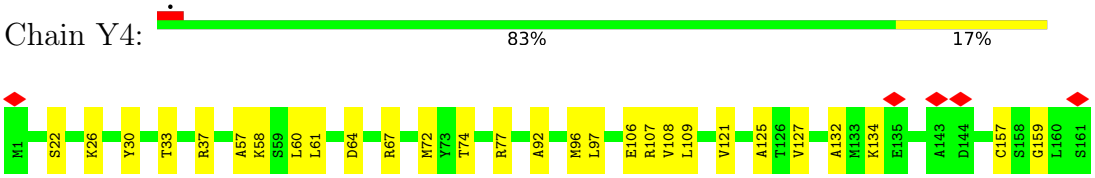
• Molecule 4: Allophycocyanin beta chain

Chain W4:



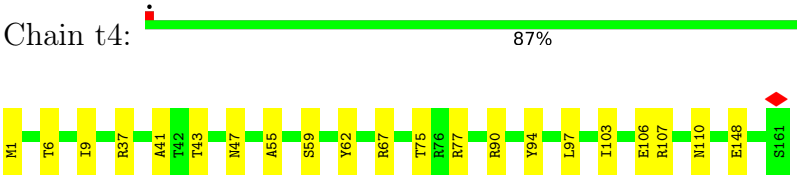
• Molecule 4: Allophycocyanin beta chain

Chain Y4:



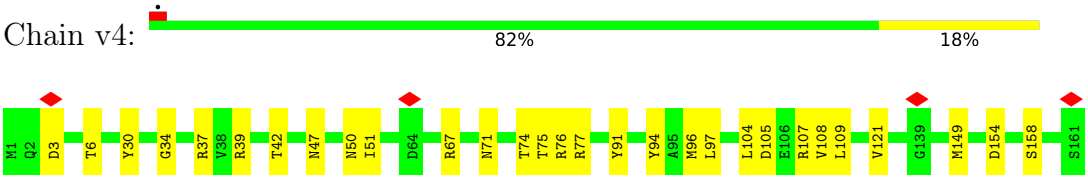
• Molecule 4: Allophycocyanin beta chain

Chain t4:



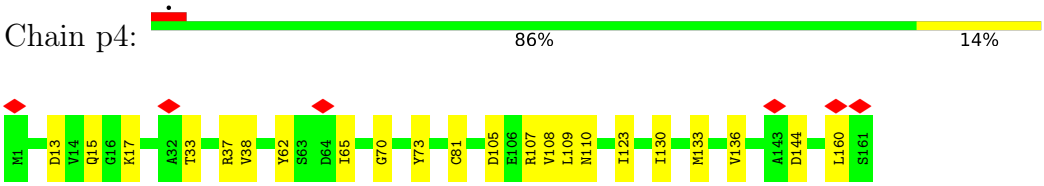
• Molecule 4: Allophycocyanin beta chain

Chain v4:



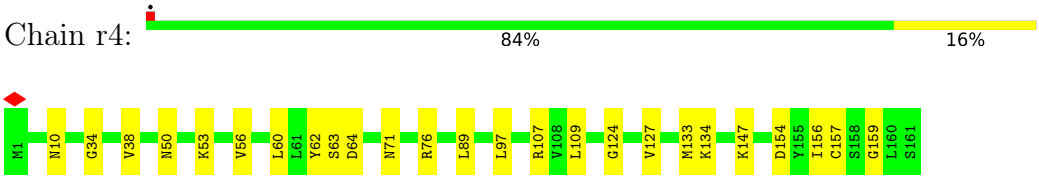
• Molecule 4: Allophycocyanin beta chain

Chain p4:



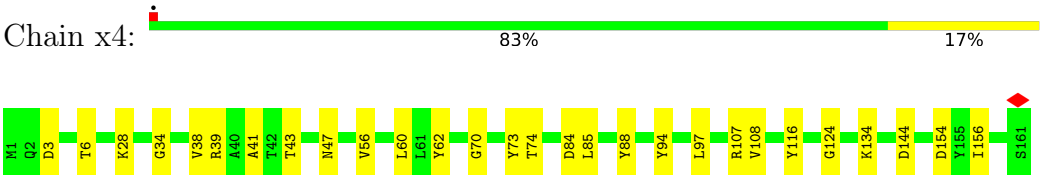
• Molecule 4: Allophycocyanin beta chain

Chain r4:



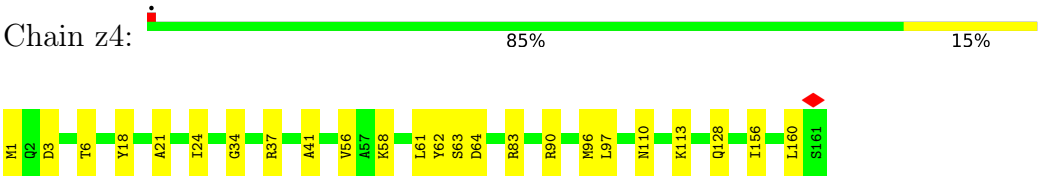
• Molecule 4: Allophycocyanin beta chain

Chain x4:



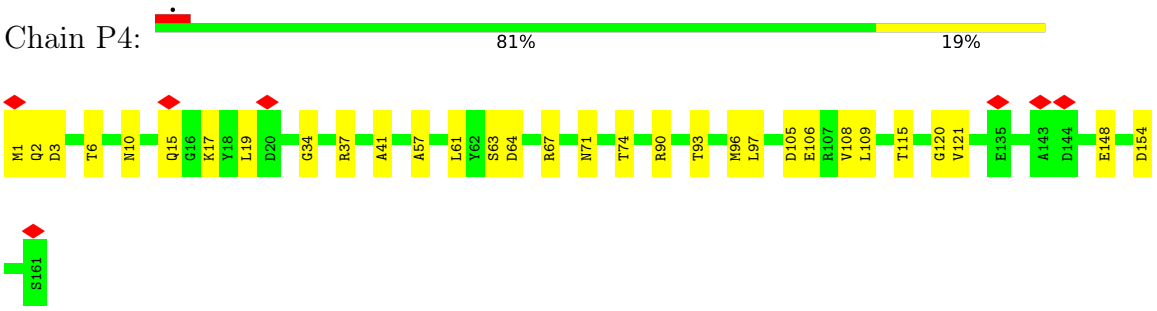
• Molecule 4: Allophycocyanin beta chain

Chain z4:



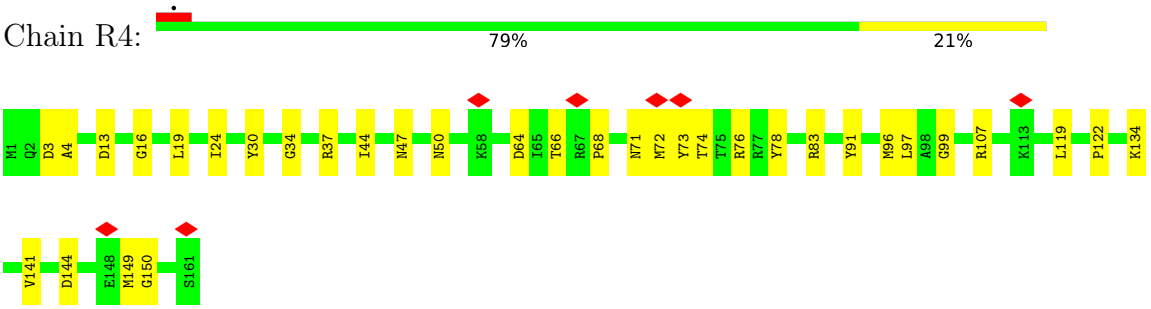
• Molecule 4: Allophycocyanin beta chain

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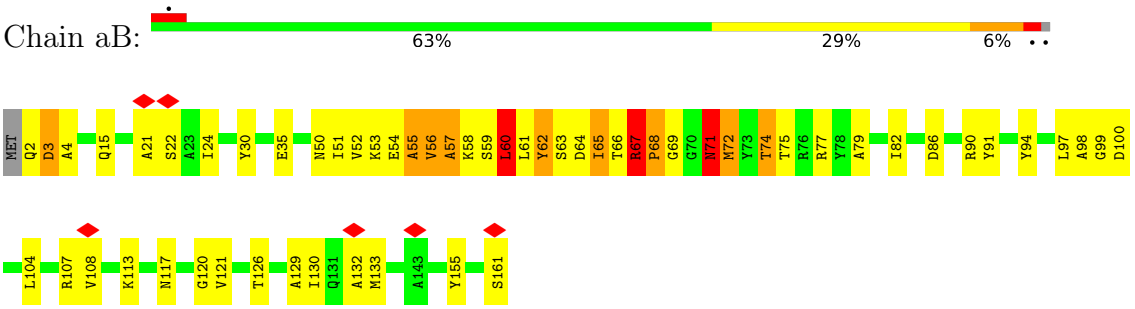
• Molecule 4: Allophycocyanin beta chain

Chain R4:



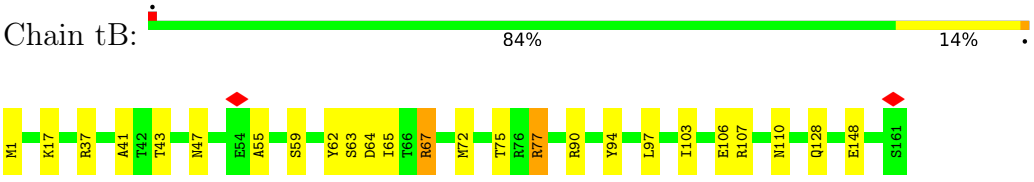
• Molecule 4: Allophycocyanin beta chain

Chain aB:



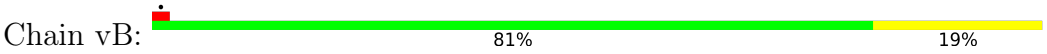
• Molecule 4: Allophycocyanin beta chain

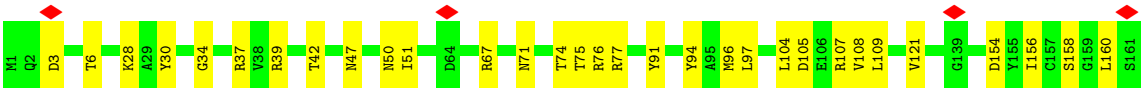
Chain tB:



• Molecule 4: Allophycocyanin beta chain

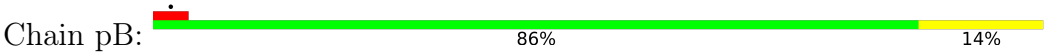
Chain vB:

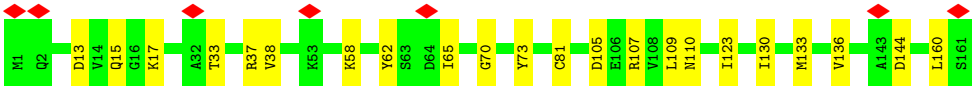




• Molecule 4: Allophycocyanin beta chain

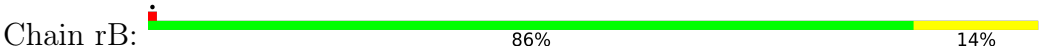
Chain pB:





• Molecule 4: Allophycocyanin beta chain

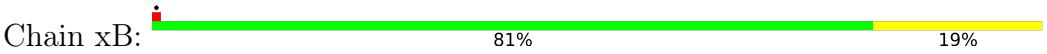
Chain rB:





• Molecule 4: Allophycocyanin beta chain

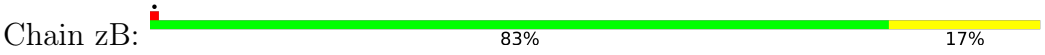
Chain xB:

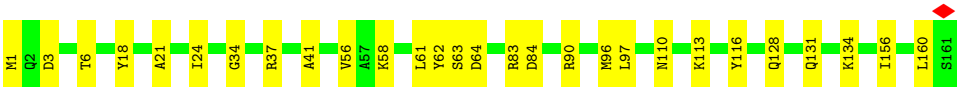




• Molecule 4: Allophycocyanin beta chain

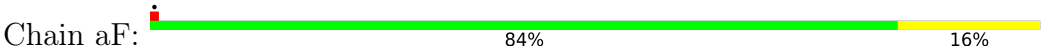
Chain zB:





• Molecule 4: Allophycocyanin beta chain

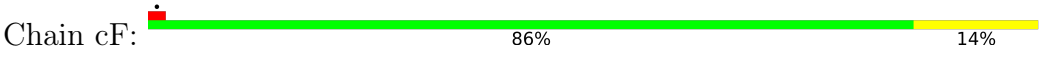
Chain aF:





• Molecule 4: Allophycocyanin beta chain

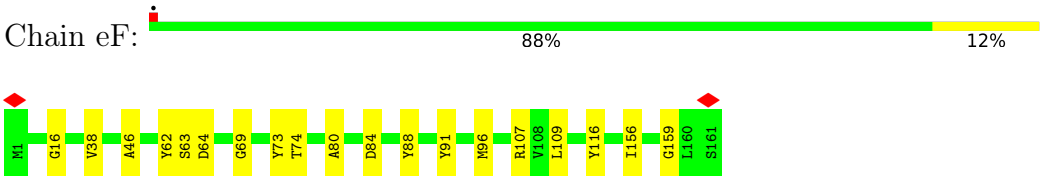
Chain cF:





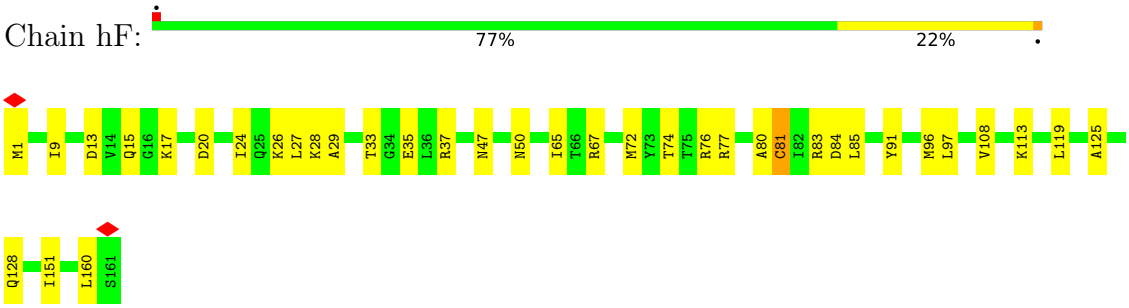
• Molecule 4: Allophycocyanin beta chain

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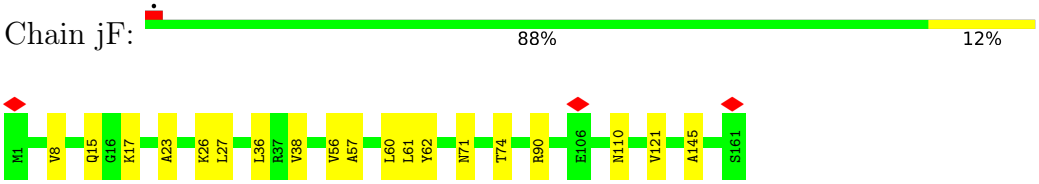
• Molecule 4: Allophycocyanin beta chain

Chain hF:



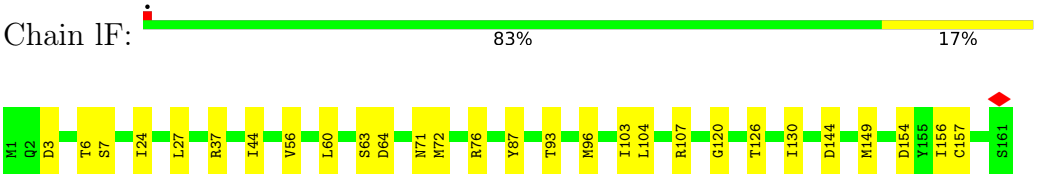
• Molecule 4: Allophycocyanin beta chain

Chain jF:



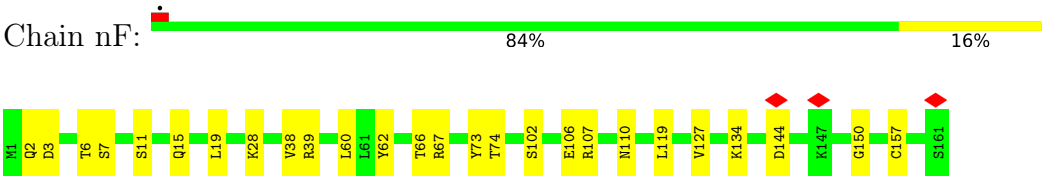
• Molecule 4: Allophycocyanin beta chain

Chain lF:



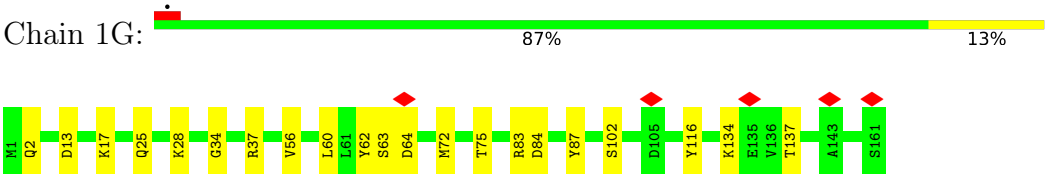
• Molecule 4: Allophycocyanin beta chain

Chain nF:



• Molecule 4: Allophycocyanin beta chain

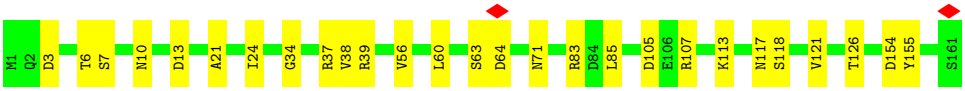
Chain 1G:



• Molecule 4: Allophycocyanin beta chain

Chain 5G:





• Molecule 4: Allophycocyanin beta chain

Chain 7G:

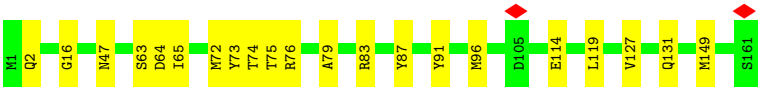




• Molecule 4: Allophycocyanin beta chain

Chain aK:

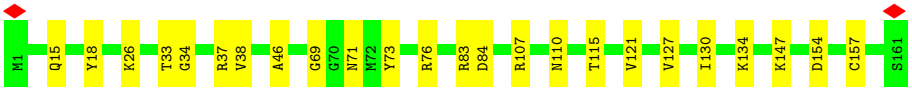




• Molecule 4: Allophycocyanin beta chain

Chain cK:

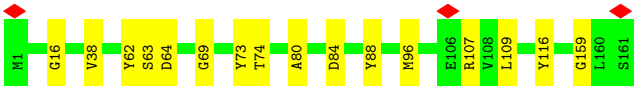




• Molecule 4: Allophycocyanin beta chain

Chain eK:

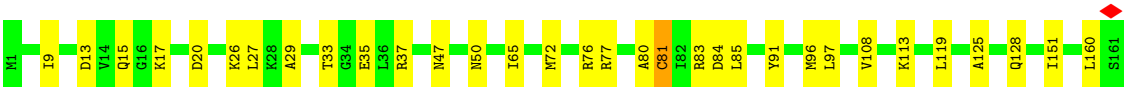




• Molecule 4: Allophycocyanin beta chain

Chain hK:

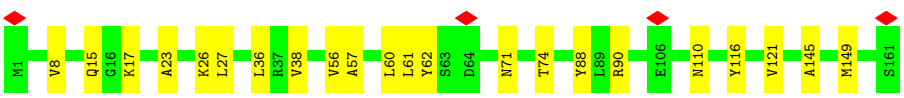




• Molecule 4: Allophycocyanin beta chain

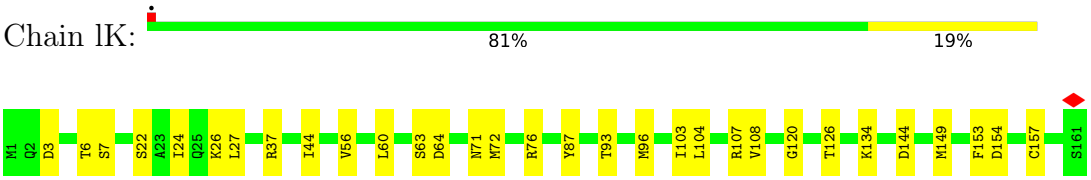
Chain jK:





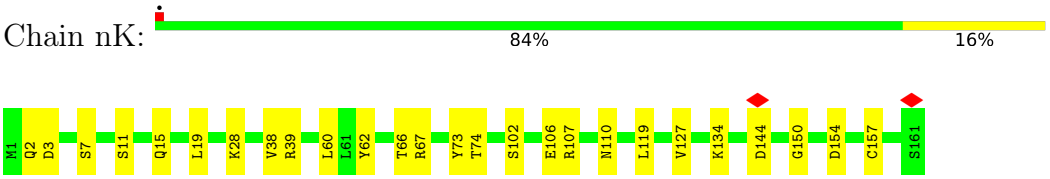
• Molecule 4: Allophycocyanin beta chain

Chain lK:



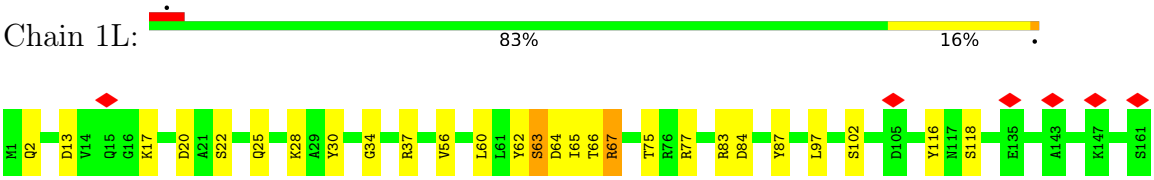
• Molecule 4: Allophycocyanin beta chain

Chain nK:



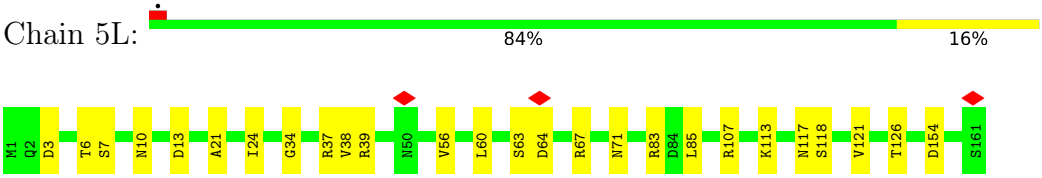
• Molecule 4: Allophycocyanin beta chain

Chain 1L:



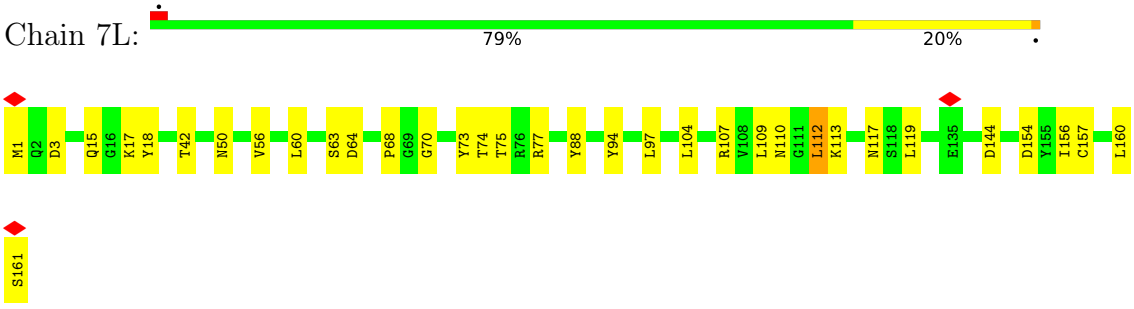
• Molecule 4: Allophycocyanin beta chain

Chain 5L:



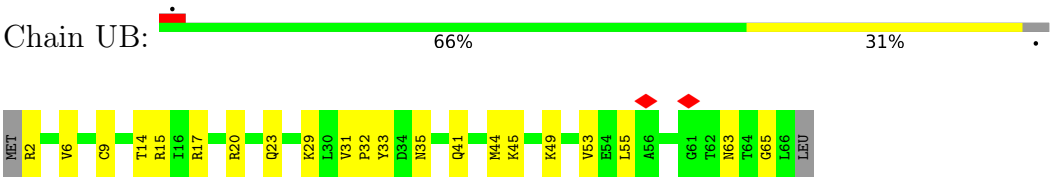
• Molecule 4: Allophycocyanin beta chain

Chain 7L:



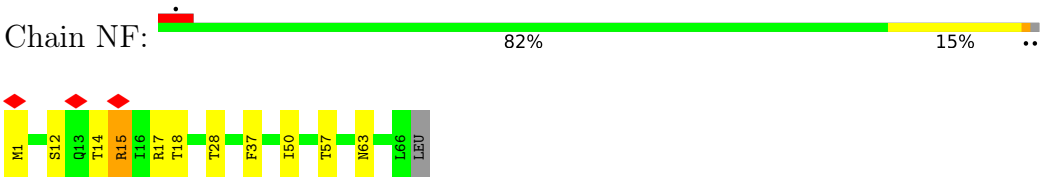
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain UB:



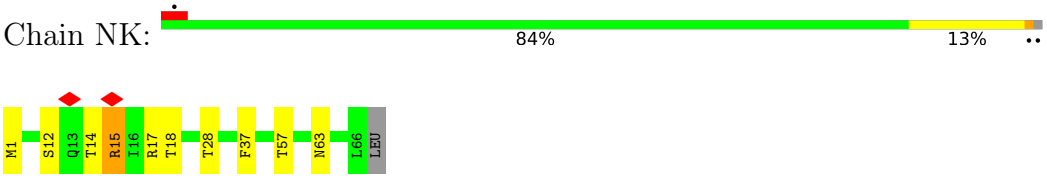
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain NF:



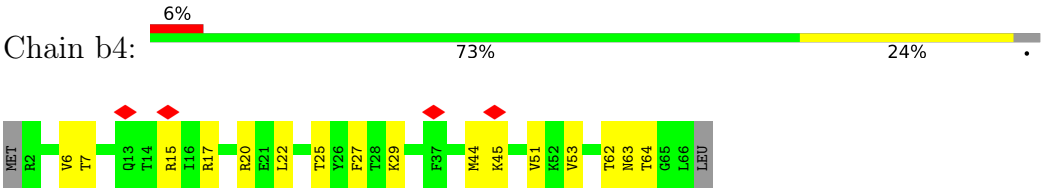
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain NK:



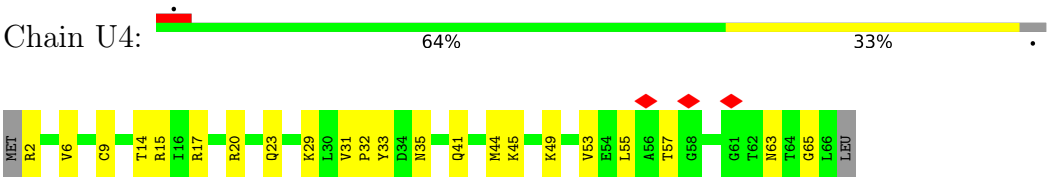
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain b4:



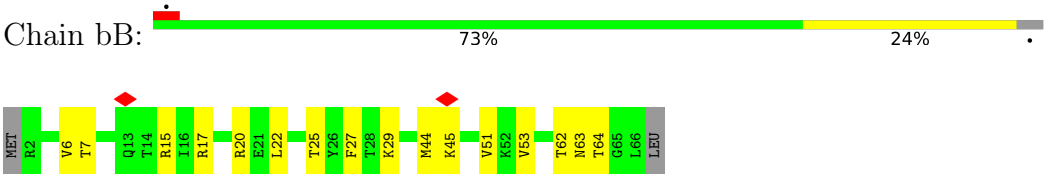
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain U4:



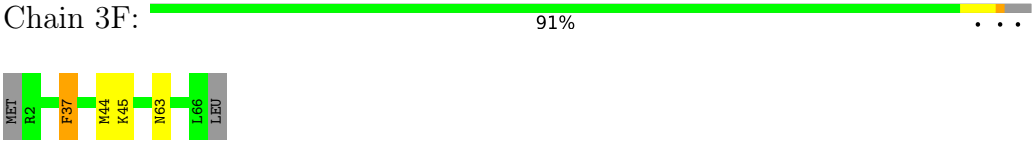
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain bB:



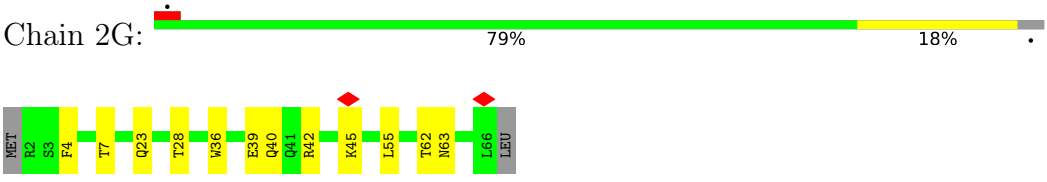
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain 3F:



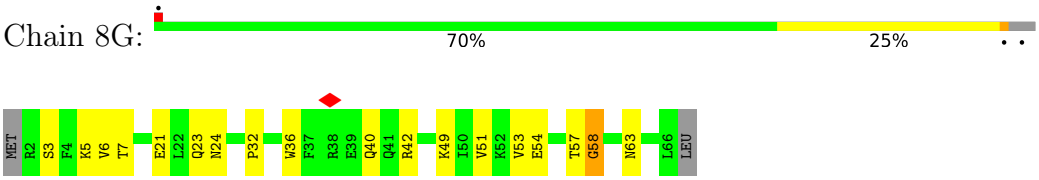
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain 2G:



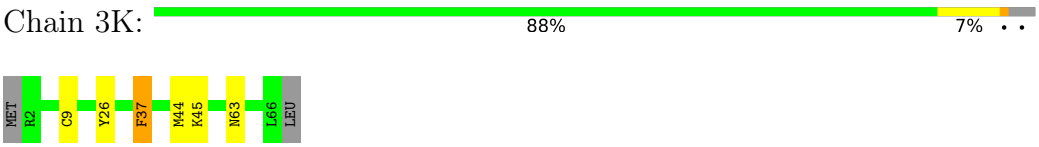
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain 8G:



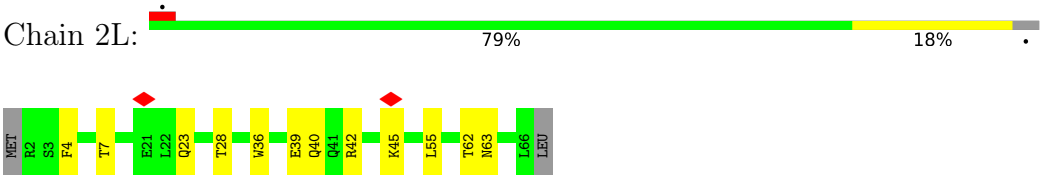
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain 3K:



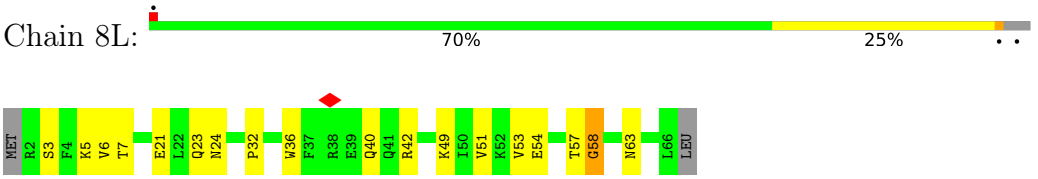
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain 2L:



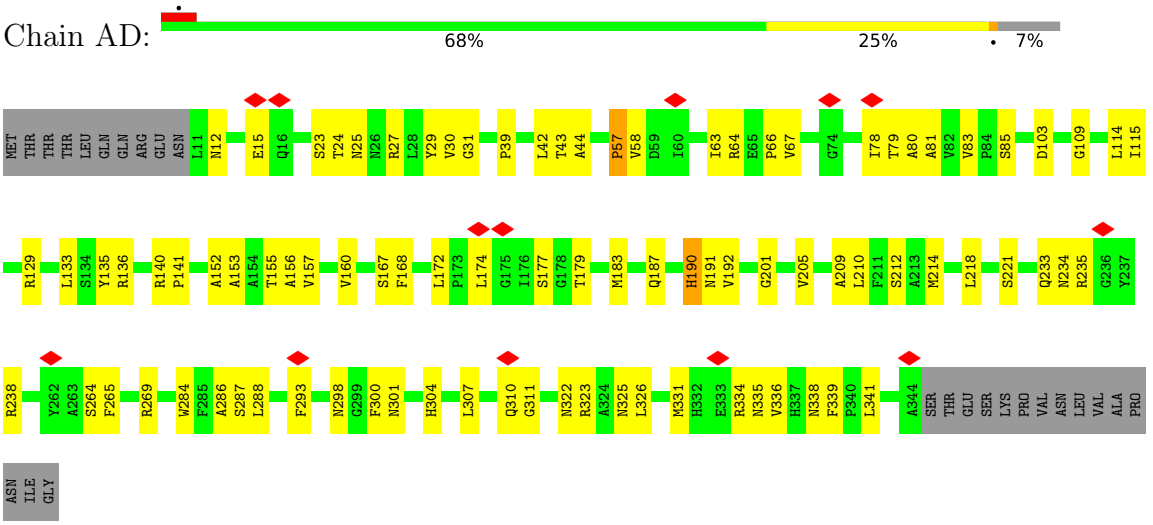
• Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain 8L:



• Molecule 6: Photosystem II protein D1

Chain AD:



• Molecule 6: Photosystem II protein D1

Chain AE:

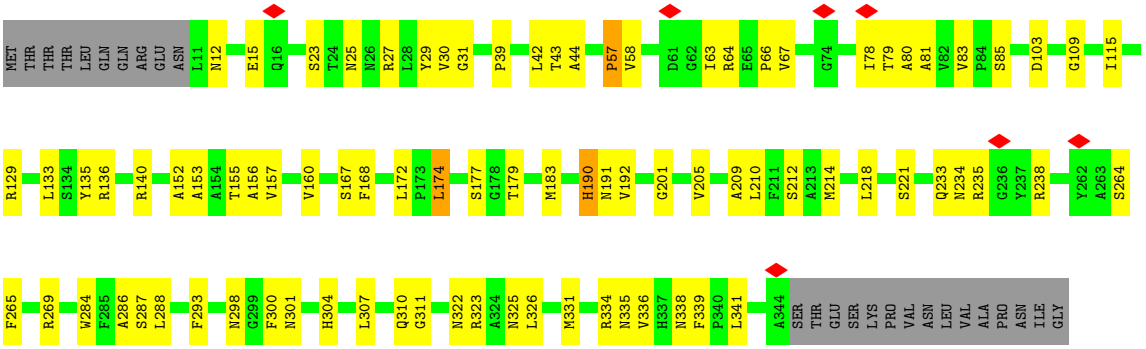




• Molecule 6: Photosystem II protein D1

Chain A1:

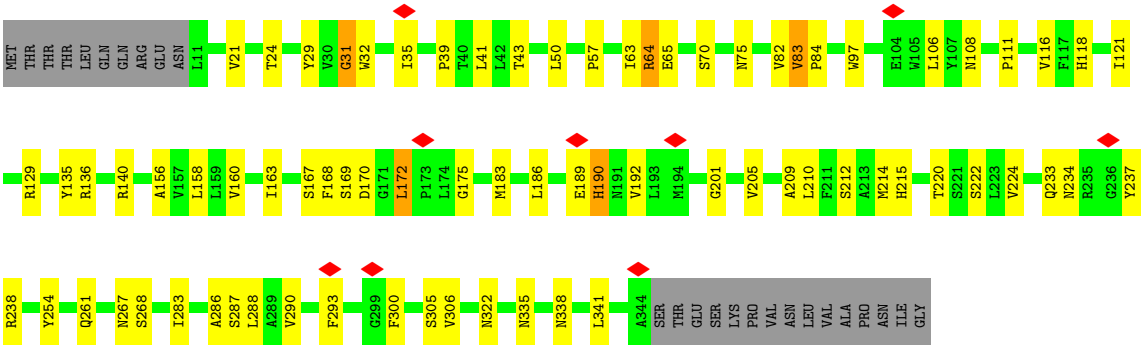




• Molecule 6: Photosystem II protein D1

Chain a1:

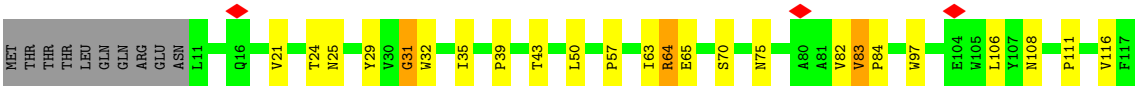


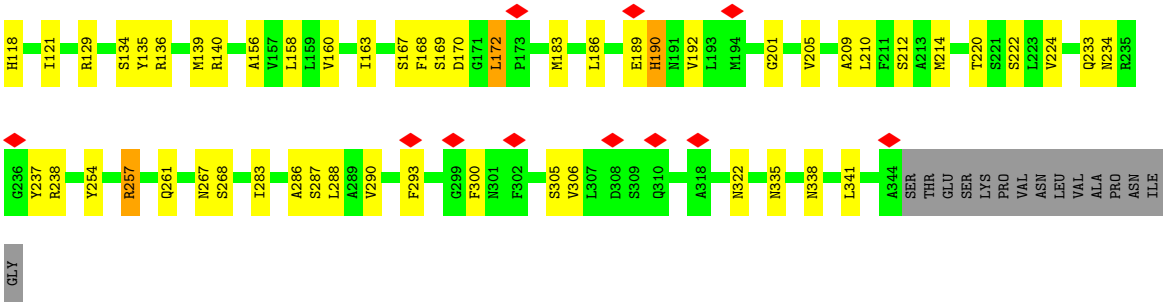


• Molecule 6: Photosystem II protein D1

Chain aD:



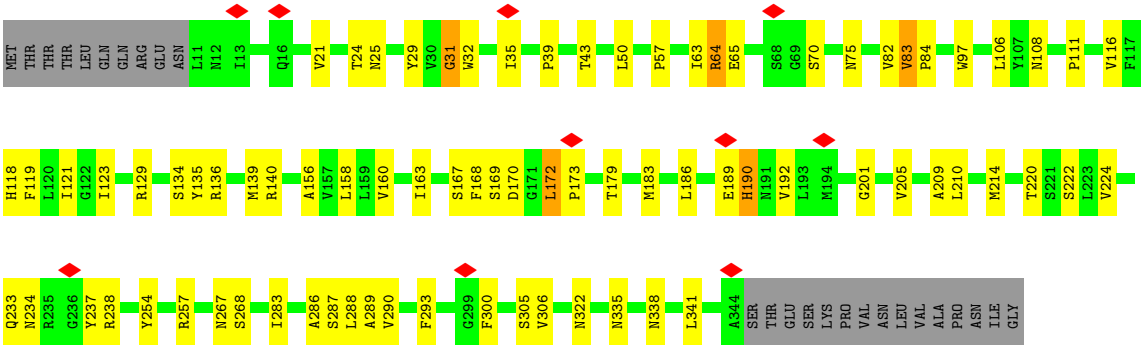




• Molecule 6: Photosystem II protein D1

Chain aE:

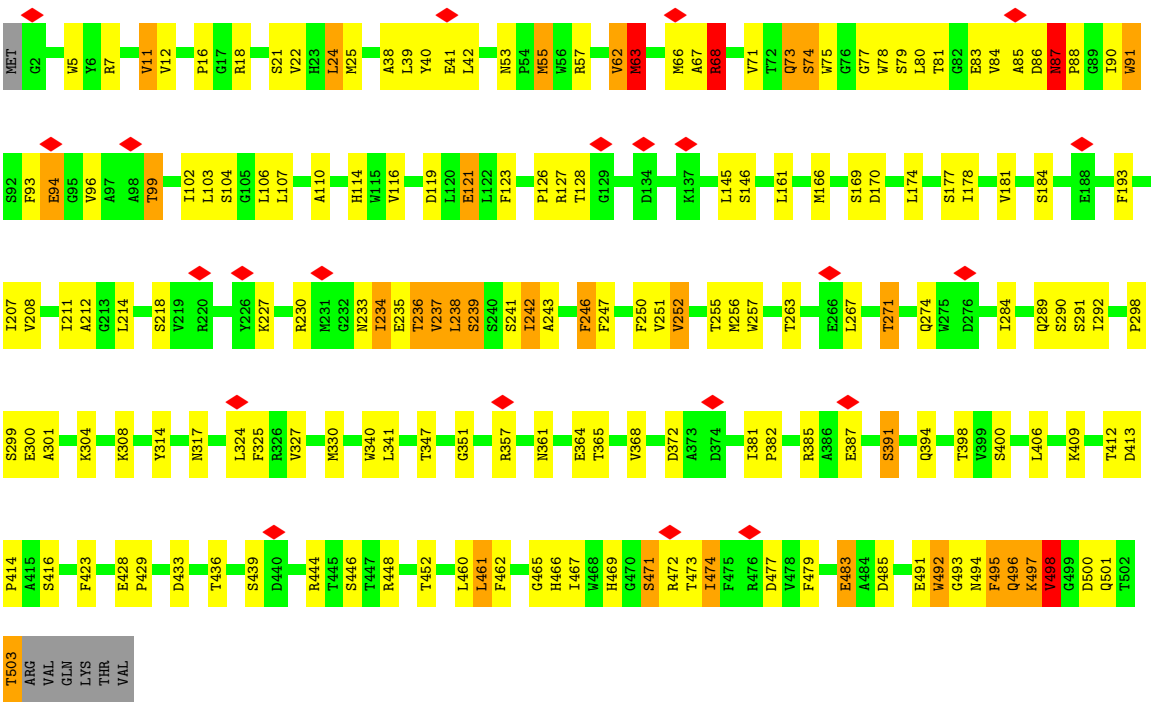




• Molecule 7: Photosystem II CP47 reaction center protein

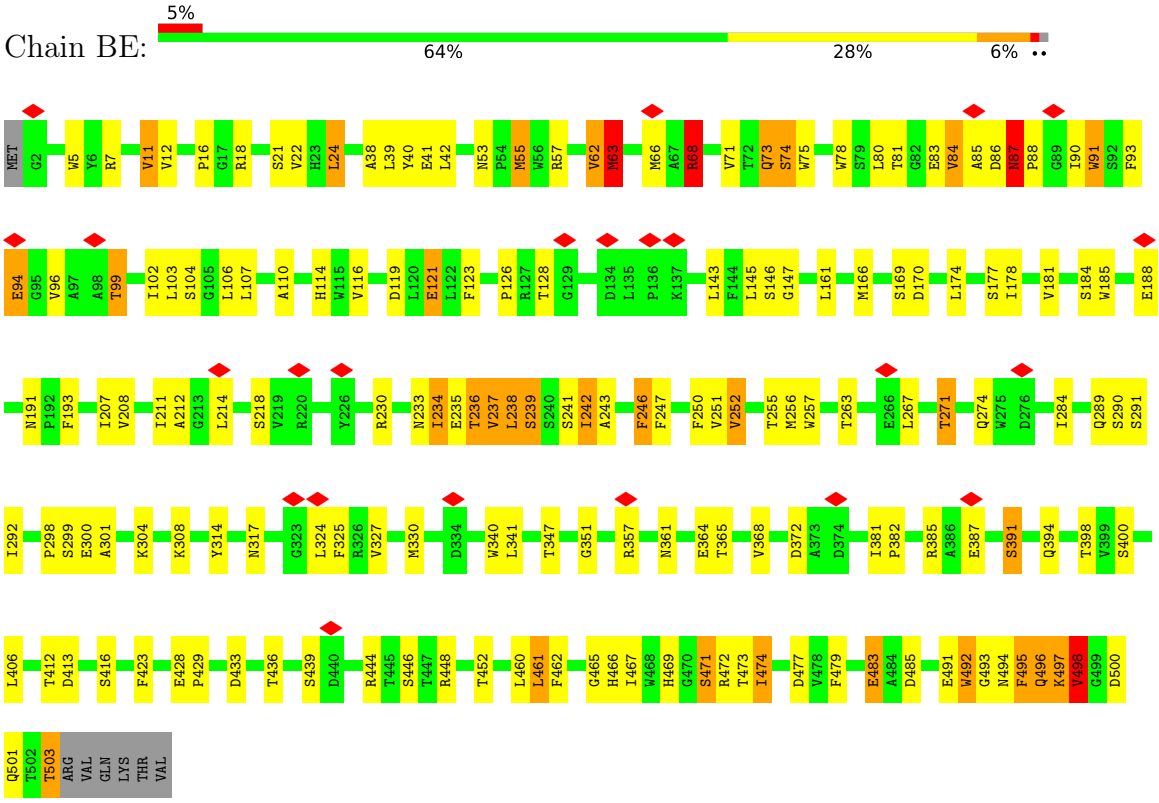
Chain BD:





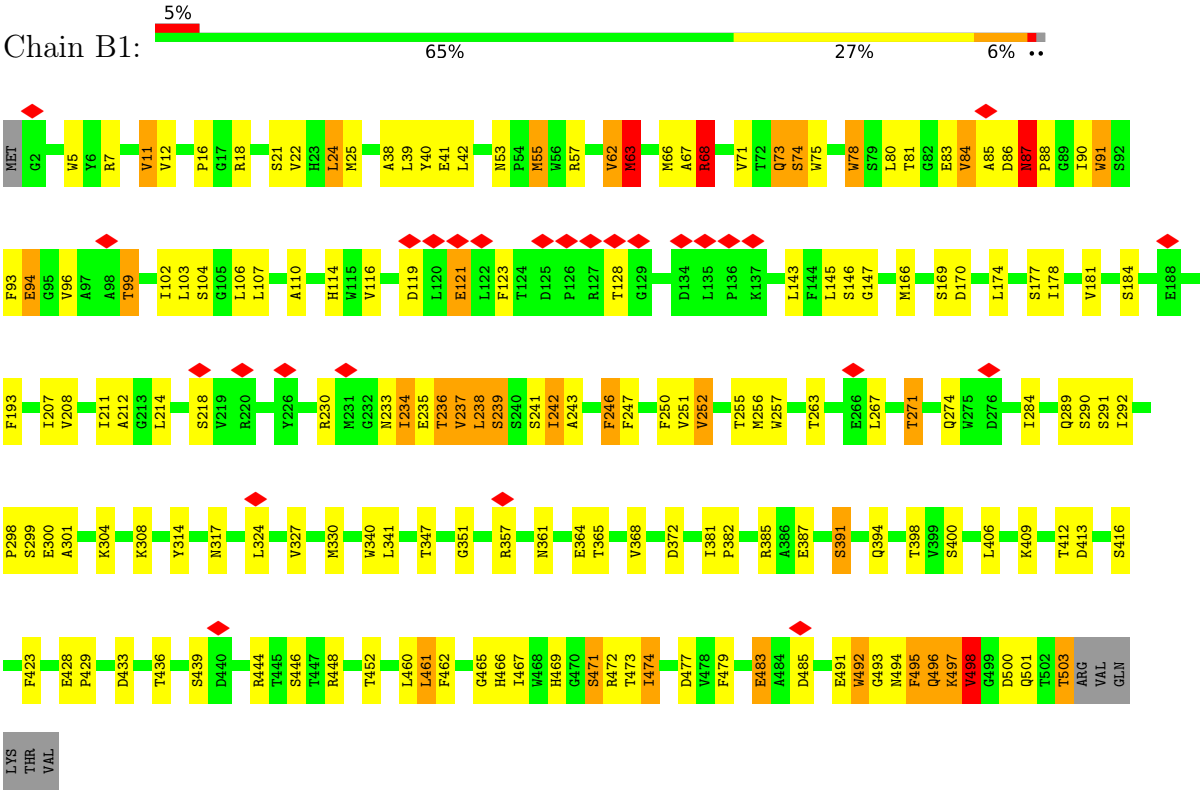
• Molecule 7: Photosystem II CP47 reaction center protein

Chain BE:



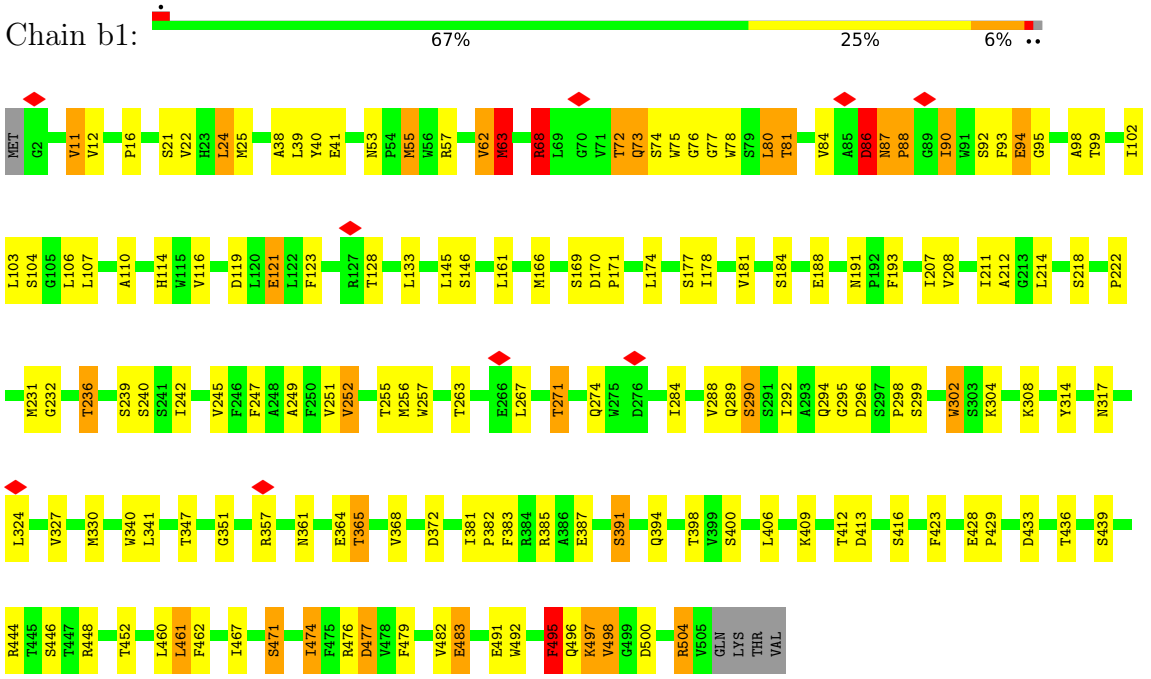
• Molecule 7: Photosystem II CP47 reaction center protein

Chain B1:



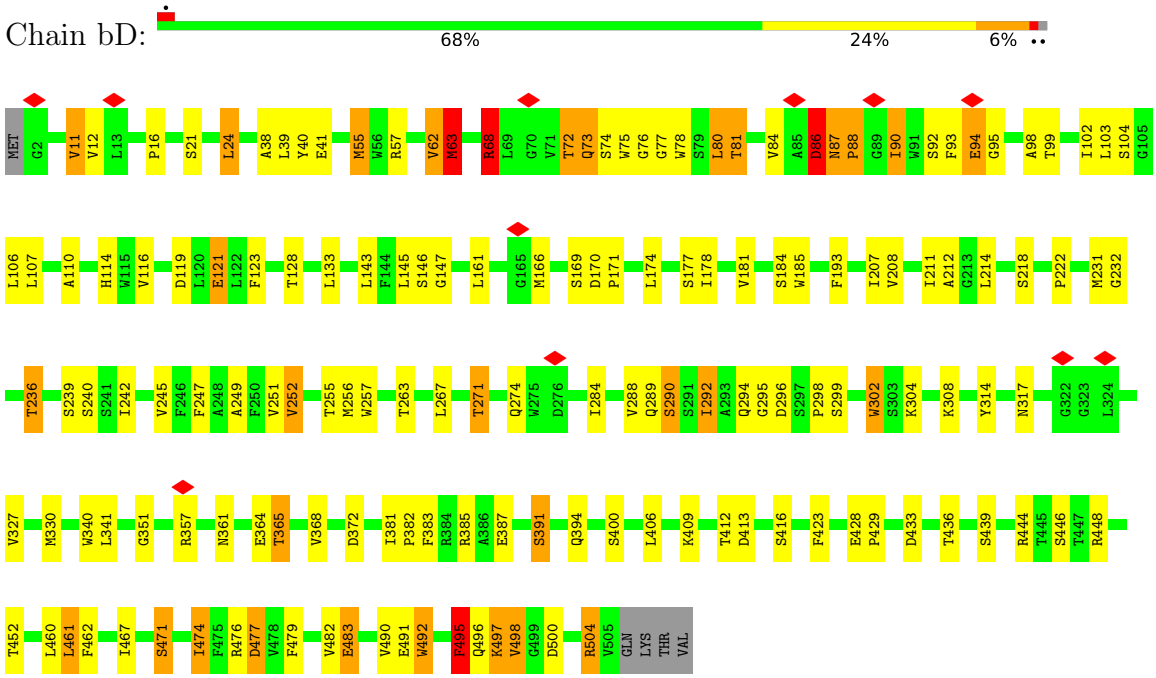
• Molecule 7: Photosystem II CP47 reaction center protein

Chain b1:



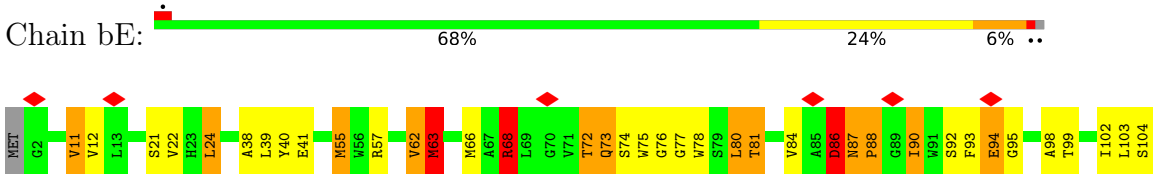
• Molecule 7: Photosystem II CP47 reaction center protein

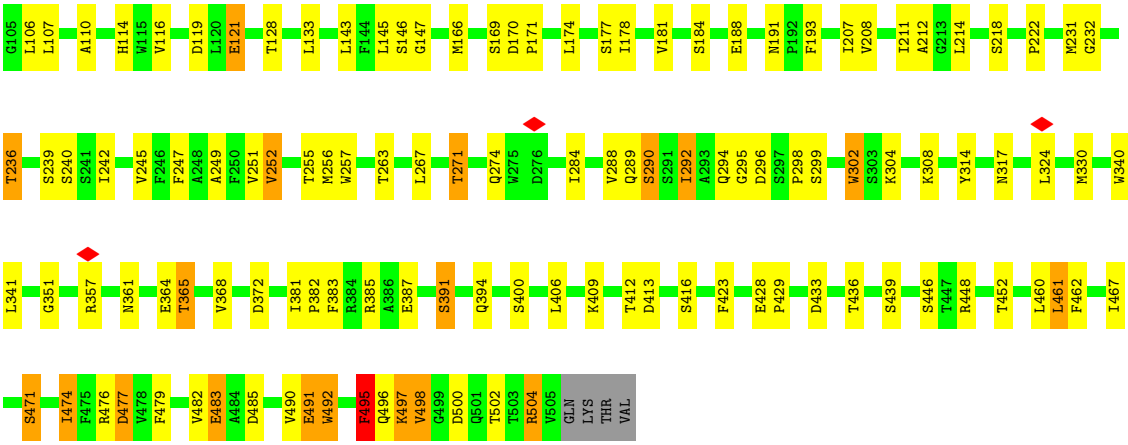
Chain bD:



• Molecule 7: Photosystem II CP47 reaction center protein

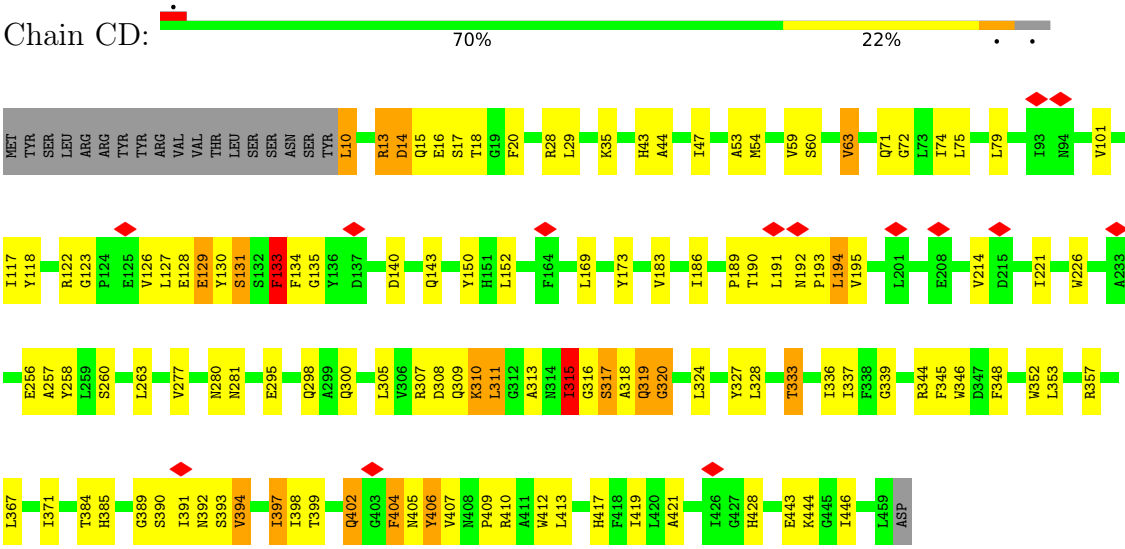
Chain bE:





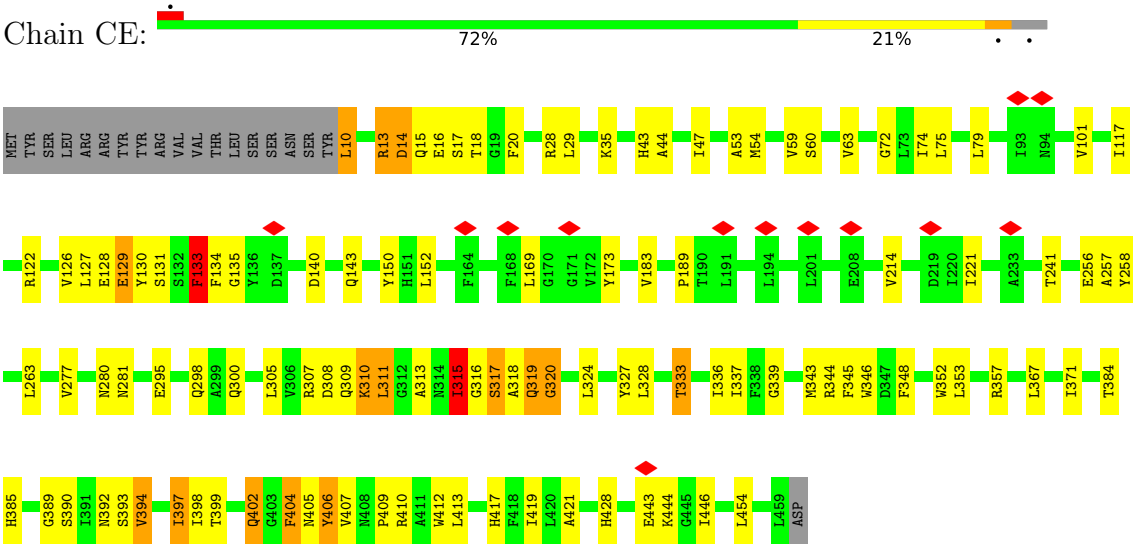
• Molecule 8: Photosystem II CP43 reaction center protein

Chain CD:



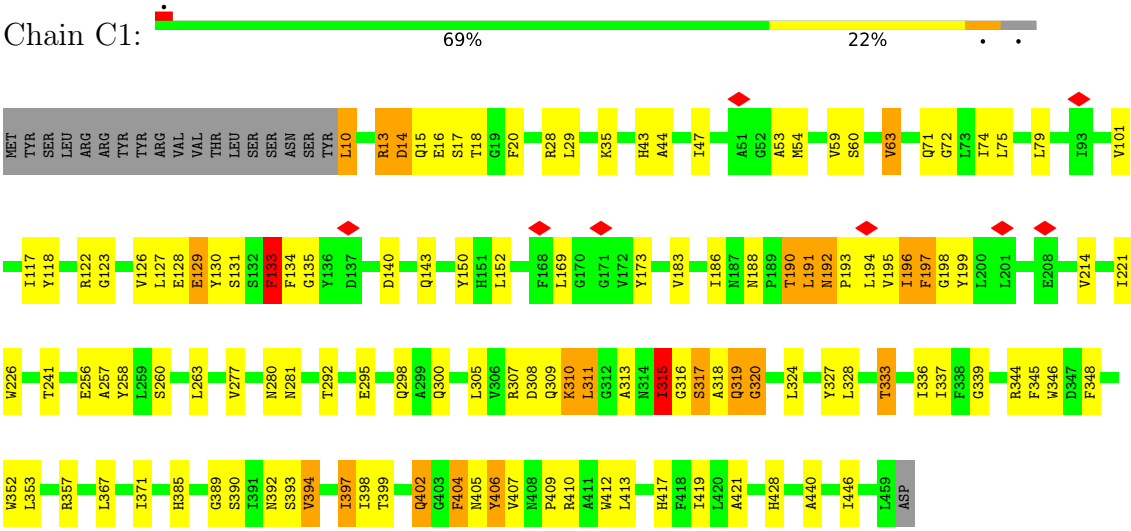
• Molecule 8: Photosystem II CP43 reaction center protein

Chain CE:



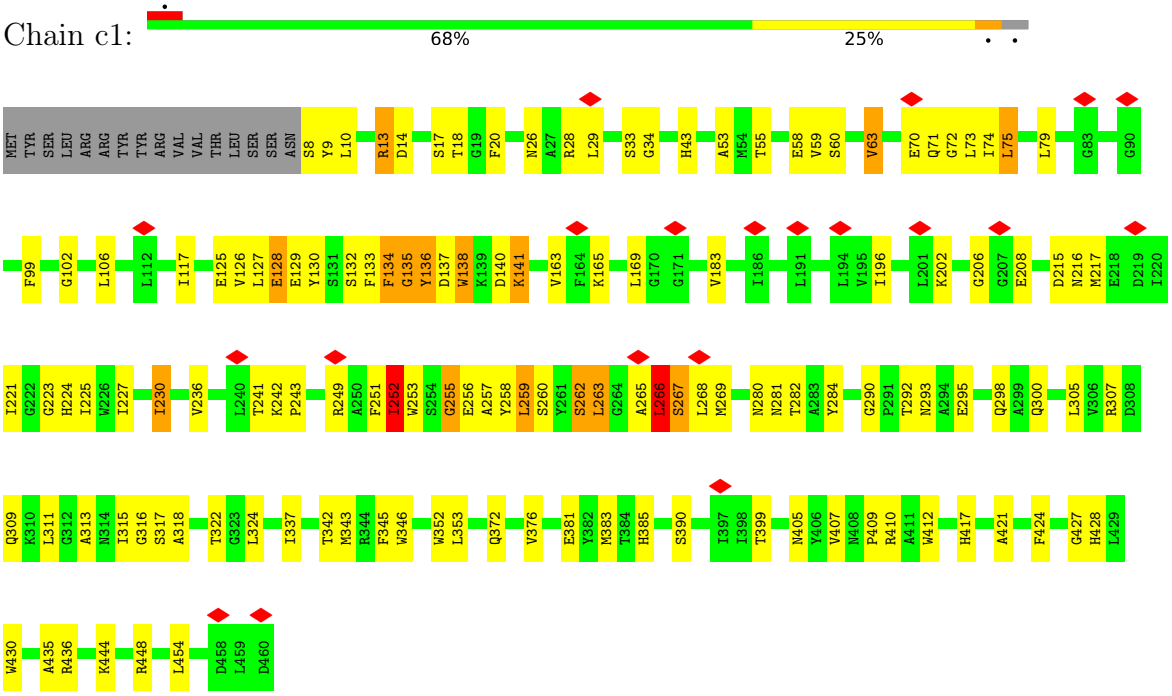
• Molecule 8: Photosystem II CP43 reaction center protein

Chain C1:



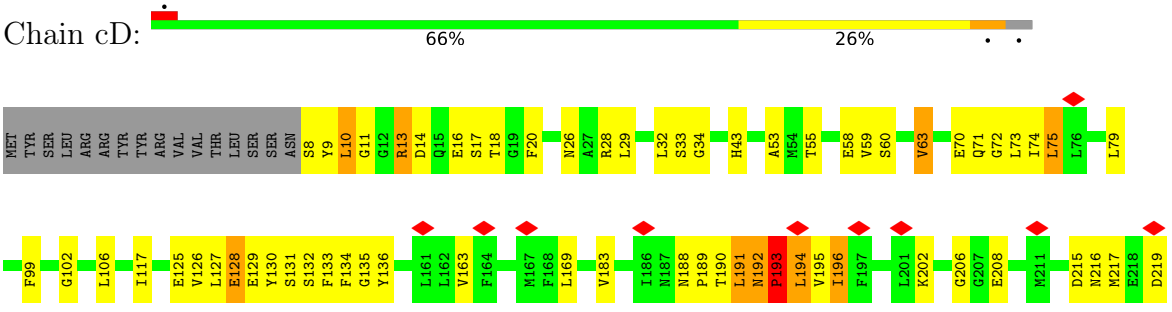
• Molecule 8: Photosystem II CP43 reaction center protein

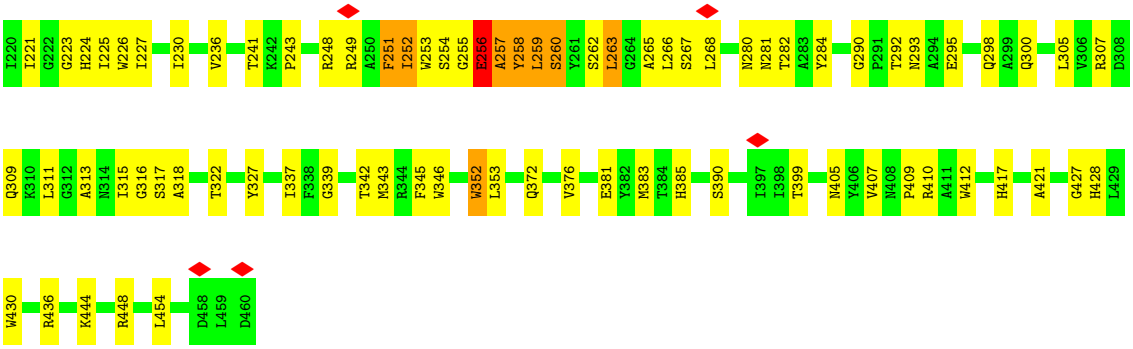
Chain c1:



• Molecule 8: Photosystem II CP43 reaction center protein

Chain cD:

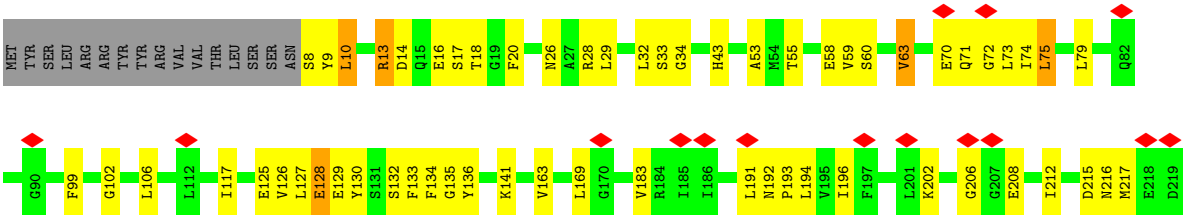




• Molecule 8: Photosystem II CP43 reaction center protein

Chain cE:

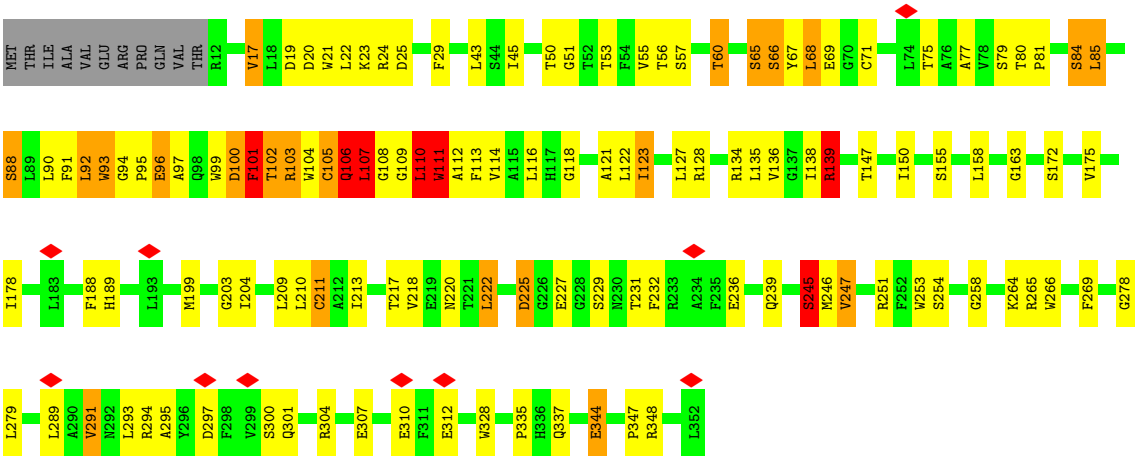




• Molecule 9: Photosystem II D2 protein

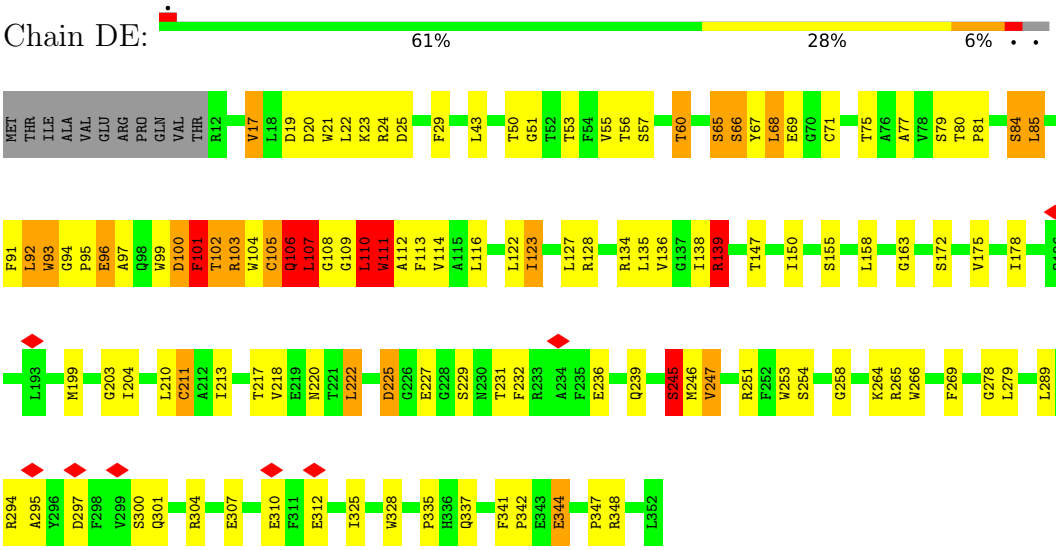
Chain DD:





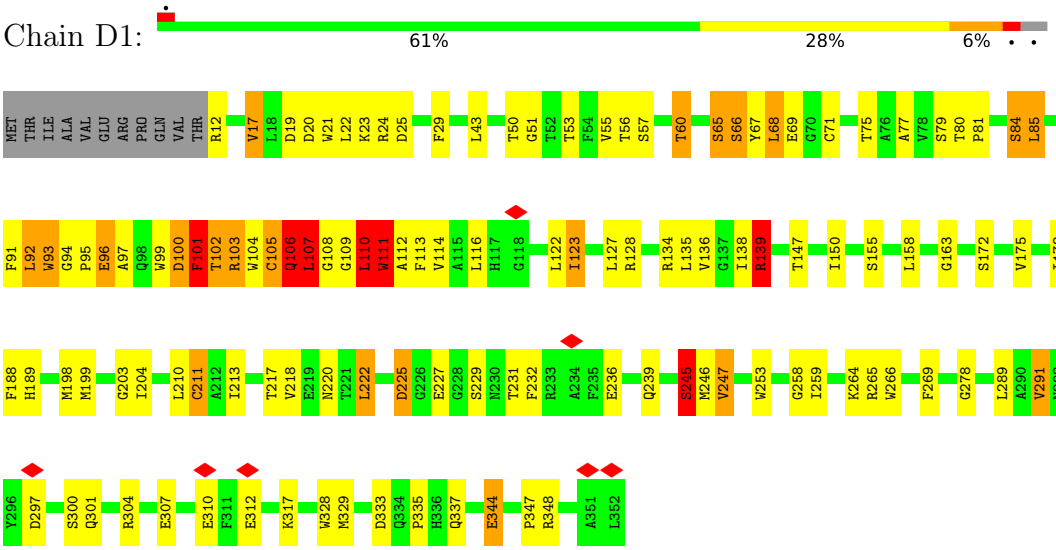
• Molecule 9: Photosystem II D2 protein

Chain DE:



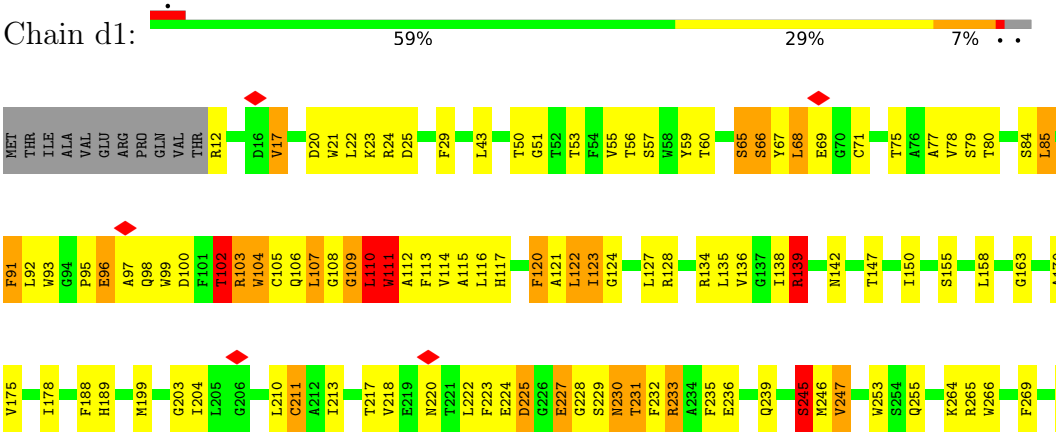
• Molecule 9: Photosystem II D2 protein

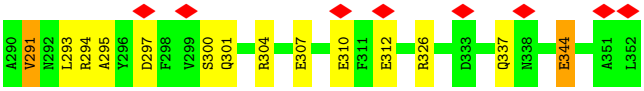
Chain D1:



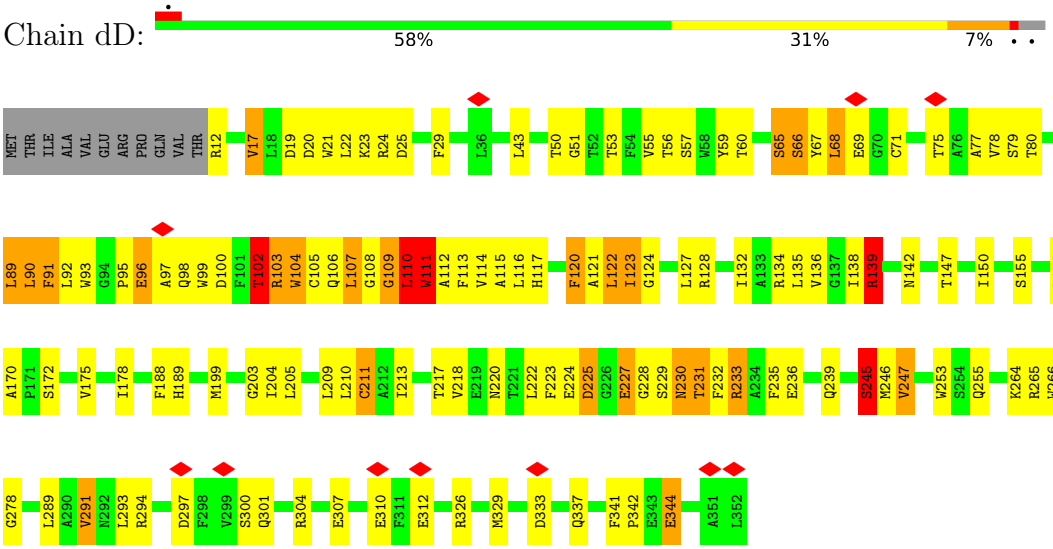
• Molecule 9: Photosystem II D2 protein

Chain d1:

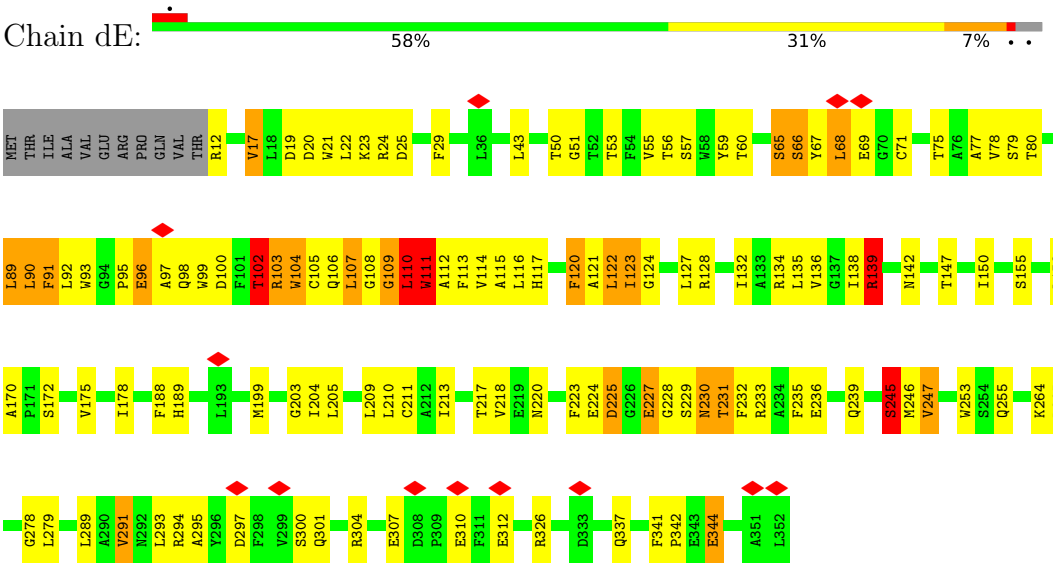




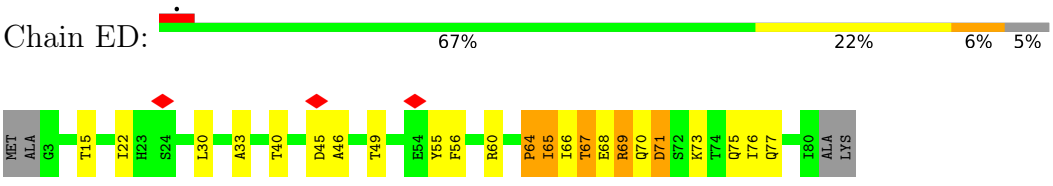
• Molecule 9: Photosystem II D2 protein



• Molecule 9: Photosystem II D2 protein

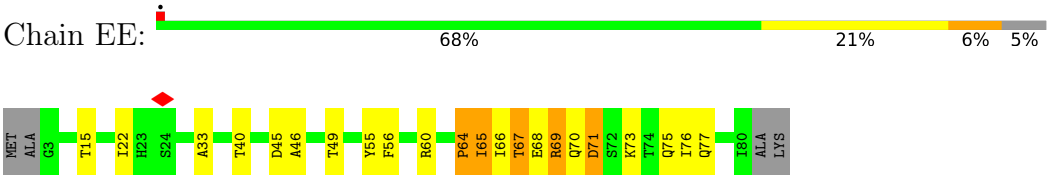


• Molecule 10: Cytochrome b559 subunit alpha



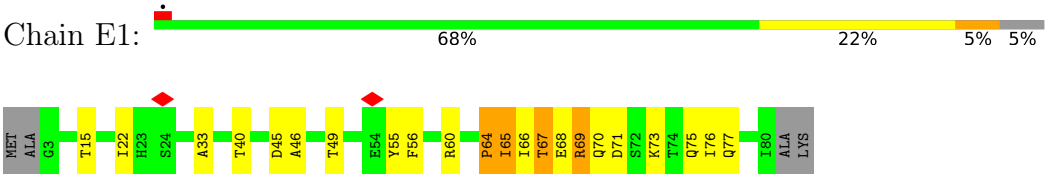
• Molecule 10: Cytochrome b559 subunit alpha

Chain EE:



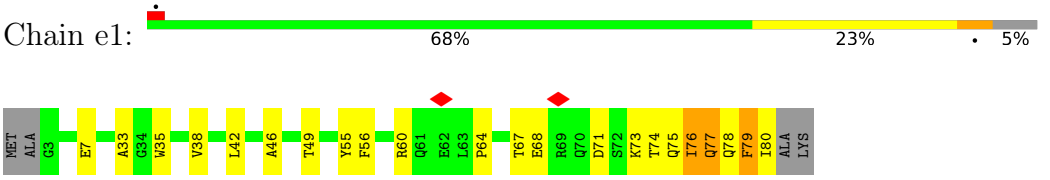
• Molecule 10: Cytochrome b559 subunit alpha

Chain E1:



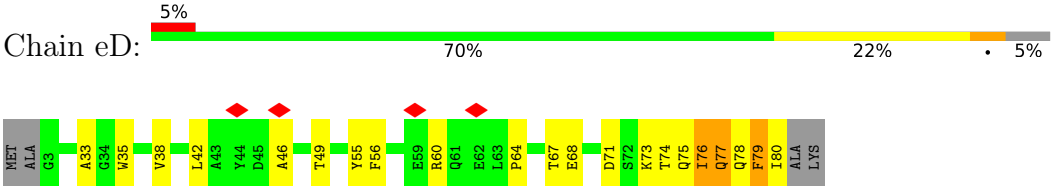
• Molecule 10: Cytochrome b559 subunit alpha

Chain e1:



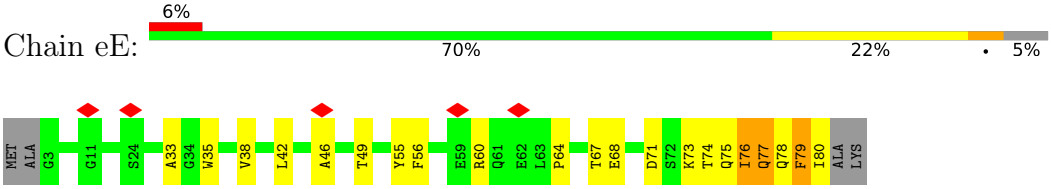
• Molecule 10: Cytochrome b559 subunit alpha

Chain eD:



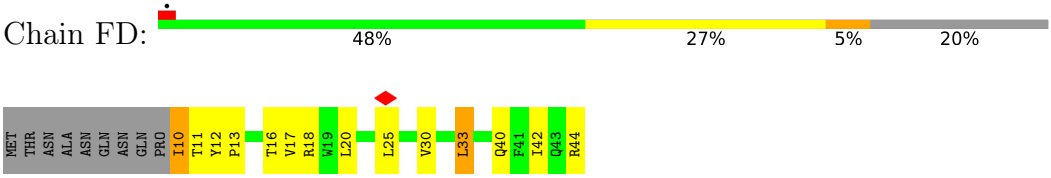
• Molecule 10: Cytochrome b559 subunit alpha

Chain eE:



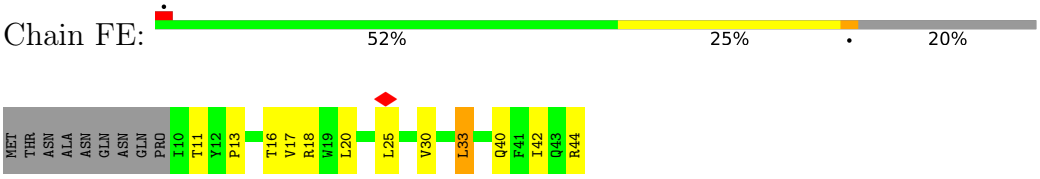
• Molecule 11: Cytochrome b559 subunit beta

Chain FD:



• Molecule 11: Cytochrome b559 subunit beta

Chain FE:



• Molecule 11: Cytochrome b559 subunit beta

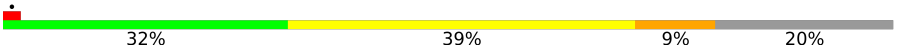
Chain F1:

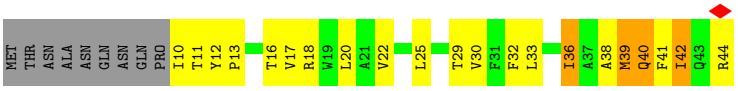




• Molecule 11: Cytochrome b559 subunit beta

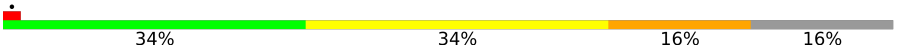
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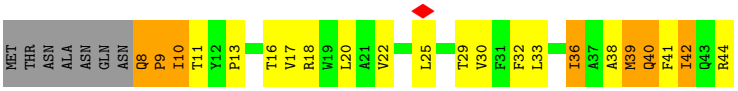




• Molecule 11: Cytochrome b559 subunit beta

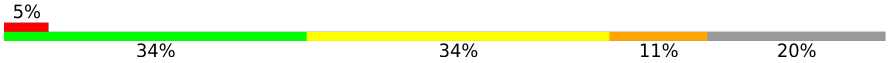
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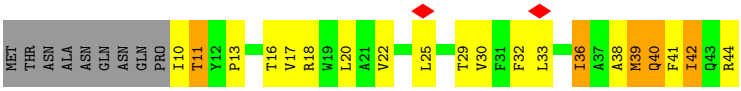




• Molecule 11: Cytochrome b559 subunit beta

Chain fE:

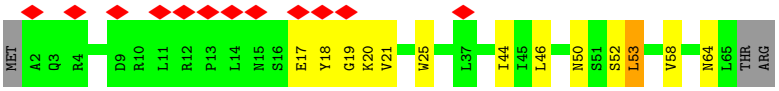




• Molecule 12: Photosystem II reaction center protein H

Chain HD:

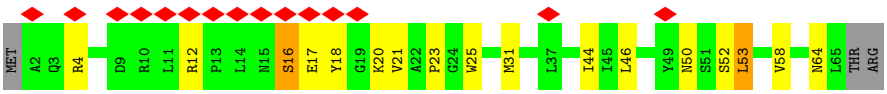




• Molecule 12: Photosystem II reaction center protein H

Chain HE:

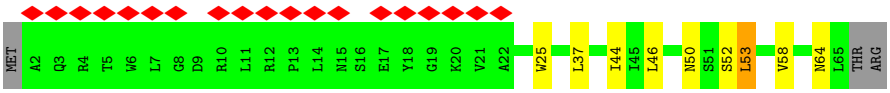




• Molecule 12: Photosystem II reaction center protein H

Chain H1:

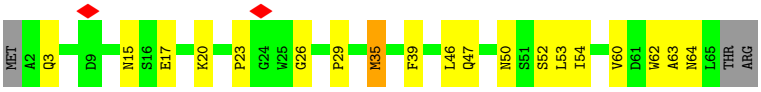




• Molecule 12: Photosystem II reaction center protein H

Chain h1:

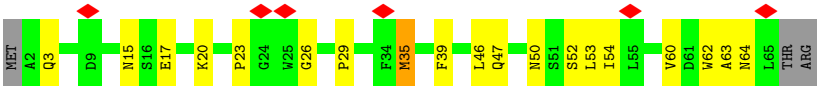




• Molecule 12: Photosystem II reaction center protein H

Chain hD:

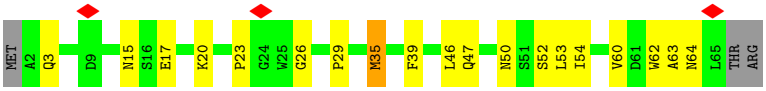




• Molecule 12: Photosystem II reaction center protein H

Chain hE:

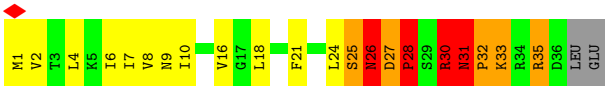




• Molecule 13: Photosystem II reaction center protein I

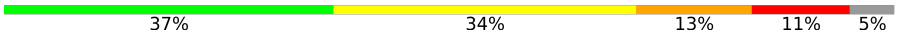
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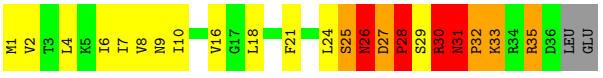




• Molecule 13: Photosystem II reaction center protein I

Chain IE:

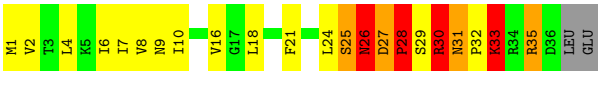




• Molecule 13: Photosystem II reaction center protein I

Chain I1:





• Molecule 13: Photosystem II reaction center protein I

Chain i1:

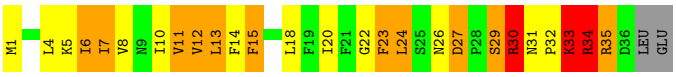




• Molecule 13: Photosystem II reaction center protein I

Chain iD:

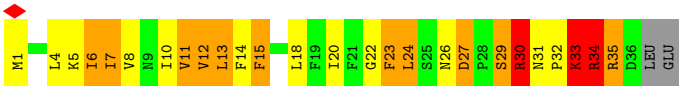




• Molecule 13: Photosystem II reaction center protein I

Chain iE:

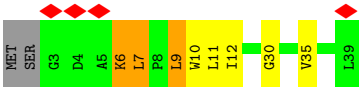




• Molecule 14: Photosystem II reaction center protein J

Chain JD:

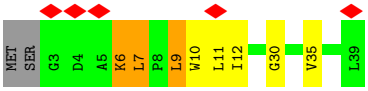




• Molecule 14: Photosystem II reaction center protein J

Chain JE:





• Molecule 14: Photosystem II reaction center protein J

Chain J1:

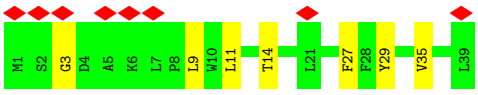




• Molecule 14: Photosystem II reaction center protein J

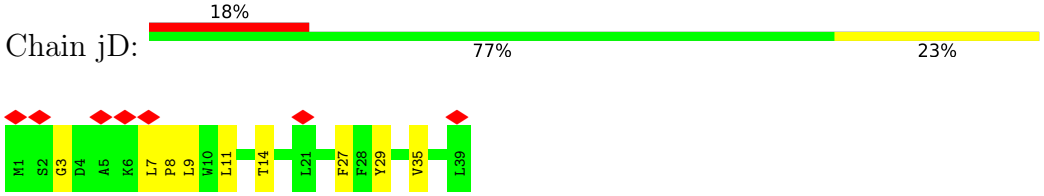
Chain j1:





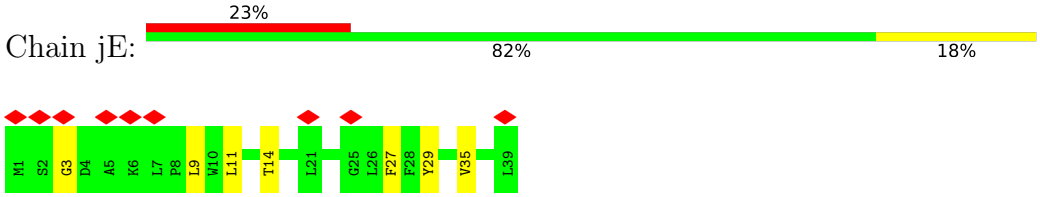
• Molecule 14: Photosystem II reaction center protein J

Chain jD:



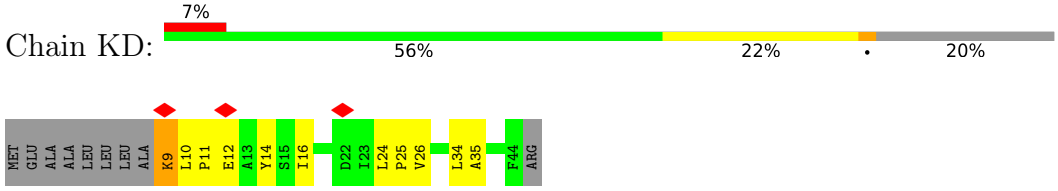
• Molecule 14: Photosystem II reaction center protein J

Chain jE:



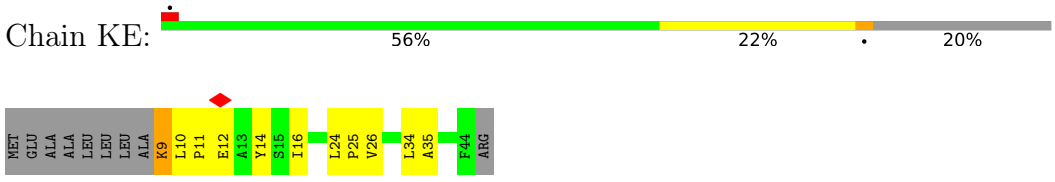
• Molecule 15: Photosystem II reaction center protein K

Chain KD:



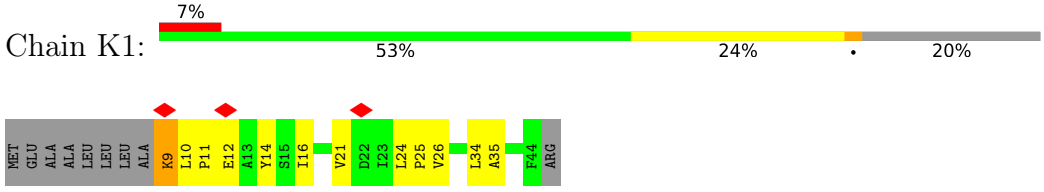
• Molecule 15: Photosystem II reaction center protein K

Chain KE:



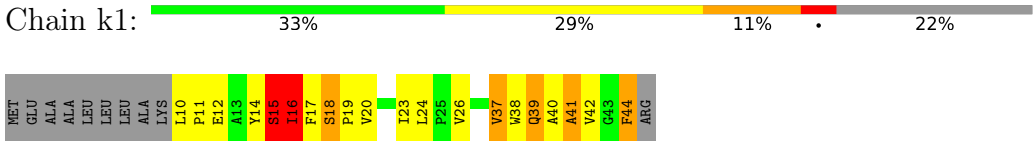
• Molecule 15: Photosystem II reaction center protein K

Chain K1:



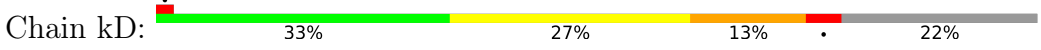
• Molecule 15: Photosystem II reaction center protein K

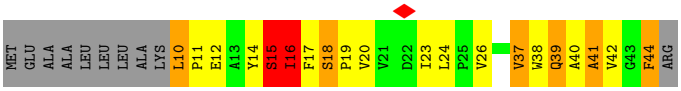
Chain k1:



• Molecule 15: Photosystem II reaction center protein K

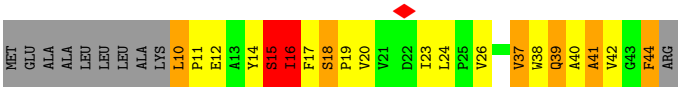
Chain kD:





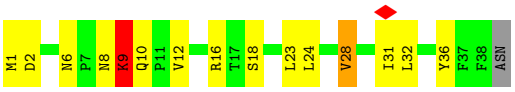
• Molecule 15: Photosystem II reaction center protein K





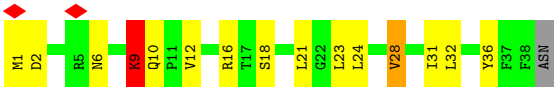
• Molecule 16: Photosystem II reaction center protein L





• Molecule 16: Photosystem II reaction center protein L





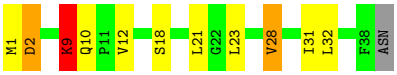
• Molecule 16: Photosystem II reaction center protein L





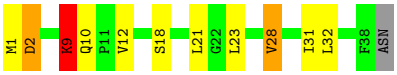
• Molecule 16: Photosystem II reaction center protein L





• Molecule 16: Photosystem II reaction center protein L





• Molecule 16: Photosystem II reaction center protein L

Chain lE:

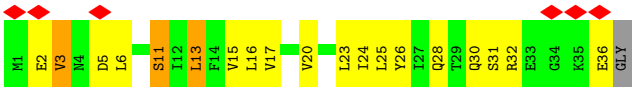




• Molecule 17: Photosystem II reaction center protein M

Chain MD:

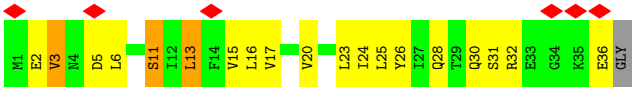




• Molecule 17: Photosystem II reaction center protein M

Chain ME:

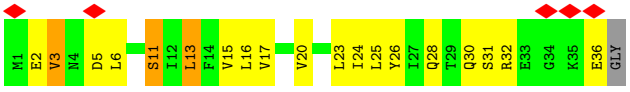




• Molecule 17: Photosystem II reaction center protein M

Chain M1:

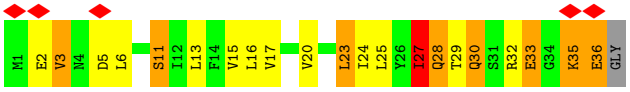




• Molecule 17: Photosystem II reaction center protein M

Chain m1:

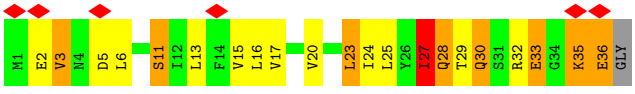




• Molecule 17: Photosystem II reaction center protein M

Chain mD:





• Molecule 17: Photosystem II reaction center protein M

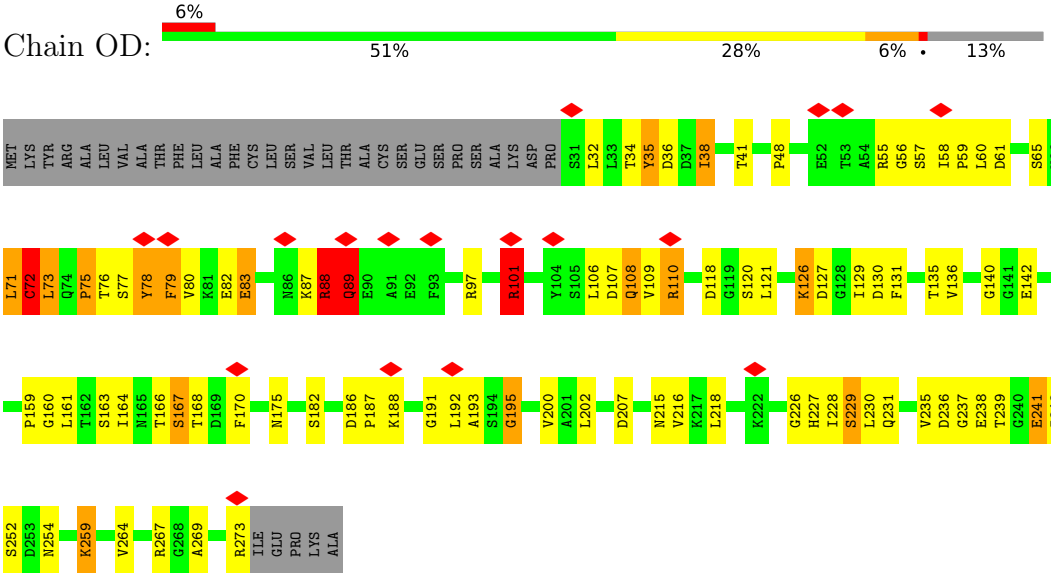
Chain mE:





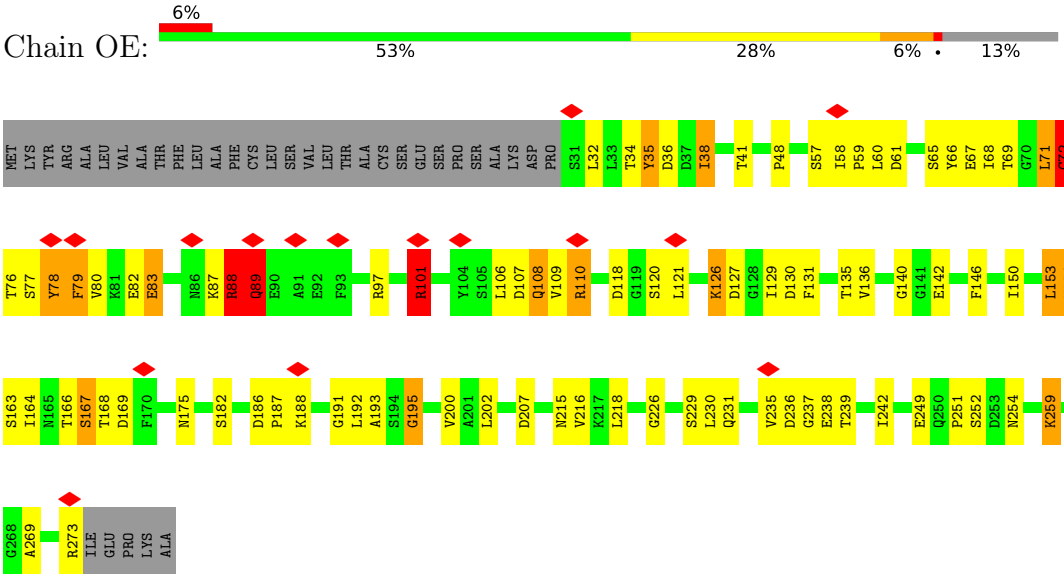
• Molecule 18: Photosystem II extrinsic protein O

Chain OD:



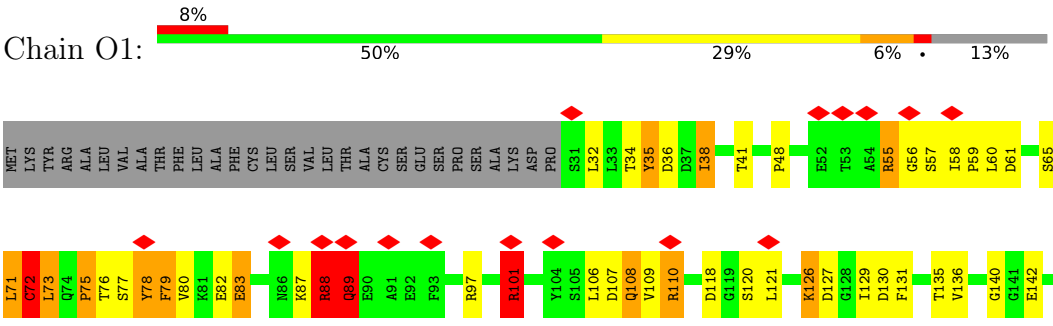
• Molecule 18: Photosystem II extrinsic protein O

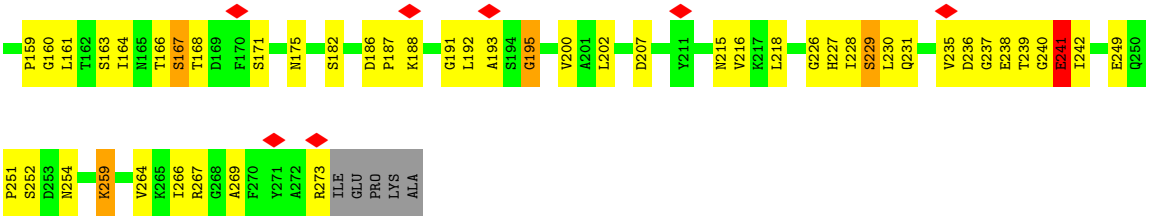
Chain OE:



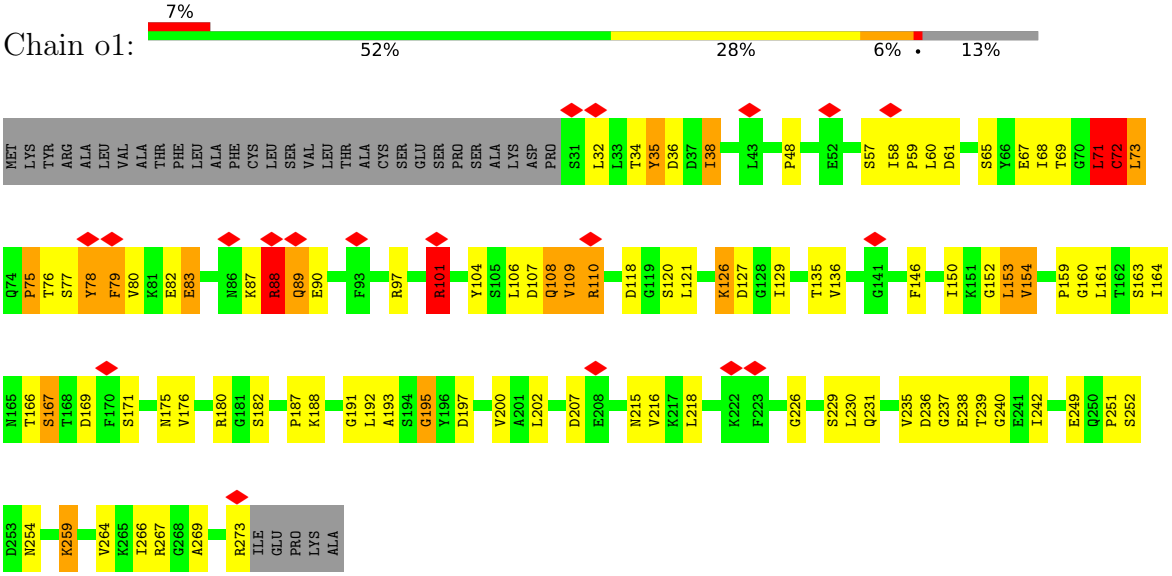
• Molecule 18: Photosystem II extrinsic protein O

Chain O1:

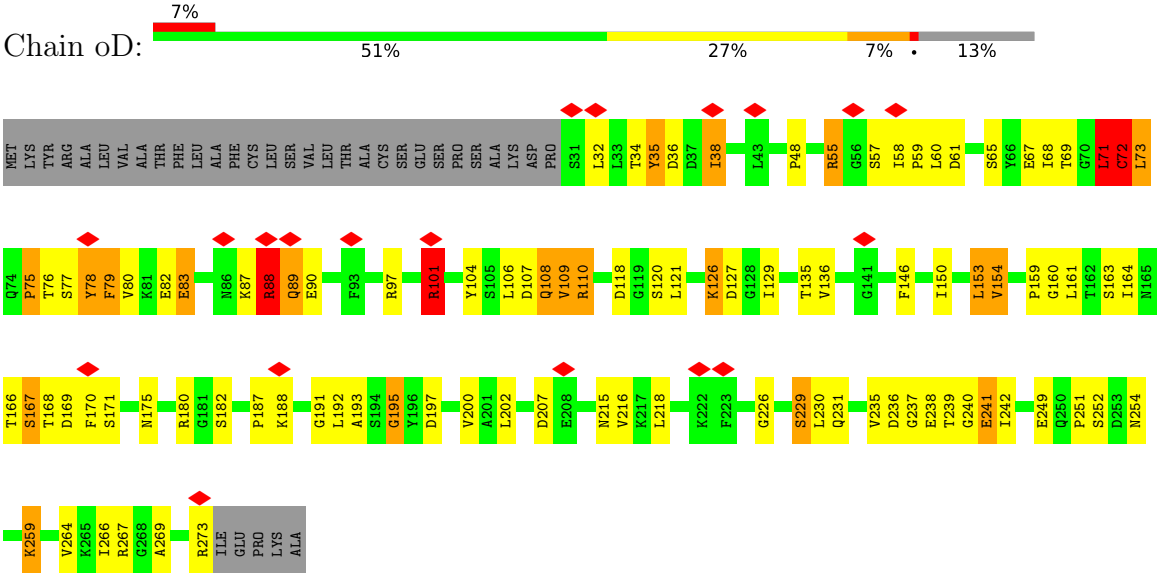




• Molecule 18: Photosystem II extrinsic protein O

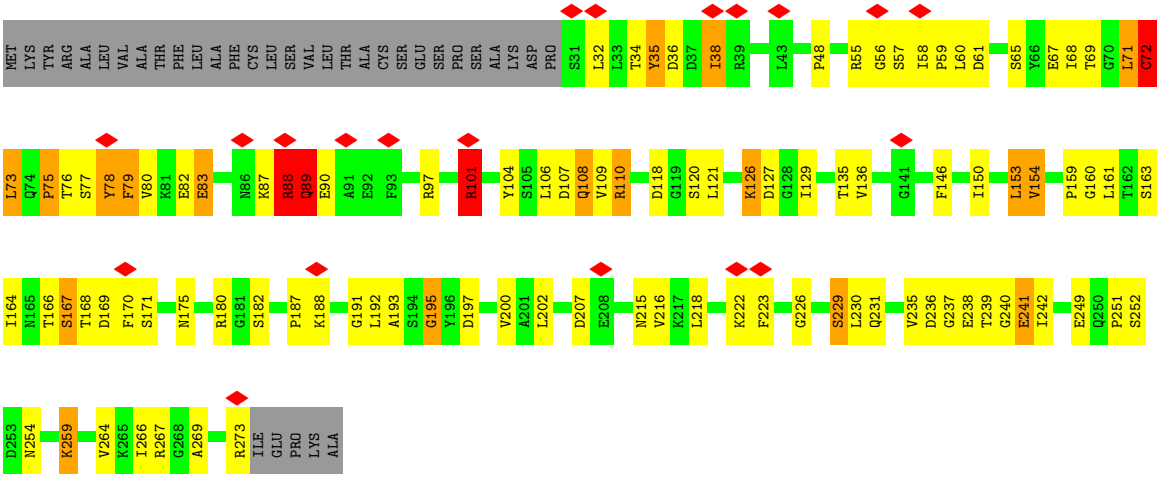


• Molecule 18: Photosystem II extrinsic protein O



• Molecule 18: Photosystem II extrinsic protein O

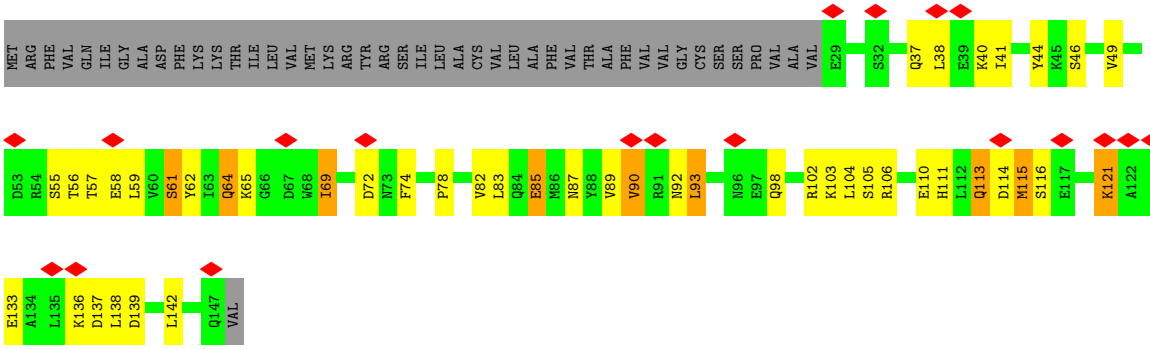




• Molecule 19: PsbQ protein

Chain QD:

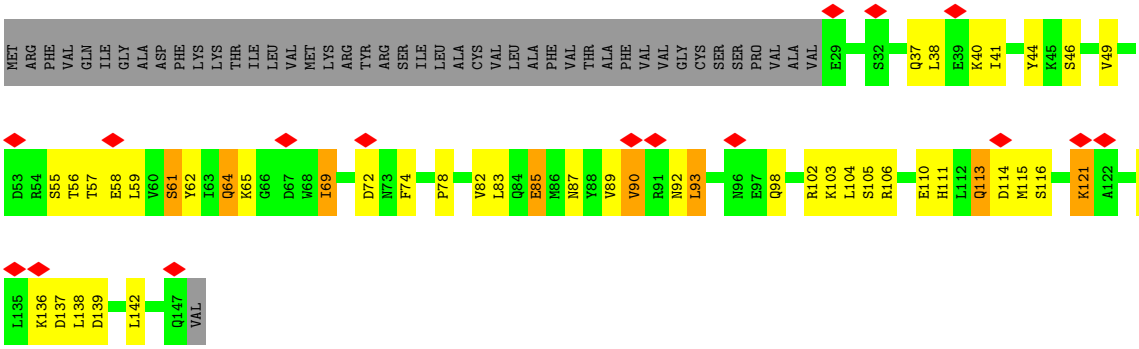




• Molecule 19: PsbQ protein

Chain QE:

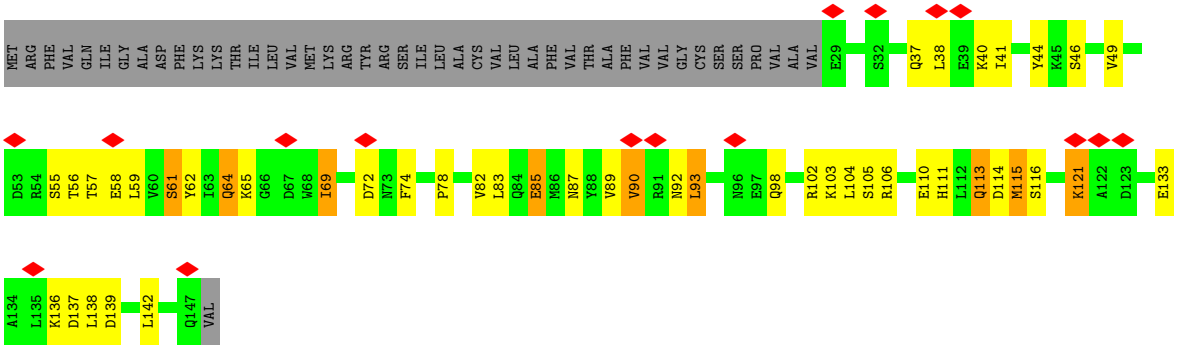




• Molecule 19: PsbQ protein

Chain Q1:

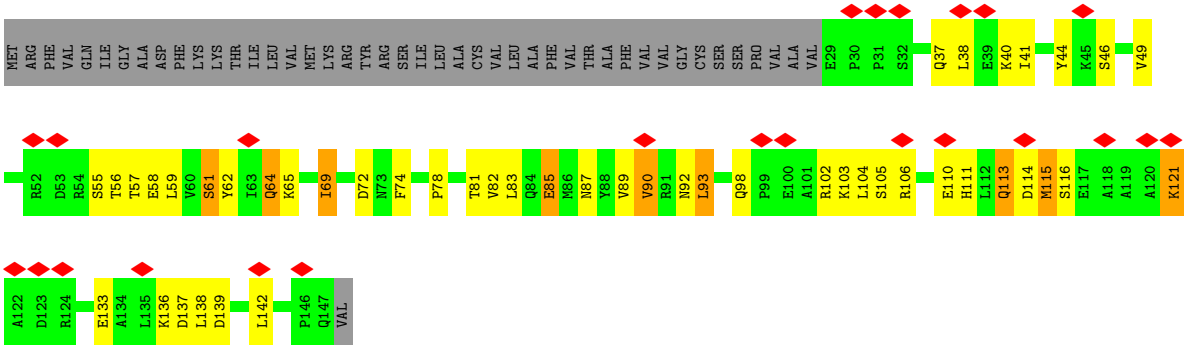




• Molecule 19: PsbQ protein

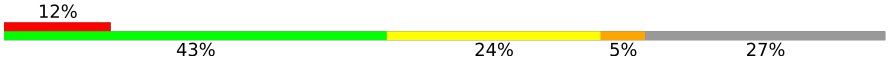
Chain q1:

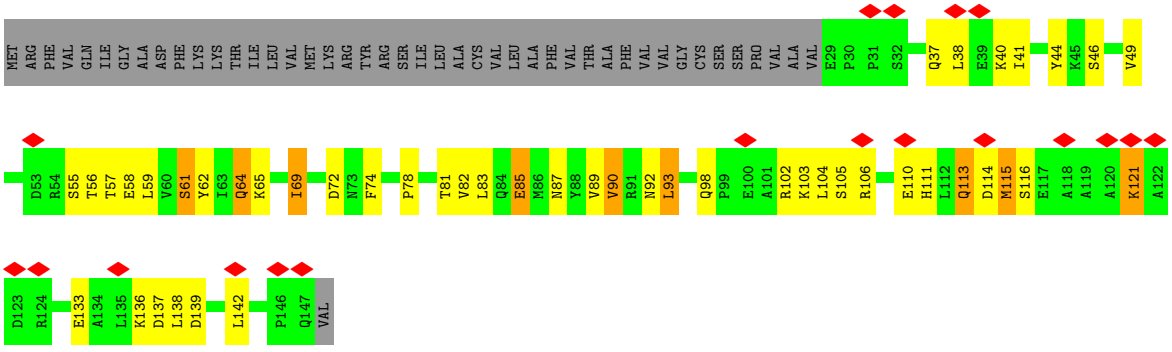




• Molecule 19: PsbQ protein

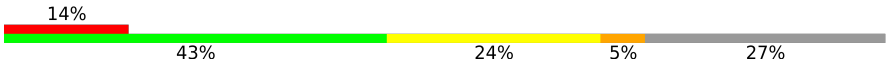
Chain qD:

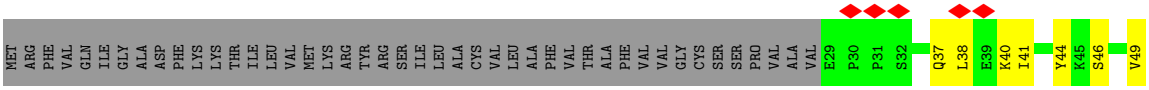


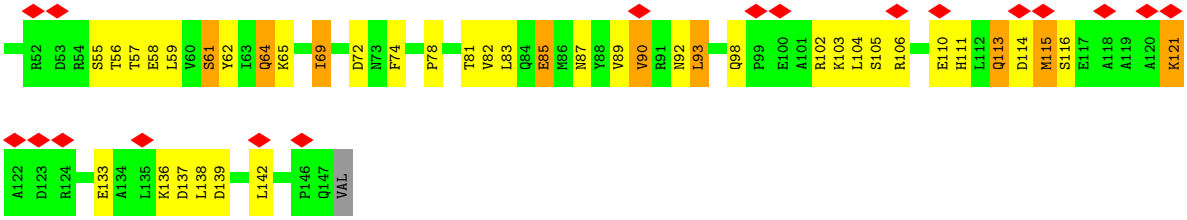


• Molecule 19: PsbQ protein

Chain qE:



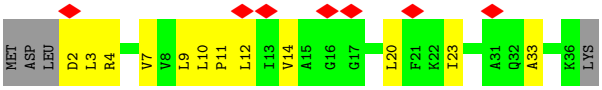




• Molecule 20: Photosystem II reaction center protein Y

Chain RD:





• Molecule 20: Photosystem II reaction center protein Y

Chain RE:





• Molecule 20: Photosystem II reaction center protein Y

Chain R1:

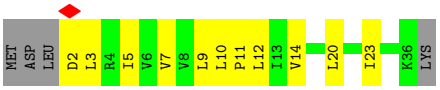




• Molecule 20: Photosystem II reaction center protein Y

Chain r1:

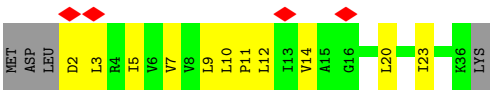




• Molecule 20: Photosystem II reaction center protein Y

Chain rD:

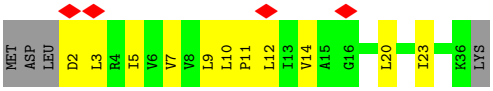




• Molecule 20: Photosystem II reaction center protein Y

Chain rE:

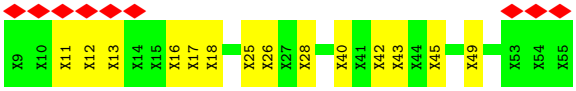




• Molecule 21: LPP1

Chain SD:

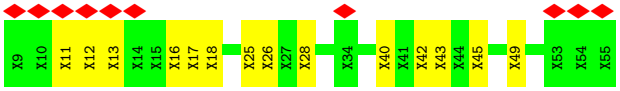




• Molecule 21: LPP1

Chain SE:

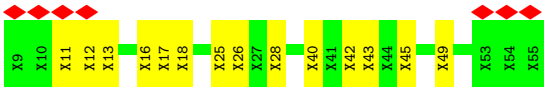




• Molecule 21: LPP1

Chain S1:

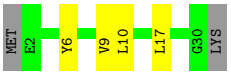




• Molecule 22: Photosystem II reaction center protein T

Chain TD:

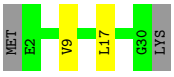




• Molecule 22: Photosystem II reaction center protein T

Chain TE:

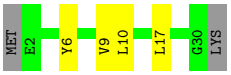




• Molecule 22: Photosystem II reaction center protein T

Chain T1:

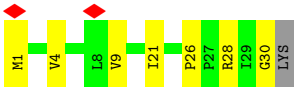




• Molecule 22: Photosystem II reaction center protein T

Chain t1:

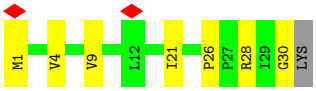




• Molecule 22: Photosystem II reaction center protein T

Chain tD:

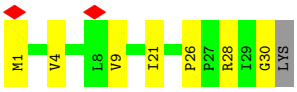




• Molecule 22: Photosystem II reaction center protein T

Chain tE:





• Molecule 23: PsbU

Chain UD:





• Molecule 23: PsbU

Chain UE:

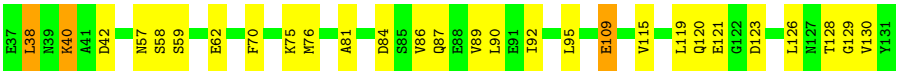




• Molecule 23: PsbU

Chain U1:

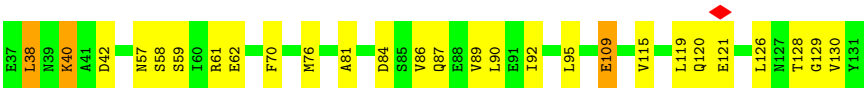




• Molecule 23: PsbU

Chain u1:

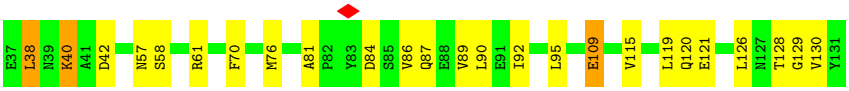




• Molecule 23: PsbU

Chain uD:

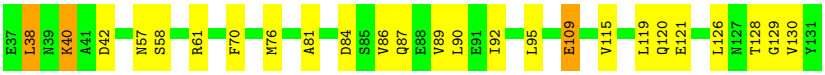




• Molecule 23: PsbU

Chain uE:

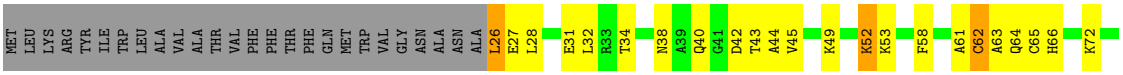




• Molecule 24: Photosystem II extrinsic protein V

Chain VD:



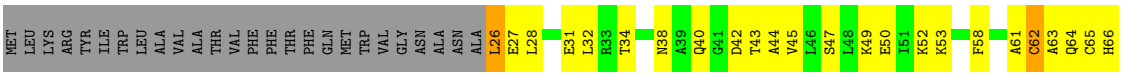




• Molecule 24: Photosystem II extrinsic protein V

Chain VE:



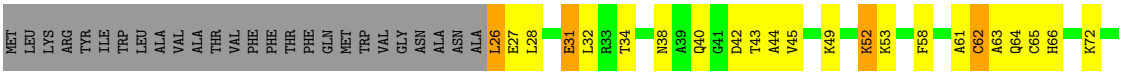




• Molecule 24: Photosystem II extrinsic protein V

Chain V1:



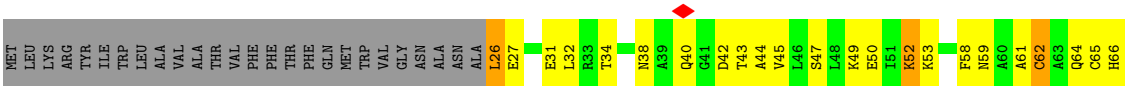




• Molecule 24: Photosystem II extrinsic protein V

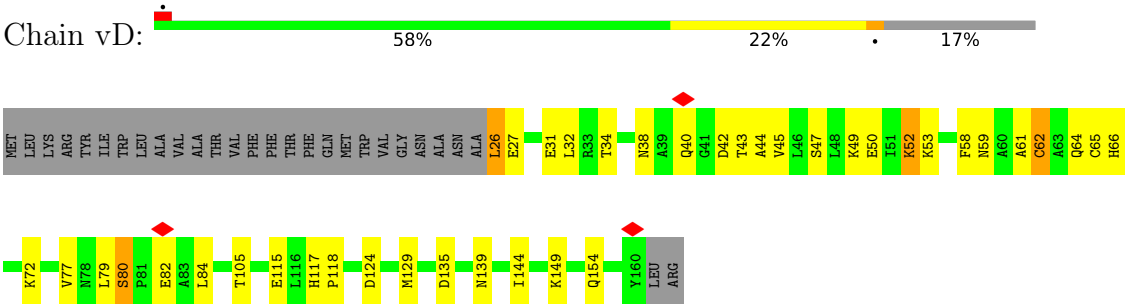
Chain v1:



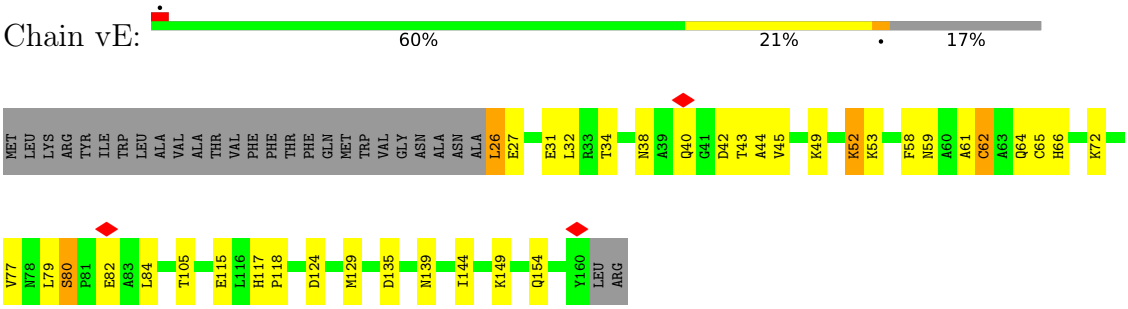




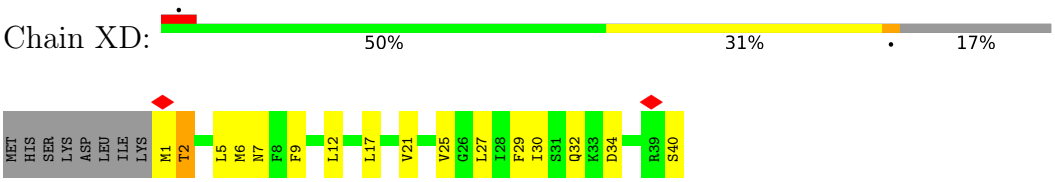
• Molecule 24: Photosystem II extrinsic protein V



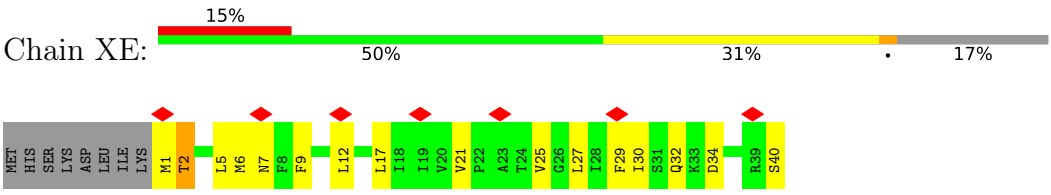
• Molecule 24: Photosystem II extrinsic protein V



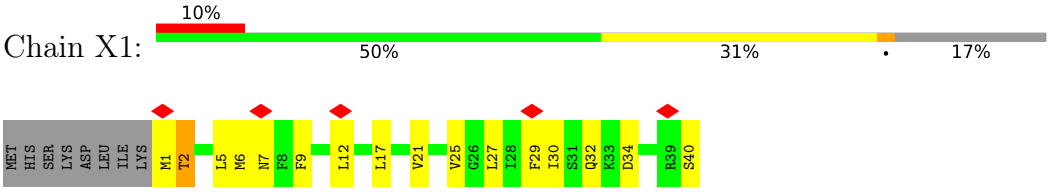
• Molecule 25: Photosystem II reaction center protein X



• Molecule 25: Photosystem II reaction center protein X



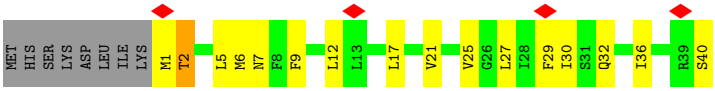
• Molecule 25: Photosystem II reaction center protein X



• Molecule 25: Photosystem II reaction center protein X

Chain x1:

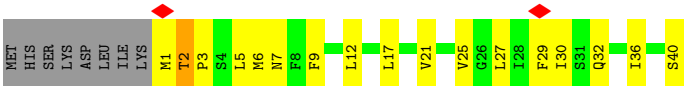




• Molecule 25: Photosystem II reaction center protein X

Chain xD:

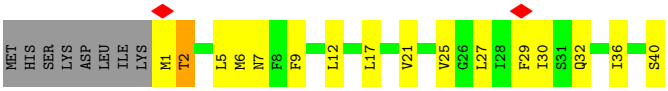




• Molecule 25: Photosystem II reaction center protein X

Chain xE:

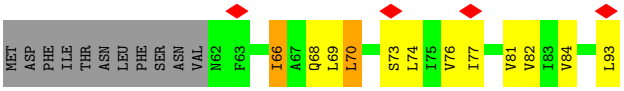




• Molecule 26: Photosystem II reaction center protein Psb30

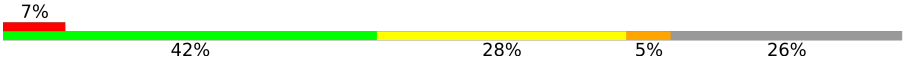
Chain YD:

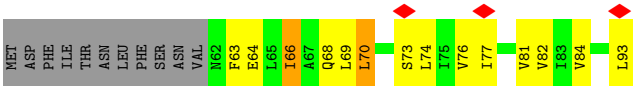




• Molecule 26: Photosystem II reaction center protein Psb30

Chain YE:

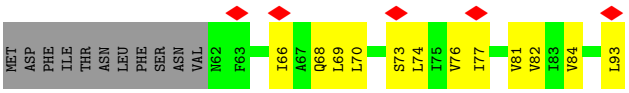




• Molecule 26: Photosystem II reaction center protein Psb30

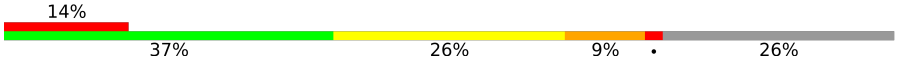
Chain Y1:

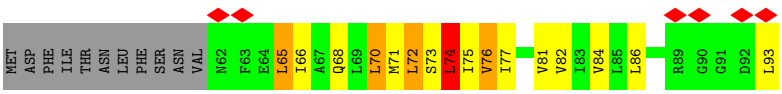




• Molecule 26: Photosystem II reaction center protein Psb30

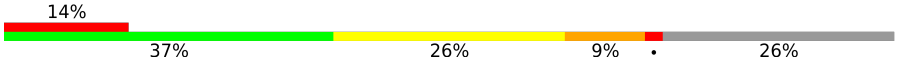
Chain y1:





• Molecule 26: Photosystem II reaction center protein Psb30

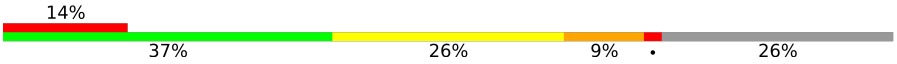
Chain yD:





• Molecule 26: Photosystem II reaction center protein Psb30

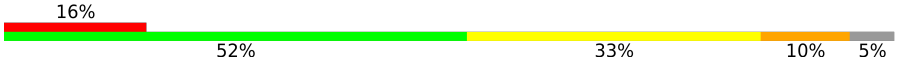
Chain yE:

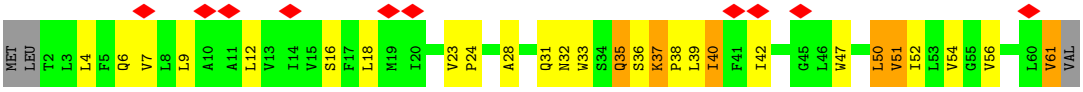




• Molecule 27: Photosystem II reaction center protein Z

Chain ZD:

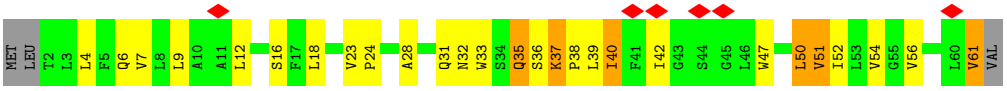




• Molecule 27: Photosystem II reaction center protein Z

Chain ZE:

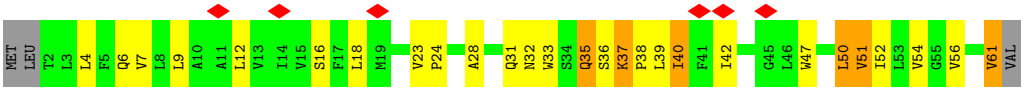




• Molecule 27: Photosystem II reaction center protein Z

Chain Z1:

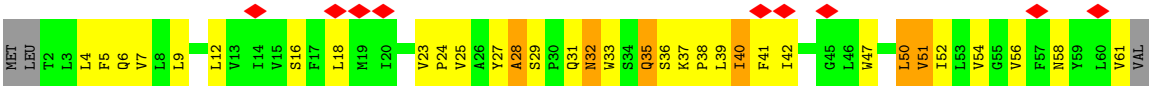




• Molecule 27: Photosystem II reaction center protein Z

Chain z1:

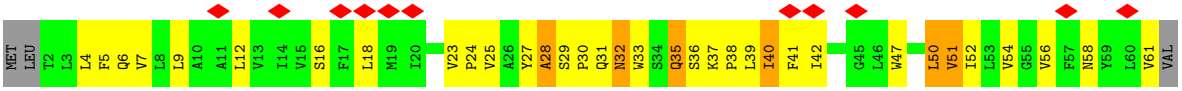




• Molecule 27: Photosystem II reaction center protein Z

Chain zD:

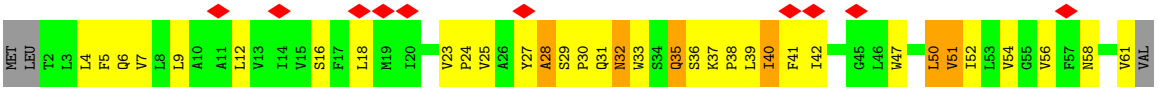




• Molecule 27: Photosystem II reaction center protein Z

Chain zE:

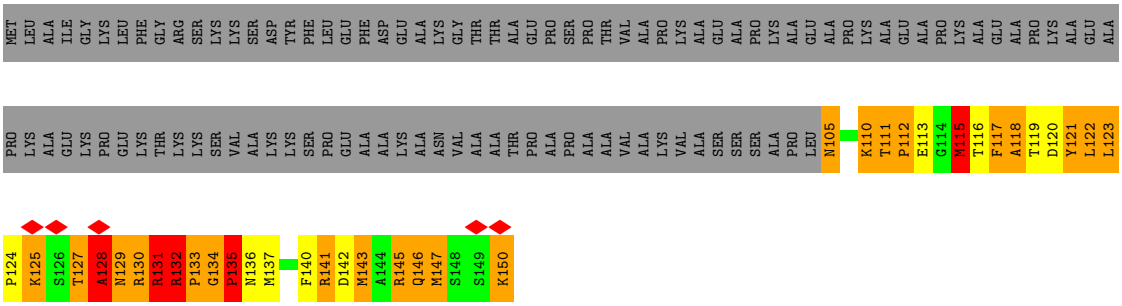




• Molecule 28: LPP2

Chain EF:

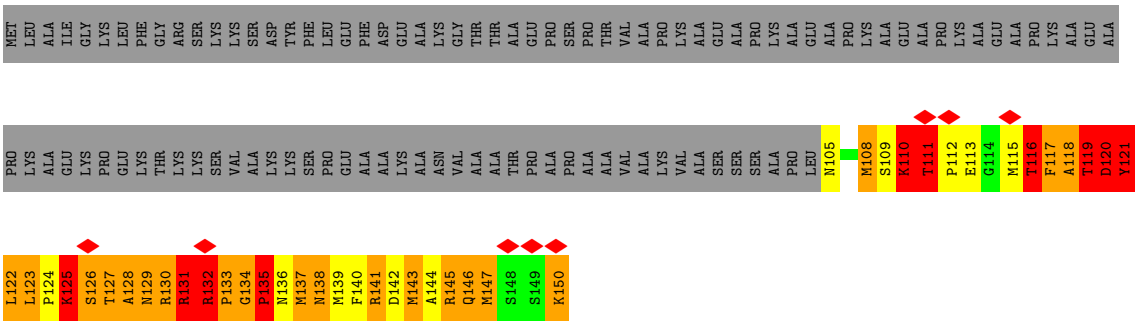




• Molecule 28: LPP2

Chain BG:

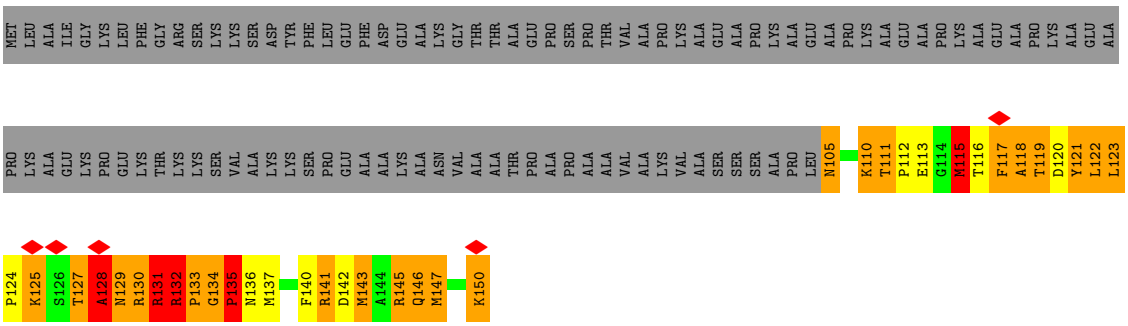




• Molecule 28: LPP2

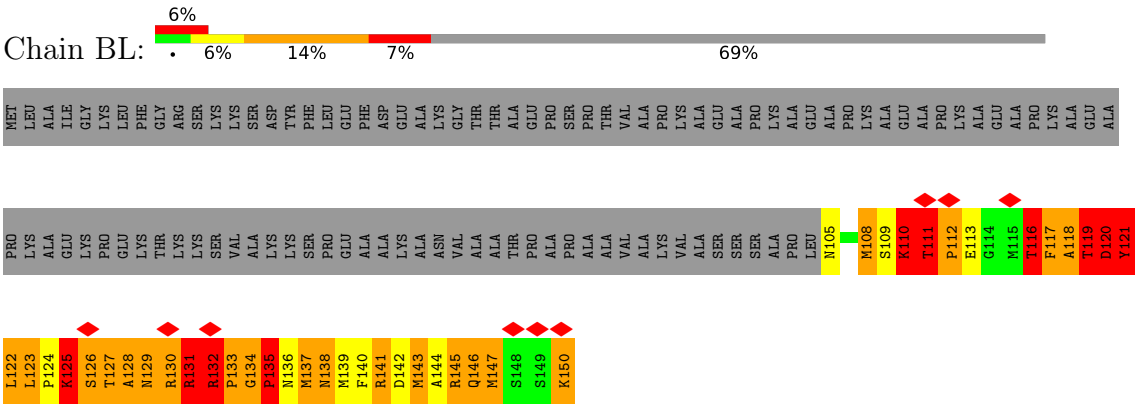
Chain EK:





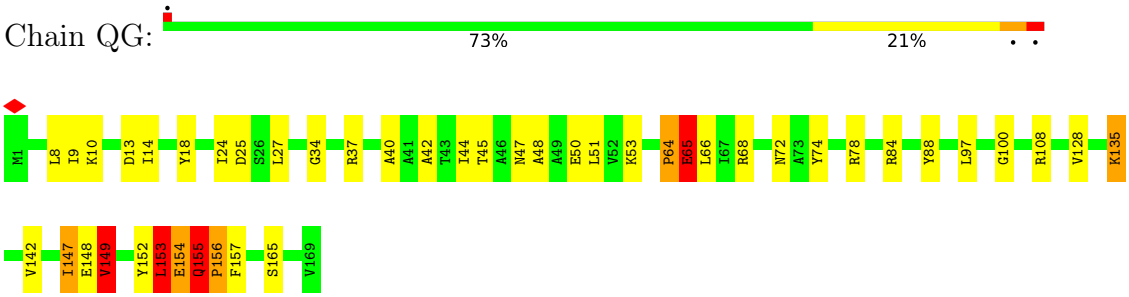
• Molecule 28: LPP2

Chain BL:



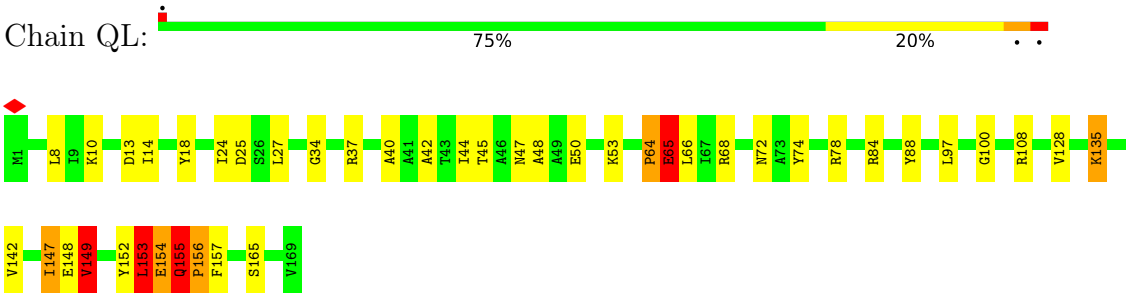
• Molecule 29: Allophycocyanin beta-18 subunit

Chain QG:



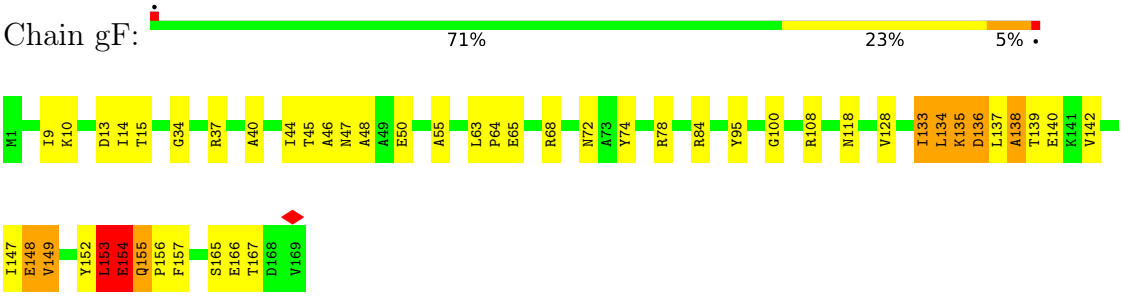
• Molecule 29: Allophycocyanin beta-18 subunit

Chain QL:



• Molecule 29: Allophycocyanin beta-18 subunit

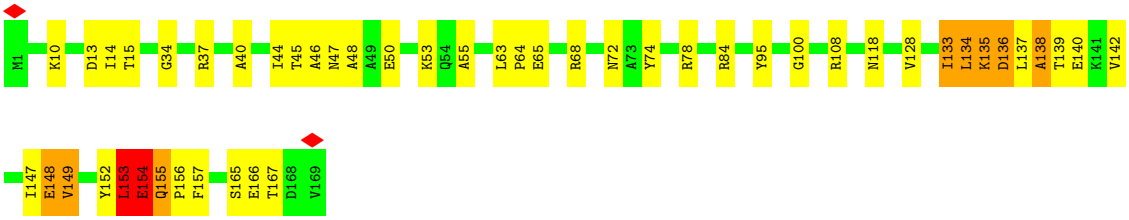
Chain gF:



• Molecule 29: Allophycocyanin beta-18 subunit

Chain gK:

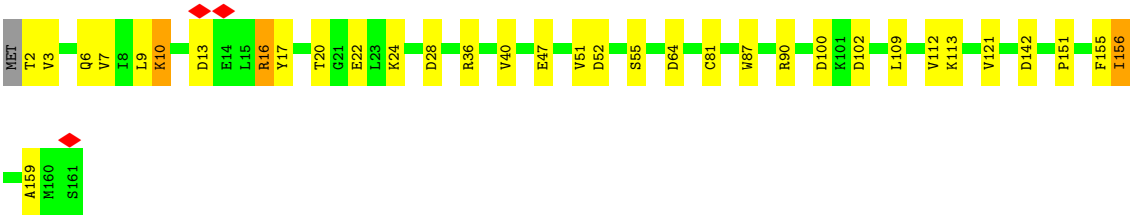




• Molecule 30: Allophycocyanin-B alpha subunit

Chain VG:

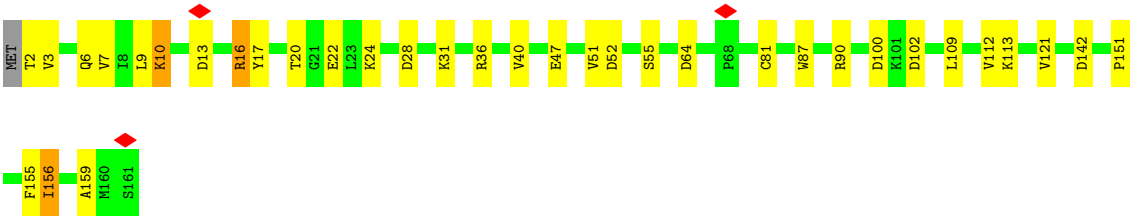




• Molecule 30: Allophycocyanin-B alpha subunit

Chain VL:

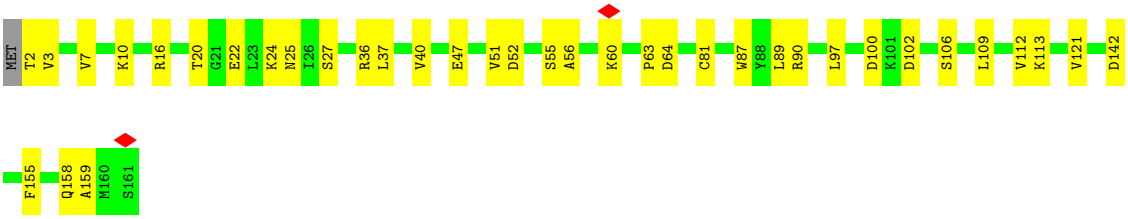




• Molecule 30: Allophycocyanin-B alpha subunit

Chain mF:

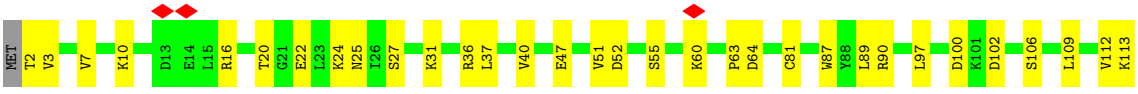


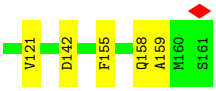


• Molecule 30: Allophycocyanin-B alpha subunit

Chain mK:



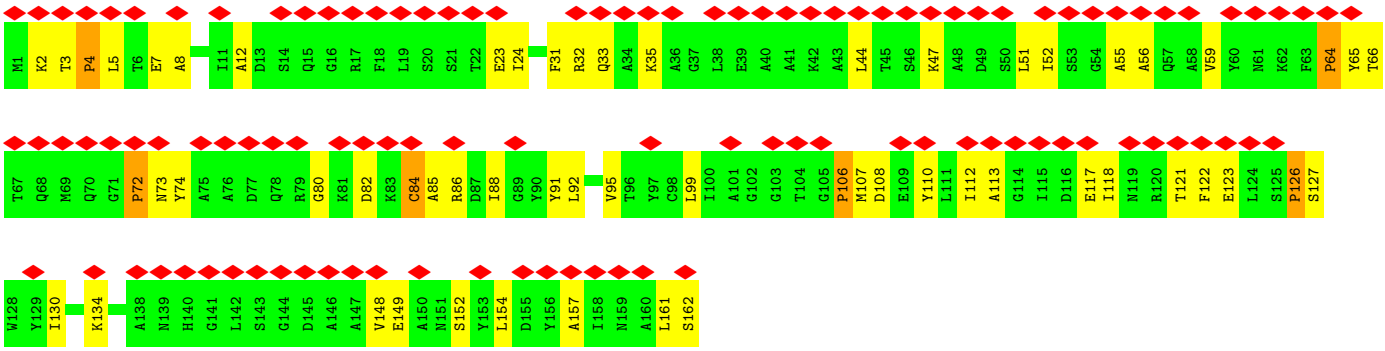




• Molecule 31: C-phycocyanin alpha subunit

Chain b2:

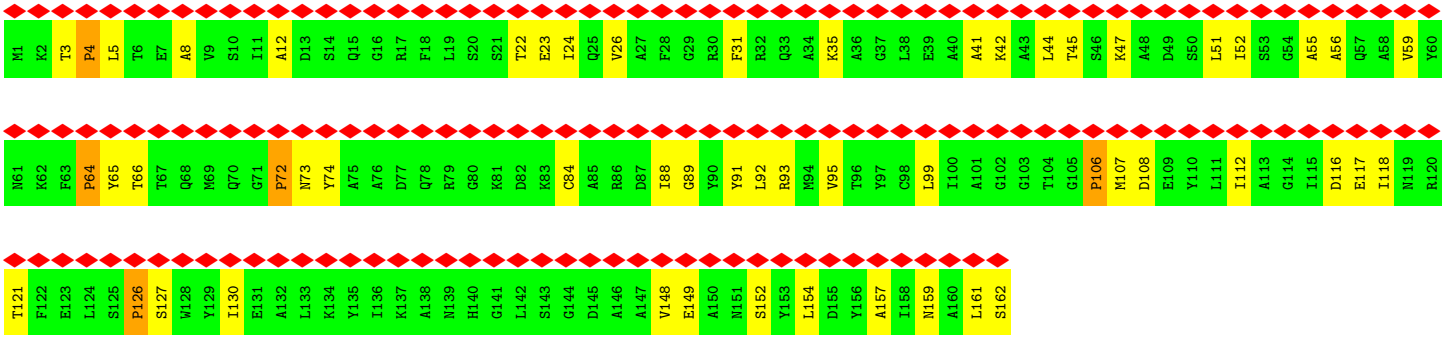




• Molecule 31: C-phycocyanin alpha subunit

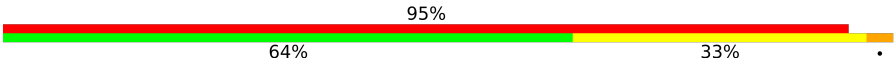
Chain d2:

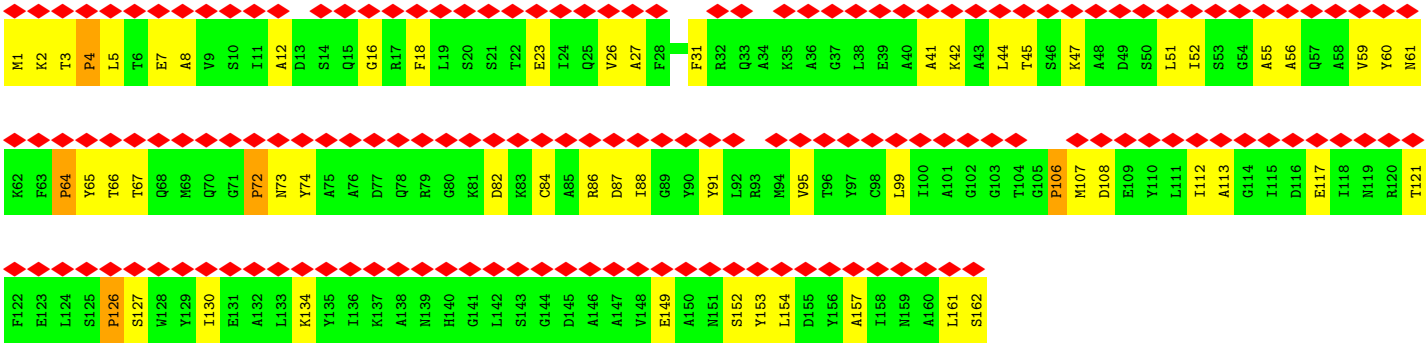




• Molecule 31: C-phycocyanin alpha subunit

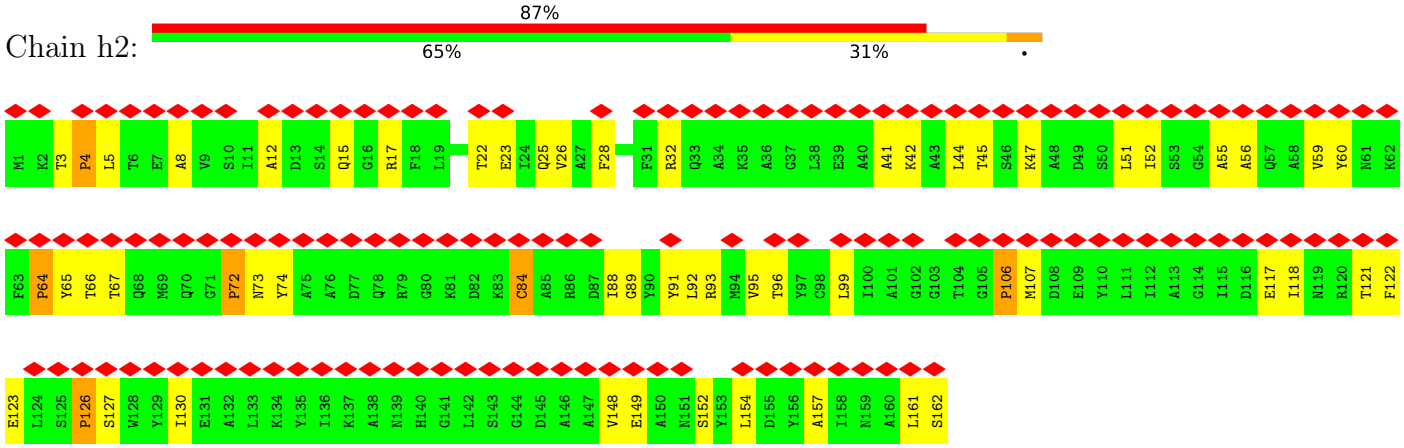
Chain f2:





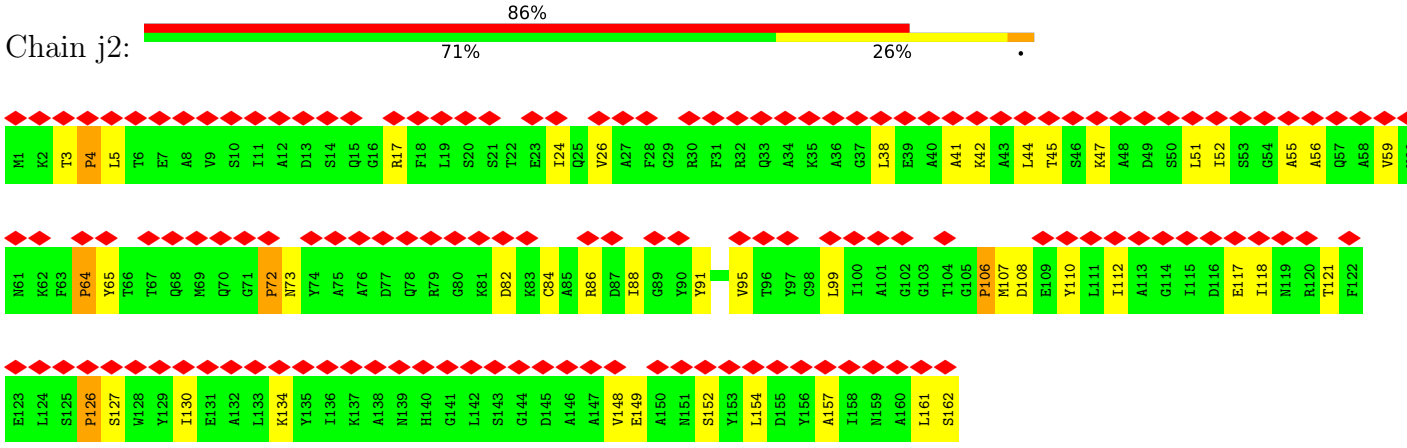
• Molecule 31: C-phycocyanin alpha subunit

Chain h2:



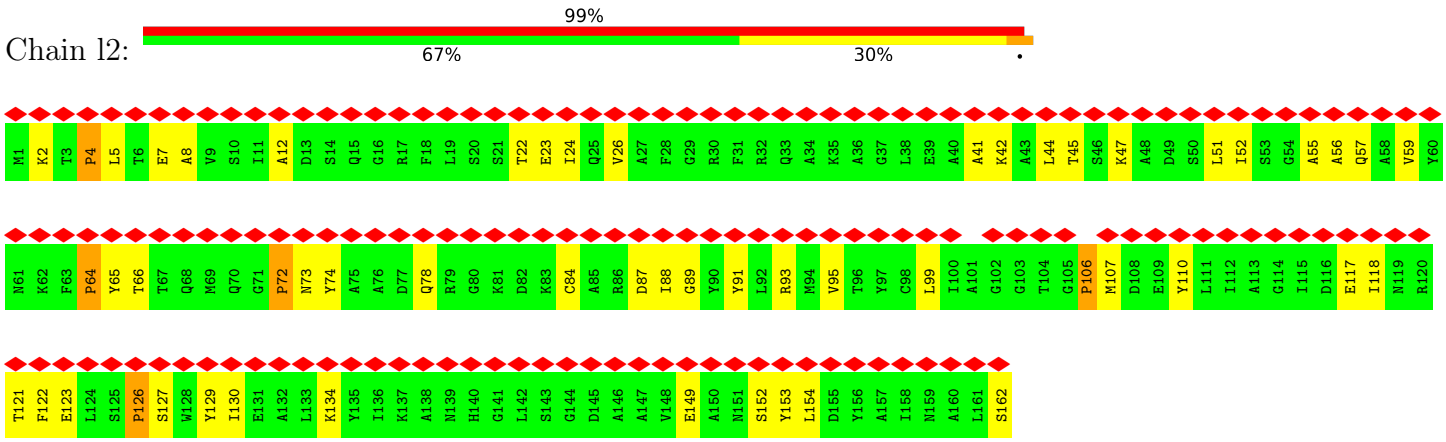
• Molecule 31: C-phycocyanin alpha subunit

Chain j2:



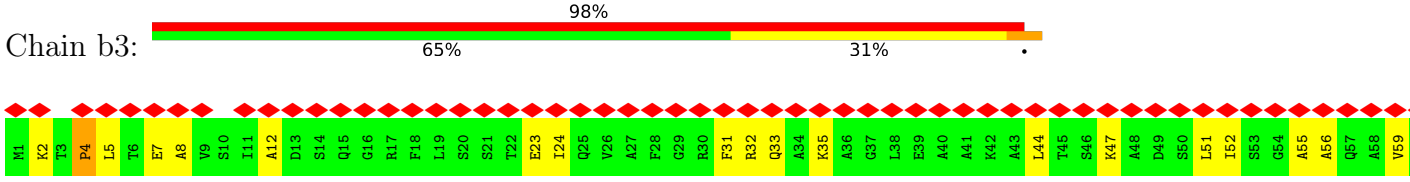
• Molecule 31: C-phycocyanin alpha subunit

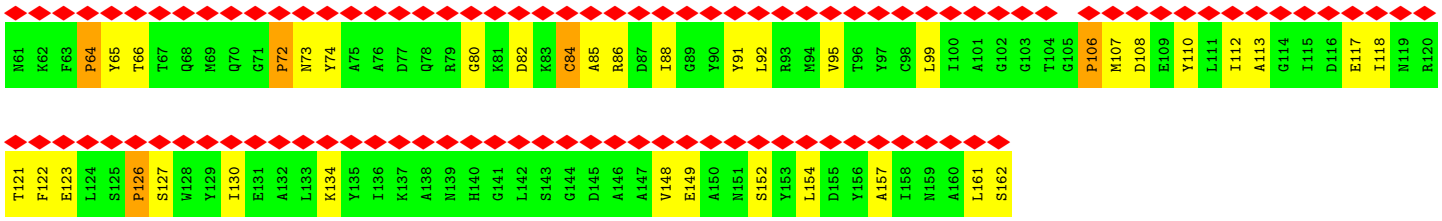
Chain l2:



• Molecule 31: C-phycocyanin alpha subunit

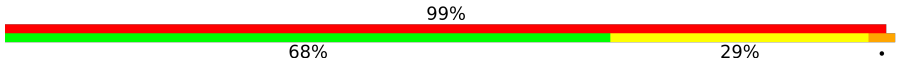
Chain b3:

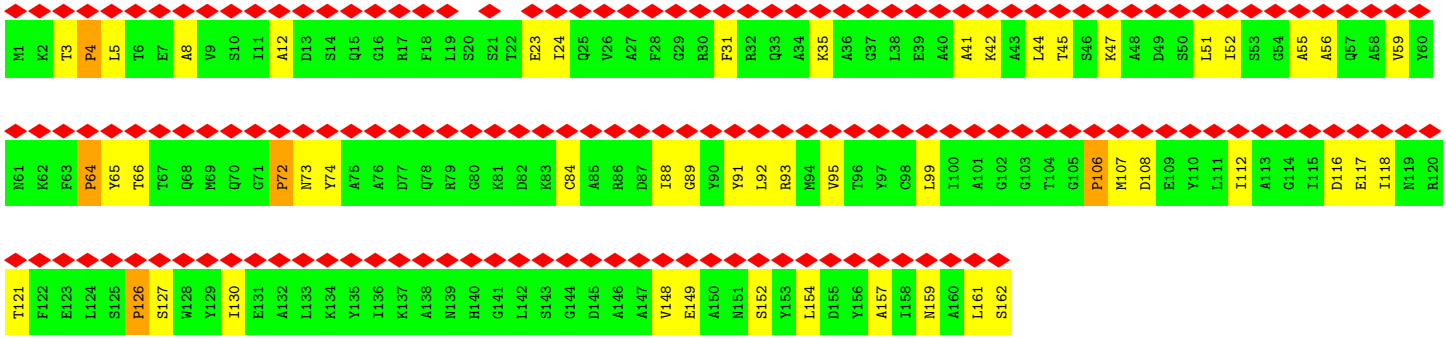




• Molecule 31: C-phycocyanin alpha subunit

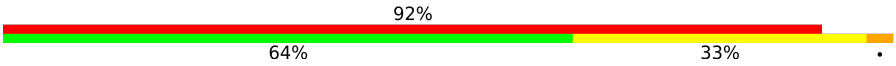
Chain d3:





• Molecule 31: C-phycocyanin alpha subunit

Chain f3:

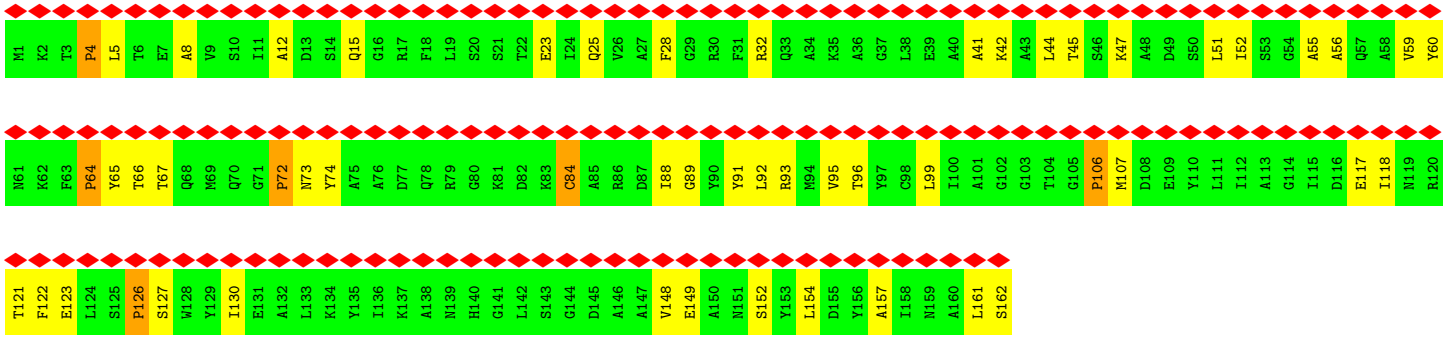




• Molecule 31: C-phycocyanin alpha subunit

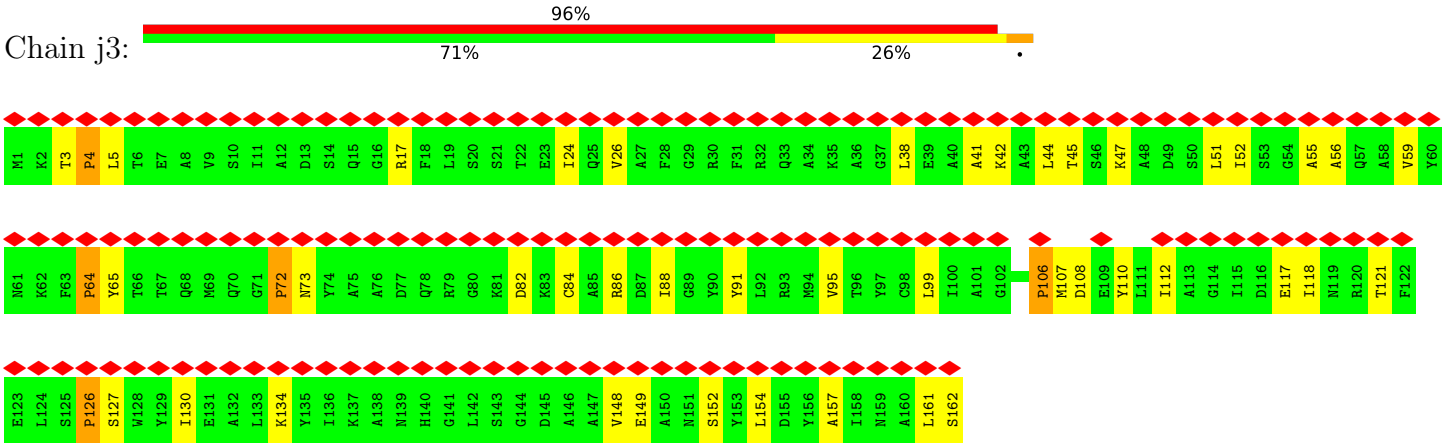
Chain h3:





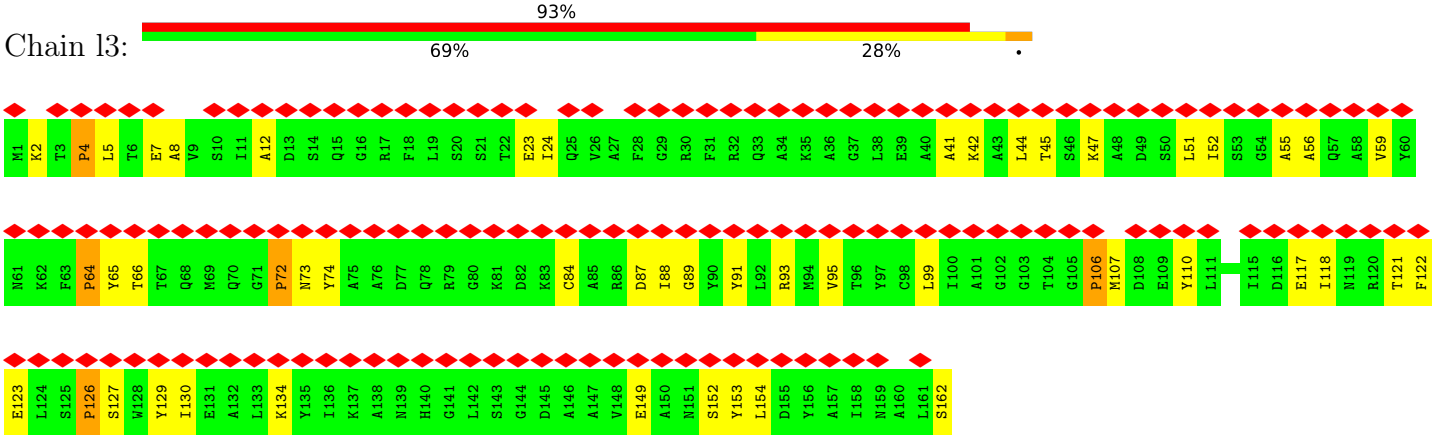
• Molecule 31: C-phycocyanin alpha subunit

Chain j3:



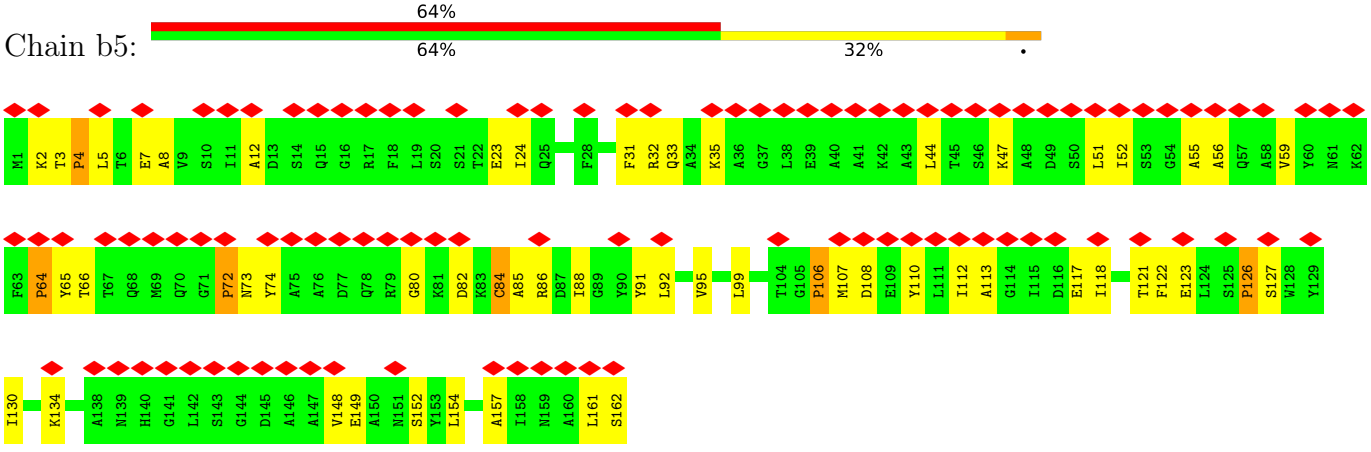
• Molecule 31: C-phycocyanin alpha subunit

Chain l3:



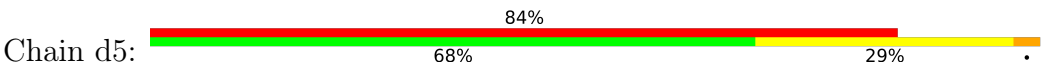
• Molecule 31: C-phycocyanin alpha subunit

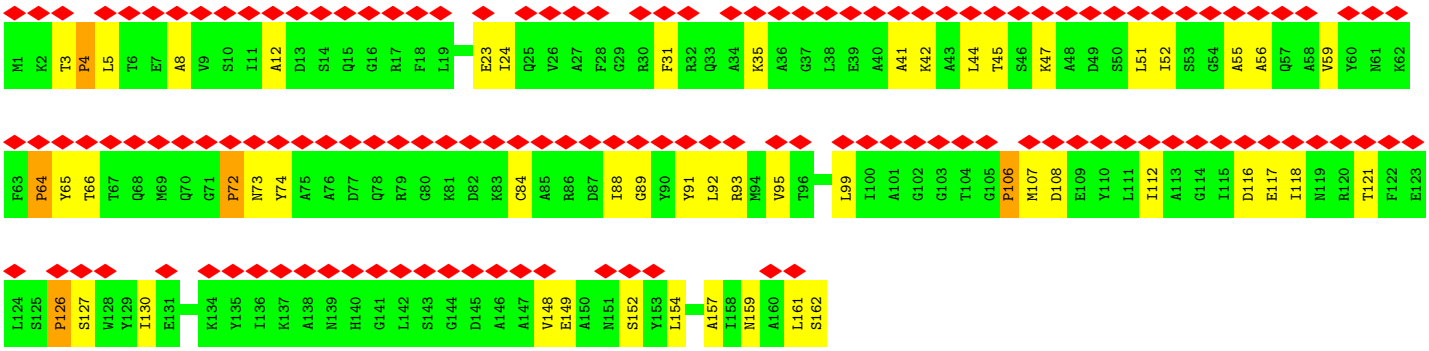
Chain b5:



• Molecule 31: C-phycocyanin alpha subunit

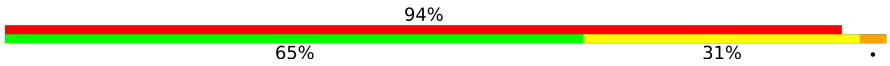
Chain d5:

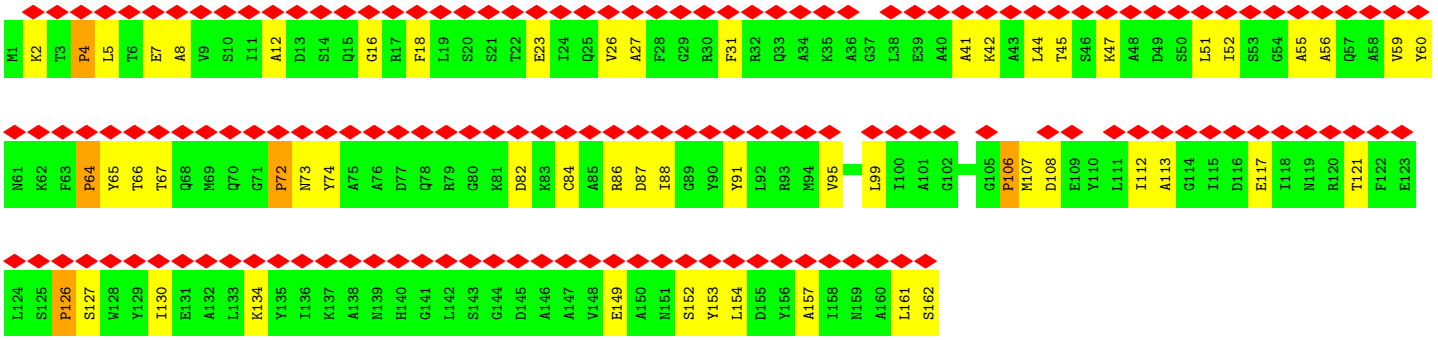




• Molecule 31: C-phycocyanin alpha subunit

Chain f5:

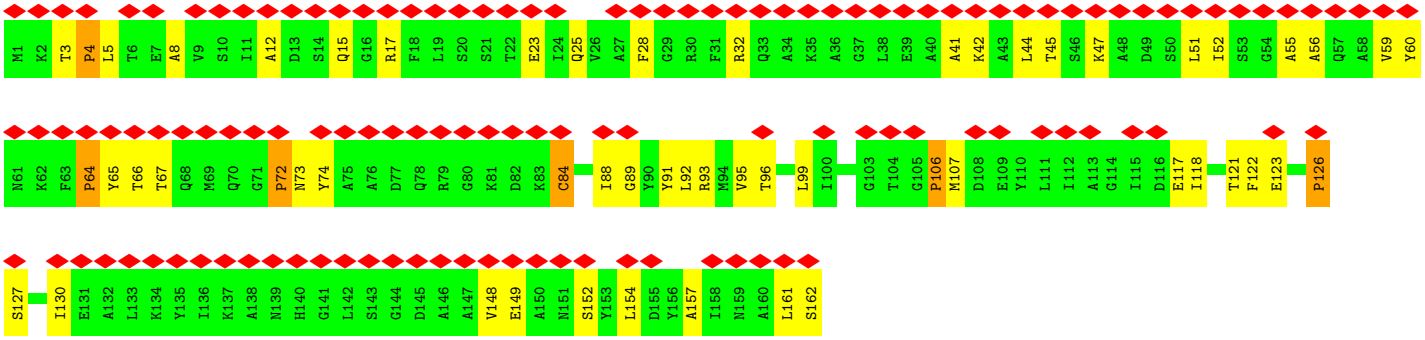




• Molecule 31: C-phycocyanin alpha subunit

Chain h5:

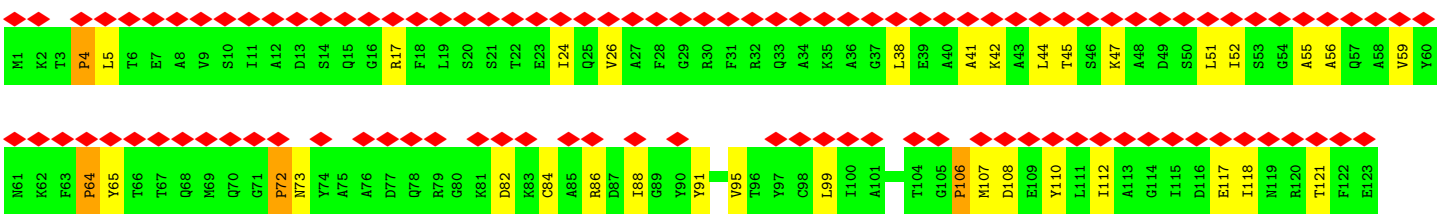


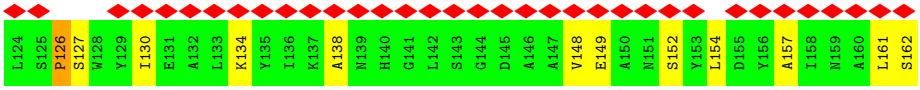


• Molecule 31: C-phycocyanin alpha subunit

Chain j5:

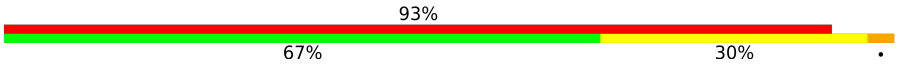


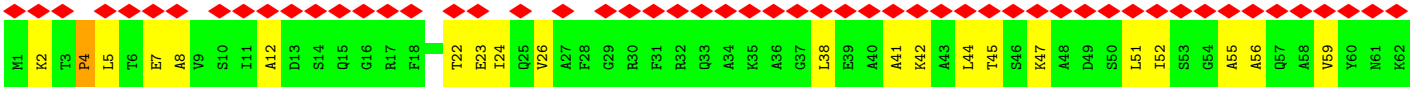


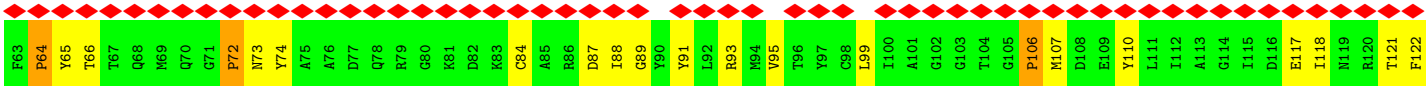


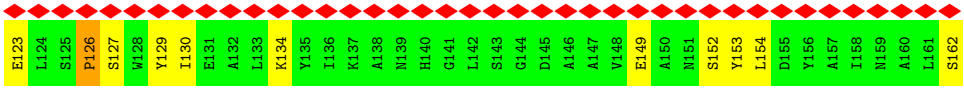
• Molecule 31: C-phycocyanin alpha subunit

Chain l5:





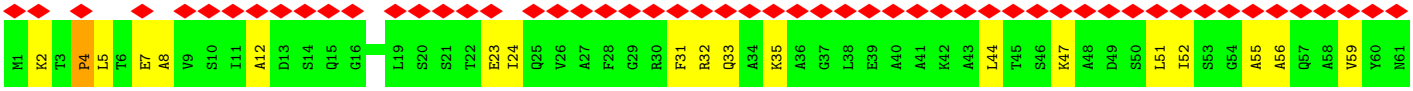


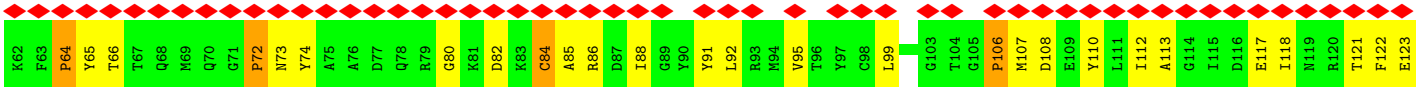


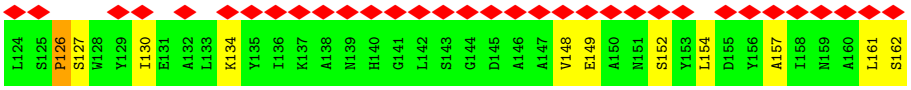
• Molecule 31: C-phycocyanin alpha subunit

Chain b6:



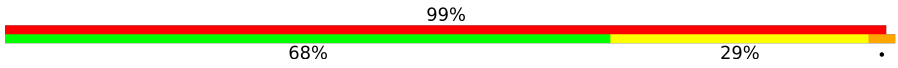


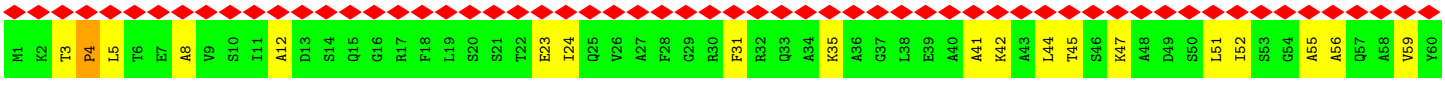


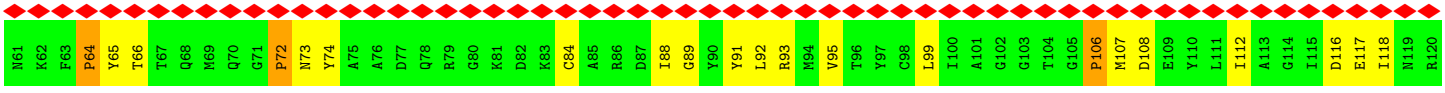


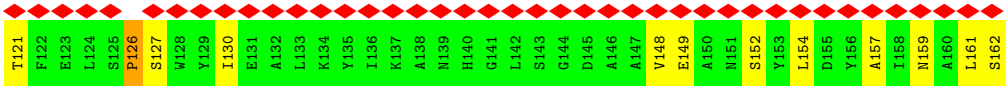
• Molecule 31: C-phycocyanin alpha subunit

Chain d6:



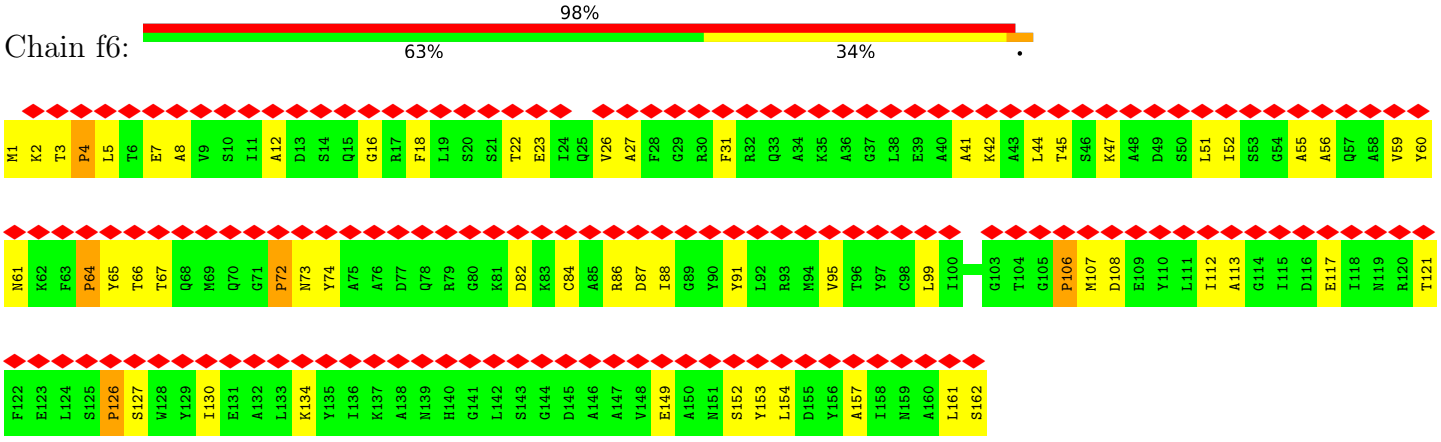






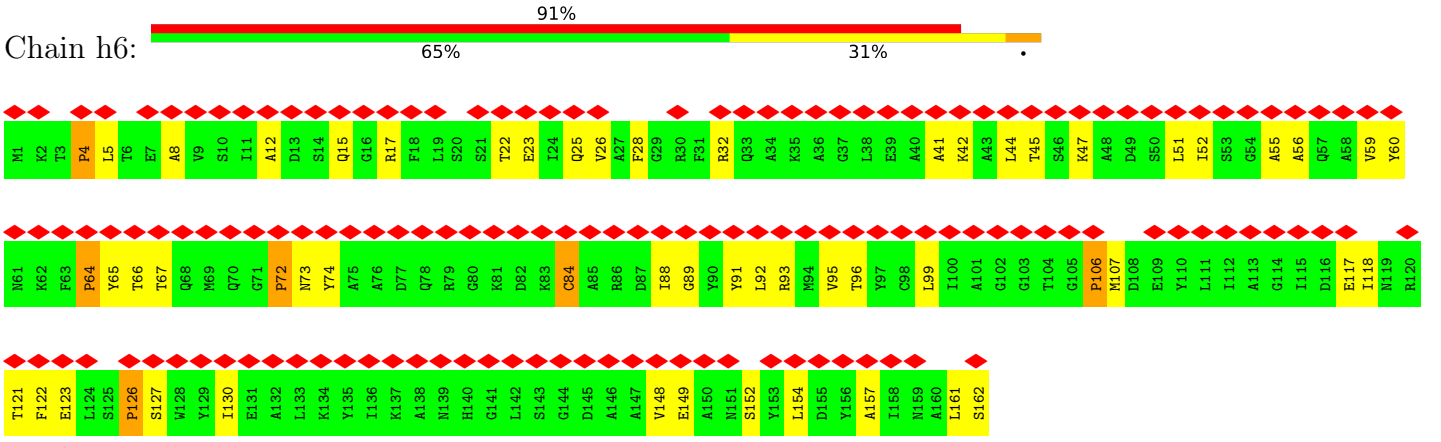
• Molecule 31: C-phycocyanin alpha subunit

Chain f6:



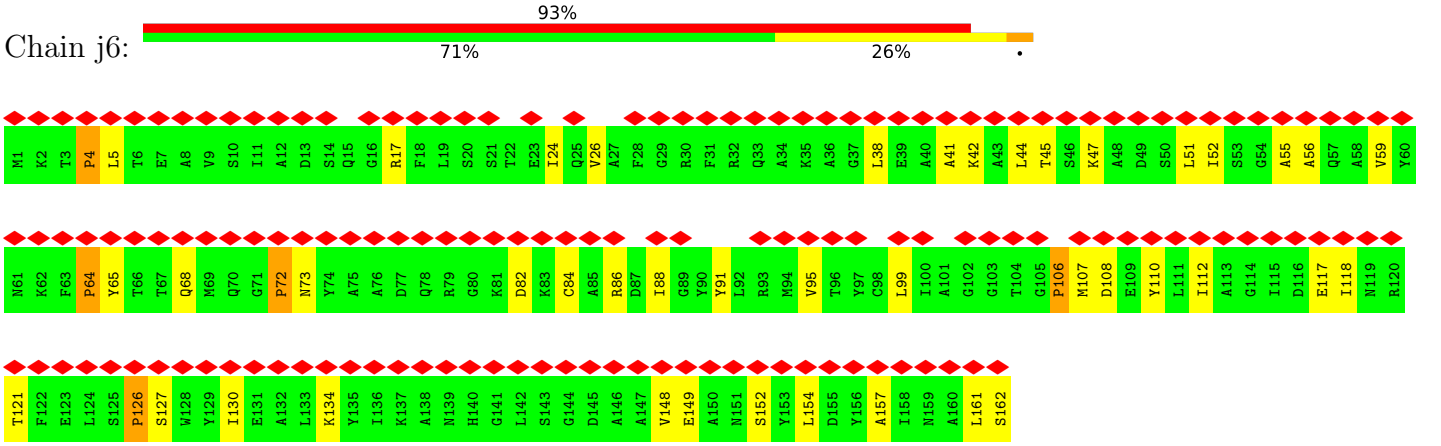
• Molecule 31: C-phycocyanin alpha subunit

Chain h6:



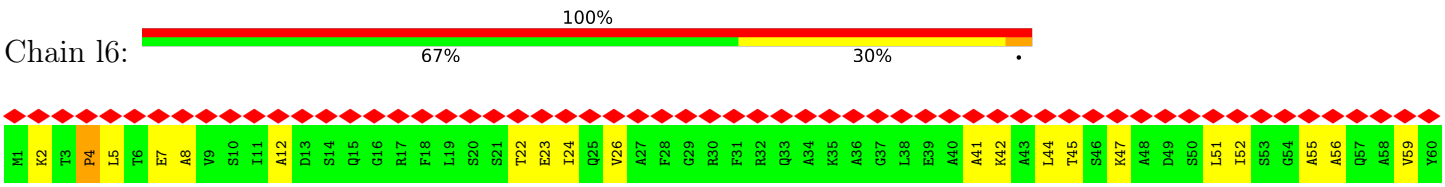
• Molecule 31: C-phycocyanin alpha subunit

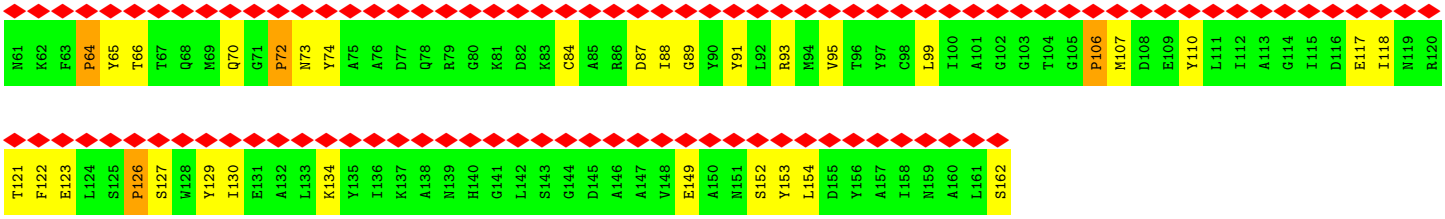
Chain j6:



• Molecule 31: C-phycocyanin alpha subunit

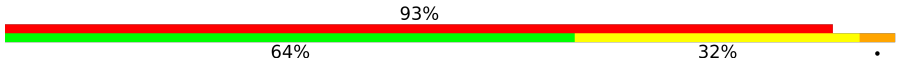
Chain l6:

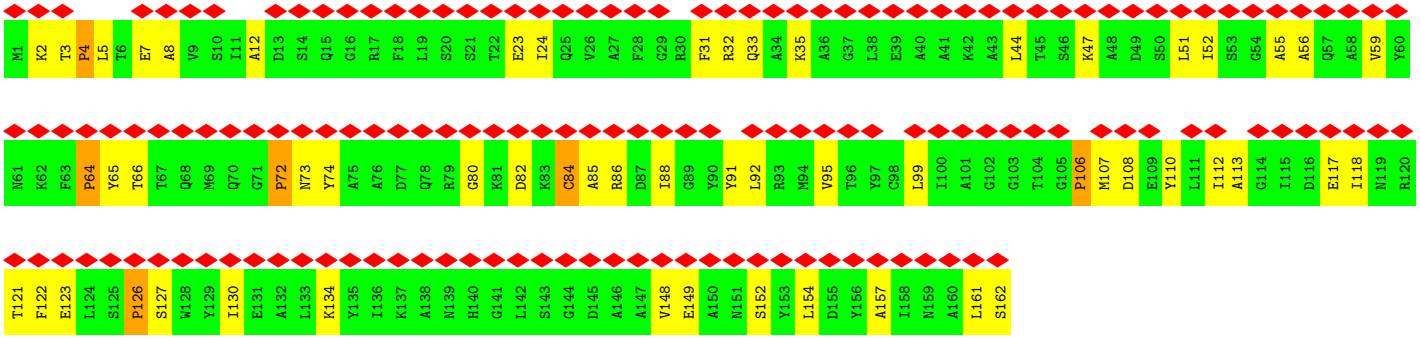




• Molecule 31: C-phycocyanin alpha subunit

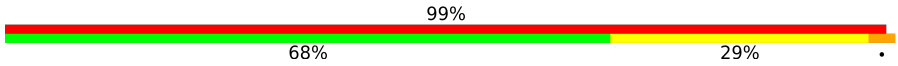
Chain b7:

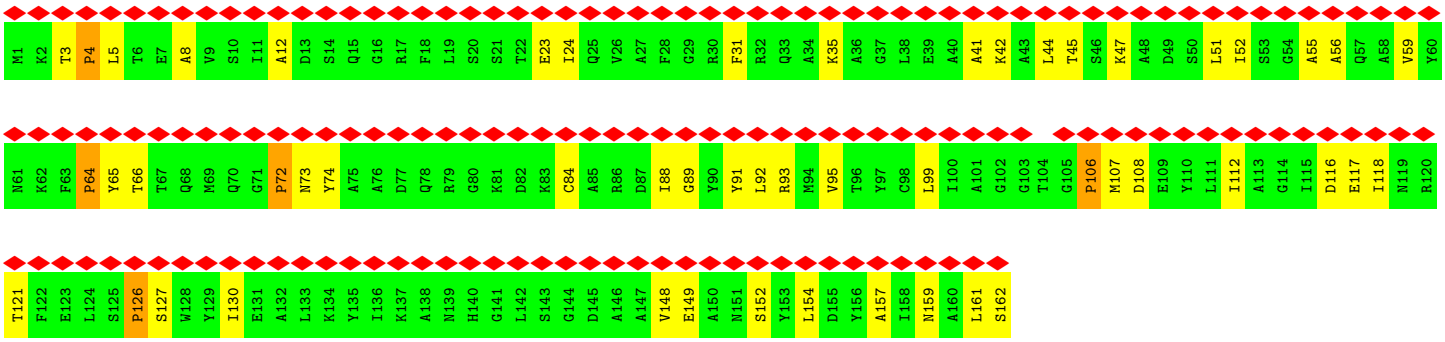




• Molecule 31: C-phycocyanin alpha subunit

Chain d7:

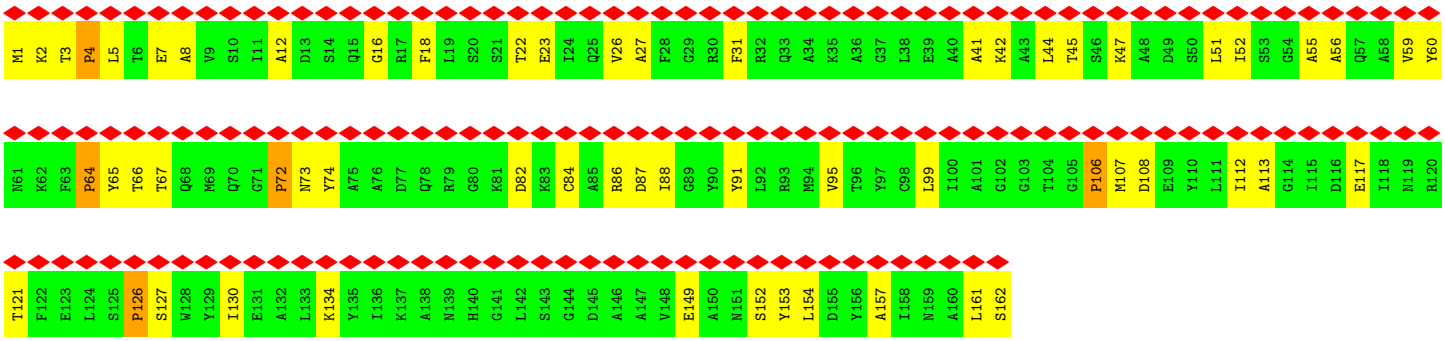




• Molecule 31: C-phycocyanin alpha subunit

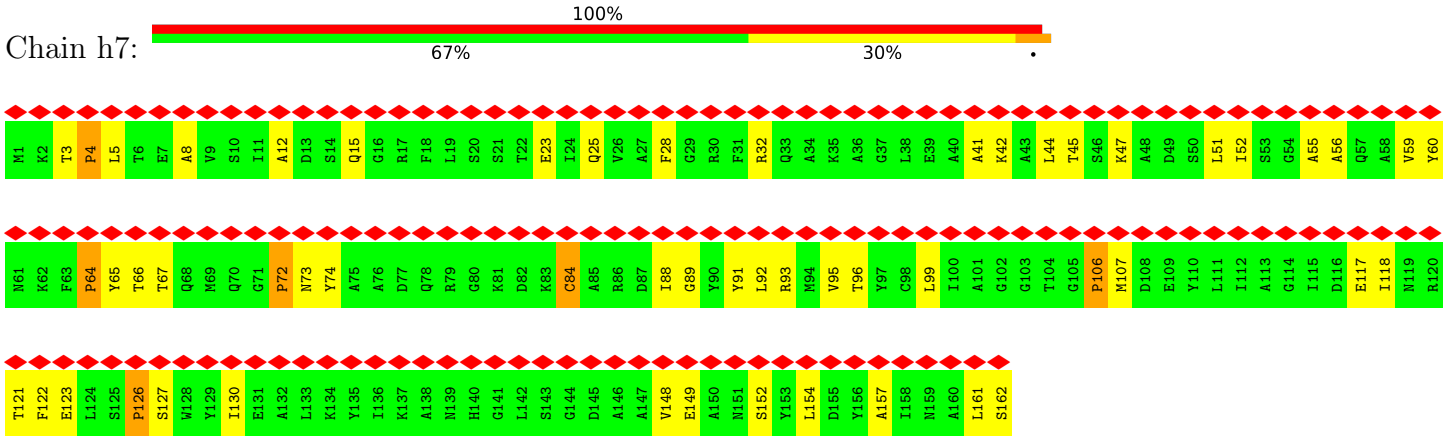
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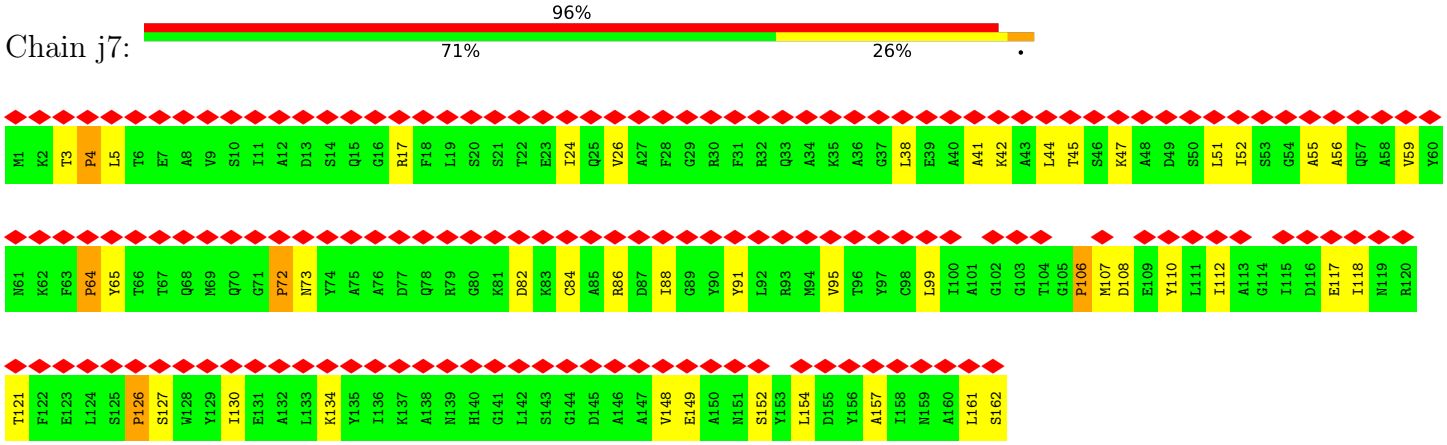
• Molecule 31: C-phycocyanin alpha subunit

Chain h7:



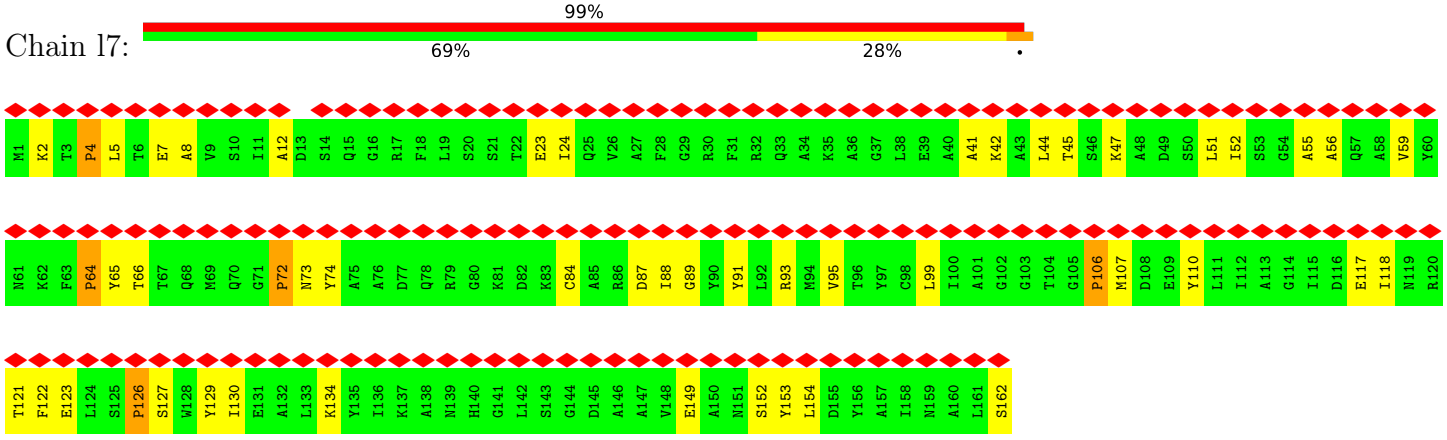
• Molecule 31: C-phycocyanin alpha subunit

Chain j7:



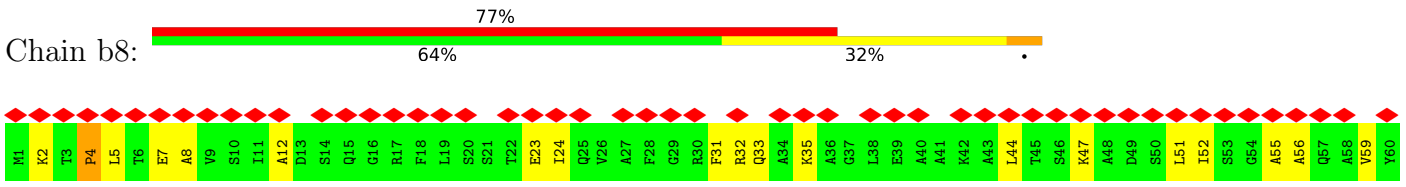
• Molecule 31: C-phycocyanin alpha subunit

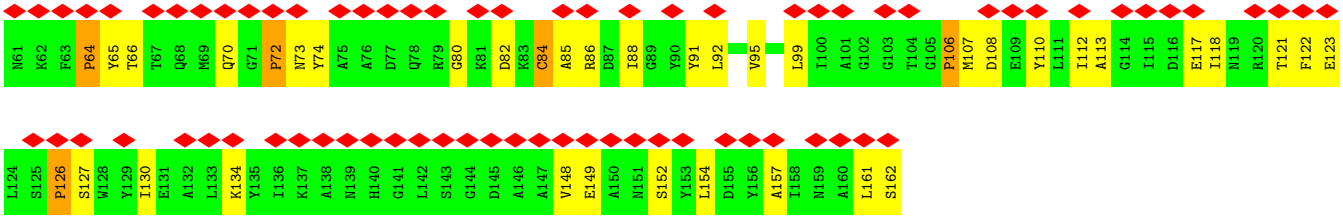
Chain l7:



• Molecule 31: C-phycocyanin alpha subunit

Chain b8:

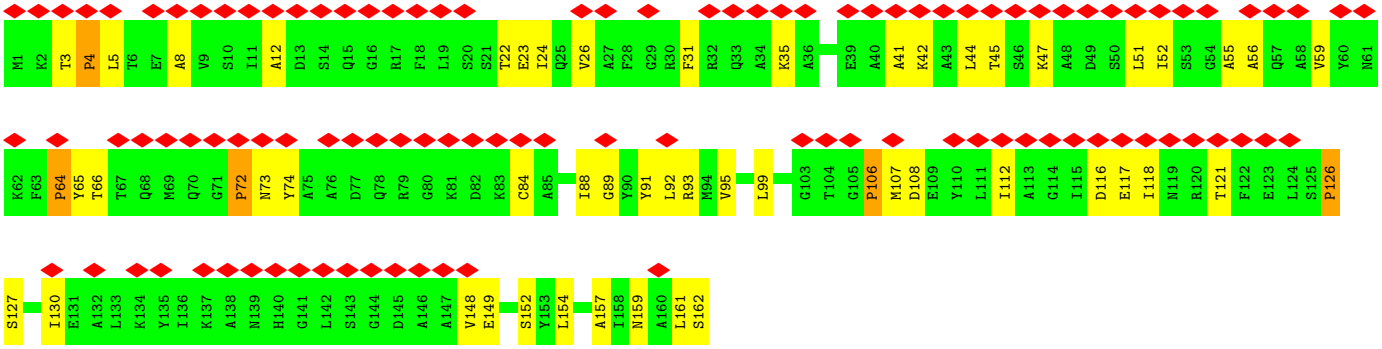




• Molecule 31: C-phycocyanin alpha subunit

Chain d8:

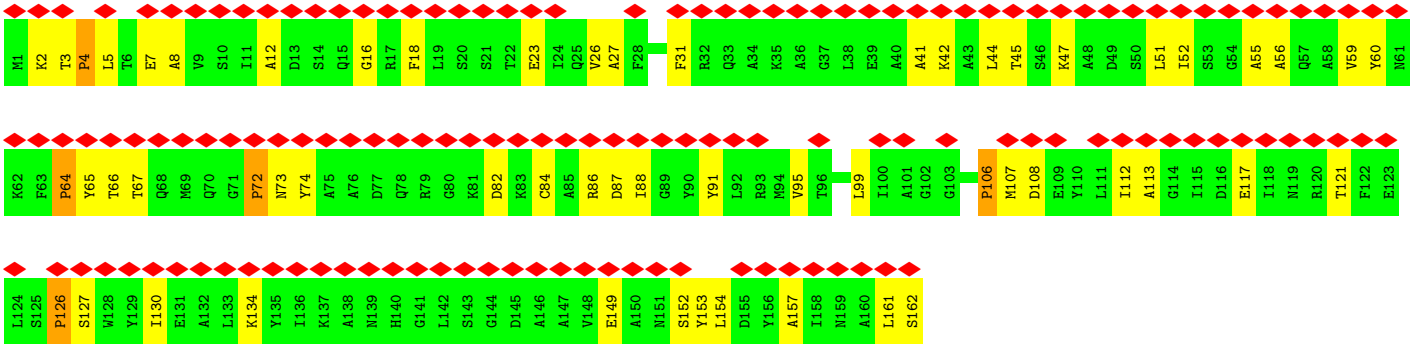




• Molecule 31: C-phycocyanin alpha subunit

Chain f8:

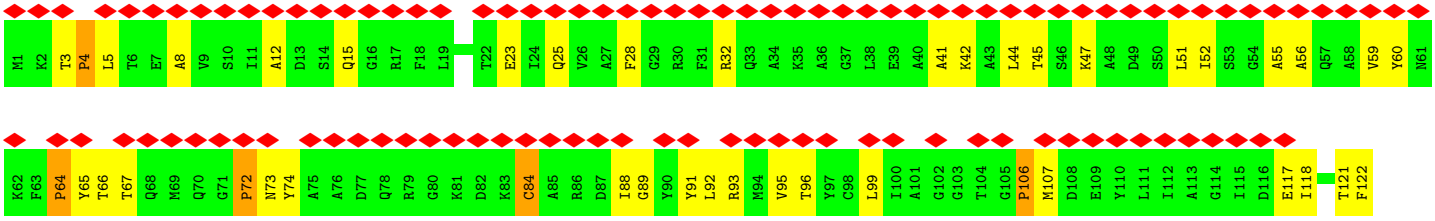


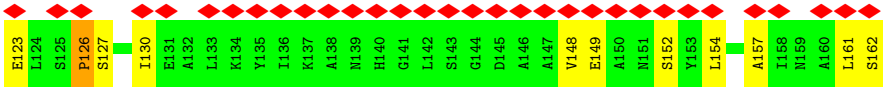


• Molecule 31: C-phycocyanin alpha subunit

Chain h8:



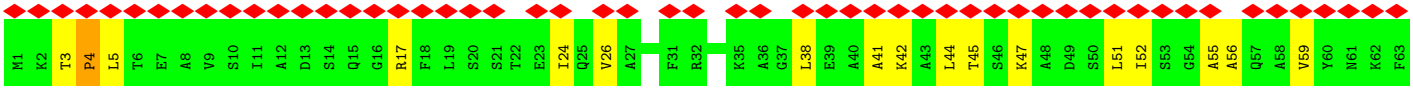


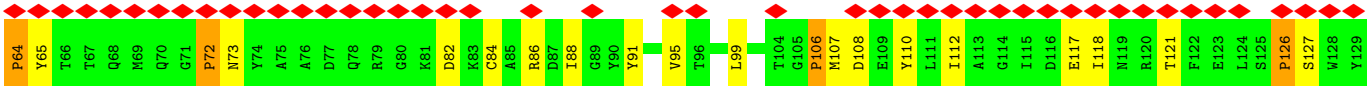


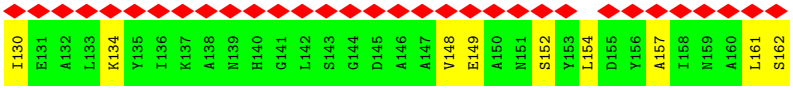
• Molecule 31: C-phycocyanin alpha subunit

Chain j8:





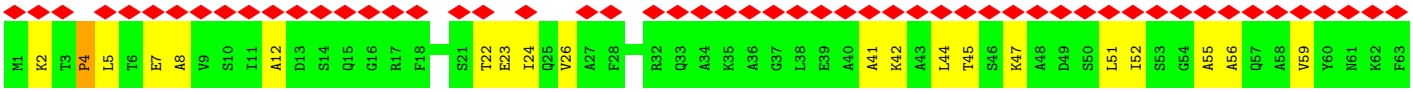


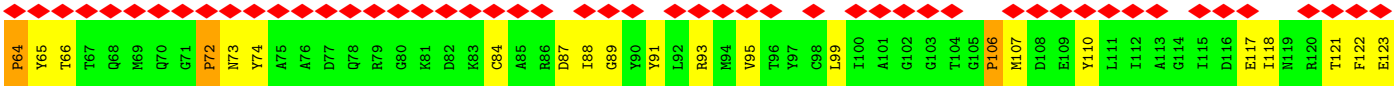


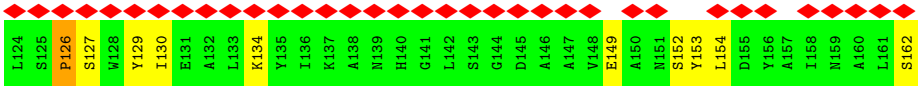
• Molecule 31: C-phycocyanin alpha subunit

Chain l8:





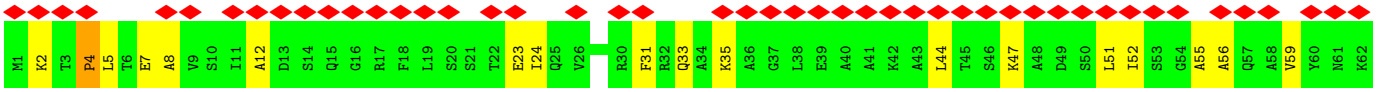


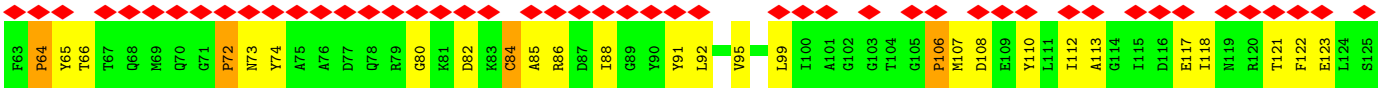


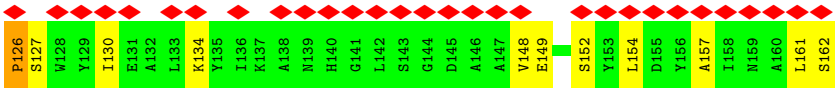
• Molecule 31: C-phycocyanin alpha subunit

Chain b9:



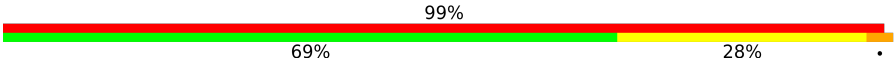


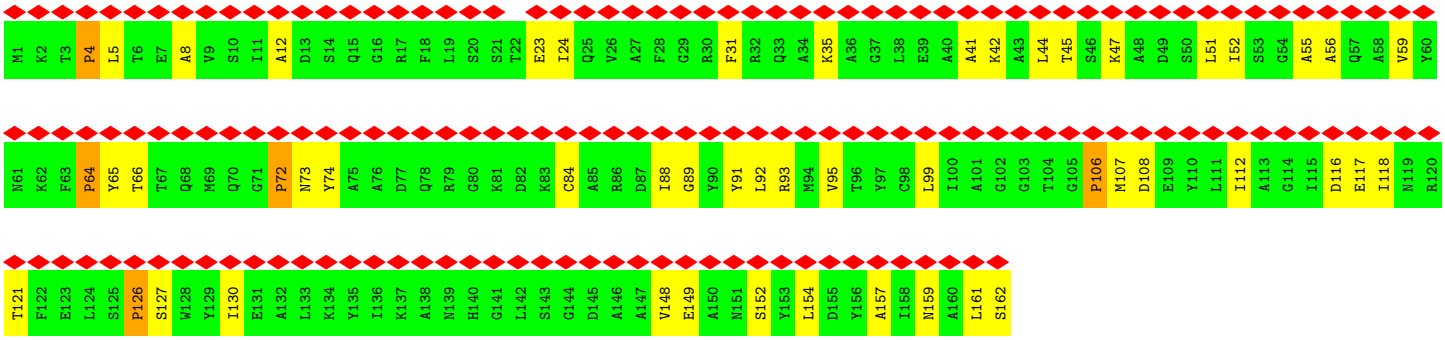




• Molecule 31: C-phycocyanin alpha subunit

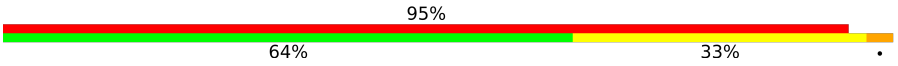
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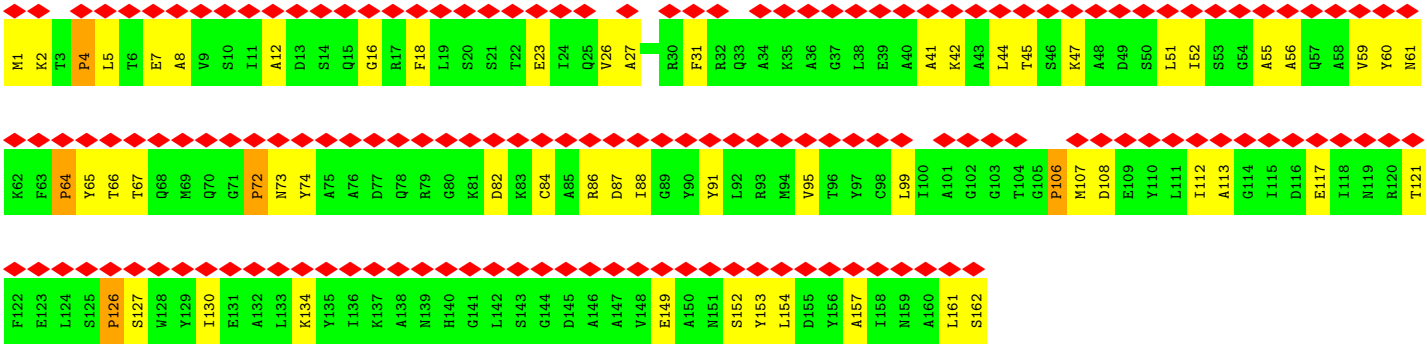




• Molecule 31: C-phycocyanin alpha subunit

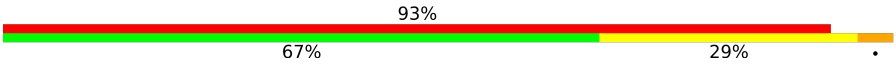
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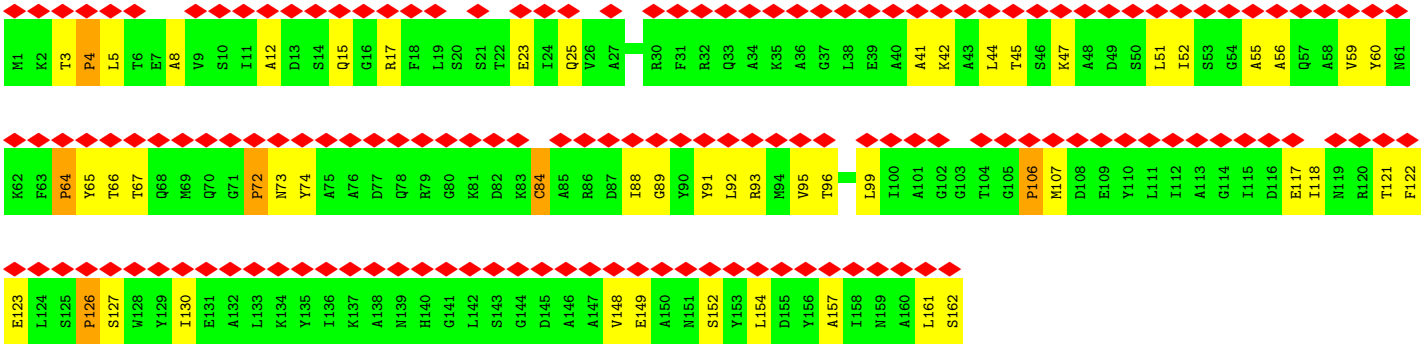




• Molecule 31: C-phycocyanin alpha subunit

Chain h9:

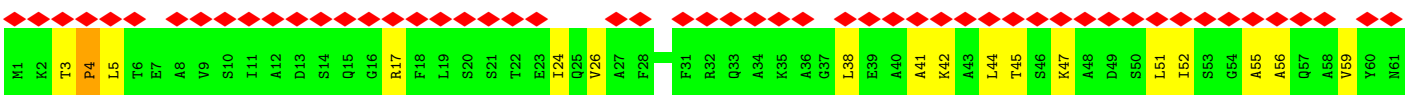


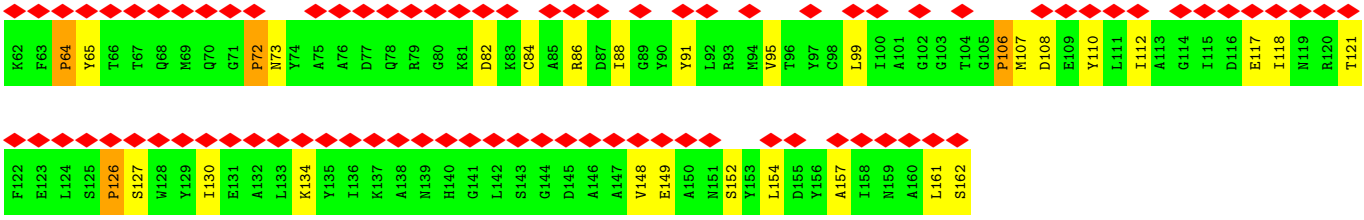


• Molecule 31: C-phycocyanin alpha subunit

Chain j9:



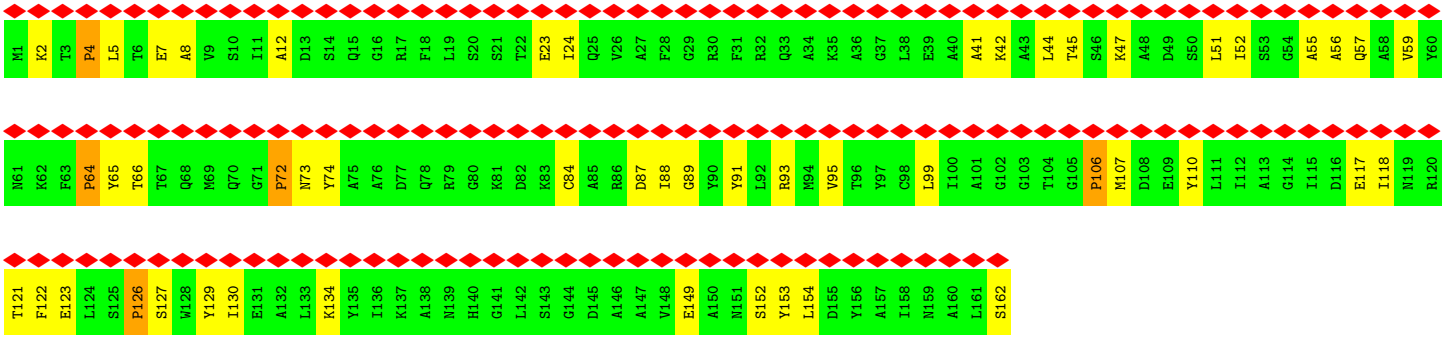




• Molecule 31: C-phycocyanin alpha subunit

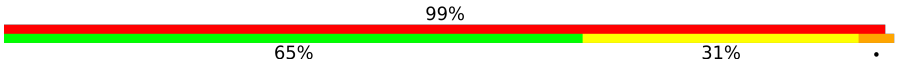
Chain l9:

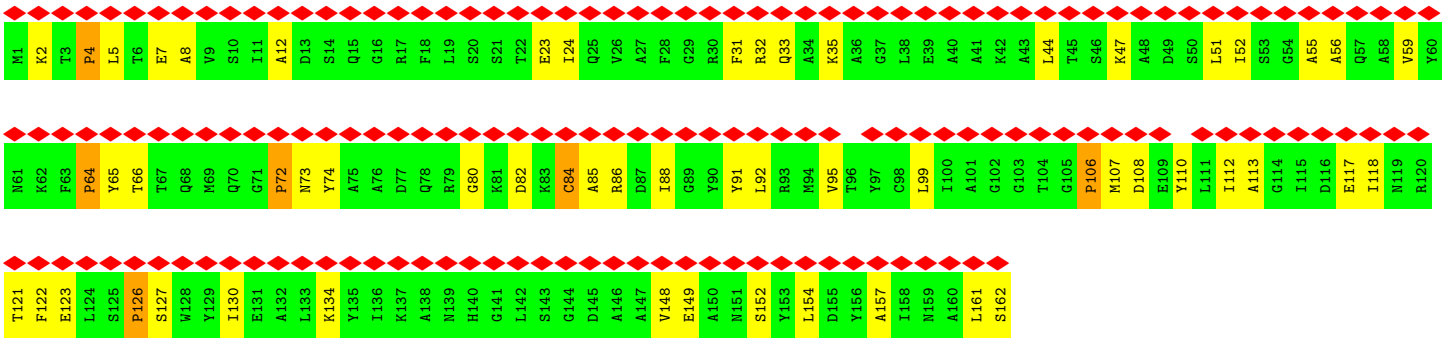




• Molecule 31: C-phycocyanin alpha subunit

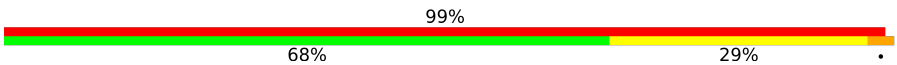
Chain bA:

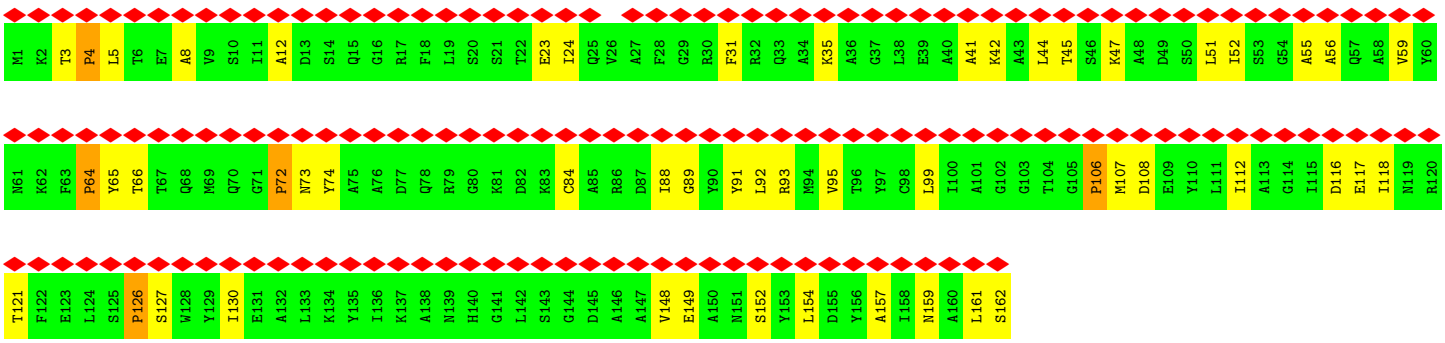




• Molecule 31: C-phycocyanin alpha subunit

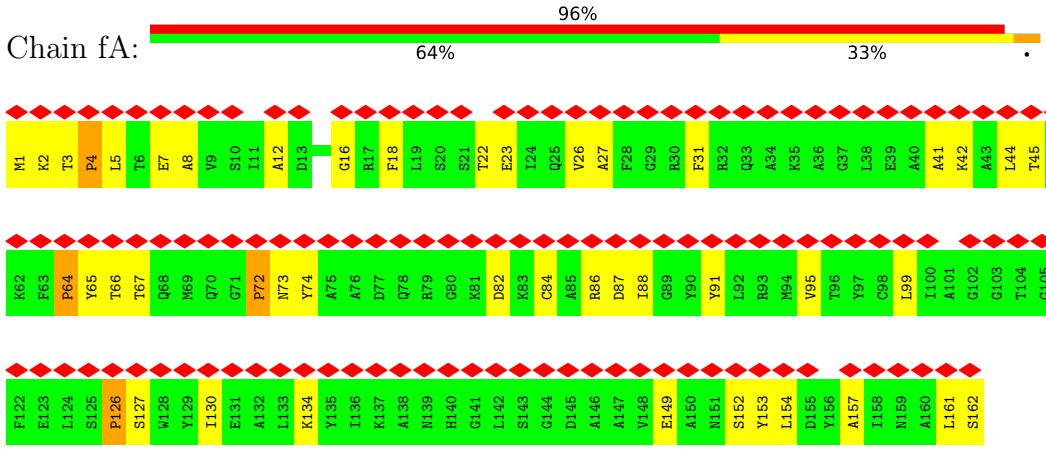
Chain dA:





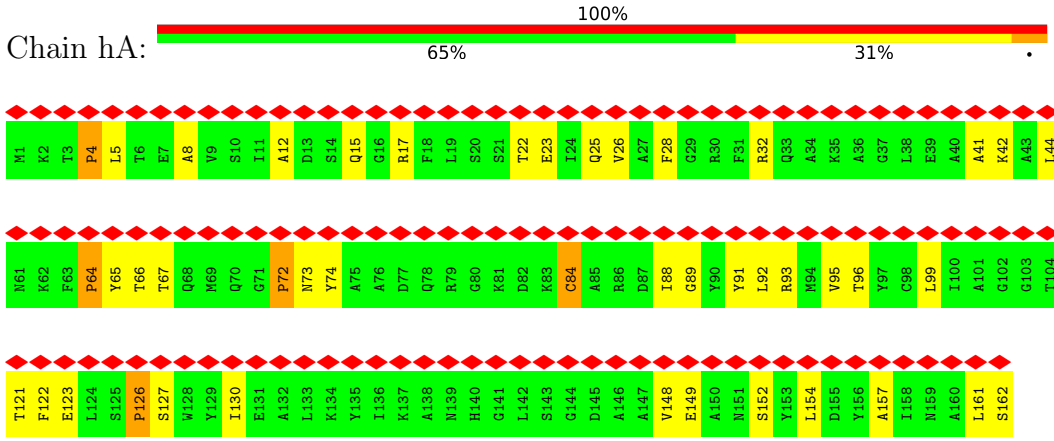
• Molecule 31: C-phycocyanin alpha subunit

Chain fA:



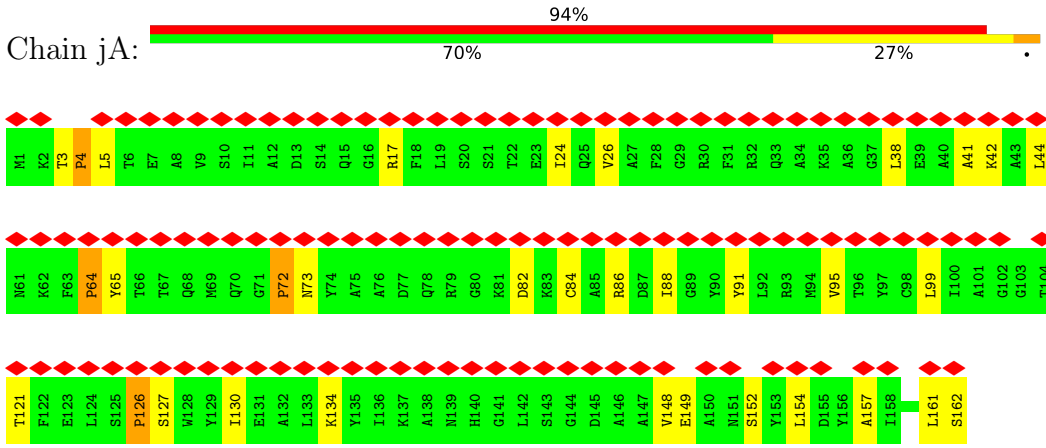
• Molecule 31: C-phycocyanin alpha subunit

Chain hA:



• Molecule 31: C-phycocyanin alpha subunit

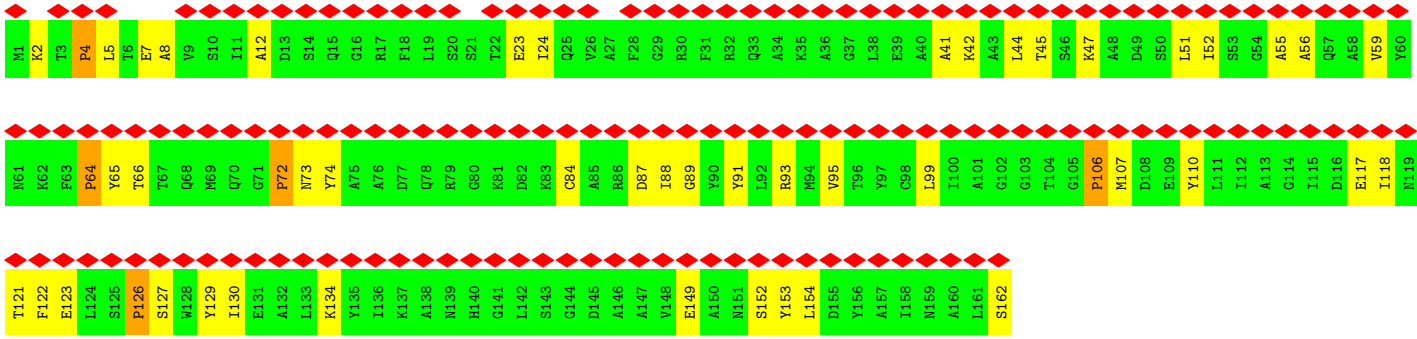
Chain jA:



• Molecule 31: C-phycocyanin alpha subunit

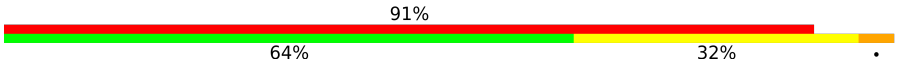
Chain lA:





• Molecule 31: C-phycocyanin alpha subunit

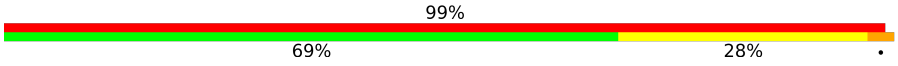
Chain bC:





• Molecule 31: C-phycocyanin alpha subunit

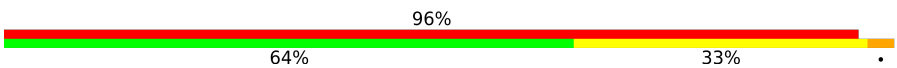
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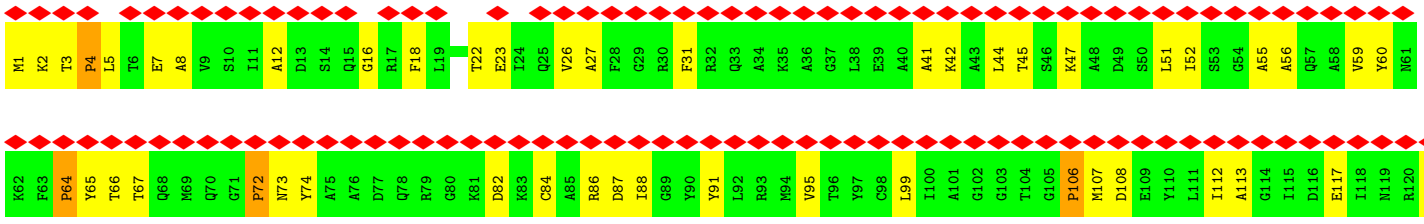


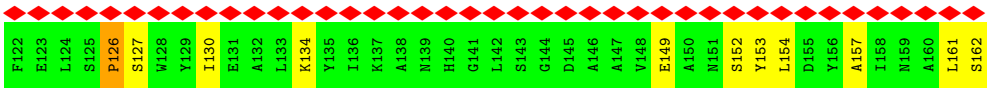


• Molecule 31: C-phycocyanin alpha subunit

Chain fC:

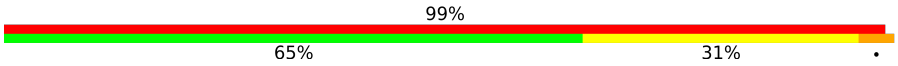


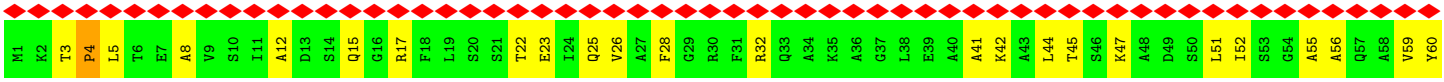


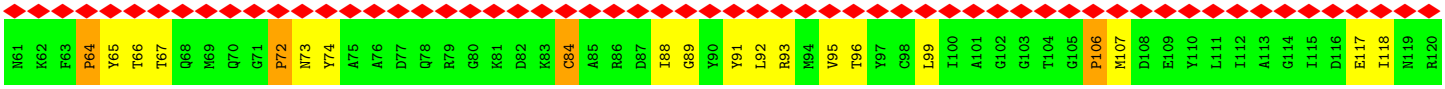


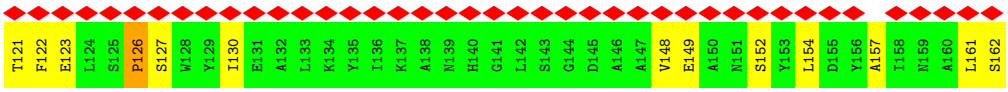
• Molecule 31: C-phycocyanin alpha subunit

Chain hC:



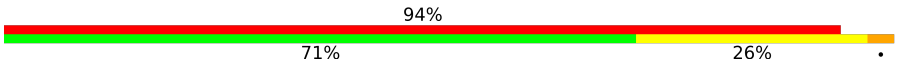


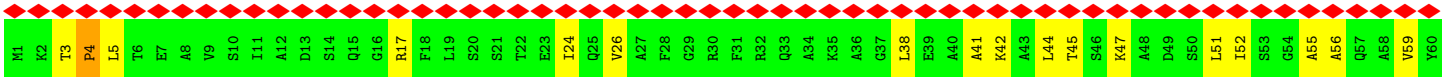


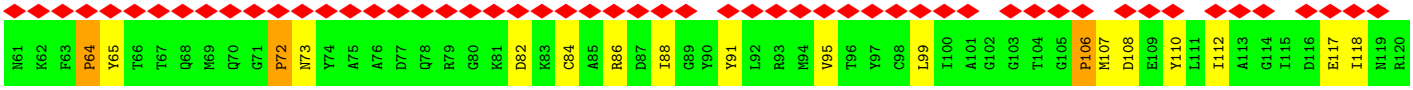


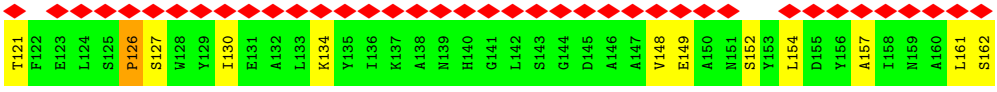
• Molecule 31: C-phycocyanin alpha subunit

Chain jC:



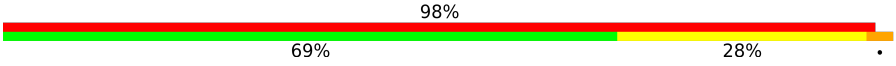


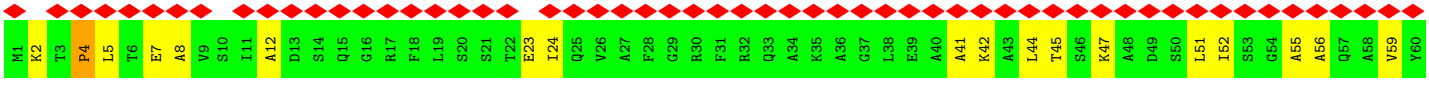


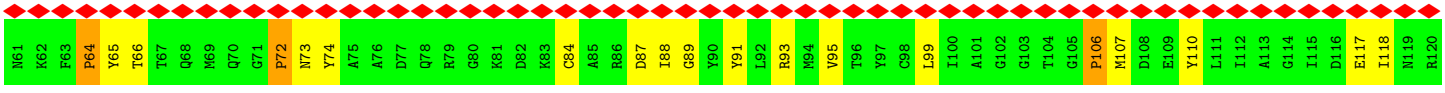


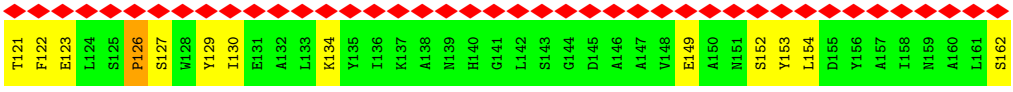
• Molecule 31: C-phycocyanin alpha subunit

Chain lC:



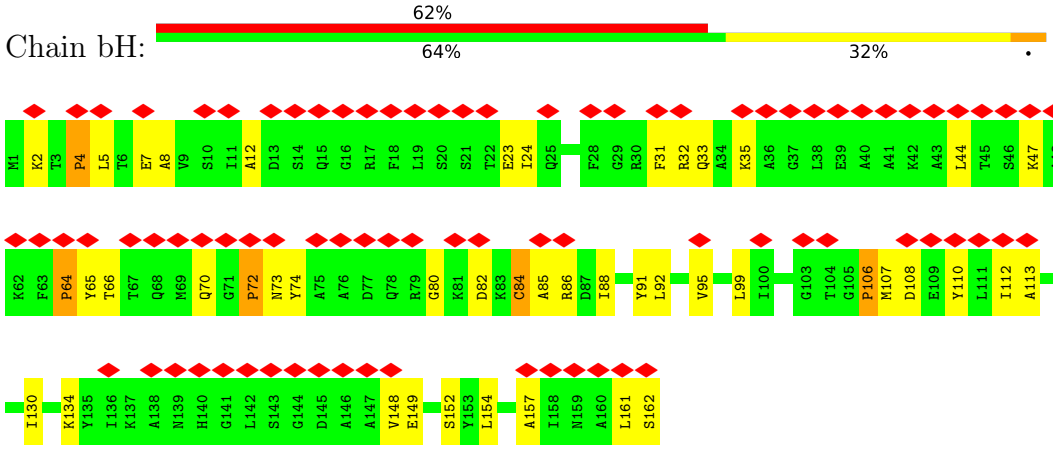






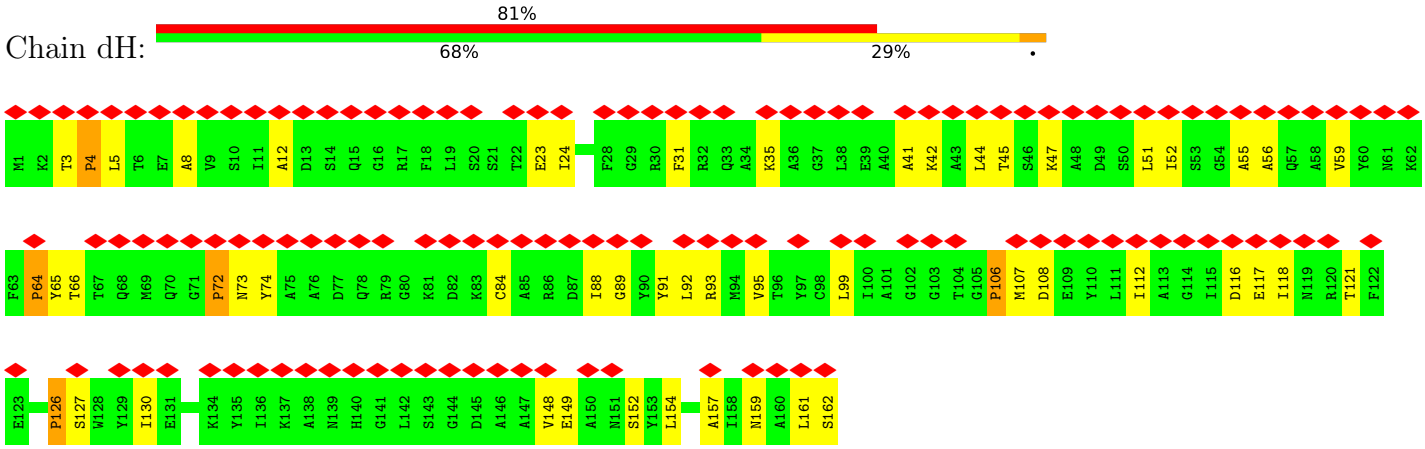
• Molecule 31: C-phycocyanin alpha subunit

Chain bH:



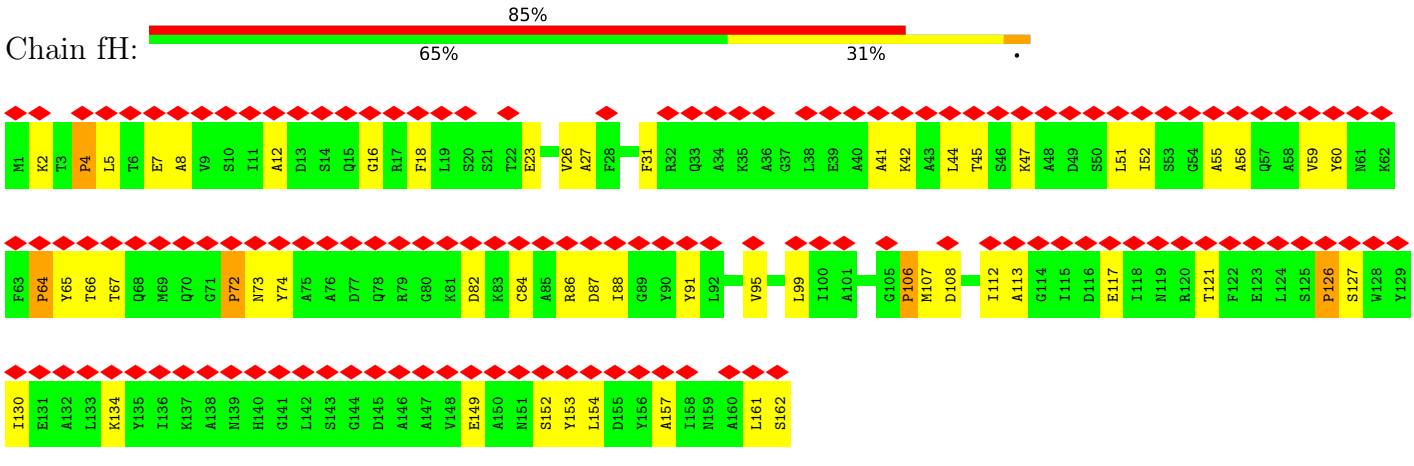
• Molecule 31: C-phycocyanin alpha subunit

Chain dH:



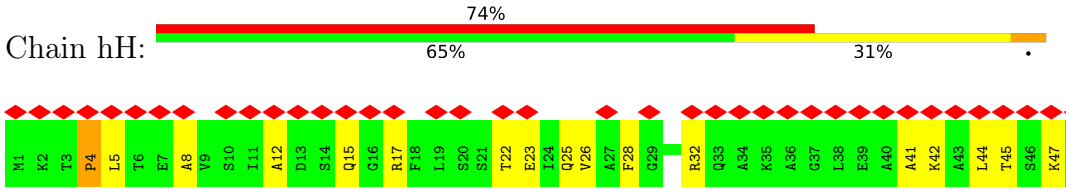
• Molecule 31: C-phycocyanin alpha subunit

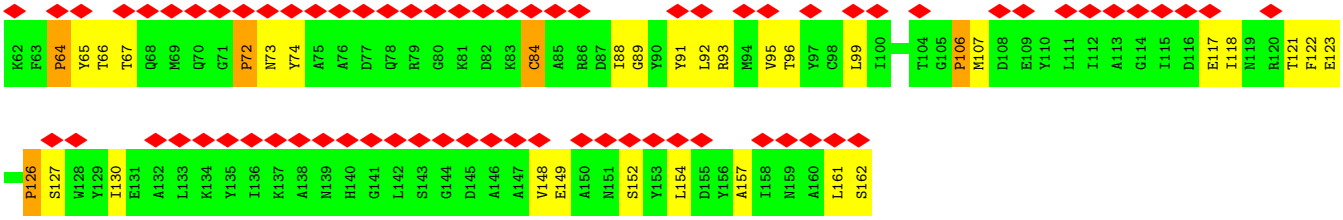
Chain fH:



• Molecule 31: C-phycocyanin alpha subunit

Chain hH:

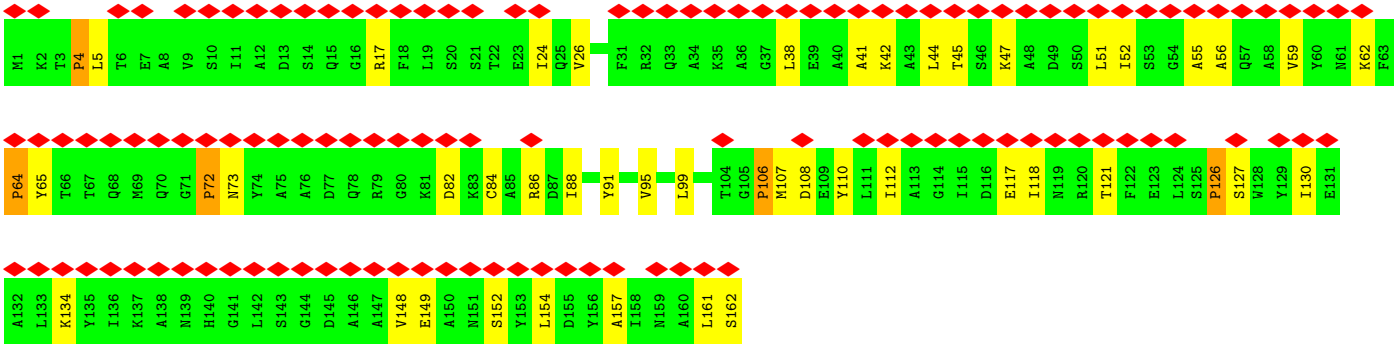




• Molecule 31: C-phycocyanin alpha subunit

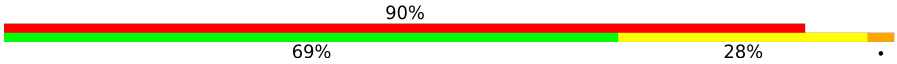
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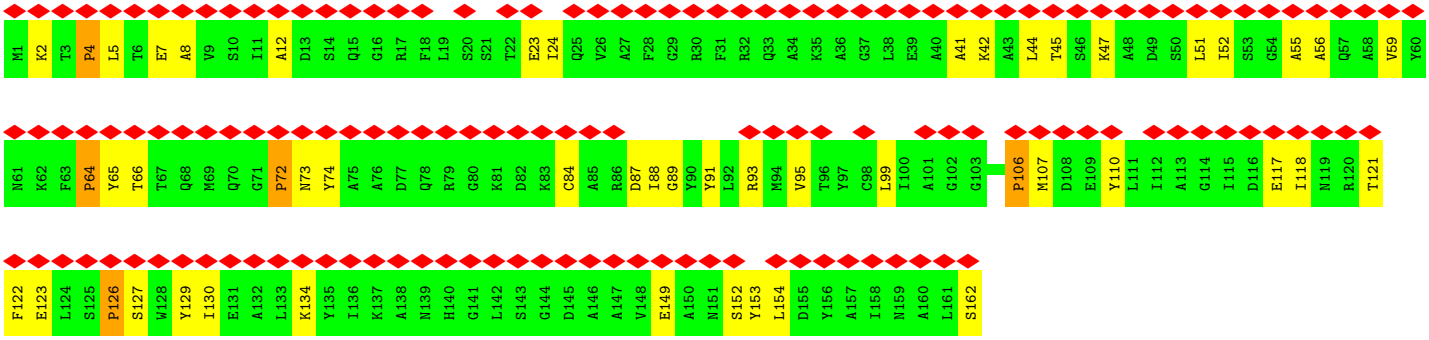




• Molecule 31: C-phycocyanin alpha subunit

Chain lH:

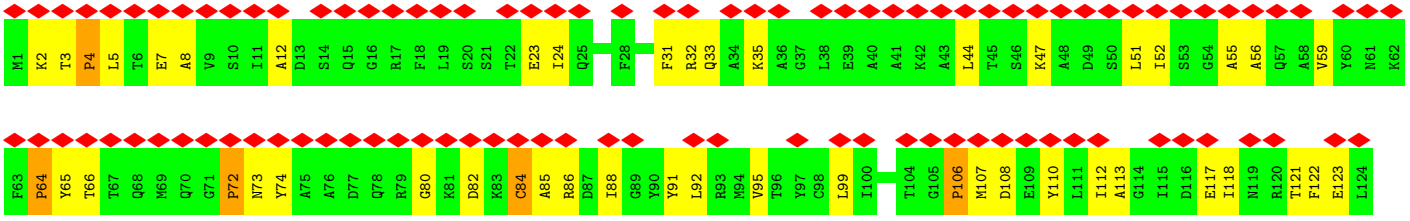


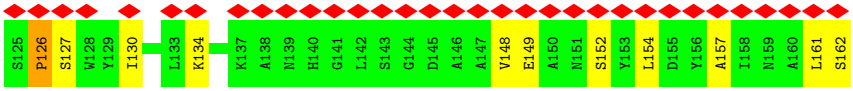


• Molecule 31: C-phycocyanin alpha subunit

Chain bI:

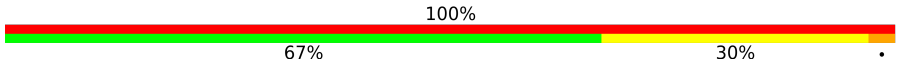


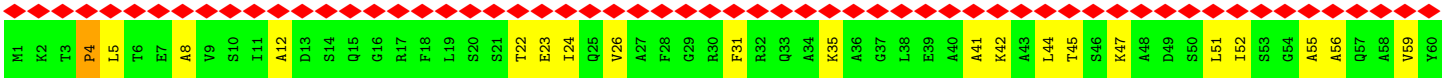


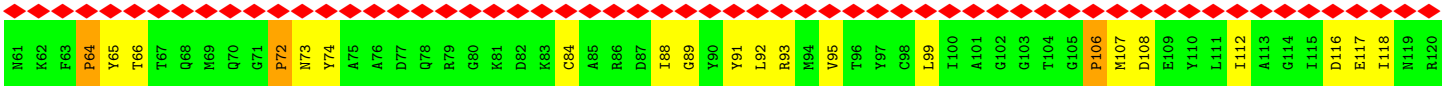


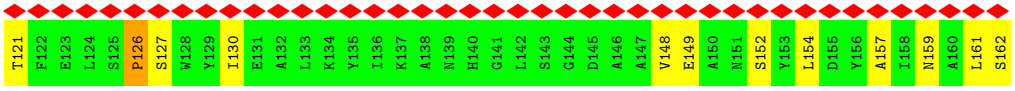
• Molecule 31: C-phycocyanin alpha subunit

Chain dI:



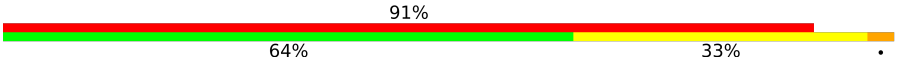


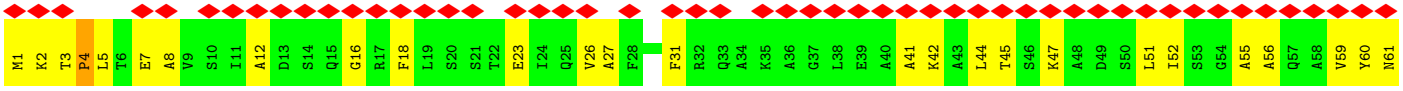


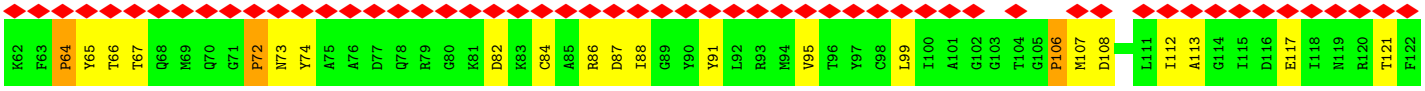


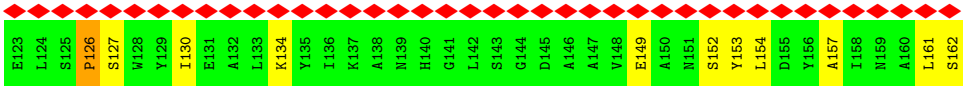
• Molecule 31: C-phycocyanin alpha subunit

Chain fI:



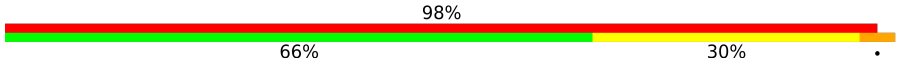


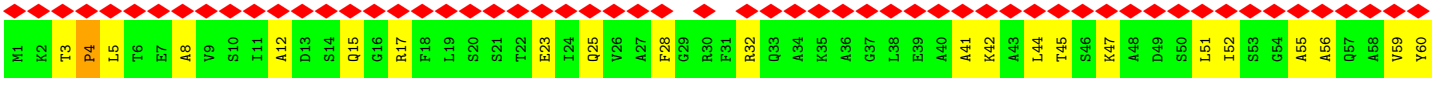


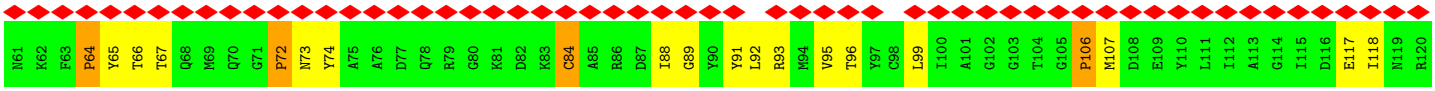


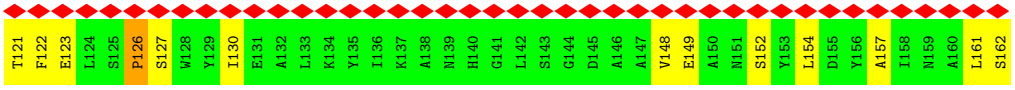
• Molecule 31: C-phycocyanin alpha subunit

Chain hI:



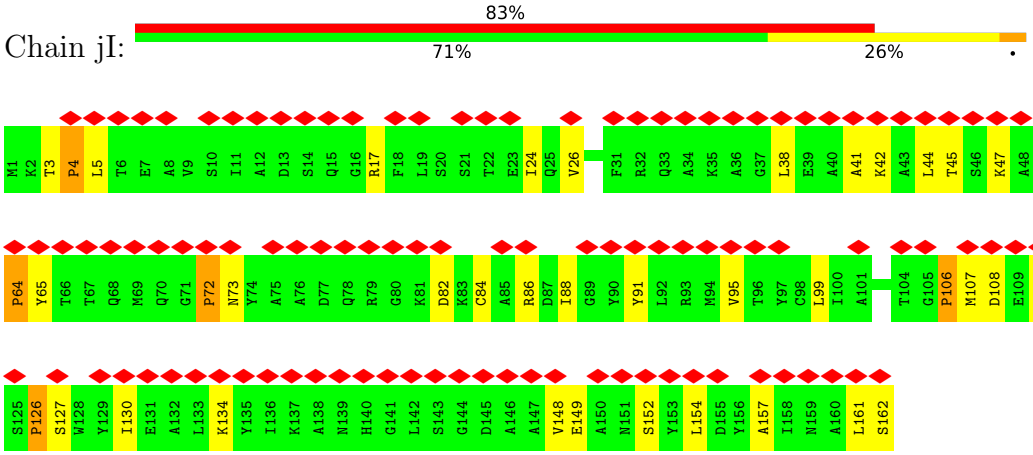






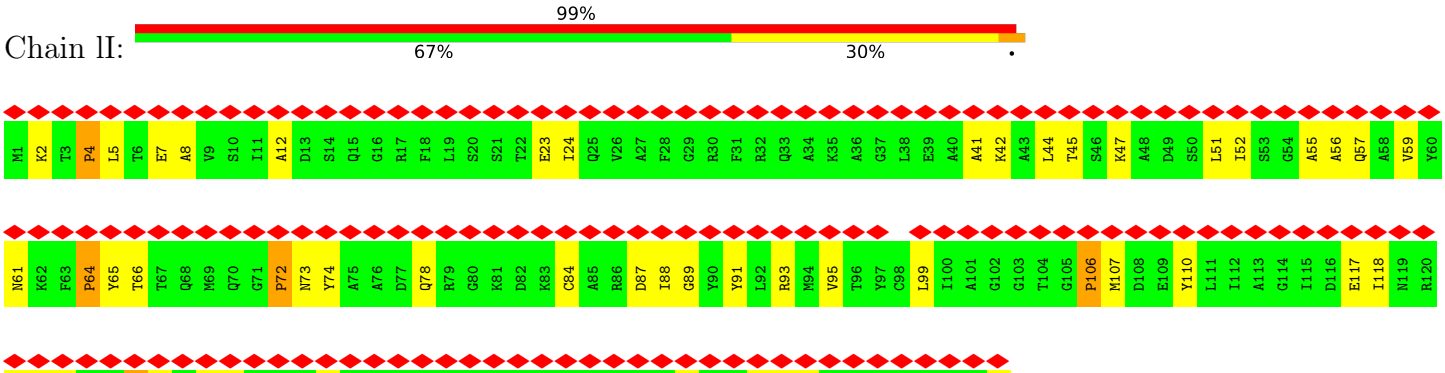
• Molecule 31: C-phycocyanin alpha subunit

Chain jI:



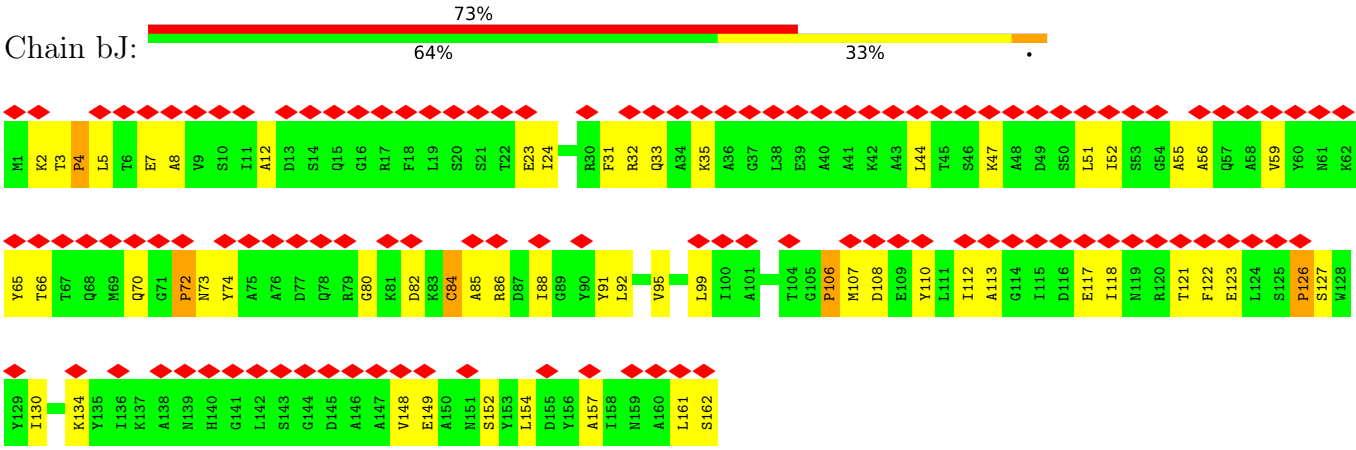
• Molecule 31: C-phycocyanin alpha subunit

Chain lI:



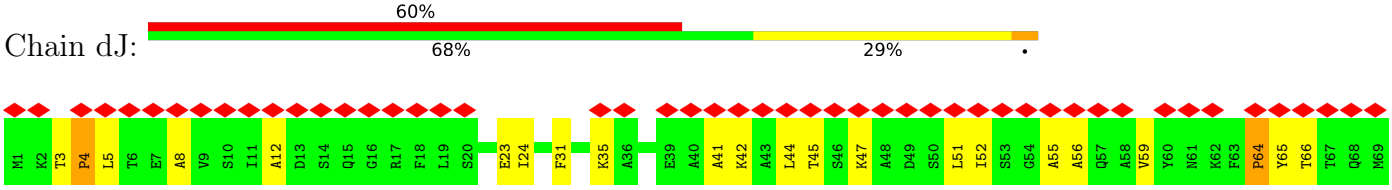
• Molecule 31: C-phycocyanin alpha subunit

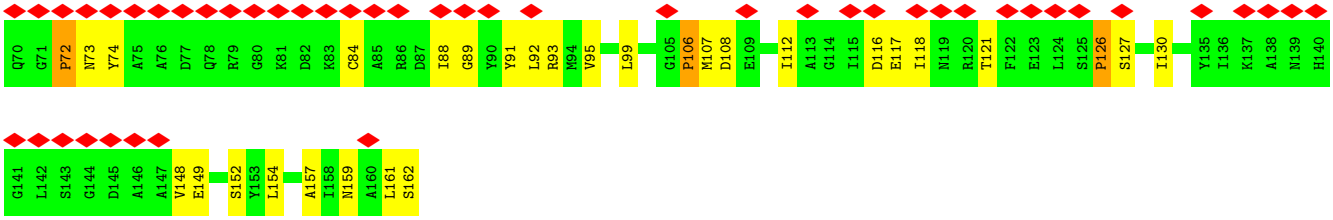
Chain bJ:



• Molecule 31: C-phycocyanin alpha subunit

Chain dJ:

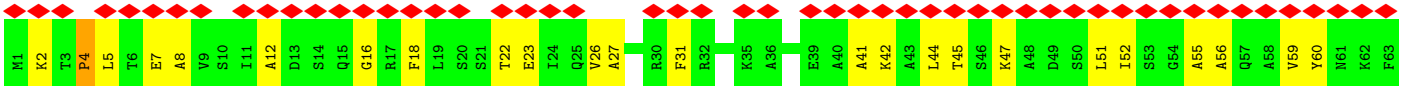


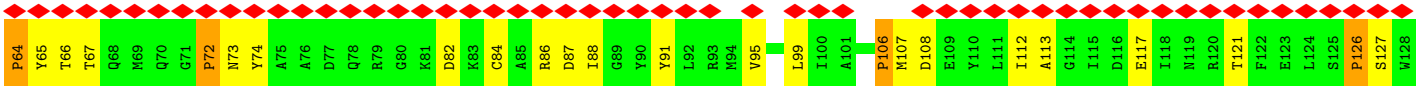


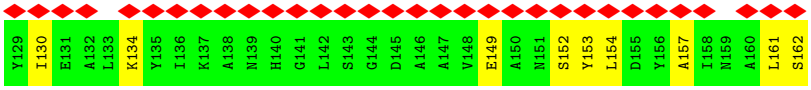
• Molecule 31: C-phycocyanin alpha subunit

Chain fJ:





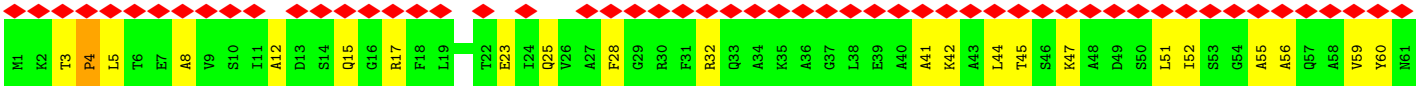




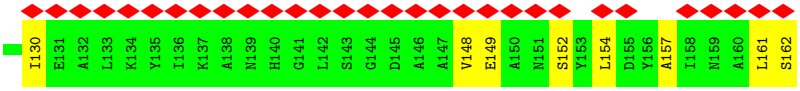
• Molecule 31: C-phycocyanin alpha subunit

Chain hJ:





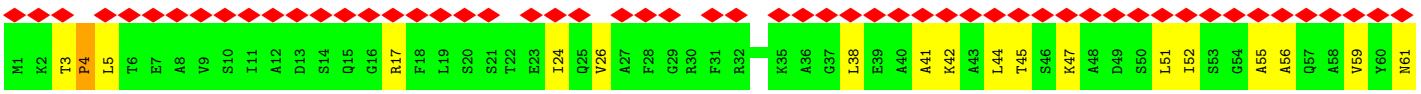


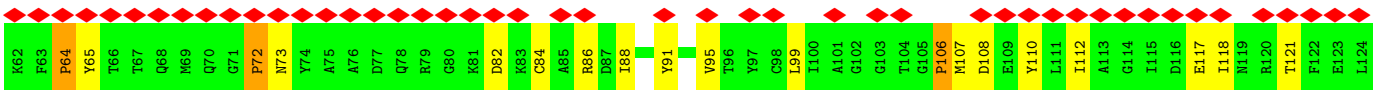


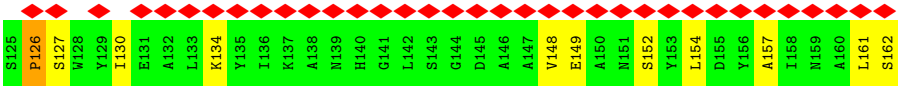
• Molecule 31: C-phycocyanin alpha subunit

Chain jJ:





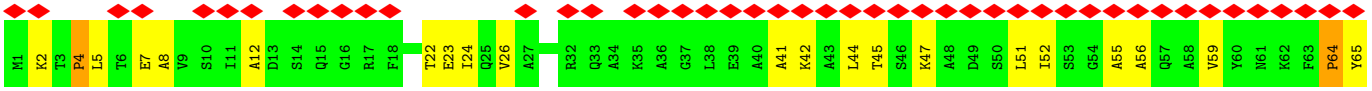


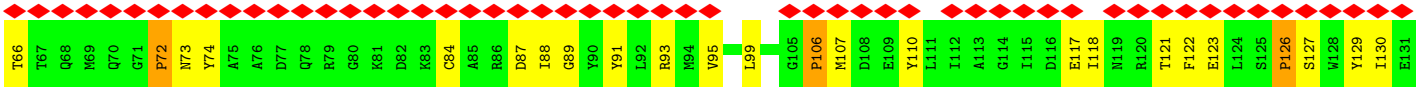


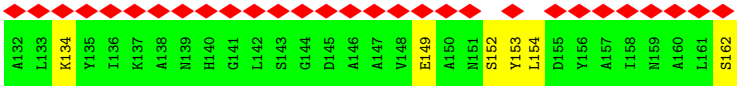
• Molecule 31: C-phycocyanin alpha subunit

Chain lJ:



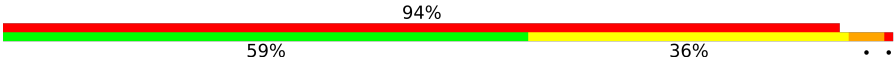


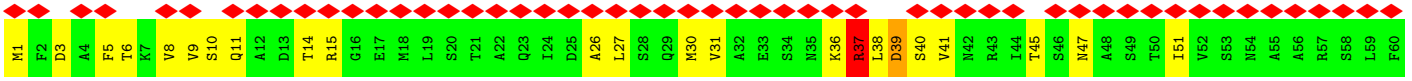


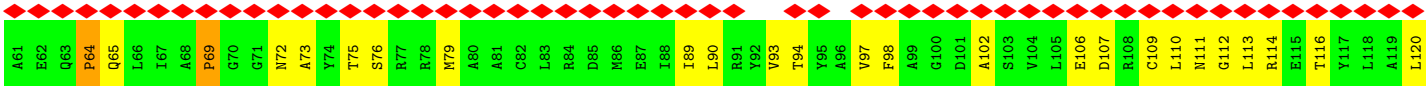


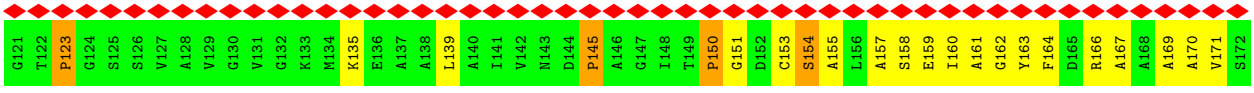
• Molecule 32: Phycocyanin beta subunit

Chain c2:



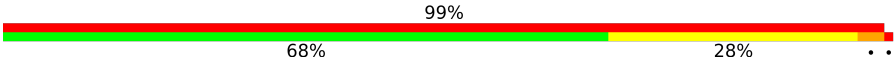


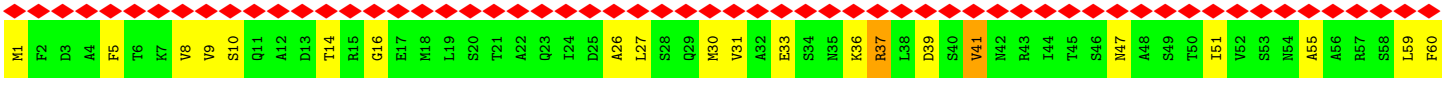


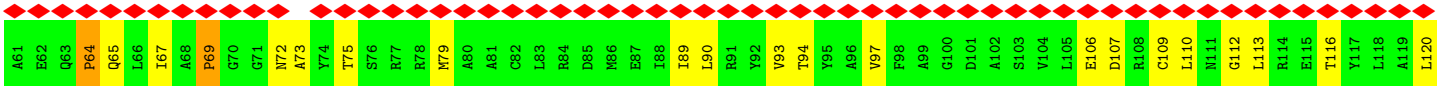


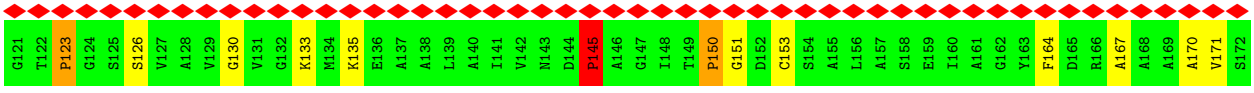
• Molecule 32: Phycocyanin beta subunit

Chain e2:



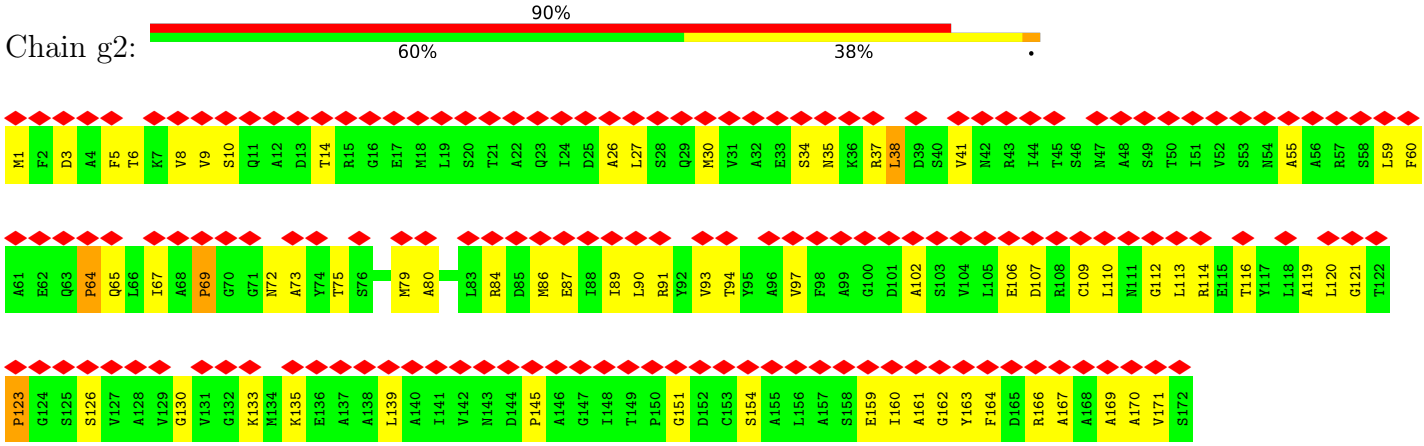






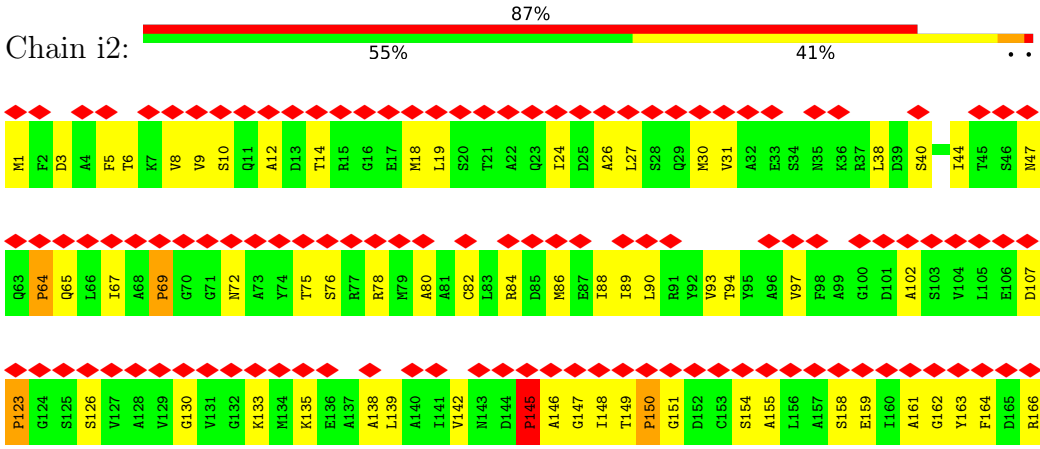
• Molecule 32: Phycocyanin beta subunit

Chain g2:



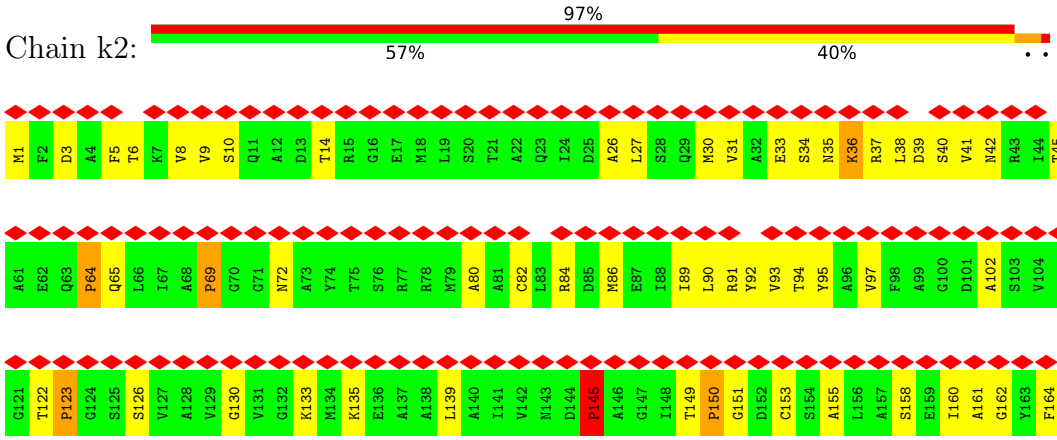
• Molecule 32: Phycocyanin beta subunit

Chain i2:



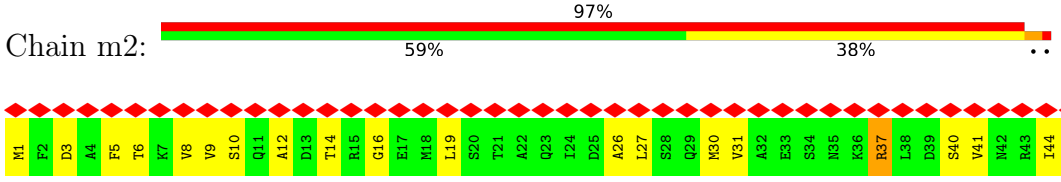
• Molecule 32: Phycocyanin beta subunit

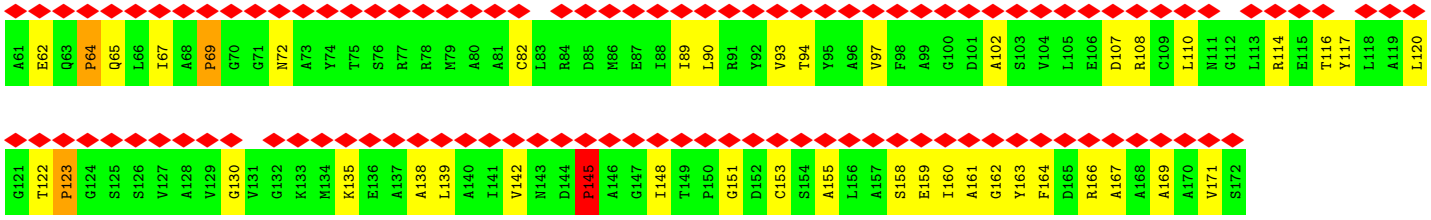
Chain k2:



• Molecule 32: Phycocyanin beta subunit

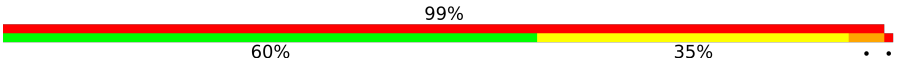
Chain m2:

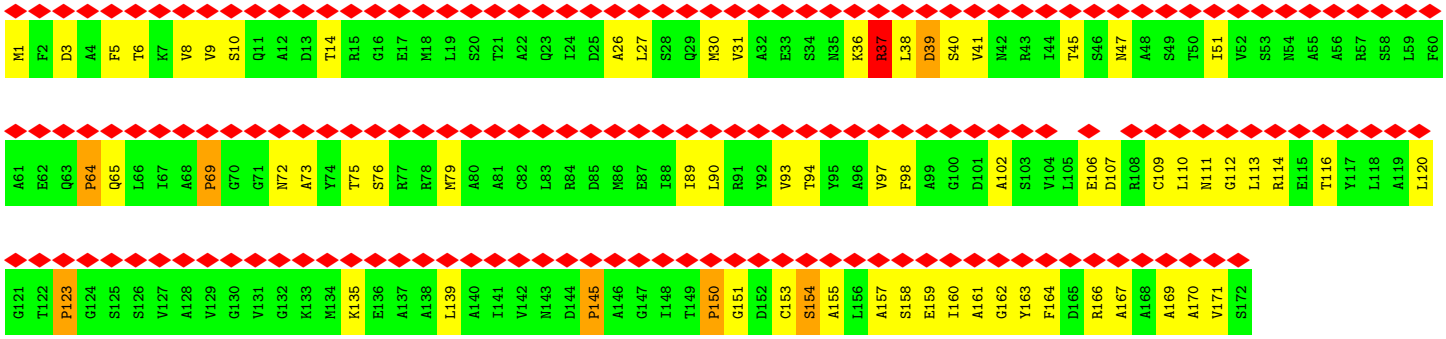




• Molecule 32: Phycocyanin beta subunit

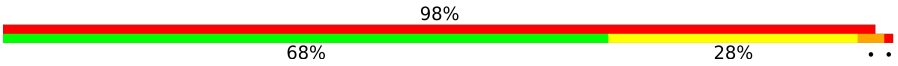
Chain c3:

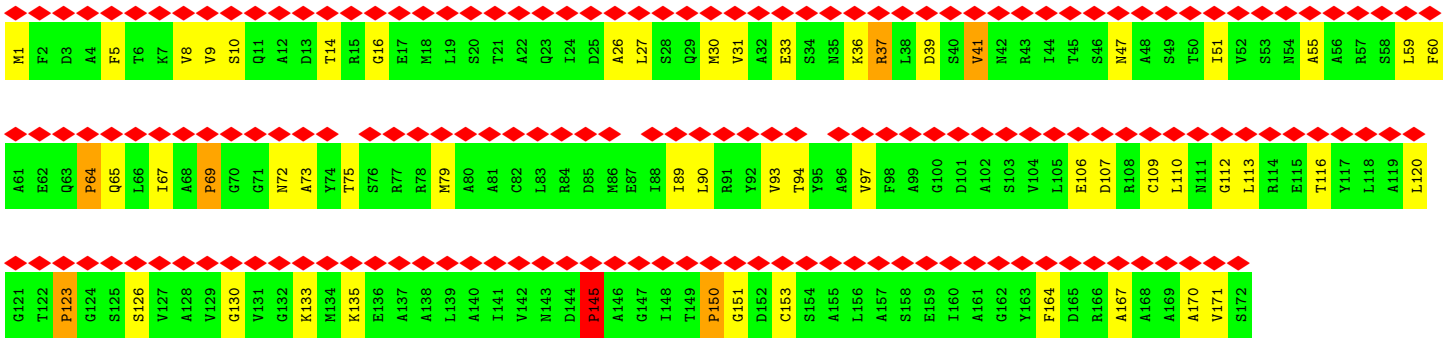




• Molecule 32: Phycocyanin beta subunit

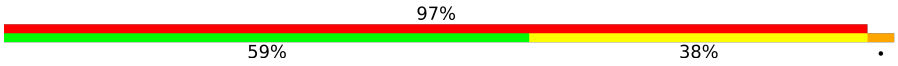
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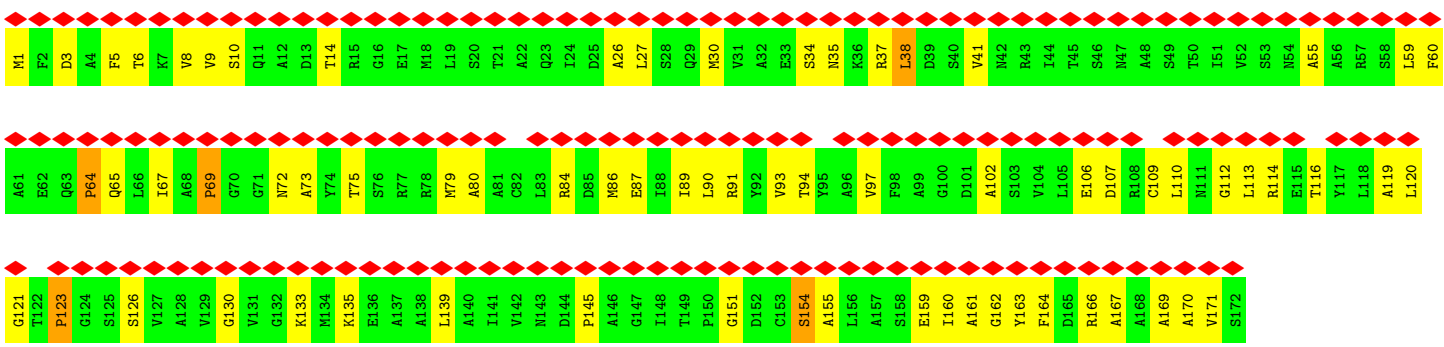




• Molecule 32: Phycocyanin beta subunit

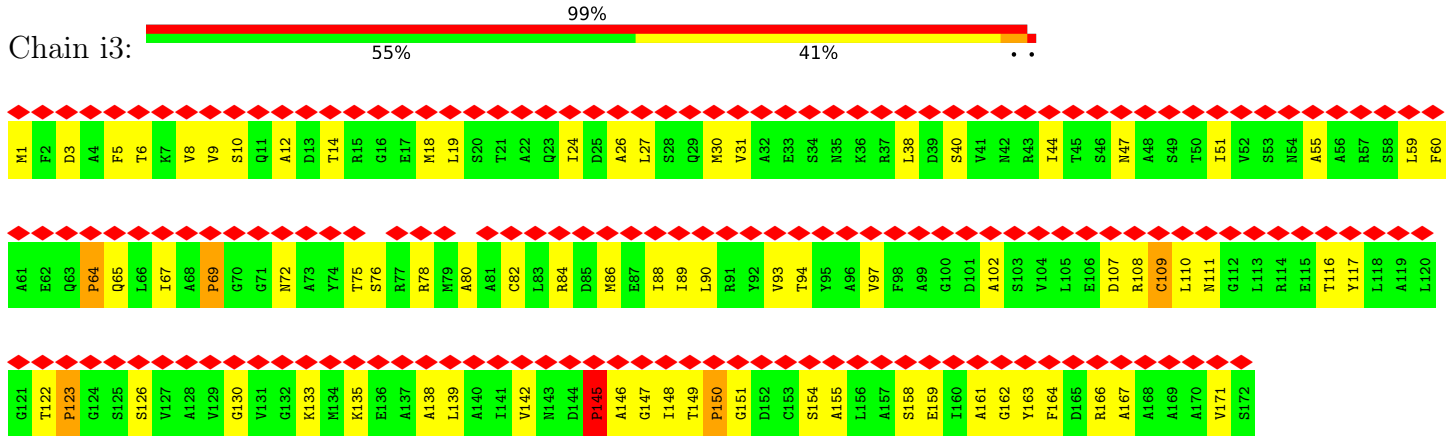
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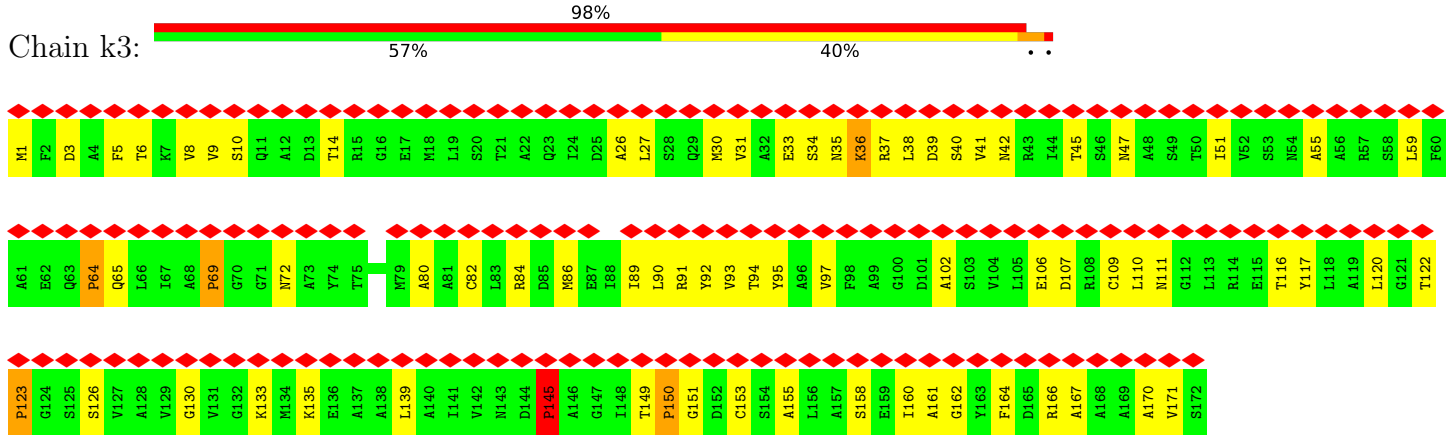
• Molecule 32: Phycocyanin beta subunit

Chain i3:



• Molecule 32: Phycocyanin beta subunit

Chain k3:



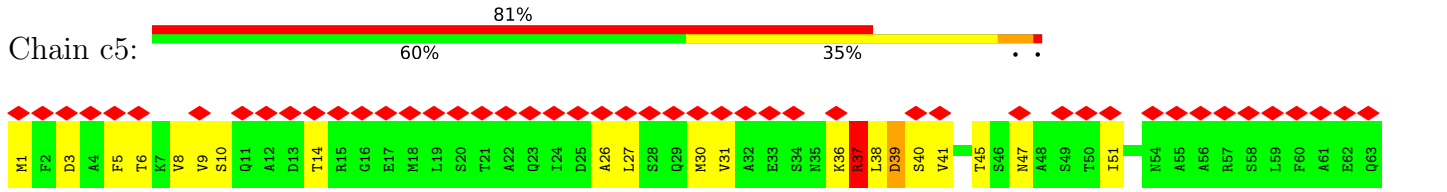
• Molecule 32: Phycocyanin beta subunit

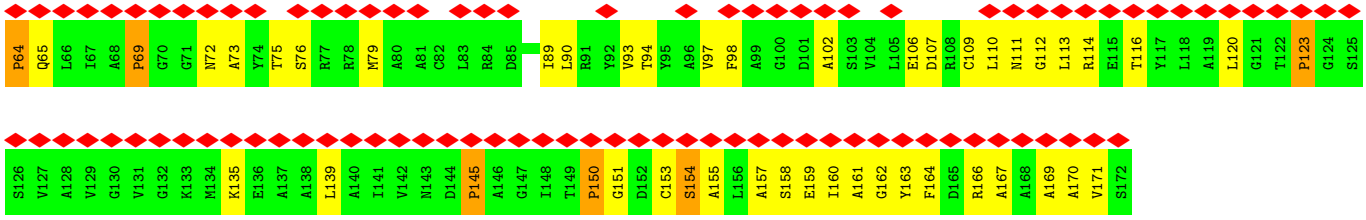
Chain m3:



• Molecule 32: Phycocyanin beta subunit

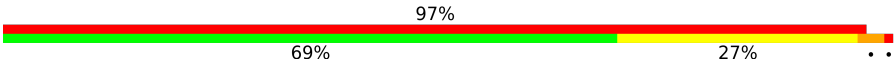
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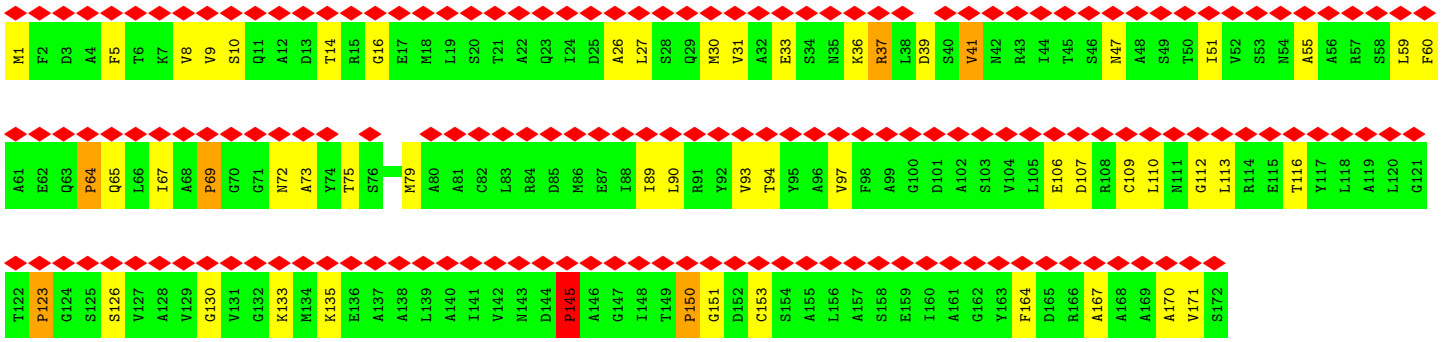




• Molecule 32: Phycocyanin beta subunit

Chain e5:

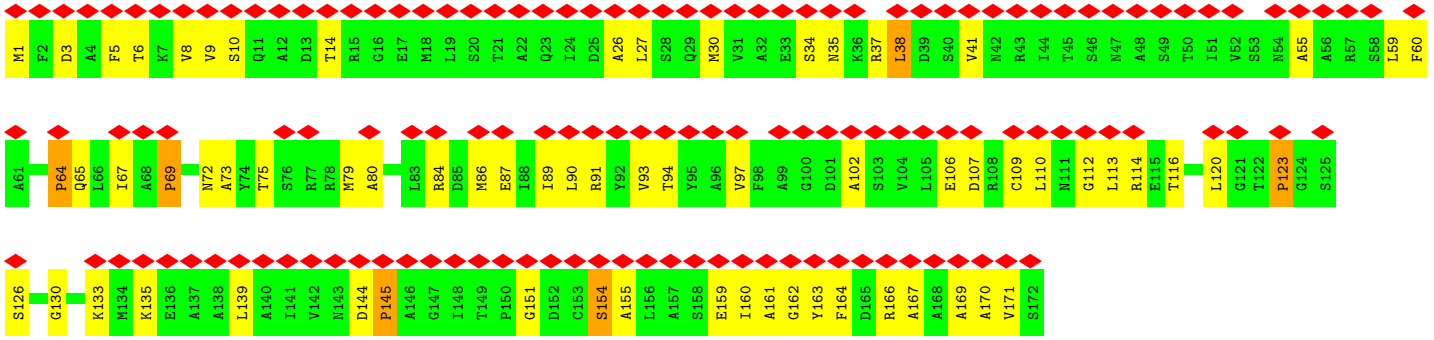




• Molecule 32: Phycocyanin beta subunit

Chain g5:

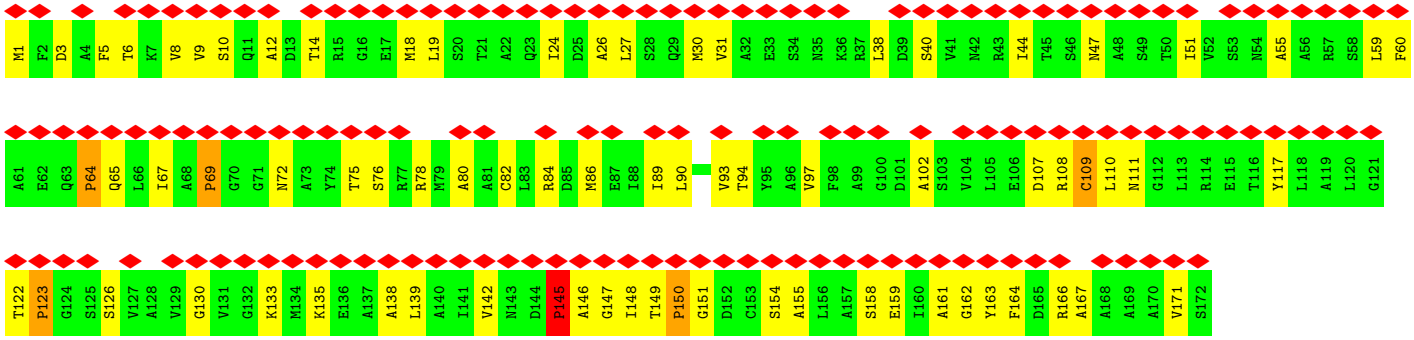




• Molecule 32: Phycocyanin beta subunit

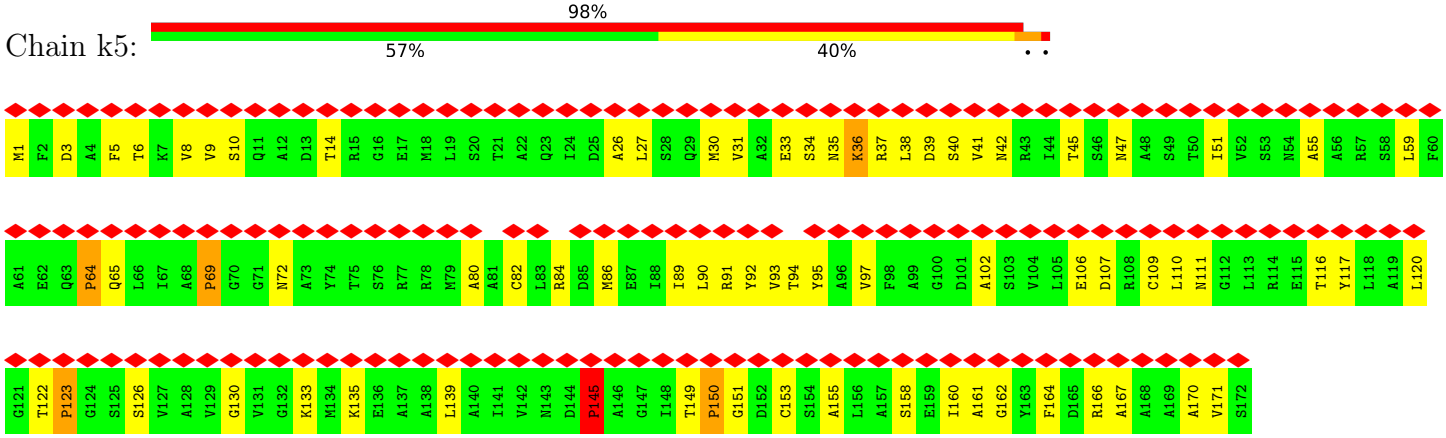
Chain i5:





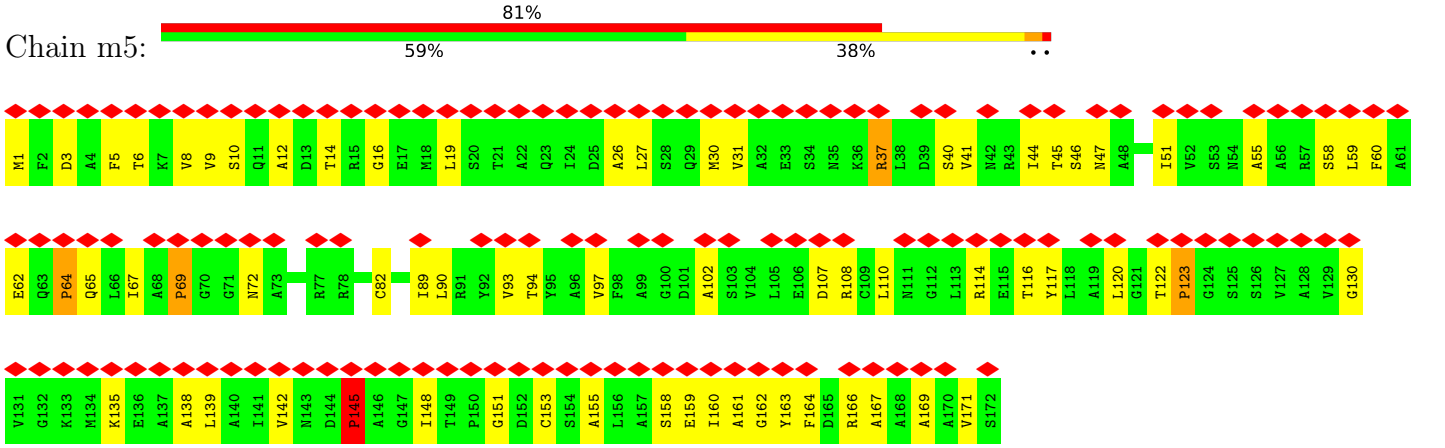
• Molecule 32: Phycocyanin beta subunit

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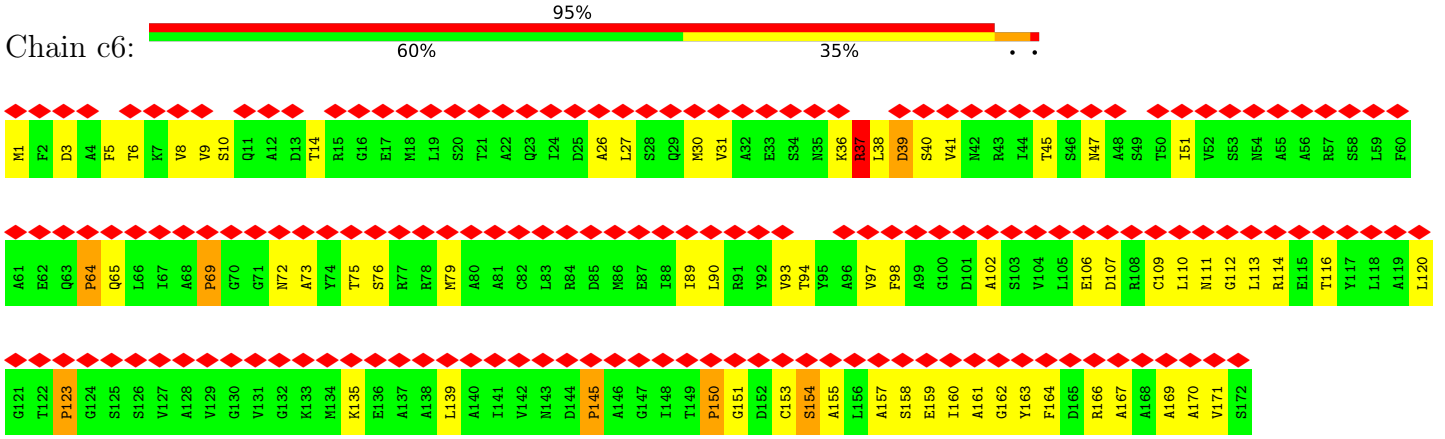
• Molecule 32: Phycocyanin beta subunit

Chain m5:



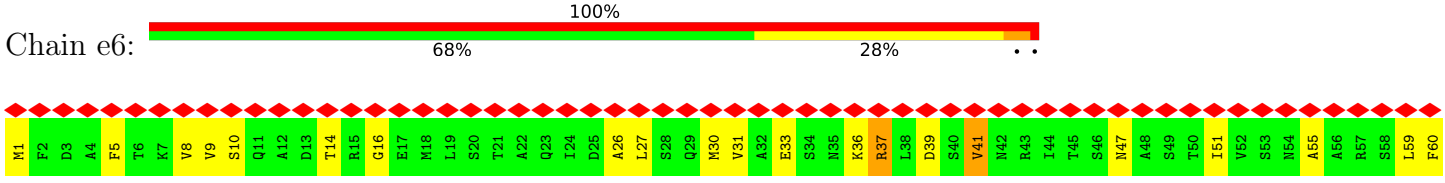
• Molecule 32: Phycocyanin beta subunit

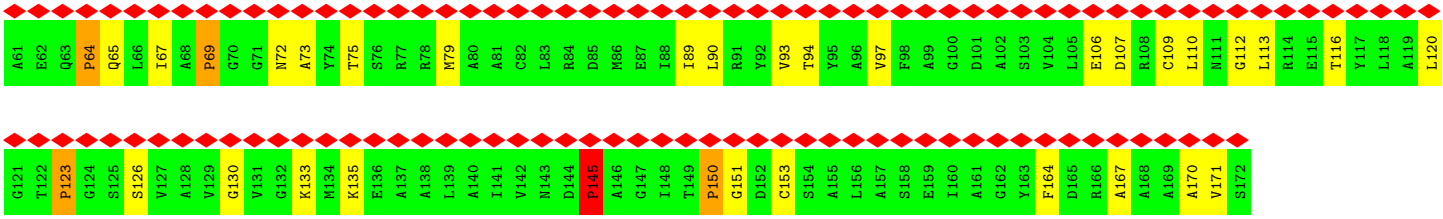
Chain c6:



• Molecule 32: Phycocyanin beta subunit

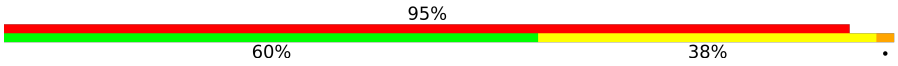
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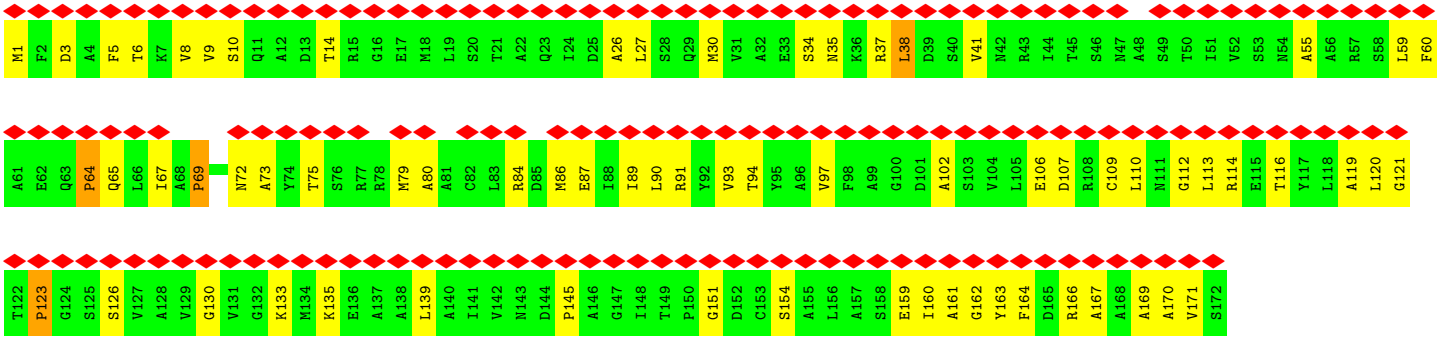




• Molecule 32: Phycocyanin beta subunit

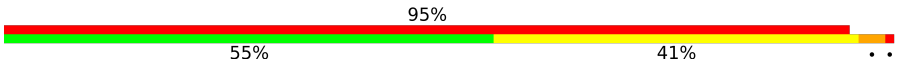
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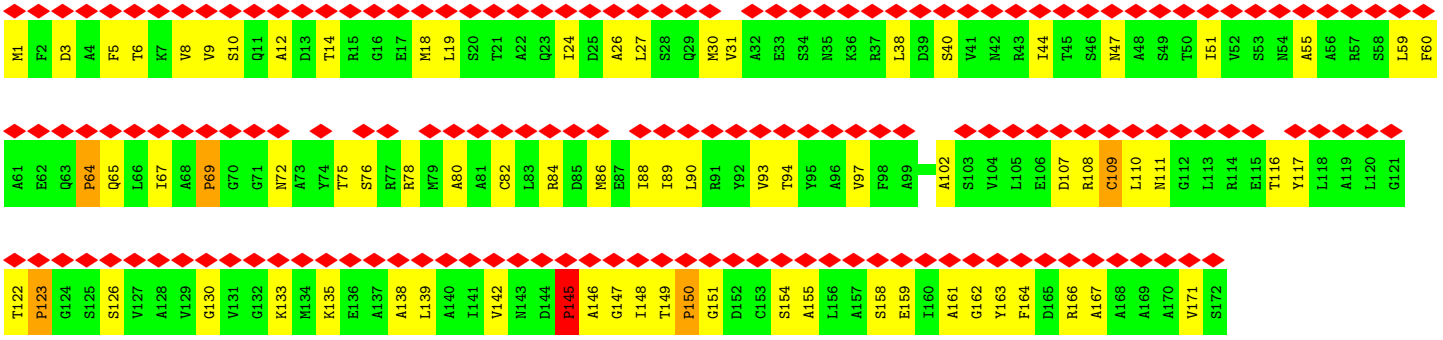




• Molecule 32: Phycocyanin beta subunit

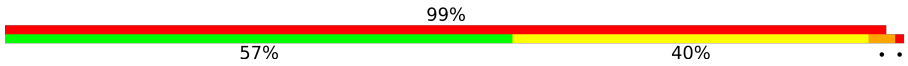
Chain i6:

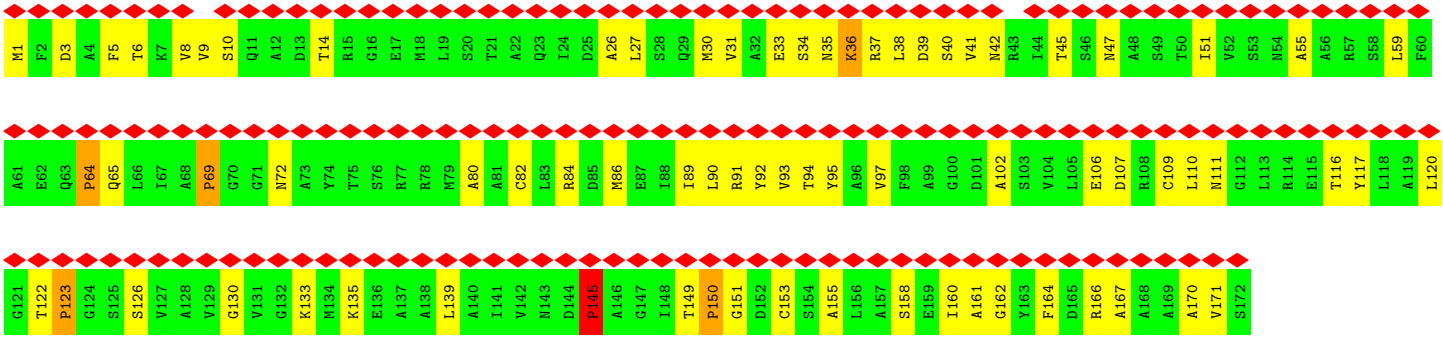




• Molecule 32: Phycocyanin beta subunit

Chain k6:

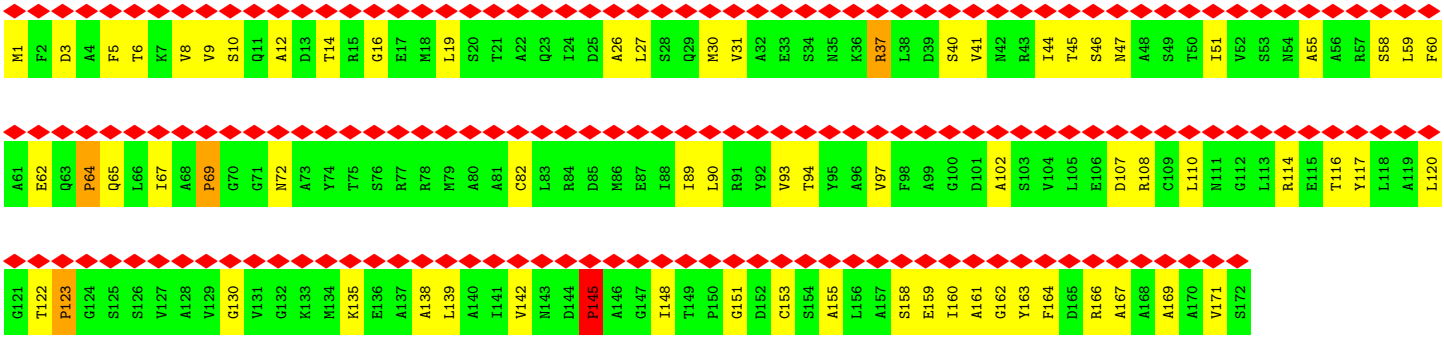




• Molecule 32: Phycocyanin beta subunit

Chain m6:

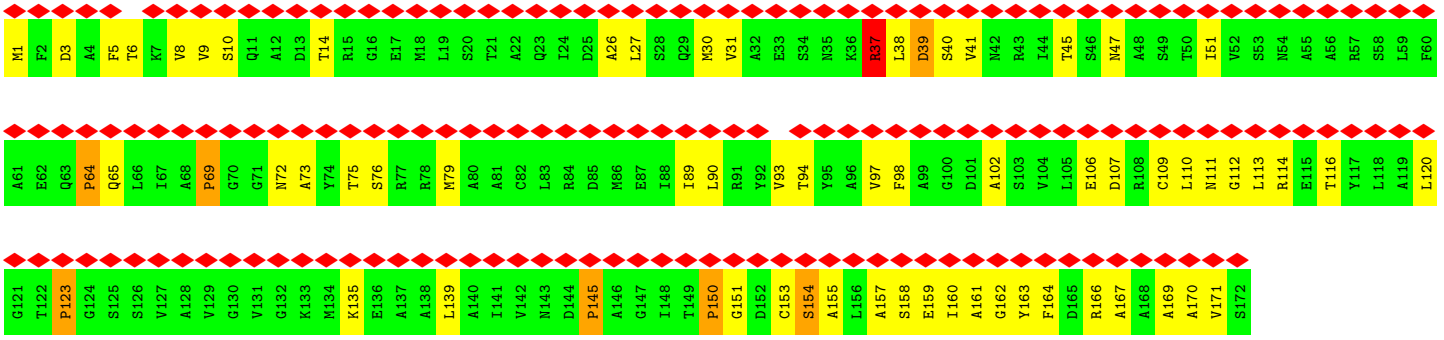




• Molecule 32: Phycocyanin beta subunit

Chain c7:

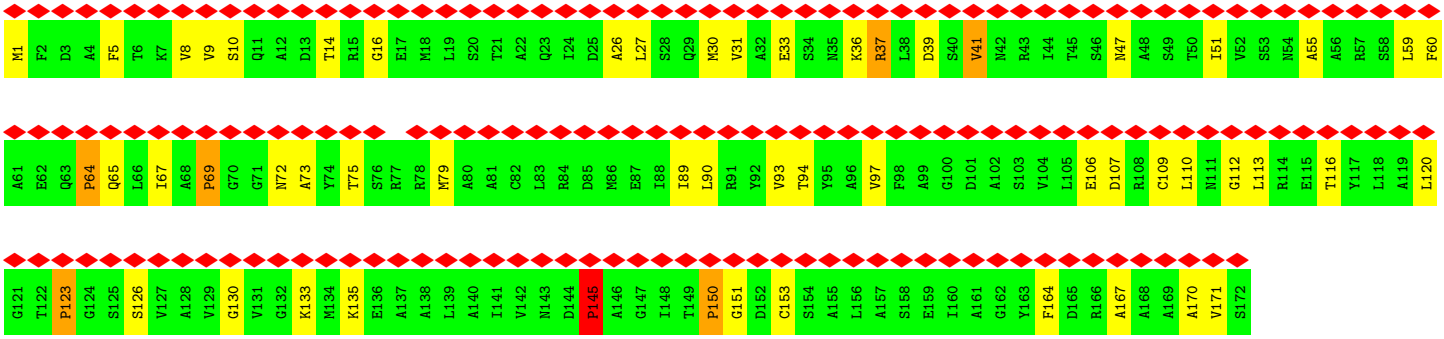




• Molecule 32: Phycocyanin beta subunit

Chain e7:

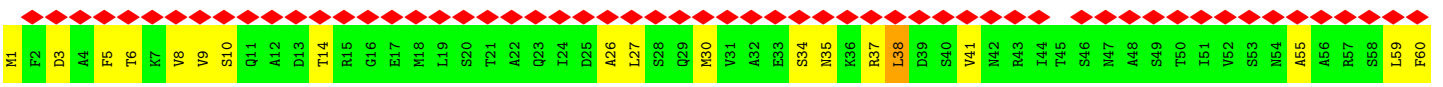


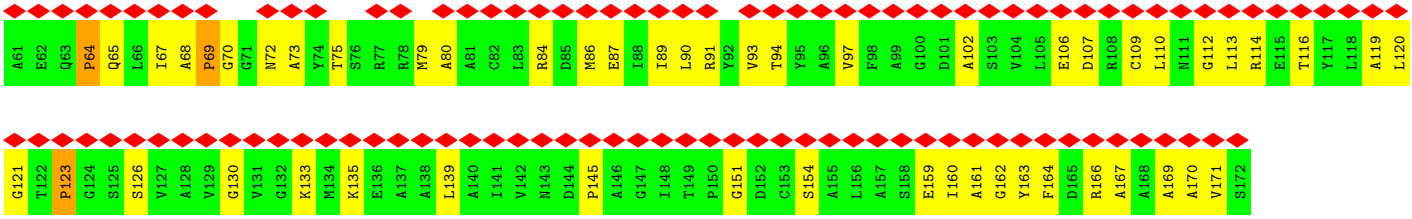


• Molecule 32: Phycocyanin beta subunit

Chain g7:

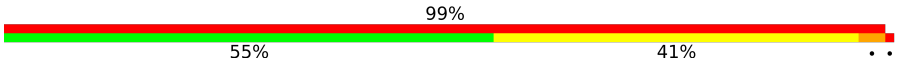


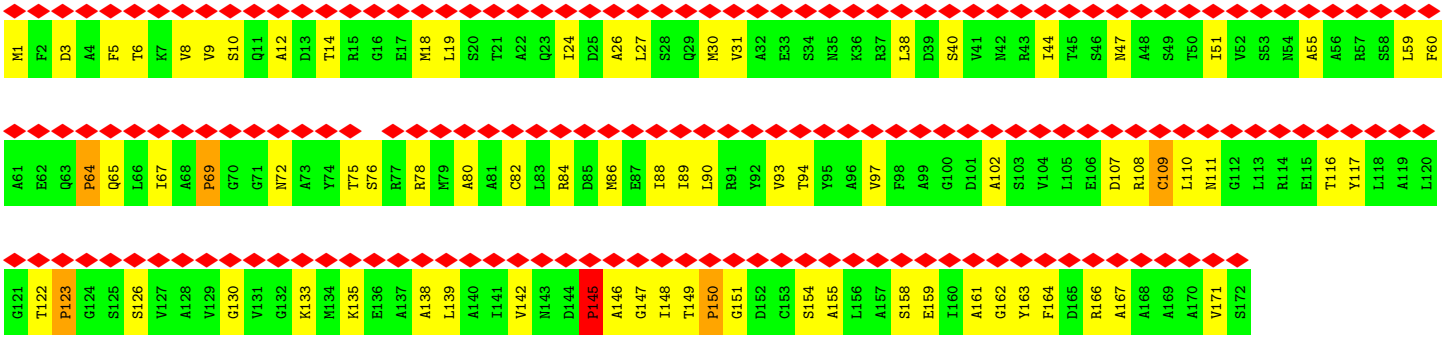




• Molecule 32: Phycocyanin beta subunit

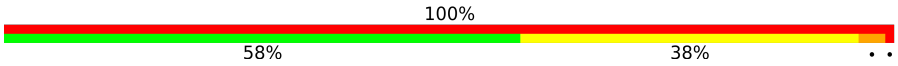
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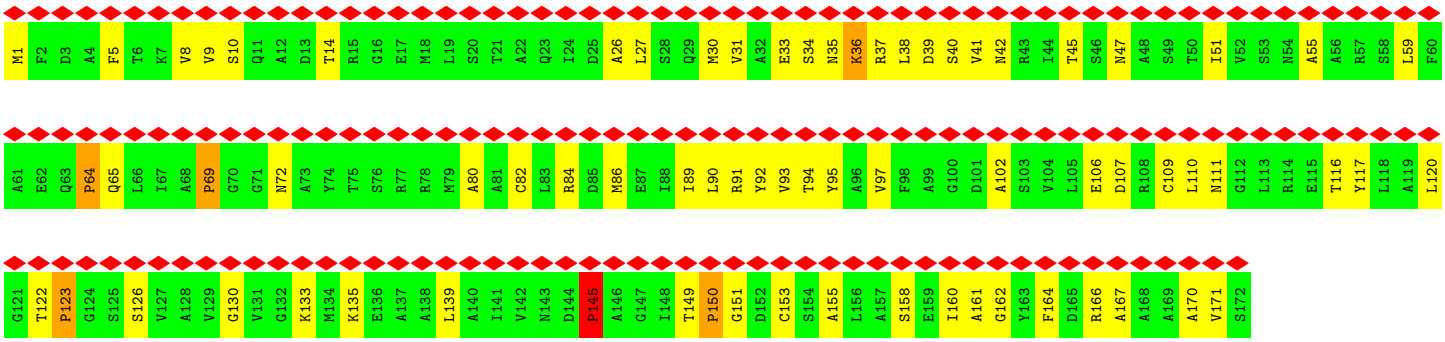




• Molecule 32: Phycocyanin beta subunit

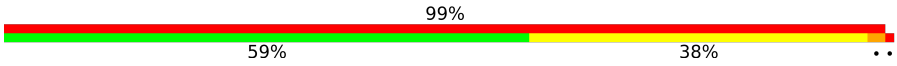
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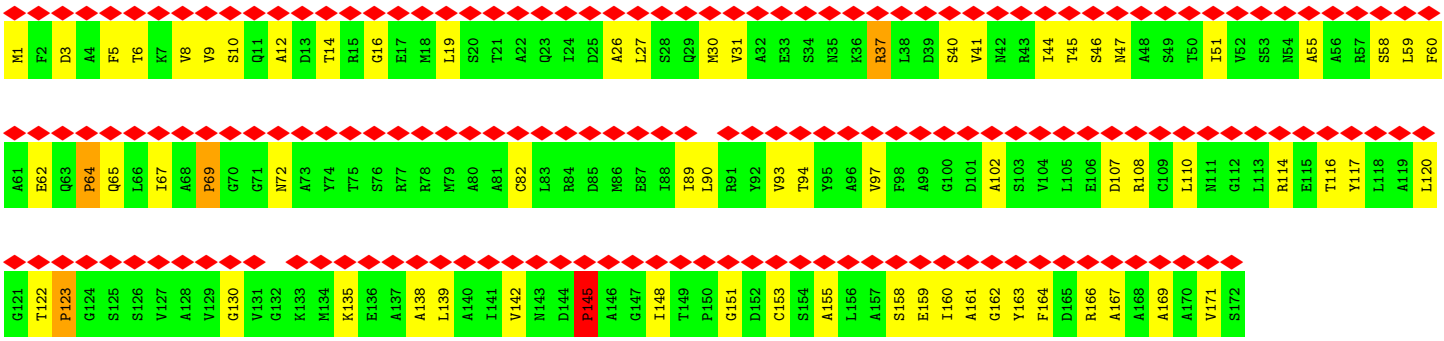




• Molecule 32: Phycocyanin beta subunit

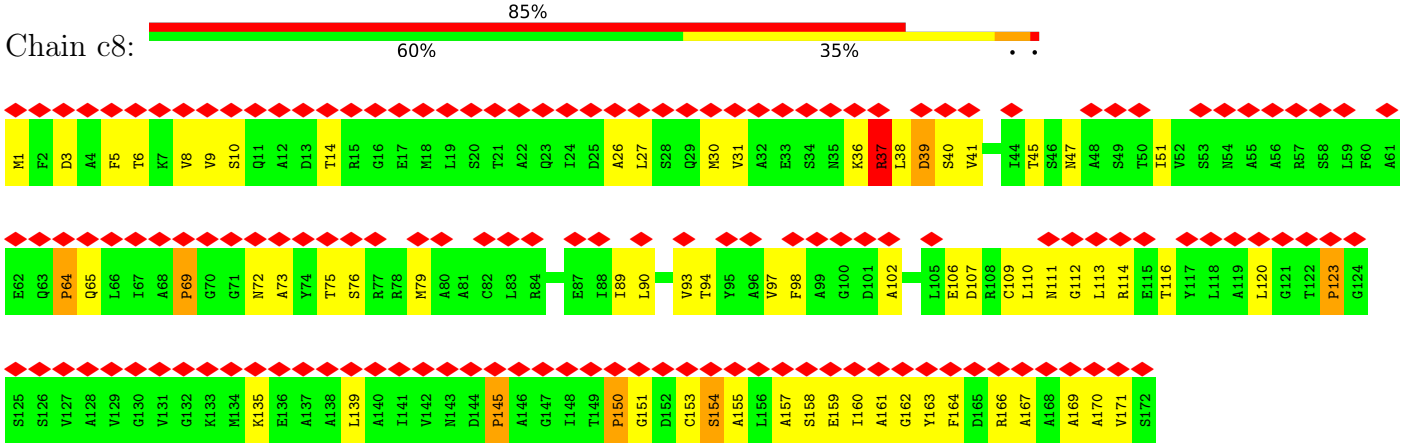
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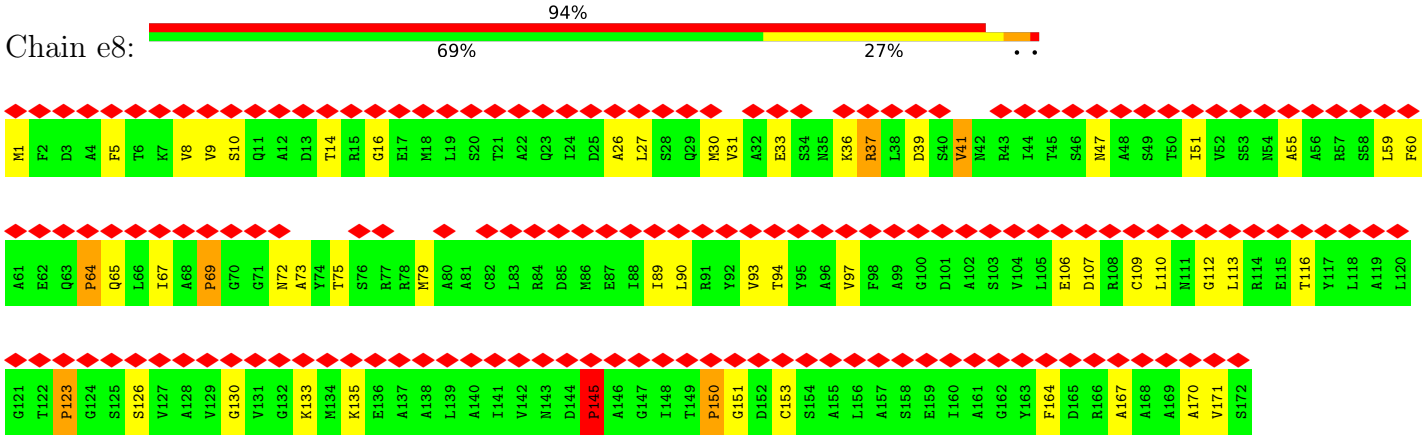
• Molecule 32: Phycocyanin beta subunit

Chain c8:



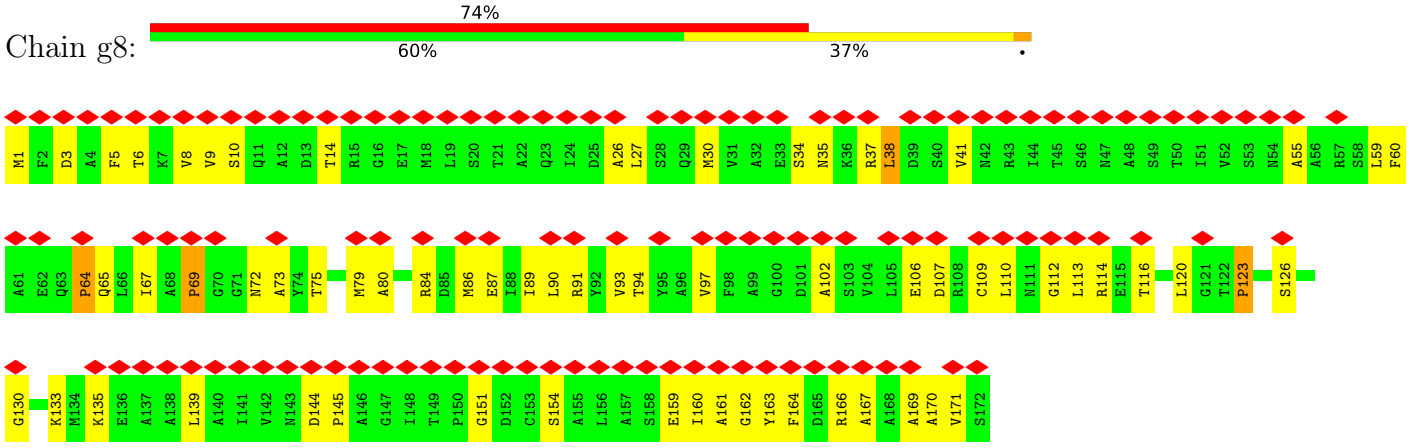
• Molecule 32: Phycocyanin beta subunit

Chain e8:



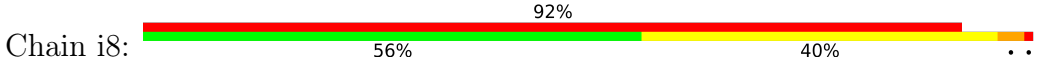
• Molecule 32: Phycocyanin beta subunit

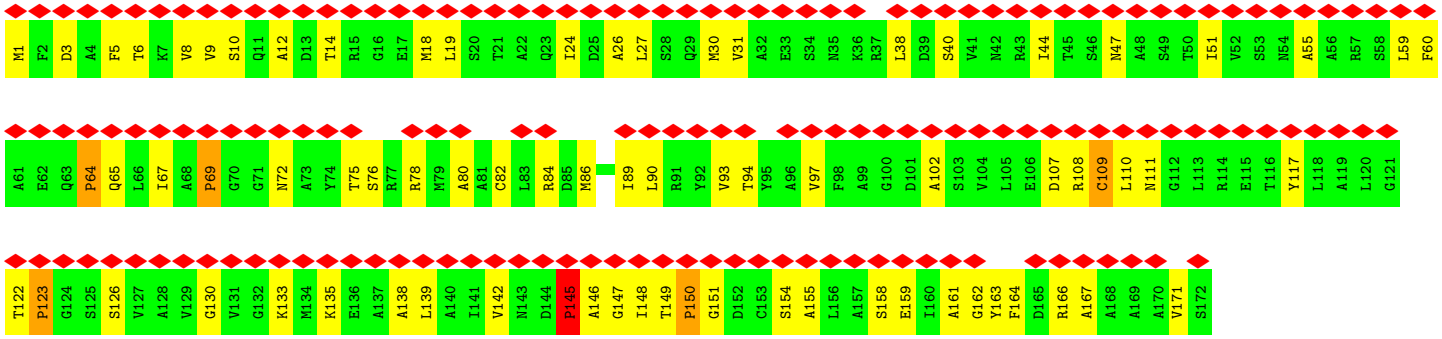
Chain g8:



• Molecule 32: Phycocyanin beta subunit

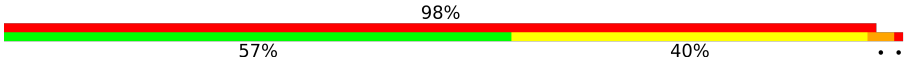
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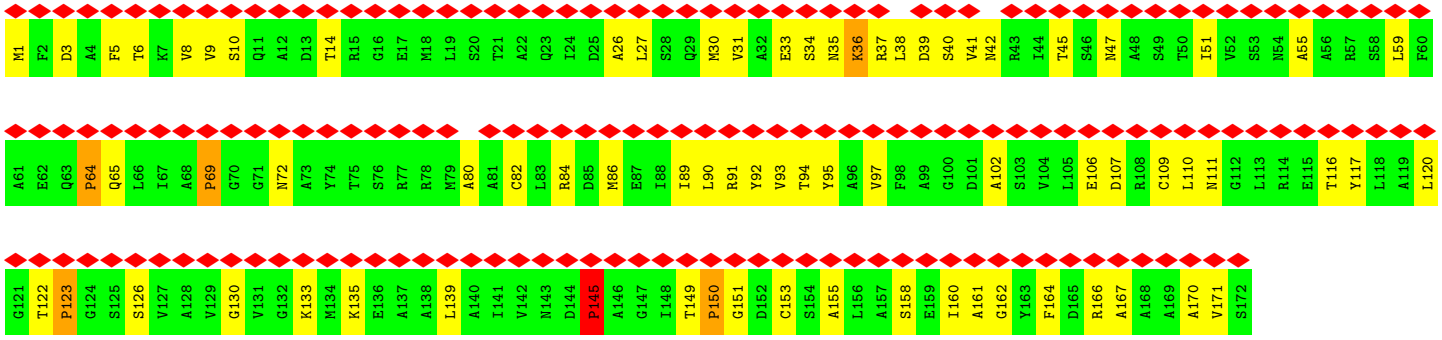




• Molecule 32: Phycocyanin beta subunit

Chain k8:

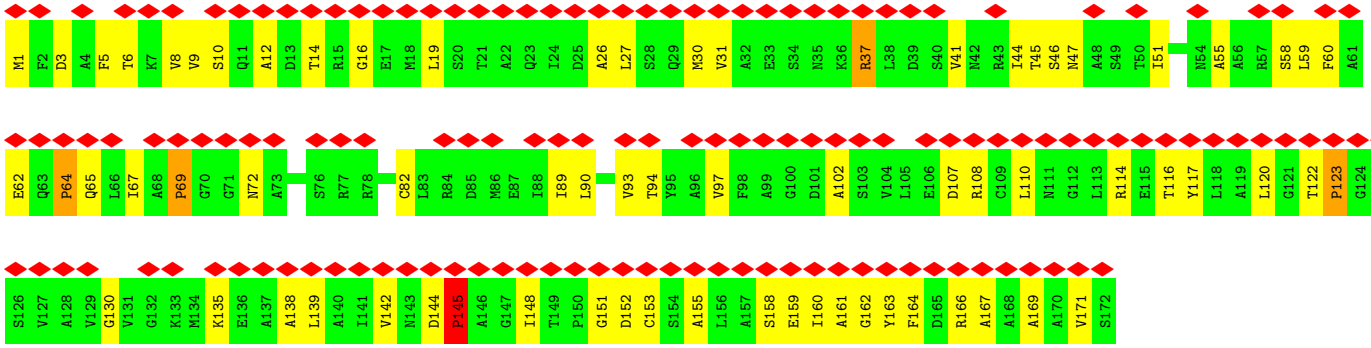




• Molecule 32: Phycocyanin beta subunit

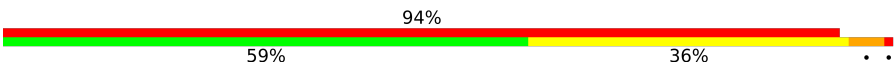
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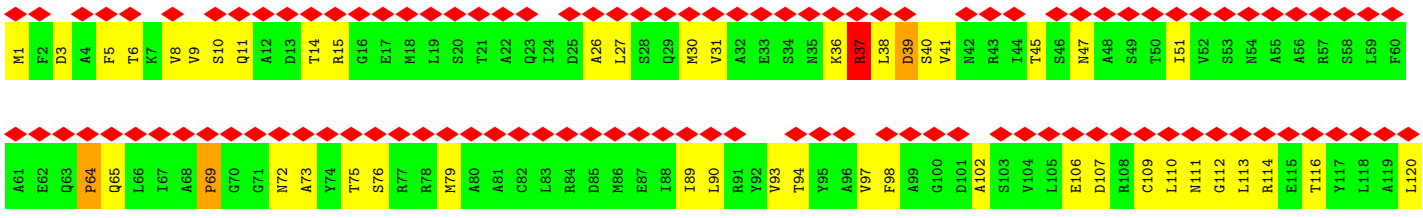


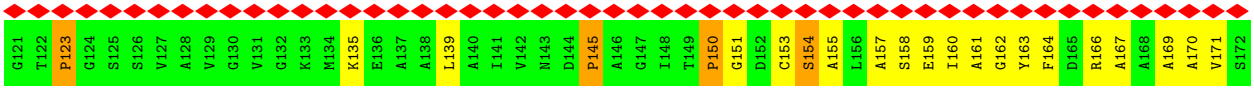


• Molecule 32: Phycocyanin beta subunit

Chain c9:

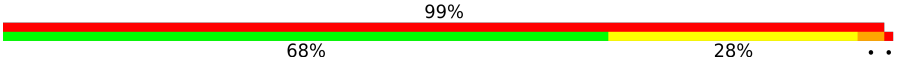


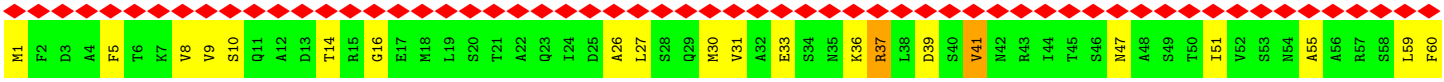


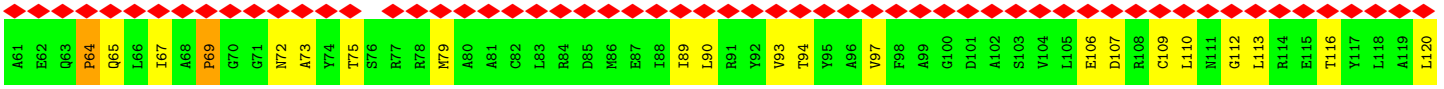


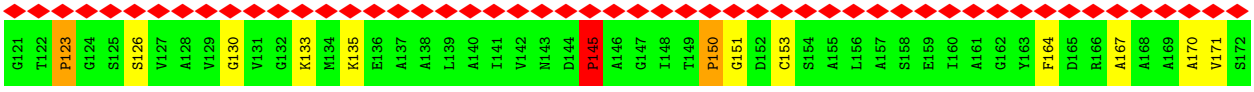
• Molecule 32: Phycocyanin beta subunit

Chain e9:



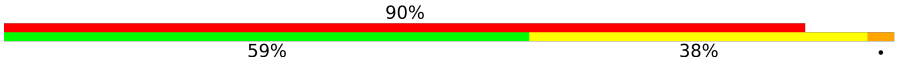


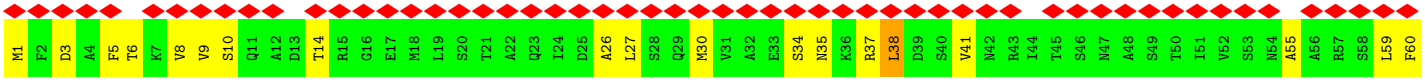


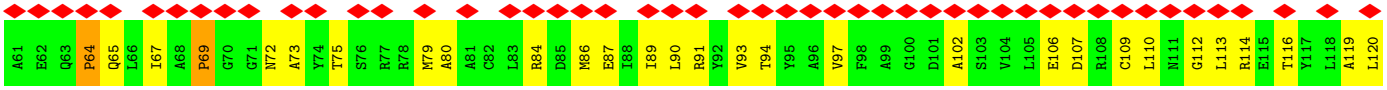


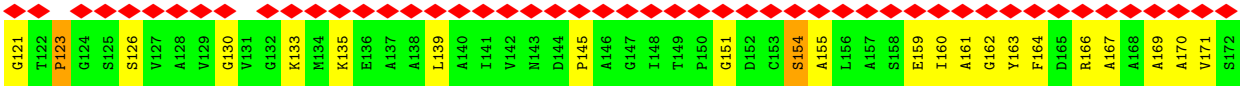
• Molecule 32: Phycocyanin beta subunit

Chain g9:





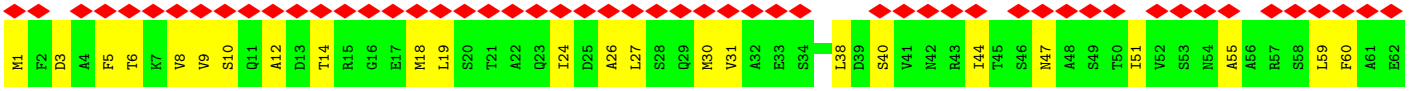


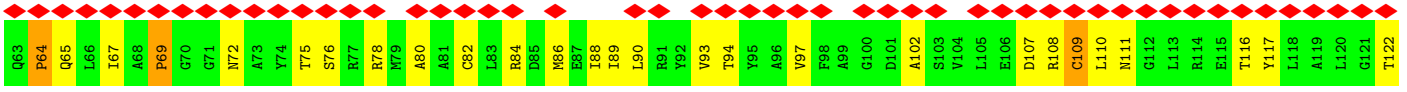


• Molecule 32: Phycocyanin beta subunit

Chain i9:



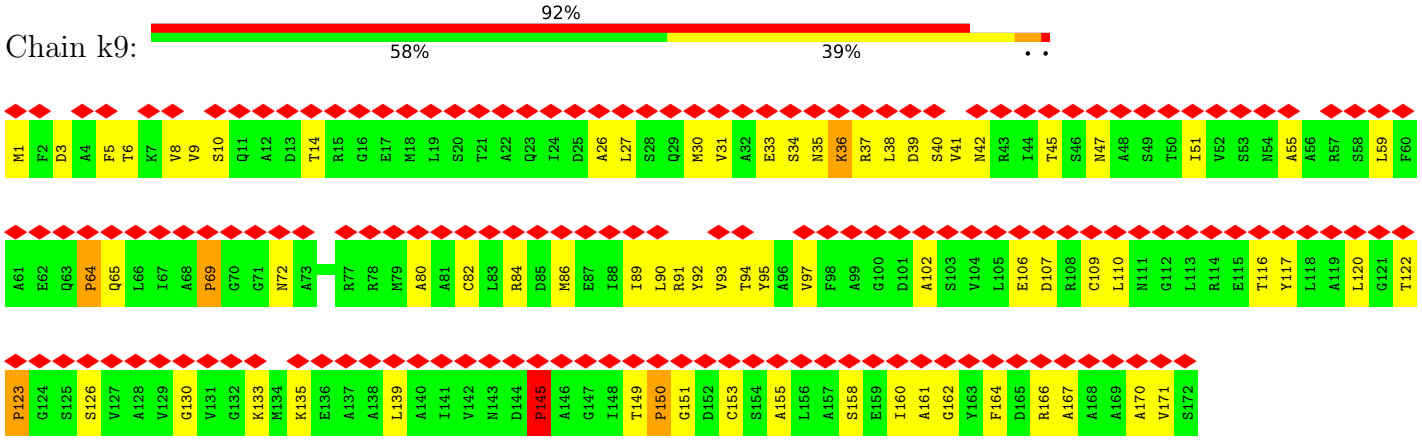






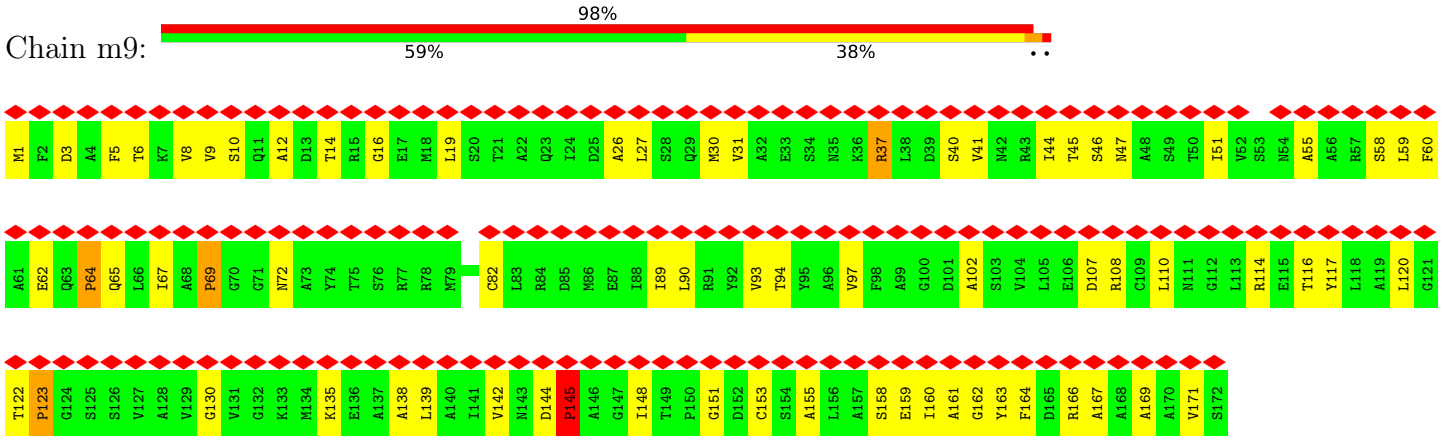
• Molecule 32: Phycocyanin beta subunit

Chain k9:



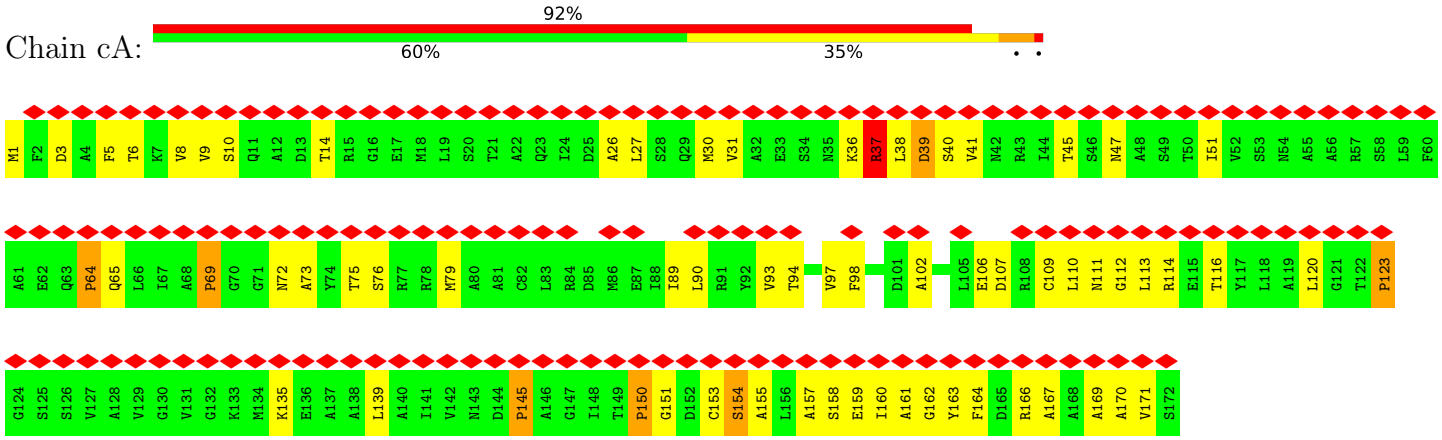
• Molecule 32: Phycocyanin beta subunit

Chain m9:



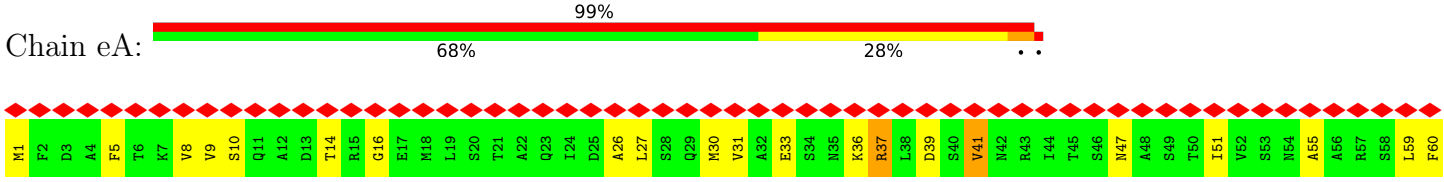
• Molecule 32: Phycocyanin beta subunit

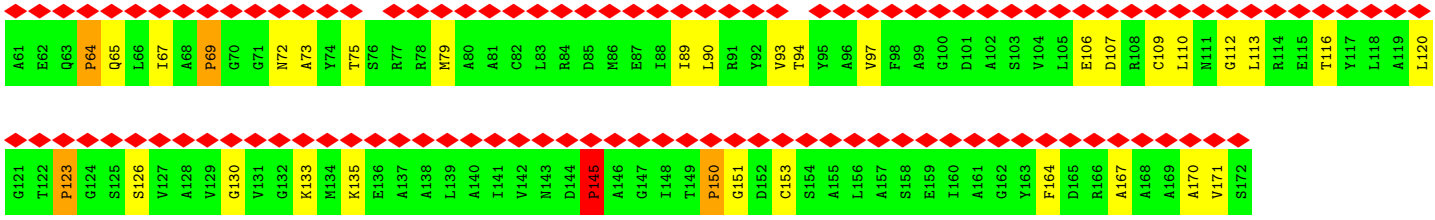
Chain cA:



• Molecule 32: Phycocyanin beta subunit

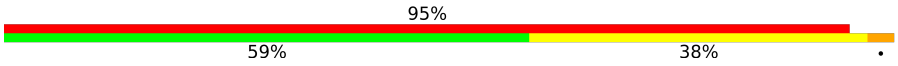
Chain eA:

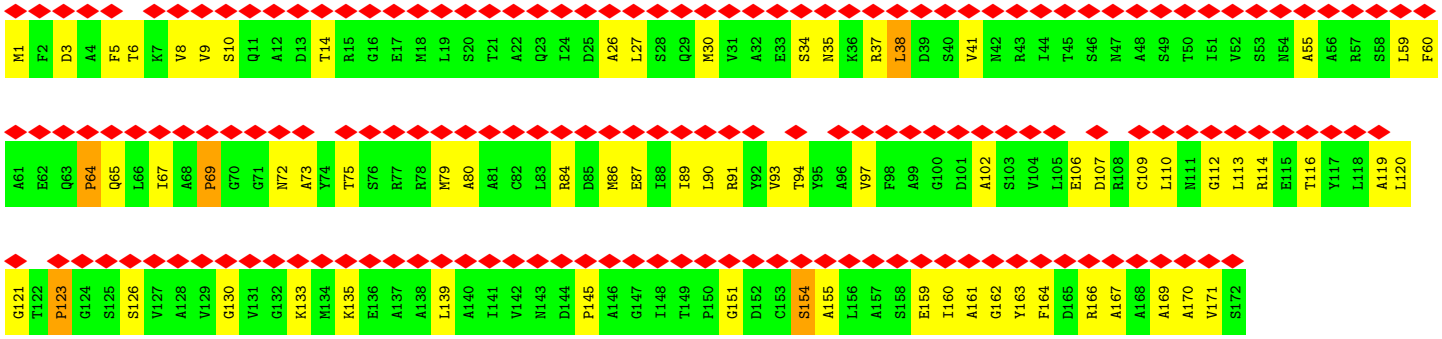




• Molecule 32: Phycocyanin beta subunit

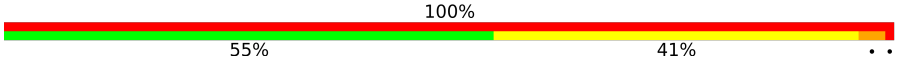
Chain gA:

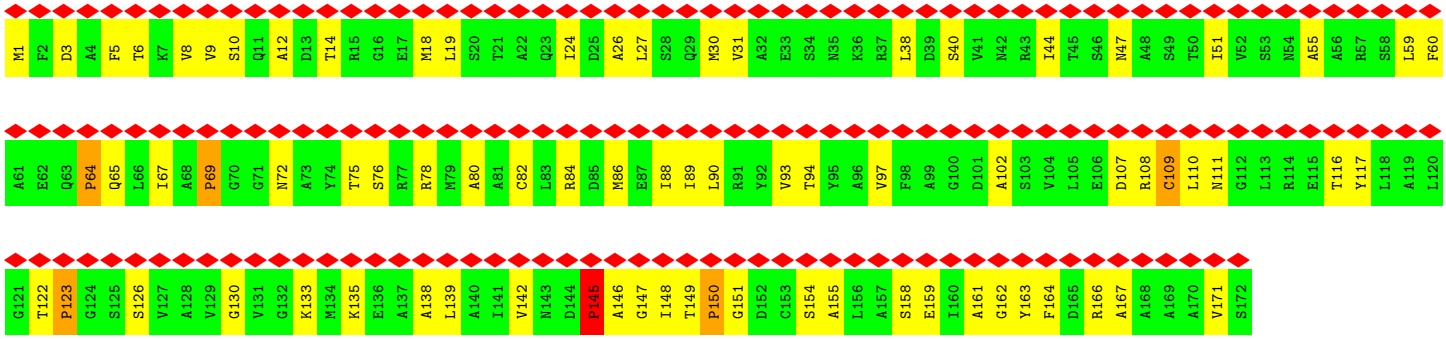




• Molecule 32: Phycocyanin beta subunit

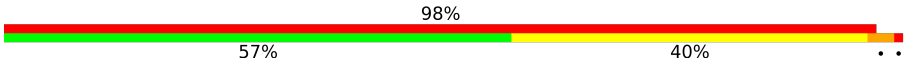
Chain iA:

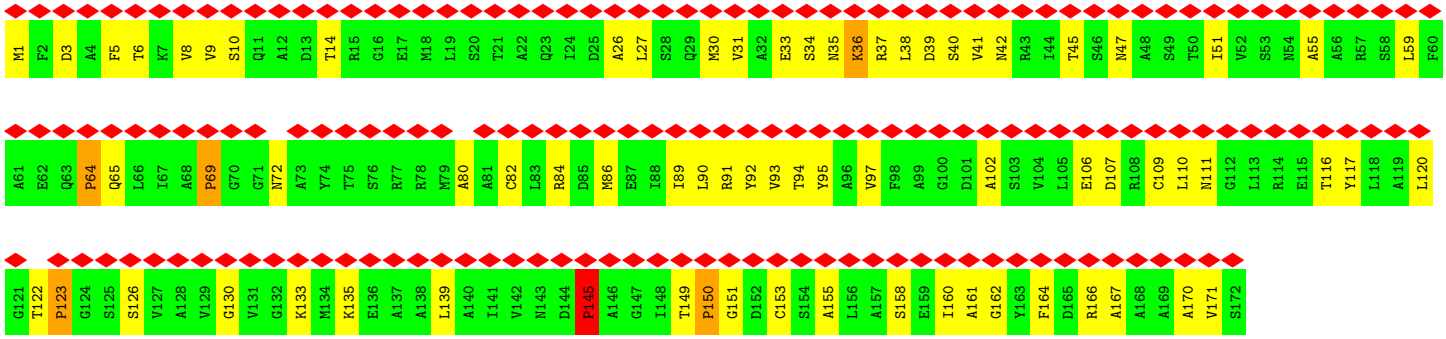




• Molecule 32: Phycocyanin beta subunit

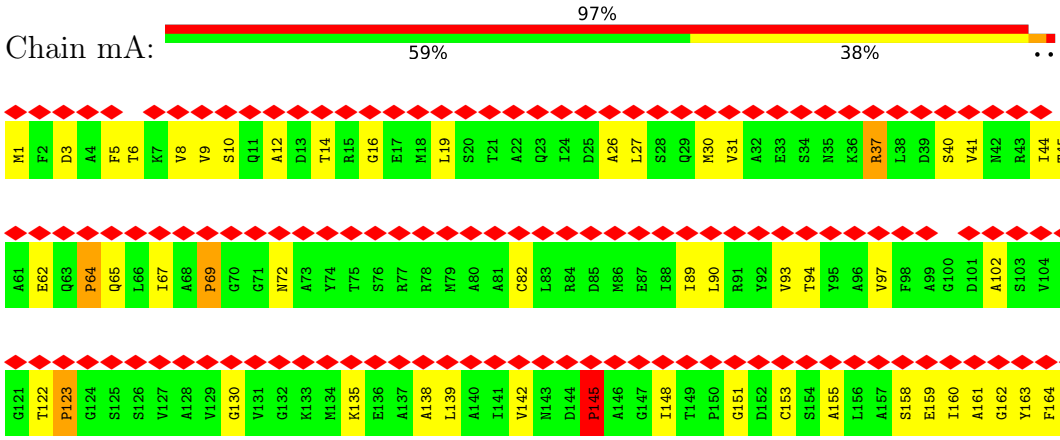
Chain kA:





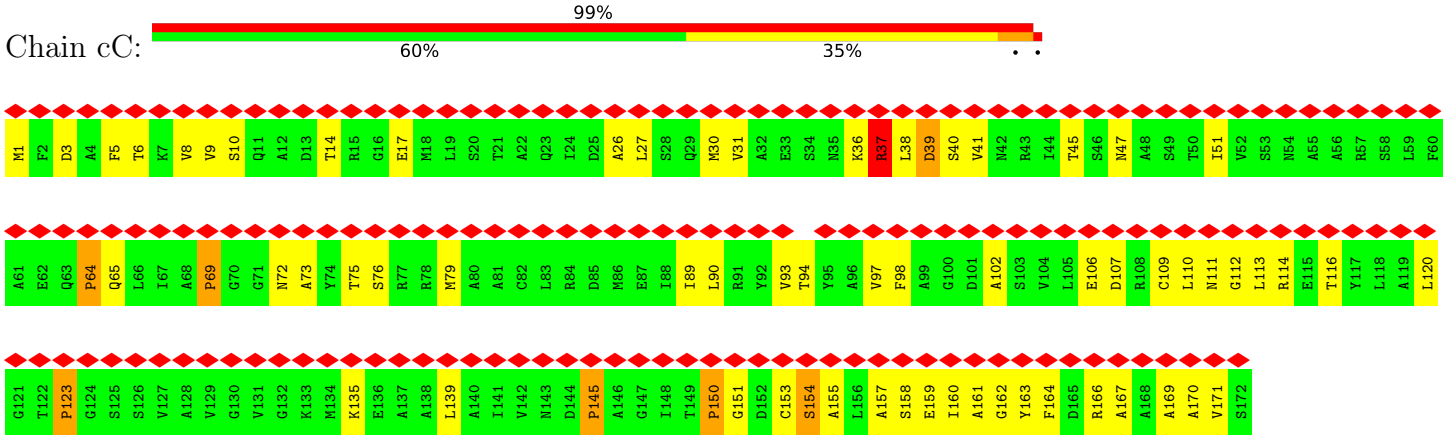
• Molecule 32: Phycocyanin beta subunit

Chain mA:



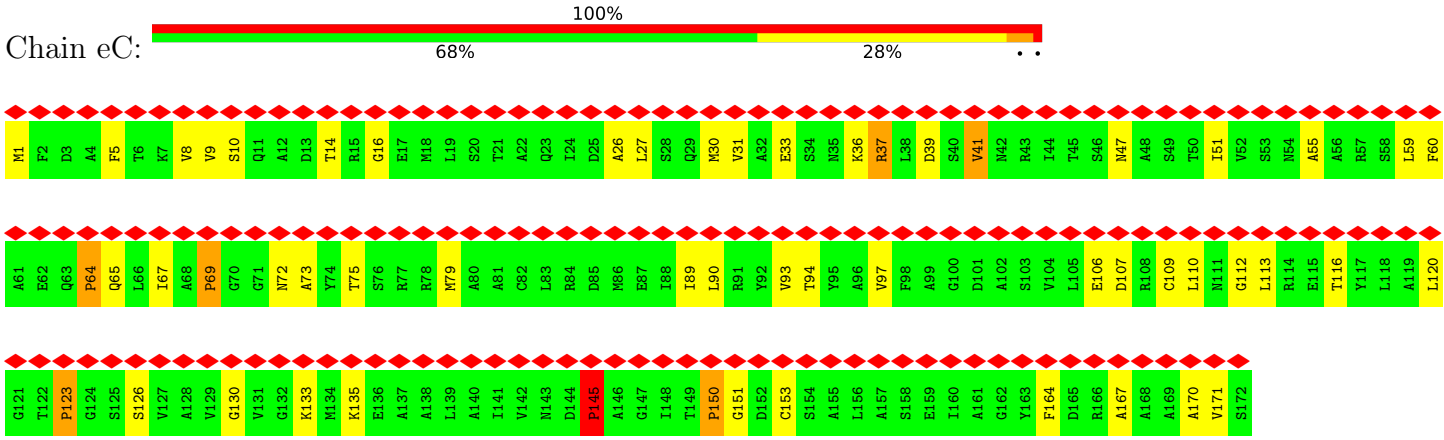
• Molecule 32: Phycocyanin beta subunit

Chain cC:



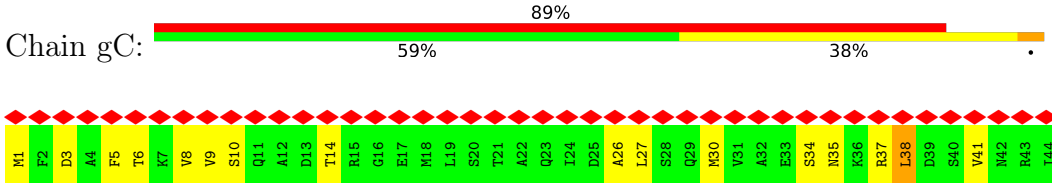
• Molecule 32: Phycocyanin beta subunit

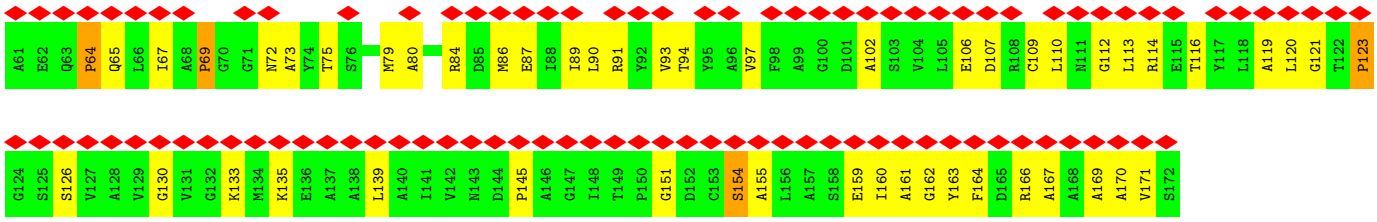
Chain eC:



• Molecule 32: Phycocyanin beta subunit

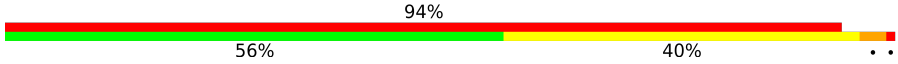
Chain gC:





• Molecule 32: Phycocyanin beta subunit

Chain iC:

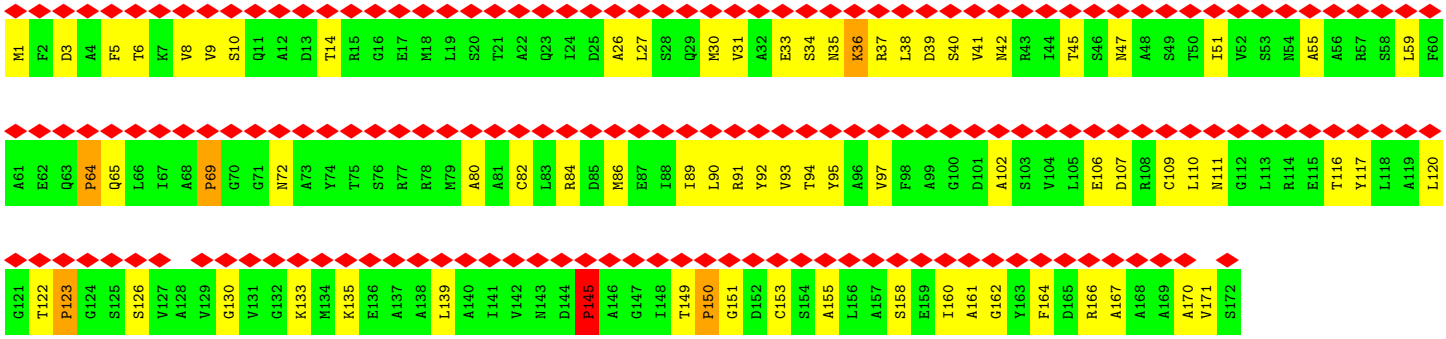




• Molecule 32: Phycocyanin beta subunit

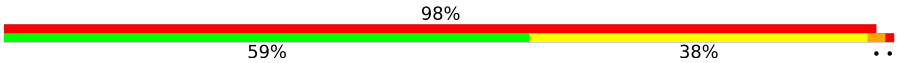
Chain kC:

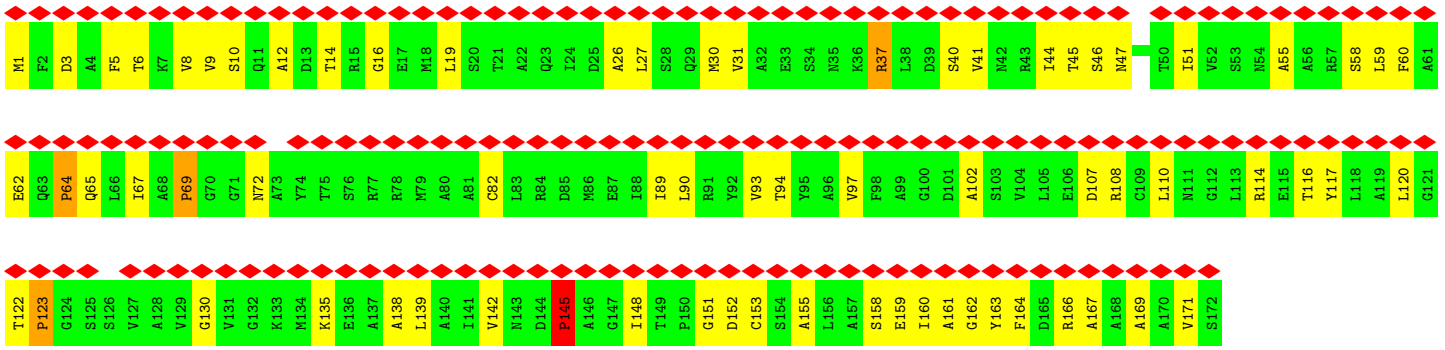




• Molecule 32: Phycocyanin beta subunit

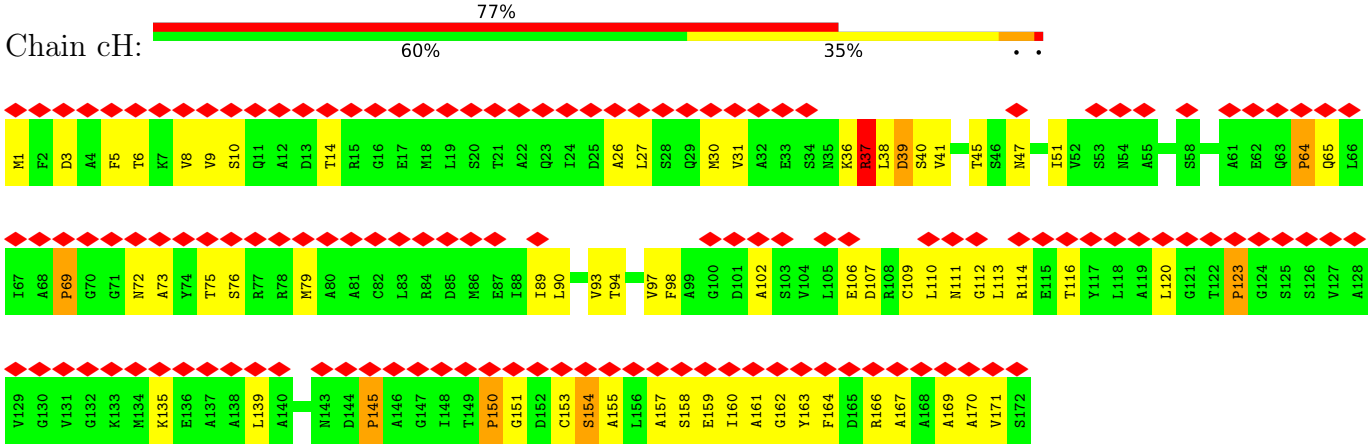
Chain mC:





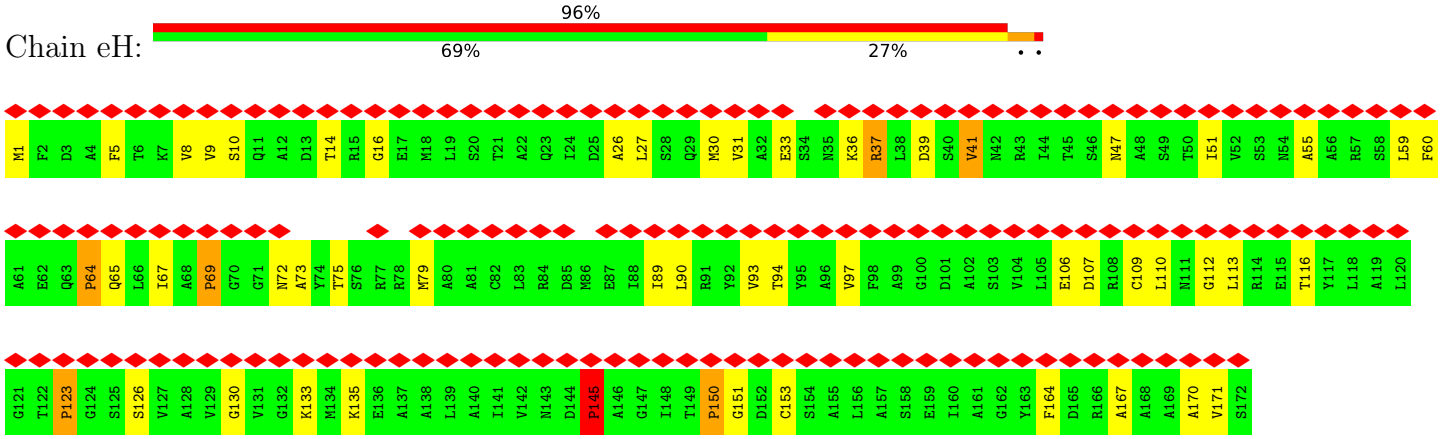
• Molecule 32: Phycocyanin beta subunit

Chain cH:



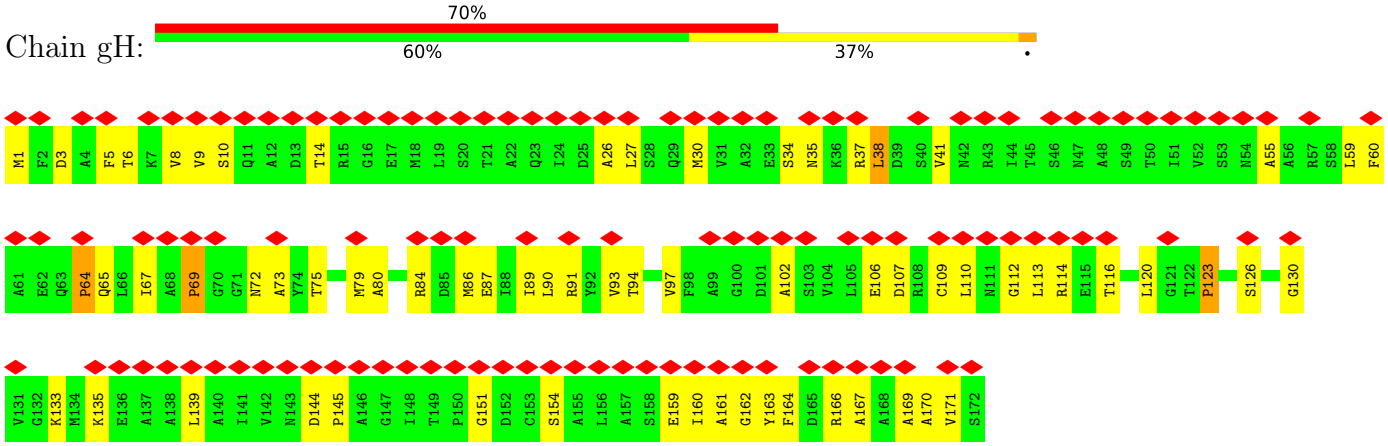
• Molecule 32: Phycocyanin beta subunit

Chain eH:



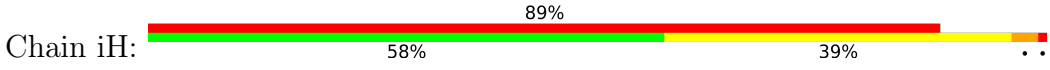
• Molecule 32: Phycocyanin beta subunit

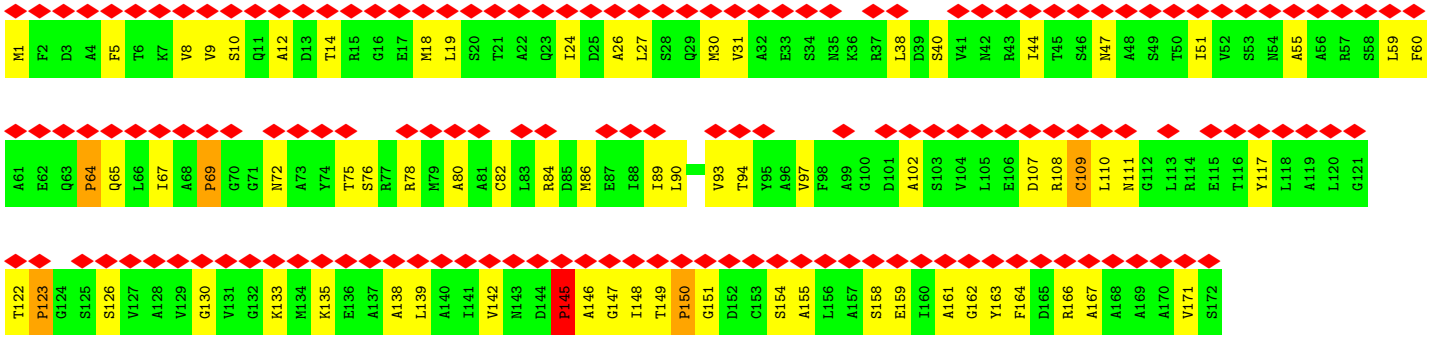
Chain gH:



• Molecule 32: Phycocyanin beta subunit

Chain iH:

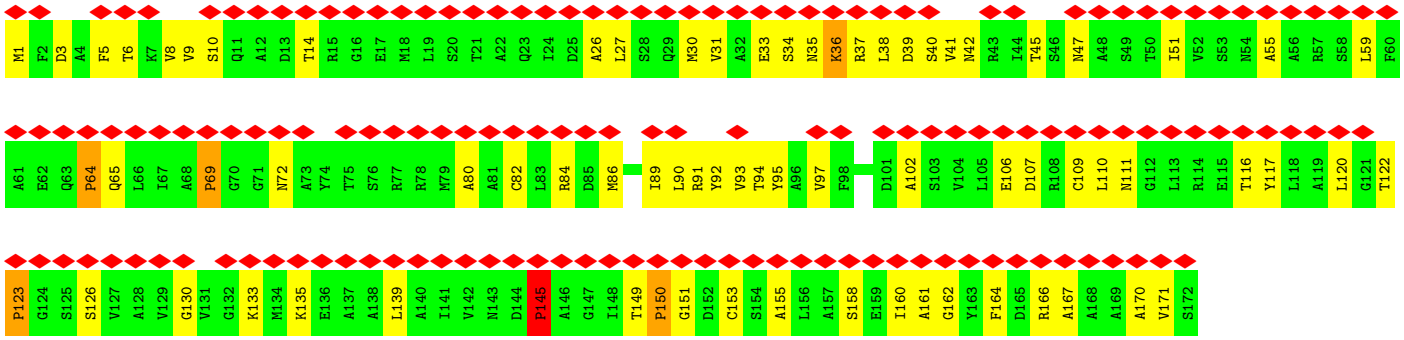




• Molecule 32: Phycocyanin beta subunit

Chain kH:

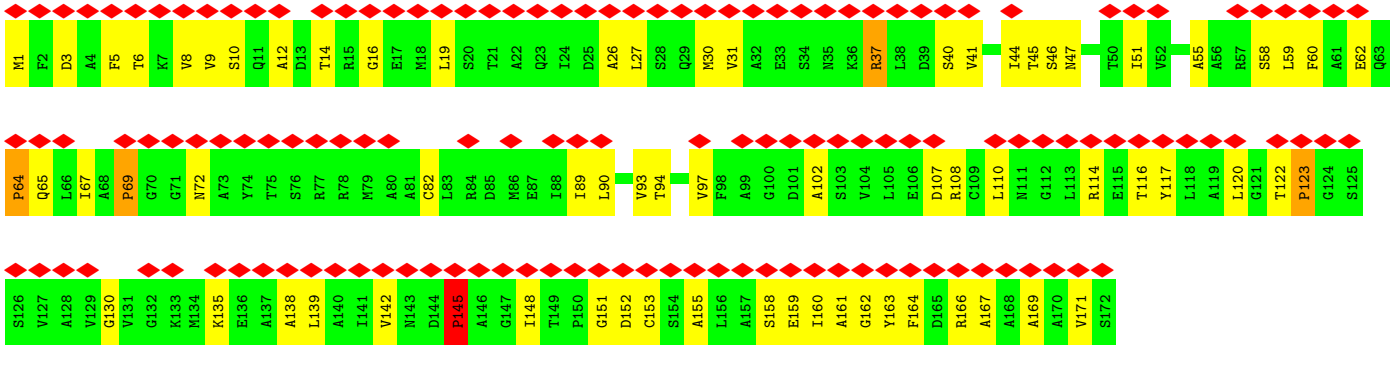




• Molecule 32: Phycocyanin beta subunit

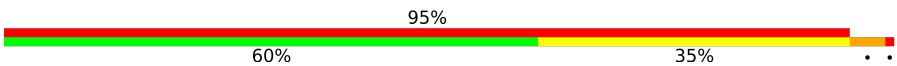
Chain mH:



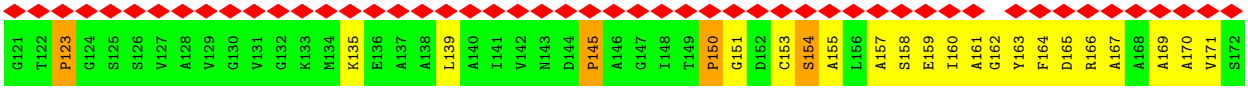


• Molecule 32: Phycocyanin beta subunit

Chain cI:



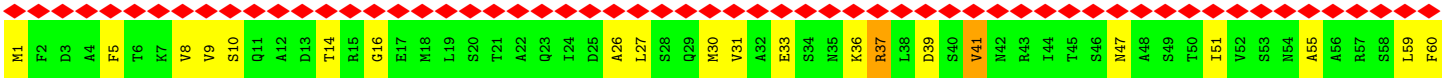


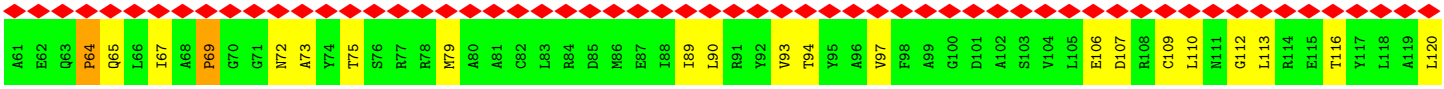


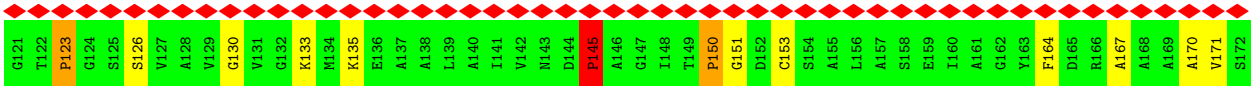
• Molecule 32: Phycocyanin beta subunit

Chain eI:



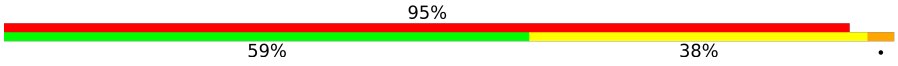


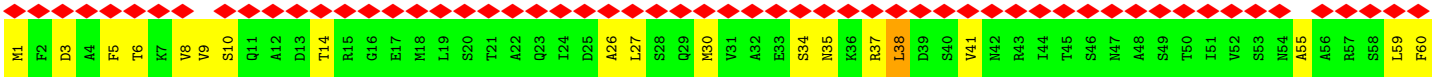


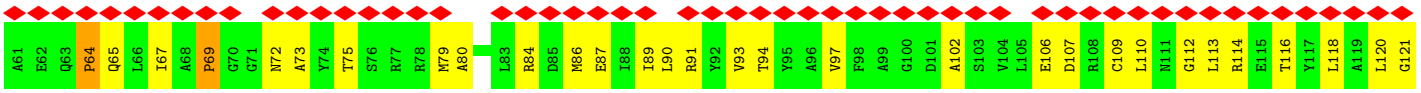


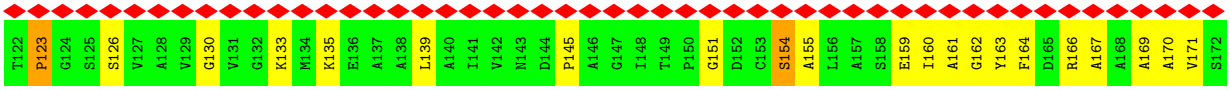
• Molecule 32: Phycocyanin beta subunit

Chain gI:





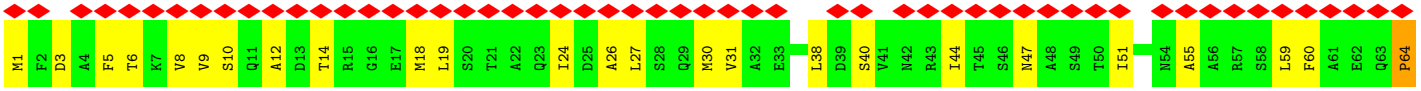


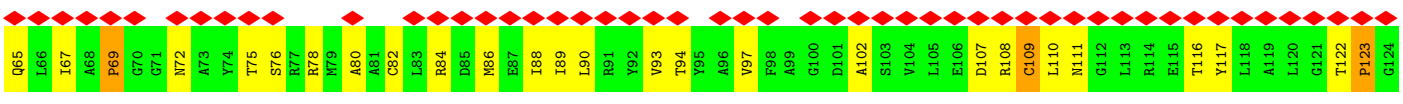


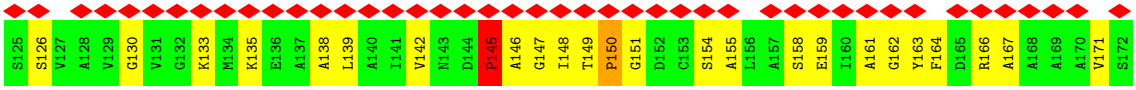
• Molecule 32: Phycocyanin beta subunit

Chain iI:



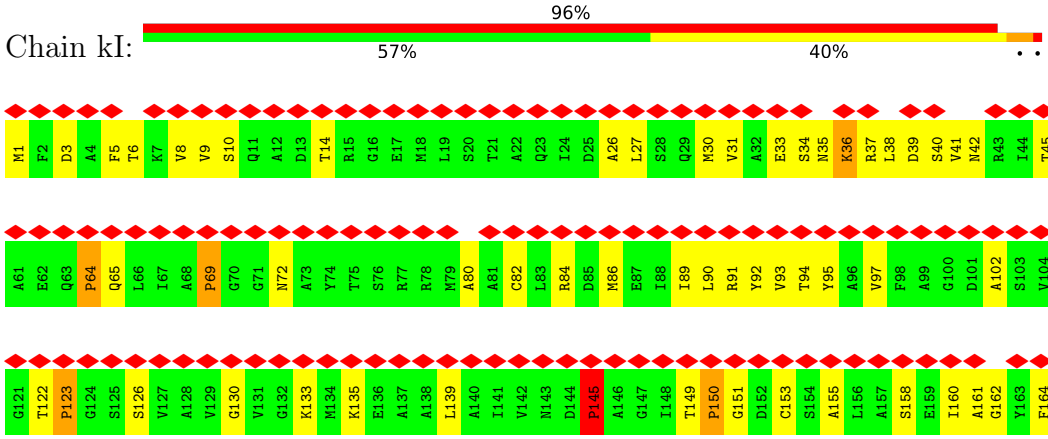






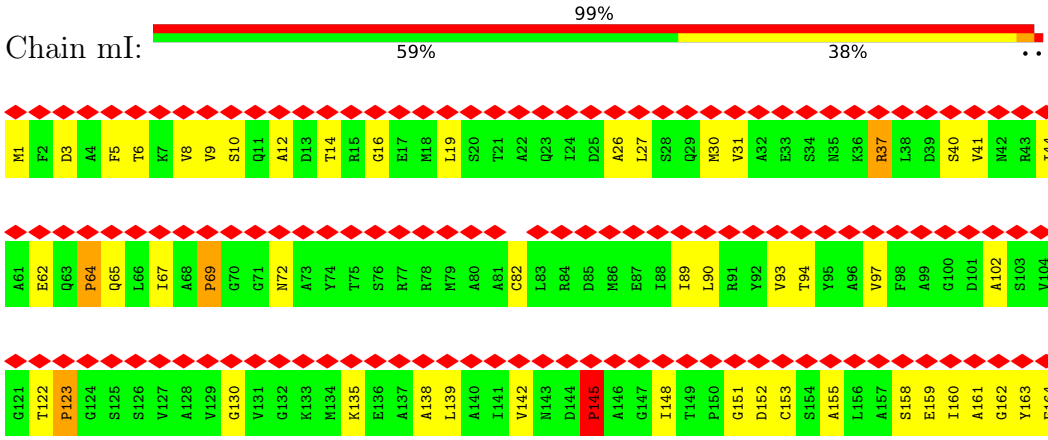
• Molecule 32: Phycocyanin beta subunit

Chain kI:



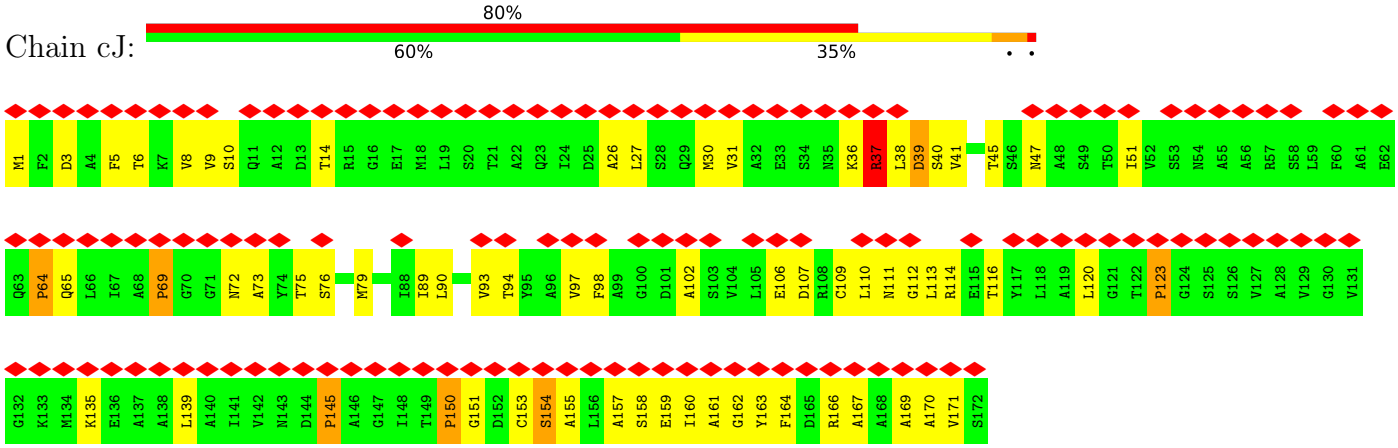
• Molecule 32: Phycocyanin beta subunit

Chain mI:



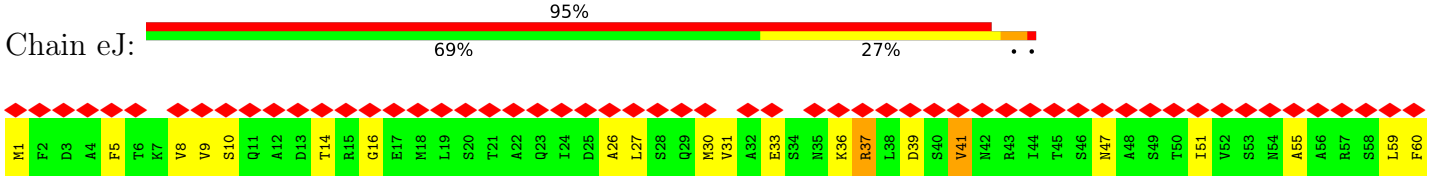
• Molecule 32: Phycocyanin beta subunit

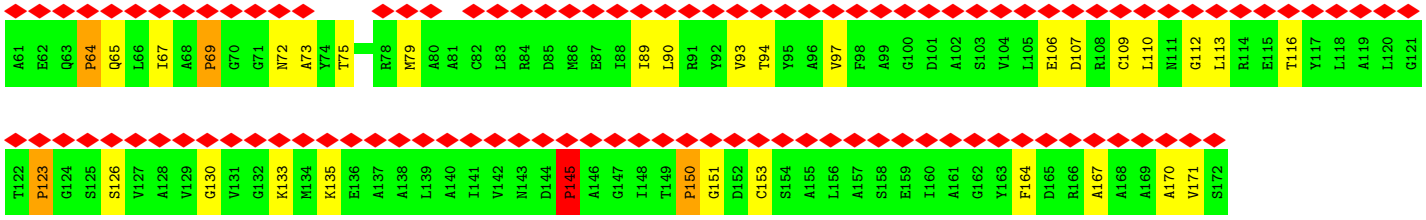
Chain cJ:



• Molecule 32: Phycocyanin beta subunit

Chain eJ:

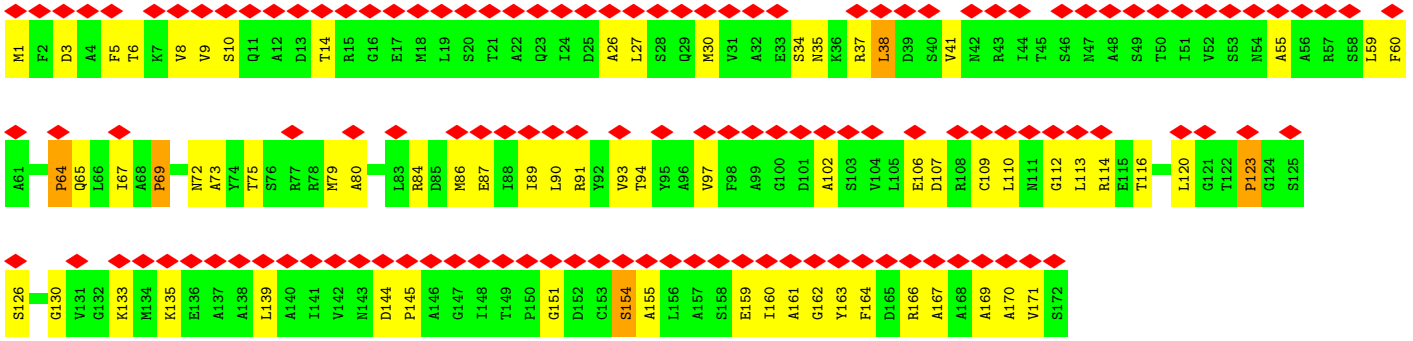




• Molecule 32: Phycocyanin beta subunit

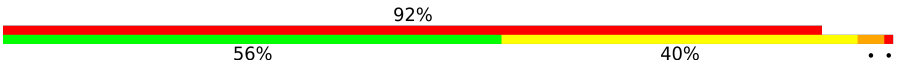
Chain gJ:

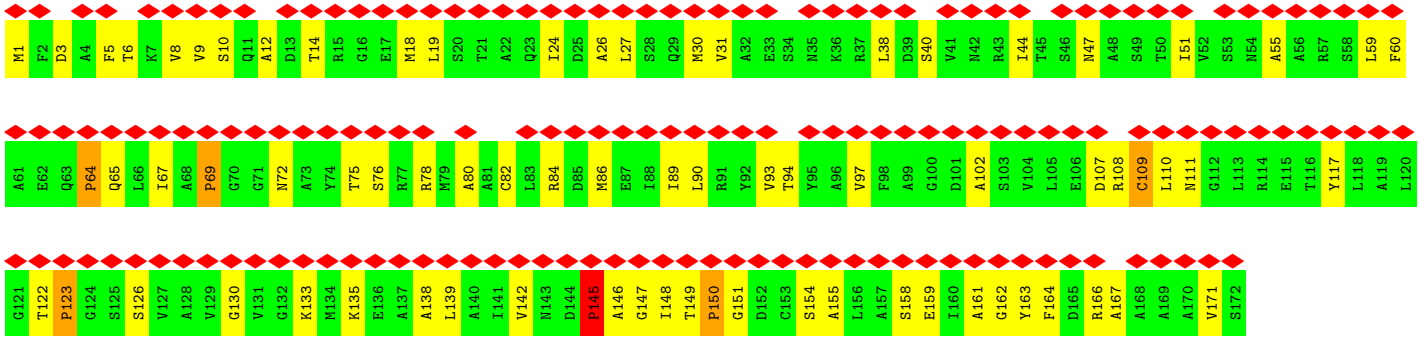




• Molecule 32: Phycocyanin beta subunit

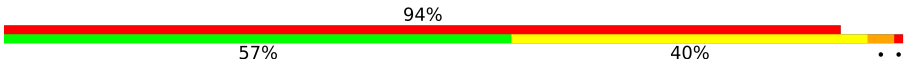
Chain iJ:

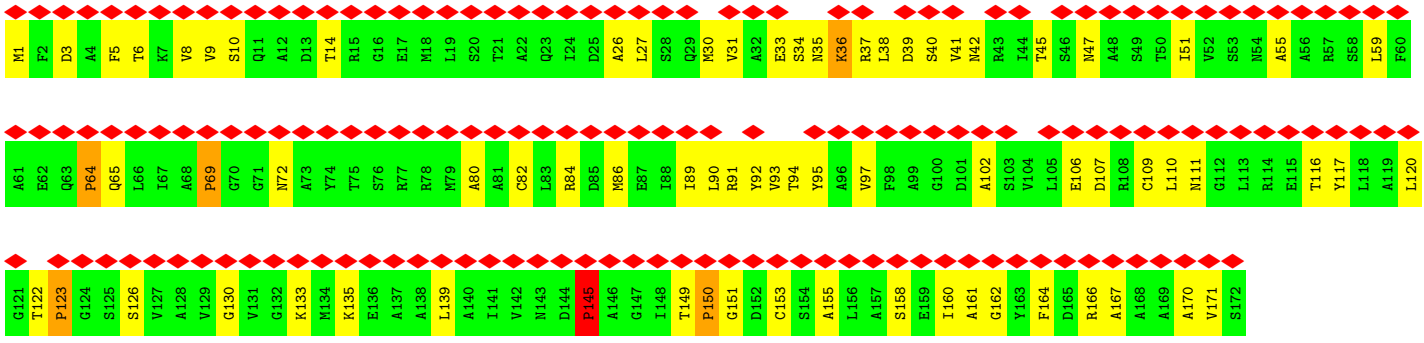




• Molecule 32: Phycocyanin beta subunit

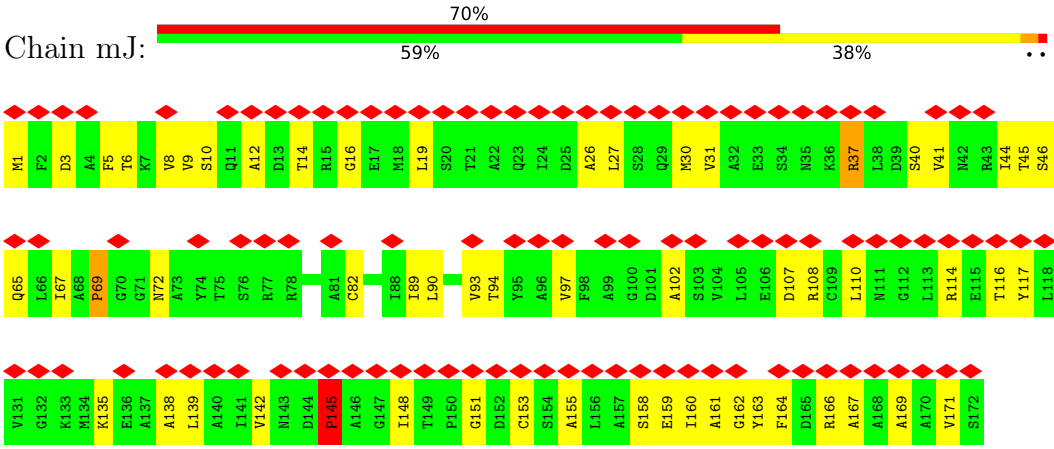
Chain kJ:





• Molecule 32: Phycocyanin beta subunit

Chain mJ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168000	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 ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	6000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.723	Depositor
Minimum map value	-1.208	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	652.8, 652.8, 652.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.632, 1.632, 1.632	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: PL9, PHO, HEM, BCT, LHG, CA, OEX, SQD, FE2, CL, BCR, CLA, LMG, LMT, DGD, CYC

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	B2	0.81	0/1991	1.46	20/2706 (0.7%)
1	B3	0.78	0/1984	1.34	12/2698 (0.4%)
1	B5	0.79	0/1899	1.44	22/2590 (0.8%)
1	B6	0.79	0/1994	1.43	20/2710 (0.7%)
1	B7	0.77	0/1991	1.31	11/2707 (0.4%)
1	B8	0.79	0/1892	1.44	22/2581 (0.9%)
1	B9	0.80	0/1991	1.39	19/2707 (0.7%)
1	BA	0.77	0/1997	1.31	12/2714 (0.4%)
1	BC	0.77	0/1990	1.33	13/2705 (0.5%)
1	BH	0.79	0/1892	1.44	22/2581 (0.9%)
1	BI	0.82	0/1971	1.52	22/2679 (0.8%)
1	BJ	0.79	0/1899	1.44	22/2590 (0.8%)
2	B4	0.46	1/7144 (0.0%)	0.81	23/9652 (0.2%)
2	BB	0.47	1/7144 (0.0%)	0.82	24/9652 (0.2%)
2	C4	0.45	1/6986 (0.0%)	0.76	11/9441 (0.1%)
2	CB	0.45	1/6986 (0.0%)	0.76	11/9441 (0.1%)
3	4G	0.33	0/1220	0.66	0/1649
3	4L	0.33	0/1220	0.66	0/1649
3	6G	0.40	0/1224	0.75	3/1653 (0.2%)
3	6L	0.40	0/1224	0.75	3/1653 (0.2%)
3	9F	0.32	0/1224	0.55	0/1653
3	9K	0.32	0/1224	0.55	0/1653
3	AG	0.35	0/1224	0.63	0/1653
3	AL	0.35	0/1224	0.63	0/1653
3	GG	0.38	0/1224	0.63	0/1653
3	GL	0.38	0/1224	0.63	0/1653
3	IG	0.40	0/1221	0.90	6/1649 (0.4%)
3	IL	0.40	0/1218	1.00	11/1646 (0.7%)
3	JF	0.38	0/1218	0.66	1/1646 (0.1%)
3	JK	0.38	0/1224	0.69	2/1653 (0.1%)
3	KG	0.39	0/1218	0.62	0/1646
3	KL	0.39	0/1218	0.62	0/1646

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	LF	0.37	0/1224	0.63	1/1653 (0.1%)
3	LK	0.37	0/1224	0.63	1/1653 (0.1%)
3	NG	0.33	0/1218	0.61	0/1646
3	NL	0.33	0/1218	0.61	0/1646
3	O4	0.30	0/1218	0.66	0/1646
3	OB	0.31	0/1214	0.67	0/1642
3	PG	0.41	0/1224	0.64	0/1653
3	PL	0.41	0/1224	0.64	0/1653
3	Q4	0.27	0/1224	0.55	0/1653
3	QB	0.27	0/1220	0.55	0/1648
3	RG	0.32	0/1224	0.55	0/1653
3	RL	0.32	0/1224	0.56	0/1653
3	S4	0.29	0/1224	0.61	0/1653
3	SB	0.30	0/1224	0.61	0/1653
3	TG	0.32	0/1218	0.58	1/1646 (0.1%)
3	TL	0.32	0/1218	0.58	1/1646 (0.1%)
3	V4	0.28	0/1220	0.61	0/1649
3	VB	0.28	0/1220	0.61	0/1649
3	X4	0.29	0/1211	0.58	0/1637
3	XB	0.29	0/1218	0.58	0/1646
3	XF	0.34	0/1224	0.76	5/1653 (0.3%)
3	XK	0.34	0/1224	0.72	3/1653 (0.2%)
3	Z4	0.29	0/1224	0.64	1/1653 (0.1%)
3	ZB	0.29	0/1224	0.65	1/1653 (0.1%)
3	ZF	0.34	0/1224	0.54	0/1653
3	ZK	0.34	0/1224	0.54	0/1653
3	bF	0.36	0/1224	0.59	1/1653 (0.1%)
3	bK	0.36	0/1224	0.59	1/1653 (0.1%)
3	dF	0.34	0/1220	0.60	0/1649
3	dK	0.34	0/1220	0.60	0/1649
3	fF	0.41	0/1224	0.66	0/1653
3	fK	0.41	0/1224	0.66	0/1653
3	iF	0.33	0/1224	0.57	0/1653
3	iK	0.33	0/1224	0.57	0/1653
3	kF	0.33	0/1224	0.63	1/1653 (0.1%)
3	kK	0.33	0/1224	0.63	1/1653 (0.1%)
3	o4	0.33	0/1220	0.74	4/1648 (0.2%)
3	oB	0.33	0/1214	0.71	3/1641 (0.2%)
3	q4	0.31	0/1212	0.62	1/1637 (0.1%)
3	qB	0.31	0/1212	0.62	1/1637 (0.1%)
3	s4	0.38	0/1224	0.65	1/1653 (0.1%)
3	sB	0.38	0/1224	0.65	1/1653 (0.1%)
3	u4	0.30	0/1214	0.62	0/1642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	uB	0.30	0/1214	0.62	0/1642
3	w4	0.29	0/1211	0.52	0/1638
3	wB	0.31	0/1224	0.53	0/1653
3	y4	0.39	0/1224	0.59	0/1653
3	yB	0.39	0/1224	0.59	0/1653
4	1G	0.32	0/1230	0.60	0/1665
4	1L	0.36	0/1230	0.62	0/1665
4	5G	0.35	0/1230	0.53	0/1665
4	5L	0.35	0/1230	0.53	0/1665
4	7G	0.40	0/1230	0.67	1/1665 (0.1%)
4	7L	0.40	0/1230	0.68	1/1665 (0.1%)
4	HG	0.39	0/1224	0.57	1/1658 (0.1%)
4	HL	0.39	0/1224	0.57	1/1658 (0.1%)
4	IF	0.35	0/1230	0.72	1/1665 (0.1%)
4	IK	0.36	0/1230	0.71	0/1665
4	JG	0.42	0/1230	0.61	0/1665
4	JL	0.42	0/1230	0.61	0/1665
4	KF	0.39	0/1230	0.56	0/1665
4	KK	0.39	0/1230	0.56	0/1665
4	LG	0.52	0/1230	0.74	2/1665 (0.1%)
4	LL	0.52	0/1230	0.74	2/1665 (0.1%)
4	MF	0.38	0/1230	0.62	1/1665 (0.1%)
4	MG	0.37	0/1226	0.56	0/1660
4	MK	0.38	0/1230	0.62	1/1665 (0.1%)
4	ML	0.37	0/1226	0.56	0/1660
4	OG	0.41	0/1230	0.63	0/1665
4	OL	0.41	0/1230	0.63	0/1665
4	P4	0.30	0/1230	0.57	0/1665
4	PB	0.30	0/1230	0.57	0/1665
4	R4	0.29	0/1230	0.56	0/1665
4	RB	0.30	0/1230	0.56	0/1665
4	SG	0.32	0/1230	0.55	0/1665
4	SL	0.32	0/1230	0.56	0/1665
4	T4	0.28	0/1230	0.53	0/1665
4	TB	0.29	0/1230	0.58	1/1665 (0.1%)
4	UG	0.32	0/1230	0.54	0/1665
4	UL	0.32	0/1230	0.54	0/1665
4	W4	0.28	0/1230	0.54	0/1665
4	WB	0.29	0/1230	0.55	0/1665
4	WG	0.37	0/1230	0.58	0/1665
4	WL	0.37	0/1230	0.58	0/1665
4	Y4	0.30	0/1230	0.63	2/1665 (0.1%)
4	YB	0.31	0/1230	0.63	2/1665 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	YF	0.40	0/1230	0.67	3/1665 (0.2%)
4	YK	0.40	0/1230	0.67	3/1665 (0.2%)
4	a4	0.44	0/1214	0.83	2/1644 (0.1%)
4	aB	0.43	0/1211	0.82	3/1640 (0.2%)
4	aF	0.45	0/1230	0.67	1/1665 (0.1%)
4	aK	0.45	0/1230	0.67	1/1665 (0.1%)
4	cF	0.39	0/1230	0.60	1/1665 (0.1%)
4	cK	0.39	0/1230	0.60	1/1665 (0.1%)
4	eF	0.41	0/1230	0.61	0/1665
4	eK	0.41	0/1230	0.61	0/1665
4	hF	0.38	0/1230	0.55	0/1665
4	hK	0.37	0/1224	0.54	0/1658
4	jF	0.32	0/1227	0.52	0/1662
4	jK	0.33	0/1227	0.52	0/1662
4	lF	0.31	0/1230	0.52	0/1665
4	lK	0.32	0/1230	0.52	0/1665
4	nF	0.37	0/1230	0.62	2/1665 (0.1%)
4	nK	0.37	0/1230	0.62	2/1665 (0.1%)
4	p4	0.32	0/1224	0.59	0/1658
4	pB	0.32	0/1224	0.59	0/1658
4	r4	0.40	0/1230	0.55	0/1665
4	rB	0.40	0/1230	0.55	0/1665
4	t4	0.42	1/1230 (0.1%)	0.60	2/1665 (0.1%)
4	tB	0.42	1/1230 (0.1%)	0.60	2/1665 (0.1%)
4	v4	0.32	0/1230	0.59	0/1665
4	vB	0.33	0/1230	0.59	0/1665
4	x4	0.40	0/1230	0.59	0/1665
4	xB	0.40	0/1230	0.59	0/1665
4	z4	0.33	0/1224	0.56	0/1658
4	zB	0.33	0/1224	0.56	0/1658
5	2G	0.39	0/536	0.71	0/720
5	2L	0.39	0/536	0.71	0/720
5	3F	0.48	0/536	0.78	1/720 (0.1%)
5	3K	0.48	0/536	0.78	1/720 (0.1%)
5	8G	0.53	1/536 (0.2%)	0.95	2/720 (0.3%)
5	8L	0.54	1/536 (0.2%)	0.95	2/720 (0.3%)
5	NF	0.43	0/544	0.85	3/730 (0.4%)
5	NK	0.44	0/544	0.85	3/730 (0.4%)
5	U4	0.34	0/536	0.69	0/720
5	UB	0.34	0/536	0.69	0/720
5	b4	0.33	0/536	0.65	0/720
5	bB	0.33	0/536	0.65	0/720
6	A1	0.41	0/2695	0.78	3/3681 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	AD	0.41	0/2687	0.78	3/3670 (0.1%)
6	AE	0.41	0/2687	0.78	3/3670 (0.1%)
6	a1	0.43	0/2693	0.74	3/3679 (0.1%)
6	aD	0.43	0/2699	0.75	3/3686 (0.1%)
6	aE	0.43	0/2699	0.75	3/3686 (0.1%)
7	B1	0.54	2/4059 (0.0%)	0.85	12/5531 (0.2%)
7	BD	0.54	1/4063 (0.0%)	0.84	11/5536 (0.2%)
7	BE	0.54	1/4057 (0.0%)	0.84	11/5529 (0.2%)
7	b1	0.43	0/4079	0.80	10/5557 (0.2%)
7	bD	0.43	0/4079	0.80	10/5557 (0.2%)
7	bE	0.43	0/4079	0.80	10/5557 (0.2%)
8	C1	0.39	0/3597	0.84	14/4895 (0.3%)
8	CD	0.37	0/3597	0.79	12/4895 (0.2%)
8	CE	0.37	0/3597	0.79	12/4895 (0.2%)
8	c1	0.44	0/3595	0.86	13/4894 (0.3%)
8	cD	0.45	0/3591	0.87	14/4890 (0.3%)
8	cE	0.43	0/3593	0.86	15/4891 (0.3%)
9	D1	0.59	2/2810 (0.1%)	0.97	20/3833 (0.5%)
9	DD	0.59	2/2810 (0.1%)	0.97	20/3833 (0.5%)
9	DE	0.59	2/2810 (0.1%)	0.97	20/3833 (0.5%)
9	d1	0.62	1/2806 (0.0%)	1.05	19/3828 (0.5%)
9	dD	0.62	1/2806 (0.0%)	1.05	19/3828 (0.5%)
9	dE	0.62	1/2806 (0.0%)	1.05	19/3828 (0.5%)
10	E1	0.35	0/652	0.90	3/889 (0.3%)
10	ED	0.35	0/652	0.90	3/889 (0.3%)
10	EE	0.35	0/652	0.90	3/889 (0.3%)
10	e1	0.40	0/652	0.77	1/889 (0.1%)
10	eD	0.40	0/652	0.77	1/889 (0.1%)
10	eE	0.40	0/652	0.77	1/889 (0.1%)
11	F1	0.43	0/292	0.83	1/400 (0.2%)
11	FD	0.44	0/292	0.83	1/400 (0.2%)
11	FE	0.43	0/292	0.83	1/400 (0.2%)
11	f1	0.55	0/292	1.20	4/400 (1.0%)
11	fD	0.57	0/309	1.24	5/424 (1.2%)
11	fE	0.53	0/292	1.17	4/400 (1.0%)
12	H1	0.34	0/526	0.91	1/717 (0.1%)
12	HD	0.34	0/518	0.91	1/708 (0.1%)
12	HE	0.40	0/518	0.94	1/708 (0.1%)
12	h1	0.40	0/526	0.80	1/717 (0.1%)
12	hD	0.40	0/526	0.80	1/717 (0.1%)
12	hE	0.40	0/526	0.80	1/717 (0.1%)
13	I1	0.94	1/300 (0.3%)	1.34	7/404 (1.7%)
13	ID	0.96	1/300 (0.3%)	1.45	6/404 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	IE	0.95	1/300 (0.3%)	1.45	6/404 (1.5%)
13	i1	0.65	0/296	1.12	3/400 (0.8%)
13	iD	0.65	0/296	1.12	3/400 (0.8%)
13	iE	0.65	0/296	1.12	3/400 (0.8%)
14	J1	0.33	0/268	0.74	0/367
14	JD	0.33	0/268	0.74	0/367
14	JE	0.33	0/268	0.74	0/367
14	j1	0.32	0/282	0.77	0/385
14	jD	0.31	0/282	0.77	0/385
14	jE	0.31	0/282	0.77	0/385
15	K1	0.43	0/297	0.94	0/409
15	KD	0.42	0/297	0.94	0/409
15	KE	0.42	0/297	0.94	0/409
15	k1	0.44	0/288	0.99	0/398
15	kD	0.44	0/288	0.99	0/398
15	kE	0.44	0/288	0.99	0/398
16	L1	0.40	0/322	0.84	1/434 (0.2%)
16	LD	0.39	0/322	0.84	1/434 (0.2%)
16	LE	0.39	0/322	0.84	1/434 (0.2%)
16	l1	0.40	0/322	0.84	1/434 (0.2%)
16	lD	0.39	0/322	0.84	1/434 (0.2%)
16	lE	0.40	0/322	0.84	1/434 (0.2%)
17	M1	0.44	0/290	0.84	0/392
17	MD	0.44	0/290	0.84	0/392
17	ME	0.44	0/290	0.84	0/392
17	m1	0.59	0/290	0.98	1/392 (0.3%)
17	mD	0.59	0/290	0.98	1/392 (0.3%)
17	mE	0.59	0/290	0.98	1/392 (0.3%)
18	O1	0.43	0/1893	1.11	7/2571 (0.3%)
18	OD	0.43	0/1893	1.11	7/2571 (0.3%)
18	OE	0.43	0/1893	1.10	6/2571 (0.2%)
18	o1	0.43	0/1893	1.10	6/2571 (0.2%)
18	oD	0.43	0/1893	1.11	7/2571 (0.3%)
18	oE	0.43	0/1893	1.11	7/2571 (0.3%)
19	Q1	0.38	0/985	0.91	3/1332 (0.2%)
19	QD	0.38	0/985	0.91	3/1332 (0.2%)
19	QE	0.38	0/985	0.91	3/1332 (0.2%)
19	q1	0.38	0/985	0.91	3/1332 (0.2%)
19	qD	0.38	0/985	0.91	3/1332 (0.2%)
19	qE	0.38	0/985	0.91	3/1332 (0.2%)
20	R1	0.32	0/264	0.85	0/357
20	RD	0.32	0/264	0.85	2/357 (0.6%)
20	RE	0.32	0/264	0.85	2/357 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	r1	0.33	0/264	0.84	0/357
20	rD	0.33	0/264	0.85	0/357
20	rE	0.33	0/264	0.85	0/357
22	T1	0.33	0/230	0.69	0/313
22	TD	0.32	0/230	0.69	0/313
22	TE	0.33	0/230	0.69	0/313
22	t1	0.31	0/238	0.56	0/323
22	tD	0.31	0/238	0.56	0/323
22	tE	0.31	0/238	0.56	0/323
23	U1	0.35	0/769	0.89	4/1040 (0.4%)
23	UD	0.35	0/769	0.89	4/1040 (0.4%)
23	UE	0.35	0/769	0.89	4/1040 (0.4%)
23	u1	0.35	0/769	0.89	4/1040 (0.4%)
23	uD	0.34	0/769	0.89	4/1040 (0.4%)
23	uE	0.35	0/769	0.89	4/1040 (0.4%)
24	V1	0.33	0/1064	0.73	1/1447 (0.1%)
24	VD	0.33	0/1064	0.74	1/1447 (0.1%)
24	VE	0.33	0/1064	0.74	1/1447 (0.1%)
24	v1	0.32	0/1064	0.72	1/1447 (0.1%)
24	vD	0.32	0/1064	0.72	1/1447 (0.1%)
24	vE	0.32	0/1064	0.72	1/1447 (0.1%)
25	X1	0.32	0/318	0.75	0/429
25	XD	0.32	0/318	0.75	0/429
25	XE	0.32	0/318	0.75	0/429
25	x1	0.33	0/318	0.75	0/429
25	xD	0.33	0/318	0.75	0/429
25	xE	0.33	0/318	0.75	0/429
26	Y1	0.35	0/241	0.84	0/327
26	YD	0.35	0/241	0.84	0/327
26	YE	0.35	0/241	0.84	0/327
26	y1	0.35	0/241	0.81	0/327
26	yD	0.35	0/241	0.79	0/327
26	yE	0.35	0/241	0.79	0/327
27	Z1	0.40	0/473	0.85	0/651
27	ZD	0.40	0/473	0.85	0/651
27	ZE	0.40	0/473	0.85	0/651
27	z1	0.57	0/473	0.96	3/651 (0.5%)
27	zD	0.57	0/473	0.96	3/651 (0.5%)
27	zE	0.57	0/473	0.95	3/651 (0.5%)
28	BG	0.78	0/363	1.99	17/483 (3.5%)
28	BL	0.78	0/363	1.99	17/483 (3.5%)
28	EF	0.83	0/360	1.90	16/480 (3.3%)
28	EK	0.83	0/360	1.90	17/480 (3.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	QG	0.52	0/1316	0.82	2/1790 (0.1%)
29	QL	0.51	0/1316	0.81	2/1790 (0.1%)
29	gF	0.51	0/1316	0.82	3/1790 (0.2%)
29	gK	0.51	0/1316	0.82	3/1790 (0.2%)
30	VG	0.40	0/1274	0.70	1/1720 (0.1%)
30	VL	0.41	0/1274	0.70	1/1720 (0.1%)
30	mF	0.39	0/1274	0.69	1/1720 (0.1%)
30	mK	0.39	0/1274	0.69	1/1720 (0.1%)
31	b2	0.39	0/1060	0.82	5/1446 (0.3%)
31	b3	0.39	0/1060	0.82	5/1446 (0.3%)
31	b5	0.39	0/1060	0.82	5/1446 (0.3%)
31	b6	0.39	0/1060	0.82	5/1446 (0.3%)
31	b7	0.39	0/1060	0.82	5/1446 (0.3%)
31	b8	0.39	0/1060	0.82	5/1446 (0.3%)
31	b9	0.39	0/1060	0.82	5/1446 (0.3%)
31	bA	0.39	0/1060	0.82	5/1446 (0.3%)
31	bC	0.39	0/1060	0.82	5/1446 (0.3%)
31	bH	0.39	0/1060	0.82	5/1446 (0.3%)
31	bI	0.39	0/1060	0.82	5/1446 (0.3%)
31	bJ	0.39	0/1060	0.82	5/1446 (0.3%)
31	d2	0.40	0/1019	0.83	5/1397 (0.4%)
31	d3	0.40	0/1019	0.83	5/1397 (0.4%)
31	d5	0.40	0/1019	0.83	5/1397 (0.4%)
31	d6	0.40	0/1019	0.83	5/1397 (0.4%)
31	d7	0.40	0/1019	0.83	5/1397 (0.4%)
31	d8	0.40	0/1019	0.83	5/1397 (0.4%)
31	d9	0.40	0/1019	0.83	5/1397 (0.4%)
31	dA	0.40	0/1019	0.83	5/1397 (0.4%)
31	dC	0.40	0/1019	0.83	5/1397 (0.4%)
31	dH	0.40	0/1019	0.83	5/1397 (0.4%)
31	dI	0.40	0/1019	0.83	5/1397 (0.4%)
31	dJ	0.40	0/1019	0.83	5/1397 (0.4%)
31	f2	0.39	0/1039	0.82	5/1424 (0.4%)
31	f3	0.39	0/1039	0.82	5/1424 (0.4%)
31	f5	0.39	0/1039	0.82	5/1424 (0.4%)
31	f6	0.39	0/1039	0.82	5/1424 (0.4%)
31	f7	0.39	0/1039	0.82	5/1424 (0.4%)
31	f8	0.39	0/1039	0.82	5/1424 (0.4%)
31	f9	0.39	0/1039	0.82	5/1424 (0.4%)
31	fA	0.39	0/1039	0.82	5/1424 (0.4%)
31	fC	0.39	0/1039	0.82	5/1424 (0.4%)
31	fH	0.39	0/1039	0.82	5/1424 (0.4%)
31	fI	0.39	0/1039	0.82	5/1424 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	fJ	0.39	0/1039	0.82	5/1424 (0.4%)
31	h2	0.39	0/1051	0.82	5/1437 (0.3%)
31	h3	0.39	0/1051	0.82	5/1437 (0.3%)
31	h5	0.39	0/1051	0.82	5/1437 (0.3%)
31	h6	0.39	0/1051	0.82	5/1437 (0.3%)
31	h7	0.39	0/1051	0.82	5/1437 (0.3%)
31	h8	0.39	0/1051	0.82	5/1437 (0.3%)
31	h9	0.39	0/1045	0.82	5/1430 (0.3%)
31	hA	0.39	0/1051	0.82	5/1437 (0.3%)
31	hC	0.39	0/1051	0.82	5/1437 (0.3%)
31	hH	0.39	0/1051	0.82	5/1437 (0.3%)
31	hI	0.39	0/1051	0.82	5/1437 (0.3%)
31	hJ	0.39	0/1051	0.82	5/1437 (0.3%)
31	j2	0.39	0/1037	0.83	5/1419 (0.4%)
31	j3	0.39	0/1037	0.83	5/1419 (0.4%)
31	j5	0.39	0/1037	0.83	5/1419 (0.4%)
31	j6	0.40	0/1037	0.83	5/1419 (0.4%)
31	j7	0.39	0/1037	0.83	5/1419 (0.4%)
31	j8	0.39	0/1037	0.83	5/1419 (0.4%)
31	j9	0.39	0/1037	0.83	5/1419 (0.4%)
31	jA	0.39	0/1037	0.83	5/1419 (0.4%)
31	jC	0.39	0/1037	0.83	5/1419 (0.4%)
31	jH	0.39	0/1037	0.83	5/1419 (0.4%)
31	jI	0.40	0/1037	0.83	5/1419 (0.4%)
31	jJ	0.39	0/1037	0.83	5/1419 (0.4%)
31	l2	0.39	0/1070	0.81	5/1464 (0.3%)
31	l3	0.39	0/1070	0.82	5/1464 (0.3%)
31	l5	0.38	0/1070	0.82	5/1464 (0.3%)
31	l6	0.39	0/1070	0.81	5/1464 (0.3%)
31	l7	0.39	0/1070	0.82	5/1464 (0.3%)
31	l8	0.39	0/1070	0.81	5/1464 (0.3%)
31	l9	0.39	0/1070	0.82	5/1464 (0.3%)
31	lA	0.39	0/1070	0.82	5/1464 (0.3%)
31	lC	0.39	0/1070	0.82	5/1464 (0.3%)
31	lH	0.38	0/1070	0.82	5/1464 (0.3%)
31	lI	0.39	0/1070	0.82	5/1464 (0.3%)
31	lJ	0.39	0/1070	0.82	5/1464 (0.3%)
32	c2	0.39	0/1083	1.00	8/1488 (0.5%)
32	c3	0.39	0/1083	1.00	8/1488 (0.5%)
32	c5	0.39	0/1083	1.00	8/1488 (0.5%)
32	c6	0.39	0/1083	1.00	8/1488 (0.5%)
32	c7	0.39	0/1083	1.00	8/1488 (0.5%)
32	c8	0.39	0/1083	1.00	8/1488 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c9	0.39	0/1083	1.00	8/1488 (0.5%)
32	cA	0.39	0/1083	1.00	8/1488 (0.5%)
32	cC	0.39	0/1083	1.00	8/1488 (0.5%)
32	cH	0.39	0/1083	1.00	8/1488 (0.5%)
32	cI	0.39	0/1080	1.01	8/1484 (0.5%)
32	cJ	0.39	0/1083	1.00	8/1488 (0.5%)
32	e2	0.39	0/1069	0.92	9/1467 (0.6%)
32	e3	0.39	0/1069	0.92	9/1467 (0.6%)
32	e5	0.39	0/1069	0.92	9/1467 (0.6%)
32	e6	0.39	0/1069	0.92	9/1467 (0.6%)
32	e7	0.39	0/1069	0.92	9/1467 (0.6%)
32	e8	0.39	0/1069	0.92	9/1467 (0.6%)
32	e9	0.39	0/1069	0.92	9/1467 (0.6%)
32	eA	0.39	0/1069	0.92	9/1467 (0.6%)
32	eC	0.39	0/1069	0.92	9/1467 (0.6%)
32	eH	0.39	0/1069	0.92	9/1467 (0.6%)
32	eI	0.39	0/1069	0.92	9/1467 (0.6%)
32	eJ	0.39	0/1069	0.92	9/1467 (0.6%)
32	g2	0.40	0/1094	0.84	5/1498 (0.3%)
32	g3	0.40	0/1094	0.84	5/1498 (0.3%)
32	g5	0.40	0/1094	0.84	5/1498 (0.3%)
32	g6	0.40	0/1094	0.84	5/1498 (0.3%)
32	g7	0.40	0/1094	0.84	5/1498 (0.3%)
32	g8	0.40	0/1094	0.84	5/1498 (0.3%)
32	g9	0.40	0/1094	0.84	5/1498 (0.3%)
32	gA	0.40	0/1094	0.84	5/1498 (0.3%)
32	gC	0.40	0/1094	0.84	5/1498 (0.3%)
32	gH	0.40	0/1094	0.84	5/1498 (0.3%)
32	gI	0.40	0/1091	0.84	5/1494 (0.3%)
32	gJ	0.40	0/1094	0.84	5/1498 (0.3%)
32	i2	0.41	0/1093	0.99	12/1497 (0.8%)
32	i3	0.41	0/1093	0.99	12/1497 (0.8%)
32	i5	0.41	0/1093	0.99	12/1497 (0.8%)
32	i6	0.41	0/1093	0.98	12/1497 (0.8%)
32	i7	0.41	0/1093	0.98	12/1497 (0.8%)
32	i8	0.41	0/1093	0.98	12/1497 (0.8%)
32	i9	0.41	0/1093	0.98	12/1497 (0.8%)
32	iA	0.41	0/1093	0.99	12/1497 (0.8%)
32	iC	0.41	0/1093	0.98	12/1497 (0.8%)
32	iH	0.41	0/1093	0.99	12/1497 (0.8%)
32	iI	0.41	0/1093	0.99	12/1497 (0.8%)
32	iJ	0.41	0/1093	0.98	12/1497 (0.8%)
32	k2	0.38	0/1110	0.88	6/1520 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	k3	0.38	0/1110	0.88	6/1520 (0.4%)
32	k5	0.37	0/1110	0.88	6/1520 (0.4%)
32	k6	0.37	0/1110	0.88	6/1520 (0.4%)
32	k7	0.37	0/1110	0.88	6/1520 (0.4%)
32	k8	0.37	0/1110	0.88	6/1520 (0.4%)
32	k9	0.37	0/1110	0.88	6/1520 (0.4%)
32	kA	0.38	0/1110	0.88	6/1520 (0.4%)
32	kC	0.37	0/1110	0.88	6/1520 (0.4%)
32	kH	0.37	0/1110	0.88	6/1520 (0.4%)
32	kI	0.37	0/1110	0.88	6/1520 (0.4%)
32	kJ	0.38	0/1110	0.88	6/1520 (0.4%)
32	m2	0.39	0/1104	0.93	8/1514 (0.5%)
32	m3	0.39	0/1104	0.93	8/1514 (0.5%)
32	m5	0.39	0/1104	0.93	8/1514 (0.5%)
32	m6	0.39	0/1104	0.93	8/1514 (0.5%)
32	m7	0.39	0/1104	0.93	8/1514 (0.5%)
32	m8	0.39	0/1104	0.93	9/1514 (0.6%)
32	m9	0.39	0/1104	0.93	9/1514 (0.6%)
32	mA	0.39	0/1104	0.93	8/1514 (0.5%)
32	mC	0.39	0/1104	0.93	8/1514 (0.5%)
32	mH	0.39	0/1104	0.93	8/1514 (0.5%)
32	mI	0.39	0/1104	0.93	8/1514 (0.5%)
32	mJ	0.39	0/1104	0.93	8/1514 (0.5%)
All	All	0.43	24/519767 (0.0%)	0.84	1862/706903 (0.3%)

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	B5	0	1
1	B8	0	1
1	BC	0	1
1	BH	0	1
1	BJ	0	1
2	B4	0	5
2	BB	0	5
2	C4	0	4
2	CB	0	4
3	GG	0	1
3	GL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	s4	0	1
3	sB	0	1
4	UG	0	1
4	UL	0	1
4	WG	0	1
4	WL	0	1
4	a4	0	2
4	aB	0	2
4	x4	0	1
4	xB	0	1
5	3F	0	1
5	3K	0	1
5	U4	0	1
5	UB	0	1
6	A1	0	4
6	AD	0	4
6	AE	0	4
6	a1	0	5
6	aD	0	5
6	aE	0	5
7	B1	0	5
7	BD	0	5
7	BE	0	5
7	b1	0	5
7	bD	0	5
7	bE	0	5
8	cE	0	1
9	D1	0	2
9	DD	0	2
9	DE	0	2
9	d1	0	2
9	dD	0	2
9	dE	0	2
12	H1	0	1
12	HD	0	1
12	HE	0	1
12	h1	0	1
12	hD	0	1
12	hE	0	1
13	i1	0	2
13	iD	0	2
13	iE	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	j1	0	1
14	jD	0	1
14	jE	0	1
18	O1	0	16
18	OD	0	16
18	OE	0	16
18	o1	0	16
18	oD	0	16
18	oE	0	16
19	Q1	0	3
19	QD	0	3
19	QE	0	3
19	q1	0	3
19	qD	0	3
19	qE	0	3
23	U1	0	2
23	UD	0	2
23	UE	0	2
23	u1	0	2
23	uD	0	2
23	uE	0	2
24	V1	0	1
24	VD	0	1
24	VE	0	1
24	v1	0	2
24	vD	0	2
24	vE	0	2
28	BG	0	1
28	BL	0	1
28	EF	0	1
28	EK	0	1
29	QG	0	1
29	QL	0	1
29	gF	0	1
29	gK	0	1
32	c2	0	1
32	c3	0	1
32	c5	0	1
32	c6	0	1
32	c7	0	1
32	c8	0	1
32	c9	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	cA	0	1
32	cC	0	1
32	cH	0	1
32	cI	0	1
32	cJ	0	1
32	e2	0	1
32	e3	0	1
32	e5	0	1
32	e6	0	1
32	e7	0	1
32	e8	0	1
32	e9	0	1
32	eA	0	1
32	eC	0	1
32	eH	0	1
32	eI	0	1
32	eJ	0	1
32	g2	0	1
32	g3	0	1
32	g5	0	1
32	g6	0	1
32	g7	0	1
32	g8	0	1
32	g9	0	1
32	gA	0	1
32	gC	0	1
32	gH	0	1
32	gI	0	1
32	gJ	0	1
32	k2	0	1
32	k3	0	1
32	k5	0	1
32	k6	0	1
32	k7	0	1
32	k8	0	1
32	k9	0	1
32	kA	0	1
32	kC	0	1
32	kH	0	1
32	kI	0	1
32	kJ	0	1
All	All	0	317

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	t4	77	ARG	CD-NE	6.86	1.55	1.46
4	tB	77	ARG	CD-NE	6.84	1.55	1.46
13	I1	26	ASN	N-CA	-6.66	1.37	1.46
5	8G	58	GLY	C-N	-6.65	1.23	1.33
5	8L	58	GLY	C-N	-6.64	1.23	1.33

The worst 5 of 1862 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BI	212	GLN	C-N-CD	-18.61	48.69	125.00
1	BI	230	ARG	C-N-CD	-17.48	53.35	125.00
1	B2	230	ARG	C-N-CD	-17.47	53.35	125.00
1	B6	230	ARG	C-N-CD	-17.47	53.35	125.00
9	dE	111	TRP	CA-C-N	-16.21	98.39	120.44

There are no chirality outliers.

5 of 317 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BB	481	LYS	Peptide
2	BB	536	SER	Peptide
2	BB	732	ASN	Peptide
2	BB	733	LYS	Mainchain
2	BB	80	SER	Mainchain

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	B2	1942	0	1885	243	0
1	B3	1936	0	1882	207	0
1	B5	1856	0	1756	232	0
1	B6	1945	0	1892	210	0
1	B7	1942	0	1889	267	0
1	B8	1850	0	1750	162	0
1	B9	1942	0	1889	253	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1948	0	1900	215	0
1	BC	1942	0	1889	233	0
1	BH	1850	0	1750	171	0
1	BI	1925	0	1867	262	0
1	BJ	1856	0	1759	196	0
2	B4	7001	0	6960	329	0
2	BB	7001	0	6960	338	0
2	C4	6844	0	6825	386	0
2	CB	6844	0	6824	374	0
3	4G	1205	0	1200	51	0
3	4L	1205	0	1200	77	0
3	6G	1209	0	1214	30	0
3	6L	1209	0	1214	32	0
3	9F	1209	0	1214	7	0
3	9K	1209	0	1214	9	0
3	AG	1209	0	1213	43	0
3	AL	1209	0	1213	41	0
3	GG	1209	0	1214	10	0
3	GL	1209	0	1214	10	0
3	IG	1206	0	1208	355	0
3	IL	1203	0	1201	334	0
3	JF	1203	0	1203	84	0
3	JK	1209	0	1214	82	0
3	KG	1203	0	1203	58	0
3	KL	1203	0	1203	57	0
3	LF	1209	0	1215	10	0
3	LK	1209	0	1215	13	0
3	NG	1203	0	1203	37	0
3	NL	1203	0	1200	63	0
3	O4	1203	0	1203	64	0
3	OB	1199	0	1192	33	0
3	PG	1209	0	1214	28	0
3	PL	1209	0	1214	26	0
3	Q4	1209	0	1214	41	0
3	QB	1205	0	1208	37	0
3	RG	1209	0	1214	10	0
3	RL	1209	0	1214	11	0
3	S4	1209	0	1214	20	0
3	SB	1209	0	1214	21	0
3	TG	1203	0	1203	22	0
3	TL	1203	0	1203	22	0
3	V4	1205	0	1202	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	VB	1205	0	1202	27	0
3	X4	1196	0	1188	24	0
3	XB	1203	0	1203	63	0
3	XF	1209	0	1214	42	0
3	XK	1209	0	1214	42	0
3	Z4	1209	0	1214	16	0
3	ZB	1209	0	1214	19	0
3	ZF	1209	0	1214	100	0
3	ZK	1209	0	1214	95	0
3	bF	1209	0	1213	19	0
3	bK	1209	0	1213	17	0
3	dF	1205	0	1202	31	0
3	dK	1205	0	1202	32	0
3	fF	1209	0	1212	27	0
3	fK	1209	0	1212	29	0
3	iF	1209	0	1214	13	0
3	iK	1209	0	1214	12	0
3	kF	1209	0	1213	19	0
3	kK	1209	0	1213	18	0
3	o4	1205	0	1204	98	0
3	oB	1199	0	1196	67	0
3	q4	1198	0	1199	43	0
3	qB	1198	0	1199	41	0
3	s4	1209	0	1214	15	0
3	sB	1209	0	1214	16	0
3	u4	1199	0	1191	58	0
3	uB	1199	0	1191	68	0
3	w4	1196	0	1192	25	0
3	wB	1209	0	1214	44	0
3	y4	1209	0	1214	24	0
3	yB	1209	0	1214	24	0
4	1G	1214	0	1221	50	0
4	1L	1214	0	1223	48	0
4	5G	1214	0	1226	21	0
4	5L	1214	0	1226	24	0
4	7G	1214	0	1225	30	0
4	7L	1214	0	1225	52	0
4	HG	1208	0	1214	22	0
4	HL	1208	0	1214	21	0
4	IF	1214	0	1225	48	0
4	IK	1214	0	1225	54	0
4	JG	1214	0	1225	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	JL	1214	0	1225	93	0
4	KF	1214	0	1224	33	0
4	KK	1214	0	1224	25	0
4	LG	1214	0	1225	23	0
4	LL	1214	0	1225	21	0
4	MF	1214	0	1225	57	0
4	MG	1210	0	1221	80	0
4	MK	1214	0	1225	40	0
4	ML	1210	0	1221	74	0
4	OG	1214	0	1225	29	0
4	OL	1214	0	1225	30	0
4	P4	1214	0	1225	42	0
4	PB	1214	0	1225	43	0
4	R4	1214	0	1225	28	0
4	RB	1214	0	1225	22	0
4	SG	1214	0	1225	19	0
4	SL	1214	0	1225	21	0
4	T4	1214	0	1223	56	0
4	TB	1214	0	1225	62	0
4	UG	1214	0	1225	13	0
4	UL	1214	0	1225	15	0
4	W4	1214	0	1225	36	0
4	WB	1214	0	1225	35	0
4	WG	1214	0	1224	17	0
4	WL	1214	0	1224	18	0
4	Y4	1214	0	1225	16	0
4	YB	1214	0	1225	19	0
4	YF	1214	0	1224	145	0
4	YK	1214	0	1224	144	0
4	a4	1199	0	1205	119	0
4	aB	1196	0	1203	117	0
4	aF	1214	0	1224	29	0
4	aK	1214	0	1224	25	0
4	cF	1214	0	1225	25	0
4	cK	1214	0	1225	26	0
4	eF	1214	0	1225	16	0
4	eK	1214	0	1225	12	0
4	hF	1214	0	1224	74	0
4	hK	1208	0	1213	71	0
4	jF	1211	0	1217	13	0
4	jK	1211	0	1217	16	0
4	lF	1214	0	1224	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	lK	1214	0	1224	21	0
4	nF	1214	0	1225	24	0
4	nK	1214	0	1225	23	0
4	p4	1208	0	1213	26	0
4	pB	1208	0	1213	25	0
4	r4	1214	0	1225	30	0
4	rB	1214	0	1225	29	0
4	t4	1214	0	1225	19	0
4	tB	1214	0	1225	35	0
4	v4	1214	0	1225	34	0
4	vB	1214	0	1224	31	0
4	x4	1214	0	1225	36	0
4	xB	1214	0	1225	37	0
4	z4	1208	0	1214	37	0
4	zB	1208	0	1214	40	0
5	2G	527	0	545	11	0
5	2L	527	0	545	11	0
5	3F	527	0	545	3	0
5	3K	527	0	545	4	0
5	8G	527	0	547	20	0
5	8L	527	0	547	20	0
5	NF	535	0	558	14	0
5	NK	535	0	558	13	0
5	U4	527	0	547	18	0
5	UB	527	0	547	17	0
5	b4	527	0	547	13	0
5	bB	527	0	547	13	0
6	A1	2613	0	2525	103	0
6	AD	2606	0	2518	110	0
6	AE	2606	0	2518	116	0
6	a1	2611	0	2520	92	0
6	aD	2617	0	2531	108	0
6	aE	2617	0	2531	105	0
7	B1	3925	0	3763	191	0
7	BD	3929	0	3766	229	0
7	BE	3923	0	3756	233	0
7	b1	3945	0	3786	169	0
7	bD	3945	0	3786	179	0
7	bE	3945	0	3786	162	0
8	C1	3485	0	3404	273	0
8	CD	3485	0	3404	265	0
8	CE	3485	0	3404	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	c1	3484	0	3386	240	0
8	cD	3480	0	3374	307	0
8	cE	3482	0	3377	283	0
9	D1	2713	0	2603	143	0
9	DD	2713	0	2603	153	0
9	DE	2713	0	2603	144	0
9	d1	2709	0	2597	231	0
9	dD	2709	0	2597	240	0
9	dE	2709	0	2597	237	0
10	E1	634	0	616	45	0
10	ED	634	0	616	47	0
10	EE	634	0	616	46	0
10	e1	634	0	616	53	0
10	eD	634	0	616	52	0
10	eE	634	0	616	51	0
11	F1	283	0	295	5	0
11	FD	283	0	295	7	0
11	FE	283	0	295	6	0
11	f1	283	0	294	45	0
11	fD	299	0	309	57	0
11	fE	283	0	294	44	0
12	H1	512	0	518	8	0
12	HD	504	0	502	43	0
12	HE	504	0	503	41	0
12	h1	512	0	518	16	0
12	hD	512	0	518	16	0
12	hE	512	0	518	16	0
13	I1	294	0	316	41	0
13	ID	294	0	317	19	0
13	IE	294	0	317	21	0
13	i1	290	0	306	133	0
13	iD	290	0	306	133	0
13	iE	290	0	306	135	0
14	J1	262	0	274	22	0
14	JD	262	0	274	23	0
14	JE	262	0	274	22	0
14	j1	276	0	291	11	0
14	jD	276	0	291	12	0
14	jE	276	0	291	13	0
15	K1	286	0	297	53	0
15	KD	286	0	297	49	0
15	KE	286	0	297	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	k1	277	0	284	64	0
15	kD	277	0	284	64	0
15	kE	277	0	284	61	0
16	L1	315	0	328	11	0
16	LD	315	0	328	12	0
16	LE	315	0	328	12	0
16	l1	315	0	328	14	0
16	lD	315	0	328	14	0
16	lE	315	0	328	13	0
17	M1	286	0	301	23	0
17	MD	286	0	301	23	0
17	ME	286	0	301	23	0
17	m1	286	0	301	52	0
17	mD	286	0	301	51	0
17	mE	286	0	301	52	0
18	O1	1856	0	1821	109	0
18	OD	1856	0	1821	143	0
18	OE	1856	0	1821	60	0
18	o1	1856	0	1821	52	0
18	oD	1856	0	1820	105	0
18	oE	1856	0	1820	133	0
19	Q1	966	0	945	14	0
19	QD	966	0	945	14	0
19	QE	966	0	945	13	0
19	q1	966	0	945	15	0
19	qD	966	0	945	15	0
19	qE	966	0	945	15	0
20	R1	260	0	286	4	0
20	RD	260	0	286	4	0
20	RE	260	0	286	4	0
20	r1	260	0	286	3	0
20	rD	260	0	286	3	0
20	rE	260	0	286	3	0
21	S1	235	0	57	27	0
21	SD	235	0	57	27	0
21	SE	235	0	57	27	0
22	T1	225	0	240	3	0
22	TD	225	0	240	3	0
22	TE	225	0	240	2	0
22	t1	233	0	252	10	0
22	tD	233	0	252	10	0
22	tE	233	0	252	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	U1	755	0	752	29	0
23	UD	755	0	752	31	0
23	UE	755	0	752	29	0
23	u1	755	0	752	13	0
23	uD	755	0	752	12	0
23	uE	755	0	752	12	0
24	V1	1043	0	1036	49	0
24	VD	1043	0	1036	48	0
24	VE	1043	0	1036	46	0
24	v1	1043	0	1037	16	0
24	vD	1043	0	1037	19	0
24	vE	1043	0	1037	18	0
25	X1	313	0	349	7	0
25	XD	313	0	349	7	0
25	XE	313	0	349	7	0
25	x1	313	0	349	7	0
25	xD	313	0	349	8	0
25	xE	313	0	349	7	0
26	Y1	239	0	267	1	0
26	YD	239	0	267	2	0
26	YE	239	0	267	3	0
26	y1	239	0	267	30	0
26	yD	239	0	267	29	0
26	yE	239	0	267	26	0
27	Z1	461	0	498	38	0
27	ZD	461	0	498	38	0
27	ZE	461	0	498	38	0
27	z1	461	0	498	31	0
27	zD	461	0	498	71	0
27	zE	461	0	498	61	0
28	BG	357	0	355	219	0
28	BL	357	0	355	222	0
28	EF	354	0	347	192	0
28	EK	354	0	347	189	0
29	QG	1297	0	1293	77	0
29	QL	1297	0	1293	80	0
29	gF	1297	0	1293	84	0
29	gK	1297	0	1293	84	0
30	VG	1254	0	1271	39	0
30	VL	1254	0	1271	38	0
30	mF	1254	0	1270	51	0
30	mK	1254	0	1269	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	b2	1052	0	948	93	0
31	b3	1052	0	948	89	0
31	b5	1052	0	948	95	0
31	b6	1052	0	948	93	0
31	b7	1052	0	948	94	0
31	b8	1052	0	948	97	0
31	b9	1052	0	948	87	0
31	bA	1052	0	948	93	0
31	bC	1052	0	948	95	0
31	bH	1052	0	948	104	0
31	bI	1052	0	948	94	0
31	bJ	1052	0	948	99	0
31	d2	1013	0	884	70	0
31	d3	1013	0	884	70	0
31	d5	1013	0	884	71	0
31	d6	1013	0	884	69	0
31	d7	1013	0	884	70	0
31	d8	1013	0	884	72	0
31	d9	1013	0	884	69	0
31	dA	1013	0	884	70	0
31	dC	1013	0	884	69	0
31	dH	1013	0	884	70	0
31	dI	1013	0	884	71	0
31	dJ	1013	0	884	71	0
31	f2	1030	0	890	96	0
31	f3	1030	0	890	96	0
31	f5	1030	0	891	84	0
31	f6	1030	0	890	105	0
31	f7	1030	0	890	98	0
31	f8	1030	0	891	84	0
31	f9	1030	0	890	94	0
31	fA	1030	0	890	100	0
31	fC	1030	0	890	97	0
31	fH	1030	0	891	85	0
31	fI	1030	0	890	96	0
31	fJ	1030	0	891	86	0
31	h2	1042	0	913	100	0
31	h3	1042	0	913	99	0
31	h5	1042	0	913	102	0
31	h6	1042	0	913	104	0
31	h7	1042	0	913	100	0
31	h8	1042	0	913	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	h9	1036	0	902	98	0
31	hA	1042	0	913	103	0
31	hC	1042	0	913	102	0
31	hH	1042	0	913	101	0
31	hI	1042	0	913	101	0
31	hJ	1042	0	913	101	0
31	j2	1029	0	910	67	0
31	j3	1029	0	910	69	0
31	j5	1029	0	910	66	0
31	j6	1029	0	908	73	0
31	j7	1029	0	910	68	0
31	j8	1029	0	910	68	0
31	j9	1029	0	910	69	0
31	jA	1029	0	910	74	0
31	jC	1029	0	910	68	0
31	jH	1029	0	910	68	0
31	jI	1029	0	910	68	0
31	jJ	1029	0	910	71	0
31	l2	1059	0	921	99	0
31	l3	1059	0	921	81	0
31	l5	1059	0	921	83	0
31	l6	1059	0	921	83	0
31	l7	1059	0	921	82	0
31	l8	1059	0	921	81	0
31	l9	1059	0	921	87	0
31	lA	1059	0	921	83	0
31	lC	1059	0	921	80	0
31	lH	1059	0	921	82	0
31	lI	1059	0	921	91	0
31	lJ	1059	0	921	82	0
32	c2	1076	0	915	106	0
32	c3	1076	0	915	78	0
32	c5	1076	0	915	67	0
32	c6	1076	0	915	83	0
32	c7	1076	0	915	86	0
32	c8	1076	0	915	67	0
32	c9	1076	0	915	118	0
32	cA	1076	0	915	79	0
32	cC	1076	0	915	77	0
32	cH	1076	0	915	67	0
32	cI	1073	0	913	119	0
32	cJ	1076	0	915	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	e2	1063	0	901	70	0
32	e3	1063	0	901	71	0
32	e5	1063	0	902	62	0
32	e6	1063	0	901	72	0
32	e7	1063	0	901	72	0
32	e8	1063	0	902	62	0
32	e9	1063	0	901	69	0
32	eA	1063	0	901	71	0
32	eC	1063	0	901	69	0
32	eH	1063	0	902	62	0
32	eI	1063	0	901	71	0
32	eJ	1063	0	902	63	0
32	g2	1088	0	952	94	0
32	g3	1088	0	952	85	0
32	g5	1088	0	952	86	0
32	g6	1088	0	952	86	0
32	g7	1088	0	952	94	0
32	g8	1088	0	952	77	0
32	g9	1088	0	952	95	0
32	gA	1088	0	952	88	0
32	gC	1088	0	952	86	0
32	gH	1088	0	952	80	0
32	gI	1085	0	948	97	0
32	gJ	1088	0	952	79	0
32	i2	1086	0	939	99	0
32	i3	1086	0	939	98	0
32	i5	1086	0	939	97	0
32	i6	1086	0	939	99	0
32	i7	1086	0	939	96	0
32	i8	1086	0	939	97	0
32	i9	1086	0	939	99	0
32	iA	1086	0	939	98	0
32	iC	1086	0	939	96	0
32	iH	1086	0	939	95	0
32	iI	1086	0	939	97	0
32	iJ	1086	0	939	94	0
32	k2	1103	0	971	101	0
32	k3	1103	0	971	99	0
32	k5	1103	0	971	96	0
32	k6	1103	0	971	99	0
32	k7	1103	0	971	100	0
32	k8	1103	0	971	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	k9	1103	0	971	96	0
32	kA	1103	0	971	98	0
32	kC	1103	0	971	98	0
32	kH	1103	0	971	100	0
32	kI	1103	0	971	102	0
32	kJ	1103	0	971	102	0
32	m2	1098	0	968	82	0
32	m3	1098	0	968	81	0
32	m5	1098	0	968	84	0
32	m6	1098	0	968	82	0
32	m7	1098	0	968	82	0
32	m8	1098	0	968	84	0
32	m9	1098	0	968	82	0
32	mA	1098	0	968	83	0
32	mC	1098	0	968	81	0
32	mH	1098	0	968	83	0
32	mI	1098	0	968	83	0
32	mJ	1098	0	968	81	0
33	1G	43	0	34	3	0
33	1L	43	0	34	4	0
33	2G	43	0	35	1	0
33	2L	43	0	35	1	0
33	3F	43	0	34	3	0
33	3K	43	0	34	4	0
33	4G	43	0	37	0	0
33	4L	43	0	37	0	0
33	5G	43	0	38	3	0
33	5L	43	0	38	3	0
33	6G	43	0	37	15	0
33	6L	43	0	37	15	0
33	7G	43	0	33	2	0
33	7L	43	0	33	2	0
33	9F	43	0	37	1	0
33	9K	43	0	37	1	0
33	AG	43	0	36	3	0
33	AL	43	0	36	4	0
33	B4	86	0	73	9	0
33	BB	86	0	73	10	0
33	C4	43	0	37	1	0
33	CB	43	0	37	1	0
33	GG	43	0	38	1	0
33	GL	43	0	38	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	HG	43	0	36	2	0
33	HL	43	0	36	2	0
33	IF	43	0	34	2	0
33	IG	43	0	37	34	0
33	IK	43	0	34	2	0
33	IL	43	0	37	26	0
33	JF	43	0	34	20	0
33	JG	43	0	34	3	0
33	JK	43	0	34	23	0
33	JL	43	0	34	3	0
33	KF	43	0	33	3	0
33	KG	43	0	33	0	0
33	KK	43	0	33	3	0
33	KL	43	0	33	0	0
33	LF	43	0	34	2	0
33	LG	43	0	36	3	0
33	LK	43	0	34	2	0
33	LL	43	0	36	1	0
33	MF	43	0	33	25	0
33	MG	43	0	38	6	0
33	MK	43	0	33	25	0
33	ML	43	0	38	6	0
33	NG	43	0	35	7	0
33	NL	43	0	35	8	0
33	O4	43	0	32	2	0
33	OB	43	0	32	2	0
33	OG	43	0	35	8	0
33	OL	43	0	35	8	0
33	P4	43	0	33	2	0
33	PB	43	0	33	2	0
33	PG	43	0	38	3	0
33	PL	43	0	38	3	0
33	Q4	43	0	34	2	0
33	QB	43	0	34	2	0
33	QG	43	0	36	1	0
33	QL	43	0	36	1	0
33	R4	43	0	37	3	0
33	RB	43	0	37	3	0
33	RG	43	0	36	2	0
33	RL	43	0	36	2	0
33	S4	43	0	36	0	0
33	SB	43	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	SG	43	0	33	1	0
33	SL	43	0	33	1	0
33	T4	43	0	37	2	0
33	TB	43	0	37	2	0
33	TG	43	0	38	2	0
33	TL	43	0	38	2	0
33	V4	43	0	34	29	0
33	VB	43	0	32	22	0
33	VG	43	0	37	2	0
33	VL	43	0	37	2	0
33	W4	43	0	34	3	0
33	WB	43	0	34	3	0
33	WG	43	0	36	1	0
33	WL	43	0	36	1	0
33	X4	43	0	33	1	0
33	XB	43	0	33	1	0
33	XF	43	0	36	0	0
33	XK	43	0	36	1	0
33	Y4	43	0	33	3	0
33	YB	43	0	33	3	0
33	YF	43	0	35	53	0
33	YK	43	0	35	52	0
33	Z4	43	0	37	1	0
33	ZB	43	0	37	1	0
33	ZF	43	0	37	16	0
33	ZK	43	0	37	16	0
33	a4	43	0	30	3	0
33	aB	43	0	30	3	0
33	aF	43	0	34	2	0
33	aK	43	0	34	2	0
33	b2	43	0	38	10	0
33	b3	43	0	38	10	0
33	b5	43	0	38	11	0
33	b6	43	0	38	10	0
33	b7	43	0	38	11	0
33	b8	43	0	38	10	0
33	b9	43	0	38	10	0
33	bA	43	0	38	10	0
33	bC	43	0	38	11	0
33	bF	43	0	37	1	0
33	bH	43	0	38	10	0
33	bI	43	0	38	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	bJ	43	0	38	10	0
33	bK	43	0	37	1	0
33	c2	86	0	73	36	0
33	c3	86	0	73	36	0
33	c5	86	0	73	32	0
33	c6	86	0	73	38	0
33	c7	86	0	73	37	0
33	c8	86	0	73	34	0
33	c9	86	0	73	38	0
33	cA	86	0	73	38	0
33	cC	86	0	73	38	0
33	cF	43	0	37	2	0
33	cH	86	0	73	36	0
33	cI	86	0	73	38	0
33	cJ	86	0	73	33	0
33	cK	43	0	37	2	0
33	d2	43	0	38	6	0
33	d3	43	0	38	6	0
33	d5	43	0	38	6	0
33	d6	43	0	38	5	0
33	d7	43	0	38	6	0
33	d8	43	0	38	6	0
33	d9	43	0	38	6	0
33	dA	43	0	38	6	0
33	dC	43	0	38	6	0
33	dF	43	0	33	1	0
33	dH	43	0	38	6	0
33	dI	43	0	38	6	0
33	dJ	43	0	38	6	0
33	dK	43	0	33	1	0
33	e2	86	0	74	34	0
33	e3	86	0	74	34	0
33	e5	86	0	74	33	0
33	e6	86	0	74	35	0
33	e7	86	0	74	34	0
33	e8	86	0	74	34	0
33	e9	86	0	74	33	0
33	eA	86	0	74	33	0
33	eC	86	0	74	33	0
33	eF	43	0	35	1	0
33	eH	86	0	74	34	0
33	eI	86	0	74	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	eJ	86	0	74	35	0
33	eK	43	0	35	2	0
33	f2	43	0	37	3	0
33	f3	43	0	37	3	0
33	f5	43	0	37	3	0
33	f6	43	0	37	3	0
33	f7	43	0	37	3	0
33	f8	43	0	37	3	0
33	f9	43	0	37	3	0
33	fA	43	0	37	3	0
33	fC	43	0	37	3	0
33	fF	43	0	33	2	0
33	fH	43	0	37	4	0
33	fI	43	0	37	3	0
33	fJ	43	0	37	3	0
33	fK	43	0	33	2	0
33	g2	86	0	73	41	0
33	g3	86	0	73	41	0
33	g5	86	0	73	34	0
33	g6	86	0	73	44	0
33	g7	86	0	73	42	0
33	g8	86	0	73	33	0
33	g9	86	0	73	42	0
33	gA	86	0	73	40	0
33	gC	86	0	73	40	0
33	gF	43	0	36	1	0
33	gH	86	0	73	34	0
33	gI	86	0	73	43	0
33	gJ	86	0	73	33	0
33	gK	43	0	36	1	0
33	h2	43	0	38	12	0
33	h3	43	0	38	14	0
33	h5	43	0	38	12	0
33	h6	43	0	38	15	0
33	h7	43	0	38	14	0
33	h8	43	0	38	15	0
33	h9	43	0	38	14	0
33	hA	43	0	38	14	0
33	hC	43	0	38	13	0
33	hF	43	0	37	55	0
33	hH	43	0	38	13	0
33	hI	43	0	38	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	hJ	43	0	38	12	0
33	hK	43	0	37	54	0
33	i2	86	0	76	39	0
33	i3	86	0	76	41	0
33	i5	86	0	76	40	0
33	i6	86	0	76	40	0
33	i7	86	0	76	39	0
33	i8	86	0	76	41	0
33	i9	86	0	76	40	0
33	iA	86	0	76	40	0
33	iC	86	0	76	38	0
33	iH	86	0	76	39	0
33	iI	86	0	76	39	0
33	iJ	86	0	76	38	0
33	j2	86	0	74	41	0
33	j3	86	0	74	41	0
33	j5	86	0	74	40	0
33	j6	86	0	74	44	0
33	j7	86	0	74	44	0
33	j8	86	0	74	42	0
33	j9	86	0	74	43	0
33	jA	86	0	74	42	0
33	jC	86	0	74	42	0
33	jF	43	0	37	0	0
33	jH	86	0	74	43	0
33	jI	86	0	74	41	0
33	jJ	86	0	74	41	0
33	jK	43	0	37	0	0
33	k2	43	0	38	9	0
33	k3	43	0	38	10	0
33	k5	43	0	38	9	0
33	k6	43	0	38	9	0
33	k7	43	0	38	11	0
33	k8	43	0	38	10	0
33	k9	43	0	38	11	0
33	kA	43	0	38	9	0
33	kC	43	0	38	9	0
33	kF	43	0	37	2	0
33	kH	43	0	38	11	0
33	kI	43	0	38	11	0
33	kJ	43	0	38	10	0
33	kK	43	0	37	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	l2	43	0	38	7	0
33	l3	43	0	38	7	0
33	l5	43	0	38	7	0
33	l6	43	0	38	7	0
33	l7	43	0	38	7	0
33	l8	43	0	38	6	0
33	l9	43	0	38	7	0
33	lA	43	0	38	7	0
33	lC	43	0	38	6	0
33	lH	43	0	38	7	0
33	lI	43	0	38	7	0
33	lJ	43	0	38	7	0
33	m2	43	0	38	36	0
33	m3	43	0	38	37	0
33	m5	43	0	38	37	0
33	m6	43	0	38	38	0
33	m7	43	0	38	38	0
33	m8	43	0	38	37	0
33	m9	43	0	38	38	0
33	mA	43	0	38	37	0
33	mC	43	0	38	38	0
33	mF	43	0	37	2	0
33	mH	43	0	38	38	0
33	mI	43	0	38	38	0
33	mJ	43	0	38	38	0
33	mK	43	0	37	2	0
33	nF	86	0	74	4	0
33	nK	86	0	74	4	0
33	o4	43	0	36	1	0
33	oB	43	0	36	1	0
33	p4	43	0	34	1	0
33	pB	43	0	34	1	0
33	q4	43	0	35	4	0
33	qB	43	0	35	3	0
33	r4	43	0	37	0	0
33	rB	43	0	37	1	0
33	s4	43	0	37	4	0
33	sB	43	0	37	4	0
33	t4	43	0	36	1	0
33	tB	43	0	36	1	0
33	u4	43	0	34	4	0
33	uB	43	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	v4	43	0	32	1	0
33	vB	43	0	32	1	0
33	w4	43	0	36	0	0
33	wB	43	0	36	0	0
33	y4	43	0	37	4	0
33	yB	43	0	37	4	0
33	z4	43	0	37	1	0
33	zB	43	0	37	1	0
34	A1	10	0	0	0	0
34	AD	10	0	0	0	0
34	AE	10	0	0	0	0
34	a1	10	0	0	0	0
34	aD	10	0	0	0	0
34	aE	10	0	0	0	0
35	A1	2	0	0	2	0
35	AD	2	0	0	2	0
35	AE	2	0	0	3	0
35	a1	2	0	0	1	0
35	aD	2	0	0	1	0
35	aE	2	0	0	1	0
36	A1	111	0	105	6	0
36	AD	111	0	105	6	0
36	AE	111	0	105	6	0
36	B1	885	0	946	50	0
36	BD	885	0	946	52	0
36	BE	885	0	946	52	0
36	C1	820	0	873	37	0
36	CD	820	0	873	40	0
36	CE	820	0	873	35	0
36	D1	130	0	144	5	0
36	DD	130	0	144	6	0
36	DE	130	0	144	5	0
36	H1	125	0	131	6	0
36	HD	125	0	131	8	0
36	HE	125	0	131	6	0
36	I1	60	0	56	1	0
36	ID	60	0	56	1	0
36	IE	60	0	56	1	0
36	X1	65	0	71	2	0
36	XD	65	0	71	2	0
36	XE	65	0	71	2	0
36	a1	171	0	164	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	aD	171	0	164	19	0
36	aE	171	0	164	19	0
36	b1	820	0	871	33	0
36	bD	820	0	871	35	0
36	bE	820	0	871	30	0
36	c1	820	0	874	55	0
36	cD	765	0	825	63	0
36	cE	765	0	824	38	0
36	d1	195	0	216	20	0
36	dD	195	0	216	24	0
36	dE	195	0	216	24	0
36	h1	125	0	131	8	0
36	hD	125	0	131	7	0
36	hE	125	0	131	6	0
36	iD	55	0	49	3	0
36	iE	55	0	49	3	0
36	x1	65	0	71	7	0
36	xD	65	0	71	7	0
36	xE	65	0	71	7	0
37	A1	55	0	80	3	0
37	AD	55	0	80	4	0
37	AE	55	0	80	2	0
37	D1	55	0	78	4	0
37	DD	55	0	78	4	0
37	DE	55	0	78	3	0
37	a1	55	0	80	3	0
37	aD	55	0	80	1	0
37	aE	55	0	80	2	0
37	d1	55	0	78	3	0
37	dD	55	0	78	3	0
37	dE	55	0	78	5	0
38	A1	46	0	59	6	0
38	AD	46	0	59	6	0
38	AE	46	0	59	7	0
38	B1	38	0	40	1	0
38	BD	38	0	40	1	0
38	BE	38	0	40	1	0
38	C1	54	0	77	0	0
38	CD	54	0	77	0	0
38	CE	54	0	77	0	0
38	D1	34	0	31	1	0
38	DD	34	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	DE	34	0	31	1	0
38	L1	86	0	100	9	0
38	LD	86	0	100	10	0
38	LE	86	0	100	9	0
38	c1	54	0	77	0	0
38	cD	54	0	77	0	0
38	cE	54	0	77	1	0
38	d1	34	0	31	1	0
38	dD	34	0	31	1	0
38	dE	34	0	31	1	0
38	h1	35	0	32	2	0
38	hD	35	0	32	2	0
38	hE	35	0	32	2	0
39	A1	36	0	42	6	0
39	AD	36	0	42	7	0
39	AE	36	0	42	7	0
39	B1	51	0	71	3	0
39	BD	51	0	71	3	0
39	BE	51	0	71	3	0
39	C1	102	0	142	1	0
39	CD	102	0	142	1	0
39	CE	102	0	142	1	0
39	D1	51	0	71	1	0
39	DD	51	0	71	1	0
39	DE	51	0	71	1	0
39	J1	27	0	24	0	0
39	JD	27	0	24	0	0
39	JE	27	0	24	0	0
39	M1	36	0	42	0	0
39	MD	36	0	42	0	0
39	ME	36	0	42	0	0
39	T1	36	0	42	1	0
39	TD	36	0	42	1	0
39	TE	36	0	42	1	0
39	a1	87	0	114	4	0
39	aD	87	0	114	4	0
39	aE	87	0	114	4	0
39	b1	51	0	71	2	0
39	bD	51	0	71	2	0
39	bE	51	0	71	2	0
39	d1	51	0	71	13	0
39	dD	51	0	71	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	dE	51	0	71	13	0
39	j1	27	0	24	1	0
39	jD	27	0	24	1	0
39	jE	27	0	24	1	0
39	m1	36	0	42	10	0
39	mD	36	0	42	10	0
39	mE	36	0	42	10	0
39	t1	36	0	42	5	0
39	tD	36	0	42	5	0
39	tE	36	0	42	5	0
39	y1	51	0	71	8	0
39	yD	51	0	71	8	0
39	yE	51	0	71	8	0
40	A1	59	0	79	0	0
40	AD	59	0	79	0	0
40	AE	59	0	80	0	0
40	B1	72	0	103	23	0
40	BD	83	0	115	31	0
40	BE	83	0	115	40	0
40	C1	24	0	34	15	0
40	CD	24	0	33	23	0
40	D1	71	0	93	5	0
40	DD	71	0	93	5	0
40	DE	71	0	93	5	0
40	a1	35	0	46	1	0
40	b1	83	0	113	3	0
40	bD	83	0	113	3	0
40	bE	107	0	147	3	0
40	cD	24	0	33	33	0
40	cE	24	0	34	19	0
40	d1	71	0	94	8	0
40	dD	71	0	94	8	0
40	dE	71	0	94	8	0
40	i1	24	0	34	0	0
40	iD	24	0	34	0	0
40	iE	24	0	34	0	0
40	j1	35	0	45	1	0
40	jD	35	0	45	1	0
40	jE	35	0	45	1	0
41	A1	4	0	1	0	0
41	AD	4	0	1	0	0
41	AE	4	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	a1	4	0	1	1	0
41	aD	4	0	1	0	0
41	aE	4	0	1	0	0
42	A1	38	0	46	1	0
42	AD	38	0	46	1	0
42	AE	38	0	46	3	0
42	B1	49	0	74	3	0
42	BD	49	0	74	3	0
42	BE	49	0	74	4	0
42	D1	98	0	148	5	0
42	DD	98	0	148	5	0
42	DE	98	0	148	5	0
42	a1	38	0	46	6	0
42	aD	38	0	46	6	0
42	aE	38	0	46	6	0
42	d1	98	0	148	3	0
42	dD	98	0	148	3	0
42	dE	98	0	148	3	0
42	e1	40	0	53	1	0
42	eD	40	0	53	1	0
42	eE	40	0	53	1	0
42	l1	49	0	74	3	0
42	lD	49	0	74	3	0
42	lE	49	0	74	1	0
43	B1	120	0	163	15	0
43	BD	120	0	163	13	0
43	BE	120	0	163	12	0
43	C1	80	0	103	6	0
43	CD	120	0	159	9	0
43	CE	80	0	103	5	0
43	D1	40	0	56	1	0
43	DD	40	0	56	1	0
43	DE	40	0	56	1	0
43	I1	40	0	53	5	0
43	ID	40	0	53	6	0
43	IE	40	0	53	7	0
43	X1	40	0	50	4	0
43	XD	40	0	50	3	0
43	XE	40	0	50	3	0
43	Z1	80	0	111	3	0
43	ZD	40	0	55	3	0
43	ZE	80	0	111	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	b1	120	0	163	15	0
43	bD	120	0	163	14	0
43	bE	120	0	163	13	0
43	c1	80	0	105	36	0
43	cD	80	0	105	32	0
43	cE	80	0	105	37	0
43	d1	40	0	56	2	0
43	dD	40	0	56	2	0
43	dE	40	0	56	2	0
43	h1	40	0	49	3	0
43	hD	40	0	49	3	0
43	hE	40	0	49	3	0
43	i1	40	0	56	11	0
43	iD	40	0	56	11	0
43	iE	40	0	56	11	0
43	k1	40	0	56	4	0
43	kD	40	0	56	5	0
43	kE	40	0	56	2	0
43	z1	40	0	55	1	0
43	zD	40	0	55	2	0
43	zE	40	0	55	2	0
44	C1	109	0	133	5	0
44	CD	109	0	133	5	0
44	CE	109	0	133	6	0
44	H1	62	0	82	5	0
44	HD	62	0	82	6	0
44	HE	62	0	82	5	0
44	J1	62	0	82	2	0
44	JD	62	0	82	2	0
44	JE	62	0	82	2	0
44	c1	171	0	215	10	0
44	cD	171	0	215	10	0
44	cE	171	0	215	11	0
44	h1	62	0	82	4	0
44	hD	62	0	82	4	0
44	hE	62	0	82	4	0
45	A1	64	0	71	1	0
45	D1	64	0	72	3	0
45	DD	122	0	126	34	0
45	DE	128	0	143	22	0
45	a1	52	0	47	6	0
45	aD	64	0	71	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	aE	56	0	54	5	0
45	d1	64	0	72	3	0
45	dD	52	0	46	9	0
45	dE	56	0	52	7	0
46	D1	1	0	0	0	0
46	DD	1	0	0	0	0
46	DE	1	0	0	0	0
46	d1	1	0	0	0	0
46	dD	1	0	0	0	0
46	dE	1	0	0	0	0
47	E1	43	0	30	0	0
47	ED	43	0	30	0	0
47	EE	43	0	30	0	0
47	V1	43	0	30	2	0
47	VD	43	0	30	2	0
47	VE	43	0	30	2	0
47	f1	43	0	30	0	0
47	fD	43	0	30	0	0
47	fE	43	0	30	0	0
47	v1	43	0	30	2	0
47	vD	43	0	30	2	0
47	vE	43	0	30	2	0
48	K1	1	0	0	0	0
48	KD	1	0	0	0	0
48	KE	1	0	0	0	0
48	U1	1	0	0	0	0
48	UD	1	0	0	0	0
48	UE	1	0	0	0	0
48	V1	1	0	0	0	0
48	VD	1	0	0	0	0
48	VE	1	0	0	0	0
48	k1	1	0	0	0	0
48	kD	1	0	0	0	0
48	kE	1	0	0	0	0
48	u1	1	0	0	0	0
48	uD	1	0	0	0	0
48	uE	1	0	0	0	0
48	v1	1	0	0	0	0
48	vD	1	0	0	0	0
48	vE	1	0	0	0	0
All	All	552008	0	531827	27775	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 26.

The worst 5 of 27775 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)
32:mC:153:CYS:SG	33:mC:201:CYC:HAC2	1.19	1.76
32:mH:153:CYS:SG	33:mH:201:CYC:HAC2	1.19	1.75
32:m9:153:CYS:SG	33:m9:201:CYC:HAC2	1.19	1.74
32:m7:153:CYS:SG	33:m7:201:CYC:HAC2	1.19	1.73
40:B1:623:LMT:H11	13:i1:1:MET:SD	1.26	1.70

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	B2	238/254 (94%)	215 (90%)	14 (6%)	9 (4%)	2 20
1	B3	238/254 (94%)	218 (92%)	10 (4%)	10 (4%)	2 19
1	B5	238/254 (94%)	215 (90%)	13 (6%)	10 (4%)	2 19
1	B6	238/254 (94%)	216 (91%)	16 (7%)	6 (2%)	4 28
1	B7	238/254 (94%)	214 (90%)	12 (5%)	12 (5%)	1 15
1	B8	238/254 (94%)	215 (90%)	13 (6%)	10 (4%)	2 19
1	B9	238/254 (94%)	213 (90%)	18 (8%)	7 (3%)	3 26
1	BA	238/254 (94%)	223 (94%)	8 (3%)	7 (3%)	3 26
1	BC	238/254 (94%)	217 (91%)	10 (4%)	11 (5%)	2 17
1	BH	238/254 (94%)	215 (90%)	13 (6%)	10 (4%)	2 19
1	BI	238/254 (94%)	212 (89%)	17 (7%)	9 (4%)	2 20
1	BJ	238/254 (94%)	215 (90%)	13 (6%)	10 (4%)	2 19
2	B4	884/914 (97%)	806 (91%)	70 (8%)	8 (1%)	14 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	BB	884/914 (97%)	806 (91%)	68 (8%)	10 (1%)	11 43
2	C4	862/914 (94%)	799 (93%)	61 (7%)	2 (0%)	43 74
2	CB	862/914 (94%)	798 (93%)	62 (7%)	2 (0%)	43 74
3	4G	158/161 (98%)	152 (96%)	6 (4%)	0	100 100
3	4L	158/161 (98%)	152 (96%)	6 (4%)	0	100 100
3	6G	158/161 (98%)	152 (96%)	6 (4%)	0	100 100
3	6L	158/161 (98%)	153 (97%)	5 (3%)	0	100 100
3	9F	158/161 (98%)	151 (96%)	7 (4%)	0	100 100
3	9K	158/161 (98%)	151 (96%)	7 (4%)	0	100 100
3	AG	158/161 (98%)	150 (95%)	8 (5%)	0	100 100
3	AL	158/161 (98%)	150 (95%)	8 (5%)	0	100 100
3	GG	158/161 (98%)	154 (98%)	4 (2%)	0	100 100
3	GL	158/161 (98%)	154 (98%)	4 (2%)	0	100 100
3	IG	158/161 (98%)	149 (94%)	9 (6%)	0	100 100
3	IL	158/161 (98%)	149 (94%)	8 (5%)	1 (1%)	21 54
3	JF	158/161 (98%)	150 (95%)	8 (5%)	0	100 100
3	JK	158/161 (98%)	150 (95%)	8 (5%)	0	100 100
3	KG	158/161 (98%)	152 (96%)	6 (4%)	0	100 100
3	KL	158/161 (98%)	152 (96%)	6 (4%)	0	100 100
3	LF	158/161 (98%)	152 (96%)	6 (4%)	0	100 100
3	LK	158/161 (98%)	152 (96%)	6 (4%)	0	100 100
3	NG	158/161 (98%)	154 (98%)	4 (2%)	0	100 100
3	NL	158/161 (98%)	154 (98%)	4 (2%)	0	100 100
3	O4	158/161 (98%)	150 (95%)	8 (5%)	0	100 100
3	OB	158/161 (98%)	150 (95%)	8 (5%)	0	100 100
3	PG	158/161 (98%)	155 (98%)	3 (2%)	0	100 100
3	PL	158/161 (98%)	155 (98%)	3 (2%)	0	100 100
3	Q4	158/161 (98%)	156 (99%)	2 (1%)	0	100 100
3	QB	158/161 (98%)	156 (99%)	2 (1%)	0	100 100
3	RG	158/161 (98%)	151 (96%)	7 (4%)	0	100 100
3	RL	158/161 (98%)	151 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S4	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
3	SB	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
3	TG	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	TL	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	V4	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
3	VB	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
3	X4	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	XB	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	XF	158/161 (98%)	156 (99%)	1 (1%)	1 (1%)	21	54
3	XK	158/161 (98%)	156 (99%)	1 (1%)	1 (1%)	21	54
3	Z4	158/161 (98%)	148 (94%)	10 (6%)	0	100	100
3	ZB	158/161 (98%)	148 (94%)	10 (6%)	0	100	100
3	ZF	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
3	ZK	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
3	bF	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	bK	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	dF	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
3	dK	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
3	fF	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
3	fK	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
3	iF	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
3	iK	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
3	kF	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	kK	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	o4	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
3	oB	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
3	q4	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	qB	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
3	s4	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	21	54
3	sB	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	21	54
3	u4	158/161 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	uB	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	w4	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	wB	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	y4	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
3	yB	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
4	1G	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
4	1L	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
4	5G	159/161 (99%)	148 (93%)	11 (7%)	0	100	100
4	5L	159/161 (99%)	148 (93%)	11 (7%)	0	100	100
4	7G	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	7L	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	HG	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	HL	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	IF	159/161 (99%)	149 (94%)	9 (6%)	1 (1%)	21	54
4	IK	159/161 (99%)	148 (93%)	10 (6%)	1 (1%)	21	54
4	JG	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	JL	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	KF	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	KK	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	LG	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	LL	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	MF	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	MG	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
4	MK	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	ML	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
4	OG	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	OL	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	P4	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	PB	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	R4	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	RB	159/161 (99%)	151 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	SG	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
4	SL	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
4	T4	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	TB	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	UG	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
4	UL	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
4	W4	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	WB	159/161 (99%)	153 (96%)	5 (3%)	1 (1%)	21	54
4	WG	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	WL	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	Y4	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	YB	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	YF	159/161 (99%)	153 (96%)	5 (3%)	1 (1%)	21	54
4	YK	159/161 (99%)	153 (96%)	5 (3%)	1 (1%)	21	54
4	a4	158/161 (98%)	141 (89%)	13 (8%)	4 (2%)	4	28
4	aB	158/161 (98%)	139 (88%)	12 (8%)	7 (4%)	2	17
4	aF	159/161 (99%)	150 (94%)	8 (5%)	1 (1%)	21	54
4	aK	159/161 (99%)	150 (94%)	8 (5%)	1 (1%)	21	54
4	cF	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	cK	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	eF	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	eK	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	hF	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	hK	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	jF	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	jK	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	lF	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
4	lK	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
4	nF	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	nK	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
4	p4	159/161 (99%)	154 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	pB	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
4	r4	159/161 (99%)	149 (94%)	10 (6%)	0	100	100
4	rB	159/161 (99%)	149 (94%)	10 (6%)	0	100	100
4	t4	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	tB	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
4	v4	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	vB	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	x4	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	xB	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	z4	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
4	zB	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
5	2G	63/67 (94%)	54 (86%)	9 (14%)	0	100	100
5	2L	63/67 (94%)	54 (86%)	9 (14%)	0	100	100
5	3F	63/67 (94%)	56 (89%)	7 (11%)	0	100	100
5	3K	63/67 (94%)	56 (89%)	7 (11%)	0	100	100
5	8G	63/67 (94%)	56 (89%)	7 (11%)	0	100	100
5	8L	63/67 (94%)	56 (89%)	7 (11%)	0	100	100
5	NF	64/67 (96%)	54 (84%)	10 (16%)	0	100	100
5	NK	64/67 (96%)	54 (84%)	10 (16%)	0	100	100
5	U4	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
5	UB	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
5	b4	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
5	bB	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
6	A1	332/359 (92%)	300 (90%)	32 (10%)	0	100	100
6	AD	332/359 (92%)	300 (90%)	32 (10%)	0	100	100
6	AE	332/359 (92%)	300 (90%)	32 (10%)	0	100	100
6	a1	332/359 (92%)	305 (92%)	26 (8%)	1 (0%)	36	67
6	aD	332/359 (92%)	305 (92%)	26 (8%)	1 (0%)	36	67
6	aE	332/359 (92%)	305 (92%)	26 (8%)	1 (0%)	36	67
7	B1	500/509 (98%)	454 (91%)	44 (9%)	2 (0%)	30	62
7	BD	500/509 (98%)	454 (91%)	44 (9%)	2 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BE	500/509 (98%)	454 (91%)	44 (9%)	2 (0%)	30	62
7	b1	502/509 (99%)	450 (90%)	48 (10%)	4 (1%)	16	49
7	bD	502/509 (99%)	450 (90%)	48 (10%)	4 (1%)	16	49
7	bE	502/509 (99%)	450 (90%)	48 (10%)	4 (1%)	16	49
8	C1	448/469 (96%)	408 (91%)	37 (8%)	3 (1%)	18	51
8	CD	448/469 (96%)	411 (92%)	36 (8%)	1 (0%)	43	74
8	CE	448/469 (96%)	411 (92%)	36 (8%)	1 (0%)	43	74
8	c1	451/469 (96%)	390 (86%)	49 (11%)	12 (3%)	4	27
8	cD	451/469 (96%)	384 (85%)	56 (12%)	11 (2%)	4	29
8	cE	451/469 (96%)	392 (87%)	49 (11%)	10 (2%)	5	30
9	D1	339/352 (96%)	302 (89%)	36 (11%)	1 (0%)	36	67
9	DD	339/352 (96%)	302 (89%)	36 (11%)	1 (0%)	36	67
9	DE	339/352 (96%)	302 (89%)	36 (11%)	1 (0%)	36	67
9	d1	339/352 (96%)	300 (88%)	34 (10%)	5 (2%)	8	37
9	dD	339/352 (96%)	301 (89%)	33 (10%)	5 (2%)	8	37
9	dE	339/352 (96%)	301 (89%)	33 (10%)	5 (2%)	8	37
10	E1	76/82 (93%)	67 (88%)	9 (12%)	0	100	100
10	ED	76/82 (93%)	67 (88%)	9 (12%)	0	100	100
10	EE	76/82 (93%)	66 (87%)	10 (13%)	0	100	100
10	e1	76/82 (93%)	69 (91%)	7 (9%)	0	100	100
10	eD	76/82 (93%)	69 (91%)	7 (9%)	0	100	100
10	eE	76/82 (93%)	69 (91%)	7 (9%)	0	100	100
11	F1	33/44 (75%)	31 (94%)	2 (6%)	0	100	100
11	FD	33/44 (75%)	31 (94%)	2 (6%)	0	100	100
11	FE	33/44 (75%)	31 (94%)	2 (6%)	0	100	100
11	f1	33/44 (75%)	31 (94%)	2 (6%)	0	100	100
11	fD	35/44 (80%)	33 (94%)	2 (6%)	0	100	100
11	fE	33/44 (75%)	30 (91%)	2 (6%)	1 (3%)	3	25
12	H1	62/67 (92%)	55 (89%)	7 (11%)	0	100	100
12	HD	62/67 (92%)	55 (89%)	7 (11%)	0	100	100
12	HE	62/67 (92%)	54 (87%)	8 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	h1	62/67 (92%)	51 (82%)	11 (18%)	0	100	100
12	hD	62/67 (92%)	51 (82%)	11 (18%)	0	100	100
12	hE	62/67 (92%)	51 (82%)	11 (18%)	0	100	100
13	I1	34/38 (90%)	27 (79%)	1 (3%)	6 (18%)	0	1
13	ID	34/38 (90%)	27 (79%)	1 (3%)	6 (18%)	0	1
13	IE	34/38 (90%)	27 (79%)	1 (3%)	6 (18%)	0	1
13	i1	34/38 (90%)	29 (85%)	4 (12%)	1 (3%)	3	26
13	iD	34/38 (90%)	29 (85%)	4 (12%)	1 (3%)	3	26
13	iE	34/38 (90%)	29 (85%)	4 (12%)	1 (3%)	3	26
14	J1	35/39 (90%)	35 (100%)	0	0	100	100
14	JD	35/39 (90%)	35 (100%)	0	0	100	100
14	JE	35/39 (90%)	35 (100%)	0	0	100	100
14	j1	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
14	jD	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
14	jE	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
15	K1	34/45 (76%)	26 (76%)	8 (24%)	0	100	100
15	KD	34/45 (76%)	26 (76%)	8 (24%)	0	100	100
15	KE	34/45 (76%)	26 (76%)	8 (24%)	0	100	100
15	k1	33/45 (73%)	27 (82%)	2 (6%)	4 (12%)	0	4
15	kD	33/45 (73%)	27 (82%)	2 (6%)	4 (12%)	0	4
15	kE	33/45 (73%)	27 (82%)	2 (6%)	4 (12%)	0	4
16	L1	36/39 (92%)	33 (92%)	3 (8%)	0	100	100
16	LD	36/39 (92%)	33 (92%)	3 (8%)	0	100	100
16	LE	36/39 (92%)	33 (92%)	3 (8%)	0	100	100
16	l1	36/39 (92%)	33 (92%)	3 (8%)	0	100	100
16	lD	36/39 (92%)	33 (92%)	3 (8%)	0	100	100
16	lE	36/39 (92%)	33 (92%)	3 (8%)	0	100	100
17	M1	34/37 (92%)	26 (76%)	8 (24%)	0	100	100
17	MD	34/37 (92%)	26 (76%)	8 (24%)	0	100	100
17	ME	34/37 (92%)	26 (76%)	8 (24%)	0	100	100
17	m1	34/37 (92%)	27 (79%)	7 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	mD	34/37 (92%)	27 (79%)	7 (21%)	0	100	100
17	mE	34/37 (92%)	27 (79%)	7 (21%)	0	100	100
18	O1	241/278 (87%)	163 (68%)	73 (30%)	5 (2%)	5	31
18	OD	241/278 (87%)	163 (68%)	73 (30%)	5 (2%)	5	31
18	OE	241/278 (87%)	163 (68%)	73 (30%)	5 (2%)	5	31
18	o1	241/278 (87%)	164 (68%)	72 (30%)	5 (2%)	5	31
18	oD	241/278 (87%)	164 (68%)	72 (30%)	5 (2%)	5	31
18	oE	241/278 (87%)	164 (68%)	72 (30%)	5 (2%)	5	31
19	Q1	117/164 (71%)	104 (89%)	13 (11%)	0	100	100
19	QD	117/164 (71%)	104 (89%)	13 (11%)	0	100	100
19	QE	117/164 (71%)	104 (89%)	13 (11%)	0	100	100
19	q1	117/164 (71%)	104 (89%)	13 (11%)	0	100	100
19	qD	117/164 (71%)	103 (88%)	14 (12%)	0	100	100
19	qE	117/164 (71%)	104 (89%)	13 (11%)	0	100	100
20	R1	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
20	RD	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
20	RE	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
20	r1	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
20	rD	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
20	rE	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
22	T1	27/31 (87%)	23 (85%)	4 (15%)	0	100	100
22	TD	27/31 (87%)	23 (85%)	4 (15%)	0	100	100
22	TE	27/31 (87%)	23 (85%)	4 (15%)	0	100	100
22	t1	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
22	tD	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
22	tE	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
23	U1	93/95 (98%)	83 (89%)	10 (11%)	0	100	100
23	UD	93/95 (98%)	83 (89%)	10 (11%)	0	100	100
23	UE	93/95 (98%)	83 (89%)	10 (11%)	0	100	100
23	u1	93/95 (98%)	83 (89%)	10 (11%)	0	100	100
23	uD	93/95 (98%)	83 (89%)	10 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	uE	93/95 (98%)	83 (89%)	10 (11%)	0	100	100
24	V1	133/163 (82%)	123 (92%)	10 (8%)	0	100	100
24	VD	133/163 (82%)	123 (92%)	10 (8%)	0	100	100
24	VE	133/163 (82%)	123 (92%)	10 (8%)	0	100	100
24	v1	133/163 (82%)	121 (91%)	12 (9%)	0	100	100
24	vD	133/163 (82%)	121 (91%)	12 (9%)	0	100	100
24	vE	133/163 (82%)	121 (91%)	12 (9%)	0	100	100
25	X1	38/48 (79%)	36 (95%)	2 (5%)	0	100	100
25	XD	38/48 (79%)	36 (95%)	2 (5%)	0	100	100
25	XE	38/48 (79%)	36 (95%)	2 (5%)	0	100	100
25	x1	38/48 (79%)	36 (95%)	2 (5%)	0	100	100
25	xD	38/48 (79%)	36 (95%)	2 (5%)	0	100	100
25	xE	38/48 (79%)	36 (95%)	2 (5%)	0	100	100
26	Y1	30/43 (70%)	28 (93%)	2 (7%)	0	100	100
26	YD	30/43 (70%)	28 (93%)	2 (7%)	0	100	100
26	YE	30/43 (70%)	28 (93%)	2 (7%)	0	100	100
26	y1	30/43 (70%)	27 (90%)	2 (7%)	1 (3%)	3	23
26	yD	30/43 (70%)	27 (90%)	2 (7%)	1 (3%)	3	23
26	yE	30/43 (70%)	27 (90%)	2 (7%)	1 (3%)	3	23
27	Z1	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
27	ZD	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
27	ZE	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
27	z1	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
27	zD	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
27	zE	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
28	BG	44/150 (29%)	32 (73%)	7 (16%)	5 (11%)	0	5
28	BL	44/150 (29%)	32 (73%)	7 (16%)	5 (11%)	0	5
28	EF	44/150 (29%)	35 (80%)	7 (16%)	2 (4%)	2	17
28	EK	44/150 (29%)	35 (80%)	7 (16%)	2 (4%)	2	17
29	QG	167/169 (99%)	151 (90%)	12 (7%)	4 (2%)	4	29
29	QL	167/169 (99%)	151 (90%)	12 (7%)	4 (2%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	gF	167/169 (99%)	151 (90%)	14 (8%)	2 (1%)	10	41
29	gK	167/169 (99%)	151 (90%)	14 (8%)	2 (1%)	10	41
30	VG	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
30	VL	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
30	mF	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
30	mK	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
31	b2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	b3	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	b5	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	b6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	b7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	b8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	b9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	bA	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	bC	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	bH	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	bI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	bJ	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	d2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	d3	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	d5	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	d6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	d7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	d8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	d9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	dA	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	dC	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	dH	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	dI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	dJ	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	f2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	f3	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	f5	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	f6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	f7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	f8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	f9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	fA	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	fC	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	fH	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	fI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	fJ	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	h2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	h3	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	h5	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	h6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	h7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	h8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	h9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	hA	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	hC	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	hH	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	hI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	hJ	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	j2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	j3	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	j5	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	j6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	j7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	j8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	j9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	jA	160/162 (99%)	159 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	jC	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	jH	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	jI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	jJ	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	l2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	l3	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	l5	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	l6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	l7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	l8	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	l9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	lA	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	lC	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	lH	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	lI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
31	lJ	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
32	c2	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	c3	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	c5	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	c6	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	c7	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	c8	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	c9	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	cA	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	cC	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	cH	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	cI	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	cJ	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	41
32	e2	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	e3	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	e5	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	e6	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	e7	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	e8	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	e9	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	eA	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	eC	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	eH	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	eI	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	eJ	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	g2	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	g3	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	g5	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	g6	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	g7	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	g8	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	g9	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	gA	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	gC	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	gH	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	gI	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	gJ	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	54
32	i2	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	i3	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	i5	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	i6	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	i7	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	i8	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	i9	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	iA	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	iC	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	iH	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	iI	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	iJ	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	k2	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	k3	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	k5	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	k6	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	k7	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	k8	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	k9	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	kA	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	kC	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	kH	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	kI	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	kJ	170/172 (99%)	169 (99%)	0	1 (1%)	21	54
32	m2	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	m3	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	m5	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	m6	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	m7	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	m8	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	m9	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	mA	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	mC	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	mH	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	mI	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
32	mJ	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	54
All	All	69685/72752 (96%)	65802 (94%)	3473 (5%)	410 (1%)	23	54

5 of 410 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BA	207	VAL
1	BA	208	PRO

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Mol	Chain	Res	Type
1	BA	212	GLN
1	BA	213	PRO
1	BA	231	PRO

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	B2	208/225 (92%)	189 (91%)	19 (9%)	9 32
1	B3	208/225 (92%)	185 (89%)	23 (11%)	6 25
1	B5	190/225 (84%)	164 (86%)	26 (14%)	3 19
1	B6	209/225 (93%)	193 (92%)	16 (8%)	12 37
1	B7	209/225 (93%)	184 (88%)	25 (12%)	5 23
1	B8	189/225 (84%)	164 (87%)	25 (13%)	4 20
1	B9	209/225 (93%)	190 (91%)	19 (9%)	9 32
1	BA	210/225 (93%)	184 (88%)	26 (12%)	4 22
1	BC	209/225 (93%)	185 (88%)	24 (12%)	5 24
1	BH	189/225 (84%)	164 (87%)	25 (13%)	4 20
1	BI	206/225 (92%)	183 (89%)	23 (11%)	6 25
1	BJ	190/225 (84%)	164 (86%)	26 (14%)	3 19
2	B4	747/767 (97%)	727 (97%)	20 (3%)	39 62
2	BB	747/767 (97%)	727 (97%)	20 (3%)	39 62
2	C4	732/767 (95%)	723 (99%)	9 (1%)	63 73
2	CB	732/767 (95%)	723 (99%)	9 (1%)	63 73
3	4G	125/127 (98%)	125 (100%)	0	100 100
3	4L	125/127 (98%)	125 (100%)	0	100 100
3	6G	126/127 (99%)	123 (98%)	3 (2%)	43 64
3	6L	126/127 (99%)	123 (98%)	3 (2%)	43 64
3	9F	126/127 (99%)	126 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	9K	126/127 (99%)	126 (100%)	0	100	100
3	AG	126/127 (99%)	126 (100%)	0	100	100
3	AL	126/127 (99%)	126 (100%)	0	100	100
3	GG	126/127 (99%)	126 (100%)	0	100	100
3	GL	126/127 (99%)	126 (100%)	0	100	100
3	IG	125/127 (98%)	123 (98%)	2 (2%)	55	70
3	IL	125/127 (98%)	120 (96%)	5 (4%)	28	54
3	JF	125/127 (98%)	125 (100%)	0	100	100
3	JK	126/127 (99%)	125 (99%)	1 (1%)	73	77
3	KG	125/127 (98%)	125 (100%)	0	100	100
3	KL	125/127 (98%)	125 (100%)	0	100	100
3	LF	126/127 (99%)	126 (100%)	0	100	100
3	LK	126/127 (99%)	126 (100%)	0	100	100
3	NG	125/127 (98%)	125 (100%)	0	100	100
3	NL	125/127 (98%)	125 (100%)	0	100	100
3	O4	125/127 (98%)	125 (100%)	0	100	100
3	OB	124/127 (98%)	124 (100%)	0	100	100
3	PG	126/127 (99%)	125 (99%)	1 (1%)	73	77
3	PL	126/127 (99%)	125 (99%)	1 (1%)	73	77
3	Q4	126/127 (99%)	126 (100%)	0	100	100
3	QB	125/127 (98%)	125 (100%)	0	100	100
3	RG	126/127 (99%)	126 (100%)	0	100	100
3	RL	126/127 (99%)	126 (100%)	0	100	100
3	S4	126/127 (99%)	126 (100%)	0	100	100
3	SB	126/127 (99%)	126 (100%)	0	100	100
3	TG	125/127 (98%)	125 (100%)	0	100	100
3	TL	125/127 (98%)	125 (100%)	0	100	100
3	V4	125/127 (98%)	125 (100%)	0	100	100
3	VB	125/127 (98%)	125 (100%)	0	100	100
3	X4	123/127 (97%)	123 (100%)	0	100	100
3	XB	125/127 (98%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	XF	126/127 (99%)	125 (99%)	1 (1%)	73 77
3	XK	126/127 (99%)	125 (99%)	1 (1%)	73 77
3	Z4	126/127 (99%)	126 (100%)	0	100 100
3	ZB	126/127 (99%)	126 (100%)	0	100 100
3	ZF	126/127 (99%)	126 (100%)	0	100 100
3	ZK	126/127 (99%)	126 (100%)	0	100 100
3	bF	126/127 (99%)	126 (100%)	0	100 100
3	bK	126/127 (99%)	126 (100%)	0	100 100
3	dF	125/127 (98%)	125 (100%)	0	100 100
3	dK	125/127 (98%)	125 (100%)	0	100 100
3	fF	126/127 (99%)	126 (100%)	0	100 100
3	fK	126/127 (99%)	126 (100%)	0	100 100
3	iF	126/127 (99%)	126 (100%)	0	100 100
3	iK	126/127 (99%)	126 (100%)	0	100 100
3	kF	126/127 (99%)	126 (100%)	0	100 100
3	kK	126/127 (99%)	126 (100%)	0	100 100
3	o4	125/127 (98%)	124 (99%)	1 (1%)	73 77
3	oB	124/127 (98%)	124 (100%)	0	100 100
3	q4	124/127 (98%)	123 (99%)	1 (1%)	73 77
3	qB	124/127 (98%)	123 (99%)	1 (1%)	73 77
3	s4	126/127 (99%)	126 (100%)	0	100 100
3	sB	126/127 (99%)	126 (100%)	0	100 100
3	u4	124/127 (98%)	123 (99%)	1 (1%)	73 77
3	uB	124/127 (98%)	123 (99%)	1 (1%)	73 77
3	w4	123/127 (97%)	123 (100%)	0	100 100
3	wB	126/127 (99%)	124 (98%)	2 (2%)	55 70
3	y4	126/127 (99%)	126 (100%)	0	100 100
3	yB	126/127 (99%)	126 (100%)	0	100 100
4	1G	125/125 (100%)	125 (100%)	0	100 100
4	1L	125/125 (100%)	121 (97%)	4 (3%)	34 59
4	5G	125/125 (100%)	125 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	5L	125/125 (100%)	125 (100%)	0	100	100
4	7G	125/125 (100%)	125 (100%)	0	100	100
4	7L	125/125 (100%)	125 (100%)	0	100	100
4	HG	124/125 (99%)	124 (100%)	0	100	100
4	HL	124/125 (99%)	124 (100%)	0	100	100
4	IF	125/125 (100%)	125 (100%)	0	100	100
4	IK	125/125 (100%)	124 (99%)	1 (1%)	73	77
4	JG	125/125 (100%)	125 (100%)	0	100	100
4	JL	125/125 (100%)	125 (100%)	0	100	100
4	KF	125/125 (100%)	123 (98%)	2 (2%)	55	70
4	KK	125/125 (100%)	123 (98%)	2 (2%)	55	70
4	LG	125/125 (100%)	124 (99%)	1 (1%)	73	77
4	LL	125/125 (100%)	124 (99%)	1 (1%)	73	77
4	MF	125/125 (100%)	125 (100%)	0	100	100
4	MG	124/125 (99%)	124 (100%)	0	100	100
4	MK	125/125 (100%)	125 (100%)	0	100	100
4	ML	124/125 (99%)	124 (100%)	0	100	100
4	OG	125/125 (100%)	125 (100%)	0	100	100
4	OL	125/125 (100%)	125 (100%)	0	100	100
4	P4	125/125 (100%)	125 (100%)	0	100	100
4	PB	125/125 (100%)	125 (100%)	0	100	100
4	R4	125/125 (100%)	125 (100%)	0	100	100
4	RB	125/125 (100%)	125 (100%)	0	100	100
4	SG	125/125 (100%)	124 (99%)	1 (1%)	73	77
4	SL	125/125 (100%)	124 (99%)	1 (1%)	73	77
4	T4	125/125 (100%)	125 (100%)	0	100	100
4	TB	125/125 (100%)	124 (99%)	1 (1%)	73	77
4	UG	125/125 (100%)	125 (100%)	0	100	100
4	UL	125/125 (100%)	125 (100%)	0	100	100
4	W4	125/125 (100%)	125 (100%)	0	100	100
4	WB	125/125 (100%)	124 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	WG	125/125 (100%)	125 (100%)	0	100	100
4	WL	125/125 (100%)	125 (100%)	0	100	100
4	Y4	125/125 (100%)	125 (100%)	0	100	100
4	YB	125/125 (100%)	125 (100%)	0	100	100
4	YF	125/125 (100%)	122 (98%)	3 (2%)	43	64
4	YK	125/125 (100%)	122 (98%)	3 (2%)	43	64
4	a4	123/125 (98%)	111 (90%)	12 (10%)	7	30
4	aB	122/125 (98%)	113 (93%)	9 (7%)	13	37
4	aF	125/125 (100%)	125 (100%)	0	100	100
4	aK	125/125 (100%)	125 (100%)	0	100	100
4	cF	125/125 (100%)	125 (100%)	0	100	100
4	cK	125/125 (100%)	125 (100%)	0	100	100
4	eF	125/125 (100%)	125 (100%)	0	100	100
4	eK	125/125 (100%)	125 (100%)	0	100	100
4	hF	125/125 (100%)	123 (98%)	2 (2%)	55	70
4	hK	124/125 (99%)	123 (99%)	1 (1%)	73	77
4	jF	124/125 (99%)	124 (100%)	0	100	100
4	jK	124/125 (99%)	124 (100%)	0	100	100
4	lF	125/125 (100%)	125 (100%)	0	100	100
4	lK	125/125 (100%)	125 (100%)	0	100	100
4	nF	125/125 (100%)	125 (100%)	0	100	100
4	nK	125/125 (100%)	125 (100%)	0	100	100
4	p4	124/125 (99%)	124 (100%)	0	100	100
4	pB	124/125 (99%)	124 (100%)	0	100	100
4	r4	125/125 (100%)	125 (100%)	0	100	100
4	rB	125/125 (100%)	125 (100%)	0	100	100
4	t4	125/125 (100%)	125 (100%)	0	100	100
4	tB	125/125 (100%)	124 (99%)	1 (1%)	73	77
4	v4	125/125 (100%)	125 (100%)	0	100	100
4	vB	125/125 (100%)	125 (100%)	0	100	100
4	x4	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	xB	125/125 (100%)	125 (100%)	0	100	100
4	z4	124/125 (99%)	124 (100%)	0	100	100
4	zB	124/125 (99%)	124 (100%)	0	100	100
5	2G	58/60 (97%)	58 (100%)	0	100	100
5	2L	58/60 (97%)	58 (100%)	0	100	100
5	3F	58/60 (97%)	58 (100%)	0	100	100
5	3K	58/60 (97%)	58 (100%)	0	100	100
5	8G	58/60 (97%)	58 (100%)	0	100	100
5	8L	58/60 (97%)	58 (100%)	0	100	100
5	NF	59/60 (98%)	59 (100%)	0	100	100
5	NK	59/60 (98%)	59 (100%)	0	100	100
5	U4	58/60 (97%)	58 (100%)	0	100	100
5	UB	58/60 (97%)	58 (100%)	0	100	100
5	b4	58/60 (97%)	58 (100%)	0	100	100
5	bB	58/60 (97%)	58 (100%)	0	100	100
6	A1	269/293 (92%)	268 (100%)	1 (0%)	84	81
6	AD	268/293 (92%)	267 (100%)	1 (0%)	84	81
6	AE	268/293 (92%)	267 (100%)	1 (0%)	84	81
6	a1	269/293 (92%)	265 (98%)	4 (2%)	57	71
6	aD	270/293 (92%)	265 (98%)	5 (2%)	50	68
6	aE	270/293 (92%)	266 (98%)	4 (2%)	57	71
7	B1	397/405 (98%)	331 (83%)	66 (17%)	2	13
7	BD	398/405 (98%)	332 (83%)	66 (17%)	2	13
7	BE	397/405 (98%)	330 (83%)	67 (17%)	2	13
7	b1	399/405 (98%)	340 (85%)	59 (15%)	3	17
7	bD	399/405 (98%)	338 (85%)	61 (15%)	3	16
7	bE	399/405 (98%)	338 (85%)	61 (15%)	3	16
8	C1	346/365 (95%)	322 (93%)	24 (7%)	14	39
8	CD	346/365 (95%)	324 (94%)	22 (6%)	16	42
8	CE	346/365 (95%)	325 (94%)	21 (6%)	17	43
8	c1	344/365 (94%)	324 (94%)	20 (6%)	18	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	cD	343/365 (94%)	323 (94%)	20 (6%)	18 44
8	cE	343/365 (94%)	326 (95%)	17 (5%)	22 48
9	D1	274/285 (96%)	233 (85%)	41 (15%)	3 17
9	DD	274/285 (96%)	233 (85%)	41 (15%)	3 17
9	DE	274/285 (96%)	233 (85%)	41 (15%)	3 17
9	d1	273/285 (96%)	233 (85%)	40 (15%)	3 17
9	dD	273/285 (96%)	233 (85%)	40 (15%)	3 17
9	dE	273/285 (96%)	233 (85%)	40 (15%)	3 17
10	E1	68/70 (97%)	63 (93%)	5 (7%)	13 37
10	ED	68/70 (97%)	63 (93%)	5 (7%)	13 37
10	EE	68/70 (97%)	63 (93%)	5 (7%)	13 37
10	e1	68/70 (97%)	65 (96%)	3 (4%)	25 51
10	eD	68/70 (97%)	65 (96%)	3 (4%)	25 51
10	eE	68/70 (97%)	65 (96%)	3 (4%)	25 51
11	F1	29/37 (78%)	24 (83%)	5 (17%)	2 12
11	FD	29/37 (78%)	24 (83%)	5 (17%)	2 12
11	FE	29/37 (78%)	25 (86%)	4 (14%)	3 19
11	f1	29/37 (78%)	22 (76%)	7 (24%)	1 4
11	fD	31/37 (84%)	23 (74%)	8 (26%)	0 3
11	fE	29/37 (78%)	22 (76%)	7 (24%)	1 4
12	H1	55/58 (95%)	54 (98%)	1 (2%)	51 69
12	HD	53/58 (91%)	52 (98%)	1 (2%)	50 68
12	HE	53/58 (91%)	51 (96%)	2 (4%)	29 55
12	h1	55/58 (95%)	52 (94%)	3 (6%)	19 46
12	hD	55/58 (95%)	52 (94%)	3 (6%)	19 46
12	hE	55/58 (95%)	52 (94%)	3 (6%)	19 46
13	I1	34/36 (94%)	21 (62%)	13 (38%)	0 1
13	ID	34/36 (94%)	20 (59%)	14 (41%)	0 0
13	IE	34/36 (94%)	20 (59%)	14 (41%)	0 0
13	i1	33/36 (92%)	20 (61%)	13 (39%)	0 1
13	iD	33/36 (92%)	20 (61%)	13 (39%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	iE	33/36 (92%)	20 (61%)	13 (39%)	0 1
14	J1	25/27 (93%)	22 (88%)	3 (12%)	5 23
14	JD	25/27 (93%)	22 (88%)	3 (12%)	5 23
14	JE	25/27 (93%)	22 (88%)	3 (12%)	5 23
14	j1	27/27 (100%)	27 (100%)	0	100 100
14	jD	27/27 (100%)	27 (100%)	0	100 100
14	jE	27/27 (100%)	27 (100%)	0	100 100
15	K1	31/37 (84%)	27 (87%)	4 (13%)	4 21
15	KD	31/37 (84%)	27 (87%)	4 (13%)	4 21
15	KE	31/37 (84%)	27 (87%)	4 (13%)	4 21
15	k1	30/37 (81%)	22 (73%)	8 (27%)	0 3
15	kD	30/37 (81%)	21 (70%)	9 (30%)	0 2
15	kE	30/37 (81%)	21 (70%)	9 (30%)	0 2
16	L1	36/37 (97%)	29 (81%)	7 (19%)	1 8
16	LD	36/37 (97%)	29 (81%)	7 (19%)	1 8
16	LE	36/37 (97%)	29 (81%)	7 (19%)	1 8
16	l1	36/37 (97%)	29 (81%)	7 (19%)	1 8
16	lD	36/37 (97%)	29 (81%)	7 (19%)	1 8
16	lE	36/37 (97%)	29 (81%)	7 (19%)	1 8
17	M1	33/33 (100%)	22 (67%)	11 (33%)	0 2
17	MD	33/33 (100%)	22 (67%)	11 (33%)	0 2
17	ME	33/33 (100%)	22 (67%)	11 (33%)	0 2
17	m1	33/33 (100%)	16 (48%)	17 (52%)	0 0
17	mD	33/33 (100%)	16 (48%)	17 (52%)	0 0
17	mE	33/33 (100%)	16 (48%)	17 (52%)	0 0
18	O1	201/230 (87%)	171 (85%)	30 (15%)	3 17
18	OD	201/230 (87%)	173 (86%)	28 (14%)	3 19
18	OE	201/230 (87%)	173 (86%)	28 (14%)	3 19
18	o1	201/230 (87%)	173 (86%)	28 (14%)	3 19
18	oD	201/230 (87%)	172 (86%)	29 (14%)	3 18
18	oE	201/230 (87%)	173 (86%)	28 (14%)	3 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	Q1	106/144 (74%)	78 (74%)	28 (26%)	0 3
19	QD	106/144 (74%)	78 (74%)	28 (26%)	0 3
19	QE	106/144 (74%)	78 (74%)	28 (26%)	0 3
19	q1	106/144 (74%)	78 (74%)	28 (26%)	0 3
19	qD	106/144 (74%)	78 (74%)	28 (26%)	0 3
19	qE	106/144 (74%)	78 (74%)	28 (26%)	0 3
20	R1	26/30 (87%)	18 (69%)	8 (31%)	0 2
20	RD	26/30 (87%)	18 (69%)	8 (31%)	0 2
20	RE	26/30 (87%)	18 (69%)	8 (31%)	0 2
20	r1	26/30 (87%)	18 (69%)	8 (31%)	0 2
20	rD	26/30 (87%)	18 (69%)	8 (31%)	0 2
20	rE	26/30 (87%)	18 (69%)	8 (31%)	0 2
22	T1	23/25 (92%)	23 (100%)	0	100 100
22	TD	23/25 (92%)	23 (100%)	0	100 100
22	TE	23/25 (92%)	23 (100%)	0	100 100
22	t1	24/25 (96%)	24 (100%)	0	100 100
22	tD	24/25 (96%)	24 (100%)	0	100 100
22	tE	24/25 (96%)	24 (100%)	0	100 100
23	U1	82/82 (100%)	75 (92%)	7 (8%)	10 34
23	UD	82/82 (100%)	75 (92%)	7 (8%)	10 34
23	UE	82/82 (100%)	75 (92%)	7 (8%)	10 34
23	u1	82/82 (100%)	75 (92%)	7 (8%)	10 34
23	uD	82/82 (100%)	75 (92%)	7 (8%)	10 34
23	uE	82/82 (100%)	75 (92%)	7 (8%)	10 34
24	V1	114/137 (83%)	98 (86%)	16 (14%)	3 19
24	VD	114/137 (83%)	98 (86%)	16 (14%)	3 19
24	VE	114/137 (83%)	98 (86%)	16 (14%)	3 19
24	v1	114/137 (83%)	101 (89%)	13 (11%)	5 24
24	vD	114/137 (83%)	101 (89%)	13 (11%)	5 24
24	vE	114/137 (83%)	101 (89%)	13 (11%)	5 24
25	X1	36/44 (82%)	29 (81%)	7 (19%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	XD	36/44 (82%)	29 (81%)	7 (19%)	1	8
25	XE	36/44 (82%)	29 (81%)	7 (19%)	1	8
25	x1	36/44 (82%)	29 (81%)	7 (19%)	1	8
25	xD	36/44 (82%)	29 (81%)	7 (19%)	1	8
25	xE	36/44 (82%)	29 (81%)	7 (19%)	1	8
26	Y1	26/37 (70%)	16 (62%)	10 (38%)	0	1
26	YD	26/37 (70%)	16 (62%)	10 (38%)	0	1
26	YE	26/37 (70%)	16 (62%)	10 (38%)	0	1
26	y1	26/37 (70%)	16 (62%)	10 (38%)	0	1
26	yD	26/37 (70%)	16 (62%)	10 (38%)	0	1
26	yE	26/37 (70%)	16 (62%)	10 (38%)	0	1
27	Z1	51/54 (94%)	36 (71%)	15 (29%)	0	2
27	ZD	51/54 (94%)	36 (71%)	15 (29%)	0	2
27	ZE	51/54 (94%)	36 (71%)	15 (29%)	0	2
27	z1	51/54 (94%)	36 (71%)	15 (29%)	0	2
27	zD	51/54 (94%)	36 (71%)	15 (29%)	0	2
27	zE	51/54 (94%)	36 (71%)	15 (29%)	0	2
28	BG	39/113 (34%)	17 (44%)	22 (56%)	0	0
28	BL	39/113 (34%)	17 (44%)	22 (56%)	0	0
28	EF	38/113 (34%)	22 (58%)	16 (42%)	0	0
28	EK	38/113 (34%)	22 (58%)	16 (42%)	0	0
29	QG	135/135 (100%)	127 (94%)	8 (6%)	18	44
29	QL	135/135 (100%)	127 (94%)	8 (6%)	18	44
29	gF	135/135 (100%)	127 (94%)	8 (6%)	18	44
29	gK	135/135 (100%)	127 (94%)	8 (6%)	18	44
30	VG	135/136 (99%)	132 (98%)	3 (2%)	45	65
30	VL	135/136 (99%)	132 (98%)	3 (2%)	45	65
30	mF	135/136 (99%)	134 (99%)	1 (1%)	76	78
30	mK	135/136 (99%)	134 (99%)	1 (1%)	76	78
31	b2	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	b3	87/125 (70%)	86 (99%)	1 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	b5	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	b6	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	b7	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	b8	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	b9	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	bA	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	bC	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	bH	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	bI	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	bJ	87/125 (70%)	86 (99%)	1 (1%)	65	74
31	d2	78/125 (62%)	78 (100%)	0	100	100
31	d3	78/125 (62%)	78 (100%)	0	100	100
31	d5	78/125 (62%)	78 (100%)	0	100	100
31	d6	78/125 (62%)	78 (100%)	0	100	100
31	d7	78/125 (62%)	78 (100%)	0	100	100
31	d8	78/125 (62%)	78 (100%)	0	100	100
31	d9	78/125 (62%)	78 (100%)	0	100	100
31	dA	78/125 (62%)	78 (100%)	0	100	100
31	dC	78/125 (62%)	78 (100%)	0	100	100
31	dH	78/125 (62%)	78 (100%)	0	100	100
31	dI	78/125 (62%)	78 (100%)	0	100	100
31	dJ	78/125 (62%)	78 (100%)	0	100	100
31	f2	80/125 (64%)	80 (100%)	0	100	100
31	f3	80/125 (64%)	80 (100%)	0	100	100
31	f5	80/125 (64%)	80 (100%)	0	100	100
31	f6	80/125 (64%)	80 (100%)	0	100	100
31	f7	80/125 (64%)	80 (100%)	0	100	100
31	f8	80/125 (64%)	80 (100%)	0	100	100
31	f9	80/125 (64%)	80 (100%)	0	100	100
31	fA	80/125 (64%)	80 (100%)	0	100	100
31	fC	80/125 (64%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	fH	80/125 (64%)	80 (100%)	0	100	100
31	fI	80/125 (64%)	80 (100%)	0	100	100
31	fJ	80/125 (64%)	80 (100%)	0	100	100
31	h2	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	h3	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	h5	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	h6	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	h7	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	h8	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	h9	81/125 (65%)	80 (99%)	1 (1%)	63	73
31	hA	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	hC	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	hH	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	hI	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	hJ	82/125 (66%)	81 (99%)	1 (1%)	63	73
31	j2	81/125 (65%)	81 (100%)	0	100	100
31	j3	81/125 (65%)	81 (100%)	0	100	100
31	j5	81/125 (65%)	81 (100%)	0	100	100
31	j6	81/125 (65%)	81 (100%)	0	100	100
31	j7	81/125 (65%)	81 (100%)	0	100	100
31	j8	81/125 (65%)	81 (100%)	0	100	100
31	j9	81/125 (65%)	81 (100%)	0	100	100
31	jA	81/125 (65%)	81 (100%)	0	100	100
31	jC	81/125 (65%)	81 (100%)	0	100	100
31	jH	81/125 (65%)	81 (100%)	0	100	100
31	jI	81/125 (65%)	81 (100%)	0	100	100
31	jJ	81/125 (65%)	81 (100%)	0	100	100
31	l2	85/125 (68%)	85 (100%)	0	100	100
31	l3	85/125 (68%)	85 (100%)	0	100	100
31	l5	85/125 (68%)	85 (100%)	0	100	100
31	l6	85/125 (68%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	l7	85/125 (68%)	85 (100%)	0	100	100
31	l8	85/125 (68%)	85 (100%)	0	100	100
31	l9	85/125 (68%)	85 (100%)	0	100	100
31	lA	85/125 (68%)	85 (100%)	0	100	100
31	lC	85/125 (68%)	85 (100%)	0	100	100
31	lH	85/125 (68%)	85 (100%)	0	100	100
31	lI	85/125 (68%)	85 (100%)	0	100	100
31	lJ	85/125 (68%)	85 (100%)	0	100	100
32	c2	85/131 (65%)	85 (100%)	0	100	100
32	c3	85/131 (65%)	85 (100%)	0	100	100
32	c5	85/131 (65%)	85 (100%)	0	100	100
32	c6	85/131 (65%)	85 (100%)	0	100	100
32	c7	85/131 (65%)	85 (100%)	0	100	100
32	c8	85/131 (65%)	85 (100%)	0	100	100
32	c9	85/131 (65%)	85 (100%)	0	100	100
32	cA	85/131 (65%)	85 (100%)	0	100	100
32	cC	85/131 (65%)	85 (100%)	0	100	100
32	cH	85/131 (65%)	85 (100%)	0	100	100
32	cI	84/131 (64%)	84 (100%)	0	100	100
32	cJ	85/131 (65%)	85 (100%)	0	100	100
32	e2	83/131 (63%)	83 (100%)	0	100	100
32	e3	83/131 (63%)	83 (100%)	0	100	100
32	e5	83/131 (63%)	83 (100%)	0	100	100
32	e6	83/131 (63%)	83 (100%)	0	100	100
32	e7	83/131 (63%)	83 (100%)	0	100	100
32	e8	83/131 (63%)	83 (100%)	0	100	100
32	e9	83/131 (63%)	83 (100%)	0	100	100
32	eA	83/131 (63%)	83 (100%)	0	100	100
32	eC	83/131 (63%)	83 (100%)	0	100	100
32	eH	83/131 (63%)	83 (100%)	0	100	100
32	eI	83/131 (63%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	eJ	83/131 (63%)	83 (100%)	0	100	100
32	g2	89/131 (68%)	89 (100%)	0	100	100
32	g3	89/131 (68%)	89 (100%)	0	100	100
32	g5	89/131 (68%)	89 (100%)	0	100	100
32	g6	89/131 (68%)	89 (100%)	0	100	100
32	g7	89/131 (68%)	89 (100%)	0	100	100
32	g8	89/131 (68%)	89 (100%)	0	100	100
32	g9	89/131 (68%)	89 (100%)	0	100	100
32	gA	89/131 (68%)	89 (100%)	0	100	100
32	gC	89/131 (68%)	89 (100%)	0	100	100
32	gH	89/131 (68%)	89 (100%)	0	100	100
32	gI	88/131 (67%)	88 (100%)	0	100	100
32	gJ	89/131 (68%)	89 (100%)	0	100	100
32	i2	88/131 (67%)	88 (100%)	0	100	100
32	i3	88/131 (67%)	88 (100%)	0	100	100
32	i5	88/131 (67%)	88 (100%)	0	100	100
32	i6	88/131 (67%)	88 (100%)	0	100	100
32	i7	88/131 (67%)	88 (100%)	0	100	100
32	i8	88/131 (67%)	88 (100%)	0	100	100
32	i9	88/131 (67%)	88 (100%)	0	100	100
32	iA	88/131 (67%)	88 (100%)	0	100	100
32	iC	88/131 (67%)	88 (100%)	0	100	100
32	iH	88/131 (67%)	88 (100%)	0	100	100
32	iI	88/131 (67%)	88 (100%)	0	100	100
32	iJ	88/131 (67%)	88 (100%)	0	100	100
32	k2	94/131 (72%)	94 (100%)	0	100	100
32	k3	94/131 (72%)	94 (100%)	0	100	100
32	k5	94/131 (72%)	94 (100%)	0	100	100
32	k6	94/131 (72%)	94 (100%)	0	100	100
32	k7	94/131 (72%)	94 (100%)	0	100	100
32	k8	94/131 (72%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	k9	94/131 (72%)	94 (100%)	0	100	100
32	kA	94/131 (72%)	94 (100%)	0	100	100
32	kC	94/131 (72%)	94 (100%)	0	100	100
32	kH	94/131 (72%)	94 (100%)	0	100	100
32	kI	94/131 (72%)	94 (100%)	0	100	100
32	kJ	94/131 (72%)	94 (100%)	0	100	100
32	m2	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	m3	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	m5	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	m6	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	m7	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	m8	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	m9	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	mA	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	mC	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	mH	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	mI	93/131 (71%)	92 (99%)	1 (1%)	65	74
32	mJ	93/131 (71%)	92 (99%)	1 (1%)	65	74
All	All	49693/57880 (86%)	47338 (95%)	2355 (5%)	25	49

5 of 2355 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	hD	35	MET
26	yE	70	LEU
18	oD	71	LEU
11	fD	40	GLN
7	bE	497	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 639 such sidechains are listed below:

Mol	Chain	Res	Type
6	aD	187	GLN
3	iF	56	ASN
8	cD	142	ASN

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Mol	Chain	Res	Type
6	aD	181	ASN
7	bE	14	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)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 882 ligands modelled in this entry, 36 are monoatomic - leaving 846 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	$\#\|Z\| > 2$
33	CYC	f5	201	31	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	ZF	201	3	46,46,46	2.39	17 (36%)	61,67,67	3.13	29 (47%)
40	LMT	BE	623	7	24,24,36	1.19	4 (16%)	29,29,47	1.14	1 (3%)
33	CYC	aB	201	5,4	46,46,46	2.42	14 (30%)	61,67,67	3.14	29 (47%)
36	CLA	BD	609	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	8 (9%)
37	PL9	AD	406	-	55,55,55	0.64	1 (1%)	68,69,69	1.46	11 (16%)
36	CLA	CE	511	8	69,73,73	1.24	8 (11%)	83,113,113	1.24	11 (13%)
36	CLA	B1	609	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	8 (9%)
33	CYC	nF	201	5,4	46,46,46	2.52	18 (39%)	61,67,67	3.29	26 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	cC	202	32	46,46,46	0.81	0	61,67,67	0.81	1 (1%)
33	CYC	gI	302	32	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
39	LMG	DD	411	9	51,51,55	0.94	2 (3%)	59,59,63	1.26	5 (8%)
43	BCR	D1	406	-	41,41,41	0.71	0	56,56,56	1.82	11 (19%)
36	CLA	B1	612	-	69,73,73	1.30	11 (15%)	83,113,113	1.32	6 (7%)
33	CYC	eF	201	4	46,46,46	2.34	18 (39%)	61,67,67	3.20	27 (44%)
42	LHG	aE	411	6	37,37,48	1.04	2 (5%)	40,43,54	1.23	4 (10%)
44	DGD	CD	517	8	48,48,67	0.98	2 (4%)	62,62,81	1.27	8 (12%)
36	CLA	C1	515	-	69,73,73	1.25	10 (14%)	83,113,113	1.38	10 (12%)
39	LMG	A1	408	-	36,36,55	1.08	2 (5%)	44,44,63	1.10	5 (11%)
39	LMG	D1	410	9	51,51,55	0.95	2 (3%)	59,59,63	1.27	5 (8%)
33	CYC	j7	202	-	46,46,46	0.79	0	61,67,67	0.81	1 (1%)
33	CYC	eJ	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
39	LMG	mD	101	-	36,36,55	1.12	2 (5%)	44,44,63	1.11	3 (6%)
36	CLA	BD	603	7	69,73,73	1.33	12 (17%)	83,113,113	1.36	8 (9%)
33	CYC	bK	201	3	46,46,46	2.30	17 (36%)	61,67,67	3.20	27 (44%)
36	CLA	bE	615	7	69,73,73	1.35	9 (13%)	83,113,113	1.33	11 (13%)
36	CLA	bD	614	43	69,73,73	1.23	10 (14%)	83,113,113	1.36	8 (9%)
40	LMT	C1	520	8	24,24,36	1.12	2 (8%)	29,29,47	1.14	3 (10%)
40	LMT	bE	602	-	24,24,36	1.17	2 (8%)	29,29,47	1.02	0
43	BCR	k1	102	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
47	HEM	v1	201	24	50,50,50	1.68	9 (18%)	66,82,82	1.89	14 (21%)
43	BCR	bE	618	-	41,41,41	0.74	0	56,56,56	1.86	12 (21%)
33	CYC	e9	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
33	CYC	dK	201	3	46,46,46	2.57	19 (41%)	61,67,67	3.27	27 (44%)
39	LMG	b1	619	7	51,51,55	0.92	2 (3%)	59,59,63	1.17	3 (5%)
43	BCR	C1	516	36,8	41,41,41	0.76	0	56,56,56	2.23	18 (32%)
33	CYC	m6	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
33	CYC	kK	201	3	46,46,46	2.28	15 (32%)	61,67,67	2.92	25 (40%)
36	CLA	CE	504	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
43	BCR	XE	102	25,36	41,41,41	0.94	2 (4%)	56,56,56	2.63	19 (33%)
36	CLA	BD	613	43	69,73,73	1.24	10 (14%)	83,113,113	1.37	8 (9%)
37	PL9	DE	408	9	55,55,55	0.63	2 (3%)	68,69,69	1.62	17 (25%)
33	CYC	iJ	202	-	46,46,46	2.30	15 (32%)	61,67,67	3.88	31 (50%)
36	CLA	AD	405	-	69,73,73	1.23	9 (13%)	83,113,113	1.63	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	LHG	eE	101	-	39,39,48	1.03	2 (5%)	42,45,54	1.18	4 (9%)
33	CYC	LG	201	4,2	46,46,46	2.37	19 (41%)	61,67,67	5.02	38 (62%)
43	BCR	C1	519	-	41,41,41	0.74	0	56,56,56	1.79	14 (25%)
36	CLA	BE	612	-	69,73,73	1.29	11 (15%)	83,113,113	1.32	6 (7%)
42	LHG	AE	411	6	37,37,48	1.03	2 (5%)	40,43,54	1.18	3 (7%)
44	DGD	c1	516	8	48,48,67	0.99	2 (4%)	62,62,81	1.30	10 (16%)
45	PHO	dE	402	9	50,61,69	3.48	15 (30%)	46,89,99	3.69	16 (34%)
44	DGD	cD	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.11	6 (7%)
38	SQD	CD	501	8	53,54,54	1.18	4 (7%)	62,65,65	1.18	7 (11%)
36	CLA	c1	508	8	69,73,73	1.28	11 (15%)	83,113,113	1.39	13 (15%)
33	CYC	2G	201	5,4	46,46,46	2.33	17 (36%)	61,67,67	3.16	33 (54%)
36	CLA	AD	404	-	50,54,73	11.58	12 (24%)	60,90,113	2.06	12 (20%)
41	BCT	aD	410	46	2,3,3	1.15	0	2,3,3	4.48	2 (100%)
42	LHG	D1	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
33	CYC	c2	202	32	46,46,46	0.81	0	61,67,67	0.80	1 (1%)
43	BCR	ZE	102	-	41,41,41	0.72	0	56,56,56	1.90	13 (23%)
33	CYC	g2	202	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	32 (52%)
42	LHG	a1	412	6	37,37,48	1.04	2 (5%)	40,43,54	1.23	4 (10%)
36	CLA	cE	504	-	69,73,73	1.33	11 (15%)	83,113,113	1.48	12 (14%)
33	CYC	c8	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
33	CYC	cJ	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
37	PL9	a1	409	-	55,55,55	0.66	1 (1%)	68,69,69	1.46	12 (17%)
33	CYC	bI	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	1L	201	4	46,46,46	2.59	18 (39%)	61,67,67	3.07	25 (40%)
33	CYC	SL	201	4,2	46,46,46	2.25	16 (34%)	61,67,67	2.96	28 (45%)
36	CLA	BE	608	-	69,73,73	1.23	9 (13%)	83,113,113	1.42	8 (9%)
33	CYC	jC	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	b9	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
36	CLA	cE	503	-	69,73,73	1.26	10 (14%)	83,113,113	1.39	8 (9%)
33	CYC	QB	201	4,3	46,46,46	2.33	19 (41%)	61,67,67	2.98	28 (45%)
40	LMT	BE	619	-	24,24,36	1.13	3 (12%)	29,29,47	1.04	1 (3%)
38	SQD	h1	103	12	34,35,54	1.65	6 (17%)	43,46,65	1.91	10 (23%)
44	DGD	JE	101	-	63,63,67	0.83	2 (3%)	77,77,81	0.99	4 (5%)
44	DGD	cE	516	8	48,48,67	0.99	2 (4%)	62,62,81	1.31	10 (16%)
36	CLA	cD	511	-	69,73,73	1.27	10 (14%)	83,113,113	1.41	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	l9	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
40	LMT	B1	620	-	24,24,36	1.12	2 (8%)	29,29,47	1.14	3 (10%)
36	CLA	CE	506	8	69,73,73	1.30	11 (15%)	83,113,113	1.70	15 (18%)
33	CYC	Y4	201	5,4	46,46,46	2.22	15 (32%)	61,67,67	3.20	30 (49%)
33	CYC	3K	101	5,4	46,46,46	2.34	17 (36%)	61,67,67	3.04	29 (47%)
33	CYC	c9	202	32	46,46,46	0.81	0	61,67,67	0.80	1 (1%)
36	CLA	b1	606	7	69,73,73	1.26	10 (14%)	83,113,113	1.47	11 (13%)
33	CYC	i2	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.89	31 (50%)
43	BCR	b1	616	7,36	41,41,41	0.83	1 (2%)	56,56,56	2.51	22 (39%)
43	BCR	bE	616	7,36	41,41,41	0.82	1 (2%)	56,56,56	2.51	22 (39%)
33	CYC	l3	201	-	46,46,46	2.22	14 (30%)	61,67,67	3.37	32 (52%)
39	LMG	TE	101	-	36,36,55	1.14	2 (5%)	44,44,63	0.99	3 (6%)
36	CLA	iE	101	-	59,63,73	1.35	10 (16%)	71,101,113	1.60	8 (11%)
38	SQD	DE	414	9	33,34,54	1.48	4 (12%)	42,45,65	1.51	6 (14%)
33	CYC	zB	201	4,2	46,46,46	2.27	18 (39%)	61,67,67	3.28	35 (57%)
33	CYC	jK	201	4	46,46,46	2.27	17 (36%)	61,67,67	2.82	28 (45%)
39	LMG	CE	520	39	51,51,55	0.92	2 (3%)	59,59,63	1.07	5 (8%)
36	CLA	cE	512	-	69,73,73	1.28	11 (15%)	83,113,113	1.49	14 (16%)
36	CLA	CD	505	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	10 (12%)
33	CYC	i6	201	-	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
39	LMG	M1	101	-	36,36,55	1.11	2 (5%)	44,44,63	1.11	3 (6%)
36	CLA	CE	510	8	69,73,73	1.25	11 (15%)	83,113,113	2.20	17 (20%)
36	CLA	cE	506	8	69,73,73	1.31	11 (15%)	83,113,113	1.65	14 (16%)
36	CLA	BD	608	-	69,73,73	1.23	9 (13%)	83,113,113	1.42	9 (10%)
38	SQD	L1	101	-	42,43,54	1.35	5 (11%)	51,54,65	1.22	4 (7%)
39	LMG	aD	409	-	36,36,55	1.08	2 (5%)	44,44,63	1.06	2 (4%)
42	LHG	lD	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.06	3 (5%)
38	SQD	c1	501	8	53,54,54	1.18	4 (7%)	62,65,65	1.15	5 (8%)
36	CLA	CD	512	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	10 (12%)
33	CYC	JF	201	3	46,46,46	2.44	16 (34%)	61,67,67	2.82	23 (37%)
40	LMT	bD	602	-	24,24,36	1.16	2 (8%)	29,29,47	1.02	0
43	BCR	BD	615	7,36	41,41,41	0.82	1 (2%)	56,56,56	2.51	22 (39%)
33	CYC	p4	201	4,2	46,46,46	2.20	15 (32%)	61,67,67	3.14	29 (47%)
41	BCT	AE	410	-	2,3,3	1.14	0	2,3,3	4.50	2 (100%)
39	LMG	B1	618	7	51,51,55	0.92	2 (3%)	59,59,63	1.17	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
43	BCR	z1	101	27	41,41,41	0.72	0	56,56,56	2.17	22 (39%)
33	CYC	iI	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.88	31 (50%)
36	CLA	c1	514	-	69,73,73	1.25	11 (15%)	83,113,113	1.37	9 (10%)
45	PHO	DE	401	-	58,69,69	2.97	19 (32%)	56,99,99	3.03	25 (44%)
33	CYC	XB	201	4,3	46,46,46	2.35	16 (34%)	61,67,67	2.92	24 (39%)
33	CYC	pB	201	4,2	46,46,46	2.20	15 (32%)	61,67,67	3.14	29 (47%)
42	LHG	AD	411	6	37,37,48	1.04	2 (5%)	40,43,54	1.18	3 (7%)
44	DGD	cD	516	8	48,48,67	0.99	2 (4%)	62,62,81	1.31	10 (16%)
36	CLA	c1	510	8	69,73,73	1.28	12 (17%)	83,113,113	1.49	15 (18%)
36	CLA	bD	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	8 (9%)
33	CYC	i5	201	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
33	CYC	c7	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
33	CYC	BB	1002	2	46,46,46	2.24	17 (36%)	61,67,67	3.02	25 (40%)
33	CYC	g3	201	32	46,46,46	0.77	0	61,67,67	0.79	1 (1%)
36	CLA	b1	605	7	69,73,73	1.32	12 (17%)	83,113,113	1.35	8 (9%)
33	CYC	iH	201	-	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
33	CYC	a4	201	5,4	46,46,46	2.42	14 (30%)	61,67,67	3.14	29 (47%)
33	CYC	sB	201	3	46,46,46	2.21	15 (32%)	61,67,67	3.28	29 (47%)
36	CLA	B1	604	7	69,73,73	1.27	10 (14%)	83,113,113	1.49	11 (13%)
36	CLA	B1	606	-	64,68,73	1.31	10 (15%)	77,107,113	1.51	12 (15%)
36	CLA	CD	504	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
33	CYC	qB	201	3	46,46,46	2.21	16 (34%)	61,67,67	2.92	24 (39%)
36	CLA	bD	611	-	69,73,73	1.30	13 (18%)	83,113,113	1.52	11 (13%)
38	SQD	DD	414	9	33,34,54	1.48	4 (12%)	42,45,65	1.51	6 (14%)
38	SQD	C1	501	8	53,54,54	1.18	4 (7%)	62,65,65	1.18	7 (11%)
40	LMT	B1	623	7	24,24,36	1.20	4 (16%)	29,29,47	1.14	1 (3%)
40	LMT	cE	501	-	24,24,36	1.12	2 (8%)	29,29,47	1.14	3 (10%)
36	CLA	bE	606	7	69,73,73	1.26	10 (14%)	83,113,113	1.48	11 (13%)
38	SQD	AD	407	-	45,46,54	1.28	4 (8%)	54,57,65	1.27	4 (7%)
33	CYC	nK	201	5,4	46,46,46	2.52	17 (36%)	61,67,67	3.28	26 (42%)
33	CYC	QG	201	29	46,46,46	2.23	19 (41%)	61,67,67	3.20	30 (49%)
33	CYC	eI	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
33	CYC	AG	201	4,3	46,46,46	2.16	15 (32%)	61,67,67	3.17	29 (47%)
33	CYC	hF	201	4	46,46,46	2.57	19 (41%)	61,67,67	3.27	26 (42%)
36	CLA	C1	506	8	69,73,73	1.29	11 (15%)	83,113,113	1.69	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
42	LHG	BE	620	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
43	BCR	IE	102	13	41,41,41	0.79	0	56,56,56	2.77	18 (32%)
40	LMT	dD	413	-	22,22,36	1.16	3 (13%)	27,27,47	1.01	1 (3%)
34	OEX	AE	401	6	0,14,14	-	-	-		
33	CYC	d7	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	g7	201	32	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
39	LMG	a1	410	-	36,36,55	1.08	2 (5%)	44,44,63	1.06	2 (4%)
40	LMT	d1	412	-	25,25,36	1.11	2 (8%)	30,30,47	1.06	2 (6%)
40	LMT	DE	413	-	22,22,36	1.17	3 (13%)	27,27,47	1.03	1 (3%)
43	BCR	d1	407	-	41,41,41	0.69	0	56,56,56	1.82	12 (21%)
36	CLA	cE	510	8	69,73,73	1.28	12 (17%)	83,113,113	1.48	15 (18%)
36	CLA	CE	512	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	10 (12%)
36	CLA	BD	607	7	69,73,73	1.35	10 (14%)	83,113,113	1.72	12 (14%)
36	CLA	cE	505	-	69,73,73	1.27	10 (14%)	83,113,113	1.40	11 (13%)
42	LHG	DE	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
33	CYC	MG	201	4,2	46,46,46	2.37	16 (34%)	61,67,67	3.38	32 (52%)
33	CYC	ZK	201	3	46,46,46	2.38	18 (39%)	61,67,67	3.13	29 (47%)
44	DGD	JD	101	-	63,63,67	0.83	2 (3%)	77,77,81	0.99	4 (5%)
33	CYC	gI	301	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	32 (52%)
43	BCR	B1	616	7	41,41,41	0.70	0	56,56,56	1.88	14 (25%)
42	LHG	d1	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
36	CLA	C1	513	-	69,73,73	1.25	10 (14%)	83,113,113	1.45	10 (12%)
33	CYC	dC	201	-	46,46,46	2.23	14 (30%)	61,67,67	3.36	32 (52%)
36	CLA	h1	102	12	64,68,73	1.30	11 (17%)	77,107,113	1.40	9 (11%)
33	CYC	OL	201	4	46,46,46	2.27	17 (36%)	61,67,67	3.29	27 (44%)
33	CYC	7L	201	5,4	46,46,46	2.68	20 (43%)	61,67,67	3.32	28 (45%)
43	BCR	b1	617	7	41,41,41	0.69	0	56,56,56	1.87	13 (23%)
36	CLA	C1	505	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	10 (12%)
43	BCR	i1	101	-	41,41,41	0.77	1 (2%)	56,56,56	2.55	19 (33%)
33	CYC	j8	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
36	CLA	HE	103	43	69,73,73	1.75	10 (14%)	83,113,113	1.71	9 (10%)
40	LMT	cD	501	-	24,24,36	1.13	2 (8%)	29,29,47	1.13	3 (10%)
33	CYC	e2	202	-	46,46,46	0.77	0	61,67,67	0.79	1 (1%)
36	CLA	b1	611	-	69,73,73	1.30	13 (18%)	83,113,113	1.53	11 (13%)
42	LHG	dE	410	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LMG	tE	101	22	36,36,55	1.15	2 (5%)	44,44,63	0.99	3 (6%)
39	LMG	aE	407	-	51,51,55	0.92	2 (3%)	59,59,63	1.06	2 (3%)
33	CYC	WG	201	4	46,46,46	2.28	15 (32%)	61,67,67	2.73	24 (39%)
33	CYC	q4	201	3	46,46,46	2.21	16 (34%)	61,67,67	2.91	24 (39%)
33	CYC	k9	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
36	CLA	BE	603	7	69,73,73	1.33	12 (17%)	83,113,113	1.36	8 (9%)
36	CLA	BE	611	7	69,73,73	1.24	9 (13%)	83,113,113	1.68	13 (15%)
39	LMG	DE	411	9	51,51,55	0.94	2 (3%)	59,59,63	1.26	5 (8%)
33	CYC	JK	201	3	46,46,46	2.44	16 (34%)	61,67,67	2.82	22 (36%)
33	CYC	yB	201	3	46,46,46	2.22	15 (32%)	61,67,67	3.38	28 (45%)
43	BCR	kE	102	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
33	CYC	IG	201	3	46,46,46	2.49	17 (36%)	61,67,67	3.03	32 (52%)
42	LHG	DD	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
33	CYC	kH	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
38	SQD	cD	502	8	53,54,54	1.18	4 (7%)	62,65,65	1.15	5 (8%)
43	BCR	CD	516	36,8	41,41,41	0.76	0	56,56,56	2.24	18 (32%)
36	CLA	b1	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.38	7 (8%)
36	CLA	bE	608	-	64,68,73	1.32	10 (15%)	77,107,113	1.52	13 (16%)
33	CYC	l2	201	-	46,46,46	2.22	14 (30%)	61,67,67	3.37	32 (52%)
38	SQD	BE	621	-	37,38,54	1.44	4 (10%)	46,49,65	4.33	9 (19%)
33	CYC	g9	201	32	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
36	CLA	bE	612	7	69,73,73	1.23	8 (11%)	83,113,113	1.69	14 (16%)
39	LMG	bD	619	7	51,51,55	0.92	2 (3%)	59,59,63	1.17	3 (5%)
33	CYC	TL	201	3	46,46,46	2.29	17 (36%)	61,67,67	3.19	26 (42%)
36	CLA	B1	601	-	49,53,73	1.48	10 (20%)	59,89,113	1.64	8 (13%)
39	LMG	a1	408	-	51,51,55	0.92	2 (3%)	59,59,63	1.06	2 (3%)
43	BCR	DE	407	-	41,41,41	0.70	0	56,56,56	1.82	11 (19%)
39	LMG	j1	102	14,39	27,27,55	1.34	2 (7%)	35,35,63	1.11	2 (5%)
43	BCR	kD	102	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
36	CLA	dD	406	9	69,73,73	1.26	11 (15%)	83,113,113	1.41	12 (14%)
33	CYC	ZB	201	3	46,46,46	2.30	18 (39%)	61,67,67	2.94	23 (37%)
36	CLA	BD	605	-	69,73,73	1.28	11 (15%)	83,113,113	1.58	10 (12%)
33	CYC	jH	202	-	46,46,46	0.78	0	61,67,67	0.81	1 (1%)
36	CLA	c1	512	-	69,73,73	1.28	11 (15%)	83,113,113	1.48	14 (16%)
33	CYC	eK	201	4	46,46,46	2.34	18 (39%)	61,67,67	3.21	27 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	B1	605	-	69,73,73	1.27	11 (15%)	83,113,113	1.57	10 (12%)
43	BCR	Z1	102	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
39	LMG	ME	101	-	36,36,55	1.11	2 (5%)	44,44,63	1.11	3 (6%)
33	CYC	XF	201	3	46,46,46	2.30	16 (34%)	61,67,67	3.12	26 (42%)
33	CYC	w4	201	3	46,46,46	2.24	14 (30%)	61,67,67	2.97	24 (39%)
44	DGD	cD	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	3 (3%)
43	BCR	X1	102	25,36	41,41,41	0.94	2 (4%)	56,56,56	2.64	20 (35%)
36	CLA	bD	608	-	64,68,73	1.31	10 (15%)	77,107,113	1.51	13 (16%)
44	DGD	CE	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	5 (6%)
33	CYC	RG	201	4,3	46,46,46	2.19	14 (30%)	61,67,67	3.05	28 (45%)
39	LMG	BE	618	7	51,51,55	0.92	2 (3%)	59,59,63	1.17	3 (5%)
36	CLA	hE	102	12	64,68,73	1.30	11 (17%)	77,107,113	1.41	10 (12%)
40	LMT	AE	412	-	36,36,36	1.21	4 (11%)	47,47,47	1.16	3 (6%)
40	LMT	d1	413	-	22,22,36	1.16	3 (13%)	27,27,47	1.01	1 (3%)
33	CYC	eC	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
33	CYC	c7	202	32	46,46,46	0.81	0	61,67,67	0.81	1 (1%)
36	CLA	BE	607	7	69,73,73	1.34	10 (14%)	83,113,113	1.72	12 (14%)
40	LMT	A1	409	-	24,24,36	1.14	3 (12%)	29,29,47	1.07	1 (3%)
33	CYC	gJ	202	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
42	LHG	A1	411	6	37,37,48	1.04	2 (5%)	40,43,54	1.18	3 (7%)
43	BCR	CE	519	-	41,41,41	0.74	0	56,56,56	1.79	14 (25%)
33	CYC	gA	302	32	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
36	CLA	BD	611	7	69,73,73	1.24	9 (13%)	83,113,113	1.68	13 (15%)
33	CYC	e8	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
43	BCR	zD	101	27	41,41,41	0.72	0	56,56,56	2.17	23 (41%)
33	CYC	iA	201	-	46,46,46	0.79	0	61,67,67	0.80	1 (1%)
33	CYC	tB	1001	4,2	46,46,46	3.00	20 (43%)	61,67,67	5.93	31 (50%)
44	DGD	C1	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.08	5 (6%)
33	CYC	P4	201	4	46,46,46	2.33	16 (34%)	61,67,67	3.00	28 (45%)
39	LMG	m1	101	-	36,36,55	1.12	2 (5%)	44,44,63	1.11	3 (6%)
33	CYC	g9	202	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
36	CLA	cD	514	-	69,73,73	1.25	11 (15%)	83,113,113	1.37	9 (10%)
36	CLA	C1	511	8	69,73,73	1.24	8 (11%)	83,113,113	1.24	11 (13%)
40	LMT	D1	403	-	24,24,36	1.16	3 (12%)	29,29,47	1.00	0
42	LHG	e1	101	-	39,39,48	1.03	2 (5%)	42,45,54	1.18	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	hE	101	43	69,73,73	1.74	10 (14%)	83,113,113	1.69	12 (14%)
36	CLA	cE	507	43,8	69,73,73	1.24	8 (11%)	83,113,113	1.71	15 (18%)
33	CYC	e5	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
33	CYC	Q4	201	4,3	46,46,46	2.33	19 (41%)	61,67,67	2.99	28 (45%)
33	CYC	mI	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
33	CYC	OB	201	3	46,46,46	2.31	16 (34%)	61,67,67	2.80	23 (37%)
36	CLA	C1	514	-	54,58,73	1.41	10 (18%)	65,95,113	1.42	6 (9%)
39	LMG	JE	102	14,39	27,27,55	1.31	2 (7%)	35,35,63	1.06	1 (2%)
40	LMT	jD	101	-	36,36,36	1.22	5 (13%)	47,47,47	1.25	6 (12%)
33	CYC	cA	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
36	CLA	cD	510	8	69,73,73	1.28	12 (17%)	83,113,113	1.48	15 (18%)
34	OEX	a1	402	6	0,14,14	-	-	-		
33	CYC	hI	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
43	BCR	hE	105	12,25,36	41,41,41	0.93	2 (4%)	56,56,56	2.64	19 (33%)
36	CLA	b1	612	7	69,73,73	1.24	8 (11%)	83,113,113	1.68	14 (16%)
40	LMT	bD	620	-	24,24,36	1.11	2 (8%)	29,29,47	1.04	1 (3%)
36	CLA	DE	406	9	69,73,73	1.25	10 (14%)	83,113,113	1.39	12 (14%)
36	CLA	b1	608	-	64,68,73	1.31	10 (15%)	77,107,113	1.52	13 (16%)
33	CYC	i5	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.89	31 (50%)
36	CLA	BE	602	7	69,73,73	1.22	11 (15%)	83,113,113	1.56	9 (10%)
39	LMG	t1	101	22	36,36,55	1.15	2 (5%)	44,44,63	0.99	3 (6%)
33	CYC	g3	202	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
33	CYC	f3	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	1G	201	4	46,46,46	2.58	18 (39%)	61,67,67	3.07	25 (40%)
33	CYC	R4	201	5,4	46,46,46	2.56	17 (36%)	61,67,67	3.25	30 (49%)
33	CYC	i9	201	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
47	HEM	ED	101	-	50,50,50	1.73	11 (22%)	66,82,82	1.84	17 (25%)
33	CYC	bC	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
38	SQD	hD	103	12	34,35,54	1.65	6 (17%)	43,46,65	1.91	10 (23%)
33	CYC	ML	201	4,2	46,46,46	2.37	16 (34%)	61,67,67	3.38	32 (52%)
33	CYC	QL	201	29	46,46,46	2.23	19 (41%)	61,67,67	3.20	30 (49%)
43	BCR	BD	617	-	41,41,41	0.73	0	56,56,56	1.86	12 (21%)
47	HEM	fE	101	-	50,50,50	1.74	11 (22%)	66,82,82	1.84	17 (25%)
33	CYC	oB	201	3	46,46,46	2.39	19 (41%)	61,67,67	3.08	26 (42%)
33	CYC	VB	201	3	46,46,46	2.38	13 (28%)	61,67,67	3.21	28 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	fC	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
36	CLA	cD	504	-	69,73,73	1.33	11 (15%)	83,113,113	1.48	12 (14%)
39	LMG	CD	522	39	51,51,55	0.92	2 (3%)	59,59,63	1.07	5 (8%)
33	CYC	h5	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
41	BCT	a1	411	46	2,3,3	1.15	0	2,3,3	4.49	2 (100%)
36	CLA	C1	503	-	69,73,73	1.24	11 (15%)	83,113,113	1.38	9 (10%)
39	LMG	aE	409	-	36,36,55	1.08	2 (5%)	44,44,63	1.07	2 (4%)
40	LMT	DD	413	-	22,22,36	1.17	3 (13%)	27,27,47	1.03	1 (3%)
42	LHG	B1	621	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
33	CYC	c3	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
33	CYC	e7	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
36	CLA	CE	507	-	59,63,73	1.37	10 (16%)	71,101,113	1.61	9 (12%)
33	CYC	g5	201	32	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
33	CYC	B4	1002	2	46,46,46	2.25	17 (36%)	61,67,67	3.02	25 (40%)
33	CYC	lI	201	-	46,46,46	2.22	14 (30%)	61,67,67	3.37	32 (52%)
36	CLA	D1	404	-	69,73,73	1.29	11 (15%)	83,113,113	1.47	6 (7%)
33	CYC	k5	201	-	46,46,46	2.30	15 (32%)	61,67,67	3.88	31 (50%)
36	CLA	cD	512	-	69,73,73	1.28	11 (15%)	83,113,113	1.49	14 (16%)
33	CYC	fH	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
36	CLA	B1	608	-	69,73,73	1.24	9 (13%)	83,113,113	1.42	9 (10%)
36	CLA	BE	606	-	64,68,73	1.30	10 (15%)	77,107,113	1.52	13 (16%)
40	LMT	b1	620	-	24,24,36	1.11	2 (8%)	29,29,47	1.04	1 (3%)
36	CLA	CD	515	-	69,73,73	1.25	10 (14%)	83,113,113	1.38	10 (12%)
36	CLA	cD	509	8	69,73,73	1.24	9 (13%)	83,113,113	2.11	12 (14%)
36	CLA	C1	507	-	59,63,73	1.36	10 (16%)	71,101,113	1.61	9 (12%)
33	CYC	l6	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
40	LMT	iD	103	-	24,24,36	1.14	2 (8%)	29,29,47	0.98	1 (3%)
33	CYC	KL	201	4,3	46,46,46	2.24	16 (34%)	61,67,67	2.92	25 (40%)
33	CYC	AL	201	4,3	46,46,46	2.17	15 (32%)	61,67,67	3.17	29 (47%)
33	CYC	j3	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	k8	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
47	HEM	VD	201	24	50,50,50	1.68	9 (18%)	66,82,82	1.90	13 (19%)
43	BCR	cD	519	-	41,41,41	0.83	0	56,56,56	2.00	16 (28%)
36	CLA	B1	607	7	69,73,73	1.34	10 (14%)	83,113,113	1.72	12 (14%)
40	LMT	jE	101	-	36,36,36	1.22	5 (13%)	47,47,47	1.25	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	KK	201	4	46,46,46	2.22	13 (28%)	61,67,67	3.23	32 (52%)
40	LMT	DE	412	-	25,25,36	1.10	2 (8%)	30,30,47	1.06	2 (6%)
33	CYC	BB	1001	4,2	46,46,46	2.36	17 (36%)	61,67,67	3.09	27 (44%)
40	LMT	CD	521	-	24,24,36	1.12	2 (8%)	29,29,47	1.14	3 (10%)
33	CYC	m2	201	-	46,46,46	0.80	0	61,67,67	0.80	1 (1%)
36	CLA	D1	405	9	69,73,73	1.25	10 (14%)	83,113,113	1.39	12 (14%)
33	CYC	TB	201	4	46,46,46	2.22	17 (36%)	61,67,67	3.21	33 (54%)
33	CYC	j6	202	-	46,46,46	0.78	0	61,67,67	0.82	1 (1%)
33	CYC	b6	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	kF	201	3	46,46,46	2.28	15 (32%)	61,67,67	2.92	25 (40%)
33	CYC	gH	202	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	32 (52%)
47	HEM	vE	201	24	50,50,50	1.68	9 (18%)	66,82,82	1.89	15 (22%)
36	CLA	DD	405	-	69,73,73	1.29	11 (15%)	83,113,113	1.48	6 (7%)
33	CYC	h9	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	b3	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	IL	201	-	46,46,46	2.49	18 (39%)	61,67,67	3.03	33 (54%)
42	LHG	eD	101	-	39,39,48	1.03	2 (5%)	42,45,54	1.18	4 (9%)
33	CYC	h6	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
36	CLA	c1	506	-	59,63,73	1.36	10 (16%)	71,101,113	1.61	9 (12%)
36	CLA	b1	604	7	69,73,73	1.23	11 (15%)	83,113,113	1.56	9 (10%)
33	CYC	cH	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
42	LHG	D1	409	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
33	CYC	lC	201	-	46,46,46	2.22	14 (30%)	61,67,67	3.37	32 (52%)
33	CYC	aK	201	4	46,46,46	2.25	15 (32%)	61,67,67	2.94	26 (42%)
33	CYC	c2	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
33	CYC	dI	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
36	CLA	C1	504	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
33	CYC	j3	202	-	46,46,46	0.78	0	61,67,67	0.81	1 (1%)
33	CYC	YF	201	4	46,46,46	2.57	19 (41%)	61,67,67	3.28	26 (42%)
33	CYC	t4	1001	4,2	46,46,46	3.00	20 (43%)	61,67,67	5.93	31 (50%)
33	CYC	k6	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
36	CLA	DD	406	9	69,73,73	1.25	10 (14%)	83,113,113	1.39	12 (14%)
36	CLA	c1	509	8	69,73,73	1.24	9 (13%)	83,113,113	2.11	11 (13%)
39	LMG	aD	407	-	51,51,55	0.92	2 (3%)	59,59,63	1.06	2 (3%)
44	DGD	c1	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	aD	405	-	69,73,73	1.25	11 (15%)	83,113,113	1.54	11 (13%)
33	CYC	VL	201	30	46,46,46	2.13	13 (28%)	61,67,67	3.21	32 (52%)
36	CLA	xE	101	25,9	69,73,73	1.23	11 (15%)	83,113,113	1.27	6 (7%)
36	CLA	c1	502	-	69,73,73	1.26	9 (13%)	83,113,113	1.40	8 (9%)
40	LMT	AE	409	-	24,24,36	1.13	3 (12%)	29,29,47	1.07	1 (3%)
36	CLA	a1	407	6	64,68,73	1.27	10 (15%)	77,107,113	1.55	12 (15%)
36	CLA	CE	509	8	69,73,73	1.24	11 (15%)	83,113,113	1.35	10 (12%)
36	CLA	cD	513	-	54,58,73	1.41	11 (20%)	65,95,113	1.45	6 (9%)
45	PHO	DE	403	9	58,69,69	2.67	16 (27%)	56,99,99	3.10	24 (42%)
36	CLA	bD	605	7	69,73,73	1.32	12 (17%)	83,113,113	1.35	8 (9%)
33	CYC	j2	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
43	BCR	cD	515	36,8	41,41,41	0.75	0	56,56,56	2.49	19 (33%)
39	LMG	bE	619	7	51,51,55	0.92	2 (3%)	59,59,63	1.17	3 (5%)
33	CYC	d6	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
43	BCR	bD	616	7,36	41,41,41	0.82	1 (2%)	56,56,56	2.51	22 (39%)
43	BCR	dD	407	-	41,41,41	0.70	0	56,56,56	1.82	13 (23%)
42	LHG	BD	620	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
33	CYC	gC	301	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	32 (52%)
33	CYC	e3	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.90	31 (50%)
33	CYC	g6	201	32	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
36	CLA	cE	508	8	69,73,73	1.28	11 (15%)	83,113,113	1.39	13 (15%)
33	CYC	hC	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
39	LMG	jE	102	14,39	27,27,55	1.35	2 (7%)	35,35,63	1.11	2 (5%)
33	CYC	7G	201	5,4	46,46,46	2.68	20 (43%)	61,67,67	3.32	28 (45%)
33	CYC	YB	201	5,4	46,46,46	2.22	15 (32%)	61,67,67	3.19	30 (49%)
33	CYC	m7	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
33	CYC	dH	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	c6	202	32	46,46,46	0.81	0	61,67,67	0.80	1 (1%)
36	CLA	CE	505	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	10 (12%)
36	CLA	cD	505	-	69,73,73	1.27	10 (14%)	83,113,113	1.40	11 (13%)
36	CLA	CD	508	43,8	69,73,73	1.28	10 (14%)	83,113,113	1.64	16 (19%)
33	CYC	eI	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
33	CYC	vB	201	4	46,46,46	2.27	16 (34%)	61,67,67	3.08	30 (49%)
33	CYC	i9	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.89	31 (50%)
36	CLA	BD	610	-	69,73,73	1.31	13 (18%)	83,113,113	1.52	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	c3	202	32	46,46,46	0.81	0	61,67,67	0.81	1 (1%)
36	CLA	CD	514	-	54,58,73	1.40	10 (18%)	65,95,113	1.41	6 (9%)
43	BCR	I1	102	13	41,41,41	0.79	0	56,56,56	2.77	18 (32%)
40	LMT	AD	412	-	36,36,36	1.21	4 (11%)	47,47,47	1.16	3 (6%)
37	PL9	dE	408	9	55,55,55	0.63	2 (3%)	68,69,69	1.62	17 (25%)
43	BCR	hD	105	12,25,36	41,41,41	0.93	2 (4%)	56,56,56	2.64	19 (33%)
33	CYC	jF	201	4	46,46,46	2.27	17 (36%)	61,67,67	2.83	28 (45%)
40	LMT	b1	601	7	36,36,36	1.34	8 (22%)	47,47,47	1.17	3 (6%)
40	LMT	dE	413	-	22,22,36	1.16	2 (9%)	27,27,47	1.01	1 (3%)
33	CYC	WL	201	4	46,46,46	2.28	15 (32%)	61,67,67	2.72	24 (39%)
33	CYC	h3	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	mK	201	30	46,46,46	2.13	13 (28%)	61,67,67	3.20	32 (52%)
33	CYC	JL	201	4,2	46,46,46	2.33	18 (39%)	61,67,67	3.17	27 (44%)
33	CYC	fJ	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
36	CLA	HE	101	12	64,68,73	1.29	11 (17%)	77,107,113	1.41	10 (12%)
33	CYC	2L	201	5,4	46,46,46	2.33	18 (39%)	61,67,67	3.16	33 (54%)
40	LMT	d1	404	-	24,24,36	1.15	2 (8%)	29,29,47	1.01	1 (3%)
47	HEM	VE	201	24	50,50,50	1.68	9 (18%)	66,82,82	1.90	14 (21%)
36	CLA	hD	102	12	64,68,73	1.30	11 (17%)	77,107,113	1.41	10 (12%)
33	CYC	f8	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
36	CLA	dD	405	-	69,73,73	1.29	11 (15%)	83,113,113	1.48	6 (7%)
40	LMT	B1	619	-	24,24,36	1.12	3 (12%)	29,29,47	1.04	1 (3%)
33	CYC	mH	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
39	LMG	CD	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.04	5 (8%)
33	CYC	j9	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	iI	201	-	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
36	CLA	BE	614	7	69,73,73	1.35	9 (13%)	83,113,113	1.33	11 (13%)
33	CYC	b8	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	4G	201	3	46,46,46	2.10	15 (32%)	61,67,67	3.50	34 (55%)
36	CLA	B1	611	7	69,73,73	1.24	9 (13%)	83,113,113	1.68	13 (15%)
36	CLA	cE	514	-	69,73,73	1.25	11 (15%)	83,113,113	1.36	9 (10%)
44	DGD	cE	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	3 (3%)
40	LMT	dD	412	-	25,25,36	1.10	2 (8%)	30,30,47	1.06	2 (6%)
45	PHO	DD	401	-	58,69,69	2.85	17 (29%)	56,99,99	3.24	25 (44%)
45	PHO	A1	412	6	58,69,69	3.10	18 (31%)	56,99,99	3.22	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	hK	201	4	46,46,46	2.57	19 (41%)	61,67,67	3.26	26 (42%)
36	CLA	C1	512	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	10 (12%)
44	DGD	CD	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.08	5 (6%)
33	CYC	e6	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
33	CYC	j5	202	-	46,46,46	0.78	0	61,67,67	0.81	1 (1%)
36	CLA	x1	101	25,9	69,73,73	1.24	11 (15%)	83,113,113	1.26	7 (8%)
33	CYC	IF	201	4	46,46,46	2.54	18 (39%)	61,67,67	3.30	29 (47%)
38	SQD	hE	103	12	34,35,54	1.65	6 (17%)	43,46,65	1.91	10 (23%)
33	CYC	jI	202	-	46,46,46	0.78	0	61,67,67	0.82	1 (1%)
33	CYC	g5	202	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	32 (52%)
36	CLA	cD	507	43,8	69,73,73	1.25	8 (11%)	83,113,113	1.71	15 (18%)
43	BCR	bD	617	7	41,41,41	0.70	0	56,56,56	1.87	14 (25%)
33	CYC	e5	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
45	PHO	aE	412	-	50,61,69	2.97	15 (30%)	46,89,99	3.48	23 (50%)
33	CYC	b5	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
39	LMG	dE	411	9	51,51,55	0.95	2 (3%)	59,59,63	1.26	5 (8%)
33	CYC	hA	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
39	LMG	TD	101	-	36,36,55	1.15	2 (5%)	44,44,63	0.99	3 (6%)
42	LHG	dD	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
45	PHO	d1	402	9	58,69,69	2.92	18 (31%)	56,99,99	3.07	22 (39%)
33	CYC	e8	201	32	46,46,46	2.31	15 (32%)	61,67,67	3.89	31 (50%)
47	HEM	V1	201	24	50,50,50	1.68	9 (18%)	66,82,82	1.91	14 (21%)
40	LMT	dE	404	-	24,24,36	1.15	2 (8%)	29,29,47	1.01	1 (3%)
36	CLA	C1	509	8	69,73,73	1.24	10 (14%)	83,113,113	1.36	10 (12%)
36	CLA	dE	405	-	69,73,73	1.29	11 (15%)	83,113,113	1.48	6 (7%)
33	CYC	i2	201	-	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
33	CYC	kC	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
33	CYC	hH	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	cI	202	32	46,46,46	0.81	0	61,67,67	0.80	1 (1%)
39	LMG	jD	102	14,39	27,27,55	1.35	2 (7%)	35,35,63	1.11	1 (2%)
37	PL9	aE	408	-	55,55,55	0.66	2 (3%)	68,69,69	1.46	12 (17%)
33	CYC	PG	201	3	46,46,46	2.28	15 (32%)	61,67,67	3.37	32 (52%)
40	LMT	BD	623	7	24,24,36	1.20	4 (16%)	29,29,47	1.14	1 (3%)
33	CYC	u4	201	4,3	46,46,46	2.35	13 (28%)	61,67,67	2.89	25 (40%)
47	HEM	fD	101	-	50,50,50	1.74	11 (22%)	66,82,82	1.84	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	OEX	A1	401	6	0,14,14	-	-	-		
33	CYC	kJ	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
36	CLA	BE	605	-	69,73,73	1.28	11 (15%)	83,113,113	1.58	10 (12%)
43	BCR	BE	615	7,36	41,41,41	0.82	1 (2%)	56,56,56	2.51	22 (39%)
33	CYC	c8	202	32	46,46,46	0.81	0	61,67,67	0.81	1 (1%)
33	CYC	lH	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
40	LMT	D1	412	-	22,22,36	1.17	3 (13%)	27,27,47	1.03	1 (3%)
36	CLA	IE	101	13,6	64,68,73	1.28	11 (17%)	77,107,113	1.39	8 (10%)
36	CLA	bE	609	7	69,73,73	1.35	10 (14%)	83,113,113	1.71	12 (14%)
33	CYC	eC	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
43	BCR	b1	618	-	41,41,41	0.73	0	56,56,56	1.86	12 (21%)
33	CYC	m8	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
33	CYC	e7	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
36	CLA	H1	101	12	64,68,73	1.30	11 (17%)	77,107,113	1.41	10 (12%)
36	CLA	XE	101	25	69,73,73	1.24	11 (15%)	83,113,113	1.26	7 (8%)
33	CYC	e3	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
33	CYC	g6	202	32	46,46,46	2.30	15 (32%)	61,67,67	3.88	32 (52%)
33	CYC	kI	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
36	CLA	DE	405	-	69,73,73	1.28	11 (15%)	83,113,113	1.47	6 (7%)
33	CYC	wB	201	3	46,46,46	2.23	14 (30%)	61,67,67	2.96	24 (39%)
39	LMG	CE	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.04	5 (8%)
39	LMG	d1	411	9	51,51,55	0.95	2 (3%)	59,59,63	1.27	5 (8%)
33	CYC	jA	202	-	46,46,46	0.78	0	61,67,67	0.81	1 (1%)
39	LMG	T1	101	-	36,36,55	1.15	2 (5%)	44,44,63	0.99	3 (6%)
33	CYC	C4	1001	2	46,46,46	2.24	18 (39%)	61,67,67	3.02	25 (40%)
33	CYC	GG	201	4,3	46,46,46	2.24	16 (34%)	61,67,67	3.18	27 (44%)
39	LMG	AD	408	-	36,36,55	1.09	2 (5%)	44,44,63	1.10	5 (11%)
43	BCR	bD	618	-	41,41,41	0.74	0	56,56,56	1.86	13 (23%)
33	CYC	OG	201	4	46,46,46	2.26	17 (36%)	61,67,67	3.29	27 (44%)
36	CLA	cD	506	8	69,73,73	1.31	11 (15%)	83,113,113	1.65	14 (16%)
36	CLA	d1	405	-	69,73,73	1.30	11 (15%)	83,113,113	1.48	6 (7%)
36	CLA	bE	603	-	49,53,73	1.48	10 (20%)	59,89,113	1.61	8 (13%)
33	CYC	k3	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
33	CYC	eA	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
38	SQD	d1	414	9	33,34,54	1.48	4 (12%)	42,45,65	1.52	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	DGD	c1	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.11	6 (7%)
43	BCR	iD	102	-	41,41,41	0.78	1 (2%)	56,56,56	2.55	19 (33%)
36	CLA	I1	101	13,6	64,68,73	1.28	11 (17%)	77,107,113	1.39	8 (10%)
33	CYC	b2	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
36	CLA	aE	405	-	69,73,73	1.25	11 (15%)	83,113,113	1.54	10 (12%)
40	LMT	iE	103	-	24,24,36	1.14	2 (8%)	29,29,47	0.98	1 (3%)
42	LHG	dD	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
36	CLA	BD	602	7	69,73,73	1.22	11 (15%)	83,113,113	1.57	9 (10%)
37	PL9	A1	406	-	55,55,55	0.64	1 (1%)	68,69,69	1.47	11 (16%)
33	CYC	d3	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
42	LHG	DE	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
43	BCR	h1	105	12,25,36	41,41,41	0.93	2 (4%)	56,56,56	2.64	19 (33%)
33	CYC	9F	201	3	46,46,46	2.18	16 (34%)	61,67,67	3.00	24 (39%)
33	CYC	cK	201	4	46,46,46	2.17	18 (39%)	61,67,67	3.20	30 (49%)
36	CLA	BE	604	7	69,73,73	1.26	10 (14%)	83,113,113	1.48	12 (14%)
33	CYC	bJ	201	-	46,46,46	2.23	14 (30%)	61,67,67	3.36	32 (52%)
40	LMT	dE	412	-	25,25,36	1.11	2 (8%)	30,30,47	1.06	2 (6%)
36	CLA	bD	613	-	69,73,73	1.29	11 (15%)	83,113,113	1.33	6 (7%)
43	BCR	c1	519	-	41,41,41	0.83	0	56,56,56	2.01	16 (28%)
36	CLA	xD	101	25,9	69,73,73	1.23	11 (15%)	83,113,113	1.26	6 (7%)
43	BCR	dE	407	-	41,41,41	0.70	0	56,56,56	1.82	13 (23%)
47	HEM	EE	101	-	50,50,50	1.73	11 (22%)	66,82,82	1.83	16 (24%)
36	CLA	bD	612	7	69,73,73	1.24	8 (11%)	83,113,113	1.69	14 (16%)
39	LMG	BD	618	7	51,51,55	0.92	2 (3%)	59,59,63	1.17	3 (5%)
36	CLA	a1	406	-	69,73,73	1.25	11 (15%)	83,113,113	1.54	11 (13%)
42	LHG	d1	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
36	CLA	h1	101	43	69,73,73	1.75	10 (14%)	83,113,113	1.70	9 (10%)
33	CYC	jI	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
44	DGD	HE	102	-	63,63,67	0.85	2 (3%)	77,77,81	1.04	4 (5%)
36	CLA	aE	404	-	50,54,73	11.59	11 (22%)	60,90,113	1.61	8 (13%)
33	CYC	c5	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
36	CLA	AE	405	-	69,73,73	1.23	9 (13%)	83,113,113	1.63	14 (16%)
42	LHG	aD	411	6	37,37,48	1.04	2 (5%)	40,43,54	1.23	4 (10%)
36	CLA	C1	510	8	69,73,73	1.25	11 (15%)	83,113,113	2.19	17 (20%)
36	CLA	BD	601	-	49,53,73	1.47	10 (20%)	59,89,113	1.64	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	SQD	dD	414	9	33,34,54	1.48	4 (12%)	42,45,65	1.52	6 (14%)
33	CYC	PL	201	3	46,46,46	2.28	15 (32%)	61,67,67	3.37	32 (52%)
36	CLA	BD	606	-	64,68,73	1.31	10 (15%)	77,107,113	1.51	13 (16%)
33	CYC	LK	201	4,3	46,46,46	2.34	17 (36%)	61,67,67	3.10	23 (37%)
36	CLA	cD	503	-	69,73,73	1.26	10 (14%)	83,113,113	1.39	8 (9%)
33	CYC	6G	201	3	46,46,46	2.23	18 (39%)	61,67,67	3.21	29 (47%)
44	DGD	hE	104	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	6 (7%)
33	CYC	s4	201	3	46,46,46	2.21	15 (32%)	61,67,67	3.27	29 (47%)
33	CYC	h2	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	SB	201	4,3	46,46,46	2.35	14 (30%)	61,67,67	2.64	28 (45%)
33	CYC	i8	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.89	31 (50%)
33	CYC	lJ	201	-	46,46,46	2.22	14 (30%)	61,67,67	3.37	32 (52%)
33	CYC	LL	201	4,2	46,46,46	2.37	19 (41%)	61,67,67	5.02	37 (60%)
33	CYC	kA	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
43	BCR	CD	520	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
43	BCR	ZD	101	27	41,41,41	0.73	0	56,56,56	2.17	23 (41%)
38	SQD	BD	621	-	37,38,54	1.43	4 (10%)	46,49,65	4.33	9 (19%)
40	LMT	D1	411	-	25,25,36	1.10	2 (8%)	30,30,47	1.06	2 (6%)
36	CLA	c1	507	43,8	69,73,73	1.26	9 (13%)	83,113,113	1.72	15 (18%)
33	CYC	e6	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
43	BCR	c1	515	36,8	41,41,41	0.76	0	56,56,56	2.49	20 (35%)
36	CLA	b1	603	-	49,53,73	1.46	10 (20%)	59,89,113	1.61	9 (15%)
37	PL9	DD	408	9	55,55,55	0.63	2 (3%)	68,69,69	1.62	17 (25%)
33	CYC	nF	202	4,3	46,46,46	2.28	17 (36%)	61,67,67	2.76	25 (40%)
36	CLA	bE	604	7	69,73,73	1.23	11 (15%)	83,113,113	1.57	9 (10%)
41	BCT	A1	410	-	2,3,3	1.15	0	2,3,3	4.49	2 (100%)
33	CYC	bA	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
39	LMG	C1	521	39	51,51,55	0.92	2 (3%)	59,59,63	1.07	5 (8%)
33	CYC	j6	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	gH	201	32	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
33	CYC	LF	201	4,3	46,46,46	2.34	17 (36%)	61,67,67	3.10	23 (37%)
33	CYC	l5	201	-	46,46,46	2.22	14 (30%)	61,67,67	3.37	32 (52%)
36	CLA	c1	513	-	54,58,73	1.41	11 (20%)	65,95,113	1.47	6 (9%)
33	CYC	W4	201	4	46,46,46	2.22	15 (32%)	61,67,67	3.03	29 (47%)
33	CYC	jA	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LMG	yD	101	39	51,51,55	0.90	2 (3%)	59,59,63	1.08	5 (8%)
33	CYC	TG	201	3	46,46,46	2.30	17 (36%)	61,67,67	3.19	26 (42%)
33	CYC	y4	201	3	46,46,46	2.22	15 (32%)	61,67,67	3.38	28 (45%)
36	CLA	CD	506	8	69,73,73	1.29	11 (15%)	83,113,113	1.69	15 (18%)
36	CLA	c1	511	-	69,73,73	1.27	9 (13%)	83,113,113	1.41	6 (7%)
45	PHO	dD	402	9	46,57,69	3.58	15 (32%)	41,84,99	3.15	15 (36%)
47	HEM	vD	201	24	50,50,50	1.68	9 (18%)	66,82,82	1.89	14 (21%)
36	CLA	A1	405	-	69,73,73	1.23	9 (13%)	83,113,113	1.63	14 (16%)
33	CYC	j8	202	-	46,46,46	0.78	0	61,67,67	0.81	1 (1%)
33	CYC	c5	202	32	46,46,46	0.80	0	61,67,67	0.80	1 (1%)
33	CYC	jJ	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
45	PHO	aD	412	6	58,69,69	2.95	20 (34%)	56,99,99	3.06	23 (41%)
36	CLA	BD	614	7	69,73,73	1.35	9 (13%)	83,113,113	1.33	11 (13%)
44	DGD	HD	102	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	4 (5%)
33	CYC	d9	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	h7	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
36	CLA	CD	503	-	69,73,73	1.24	11 (15%)	83,113,113	1.38	9 (10%)
33	CYC	i6	202	-	46,46,46	2.31	16 (34%)	61,67,67	3.89	31 (50%)
40	LMT	a1	401	-	36,36,36	1.28	5 (13%)	47,47,47	1.15	1 (2%)
33	CYC	eH	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
33	CYC	RB	201	5,4	46,46,46	2.55	17 (36%)	61,67,67	3.25	30 (49%)
33	CYC	b7	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
45	PHO	a1	413	-	46,57,69	3.57	15 (32%)	41,84,99	3.65	21 (51%)
36	CLA	bD	615	7	69,73,73	1.35	9 (13%)	83,113,113	1.33	11 (13%)
33	CYC	fF	201	3	46,46,46	2.28	17 (36%)	61,67,67	3.12	28 (45%)
33	CYC	bH	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	j7	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
40	LMT	bE	601	7	36,36,36	1.34	8 (22%)	47,47,47	1.17	3 (6%)
33	CYC	mJ	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
33	CYC	HG	201	4,2	46,46,46	2.16	15 (32%)	61,67,67	3.76	33 (54%)
36	CLA	dE	403	-	69,73,73	1.24	9 (13%)	83,113,113	1.40	9 (10%)
33	CYC	JG	201	4,2	46,46,46	2.33	18 (39%)	61,67,67	3.17	27 (44%)
33	CYC	5L	201	5,4	46,46,46	2.27	17 (36%)	61,67,67	3.25	33 (54%)
33	CYC	CB	1001	2	46,46,46	2.25	18 (39%)	61,67,67	3.02	24 (39%)
36	CLA	HD	103	43	69,73,73	1.75	10 (14%)	83,113,113	1.71	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	PHO	DD	403	9	51,62,69	3.23	19 (37%)	47,90,99	3.11	24 (51%)
33	CYC	i7	201	-	46,46,46	0.79	0	61,67,67	0.80	1 (1%)
37	PL9	D1	407	9	55,55,55	0.63	1 (1%)	68,69,69	1.62	17 (25%)
33	CYC	m5	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
33	CYC	cI	201	-	46,46,46	2.30	15 (32%)	61,67,67	3.87	31 (50%)
36	CLA	bE	607	-	69,73,73	1.27	11 (15%)	83,113,113	1.58	10 (12%)
33	CYC	rB	201	4,2	46,46,46	2.21	18 (39%)	61,67,67	3.18	33 (54%)
33	CYC	r4	201	4,2	46,46,46	2.21	18 (39%)	61,67,67	3.18	34 (55%)
33	CYC	cC	201	-	46,46,46	2.30	15 (32%)	61,67,67	3.86	31 (50%)
33	CYC	f6	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
38	SQD	LD	102	-	42,43,54	1.35	5 (11%)	51,54,65	1.22	4 (7%)
38	SQD	AE	407	-	45,46,54	1.28	4 (8%)	54,57,65	1.27	4 (7%)
42	LHG	DD	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
33	CYC	mF	201	30	46,46,46	2.13	13 (28%)	61,67,67	3.20	32 (52%)
36	CLA	bE	610	-	69,73,73	1.25	10 (14%)	83,113,113	1.39	8 (9%)
41	BCT	AD	410	-	2,3,3	1.15	0	2,3,3	4.50	2 (100%)
37	PL9	dD	408	9	55,55,55	0.63	2 (3%)	68,69,69	1.62	17 (25%)
36	CLA	HD	101	12	64,68,73	1.29	11 (17%)	77,107,113	1.41	10 (12%)
36	CLA	b1	614	43	69,73,73	1.22	10 (14%)	83,113,113	1.37	8 (9%)
33	CYC	e2	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
33	CYC	g2	201	32	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
33	CYC	k7	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.88	31 (50%)
36	CLA	b1	609	7	69,73,73	1.35	10 (14%)	83,113,113	1.70	12 (14%)
33	CYC	V4	201	3	46,46,46	2.38	13 (28%)	61,67,67	3.22	28 (45%)
33	CYC	mA	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
40	LMT	bE	621	-	24,24,36	1.12	2 (8%)	29,29,47	1.14	3 (10%)
33	CYC	MF	201	5,4	46,46,46	2.28	17 (36%)	61,67,67	3.21	30 (49%)
38	SQD	LE	102	-	42,43,54	1.35	5 (11%)	51,54,65	1.23	4 (7%)
43	BCR	B1	615	7,36	41,41,41	0.82	1 (2%)	56,56,56	2.51	22 (39%)
36	CLA	BE	610	-	69,73,73	1.31	13 (18%)	83,113,113	1.52	12 (14%)
40	LMT	dD	404	-	24,24,36	1.15	2 (8%)	29,29,47	1.01	2 (6%)
33	CYC	WB	201	4	46,46,46	2.22	15 (32%)	61,67,67	3.03	29 (47%)
47	HEM	f1	101	-	50,50,50	1.74	11 (22%)	66,82,82	1.85	17 (25%)
36	CLA	B1	603	7	69,73,73	1.33	12 (17%)	83,113,113	1.37	8 (9%)
33	CYC	MK	201	5,4	46,46,46	2.28	17 (36%)	61,67,67	3.20	30 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	mC	201	-	46,46,46	0.80	0	61,67,67	0.79	1 (1%)
33	CYC	i3	201	-	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
40	LMT	i1	102	-	24,24,36	1.15	2 (8%)	29,29,47	0.98	1 (3%)
33	CYC	d8	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
40	LMT	DD	404	-	24,24,36	1.16	3 (12%)	29,29,47	1.01	1 (3%)
36	CLA	BD	604	7	69,73,73	1.26	10 (14%)	83,113,113	1.48	11 (13%)
36	CLA	b1	615	7	69,73,73	1.34	9 (13%)	83,113,113	1.33	11 (13%)
33	CYC	iA	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.89	31 (50%)
38	SQD	cE	502	8	53,54,54	1.18	4 (7%)	62,65,65	1.15	5 (8%)
36	CLA	cE	509	8	69,73,73	1.24	9 (13%)	83,113,113	2.11	12 (14%)
43	BCR	bE	617	7	41,41,41	0.70	0	56,56,56	1.87	14 (25%)
45	PHO	D1	402	9	58,69,69	2.68	15 (25%)	56,99,99	3.07	25 (44%)
33	CYC	SG	201	4,2	46,46,46	2.25	16 (34%)	61,67,67	2.97	28 (45%)
33	CYC	cA	202	32	46,46,46	0.81	0	61,67,67	0.80	1 (1%)
39	LMG	dD	411	9	51,51,55	0.95	2 (3%)	59,59,63	1.27	5 (8%)
40	LMT	A1	413	-	36,36,36	1.21	4 (11%)	47,47,47	1.16	3 (6%)
43	BCR	DD	407	-	41,41,41	0.71	0	56,56,56	1.82	12 (21%)
43	BCR	iE	102	-	41,41,41	0.78	1 (2%)	56,56,56	2.55	19 (33%)
33	CYC	S4	201	4,3	46,46,46	2.35	14 (30%)	61,67,67	2.64	29 (47%)
47	HEM	E1	101	-	50,50,50	1.73	11 (22%)	66,82,82	1.83	17 (25%)
36	CLA	aD	406	6	64,68,73	1.27	10 (15%)	77,107,113	1.54	12 (15%)
33	CYC	cJ	202	32	46,46,46	0.81	0	61,67,67	0.80	1 (1%)
33	CYC	iH	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.89	31 (50%)
36	CLA	b1	607	-	69,73,73	1.26	11 (15%)	83,113,113	1.58	10 (12%)
39	LMG	AE	408	-	36,36,55	1.09	2 (5%)	44,44,63	1.10	5 (11%)
33	CYC	KG	201	4,3	46,46,46	2.24	16 (34%)	61,67,67	2.92	25 (40%)
33	CYC	g8	201	32	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
43	BCR	BE	617	-	41,41,41	0.73	0	56,56,56	1.86	12 (21%)
33	CYC	jJ	202	-	46,46,46	0.78	0	61,67,67	0.81	1 (1%)
36	CLA	aE	406	6	64,68,73	1.27	10 (15%)	77,107,113	1.55	12 (15%)
33	CYC	NG	201	3	46,46,46	2.12	14 (30%)	61,67,67	3.10	27 (44%)
36	CLA	bE	605	7	69,73,73	1.33	12 (17%)	83,113,113	1.34	8 (9%)
40	LMT	bD	601	7	36,36,36	1.34	8 (22%)	47,47,47	1.17	3 (6%)
43	BCR	CE	516	36,8	41,41,41	0.76	0	56,56,56	2.24	18 (32%)
36	CLA	ID	101	13,6	64,68,73	1.28	11 (17%)	77,107,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	CE	508	43,8	69,73,73	1.28	10 (14%)	83,113,113	1.64	15 (18%)
33	CYC	v4	201	4	46,46,46	2.27	16 (34%)	61,67,67	3.08	30 (49%)
33	CYC	i3	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.89	31 (50%)
43	BCR	cE	515	36,8	41,41,41	0.75	0	56,56,56	2.49	20 (35%)
33	CYC	d5	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.36	32 (52%)
36	CLA	bE	614	43	69,73,73	1.23	10 (14%)	83,113,113	1.36	8 (9%)
36	CLA	CD	510	8	69,73,73	1.24	11 (15%)	83,113,113	2.20	17 (20%)
36	CLA	c1	505	8	69,73,73	1.31	11 (15%)	83,113,113	1.65	14 (16%)
33	CYC	gJ	201	32	46,46,46	0.77	0	61,67,67	0.80	1 (1%)
36	CLA	iD	101	-	59,63,73	1.35	10 (16%)	71,101,113	1.60	9 (12%)
39	LMG	y1	101	39	51,51,55	0.91	2 (3%)	59,59,63	1.08	5 (8%)
33	CYC	O4	201	3	46,46,46	2.31	16 (34%)	61,67,67	2.80	23 (37%)
36	CLA	dD	403	-	69,73,73	1.24	8 (11%)	83,113,113	1.41	9 (10%)
40	LMT	DE	404	-	24,24,36	1.16	3 (12%)	29,29,47	1.01	1 (3%)
36	CLA	C1	508	43,8	69,73,73	1.28	11 (15%)	83,113,113	1.65	16 (19%)
40	LMT	b1	602	-	24,24,36	1.16	2 (8%)	29,29,47	1.02	0
33	CYC	cH	202	32	46,46,46	0.81	0	61,67,67	0.80	1 (1%)
36	CLA	bD	609	7	69,73,73	1.35	10 (14%)	83,113,113	1.70	12 (14%)
36	CLA	B1	602	7	69,73,73	1.22	11 (15%)	83,113,113	1.56	9 (10%)
38	SQD	CE	501	8	53,54,54	1.18	4 (7%)	62,65,65	1.18	7 (11%)
33	CYC	B4	1001	4,2	46,46,46	2.36	17 (36%)	61,67,67	3.10	27 (44%)
43	BCR	ZE	101	27	41,41,41	0.72	0	56,56,56	2.17	23 (41%)
43	BCR	zE	101	27	41,41,41	0.72	0	56,56,56	2.17	22 (39%)
40	LMT	BD	622	-	36,36,36	1.28	5 (13%)	47,47,47	1.15	1 (2%)
37	PL9	aD	408	-	55,55,55	0.66	1 (1%)	68,69,69	1.46	12 (17%)
33	CYC	d2	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	i7	202	-	46,46,46	2.30	16 (34%)	61,67,67	3.88	31 (50%)
33	CYC	fI	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.38	32 (52%)
36	CLA	b1	613	-	69,73,73	1.29	11 (15%)	83,113,113	1.32	6 (7%)
36	CLA	BD	612	-	69,73,73	1.29	11 (15%)	83,113,113	1.32	6 (7%)
36	CLA	BE	601	-	49,53,73	1.48	10 (20%)	59,89,113	1.64	8 (13%)
44	DGD	H1	102	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	4 (5%)
36	CLA	aD	404	-	50,54,73	11.60	11 (22%)	60,90,113	1.61	8 (13%)
33	CYC	NL	201	3	46,46,46	2.12	14 (30%)	61,67,67	3.10	27 (44%)
33	CYC	IK	201	4	46,46,46	2.54	18 (39%)	61,67,67	3.30	31 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	eA	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
36	CLA	c1	503	-	69,73,73	1.33	11 (15%)	83,113,113	1.48	12 (14%)
36	CLA	hD	101	43	69,73,73	1.75	10 (14%)	83,113,113	1.70	11 (13%)
36	CLA	bD	606	7	69,73,73	1.26	10 (14%)	83,113,113	1.48	11 (13%)
44	DGD	CE	517	8	48,48,67	0.97	2 (4%)	62,62,81	1.27	8 (12%)
38	SQD	B1	622	-	37,38,54	1.43	4 (10%)	46,49,65	4.33	9 (19%)
36	CLA	BE	613	43	69,73,73	1.24	10 (14%)	83,113,113	1.37	7 (8%)
36	CLA	B1	614	7	69,73,73	1.35	9 (13%)	83,113,113	1.33	11 (13%)
39	LMG	yE	101	39	51,51,55	0.90	2 (3%)	59,59,63	1.08	4 (6%)
44	DGD	hD	104	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	6 (7%)
33	CYC	iC	201	-	46,46,46	0.79	0	61,67,67	0.79	1 (1%)
38	SQD	LD	101	-	42,43,54	1.34	5 (11%)	51,54,65	1.22	4 (7%)
39	LMG	J1	102	14,39	27,27,55	1.30	2 (7%)	35,35,63	1.06	1 (2%)
33	CYC	RL	201	4,3	46,46,46	2.19	14 (30%)	61,67,67	3.04	28 (45%)
33	CYC	XK	201	3	46,46,46	2.30	16 (34%)	61,67,67	3.11	27 (44%)
33	CYC	m3	201	-	46,46,46	0.80	0	61,67,67	0.80	1 (1%)
33	CYC	3F	101	5,4	46,46,46	2.35	17 (36%)	61,67,67	3.05	29 (47%)
33	CYC	6L	201	3	46,46,46	2.23	18 (39%)	61,67,67	3.21	29 (47%)
44	DGD	C1	517	8	48,48,67	0.98	2 (4%)	62,62,81	1.27	8 (12%)
36	CLA	d1	406	9	69,73,73	1.26	11 (15%)	83,113,113	1.41	12 (14%)
33	CYC	VG	201	30	46,46,46	2.13	13 (28%)	61,67,67	3.21	32 (52%)
33	CYC	f9	201	31	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	lA	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	hJ	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.36	32 (52%)
33	CYC	jC	202	-	46,46,46	0.78	0	61,67,67	0.82	1 (1%)
33	CYC	gC	302	32	46,46,46	0.78	0	61,67,67	0.80	1 (1%)
36	CLA	CD	509	8	69,73,73	1.24	11 (15%)	83,113,113	1.35	10 (12%)
33	CYC	5G	201	5,4	46,46,46	2.27	17 (36%)	61,67,67	3.25	33 (54%)
42	LHG	lE	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
33	CYC	dA	201	-	46,46,46	2.22	14 (30%)	61,67,67	3.37	32 (52%)
33	CYC	gA	301	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
33	CYC	l7	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	HL	201	4,2	46,46,46	2.15	15 (32%)	61,67,67	3.76	33 (54%)
43	BCR	XD	102	25,36	41,41,41	0.93	2 (4%)	56,56,56	2.63	20 (35%)
36	CLA	CE	514	-	54,58,73	1.40	10 (18%)	65,95,113	1.41	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	CLA	dE	406	9	69,73,73	1.26	11 (15%)	83,113,113	1.41	12 (14%)
33	CYC	4L	201	3	46,46,46	2.10	14 (30%)	61,67,67	3.50	34 (55%)
36	CLA	bD	607	-	69,73,73	1.27	11 (15%)	83,113,113	1.58	10 (12%)
43	BCR	BD	616	7	41,41,41	0.69	0	56,56,56	1.87	14 (25%)
33	CYC	9K	201	3	46,46,46	2.18	16 (34%)	61,67,67	3.01	24 (39%)
33	CYC	e9	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
33	CYC	YK	201	4	46,46,46	2.57	19 (41%)	61,67,67	3.27	26 (42%)
33	CYC	gF	201	29	46,46,46	2.23	19 (41%)	61,67,67	3.22	29 (47%)
37	PL9	AE	406	-	55,55,55	0.64	1 (1%)	68,69,69	1.46	11 (16%)
33	CYC	T4	201	4	46,46,46	2.22	17 (36%)	61,67,67	3.20	33 (54%)
38	SQD	L1	102	-	42,43,54	1.35	5 (11%)	51,54,65	1.23	4 (7%)
33	CYC	dJ	201	-	46,46,46	2.23	14 (30%)	61,67,67	3.37	32 (52%)
36	CLA	c1	504	-	69,73,73	1.27	9 (13%)	83,113,113	1.41	11 (13%)
36	CLA	cE	513	-	54,58,73	1.41	11 (20%)	65,95,113	1.46	6 (9%)
38	SQD	dE	414	9	33,34,54	1.48	4 (12%)	42,45,65	1.52	6 (14%)
39	LMG	mE	101	-	36,36,55	1.12	2 (5%)	44,44,63	1.11	3 (6%)
33	CYC	k2	201	-	46,46,46	2.30	16 (34%)	61,67,67	3.89	31 (50%)
33	CYC	X4	201	4,3	46,46,46	2.35	16 (34%)	61,67,67	2.92	24 (39%)
36	CLA	AE	404	-	50,54,73	11.58	12 (24%)	60,90,113	2.06	12 (20%)
33	CYC	Z4	201	3	46,46,46	2.30	18 (39%)	61,67,67	2.94	23 (37%)
36	CLA	A1	404	-	50,54,73	11.58	12 (24%)	60,90,113	2.07	12 (20%)
39	LMG	JD	102	14,39	27,27,55	1.30	2 (7%)	35,35,63	1.06	1 (2%)
33	CYC	m9	201	-	46,46,46	0.79	0	61,67,67	0.80	1 (1%)
36	CLA	bE	613	-	69,73,73	1.29	11 (15%)	83,113,113	1.33	6 (7%)
33	CYC	j2	202	-	46,46,46	0.78	0	61,67,67	0.82	1 (1%)
33	CYC	aF	201	4	46,46,46	2.25	15 (32%)	61,67,67	2.94	26 (42%)
33	CYC	g8	202	32	46,46,46	2.31	15 (32%)	61,67,67	3.89	32 (52%)
33	CYC	eJ	201	32	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
43	BCR	Z1	101	27	41,41,41	0.73	0	56,56,56	2.16	23 (41%)
36	CLA	CD	511	8	69,73,73	1.25	8 (11%)	83,113,113	1.24	11 (13%)
33	CYC	iC	202	-	46,46,46	2.30	15 (32%)	61,67,67	3.89	31 (50%)
36	CLA	CE	515	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	10 (12%)
39	LMG	MD	101	-	36,36,55	1.11	2 (5%)	44,44,63	1.11	3 (6%)
43	BCR	CD	519	-	41,41,41	0.74	0	56,56,56	1.79	14 (25%)
37	PL9	d1	408	9	55,55,55	0.63	2 (3%)	68,69,69	1.62	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	CYC	f2	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.38	32 (52%)
33	CYC	l8	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.38	32 (52%)
33	CYC	h8	201	-	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
40	LMT	BE	622	-	36,36,36	1.28	5 (13%)	47,47,47	1.15	1 (2%)
33	CYC	PB	201	4	46,46,46	2.33	16 (34%)	61,67,67	2.99	28 (45%)
42	LHG	dE	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	2 (3%)
33	CYC	o4	201	3	46,46,46	2.39	19 (41%)	61,67,67	3.09	26 (42%)
40	LMT	BD	619	-	24,24,36	1.12	3 (12%)	29,29,47	1.04	1 (3%)
33	CYC	i8	201	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
39	LMG	C1	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.04	5 (8%)
36	CLA	XD	101	25	69,73,73	1.24	11 (15%)	83,113,113	1.27	7 (8%)
33	CYC	fA	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	iJ	201	-	46,46,46	0.79	0	61,67,67	0.80	1 (1%)
36	CLA	CE	503	-	69,73,73	1.24	11 (15%)	83,113,113	1.38	9 (10%)
38	SQD	A1	407	-	45,46,54	1.28	4 (8%)	54,57,65	1.27	4 (7%)
33	CYC	KF	201	4	46,46,46	2.22	13 (28%)	61,67,67	3.24	32 (52%)
36	CLA	bD	603	-	49,53,73	1.47	10 (20%)	59,89,113	1.61	8 (13%)
36	CLA	bD	604	7	69,73,73	1.23	11 (15%)	83,113,113	1.57	9 (10%)
34	OEX	aE	401	6	0,14,14	-	-	-		
40	LMT	DD	412	-	25,25,36	1.11	2 (8%)	30,30,47	1.06	2 (6%)
33	CYC	j9	202	-	46,46,46	0.78	0	61,67,67	0.81	1 (1%)
36	CLA	cD	508	8	69,73,73	1.28	11 (15%)	83,113,113	1.39	13 (15%)
41	BCT	aE	410	46	2,3,3	1.15	0	2,3,3	4.48	2 (100%)
33	CYC	j5	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
36	CLA	X1	101	25	69,73,73	1.25	11 (15%)	83,113,113	1.26	6 (7%)
33	CYC	jH	201	-	46,46,46	2.22	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	GL	201	4,3	46,46,46	2.25	16 (34%)	61,67,67	3.19	27 (44%)
38	SQD	LE	101	-	42,43,54	1.34	5 (11%)	51,54,65	1.22	4 (7%)
36	CLA	B1	613	43	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)
36	CLA	B1	610	-	69,73,73	1.31	13 (18%)	83,113,113	1.52	11 (13%)
43	BCR	ID	102	13	41,41,41	0.79	0	56,56,56	2.77	18 (32%)
33	CYC	dF	201	3	46,46,46	2.58	19 (41%)	61,67,67	3.28	27 (44%)
33	CYC	eH	202	-	46,46,46	0.78	0	61,67,67	0.79	1 (1%)
33	CYC	z4	201	4,2	46,46,46	2.27	18 (39%)	61,67,67	3.28	35 (57%)
33	CYC	uB	201	4,3	46,46,46	2.35	13 (28%)	61,67,67	2.89	25 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	OEX	AD	401	6	0,14,14	-	-	-		
34	OEX	aD	401	6	0,14,14	-	-	-		
44	DGD	cE	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.11	6 (7%)
44	DGD	h1	104	-	63,63,67	0.87	2 (3%)	77,77,81	1.14	6 (7%)
33	CYC	gK	201	29	46,46,46	2.23	19 (41%)	61,67,67	3.22	30 (49%)
44	DGD	J1	101	-	63,63,67	0.83	2 (3%)	77,77,81	0.99	4 (5%)
33	CYC	cF	201	4	46,46,46	2.16	18 (39%)	61,67,67	3.19	30 (49%)
40	LMT	j1	101	-	36,36,36	1.23	5 (13%)	47,47,47	1.24	6 (12%)
43	BCR	B1	617	-	41,41,41	0.73	0	56,56,56	1.86	12 (21%)
36	CLA	BE	609	-	69,73,73	1.25	10 (14%)	83,113,113	1.38	8 (9%)
33	CYC	c6	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
33	CYC	f7	201	31	46,46,46	2.23	15 (32%)	61,67,67	3.37	32 (52%)
33	CYC	nK	202	4,3	46,46,46	2.28	17 (36%)	61,67,67	2.75	25 (40%)
36	CLA	d1	403	-	69,73,73	1.24	9 (13%)	83,113,113	1.41	9 (10%)
36	CLA	bE	611	-	69,73,73	1.30	13 (18%)	83,113,113	1.52	10 (12%)
38	SQD	D1	413	9	33,34,54	1.48	4 (12%)	42,45,65	1.52	6 (14%)
36	CLA	H1	103	43	69,73,73	1.75	10 (14%)	83,113,113	1.71	9 (10%)
40	LMT	AD	409	-	24,24,36	1.14	3 (12%)	29,29,47	1.07	1 (3%)
33	CYC	fK	201	3	46,46,46	2.28	17 (36%)	61,67,67	3.12	28 (45%)
40	LMT	bE	620	-	24,24,36	1.11	2 (8%)	29,29,47	1.04	1 (3%)
36	CLA	cE	511	-	69,73,73	1.28	9 (13%)	83,113,113	1.41	6 (7%)
42	LHG	l1	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.05	3 (5%)
36	CLA	CE	513	-	69,73,73	1.25	10 (14%)	83,113,113	1.44	9 (10%)
43	BCR	BE	616	7	41,41,41	0.69	0	56,56,56	1.88	14 (25%)
33	CYC	c9	201	-	46,46,46	2.29	15 (32%)	61,67,67	3.86	31 (50%)
33	CYC	bF	201	3	46,46,46	2.30	17 (36%)	61,67,67	3.20	27 (44%)
36	CLA	a1	405	-	50,54,73	11.60	12 (24%)	60,90,113	1.61	8 (13%)
43	BCR	cE	519	-	41,41,41	0.83	0	56,56,56	2.01	16 (28%)
39	LMG	tD	101	22	36,36,55	1.15	2 (5%)	44,44,63	0.99	3 (6%)
36	CLA	CD	507	-	59,63,73	1.36	10 (16%)	71,101,113	1.61	9 (12%)
36	CLA	CD	513	-	69,73,73	1.25	10 (14%)	83,113,113	1.45	10 (12%)
33	CYC	g7	202	32	46,46,46	2.31	15 (32%)	61,67,67	3.89	31 (50%)

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
33	CYC	f5	201	31	-	12/26/74/74	0/4/4/4
33	CYC	ZF	201	3	-	10/26/74/74	0/4/4/4
40	LMT	BE	623	7	-	8/15/35/61	0/1/1/2
33	CYC	aB	201	5,4	-	9/26/74/74	0/4/4/4
36	CLA	BD	609	-	-	17/39/115/115	-
37	PL9	AD	406	-	-	14/53/73/73	0/1/1/1
36	CLA	CE	511	8	-	21/39/115/115	-
36	CLA	B1	609	-	-	17/39/115/115	-
33	CYC	nF	201	5,4	-	6/26/74/74	0/4/4/4
33	CYC	cC	202	32	-	12/26/74/74	0/4/4/4
33	CYC	gI	302	32	-	12/26/74/74	0/4/4/4
39	LMG	DD	411	9	-	12/46/66/70	0/1/1/1
43	BCR	D1	406	-	-	7/29/63/63	0/2/2/2
36	CLA	B1	612	-	-	17/39/115/115	-
33	CYC	eF	201	4	-	10/26/74/74	0/4/4/4
42	LHG	aE	411	6	-	12/42/42/53	-
44	DGD	CD	517	8	-	15/36/76/95	0/2/2/2
36	CLA	C1	515	-	-	16/39/115/115	-
39	LMG	A1	408	-	-	9/31/51/70	0/1/1/1
39	LMG	D1	410	9	-	12/46/66/70	0/1/1/1
33	CYC	j7	202	-	-	12/26/74/74	0/4/4/4
33	CYC	eJ	202	-	-	12/26/74/74	0/4/4/4
39	LMG	mD	101	-	-	9/31/51/70	0/1/1/1
36	CLA	BD	603	7	-	18/39/115/115	-
33	CYC	bK	201	3	-	10/26/74/74	0/4/4/4
36	CLA	bE	615	7	-	14/39/115/115	-
36	CLA	bD	614	43	-	16/39/115/115	-
40	LMT	C1	520	8	-	8/15/35/61	0/1/1/2
40	LMT	bE	602	-	-	6/15/35/61	0/1/1/2
43	BCR	k1	102	-	-	2/29/63/63	0/2/2/2
47	HEM	v1	201	24	-	7/14/54/54	-
43	BCR	bE	618	-	-	4/29/63/63	0/2/2/2
33	CYC	e9	202	-	-	12/26/74/74	0/4/4/4
33	CYC	dK	201	3	-	7/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LMG	b1	619	7	-	7/46/66/70	0/1/1/1
43	BCR	C1	516	36,8	-	10/29/63/63	0/2/2/2
33	CYC	m6	201	-	-	12/26/74/74	0/4/4/4
33	CYC	kK	201	3	-	8/26/74/74	0/4/4/4
36	CLA	CE	504	-	-	10/39/115/115	-
43	BCR	XE	102	25,36	-	7/29/63/63	0/2/2/2
36	CLA	BD	613	43	-	16/39/115/115	-
37	PL9	DE	408	9	-	8/53/73/73	0/1/1/1
33	CYC	iJ	202	-	-	8/26/74/74	0/4/4/4
36	CLA	AD	405	-	-	14/39/115/115	-
42	LHG	eE	101	-	-	16/44/44/53	-
33	CYC	LG	201	4,2	-	10/26/74/74	0/4/4/4
43	BCR	C1	519	-	-	2/29/63/63	0/2/2/2
36	CLA	BE	612	-	-	17/39/115/115	-
42	LHG	AE	411	6	-	10/42/42/53	-
44	DGD	c1	516	8	-	15/36/76/95	0/2/2/2
45	PHO	dE	402	9	-	13/28/94/103	0/5/6/6
44	DGD	cD	518	-	-	12/51/91/95	0/2/2/2
38	SQD	CD	501	8	-	10/49/69/69	0/1/1/1
36	CLA	c1	508	8	-	9/39/115/115	-
33	CYC	2G	201	5,4	-	8/26/74/74	0/4/4/4
36	CLA	AD	404	-	-	6/17/93/115	-
42	LHG	D1	408	-	-	13/53/53/53	-
43	BCR	ZE	102	-	-	2/29/63/63	0/2/2/2
33	CYC	c2	202	32	-	12/26/74/74	0/4/4/4
33	CYC	g2	202	32	-	8/26/74/74	0/4/4/4
42	LHG	a1	412	6	-	12/42/42/53	-
36	CLA	cE	504	-	-	11/39/115/115	-
33	CYC	c8	201	-	-	8/26/74/74	0/4/4/4
33	CYC	cJ	201	-	-	8/26/74/74	0/4/4/4
37	PL9	a1	409	-	-	15/53/73/73	0/1/1/1
33	CYC	bI	201	-	-	12/26/74/74	0/4/4/4
33	CYC	1L	201	4	-	11/26/74/74	0/4/4/4
33	CYC	SL	201	4,2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	BE	608	-	-	14/39/115/115	-
33	CYC	jC	201	-	-	12/26/74/74	0/4/4/4
33	CYC	b9	201	-	-	12/26/74/74	0/4/4/4
36	CLA	cE	503	-	-	14/39/115/115	-
33	CYC	QB	201	4,3	-	8/26/74/74	0/4/4/4
40	LMT	BE	619	-	-	6/15/35/61	0/1/1/2
38	SQD	h1	103	12	-	17/30/50/69	0/1/1/1
44	DGD	JE	101	-	-	10/51/91/95	0/2/2/2
44	DGD	cE	516	8	-	15/36/76/95	0/2/2/2
36	CLA	cD	511	-	-	15/39/115/115	-
33	CYC	l9	201	-	-	12/26/74/74	0/4/4/4
40	LMT	B1	620	-	-	8/15/35/61	0/1/1/2
36	CLA	CE	506	8	-	17/39/115/115	-
33	CYC	Y4	201	5,4	-	11/26/74/74	0/4/4/4
33	CYC	3K	101	5,4	-	9/26/74/74	0/4/4/4
33	CYC	c9	202	32	-	12/26/74/74	0/4/4/4
36	CLA	b1	606	7	-	18/39/115/115	-
33	CYC	i2	202	-	-	8/26/74/74	0/4/4/4
43	BCR	b1	616	7,36	-	7/29/63/63	0/2/2/2
43	BCR	bE	616	7,36	-	7/29/63/63	0/2/2/2
33	CYC	l3	201	-	-	12/26/74/74	0/4/4/4
39	LMG	TE	101	-	-	7/31/51/70	0/1/1/1
36	CLA	iE	101	-	-	12/27/103/115	-
38	SQD	DE	414	9	-	10/29/49/69	0/1/1/1
33	CYC	zB	201	4,2	-	7/26/74/74	0/4/4/4
33	CYC	jK	201	4	-	8/26/74/74	0/4/4/4
39	LMG	CE	520	39	-	11/46/66/70	0/1/1/1
36	CLA	cE	512	-	-	15/39/115/115	-
36	CLA	CD	505	-	-	8/39/115/115	-
33	CYC	i6	201	-	-	12/26/74/74	0/4/4/4
39	LMG	M1	101	-	-	9/31/51/70	0/1/1/1
36	CLA	CE	510	8	-	8/39/115/115	-
36	CLA	cE	506	8	-	16/39/115/115	-
36	CLA	BD	608	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SQD	L1	101	-	-	11/38/58/69	0/1/1/1
39	LMG	aD	409	-	-	12/31/51/70	0/1/1/1
42	LHG	lD	101	-	-	20/53/53/53	-
38	SQD	c1	501	8	-	17/49/69/69	0/1/1/1
36	CLA	CD	512	-	-	17/39/115/115	-
33	CYC	JF	201	3	-	8/26/74/74	0/4/4/4
40	LMT	bD	602	-	-	6/15/35/61	0/1/1/2
43	BCR	BD	615	7,36	-	7/29/63/63	0/2/2/2
33	CYC	p4	201	4,2	-	9/26/74/74	0/4/4/4
39	LMG	B1	618	7	-	7/46/66/70	0/1/1/1
43	BCR	z1	101	27	-	12/29/63/63	0/2/2/2
33	CYC	iI	202	-	-	8/26/74/74	0/4/4/4
36	CLA	c1	514	-	-	15/39/115/115	-
45	PHO	DE	401	-	-	20/37/103/103	0/5/6/6
33	CYC	XB	201	4,3	-	8/26/74/74	0/4/4/4
33	CYC	pB	201	4,2	-	9/26/74/74	0/4/4/4
42	LHG	AD	411	6	-	10/42/42/53	-
44	DGD	cD	516	8	-	15/36/76/95	0/2/2/2
36	CLA	c1	510	8	-	23/39/115/115	-
36	CLA	bD	610	-	-	17/39/115/115	-
33	CYC	i5	201	-	-	12/26/74/74	0/4/4/4
33	CYC	c7	201	-	-	8/26/74/74	0/4/4/4
33	CYC	BB	1002	2	-	6/26/74/74	0/4/4/4
33	CYC	g3	201	32	-	12/26/74/74	0/4/4/4
36	CLA	b1	605	7	-	18/39/115/115	-
33	CYC	iH	201	-	-	12/26/74/74	0/4/4/4
33	CYC	a4	201	5,4	-	10/26/74/74	0/4/4/4
33	CYC	sB	201	3	-	9/26/74/74	0/4/4/4
36	CLA	B1	604	7	-	18/39/115/115	-
36	CLA	B1	606	-	-	12/33/109/115	-
36	CLA	CD	504	-	-	10/39/115/115	-
33	CYC	qB	201	3	-	8/26/74/74	0/4/4/4
36	CLA	bD	611	-	-	20/39/115/115	-
38	SQD	DD	414	9	-	10/29/49/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SQD	C1	501	8	-	10/49/69/69	0/1/1/1
40	LMT	B1	623	7	-	8/15/35/61	0/1/1/2
40	LMT	cE	501	-	-	8/15/35/61	0/1/1/2
36	CLA	bE	606	7	-	18/39/115/115	-
38	SQD	AD	407	-	-	19/41/61/69	0/1/1/1
33	CYC	nK	201	5,4	-	6/26/74/74	0/4/4/4
33	CYC	QG	201	29	-	9/26/74/74	0/4/4/4
33	CYC	eI	201	32	-	8/26/74/74	0/4/4/4
33	CYC	AG	201	4,3	-	8/26/74/74	0/4/4/4
33	CYC	hF	201	4	-	7/26/74/74	0/4/4/4
36	CLA	C1	506	8	-	17/39/115/115	-
42	LHG	BE	620	-	-	20/53/53/53	-
43	BCR	IE	102	13	-	10/29/63/63	0/2/2/2
40	LMT	dD	413	-	-	8/13/33/61	0/1/1/2
33	CYC	d7	201	-	-	12/26/74/74	0/4/4/4
33	CYC	g7	201	32	-	12/26/74/74	0/4/4/4
39	LMG	a1	410	-	-	12/31/51/70	0/1/1/1
40	LMT	d1	412	-	-	10/17/37/61	0/1/1/2
40	LMT	DE	413	-	-	6/13/33/61	0/1/1/2
43	BCR	d1	407	-	-	7/29/63/63	0/2/2/2
36	CLA	cE	510	8	-	23/39/115/115	-
36	CLA	CE	512	-	-	17/39/115/115	-
36	CLA	BD	607	7	-	15/39/115/115	-
36	CLA	cE	505	-	-	8/39/115/115	-
42	LHG	DE	410	-	-	17/53/53/53	-
33	CYC	MG	201	4,2	-	13/26/74/74	0/4/4/4
33	CYC	ZK	201	3	-	10/26/74/74	0/4/4/4
44	DGD	JD	101	-	-	10/51/91/95	0/2/2/2
33	CYC	gI	301	32	-	8/26/74/74	0/4/4/4
43	BCR	B1	616	7	-	2/29/63/63	0/2/2/2
42	LHG	d1	410	-	-	17/53/53/53	-
36	CLA	C1	513	-	-	14/39/115/115	-
33	CYC	dC	201	-	-	12/26/74/74	0/4/4/4
36	CLA	h1	102	12	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	OL	201	4	-	7/26/74/74	0/4/4/4
33	CYC	7L	201	5,4	-	12/26/74/74	0/4/4/4
43	BCR	b1	617	7	-	2/29/63/63	0/2/2/2
36	CLA	C1	505	-	-	8/39/115/115	-
43	BCR	i1	101	-	-	6/29/63/63	0/2/2/2
33	CYC	j8	201	-	-	12/26/74/74	0/4/4/4
36	CLA	HE	103	43	-	13/39/115/115	-
40	LMT	cD	501	-	-	8/15/35/61	0/1/1/2
33	CYC	e2	202	-	-	12/26/74/74	0/4/4/4
36	CLA	b1	611	-	-	20/39/115/115	-
42	LHG	dE	410	-	-	17/53/53/53	-
39	LMG	tE	101	22	-	7/31/51/70	0/1/1/1
39	LMG	aE	407	-	-	9/46/66/70	0/1/1/1
33	CYC	WG	201	4	-	6/26/74/74	0/4/4/4
33	CYC	q4	201	3	-	8/26/74/74	0/4/4/4
33	CYC	k9	201	-	-	8/26/74/74	0/4/4/4
36	CLA	BE	603	7	-	18/39/115/115	-
36	CLA	BE	611	7	-	17/39/115/115	-
39	LMG	DE	411	9	-	12/46/66/70	0/1/1/1
33	CYC	JK	201	3	-	8/26/74/74	0/4/4/4
33	CYC	yB	201	3	-	10/26/74/74	0/4/4/4
43	BCR	kE	102	-	-	2/29/63/63	0/2/2/2
33	CYC	IG	201	3	-	7/26/74/74	0/4/4/4
42	LHG	DD	409	-	-	13/53/53/53	-
33	CYC	kH	201	-	-	8/26/74/74	0/4/4/4
38	SQD	cD	502	8	-	17/49/69/69	0/1/1/1
43	BCR	CD	516	36,8	-	10/29/63/63	0/2/2/2
36	CLA	b1	610	-	-	17/39/115/115	-
36	CLA	bE	608	-	-	12/33/109/115	-
33	CYC	l2	201	-	-	12/26/74/74	0/4/4/4
38	SQD	BE	621	-	-	14/33/53/69	0/1/1/1
33	CYC	g9	201	32	-	12/26/74/74	0/4/4/4
36	CLA	bE	612	7	-	17/39/115/115	-
39	LMG	bD	619	7	-	7/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	TL	201	3	-	9/26/74/74	0/4/4/4
36	CLA	B1	601	-	-	9/15/91/115	-
39	LMG	a1	408	-	-	9/46/66/70	0/1/1/1
43	BCR	DE	407	-	-	7/29/63/63	0/2/2/2
39	LMG	j1	102	14,39	-	13/22/42/70	0/1/1/1
43	BCR	kD	102	-	-	2/29/63/63	0/2/2/2
36	CLA	dD	406	9	-	13/39/115/115	-
33	CYC	ZB	201	3	-	6/26/74/74	0/4/4/4
36	CLA	BD	605	-	-	11/39/115/115	-
33	CYC	jH	202	-	-	12/26/74/74	0/4/4/4
36	CLA	c1	512	-	-	15/39/115/115	-
33	CYC	eK	201	4	-	10/26/74/74	0/4/4/4
36	CLA	B1	605	-	-	11/39/115/115	-
43	BCR	Z1	102	-	-	2/29/63/63	0/2/2/2
39	LMG	ME	101	-	-	9/31/51/70	0/1/1/1
33	CYC	XF	201	3	-	12/26/74/74	0/4/4/4
33	CYC	w4	201	3	-	12/26/74/74	0/4/4/4
44	DGD	cD	517	-	-	17/51/91/95	0/2/2/2
43	BCR	X1	102	25,36	-	7/29/63/63	0/2/2/2
36	CLA	bD	608	-	-	12/33/109/115	-
44	DGD	CE	518	-	-	19/51/91/95	0/2/2/2
33	CYC	RG	201	4,3	-	10/26/74/74	0/4/4/4
39	LMG	BE	618	7	-	7/46/66/70	0/1/1/1
36	CLA	hE	102	12	-	12/33/109/115	-
40	LMT	AE	412	-	-	14/21/61/61	0/2/2/2
40	LMT	d1	413	-	-	8/13/33/61	0/1/1/2
33	CYC	eC	202	-	-	12/26/74/74	0/4/4/4
33	CYC	c7	202	32	-	12/26/74/74	0/4/4/4
36	CLA	BE	607	7	-	15/39/115/115	-
40	LMT	A1	409	-	-	7/15/35/61	0/1/1/2
33	CYC	gJ	202	32	-	8/26/74/74	0/4/4/4
42	LHG	A1	411	6	-	10/42/42/53	-
43	BCR	CE	519	-	-	2/29/63/63	0/2/2/2
33	CYC	gA	302	32	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	BD	611	7	-	17/39/115/115	-
33	CYC	e8	202	-	-	12/26/74/74	0/4/4/4
43	BCR	zD	101	27	-	12/29/63/63	0/2/2/2
33	CYC	iA	201	-	-	12/26/74/74	0/4/4/4
33	CYC	tB	1001	4,2	-	16/26/74/74	0/4/4/4
44	DGD	C1	518	-	-	19/51/91/95	0/2/2/2
33	CYC	P4	201	4	-	11/26/74/74	0/4/4/4
39	LMG	m1	101	-	-	9/31/51/70	0/1/1/1
33	CYC	g9	202	32	-	8/26/74/74	0/4/4/4
36	CLA	cD	514	-	-	15/39/115/115	-
36	CLA	C1	511	8	-	21/39/115/115	-
40	LMT	D1	403	-	-	8/15/35/61	0/1/1/2
42	LHG	e1	101	-	-	16/44/44/53	-
36	CLA	hE	101	43	-	13/39/115/115	-
36	CLA	cE	507	43,8	-	20/39/115/115	-
33	CYC	e5	202	-	-	12/26/74/74	0/4/4/4
33	CYC	Q4	201	4,3	-	8/26/74/74	0/4/4/4
33	CYC	mI	201	-	-	12/26/74/74	0/4/4/4
33	CYC	OB	201	3	-	9/26/74/74	0/4/4/4
36	CLA	C1	514	-	-	7/21/97/115	-
39	LMG	JE	102	14,39	-	9/22/42/70	0/1/1/1
40	LMT	jD	101	-	-	11/21/61/61	0/2/2/2
33	CYC	cA	201	-	-	8/26/74/74	0/4/4/4
36	CLA	cD	510	8	-	23/39/115/115	-
33	CYC	hI	201	-	-	12/26/74/74	0/4/4/4
43	BCR	hE	105	12,25,36	-	7/29/63/63	0/2/2/2
36	CLA	b1	612	7	-	17/39/115/115	-
40	LMT	bD	620	-	-	6/15/35/61	0/1/1/2
36	CLA	DE	406	9	-	13/39/115/115	-
36	CLA	b1	608	-	-	12/33/109/115	-
33	CYC	i5	202	-	-	8/26/74/74	0/4/4/4
36	CLA	BE	602	7	-	16/39/115/115	-
39	LMG	t1	101	22	-	7/31/51/70	0/1/1/1
33	CYC	g3	202	32	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	f3	201	31	-	12/26/74/74	0/4/4/4
33	CYC	1G	201	4	-	11/26/74/74	0/4/4/4
33	CYC	R4	201	5,4	-	9/26/74/74	0/4/4/4
33	CYC	i9	201	-	-	12/26/74/74	0/4/4/4
47	HEM	ED	101	-	-	10/14/54/54	-
33	CYC	bC	201	-	-	12/26/74/74	0/4/4/4
38	SQD	hD	103	12	-	17/30/50/69	0/1/1/1
33	CYC	ML	201	4,2	-	13/26/74/74	0/4/4/4
33	CYC	QL	201	29	-	9/26/74/74	0/4/4/4
43	BCR	BD	617	-	-	4/29/63/63	0/2/2/2
47	HEM	fE	101	-	-	10/14/54/54	-
33	CYC	oB	201	3	-	11/26/74/74	0/4/4/4
33	CYC	VB	201	3	-	14/26/74/74	0/4/4/4
33	CYC	fC	201	31	-	12/26/74/74	0/4/4/4
36	CLA	cD	504	-	-	11/39/115/115	-
39	LMG	CD	522	39	-	11/46/66/70	0/1/1/1
33	CYC	h5	201	-	-	12/26/74/74	0/4/4/4
36	CLA	C1	503	-	-	17/39/115/115	-
39	LMG	aE	409	-	-	12/31/51/70	0/1/1/1
40	LMT	DD	413	-	-	6/13/33/61	0/1/1/2
42	LHG	B1	621	-	-	20/53/53/53	-
33	CYC	c3	201	-	-	8/26/74/74	0/4/4/4
33	CYC	e7	202	-	-	12/26/74/74	0/4/4/4
36	CLA	CE	507	-	-	16/27/103/115	-
33	CYC	g5	201	32	-	12/26/74/74	0/4/4/4
33	CYC	B4	1002	2	-	6/26/74/74	0/4/4/4
33	CYC	lI	201	-	-	12/26/74/74	0/4/4/4
36	CLA	D1	404	-	-	13/39/115/115	-
33	CYC	k5	201	-	-	8/26/74/74	0/4/4/4
36	CLA	cD	512	-	-	15/39/115/115	-
33	CYC	fH	201	31	-	12/26/74/74	0/4/4/4
36	CLA	B1	608	-	-	14/39/115/115	-
36	CLA	BE	606	-	-	12/33/109/115	-
40	LMT	b1	620	-	-	6/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	CD	515	-	-	16/39/115/115	-
36	CLA	cD	509	8	-	8/39/115/115	-
36	CLA	C1	507	-	-	16/27/103/115	-
33	CYC	l6	201	-	-	12/26/74/74	0/4/4/4
40	LMT	iD	103	-	-	7/15/35/61	0/1/1/2
33	CYC	KL	201	4,3	-	9/26/74/74	0/4/4/4
33	CYC	AL	201	4,3	-	8/26/74/74	0/4/4/4
33	CYC	j3	201	-	-	12/26/74/74	0/4/4/4
33	CYC	k8	201	-	-	8/26/74/74	0/4/4/4
47	HEM	VD	201	24	-	7/14/54/54	-
43	BCR	cD	519	-	-	3/29/63/63	0/2/2/2
36	CLA	B1	607	7	-	15/39/115/115	-
40	LMT	jE	101	-	-	11/21/61/61	0/2/2/2
33	CYC	KK	201	4	-	9/26/74/74	0/4/4/4
40	LMT	DE	412	-	-	10/17/37/61	0/1/1/2
33	CYC	BB	1001	4,2	-	13/26/74/74	0/4/4/4
40	LMT	CD	521	-	-	8/15/35/61	0/1/1/2
33	CYC	m2	201	-	-	12/26/74/74	0/4/4/4
36	CLA	D1	405	9	-	13/39/115/115	-
33	CYC	TB	201	4	-	11/26/74/74	0/4/4/4
33	CYC	j6	202	-	-	12/26/74/74	0/4/4/4
33	CYC	b6	201	-	-	12/26/74/74	0/4/4/4
33	CYC	kF	201	3	-	8/26/74/74	0/4/4/4
33	CYC	gH	202	32	-	8/26/74/74	0/4/4/4
47	HEM	vE	201	24	-	7/14/54/54	-
36	CLA	DD	405	-	-	13/39/115/115	-
33	CYC	h9	201	-	-	12/26/74/74	0/4/4/4
33	CYC	b3	201	-	-	12/26/74/74	0/4/4/4
33	CYC	IL	201	-	-	7/26/74/74	0/4/4/4
42	LHG	eD	101	-	-	16/44/44/53	-
33	CYC	h6	201	-	-	12/26/74/74	0/4/4/4
36	CLA	c1	506	-	-	12/27/103/115	-
36	CLA	b1	604	7	-	16/39/115/115	-
33	CYC	cH	201	-	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	LHG	D1	409	-	-	17/53/53/53	-
33	CYC	lC	201	-	-	12/26/74/74	0/4/4/4
33	CYC	aK	201	4	-	10/26/74/74	0/4/4/4
33	CYC	c2	201	-	-	8/26/74/74	0/4/4/4
33	CYC	dI	201	-	-	12/26/74/74	0/4/4/4
36	CLA	C1	504	-	-	10/39/115/115	-
33	CYC	j3	202	-	-	12/26/74/74	0/4/4/4
33	CYC	YF	201	4	-	7/26/74/74	0/4/4/4
33	CYC	t4	1001	4,2	-	16/26/74/74	0/4/4/4
33	CYC	k6	201	-	-	8/26/74/74	0/4/4/4
36	CLA	DD	406	9	-	13/39/115/115	-
36	CLA	c1	509	8	-	8/39/115/115	-
39	LMG	aD	407	-	-	9/46/66/70	0/1/1/1
44	DGD	c1	517	-	-	17/51/91/95	0/2/2/2
36	CLA	aD	405	-	-	16/39/115/115	-
33	CYC	VL	201	30	-	12/26/74/74	0/4/4/4
36	CLA	xE	101	25,9	-	22/39/115/115	-
36	CLA	c1	502	-	-	14/39/115/115	-
40	LMT	AE	409	-	-	7/15/35/61	0/1/1/2
36	CLA	a1	407	6	-	16/33/109/115	-
36	CLA	CE	509	8	-	15/39/115/115	-
36	CLA	cD	513	-	-	9/21/97/115	-
45	PHO	DE	403	9	-	18/37/103/103	0/5/6/6
36	CLA	bD	605	7	-	18/39/115/115	-
33	CYC	j2	201	-	-	12/26/74/74	0/4/4/4
43	BCR	cD	515	36,8	-	12/29/63/63	0/2/2/2
39	LMG	bE	619	7	-	7/46/66/70	0/1/1/1
33	CYC	d6	201	-	-	12/26/74/74	0/4/4/4
43	BCR	bD	616	7,36	-	7/29/63/63	0/2/2/2
43	BCR	dD	407	-	-	7/29/63/63	0/2/2/2
42	LHG	BD	620	-	-	20/53/53/53	-
33	CYC	gC	301	32	-	8/26/74/74	0/4/4/4
33	CYC	e3	201	32	-	8/26/74/74	0/4/4/4
33	CYC	g6	201	32	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	cE	508	8	-	9/39/115/115	-
33	CYC	hC	201	-	-	12/26/74/74	0/4/4/4
39	LMG	jE	102	14,39	-	13/22/42/70	0/1/1/1
33	CYC	7G	201	5,4	-	12/26/74/74	0/4/4/4
33	CYC	YB	201	5,4	-	11/26/74/74	0/4/4/4
33	CYC	m7	201	-	-	12/26/74/74	0/4/4/4
33	CYC	dH	201	-	-	12/26/74/74	0/4/4/4
33	CYC	c6	202	32	-	12/26/74/74	0/4/4/4
36	CLA	CE	505	-	-	8/39/115/115	-
36	CLA	cD	505	-	-	8/39/115/115	-
36	CLA	CD	508	43,8	-	15/39/115/115	-
33	CYC	eI	202	-	-	12/26/74/74	0/4/4/4
33	CYC	vB	201	4	-	7/26/74/74	0/4/4/4
33	CYC	i9	202	-	-	8/26/74/74	0/4/4/4
36	CLA	BD	610	-	-	20/39/115/115	-
33	CYC	c3	202	32	-	12/26/74/74	0/4/4/4
36	CLA	CD	514	-	-	7/21/97/115	-
43	BCR	I1	102	13	-	10/29/63/63	0/2/2/2
40	LMT	AD	412	-	-	14/21/61/61	0/2/2/2
37	PL9	dE	408	9	-	8/53/73/73	0/1/1/1
43	BCR	hD	105	12,25,36	-	7/29/63/63	0/2/2/2
33	CYC	jF	201	4	-	8/26/74/74	0/4/4/4
40	LMT	b1	601	7	-	9/21/61/61	0/2/2/2
40	LMT	dE	413	-	-	8/13/33/61	0/1/1/2
33	CYC	WL	201	4	-	6/26/74/74	0/4/4/4
33	CYC	h3	201	-	-	12/26/74/74	0/4/4/4
33	CYC	mK	201	30	-	12/26/74/74	0/4/4/4
33	CYC	JL	201	4,2	-	9/26/74/74	0/4/4/4
33	CYC	fJ	201	31	-	12/26/74/74	0/4/4/4
36	CLA	HE	101	12	-	12/33/109/115	-
33	CYC	2L	201	5,4	-	8/26/74/74	0/4/4/4
40	LMT	d1	404	-	-	8/15/35/61	0/1/1/2
47	HEM	VE	201	24	-	7/14/54/54	-
36	CLA	hD	102	12	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	f8	201	31	-	12/26/74/74	0/4/4/4
36	CLA	dD	405	-	-	13/39/115/115	-
40	LMT	B1	619	-	-	6/15/35/61	0/1/1/2
33	CYC	mH	201	-	-	12/26/74/74	0/4/4/4
39	LMG	CD	502	-	-	13/46/66/70	0/1/1/1
33	CYC	j9	201	-	-	12/26/74/74	0/4/4/4
33	CYC	iI	201	-	-	12/26/74/74	0/4/4/4
36	CLA	BE	614	7	-	14/39/115/115	-
33	CYC	b8	201	-	-	12/26/74/74	0/4/4/4
33	CYC	4G	201	3	-	9/26/74/74	0/4/4/4
36	CLA	B1	611	7	-	17/39/115/115	-
36	CLA	cE	514	-	-	15/39/115/115	-
44	DGD	cE	517	-	-	17/51/91/95	0/2/2/2
40	LMT	dD	412	-	-	10/17/37/61	0/1/1/2
45	PHO	DD	401	-	-	18/37/103/103	0/5/6/6
45	PHO	A1	412	6	-	20/37/103/103	0/5/6/6
33	CYC	hK	201	4	-	7/26/74/74	0/4/4/4
36	CLA	C1	512	-	-	17/39/115/115	-
44	DGD	CD	518	-	-	19/51/91/95	0/2/2/2
33	CYC	e6	202	-	-	12/26/74/74	0/4/4/4
33	CYC	j5	202	-	-	12/26/74/74	0/4/4/4
36	CLA	x1	101	25,9	-	22/39/115/115	-
33	CYC	IF	201	4	-	10/26/74/74	0/4/4/4
38	SQD	hE	103	12	-	17/30/50/69	0/1/1/1
33	CYC	jI	202	-	-	12/26/74/74	0/4/4/4
33	CYC	g5	202	32	-	8/26/74/74	0/4/4/4
36	CLA	cD	507	43,8	-	20/39/115/115	-
43	BCR	bD	617	7	-	2/29/63/63	0/2/2/2
33	CYC	e5	201	32	-	8/26/74/74	0/4/4/4
45	PHO	aE	412	-	-	13/28/94/103	0/5/6/6
33	CYC	b5	201	-	-	12/26/74/74	0/4/4/4
39	LMG	dE	411	9	-	12/46/66/70	0/1/1/1
33	CYC	hA	201	-	-	12/26/74/74	0/4/4/4
39	LMG	TD	101	-	-	7/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	LHG	dD	409	-	-	14/53/53/53	-
45	PHO	d1	402	9	-	16/37/103/103	0/5/6/6
33	CYC	e8	201	32	-	8/26/74/74	0/4/4/4
47	HEM	V1	201	24	-	7/14/54/54	-
40	LMT	dE	404	-	-	8/15/35/61	0/1/1/2
36	CLA	C1	509	8	-	15/39/115/115	-
36	CLA	dE	405	-	-	13/39/115/115	-
33	CYC	i2	201	-	-	12/26/74/74	0/4/4/4
33	CYC	kC	201	-	-	8/26/74/74	0/4/4/4
33	CYC	hH	201	-	-	12/26/74/74	0/4/4/4
33	CYC	cI	202	32	-	12/26/74/74	0/4/4/4
39	LMG	jD	102	14,39	-	13/22/42/70	0/1/1/1
37	PL9	aE	408	-	-	15/53/73/73	0/1/1/1
33	CYC	PG	201	3	-	10/26/74/74	0/4/4/4
40	LMT	BD	623	7	-	8/15/35/61	0/1/1/2
33	CYC	u4	201	4,3	-	10/26/74/74	0/4/4/4
47	HEM	fD	101	-	-	10/14/54/54	-
33	CYC	kJ	201	-	-	8/26/74/74	0/4/4/4
36	CLA	BE	605	-	-	11/39/115/115	-
43	BCR	BE	615	7,36	-	7/29/63/63	0/2/2/2
33	CYC	c8	202	32	-	12/26/74/74	0/4/4/4
33	CYC	lH	201	-	-	12/26/74/74	0/4/4/4
40	LMT	D1	412	-	-	6/13/33/61	0/1/1/2
36	CLA	IE	101	13,6	-	17/33/109/115	-
36	CLA	bE	609	7	-	15/39/115/115	-
33	CYC	eC	201	32	-	8/26/74/74	0/4/4/4
43	BCR	b1	618	-	-	4/29/63/63	0/2/2/2
33	CYC	m8	201	-	-	12/26/74/74	0/4/4/4
33	CYC	e7	201	32	-	8/26/74/74	0/4/4/4
36	CLA	H1	101	12	-	12/33/109/115	-
36	CLA	XE	101	25	-	22/39/115/115	-
33	CYC	e3	202	-	-	12/26/74/74	0/4/4/4
33	CYC	g6	202	32	-	8/26/74/74	0/4/4/4
33	CYC	kI	201	-	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	DE	405	-	-	13/39/115/115	-
33	CYC	wB	201	3	-	12/26/74/74	0/4/4/4
39	LMG	CE	502	-	-	13/46/66/70	0/1/1/1
39	LMG	d1	411	9	-	12/46/66/70	0/1/1/1
33	CYC	jA	202	-	-	12/26/74/74	0/4/4/4
39	LMG	T1	101	-	-	7/31/51/70	0/1/1/1
33	CYC	C4	1001	2	-	6/26/74/74	0/4/4/4
33	CYC	GG	201	4,3	-	8/26/74/74	0/4/4/4
39	LMG	AD	408	-	-	9/31/51/70	0/1/1/1
43	BCR	bD	618	-	-	4/29/63/63	0/2/2/2
33	CYC	OG	201	4	-	7/26/74/74	0/4/4/4
36	CLA	cD	506	8	-	16/39/115/115	-
36	CLA	d1	405	-	-	13/39/115/115	-
36	CLA	bE	603	-	-	9/15/91/115	-
33	CYC	k3	201	-	-	8/26/74/74	0/4/4/4
33	CYC	eA	202	-	-	12/26/74/74	0/4/4/4
38	SQD	d1	414	9	-	10/29/49/69	0/1/1/1
44	DGD	c1	518	-	-	12/51/91/95	0/2/2/2
43	BCR	iD	102	-	-	6/29/63/63	0/2/2/2
36	CLA	I1	101	13,6	-	17/33/109/115	-
33	CYC	b2	201	-	-	12/26/74/74	0/4/4/4
36	CLA	aE	405	-	-	16/39/115/115	-
40	LMT	iE	103	-	-	7/15/35/61	0/1/1/2
42	LHG	dD	410	-	-	17/53/53/53	-
36	CLA	BD	602	7	-	16/39/115/115	-
37	PL9	A1	406	-	-	14/53/73/73	0/1/1/1
33	CYC	d3	201	-	-	12/26/74/74	0/4/4/4
42	LHG	DE	409	-	-	14/53/53/53	-
43	BCR	h1	105	12,25,36	-	7/29/63/63	0/2/2/2
33	CYC	9F	201	3	-	7/26/74/74	0/4/4/4
33	CYC	cK	201	4	-	6/26/74/74	0/4/4/4
36	CLA	BE	604	7	-	18/39/115/115	-
33	CYC	bJ	201	-	-	12/26/74/74	0/4/4/4
40	LMT	dE	412	-	-	10/17/37/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	bD	613	-	-	17/39/115/115	-
43	BCR	c1	519	-	-	3/29/63/63	0/2/2/2
36	CLA	xD	101	25,9	-	22/39/115/115	-
43	BCR	dE	407	-	-	7/29/63/63	0/2/2/2
47	HEM	EE	101	-	-	10/14/54/54	-
36	CLA	bD	612	7	-	17/39/115/115	-
39	LMG	BD	618	7	-	7/46/66/70	0/1/1/1
36	CLA	a1	406	-	-	16/39/115/115	-
42	LHG	d1	409	-	-	14/53/53/53	-
36	CLA	h1	101	43	-	13/39/115/115	-
33	CYC	jI	201	-	-	12/26/74/74	0/4/4/4
44	DGD	HE	102	-	-	13/51/91/95	0/2/2/2
36	CLA	aE	404	-	-	5/17/93/115	-
33	CYC	c5	201	-	-	8/26/74/74	0/4/4/4
36	CLA	AE	405	-	-	14/39/115/115	-
42	LHG	aD	411	6	-	12/42/42/53	-
36	CLA	C1	510	8	-	8/39/115/115	-
36	CLA	BD	601	-	-	9/15/91/115	-
38	SQD	dD	414	9	-	10/29/49/69	0/1/1/1
33	CYC	PL	201	3	-	10/26/74/74	0/4/4/4
36	CLA	BD	606	-	-	12/33/109/115	-
33	CYC	LK	201	4,3	-	8/26/74/74	0/4/4/4
36	CLA	cD	503	-	-	14/39/115/115	-
33	CYC	6G	201	3	-	8/26/74/74	0/4/4/4
44	DGD	hE	104	-	-	13/51/91/95	0/2/2/2
33	CYC	s4	201	3	-	9/26/74/74	0/4/4/4
33	CYC	h2	201	-	-	12/26/74/74	0/4/4/4
33	CYC	SB	201	4,3	-	11/26/74/74	0/4/4/4
33	CYC	i8	202	-	-	8/26/74/74	0/4/4/4
33	CYC	lJ	201	-	-	12/26/74/74	0/4/4/4
33	CYC	LL	201	4,2	-	10/26/74/74	0/4/4/4
33	CYC	kA	201	-	-	8/26/74/74	0/4/4/4
43	BCR	CD	520	-	-	2/29/63/63	0/2/2/2
43	BCR	ZD	101	27	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SQD	BD	621	-	-	14/33/53/69	0/1/1/1
40	LMT	D1	411	-	-	10/17/37/61	0/1/1/2
36	CLA	c1	507	43,8	-	20/39/115/115	-
33	CYC	e6	201	32	-	8/26/74/74	0/4/4/4
43	BCR	c1	515	36,8	-	12/29/63/63	0/2/2/2
36	CLA	b1	603	-	-	9/15/91/115	-
37	PL9	DD	408	9	-	8/53/73/73	0/1/1/1
33	CYC	nF	202	4,3	-	7/26/74/74	0/4/4/4
36	CLA	bE	604	7	-	15/39/115/115	-
33	CYC	bA	201	-	-	12/26/74/74	0/4/4/4
39	LMG	C1	521	39	-	11/46/66/70	0/1/1/1
33	CYC	j6	201	-	-	12/26/74/74	0/4/4/4
33	CYC	gH	201	32	-	12/26/74/74	0/4/4/4
33	CYC	LF	201	4,3	-	8/26/74/74	0/4/4/4
33	CYC	l5	201	-	-	12/26/74/74	0/4/4/4
36	CLA	c1	513	-	-	9/21/97/115	-
33	CYC	W4	201	4	-	10/26/74/74	0/4/4/4
33	CYC	jA	201	-	-	12/26/74/74	0/4/4/4
39	LMG	yD	101	39	-	15/46/66/70	0/1/1/1
33	CYC	TG	201	3	-	9/26/74/74	0/4/4/4
33	CYC	y4	201	3	-	10/26/74/74	0/4/4/4
36	CLA	CD	506	8	-	17/39/115/115	-
36	CLA	c1	511	-	-	15/39/115/115	-
45	PHO	dD	402	9	-	9/23/89/103	0/5/6/6
47	HEM	vD	201	24	-	7/14/54/54	-
36	CLA	A1	405	-	-	14/39/115/115	-
33	CYC	j8	202	-	-	12/26/74/74	0/4/4/4
33	CYC	c5	202	32	-	12/26/74/74	0/4/4/4
33	CYC	jJ	201	-	-	12/26/74/74	0/4/4/4
45	PHO	aD	412	6	-	20/37/103/103	0/5/6/6
36	CLA	BD	614	7	-	14/39/115/115	-
44	DGD	HD	102	-	-	13/51/91/95	0/2/2/2
33	CYC	d9	201	-	-	12/26/74/74	0/4/4/4
33	CYC	h7	201	-	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	CD	503	-	-	17/39/115/115	-
33	CYC	i6	202	-	-	8/26/74/74	0/4/4/4
40	LMT	a1	401	-	-	8/21/61/61	0/2/2/2
33	CYC	eH	201	32	-	8/26/74/74	0/4/4/4
33	CYC	RB	201	5,4	-	9/26/74/74	0/4/4/4
33	CYC	b7	201	-	-	12/26/74/74	0/4/4/4
45	PHO	a1	413	-	-	8/23/89/103	0/5/6/6
36	CLA	bD	615	7	-	14/39/115/115	-
33	CYC	fF	201	3	-	10/26/74/74	0/4/4/4
33	CYC	bH	201	-	-	12/26/74/74	0/4/4/4
33	CYC	j7	201	-	-	12/26/74/74	0/4/4/4
40	LMT	bE	601	7	-	9/21/61/61	0/2/2/2
33	CYC	mJ	201	-	-	12/26/74/74	0/4/4/4
33	CYC	HG	201	4,2	-	7/26/74/74	0/4/4/4
36	CLA	dE	403	-	-	14/39/115/115	-
33	CYC	JG	201	4,2	-	9/26/74/74	0/4/4/4
33	CYC	5L	201	5,4	-	11/26/74/74	0/4/4/4
33	CYC	CB	1001	2	-	6/26/74/74	0/4/4/4
36	CLA	HD	103	43	-	13/39/115/115	-
45	PHO	DD	403	9	-	13/29/95/103	0/5/6/6
33	CYC	i7	201	-	-	12/26/74/74	0/4/4/4
37	PL9	D1	407	9	-	8/53/73/73	0/1/1/1
33	CYC	m5	201	-	-	12/26/74/74	0/4/4/4
33	CYC	cI	201	-	-	8/26/74/74	0/4/4/4
36	CLA	bE	607	-	-	12/39/115/115	-
33	CYC	rB	201	4,2	-	10/26/74/74	0/4/4/4
33	CYC	r4	201	4,2	-	10/26/74/74	0/4/4/4
33	CYC	cC	201	-	-	8/26/74/74	0/4/4/4
33	CYC	f6	201	31	-	12/26/74/74	0/4/4/4
38	SQD	LD	102	-	-	11/38/58/69	0/1/1/1
38	SQD	AE	407	-	-	19/41/61/69	0/1/1/1
42	LHG	DD	410	-	-	17/53/53/53	-
33	CYC	mF	201	30	-	12/26/74/74	0/4/4/4
36	CLA	bE	610	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PL9	dD	408	9	-	8/53/73/73	0/1/1/1
36	CLA	HD	101	12	-	12/33/109/115	-
36	CLA	b1	614	43	-	16/39/115/115	-
33	CYC	e2	201	32	-	8/26/74/74	0/4/4/4
33	CYC	g2	201	32	-	12/26/74/74	0/4/4/4
33	CYC	k7	201	-	-	8/26/74/74	0/4/4/4
36	CLA	b1	609	7	-	15/39/115/115	-
33	CYC	V4	201	3	-	14/26/74/74	0/4/4/4
33	CYC	mA	201	-	-	12/26/74/74	0/4/4/4
40	LMT	bE	621	-	-	8/15/35/61	0/1/1/2
33	CYC	MF	201	5,4	-	8/26/74/74	0/4/4/4
38	SQD	LE	102	-	-	11/38/58/69	0/1/1/1
43	BCR	B1	615	7,36	-	7/29/63/63	0/2/2/2
36	CLA	BE	610	-	-	20/39/115/115	-
40	LMT	dD	404	-	-	8/15/35/61	0/1/1/2
33	CYC	WB	201	4	-	10/26/74/74	0/4/4/4
47	HEM	f1	101	-	-	10/14/54/54	-
36	CLA	B1	603	7	-	18/39/115/115	-
33	CYC	MK	201	5,4	-	8/26/74/74	0/4/4/4
33	CYC	mC	201	-	-	12/26/74/74	0/4/4/4
33	CYC	i3	201	-	-	12/26/74/74	0/4/4/4
40	LMT	i1	102	-	-	7/15/35/61	0/1/1/2
33	CYC	d8	201	-	-	12/26/74/74	0/4/4/4
40	LMT	DD	404	-	-	8/15/35/61	0/1/1/2
36	CLA	BD	604	7	-	18/39/115/115	-
36	CLA	b1	615	7	-	14/39/115/115	-
33	CYC	iA	202	-	-	8/26/74/74	0/4/4/4
38	SQD	cE	502	8	-	16/49/69/69	0/1/1/1
36	CLA	cE	509	8	-	8/39/115/115	-
43	BCR	bE	617	7	-	2/29/63/63	0/2/2/2
45	PHO	D1	402	9	-	17/37/103/103	0/5/6/6
33	CYC	SG	201	4,2	-	8/26/74/74	0/4/4/4
33	CYC	cA	202	32	-	12/26/74/74	0/4/4/4
39	LMG	dD	411	9	-	12/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	LMT	A1	413	-	-	14/21/61/61	0/2/2/2
43	BCR	DD	407	-	-	7/29/63/63	0/2/2/2
43	BCR	iE	102	-	-	6/29/63/63	0/2/2/2
33	CYC	S4	201	4,3	-	11/26/74/74	0/4/4/4
47	HEM	E1	101	-	-	10/14/54/54	-
36	CLA	aD	406	6	-	16/33/109/115	-
33	CYC	cJ	202	32	-	12/26/74/74	0/4/4/4
33	CYC	iH	202	-	-	8/26/74/74	0/4/4/4
36	CLA	b1	607	-	-	11/39/115/115	-
39	LMG	AE	408	-	-	9/31/51/70	0/1/1/1
33	CYC	KG	201	4,3	-	9/26/74/74	0/4/4/4
33	CYC	g8	201	32	-	12/26/74/74	0/4/4/4
43	BCR	BE	617	-	-	4/29/63/63	0/2/2/2
33	CYC	jJ	202	-	-	12/26/74/74	0/4/4/4
36	CLA	aE	406	6	-	16/33/109/115	-
33	CYC	NG	201	3	-	6/26/74/74	0/4/4/4
36	CLA	bE	605	7	-	18/39/115/115	-
40	LMT	bD	601	7	-	9/21/61/61	0/2/2/2
43	BCR	CE	516	36,8	-	10/29/63/63	0/2/2/2
36	CLA	ID	101	13,6	-	17/33/109/115	-
36	CLA	CE	508	43,8	-	15/39/115/115	-
33	CYC	v4	201	4	-	7/26/74/74	0/4/4/4
33	CYC	i3	202	-	-	8/26/74/74	0/4/4/4
43	BCR	cE	515	36,8	-	12/29/63/63	0/2/2/2
33	CYC	d5	201	-	-	12/26/74/74	0/4/4/4
36	CLA	bE	614	43	-	16/39/115/115	-
36	CLA	CD	510	8	-	8/39/115/115	-
36	CLA	c1	505	8	-	16/39/115/115	-
33	CYC	gJ	201	32	-	12/26/74/74	0/4/4/4
36	CLA	iD	101	-	-	12/27/103/115	-
39	LMG	y1	101	39	-	15/46/66/70	0/1/1/1
33	CYC	O4	201	3	-	9/26/74/74	0/4/4/4
36	CLA	dD	403	-	-	14/39/115/115	-
40	LMT	DE	404	-	-	8/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	C1	508	43,8	-	15/39/115/115	-
40	LMT	b1	602	-	-	6/15/35/61	0/1/1/2
33	CYC	cH	202	32	-	12/26/74/74	0/4/4/4
36	CLA	bD	609	7	-	15/39/115/115	-
36	CLA	B1	602	7	-	16/39/115/115	-
38	SQD	CE	501	8	-	10/49/69/69	0/1/1/1
33	CYC	B4	1001	4,2	-	13/26/74/74	0/4/4/4
43	BCR	ZE	101	27	-	12/29/63/63	0/2/2/2
43	BCR	zE	101	27	-	12/29/63/63	0/2/2/2
40	LMT	BD	622	-	-	8/21/61/61	0/2/2/2
37	PL9	aD	408	-	-	15/53/73/73	0/1/1/1
33	CYC	d2	201	-	-	12/26/74/74	0/4/4/4
33	CYC	i7	202	-	-	8/26/74/74	0/4/4/4
33	CYC	fI	201	31	-	12/26/74/74	0/4/4/4
36	CLA	b1	613	-	-	17/39/115/115	-
36	CLA	BD	612	-	-	17/39/115/115	-
36	CLA	BE	601	-	-	9/15/91/115	-
44	DGD	H1	102	-	-	13/51/91/95	0/2/2/2
36	CLA	aD	404	-	-	5/17/93/115	-
33	CYC	NL	201	3	-	6/26/74/74	0/4/4/4
33	CYC	IK	201	4	-	10/26/74/74	0/4/4/4
33	CYC	eA	201	32	-	8/26/74/74	0/4/4/4
36	CLA	c1	503	-	-	11/39/115/115	-
36	CLA	hD	101	43	-	13/39/115/115	-
36	CLA	bD	606	7	-	18/39/115/115	-
44	DGD	CE	517	8	-	15/36/76/95	0/2/2/2
38	SQD	B1	622	-	-	14/33/53/69	0/1/1/1
36	CLA	BE	613	43	-	16/39/115/115	-
36	CLA	B1	614	7	-	14/39/115/115	-
39	LMG	yE	101	39	-	15/46/66/70	0/1/1/1
44	DGD	hD	104	-	-	13/51/91/95	0/2/2/2
33	CYC	iC	201	-	-	12/26/74/74	0/4/4/4
38	SQD	LD	101	-	-	11/38/58/69	0/1/1/1
39	LMG	J1	102	14,39	-	9/22/42/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	RL	201	4,3	-	10/26/74/74	0/4/4/4
33	CYC	XK	201	3	-	12/26/74/74	0/4/4/4
33	CYC	m3	201	-	-	12/26/74/74	0/4/4/4
33	CYC	3F	101	5,4	-	9/26/74/74	0/4/4/4
33	CYC	6L	201	3	-	8/26/74/74	0/4/4/4
44	DGD	C1	517	8	-	15/36/76/95	0/2/2/2
36	CLA	d1	406	9	-	13/39/115/115	-
33	CYC	VG	201	30	-	12/26/74/74	0/4/4/4
33	CYC	f9	201	31	-	12/26/74/74	0/4/4/4
33	CYC	lA	201	-	-	12/26/74/74	0/4/4/4
33	CYC	hJ	201	-	-	12/26/74/74	0/4/4/4
33	CYC	jC	202	-	-	12/26/74/74	0/4/4/4
33	CYC	gC	302	32	-	12/26/74/74	0/4/4/4
36	CLA	CD	509	8	-	15/39/115/115	-
33	CYC	5G	201	5,4	-	11/26/74/74	0/4/4/4
42	LHG	lE	101	-	-	20/53/53/53	-
33	CYC	dA	201	-	-	12/26/74/74	0/4/4/4
33	CYC	gA	301	32	-	8/26/74/74	0/4/4/4
33	CYC	l7	201	-	-	12/26/74/74	0/4/4/4
33	CYC	HL	201	4,2	-	7/26/74/74	0/4/4/4
43	BCR	XD	102	25,36	-	7/29/63/63	0/2/2/2
36	CLA	CE	514	-	-	7/21/97/115	-
36	CLA	dE	406	9	-	13/39/115/115	-
33	CYC	4L	201	3	-	9/26/74/74	0/4/4/4
36	CLA	bD	607	-	-	11/39/115/115	-
43	BCR	BD	616	7	-	2/29/63/63	0/2/2/2
33	CYC	9K	201	3	-	7/26/74/74	0/4/4/4
33	CYC	e9	201	32	-	8/26/74/74	0/4/4/4
33	CYC	YK	201	4	-	7/26/74/74	0/4/4/4
33	CYC	gF	201	29	-	9/26/74/74	0/4/4/4
37	PL9	AE	406	-	-	14/53/73/73	0/1/1/1
33	CYC	T4	201	4	-	11/26/74/74	0/4/4/4
38	SQD	L1	102	-	-	11/38/58/69	0/1/1/1
33	CYC	dJ	201	-	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	c1	504	-	-	8/39/115/115	-
36	CLA	cE	513	-	-	9/21/97/115	-
38	SQD	dE	414	9	-	10/29/49/69	0/1/1/1
39	LMG	mE	101	-	-	9/31/51/70	0/1/1/1
33	CYC	k2	201	-	-	8/26/74/74	0/4/4/4
33	CYC	X4	201	4,3	-	8/26/74/74	0/4/4/4
36	CLA	AE	404	-	-	6/17/93/115	-
33	CYC	Z4	201	3	-	6/26/74/74	0/4/4/4
36	CLA	A1	404	-	-	6/17/93/115	-
39	LMG	JD	102	14,39	-	9/22/42/70	0/1/1/1
33	CYC	m9	201	-	-	12/26/74/74	0/4/4/4
36	CLA	bE	613	-	-	17/39/115/115	-
33	CYC	j2	202	-	-	12/26/74/74	0/4/4/4
33	CYC	aF	201	4	-	10/26/74/74	0/4/4/4
33	CYC	g8	202	32	-	8/26/74/74	0/4/4/4
33	CYC	eJ	201	32	-	8/26/74/74	0/4/4/4
43	BCR	Z1	101	27	-	12/29/63/63	0/2/2/2
36	CLA	CD	511	8	-	21/39/115/115	-
33	CYC	iC	202	-	-	8/26/74/74	0/4/4/4
36	CLA	CE	515	-	-	16/39/115/115	-
39	LMG	MD	101	-	-	9/31/51/70	0/1/1/1
43	BCR	CD	519	-	-	2/29/63/63	0/2/2/2
37	PL9	d1	408	9	-	8/53/73/73	0/1/1/1
33	CYC	f2	201	31	-	12/26/74/74	0/4/4/4
33	CYC	l8	201	-	-	12/26/74/74	0/4/4/4
33	CYC	h8	201	-	-	12/26/74/74	0/4/4/4
40	LMT	BE	622	-	-	8/21/61/61	0/2/2/2
33	CYC	PB	201	4	-	11/26/74/74	0/4/4/4
42	LHG	dE	409	-	-	14/53/53/53	-
33	CYC	o4	201	3	-	11/26/74/74	0/4/4/4
40	LMT	BD	619	-	-	6/15/35/61	0/1/1/2
33	CYC	i8	201	-	-	12/26/74/74	0/4/4/4
39	LMG	C1	502	-	-	13/46/66/70	0/1/1/1
36	CLA	XD	101	25	-	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	fA	201	31	-	12/26/74/74	0/4/4/4
33	CYC	iJ	201	-	-	12/26/74/74	0/4/4/4
36	CLA	CE	503	-	-	17/39/115/115	-
38	SQD	A1	407	-	-	19/41/61/69	0/1/1/1
33	CYC	KF	201	4	-	9/26/74/74	0/4/4/4
36	CLA	bD	603	-	-	9/15/91/115	-
36	CLA	bD	604	7	-	16/39/115/115	-
40	LMT	DD	412	-	-	10/17/37/61	0/1/1/2
33	CYC	j9	202	-	-	12/26/74/74	0/4/4/4
36	CLA	cD	508	8	-	9/39/115/115	-
33	CYC	j5	201	-	-	12/26/74/74	0/4/4/4
36	CLA	X1	101	25	-	22/39/115/115	-
33	CYC	jH	201	-	-	12/26/74/74	0/4/4/4
33	CYC	GL	201	4,3	-	8/26/74/74	0/4/4/4
38	SQD	LE	101	-	-	11/38/58/69	0/1/1/1
36	CLA	B1	613	43	-	16/39/115/115	-
36	CLA	B1	610	-	-	20/39/115/115	-
43	BCR	ID	102	13	-	10/29/63/63	0/2/2/2
33	CYC	dF	201	3	-	7/26/74/74	0/4/4/4
33	CYC	eH	202	-	-	12/26/74/74	0/4/4/4
33	CYC	z4	201	4,2	-	7/26/74/74	0/4/4/4
33	CYC	uB	201	4,3	-	10/26/74/74	0/4/4/4
44	DGD	cE	518	-	-	13/51/91/95	0/2/2/2
44	DGD	h1	104	-	-	12/51/91/95	0/2/2/2
33	CYC	gK	201	29	-	9/26/74/74	0/4/4/4
44	DGD	J1	101	-	-	10/51/91/95	0/2/2/2
33	CYC	cF	201	4	-	6/26/74/74	0/4/4/4
40	LMT	j1	101	-	-	11/21/61/61	0/2/2/2
43	BCR	B1	617	-	-	4/29/63/63	0/2/2/2
36	CLA	BE	609	-	-	17/39/115/115	-
33	CYC	c6	201	-	-	8/26/74/74	0/4/4/4
33	CYC	f7	201	31	-	12/26/74/74	0/4/4/4
33	CYC	nK	202	4,3	-	7/26/74/74	0/4/4/4
36	CLA	d1	403	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	bE	611	-	-	20/39/115/115	-
38	SQD	D1	413	9	-	10/29/49/69	0/1/1/1
36	CLA	H1	103	43	-	13/39/115/115	-
40	LMT	AD	409	-	-	7/15/35/61	0/1/1/2
33	CYC	fK	201	3	-	10/26/74/74	0/4/4/4
40	LMT	bE	620	-	-	6/15/35/61	0/1/1/2
36	CLA	cE	511	-	-	15/39/115/115	-
42	LHG	l1	101	-	-	20/53/53/53	-
36	CLA	CE	513	-	-	14/39/115/115	-
43	BCR	BE	616	7	-	2/29/63/63	0/2/2/2
33	CYC	c9	201	-	-	8/26/74/74	0/4/4/4
33	CYC	bF	201	3	-	10/26/74/74	0/4/4/4
36	CLA	a1	405	-	-	5/17/93/115	-
43	BCR	cE	519	-	-	3/29/63/63	0/2/2/2
39	LMG	tD	101	22	-	7/31/51/70	0/1/1/1
36	CLA	CD	507	-	-	16/27/103/115	-
36	CLA	CD	513	-	-	14/39/115/115	-
33	CYC	g7	202	32	-	8/26/74/74	0/4/4/4

The worst 5 of 7381 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	aD	404	CLA	O2A-C1	81.33	3.36	1.45
36	a1	405	CLA	O2A-C1	81.33	3.36	1.45
36	aE	404	CLA	O2A-C1	81.32	3.36	1.45
36	AE	404	CLA	O2A-C1	81.21	3.36	1.45
36	AD	404	CLA	O2A-C1	81.20	3.36	1.45

The worst 5 of 12730 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	BE	621	SQD	O9-S-C6	-20.40	82.70	106.94
38	BD	621	SQD	O9-S-C6	-20.39	82.70	106.94
38	B1	622	SQD	O9-S-C6	-20.38	82.71	106.94
33	t4	1001	CYC	CMD-C2D-C1D	-19.23	97.42	125.56
33	tB	1001	CYC	CMD-C2D-C1D	-19.20	97.47	125.56

There are no chirality outliers.

5 of 9373 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	BB	1001	CYC	C2C-C3C-CAC-CBC
33	BB	1001	CYC	C4C-C3C-CAC-CBC
33	OB	201	CYC	NA-C4A-CHB-C1B
33	OB	201	CYC	C3A-C4A-CHB-C1B
33	OB	201	CYC	C2C-C3C-CAC-CBC

There are no ring outliers.

756 monomers are involved in 5699 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	f5	201	CYC	3	0
33	ZF	201	CYC	16	0
40	BE	623	LMT	24	0
33	aB	201	CYC	3	0
36	BD	609	CLA	1	0
37	AD	406	PL9	4	0
36	CE	511	CLA	5	0
36	B1	609	CLA	1	0
33	nF	201	CYC	2	0
33	cC	202	CYC	34	0
33	gI	302	CYC	27	0
39	DD	411	LMG	1	0
43	D1	406	BCR	1	0
36	B1	612	CLA	7	0
33	eF	201	CYC	1	0
42	aE	411	LHG	6	0
36	C1	515	CLA	6	0
39	A1	408	LMG	6	0
39	D1	410	LMG	1	0
33	j7	202	CYC	38	0
33	eJ	202	CYC	30	0
39	mD	101	LMG	10	0
36	BD	603	CLA	6	0
33	bK	201	CYC	1	0
36	bE	615	CLA	3	0
36	bD	614	CLA	1	0
40	C1	520	LMT	15	0
40	bE	602	LMT	3	0
43	k1	102	BCR	4	0
47	v1	201	HEM	2	0
43	bE	618	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	e9	202	CYC	28	0
33	dK	201	CYC	1	0
39	b1	619	LMG	2	0
43	C1	516	BCR	1	0
33	m6	201	CYC	38	0
33	kK	201	CYC	2	0
36	CE	504	CLA	3	0
43	XE	102	BCR	3	0
36	BD	613	CLA	2	0
37	DE	408	PL9	3	0
33	iJ	202	CYC	13	0
36	AD	405	CLA	4	0
42	eE	101	LHG	1	0
33	LG	201	CYC	3	0
43	C1	519	BCR	5	0
36	BE	612	CLA	6	0
42	AE	411	LHG	3	0
44	c1	516	DGD	2	0
45	dE	402	PHO	7	0
44	cD	518	DGD	2	0
36	c1	508	CLA	2	0
33	2G	201	CYC	1	0
36	AD	404	CLA	2	0
42	D1	408	LHG	1	0
33	c2	202	CYC	32	0
43	ZE	102	BCR	3	0
33	g2	202	CYC	16	0
42	a1	412	LHG	6	0
36	cE	504	CLA	1	0
33	c8	201	CYC	1	0
33	cJ	201	CYC	1	0
37	a1	409	PL9	3	0
33	bI	201	CYC	10	0
33	1L	201	CYC	4	0
33	SL	201	CYC	1	0
36	BE	608	CLA	6	0
33	jC	201	CYC	6	0
33	b9	201	CYC	10	0
36	cE	503	CLA	3	0
33	QB	201	CYC	2	0
38	h1	103	SQD	2	0
44	JE	101	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	cE	516	DGD	3	0
36	cD	511	CLA	3	0
33	l9	201	CYC	7	0
33	Y4	201	CYC	3	0
33	3K	101	CYC	4	0
33	c9	202	CYC	34	0
36	b1	606	CLA	1	0
33	i2	202	CYC	14	0
43	b1	616	BCR	4	0
43	bE	616	BCR	3	0
33	l3	201	CYC	7	0
39	TE	101	LMG	1	0
36	iE	101	CLA	3	0
38	DE	414	SQD	1	0
33	zB	201	CYC	1	0
39	CE	520	LMG	1	0
36	cE	512	CLA	4	0
36	CD	505	CLA	6	0
33	i6	201	CYC	26	0
36	CE	510	CLA	2	0
36	cE	506	CLA	2	0
36	BD	608	CLA	6	0
38	L1	101	SQD	4	0
39	aD	409	LMG	1	0
42	lD	101	LHG	3	0
36	CD	512	CLA	1	0
33	JF	201	CYC	20	0
40	bD	602	LMT	3	0
43	BD	615	BCR	5	0
33	p4	201	CYC	1	0
39	B1	618	LMG	3	0
43	z1	101	BCR	1	0
33	iI	202	CYC	13	0
45	DE	401	PHO	19	0
33	XB	201	CYC	1	0
33	pB	201	CYC	1	0
42	AD	411	LHG	1	0
44	cD	516	DGD	2	0
36	c1	510	CLA	14	0
36	bD	610	CLA	1	0
33	i5	201	CYC	26	0
33	c7	201	CYC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	BB	1002	CYC	1	0
33	g3	201	CYC	25	0
36	b1	605	CLA	5	0
33	iH	201	CYC	25	0
33	a4	201	CYC	3	0
33	sB	201	CYC	4	0
36	B1	604	CLA	1	0
36	B1	606	CLA	10	0
36	CD	504	CLA	3	0
33	qB	201	CYC	3	0
36	bD	611	CLA	1	0
38	DD	414	SQD	1	0
40	B1	623	LMT	23	0
40	cE	501	LMT	19	0
36	bE	606	CLA	1	0
38	AD	407	SQD	6	0
33	nK	201	CYC	2	0
33	QG	201	CYC	1	0
33	eI	201	CYC	5	0
33	AG	201	CYC	3	0
33	hF	201	CYC	55	0
42	BE	620	LHG	4	0
43	IE	102	BCR	7	0
40	dD	413	LMT	7	0
33	d7	201	CYC	6	0
33	g7	201	CYC	26	0
39	a1	410	LMG	1	0
40	DE	413	LMT	5	0
43	d1	407	BCR	2	0
36	cE	510	CLA	5	0
36	CE	512	CLA	1	0
36	BD	607	CLA	3	0
36	cE	505	CLA	3	0
42	DE	410	LHG	4	0
33	MG	201	CYC	6	0
33	ZK	201	CYC	16	0
44	JD	101	DGD	2	0
33	gI	301	CYC	16	0
43	B1	616	BCR	6	0
42	d1	410	LHG	1	0
36	C1	513	CLA	12	0
33	dC	201	CYC	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	h1	102	CLA	2	0
33	OL	201	CYC	8	0
33	7L	201	CYC	2	0
43	b1	617	BCR	5	0
36	C1	505	CLA	4	0
43	i1	101	BCR	11	0
33	j8	201	CYC	6	0
36	HE	103	CLA	4	0
40	cD	501	LMT	33	0
33	e2	202	CYC	29	0
36	b1	611	CLA	1	0
42	dE	410	LHG	1	0
39	tE	101	LMG	5	0
39	aE	407	LMG	3	0
33	WG	201	CYC	1	0
33	q4	201	CYC	4	0
33	k9	201	CYC	11	0
36	BE	603	CLA	5	0
36	BE	611	CLA	6	0
39	DE	411	LMG	1	0
33	JK	201	CYC	23	0
33	yB	201	CYC	4	0
43	kE	102	BCR	2	0
33	IG	201	CYC	34	0
42	DD	409	LHG	1	0
33	kH	201	CYC	11	0
36	b1	610	CLA	1	0
36	bE	608	CLA	1	0
33	l2	201	CYC	7	0
38	BE	621	SQD	1	0
33	g9	201	CYC	26	0
36	bE	612	CLA	3	0
39	bD	619	LMG	2	0
33	TL	201	CYC	2	0
36	B1	601	CLA	1	0
39	a1	408	LMG	3	0
43	DE	407	BCR	1	0
39	j1	102	LMG	1	0
43	kD	102	BCR	5	0
36	dD	406	CLA	4	0
33	ZB	201	CYC	1	0
36	BD	605	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	jH	202	CYC	37	0
36	c1	512	CLA	3	0
33	eK	201	CYC	2	0
36	B1	605	CLA	3	0
43	Z1	102	BCR	1	0
44	cD	517	DGD	6	0
43	X1	102	BCR	4	0
36	bD	608	CLA	1	0
44	CE	518	DGD	5	0
33	RG	201	CYC	2	0
39	BE	618	LMG	3	0
36	hE	102	CLA	2	0
40	d1	413	LMT	7	0
33	eC	202	CYC	28	0
33	c7	202	CYC	33	0
36	BE	607	CLA	3	0
33	gJ	202	CYC	8	0
42	A1	411	LHG	1	0
43	CE	519	BCR	5	0
33	gA	302	CYC	25	0
36	BD	611	CLA	6	0
33	e8	202	CYC	29	0
43	zD	101	BCR	2	0
33	iA	201	CYC	26	0
33	tB	1001	CYC	1	0
44	C1	518	DGD	5	0
33	P4	201	CYC	2	0
39	m1	101	LMG	10	0
33	g9	202	CYC	16	0
36	C1	511	CLA	8	0
42	e1	101	LHG	1	0
36	hE	101	CLA	4	0
36	cE	507	CLA	4	0
33	e5	202	CYC	28	0
33	Q4	201	CYC	2	0
33	mI	201	CYC	38	0
33	OB	201	CYC	2	0
36	C1	514	CLA	3	0
40	jD	101	LMT	1	0
33	cA	201	CYC	4	0
36	cD	510	CLA	23	0
33	hI	201	CYC	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	hE	105	BCR	3	0
36	b1	612	CLA	3	0
36	DE	406	CLA	5	0
36	b1	608	CLA	1	0
33	i5	202	CYC	14	0
36	BE	602	CLA	6	0
39	t1	101	LMG	5	0
33	g3	202	CYC	16	0
33	f3	201	CYC	3	0
33	1G	201	CYC	3	0
33	R4	201	CYC	3	0
33	i9	201	CYC	26	0
33	bC	201	CYC	11	0
38	hD	103	SQD	2	0
33	ML	201	CYC	6	0
33	QL	201	CYC	1	0
43	BD	617	BCR	3	0
33	oB	201	CYC	1	0
33	VB	201	CYC	22	0
33	fC	201	CYC	3	0
36	cD	504	CLA	1	0
39	CD	522	LMG	1	0
33	h5	201	CYC	12	0
41	a1	411	BCT	1	0
36	C1	503	CLA	3	0
39	aE	409	LMG	1	0
40	DD	413	LMT	5	0
42	B1	621	LHG	3	0
33	c3	201	CYC	4	0
33	e7	202	CYC	29	0
33	g5	201	CYC	26	0
33	B4	1002	CYC	1	0
33	lI	201	CYC	7	0
33	k5	201	CYC	9	0
36	cD	512	CLA	3	0
33	fH	201	CYC	4	0
36	B1	608	CLA	5	0
36	BE	606	CLA	10	0
36	CD	515	CLA	7	0
36	cD	509	CLA	1	0
33	l6	201	CYC	7	0
33	AL	201	CYC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	j3	201	CYC	6	0
33	k8	201	CYC	10	0
47	VD	201	HEM	2	0
43	cD	519	BCR	1	0
36	B1	607	CLA	4	0
40	jE	101	LMT	1	0
33	KK	201	CYC	3	0
33	BB	1001	CYC	9	0
40	CD	521	LMT	23	0
33	m2	201	CYC	36	0
36	D1	405	CLA	5	0
33	TB	201	CYC	2	0
33	j6	202	CYC	38	0
33	b6	201	CYC	10	0
33	kF	201	CYC	2	0
33	gH	202	CYC	8	0
47	vE	201	HEM	2	0
33	h9	201	CYC	14	0
33	b3	201	CYC	10	0
33	IL	201	CYC	26	0
42	eD	101	LHG	1	0
33	h6	201	CYC	15	0
36	c1	506	CLA	5	0
36	b1	604	CLA	6	0
33	cH	201	CYC	1	0
42	D1	409	LHG	4	0
33	lC	201	CYC	6	0
33	aK	201	CYC	2	0
33	c2	201	CYC	4	0
33	dI	201	CYC	6	0
36	C1	504	CLA	3	0
33	j3	202	CYC	35	0
33	YF	201	CYC	53	0
33	t4	1001	CYC	1	0
33	k6	201	CYC	9	0
36	DD	406	CLA	6	0
36	c1	509	CLA	1	0
39	aD	407	LMG	3	0
44	c1	517	DGD	6	0
36	aD	405	CLA	2	0
33	VL	201	CYC	2	0
36	xE	101	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	c1	502	CLA	10	0
36	a1	407	CLA	16	0
36	CE	509	CLA	1	0
36	cD	513	CLA	10	0
45	DE	403	PHO	3	0
36	bD	605	CLA	6	0
33	j2	201	CYC	6	0
43	cD	515	BCR	31	0
39	bE	619	LMG	2	0
33	d6	201	CYC	5	0
43	bD	616	BCR	4	0
43	dD	407	BCR	2	0
42	BD	620	LHG	3	0
33	gC	301	CYC	15	0
33	e3	201	CYC	5	0
33	g6	201	CYC	26	0
36	cE	508	CLA	7	0
33	hC	201	CYC	13	0
39	jE	102	LMG	1	0
33	7G	201	CYC	2	0
33	YB	201	CYC	3	0
33	m7	201	CYC	38	0
33	dH	201	CYC	6	0
33	c6	202	CYC	34	0
36	CE	505	CLA	5	0
36	cD	505	CLA	3	0
36	CD	508	CLA	2	0
33	eI	202	CYC	29	0
33	vB	201	CYC	1	0
33	i9	202	CYC	14	0
36	BD	610	CLA	1	0
33	c3	202	CYC	32	0
36	CD	514	CLA	3	0
43	I1	102	BCR	5	0
37	dE	408	PL9	5	0
43	hD	105	BCR	3	0
40	dE	413	LMT	7	0
33	WL	201	CYC	1	0
33	h3	201	CYC	14	0
33	mK	201	CYC	2	0
33	JL	201	CYC	3	0
33	fJ	201	CYC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	HE	101	CLA	2	0
33	2L	201	CYC	1	0
40	d1	404	LMT	1	0
47	VE	201	HEM	2	0
36	hD	102	CLA	2	0
33	f8	201	CYC	3	0
36	dD	405	CLA	2	0
33	mH	201	CYC	38	0
33	j9	201	CYC	6	0
33	iI	201	CYC	26	0
36	BE	614	CLA	3	0
33	b8	201	CYC	10	0
36	B1	611	CLA	5	0
44	cE	517	DGD	6	0
45	DD	401	PHO	30	0
45	A1	412	PHO	1	0
33	hK	201	CYC	54	0
36	C1	512	CLA	1	0
44	CD	518	DGD	5	0
33	e6	202	CYC	30	0
33	j5	202	CYC	34	0
36	x1	101	CLA	7	0
33	IF	201	CYC	2	0
38	hE	103	SQD	2	0
33	jI	202	CYC	35	0
33	g5	202	CYC	8	0
36	cD	507	CLA	6	0
43	bD	617	BCR	5	0
33	e5	201	CYC	5	0
45	aE	412	PHO	5	0
33	b5	201	CYC	11	0
39	dE	411	LMG	13	0
33	hA	201	CYC	14	0
39	TD	101	LMG	1	0
42	dD	409	LHG	2	0
45	d1	402	PHO	3	0
33	e8	201	CYC	5	0
47	V1	201	HEM	2	0
40	dE	404	LMT	1	0
36	C1	509	CLA	1	0
36	dE	405	CLA	3	0
33	i2	201	CYC	25	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	kC	201	CYC	9	0
33	hH	201	CYC	13	0
33	cI	202	CYC	34	0
39	jD	102	LMG	1	0
37	aE	408	PL9	2	0
33	PG	201	CYC	3	0
40	BD	623	LMT	24	0
33	u4	201	CYC	4	0
33	kJ	201	CYC	10	0
36	BE	605	CLA	4	0
43	BE	615	BCR	4	0
33	c8	202	CYC	33	0
33	lH	201	CYC	7	0
40	D1	412	LMT	5	0
36	IE	101	CLA	1	0
36	bE	609	CLA	4	0
33	eC	201	CYC	5	0
43	b1	618	BCR	6	0
33	m8	201	CYC	37	0
33	e7	201	CYC	5	0
36	H1	101	CLA	2	0
36	XE	101	CLA	2	0
33	e3	202	CYC	29	0
33	g6	202	CYC	18	0
33	kI	201	CYC	11	0
39	d1	411	LMG	13	0
33	jA	202	CYC	36	0
39	T1	101	LMG	1	0
33	C4	1001	CYC	1	0
33	GG	201	CYC	1	0
39	AD	408	LMG	7	0
43	bD	618	BCR	5	0
33	OG	201	CYC	8	0
36	cD	506	CLA	2	0
36	bE	603	CLA	1	0
33	k3	201	CYC	10	0
33	eA	202	CYC	28	0
38	d1	414	SQD	1	0
44	c1	518	DGD	2	0
43	iD	102	BCR	11	0
36	I1	101	CLA	1	0
33	b2	201	CYC	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	aE	405	CLA	2	0
42	dD	410	LHG	1	0
36	BD	602	CLA	6	0
37	A1	406	PL9	3	0
33	d3	201	CYC	6	0
42	DE	409	LHG	1	0
43	h1	105	BCR	3	0
33	9F	201	CYC	1	0
33	cK	201	CYC	2	0
36	BE	604	CLA	1	0
33	bJ	201	CYC	10	0
36	bD	613	CLA	7	0
43	c1	519	BCR	1	0
36	xD	101	CLA	7	0
43	dE	407	BCR	2	0
36	bD	612	CLA	3	0
39	BD	618	LMG	3	0
36	a1	406	CLA	2	0
42	d1	409	LHG	2	0
36	h1	101	CLA	6	0
33	jI	201	CYC	6	0
44	HE	102	DGD	5	0
36	aE	404	CLA	1	0
33	c5	201	CYC	1	0
36	AE	405	CLA	4	0
42	aD	411	LHG	6	0
36	C1	510	CLA	2	0
36	BD	601	CLA	1	0
38	dD	414	SQD	1	0
33	PL	201	CYC	3	0
36	BD	606	CLA	10	0
33	LK	201	CYC	2	0
36	cD	503	CLA	4	0
33	6G	201	CYC	15	0
44	hE	104	DGD	4	0
33	s4	201	CYC	4	0
33	h2	201	CYC	12	0
33	i8	202	CYC	14	0
33	lJ	201	CYC	7	0
33	LL	201	CYC	1	0
33	kA	201	CYC	9	0
43	CD	520	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	ZD	101	BCR	3	0
38	BD	621	SQD	1	0
36	c1	507	CLA	4	0
33	e6	201	CYC	5	0
43	c1	515	BCR	35	0
36	b1	603	CLA	1	0
37	DD	408	PL9	4	0
33	nF	202	CYC	2	0
36	bE	604	CLA	6	0
33	bA	201	CYC	10	0
39	C1	521	LMG	1	0
33	j6	201	CYC	6	0
33	gH	201	CYC	26	0
33	LF	201	CYC	2	0
33	l5	201	CYC	7	0
36	c1	513	CLA	4	0
33	W4	201	CYC	3	0
33	jA	201	CYC	6	0
39	yD	101	LMG	8	0
33	TG	201	CYC	2	0
33	y4	201	CYC	4	0
36	c1	511	CLA	2	0
45	dD	402	PHO	9	0
47	vD	201	HEM	2	0
36	A1	405	CLA	4	0
33	j8	202	CYC	36	0
33	c5	202	CYC	31	0
33	jJ	201	CYC	6	0
45	aD	412	PHO	1	0
36	BD	614	CLA	3	0
44	HD	102	DGD	6	0
33	d9	201	CYC	6	0
33	h7	201	CYC	14	0
36	CD	503	CLA	3	0
33	i6	202	CYC	14	0
40	a1	401	LMT	1	0
33	eH	201	CYC	5	0
33	RB	201	CYC	3	0
33	b7	201	CYC	11	0
45	a1	413	PHO	6	0
36	bD	615	CLA	3	0
33	fF	201	CYC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	bH	201	CYC	10	0
33	j7	201	CYC	6	0
33	mJ	201	CYC	38	0
33	HG	201	CYC	2	0
36	dE	403	CLA	18	0
33	JG	201	CYC	3	0
33	5L	201	CYC	3	0
33	CB	1001	CYC	1	0
36	HD	103	CLA	6	0
45	DD	403	PHO	4	0
33	i7	201	CYC	25	0
37	D1	407	PL9	4	0
33	m5	201	CYC	37	0
33	cI	201	CYC	4	0
36	bE	607	CLA	3	0
33	rB	201	CYC	1	0
33	cC	201	CYC	4	0
33	f6	201	CYC	3	0
38	LD	102	SQD	6	0
38	AE	407	SQD	7	0
42	DD	410	LHG	4	0
33	mF	201	CYC	2	0
36	bE	610	CLA	1	0
37	dD	408	PL9	3	0
36	HD	101	CLA	2	0
36	b1	614	CLA	1	0
33	e2	201	CYC	5	0
33	g2	201	CYC	25	0
33	k7	201	CYC	11	0
36	b1	609	CLA	4	0
33	V4	201	CYC	29	0
33	mA	201	CYC	37	0
33	MF	201	CYC	25	0
38	LE	102	SQD	5	0
43	B1	615	BCR	5	0
36	BE	610	CLA	1	0
40	dD	404	LMT	1	0
33	WB	201	CYC	3	0
36	B1	603	CLA	5	0
33	MK	201	CYC	25	0
33	mC	201	CYC	38	0
33	i3	201	CYC	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	d8	201	CYC	6	0
36	BD	604	CLA	1	0
36	b1	615	CLA	3	0
33	iA	202	CYC	14	0
38	cE	502	SQD	1	0
36	cE	509	CLA	1	0
43	bE	617	BCR	5	0
45	D1	402	PHO	3	0
33	SG	201	CYC	1	0
33	cA	202	CYC	34	0
39	dD	411	LMG	13	0
43	DD	407	BCR	1	0
43	iE	102	BCR	11	0
36	aD	406	CLA	16	0
33	cJ	202	CYC	32	0
33	iH	202	CYC	14	0
36	b1	607	CLA	3	0
39	AE	408	LMG	7	0
33	g8	201	CYC	25	0
43	BE	617	BCR	3	0
33	jJ	202	CYC	35	0
36	aE	406	CLA	16	0
33	NG	201	CYC	7	0
36	bE	605	CLA	4	0
36	ID	101	CLA	1	0
36	CE	508	CLA	2	0
33	v4	201	CYC	1	0
33	i3	202	CYC	14	0
43	cE	515	BCR	35	0
33	d5	201	CYC	6	0
36	CD	510	CLA	2	0
36	c1	505	CLA	2	0
33	gJ	201	CYC	25	0
36	iD	101	CLA	3	0
39	y1	101	LMG	8	0
33	O4	201	CYC	2	0
36	dD	403	CLA	18	0
36	C1	508	CLA	2	0
40	b1	602	LMT	3	0
33	cH	202	CYC	35	0
36	bD	609	CLA	5	0
36	B1	602	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B4	1001	CYC	8	0
43	ZE	101	BCR	2	0
43	zE	101	BCR	2	0
40	BD	622	LMT	7	0
37	aD	408	PL9	1	0
33	d2	201	CYC	6	0
33	i7	202	CYC	14	0
33	fI	201	CYC	3	0
36	b1	613	CLA	7	0
36	BD	612	CLA	7	0
36	BE	601	CLA	1	0
44	H1	102	DGD	5	0
36	aD	404	CLA	1	0
33	NL	201	CYC	8	0
33	IK	201	CYC	2	0
33	eA	201	CYC	5	0
36	c1	503	CLA	7	0
36	hD	101	CLA	5	0
36	bD	606	CLA	1	0
44	CE	517	DGD	1	0
38	B1	622	SQD	1	0
36	BE	613	CLA	3	0
36	B1	614	CLA	3	0
39	yE	101	LMG	8	0
44	hD	104	DGD	4	0
33	iC	201	CYC	25	0
38	LD	101	SQD	4	0
33	RL	201	CYC	2	0
33	XK	201	CYC	1	0
33	m3	201	CYC	37	0
33	3F	101	CYC	3	0
33	6L	201	CYC	15	0
36	d1	406	CLA	2	0
33	VG	201	CYC	2	0
33	f9	201	CYC	3	0
33	lA	201	CYC	7	0
33	hJ	201	CYC	12	0
33	jC	202	CYC	36	0
33	gC	302	CYC	25	0
36	CD	509	CLA	3	0
33	5G	201	CYC	3	0
42	lE	101	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	dA	201	CYC	6	0
33	gA	301	CYC	15	0
33	l7	201	CYC	7	0
33	HL	201	CYC	2	0
43	XD	102	BCR	3	0
36	CE	514	CLA	2	0
36	dE	406	CLA	3	0
36	bD	607	CLA	3	0
43	BD	616	BCR	5	0
33	9K	201	CYC	1	0
33	e9	201	CYC	5	0
33	YK	201	CYC	52	0
33	gF	201	CYC	1	0
37	AE	406	PL9	2	0
33	T4	201	CYC	2	0
38	L1	102	SQD	5	0
33	dJ	201	CYC	6	0
36	c1	504	CLA	4	0
36	cE	513	CLA	9	0
38	dE	414	SQD	1	0
39	mE	101	LMG	10	0
33	k2	201	CYC	9	0
33	X4	201	CYC	1	0
36	AE	404	CLA	2	0
33	Z4	201	CYC	1	0
36	A1	404	CLA	2	0
33	m9	201	CYC	38	0
36	bE	613	CLA	6	0
33	j2	202	CYC	35	0
33	aF	201	CYC	2	0
33	g8	202	CYC	8	0
33	eJ	201	CYC	5	0
43	Z1	101	BCR	2	0
36	CD	511	CLA	6	0
33	iC	202	CYC	13	0
36	CE	515	CLA	6	0
43	CD	519	BCR	5	0
37	d1	408	PL9	3	0
33	f2	201	CYC	3	0
33	l8	201	CYC	6	0
33	h8	201	CYC	15	0
40	BE	622	LMT	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	PB	201	CYC	2	0
42	dE	409	LHG	2	0
33	o4	201	CYC	1	0
33	i8	201	CYC	27	0
36	XD	101	CLA	2	0
33	fA	201	CYC	3	0
33	iJ	201	CYC	25	0
36	CE	503	CLA	4	0
38	A1	407	SQD	6	0
33	KF	201	CYC	3	0
36	bD	603	CLA	1	0
36	bD	604	CLA	6	0
33	j9	202	CYC	37	0
36	cD	508	CLA	10	0
33	j5	201	CYC	6	0
36	X1	101	CLA	2	0
33	jH	201	CYC	6	0
33	GL	201	CYC	1	0
38	LE	101	SQD	4	0
36	B1	613	CLA	2	0
36	B1	610	CLA	1	0
43	ID	102	BCR	6	0
33	dF	201	CYC	1	0
33	eH	202	CYC	29	0
33	z4	201	CYC	1	0
33	uB	201	CYC	1	0
44	cE	518	DGD	2	0
44	h1	104	DGD	4	0
33	gK	201	CYC	1	0
44	J1	101	DGD	2	0
33	cF	201	CYC	2	0
40	j1	101	LMT	1	0
43	B1	617	BCR	4	0
36	BE	609	CLA	1	0
33	c6	201	CYC	4	0
33	f7	201	CYC	3	0
33	nK	202	CYC	2	0
36	d1	403	CLA	18	0
36	bE	611	CLA	1	0
38	D1	413	SQD	1	0
36	H1	103	CLA	4	0
33	fK	201	CYC	2	0

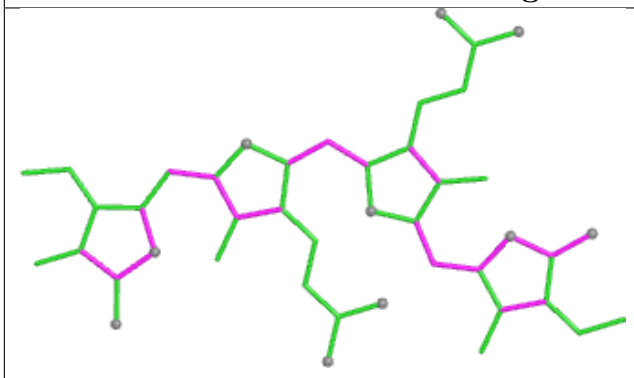
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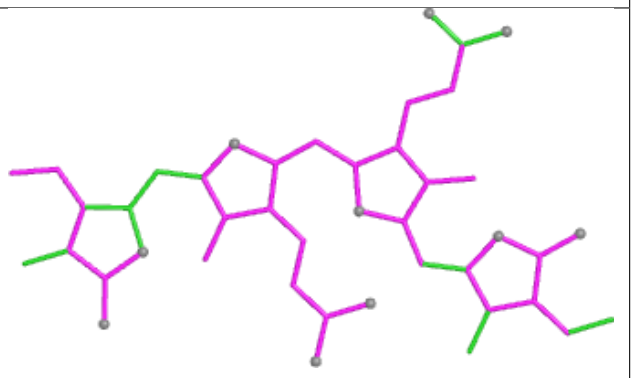
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	cE	511	CLA	2	0
42	l1	101	LHG	3	0
36	CE	513	CLA	11	0
43	BE	616	BCR	5	0
33	c9	201	CYC	4	0
33	bF	201	CYC	1	0
36	a1	405	CLA	1	0
43	cE	519	BCR	2	0
39	tD	101	LMG	5	0
36	CD	513	CLA	12	0
33	g7	202	CYC	16	0

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.

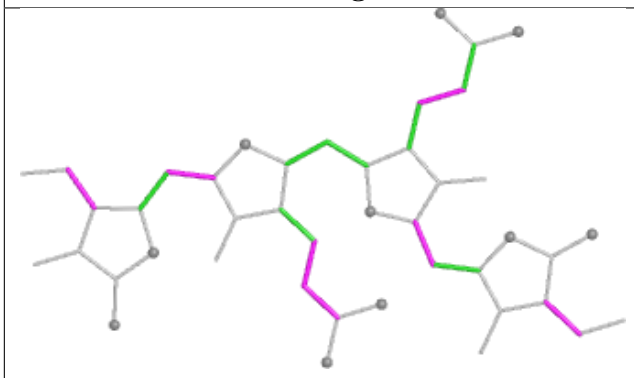
Ligand CYC f5 201



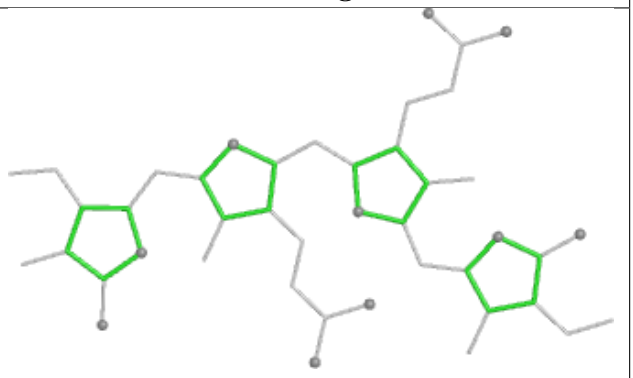
Bond lengths



Bond angles

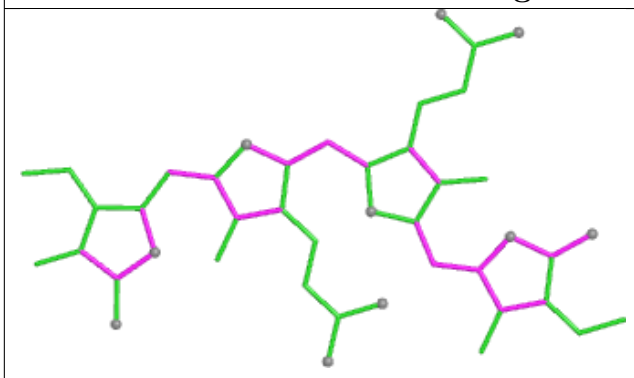


Torsions

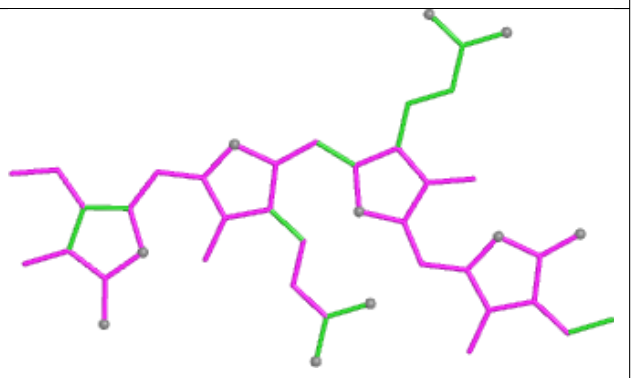


Rings

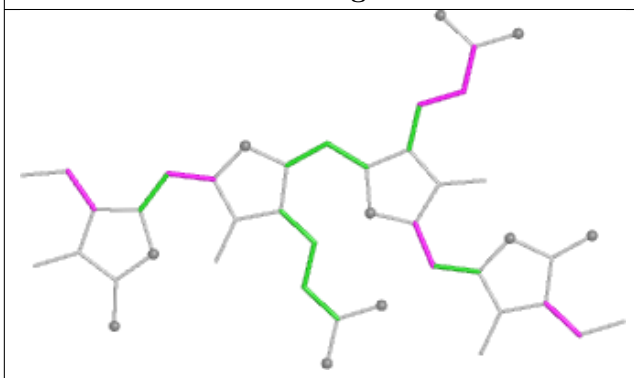
Ligand CYC ZF 201



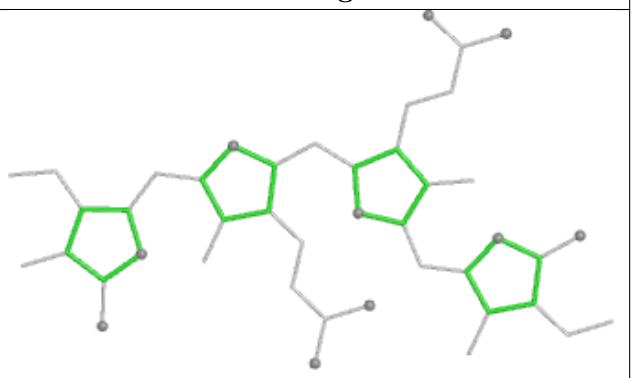
Bond lengths



Bond angles

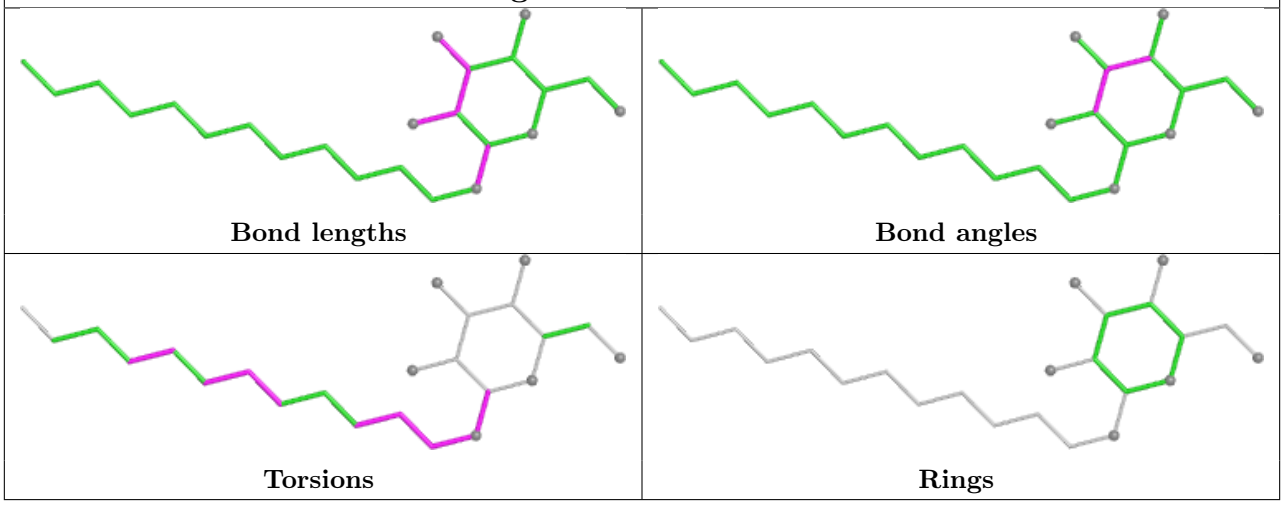


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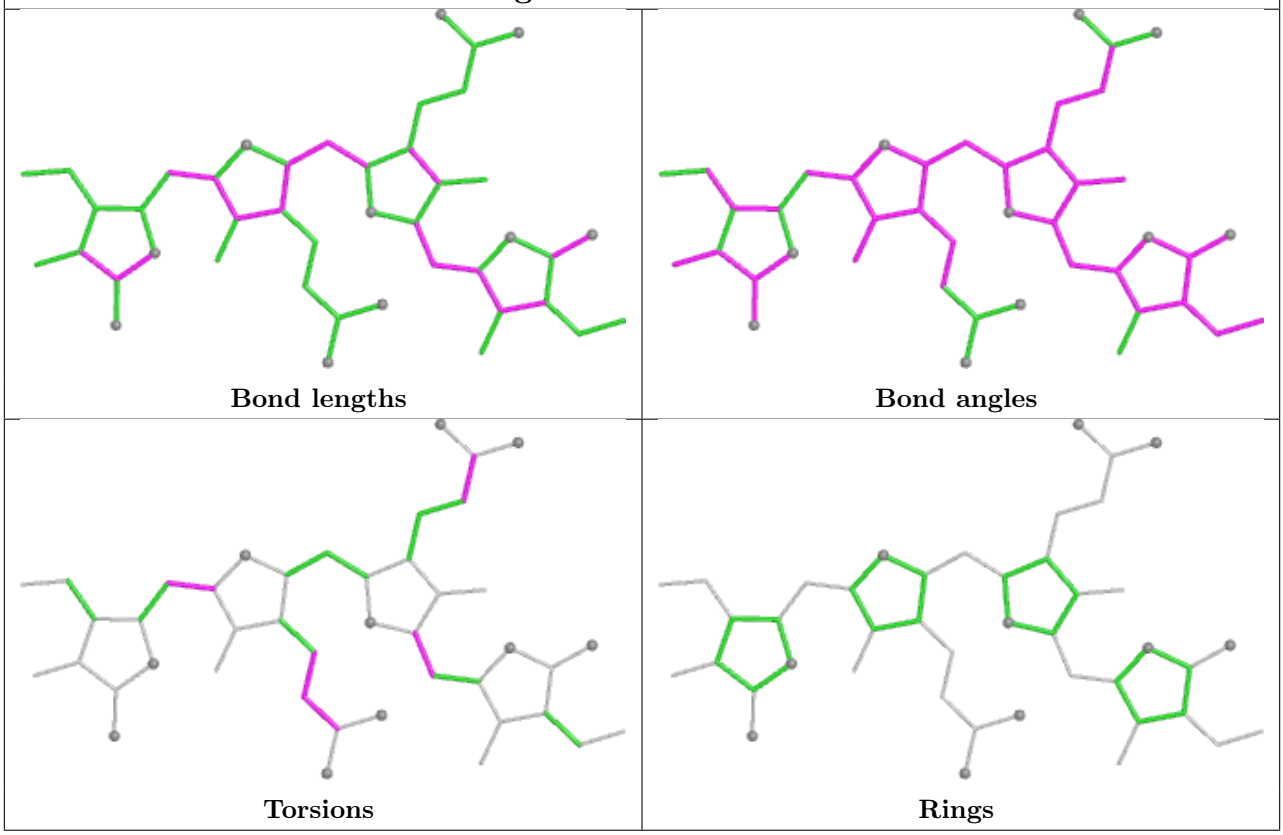


Rings

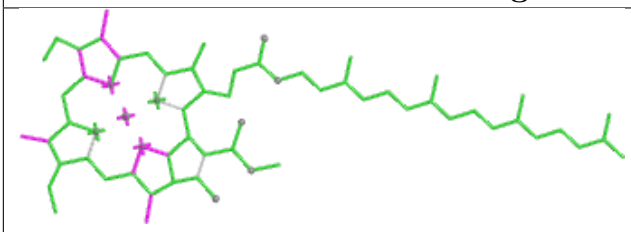
Ligand LMT BE 623



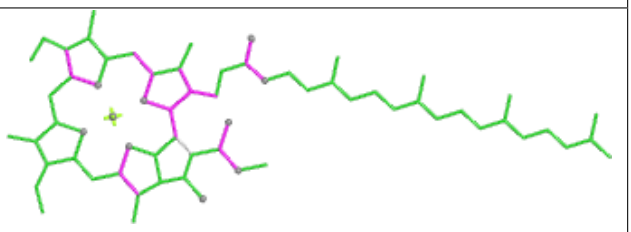
Ligand CYC aB 201



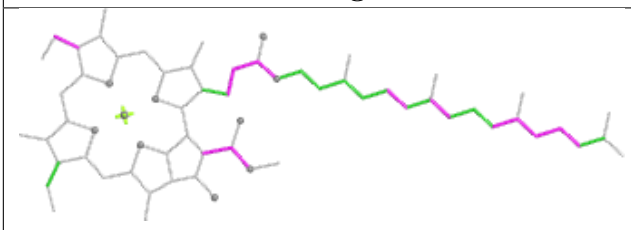
Ligand CLA BD 609



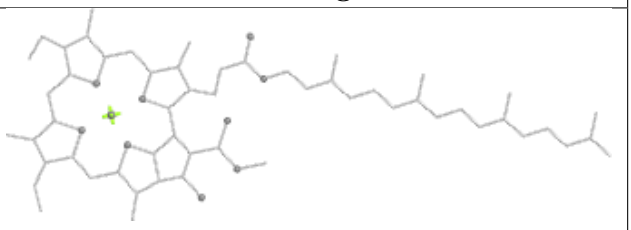
Bond lengths



Bond angles



Torsions

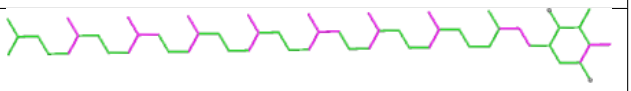


Rings

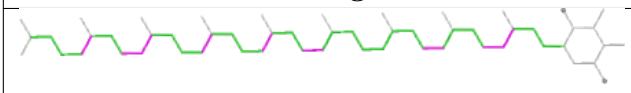
Ligand PL9 AD 406



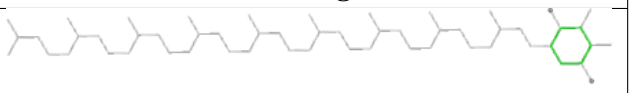
Bond lengths



Bond angles

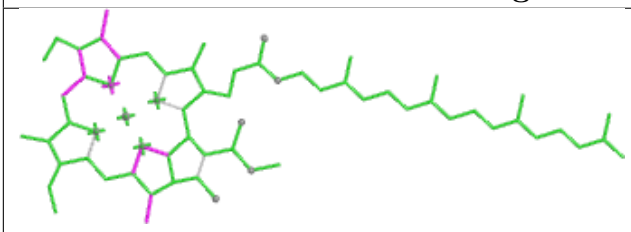


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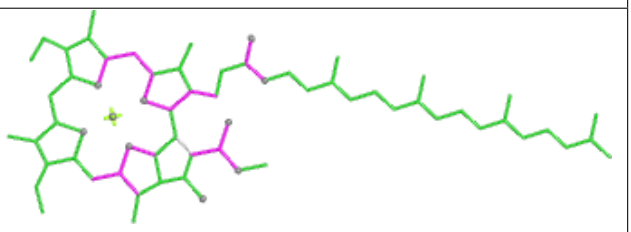


Rings

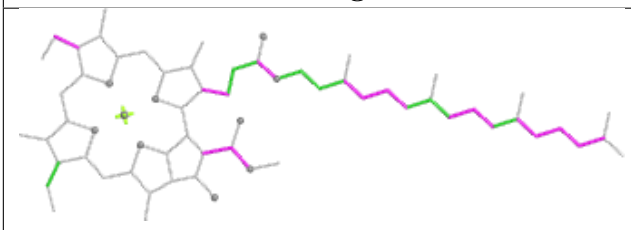
Ligand CLA CE 511



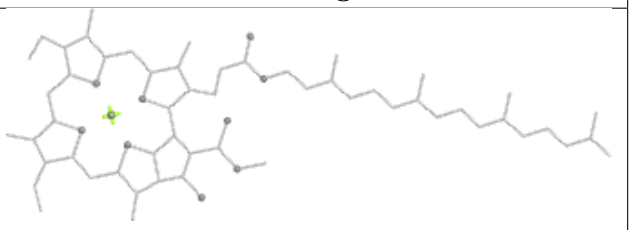
Bond lengths



Bond angles

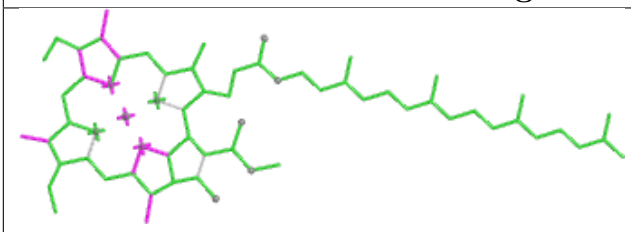


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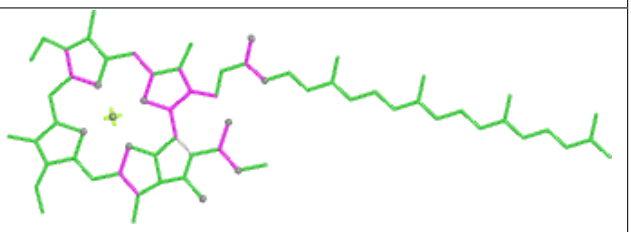


Rings

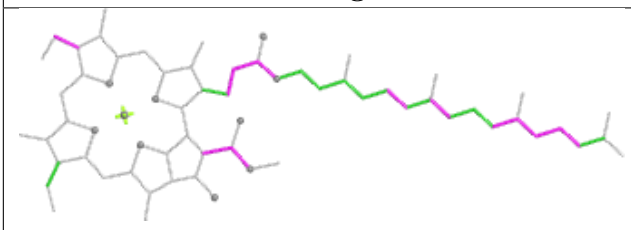
Ligand CLA B1 609



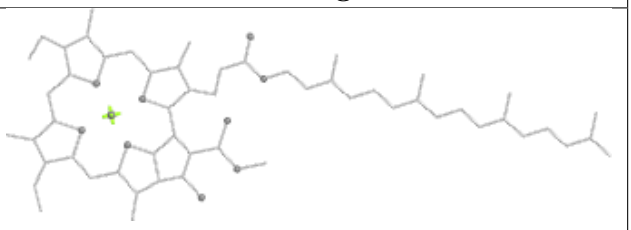
Bond lengths



Bond angles

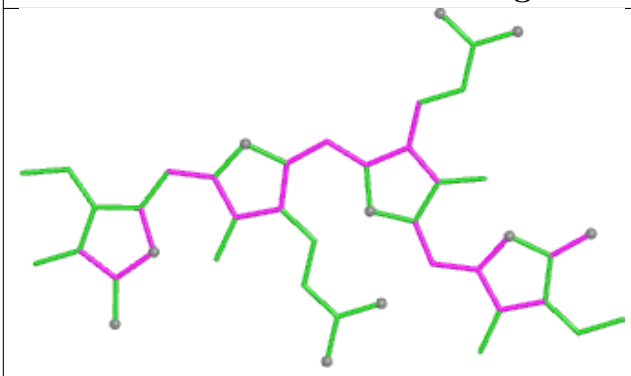


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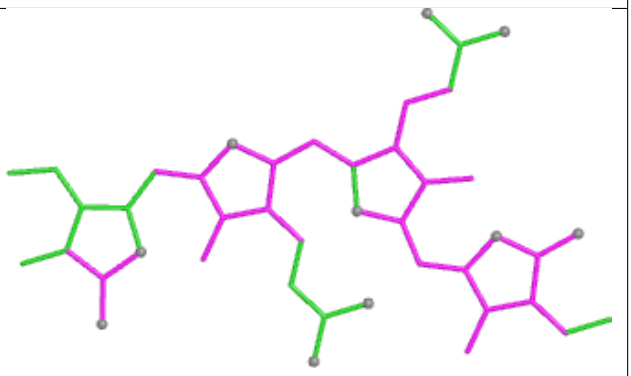


Rings

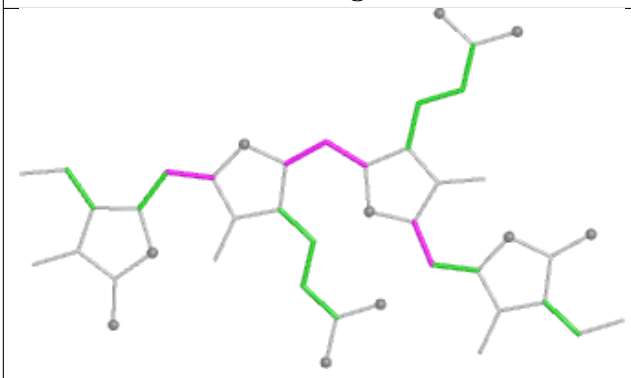
Ligand CYC nF 201



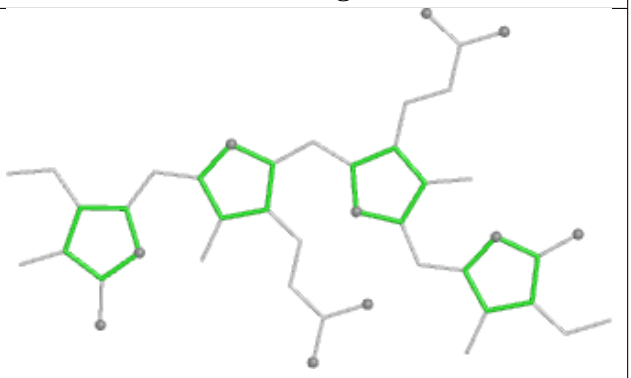
Bond lengths



Bond angles

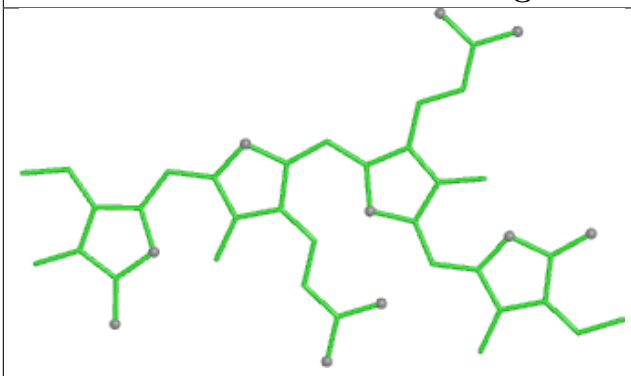


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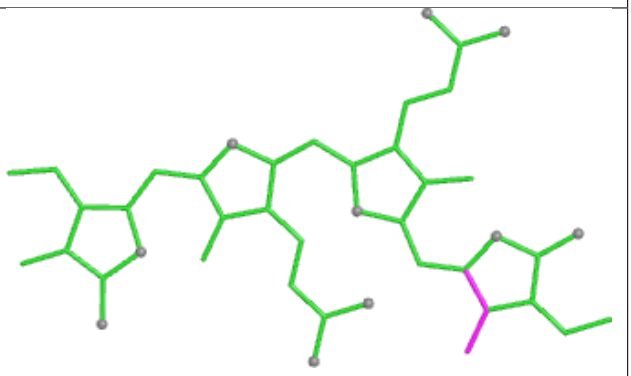


Rings

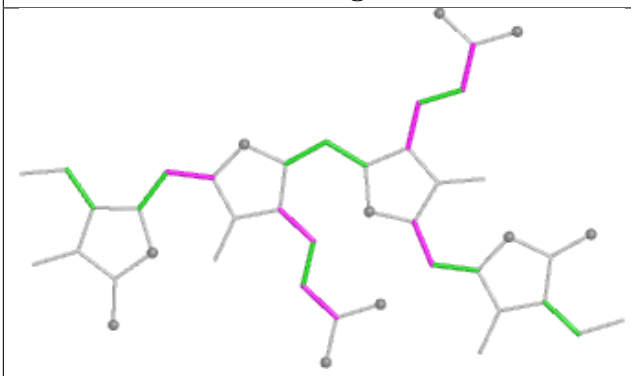
Ligand CYC cC 202



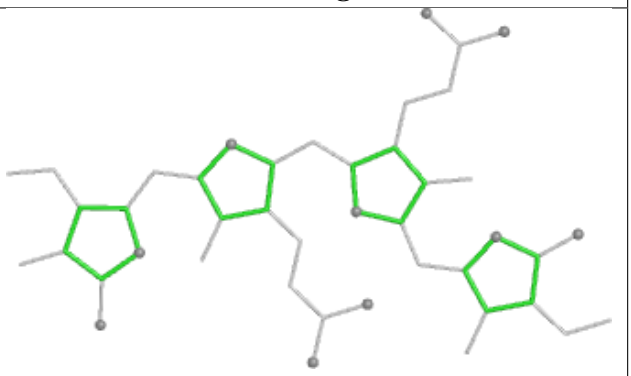
Bond lengths



Bond angles

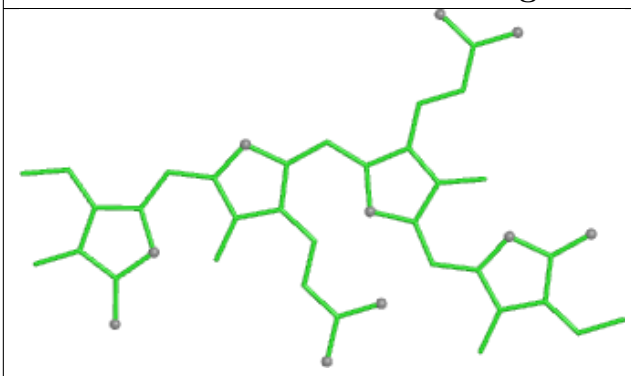


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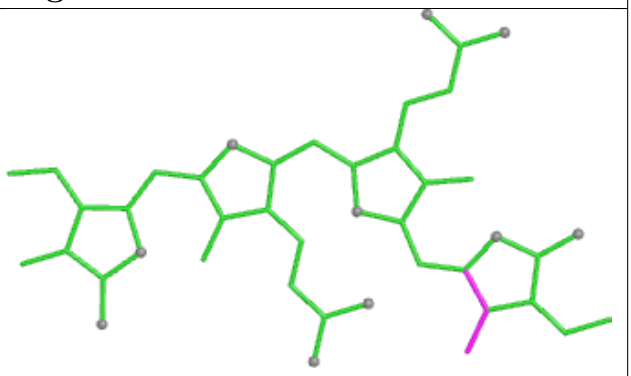


Rings

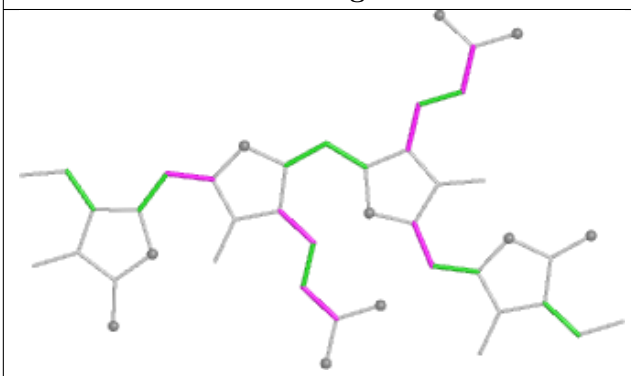
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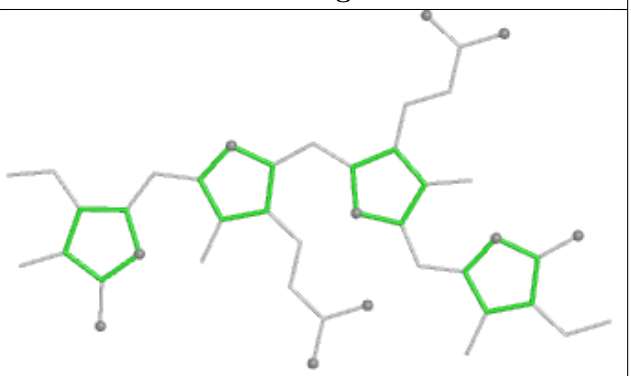
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Bond angles

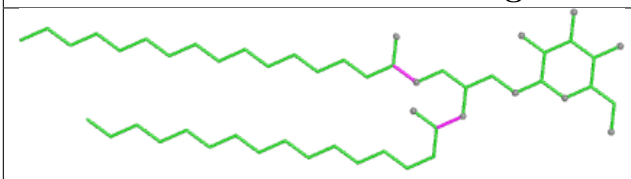


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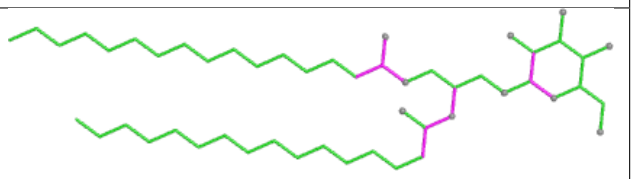


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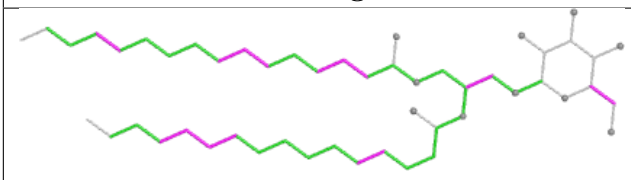
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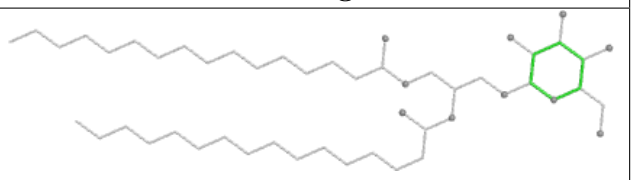
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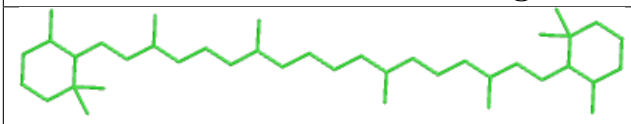


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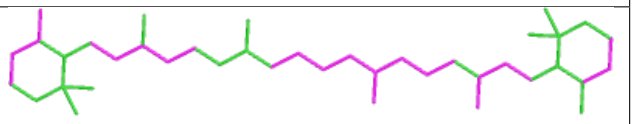


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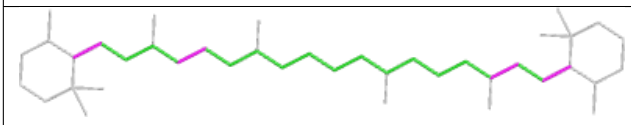
Ligand BCR D1 406



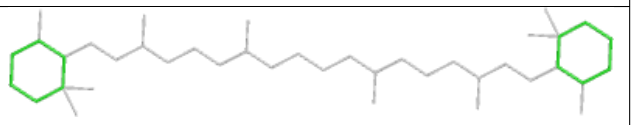
Bond lengths



Bond angles

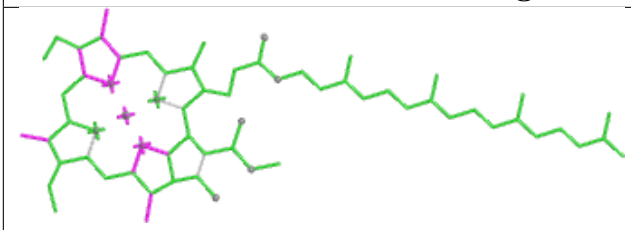


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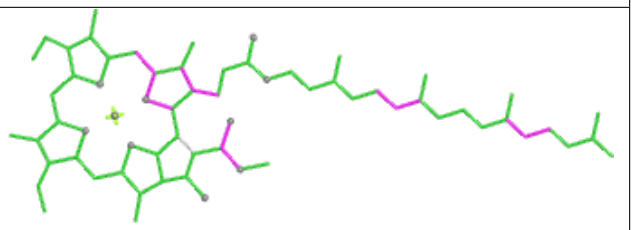


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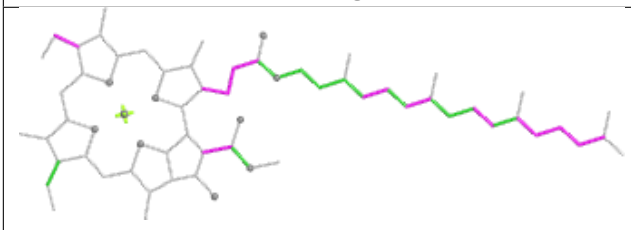
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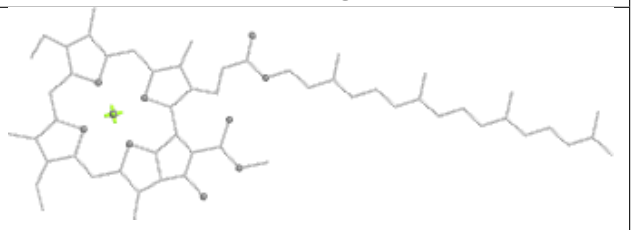
Bond lengths



Bond angles

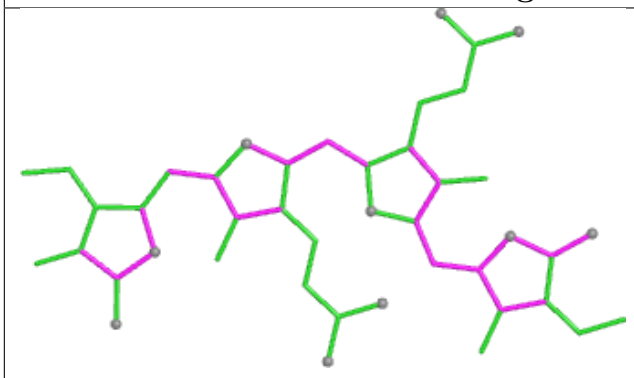


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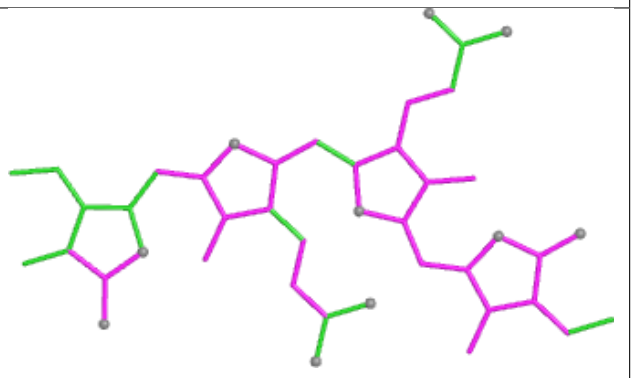


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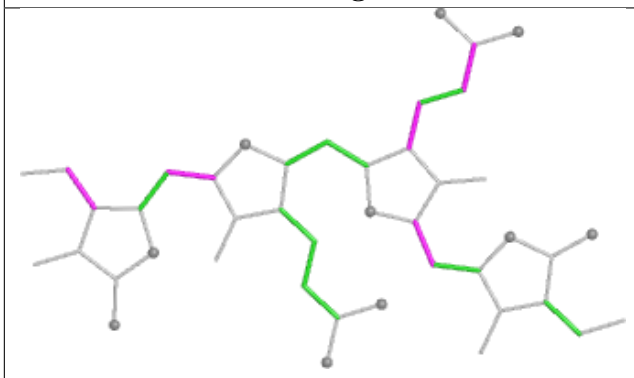
Ligand CYC eF 201



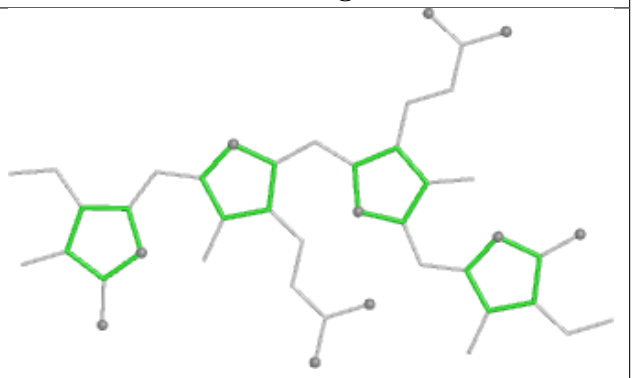
Bond lengths



Bond angles

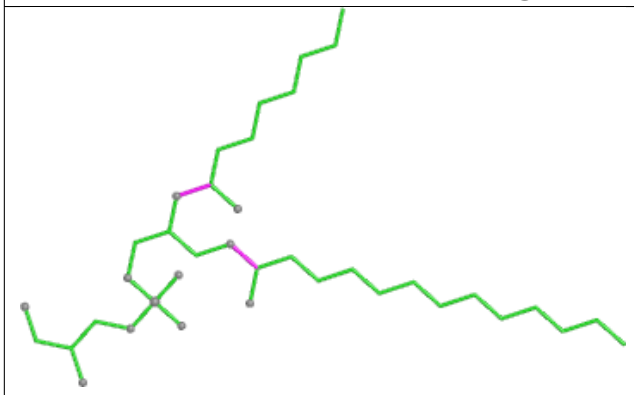


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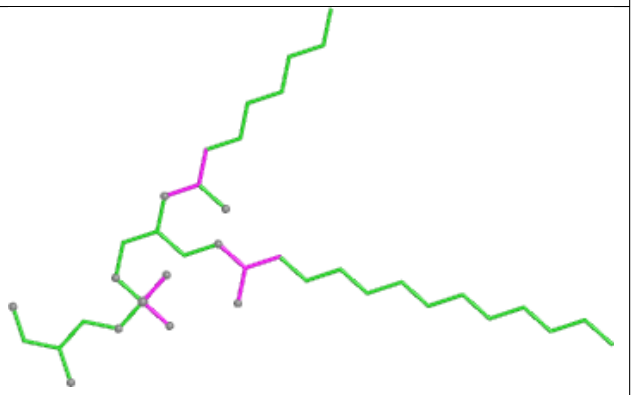


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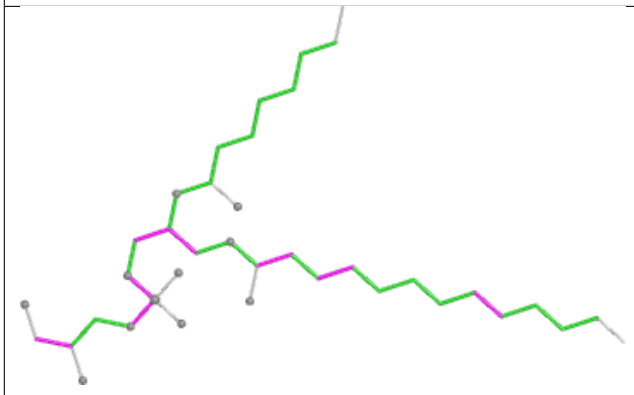
Ligand LHG aE 411



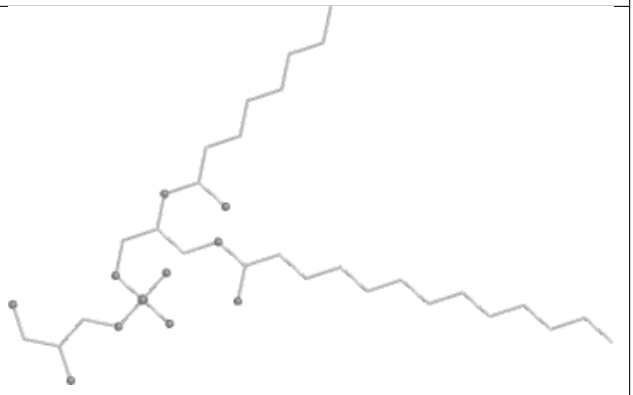
Bond lengths



Bond angles

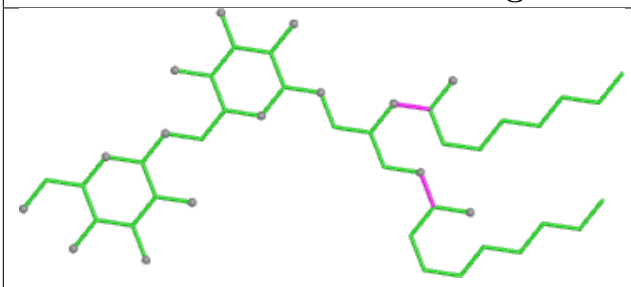


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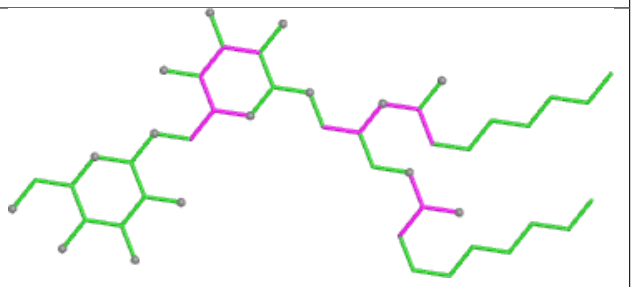


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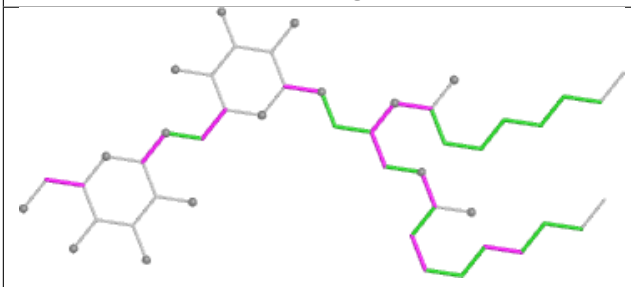
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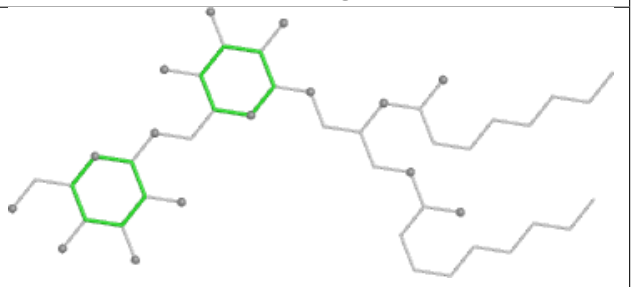
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Bond angles

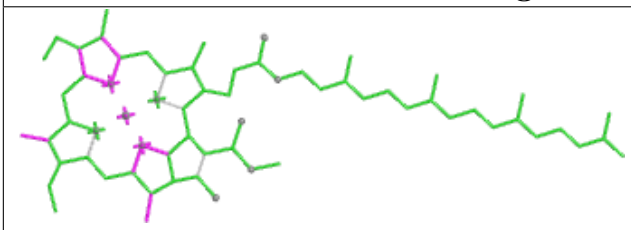


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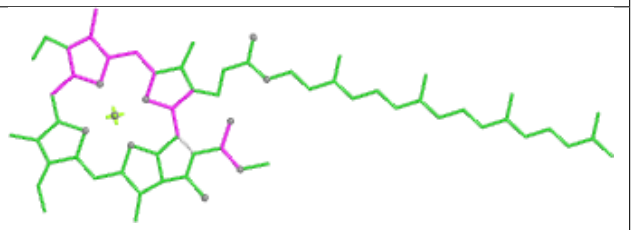


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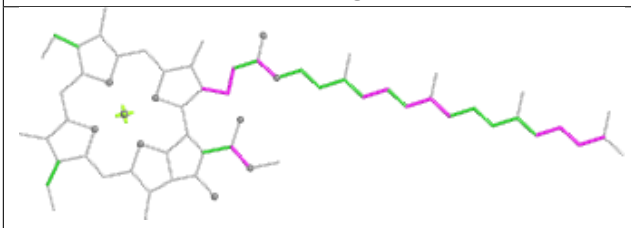
Ligand CLA C1 515



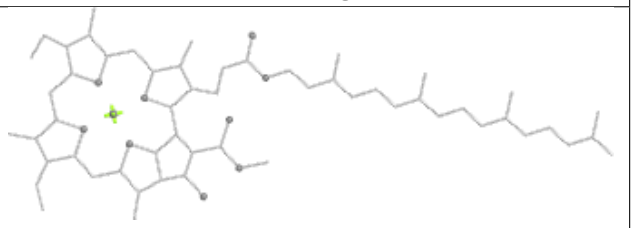
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Bond angles

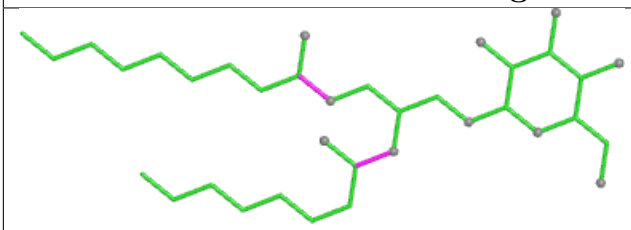


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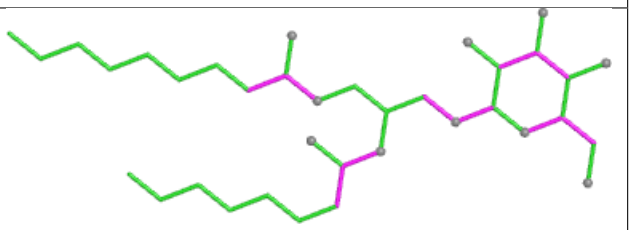


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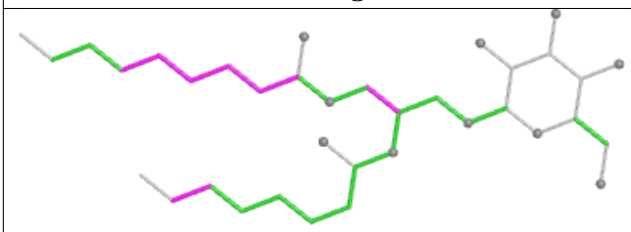
Ligand LMG A1 408



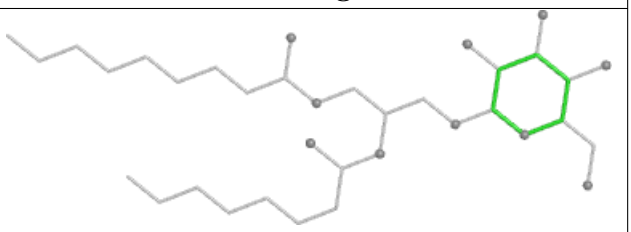
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Bond angles

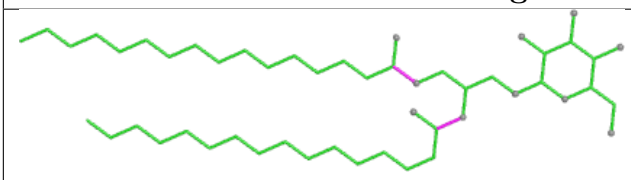


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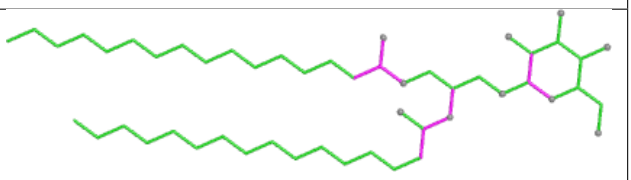


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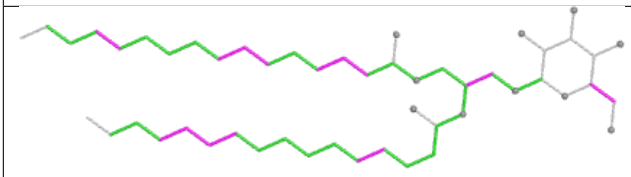
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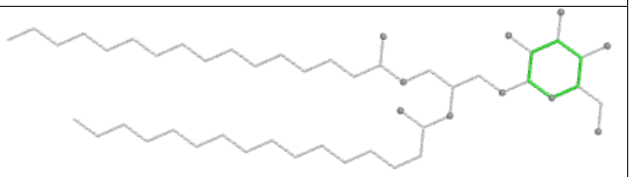
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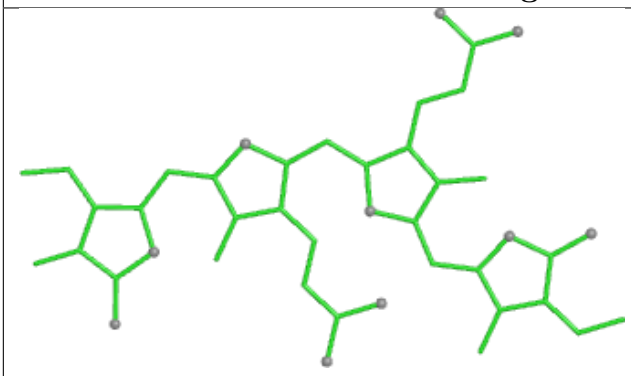


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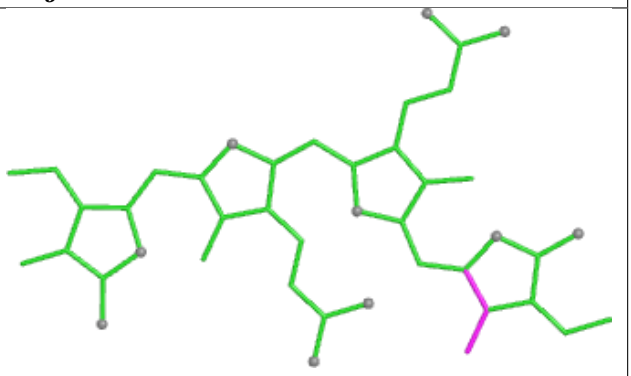


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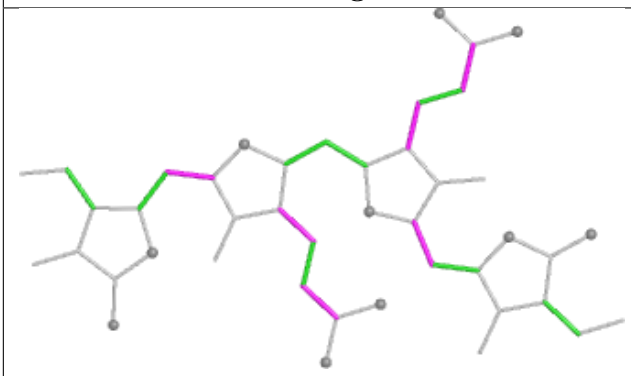
Ligand CYC j7 202



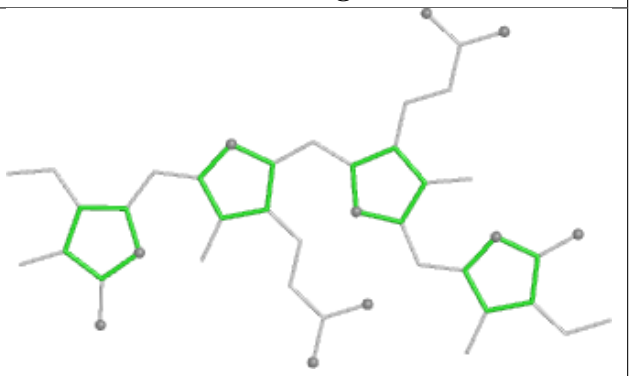
Bond lengths



Bond angles

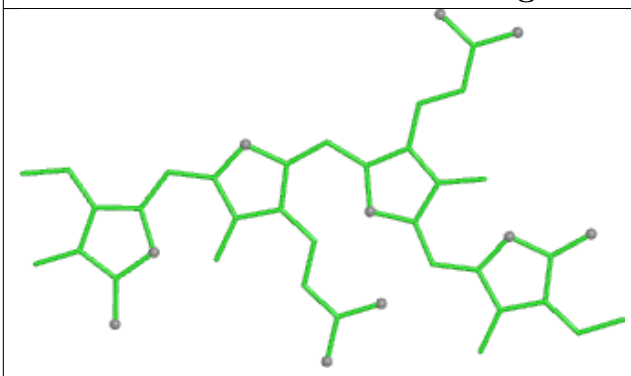


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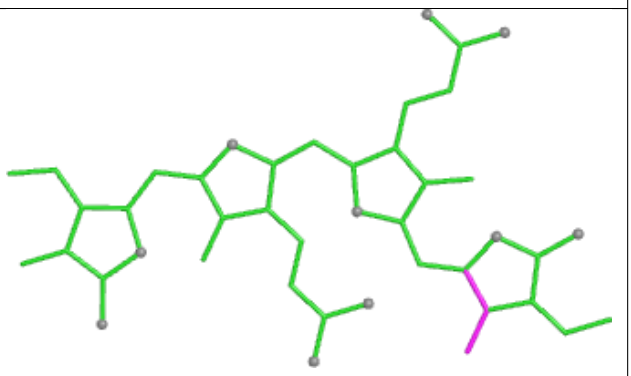


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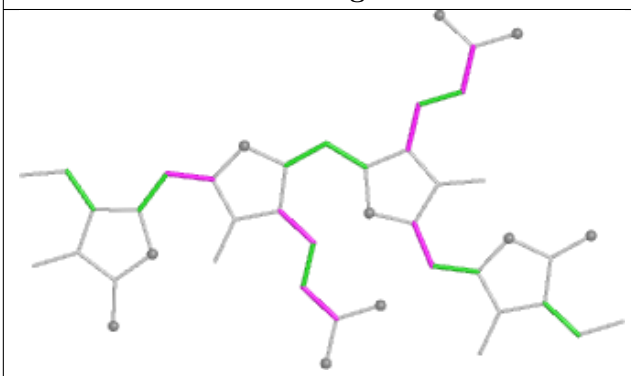
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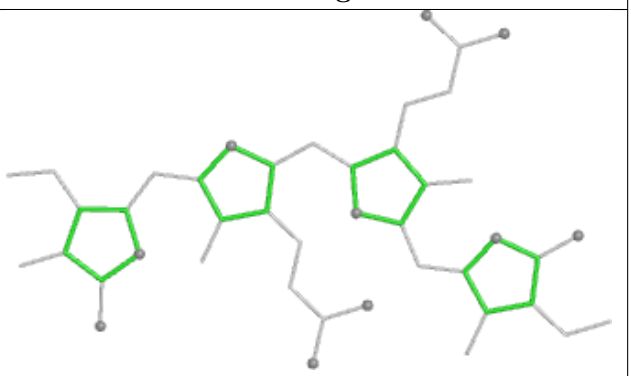
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Bond angles

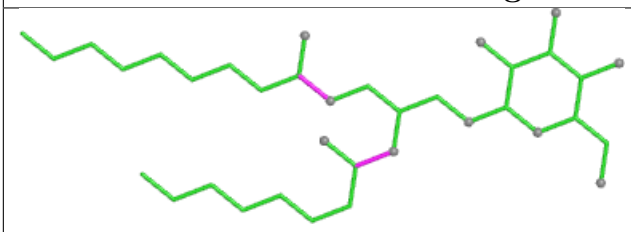


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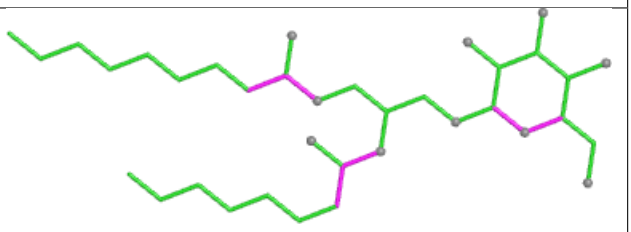


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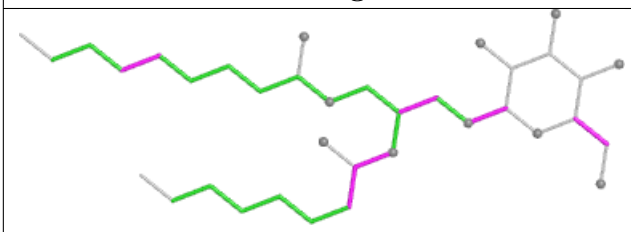
Ligand LMG mD 101



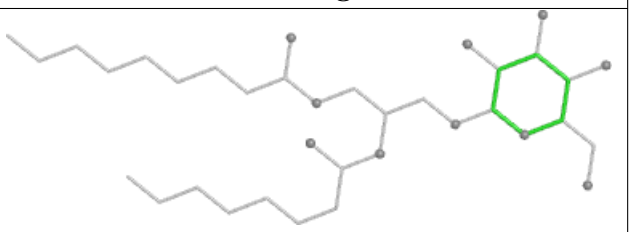
Bond lengths



Bond angles

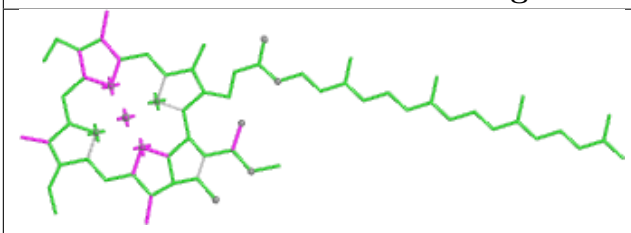


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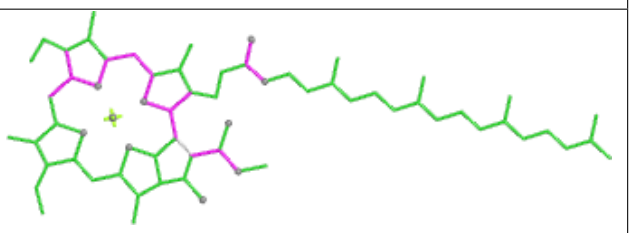


Rings

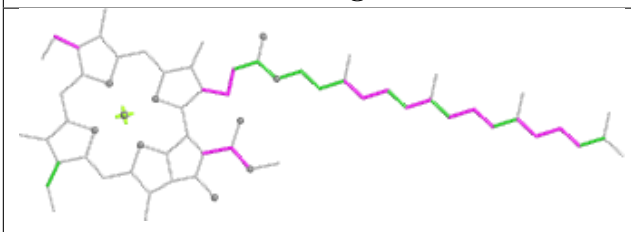
Ligand CLA BD 603



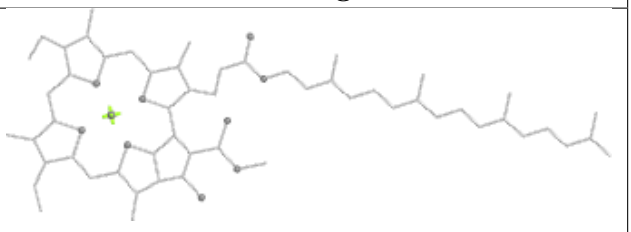
Bond lengths



Bond angles

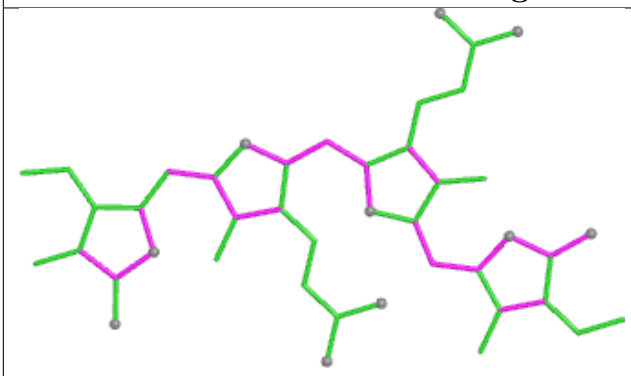


Torsions

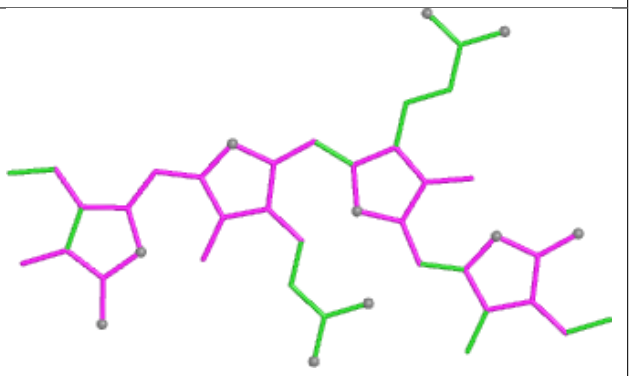


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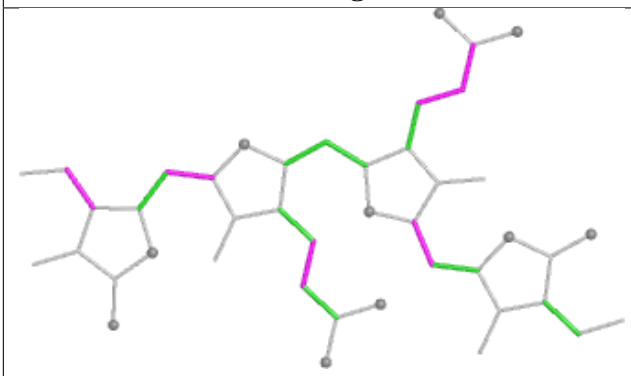
Ligand CYC bK 201



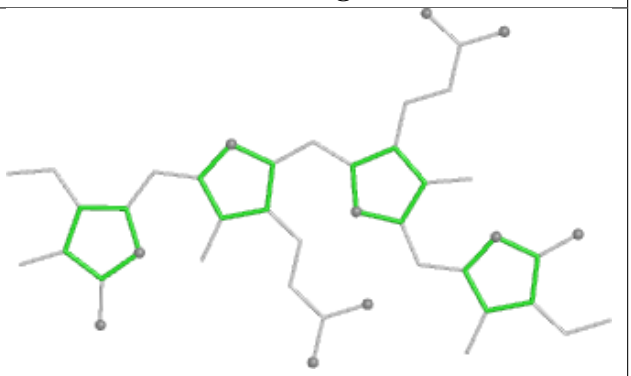
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Bond angles

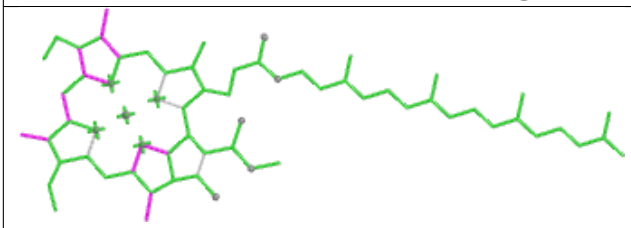


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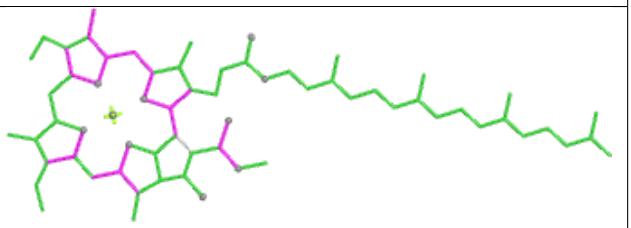


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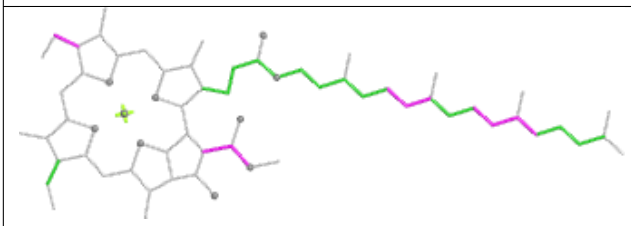
Ligand CLA bE 615



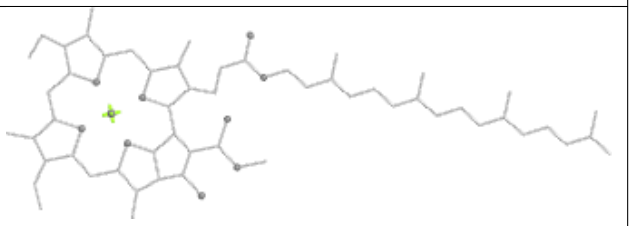
Bond lengths



Bond angles

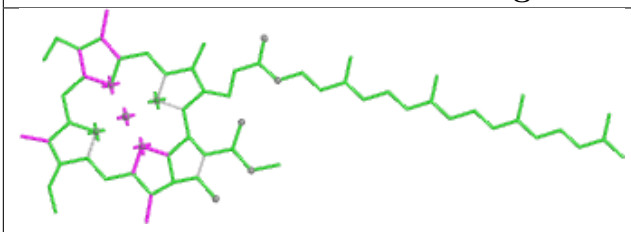


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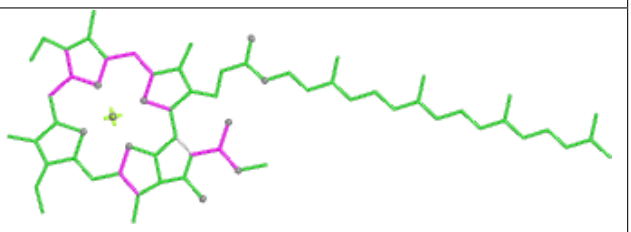


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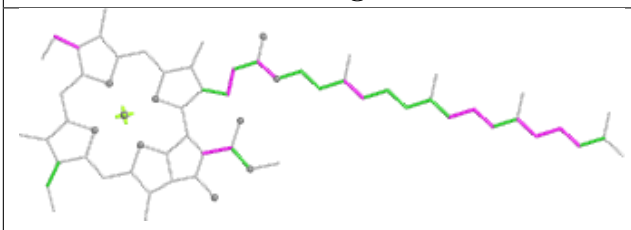
Ligand CLA bD 614



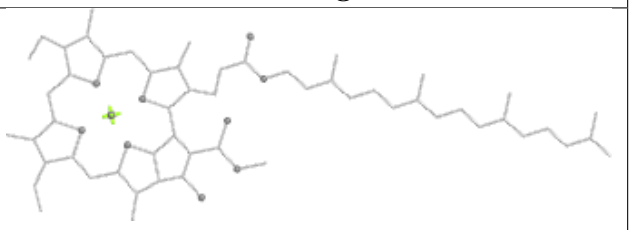
Bond lengths



Bond angles



Torsions



Rings

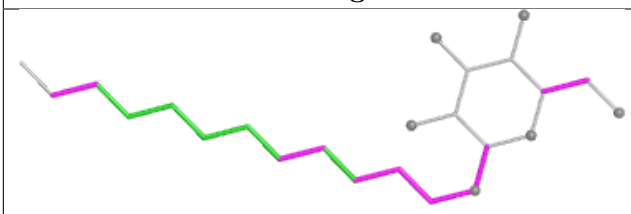
Ligand LMT C1 520



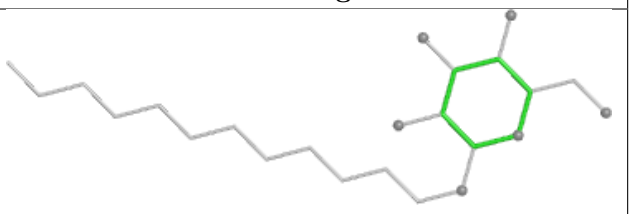
Bond lengths



Bond angles

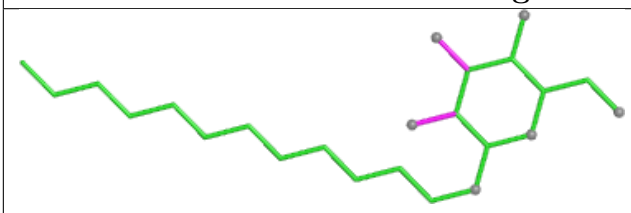


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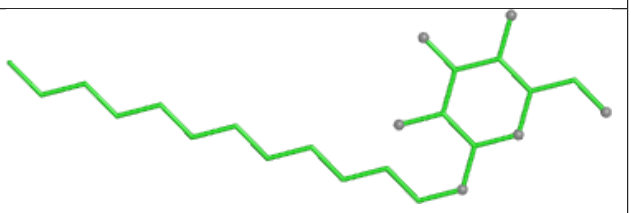


Rings

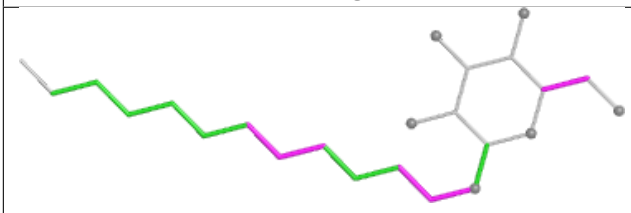
Ligand LMT bE 602



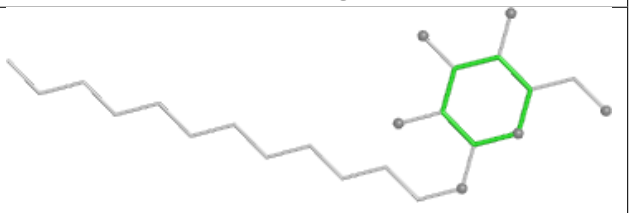
Bond lengths



Bond angles

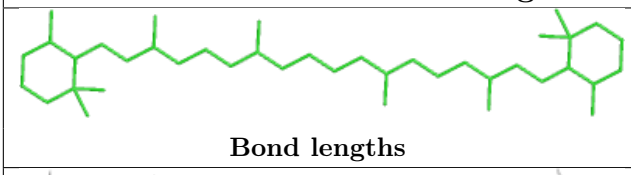


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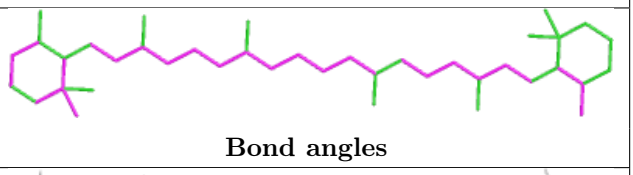


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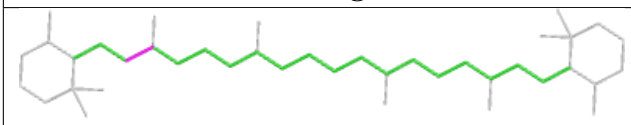
Ligand BCR k1 102



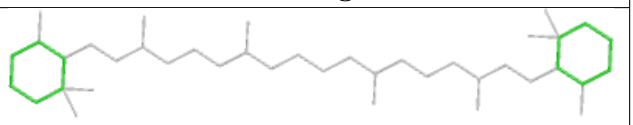
Bond lengths



Bond angles

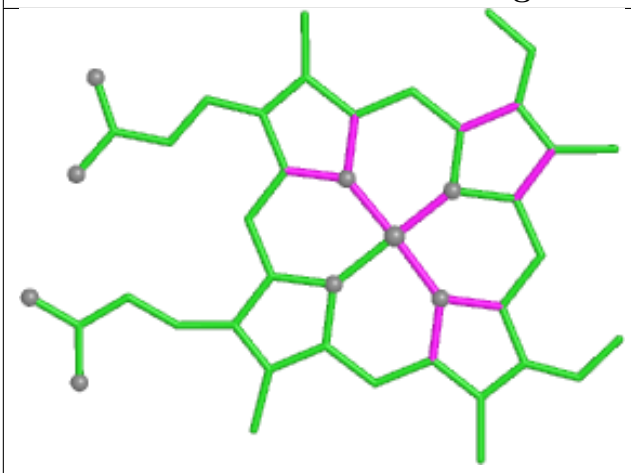


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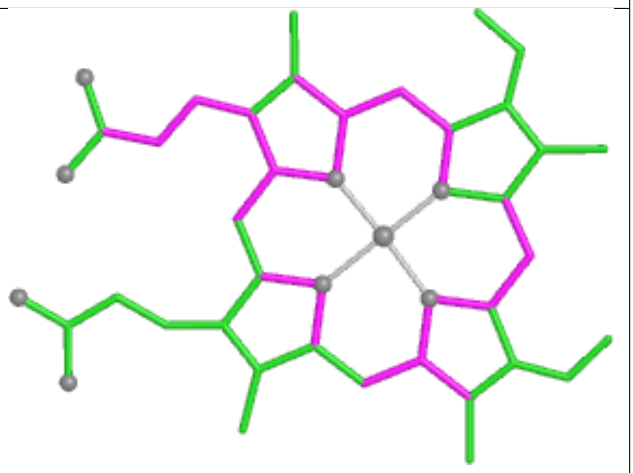


Rings

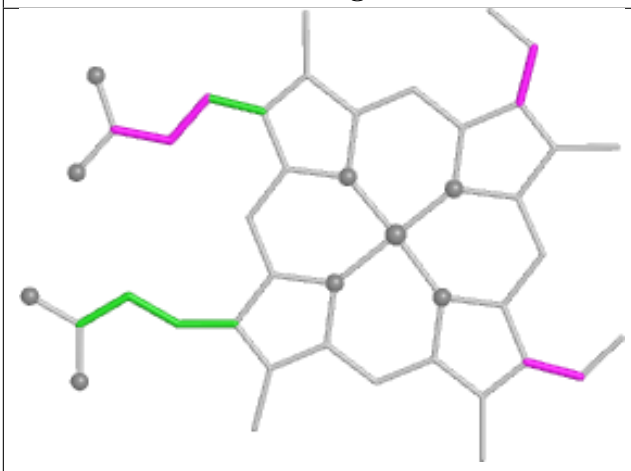
Ligand HEM v1 201



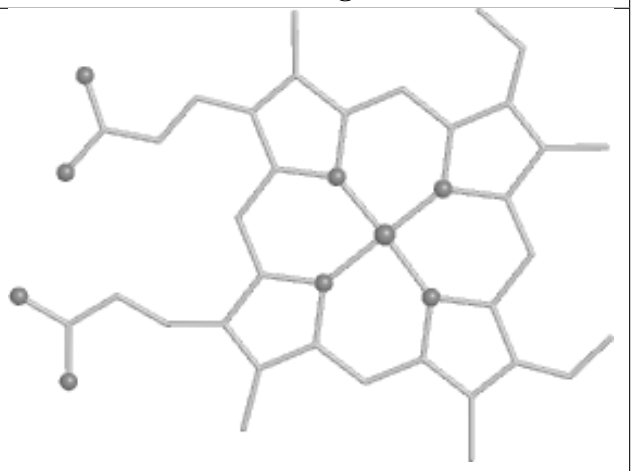
Bond lengths



Bond angles

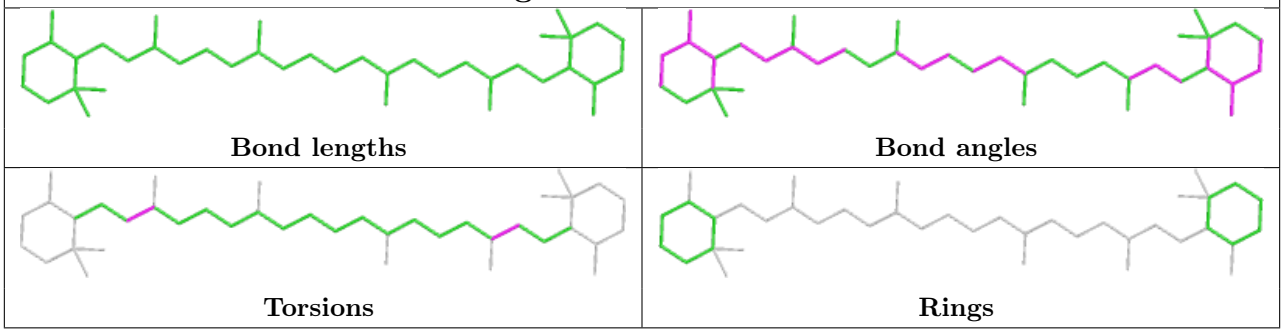


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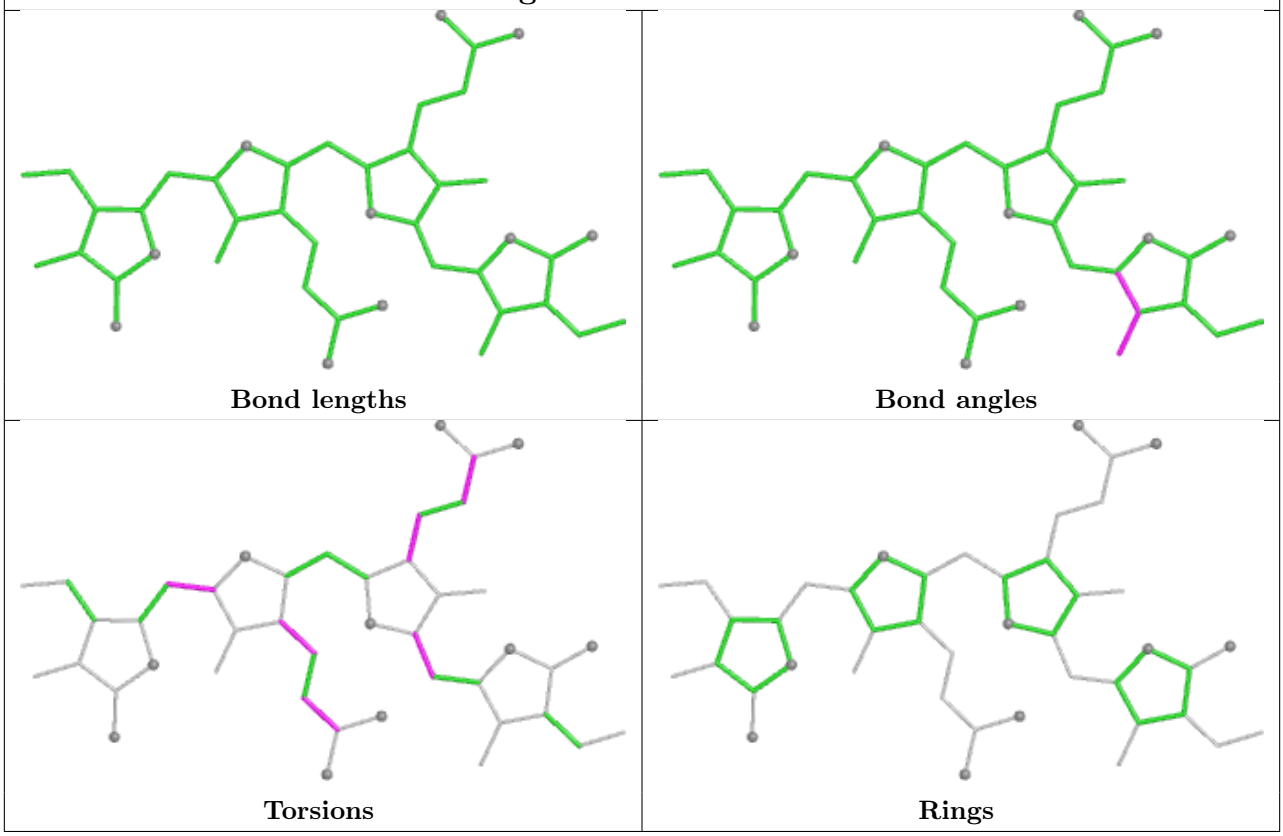


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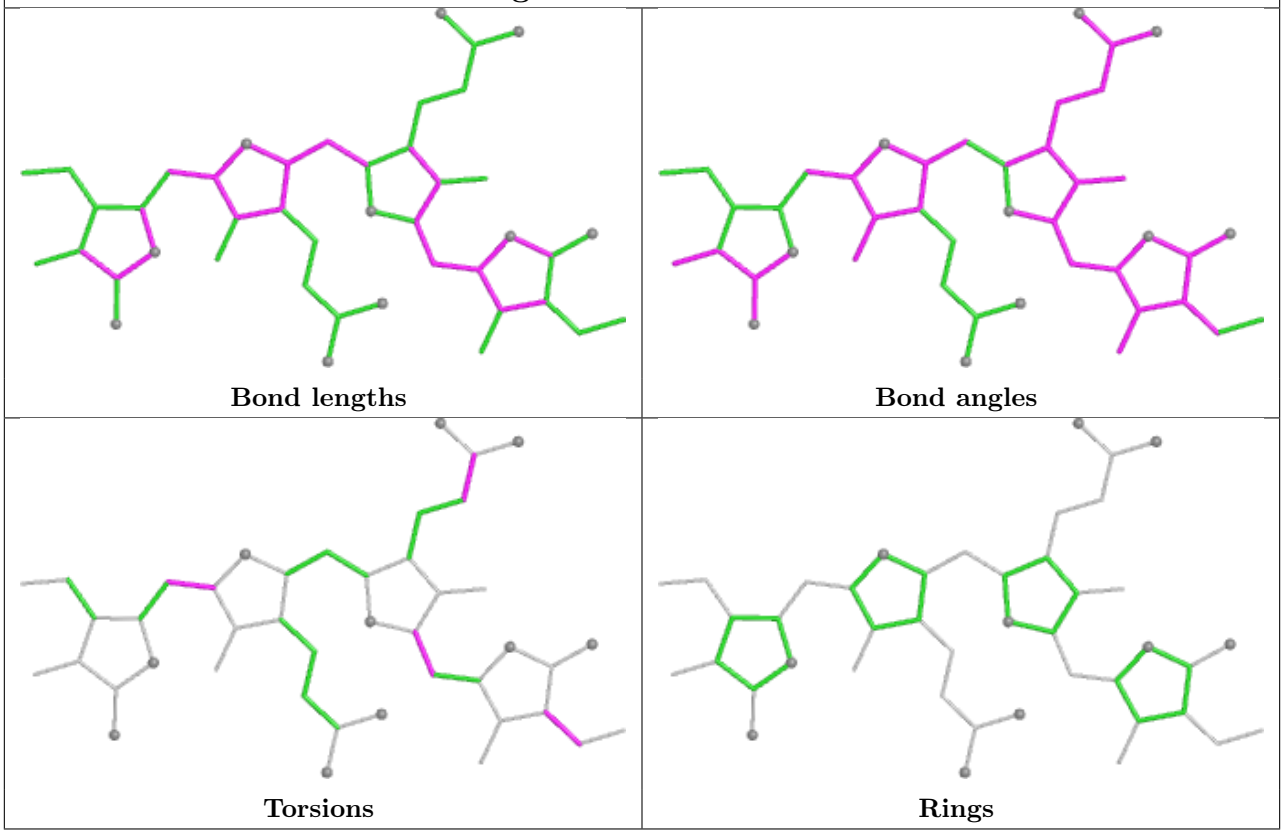
Ligand BCR bE 618



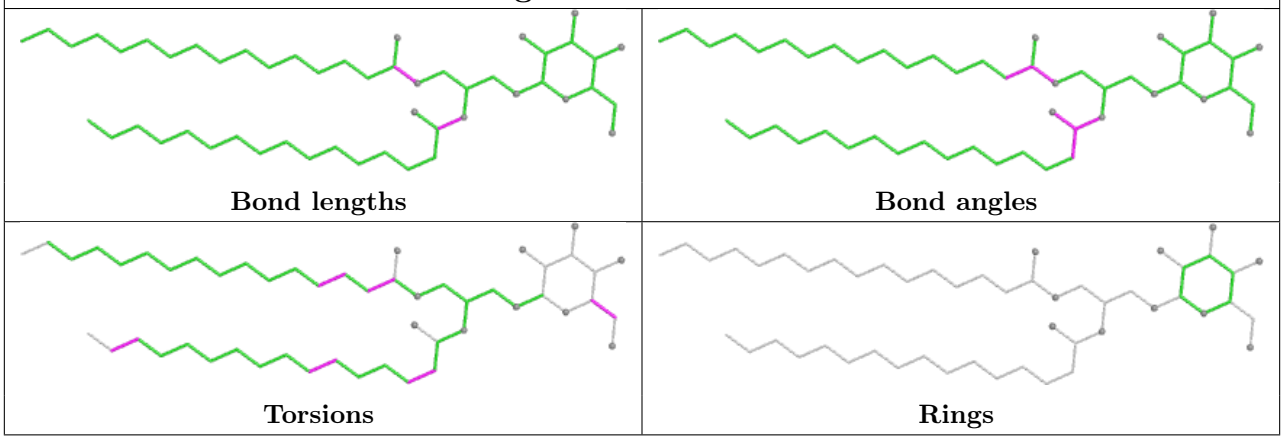
Ligand CYC e9 202



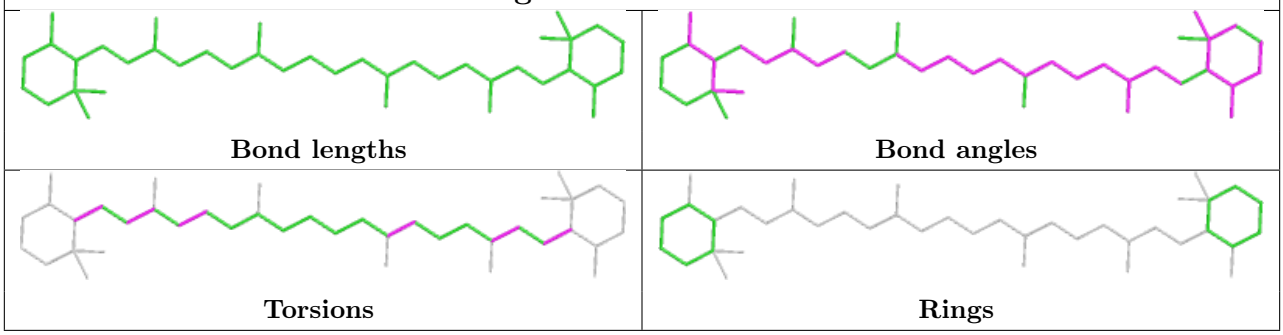
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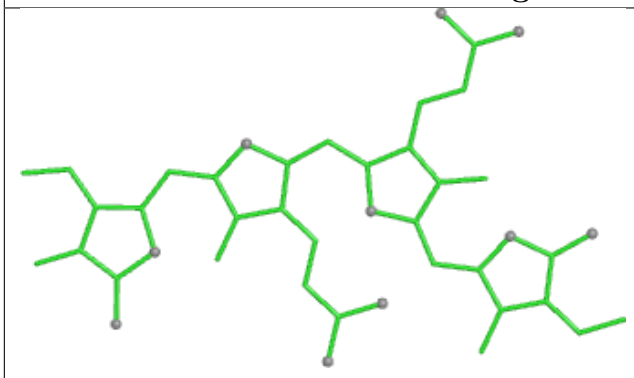
Ligand LMG b1 619



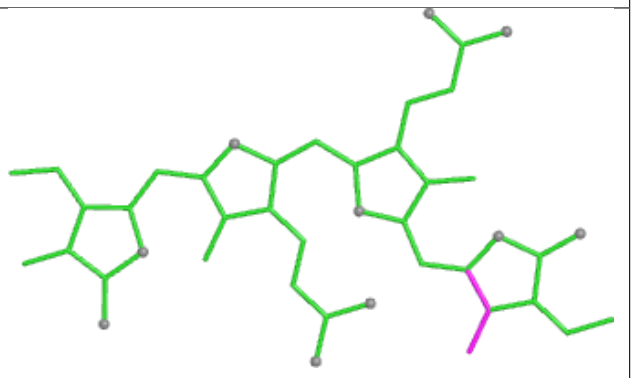
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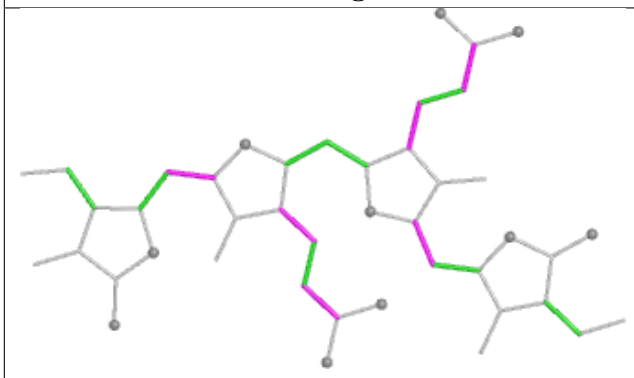
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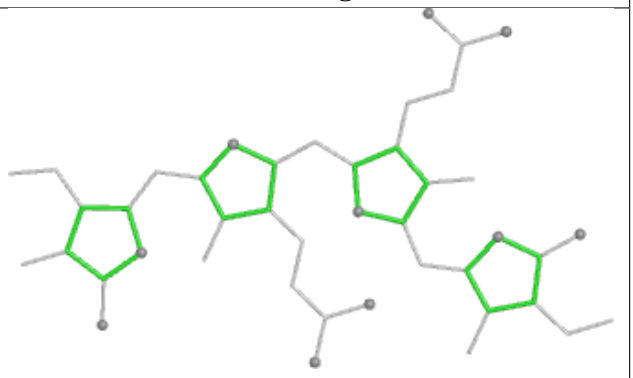
Bond lengths



Bond angles

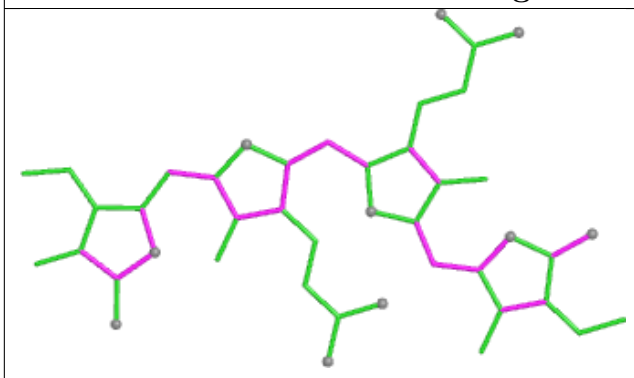


Torsions

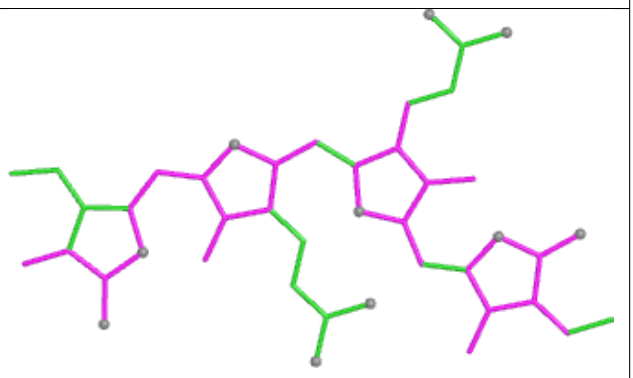


Rings

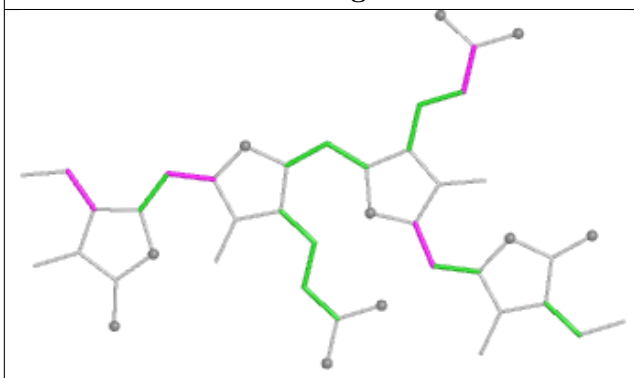
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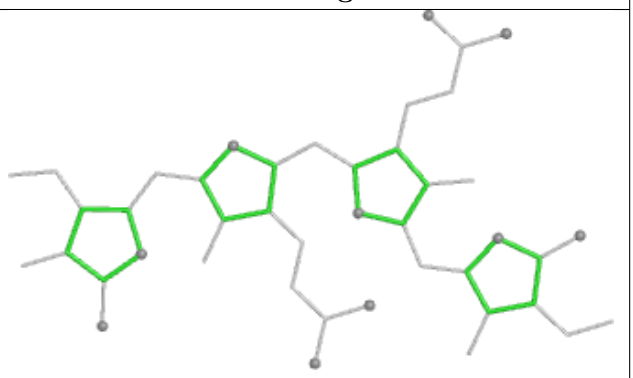
Bond lengths



Bond angles

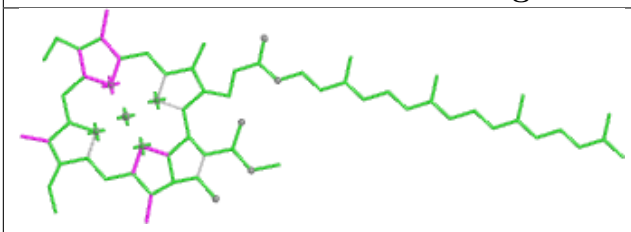


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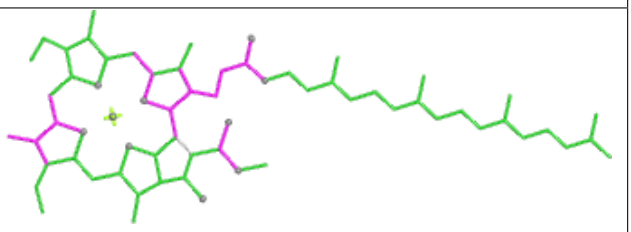


Rings

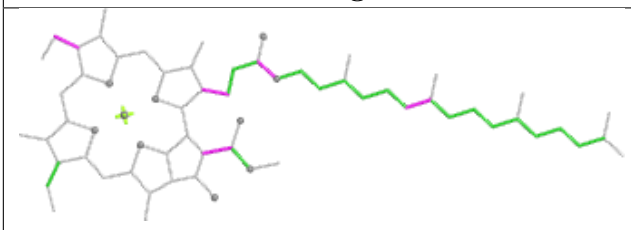
Ligand CLA CE 504



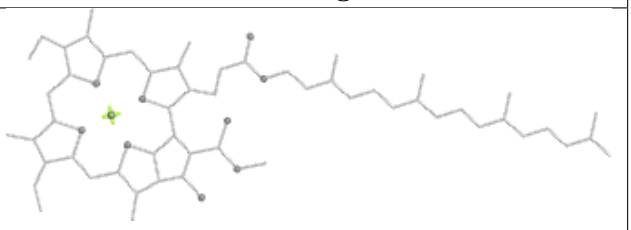
Bond lengths



Bond angles



Torsions

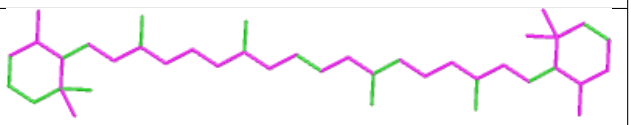


Rings

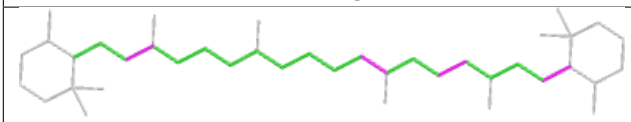
Ligand BCR XE 102



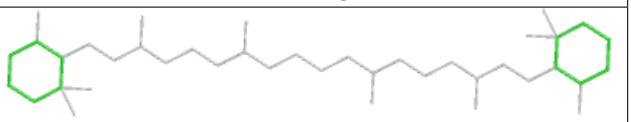
Bond lengths



Bond angles

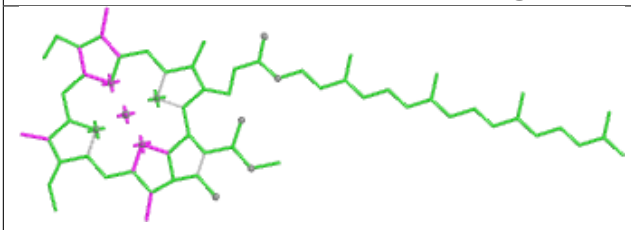


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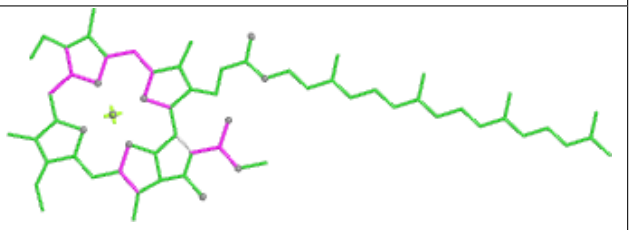


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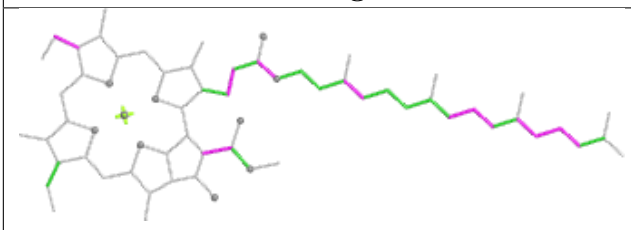
Ligand CLA BD 613



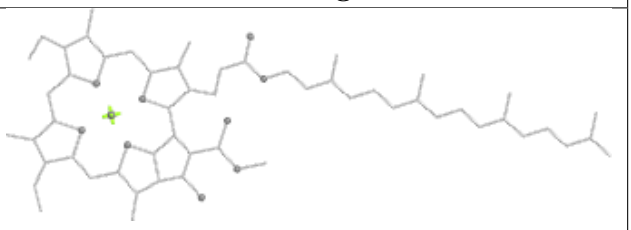
Bond lengths



Bond angles

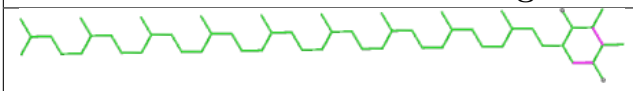


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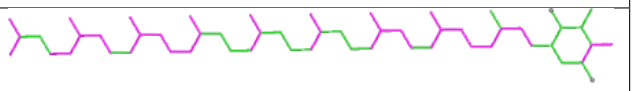


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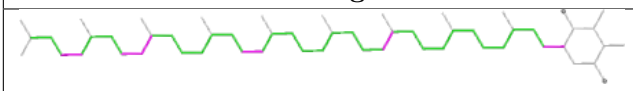
Ligand PL9 DE 408



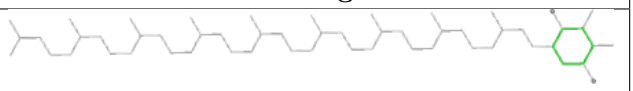
Bond lengths



Bond angles

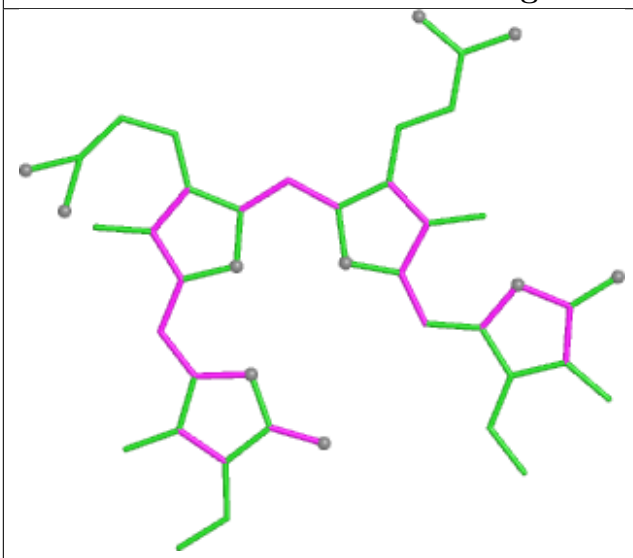


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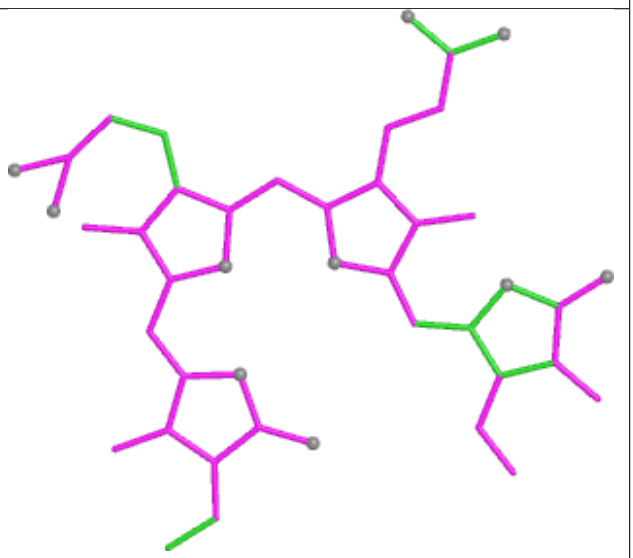


Rings

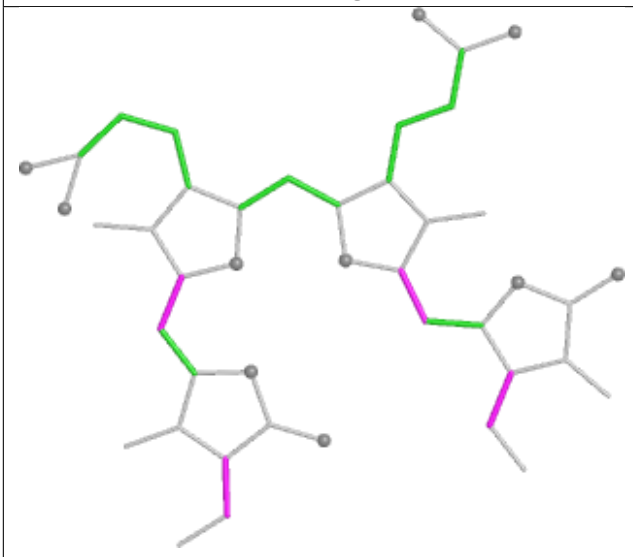
Ligand CYC iJ 202



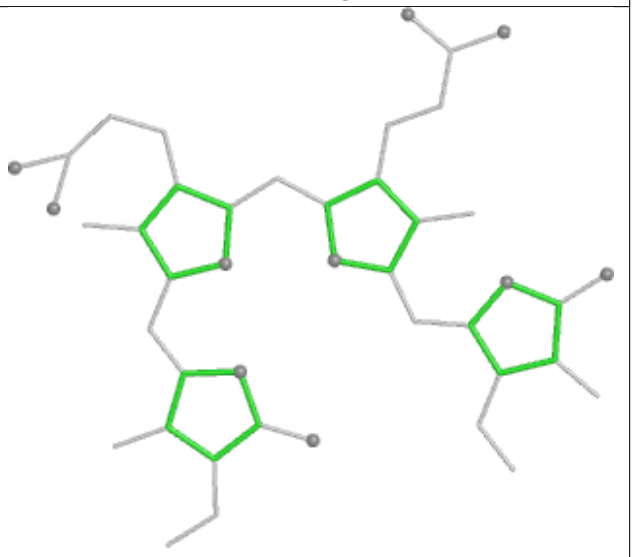
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Bond angles

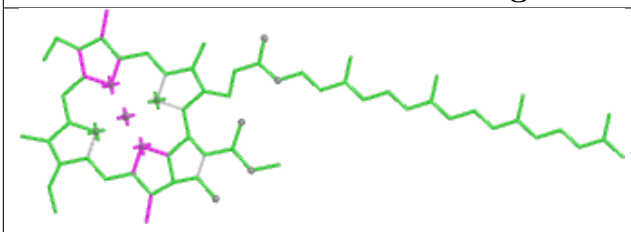


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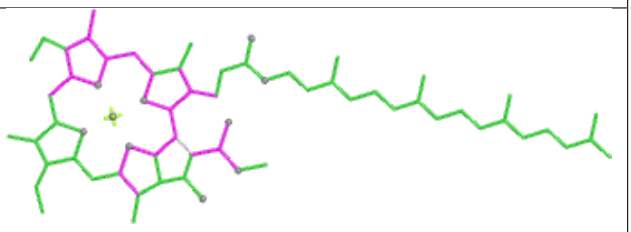


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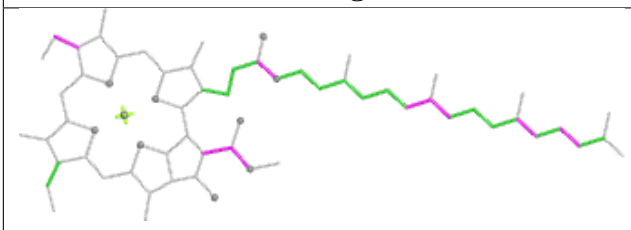
Ligand CLA AD 405



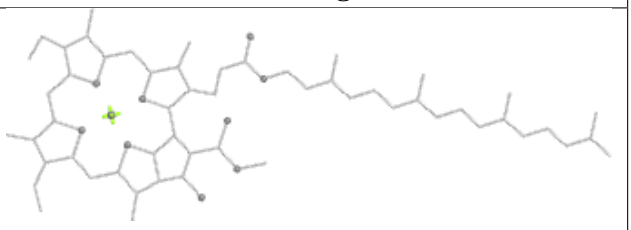
Bond lengths



Bond angles

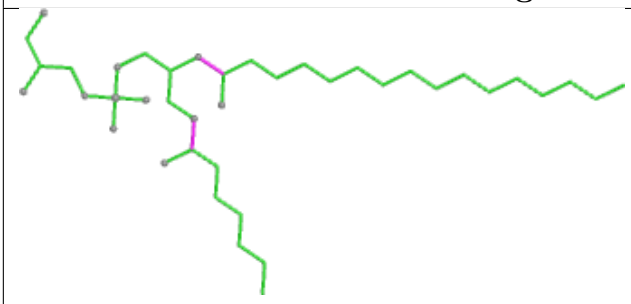


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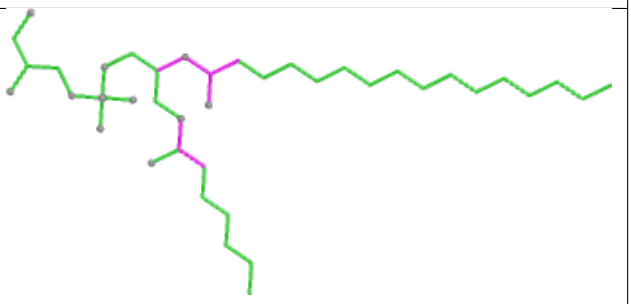


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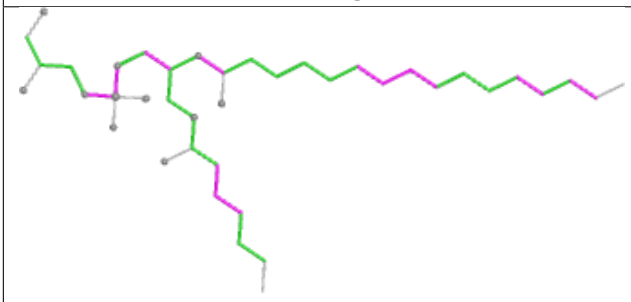
Ligand LHG eE 101



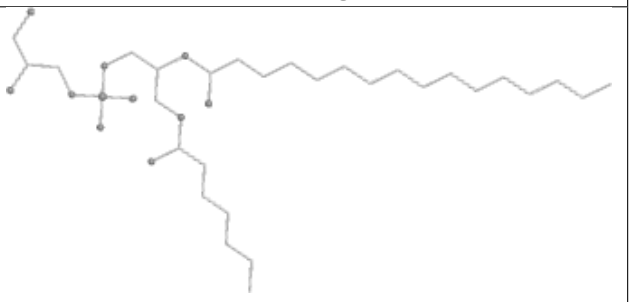
Bond lengths



Bond angles

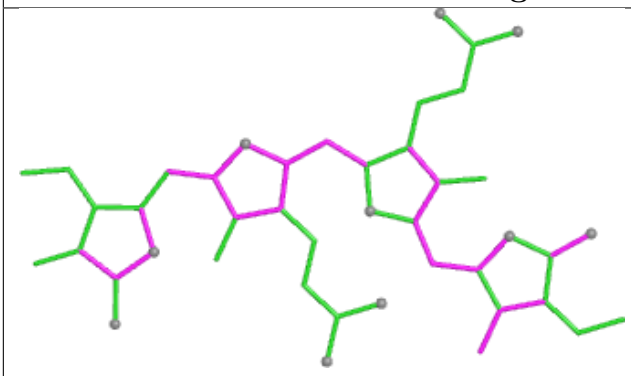


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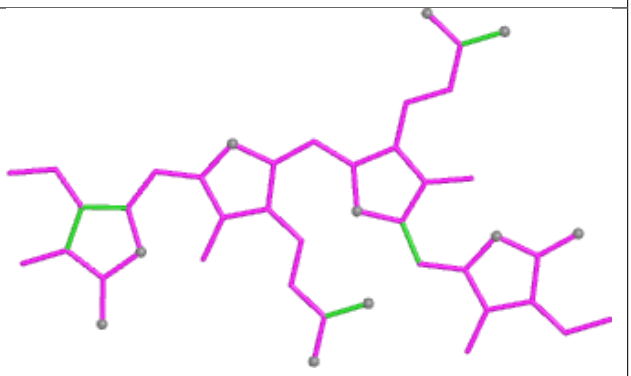


Rings

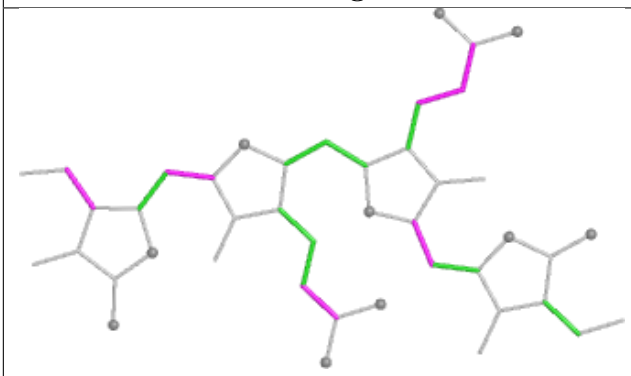
Ligand CYC LG 201



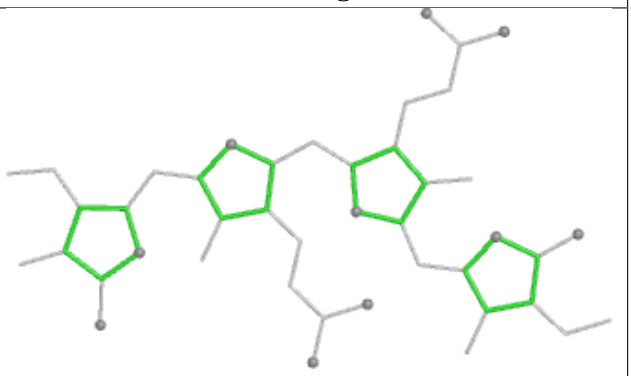
Bond lengths



Bond angles

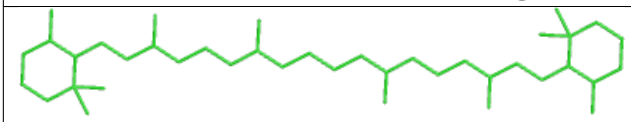


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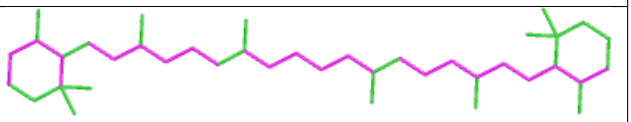


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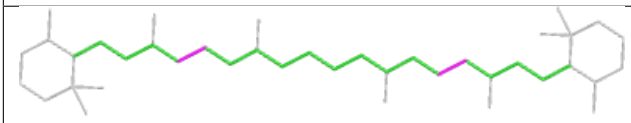
Ligand BCR C1 519



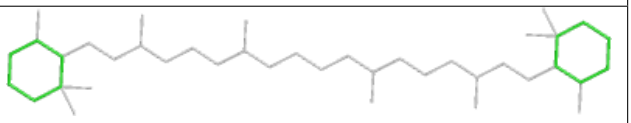
Bond lengths



Bond angles

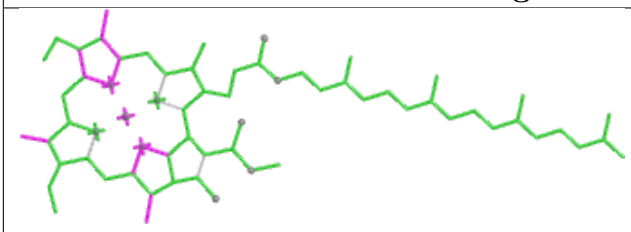


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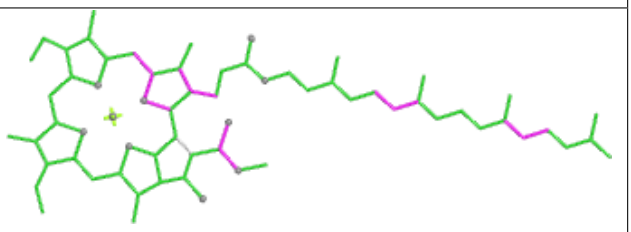


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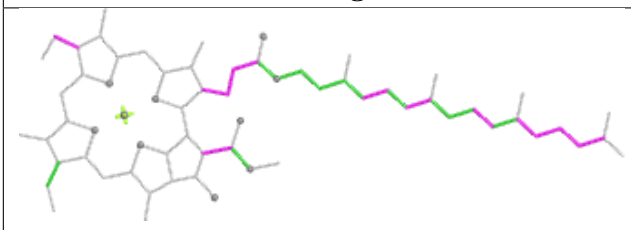
Ligand CLA BE 612



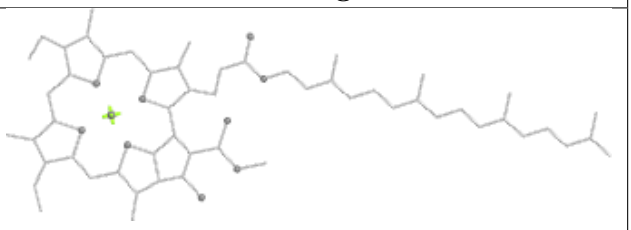
Bond lengths



Bond angles

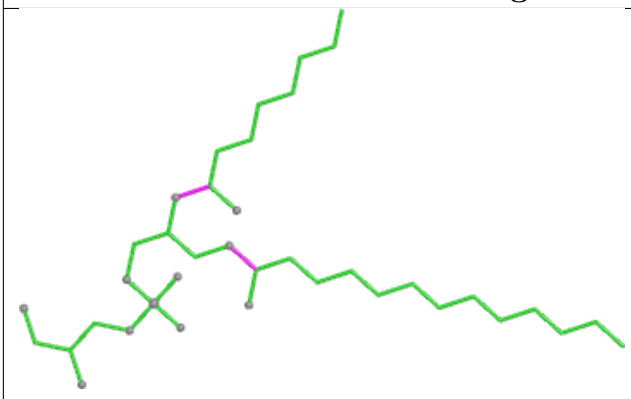


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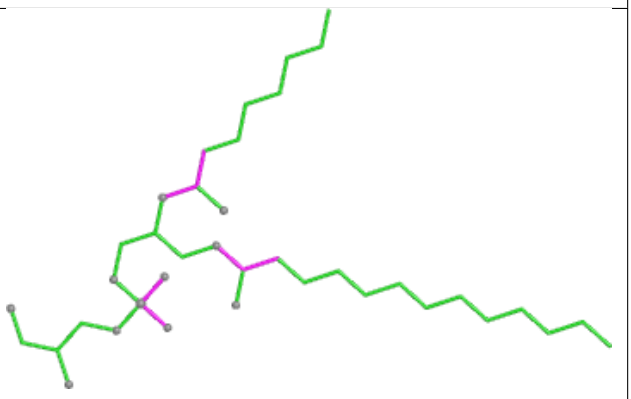


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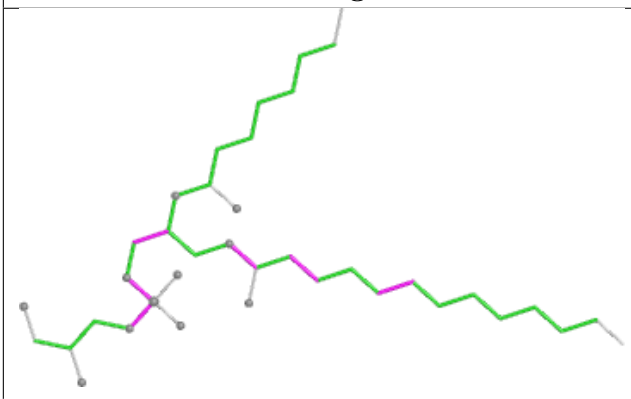
Ligand LHG AE 411



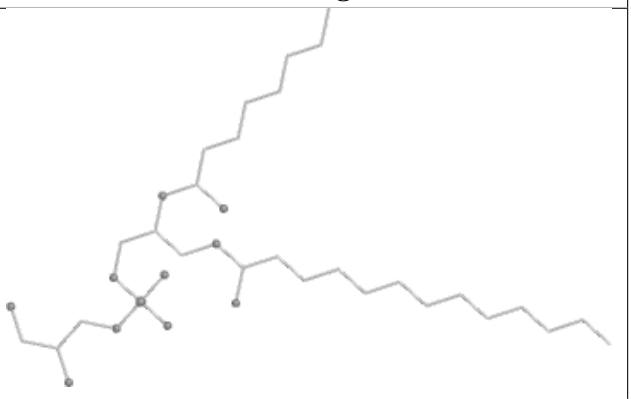
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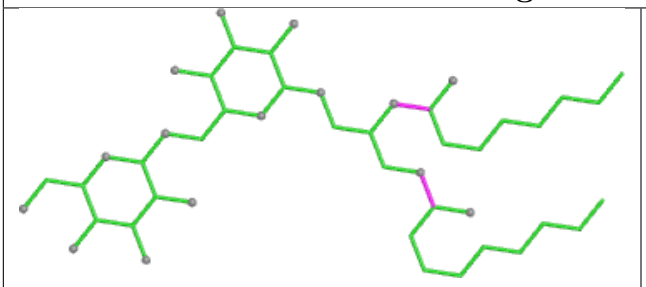


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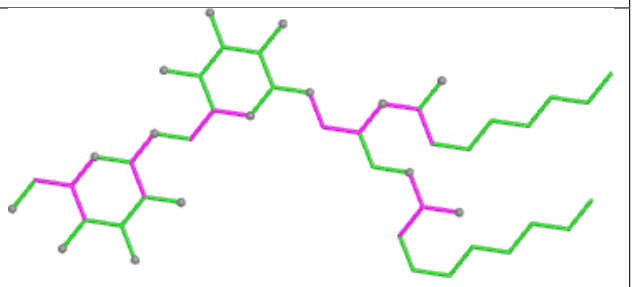


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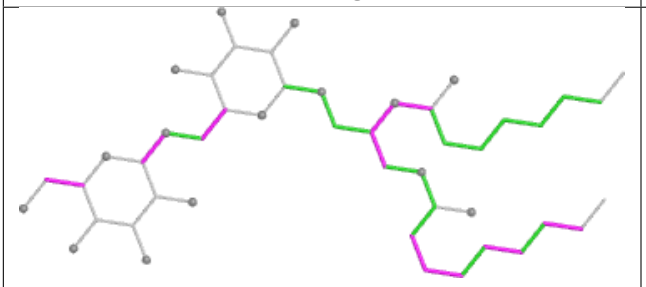
Ligand DGD c1 516



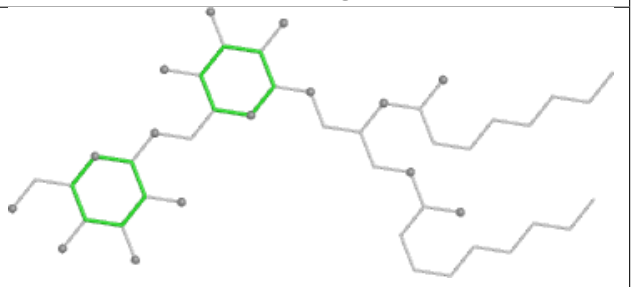
Bond lengths



Bond angles

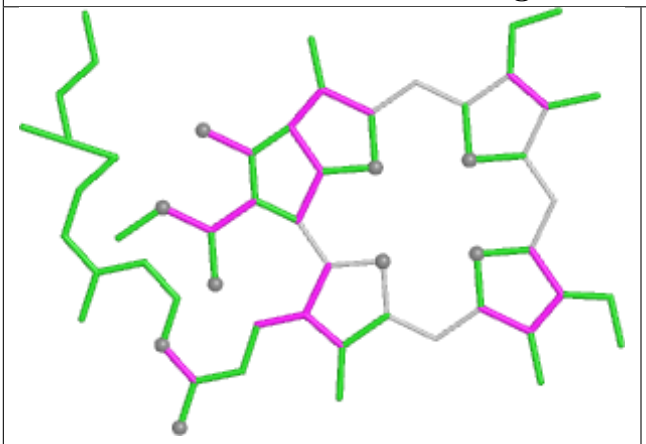


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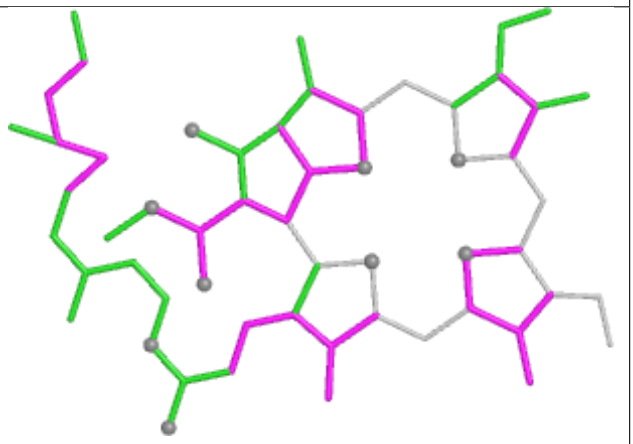


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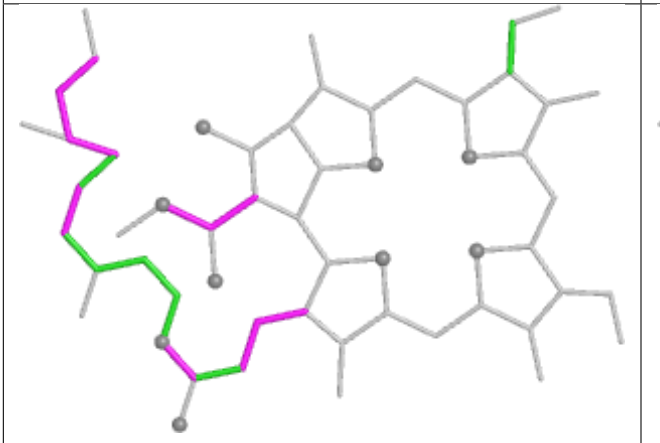
Ligand PHO dE 402



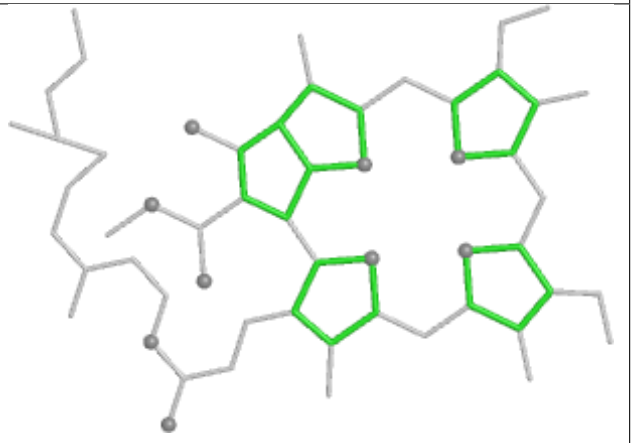
Bond lengths



Bond angles

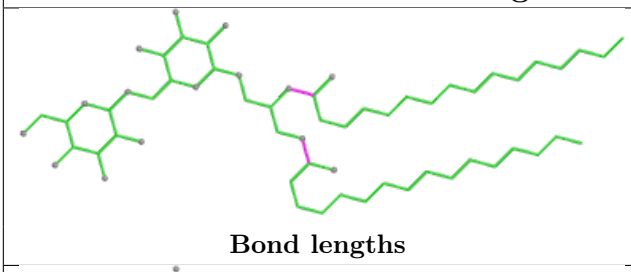


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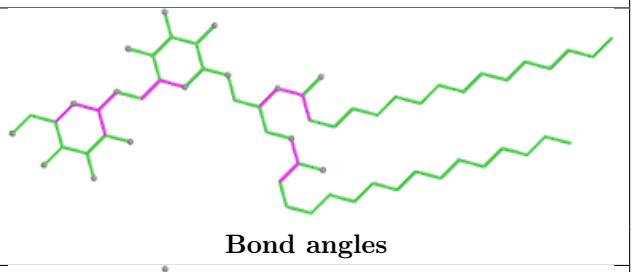


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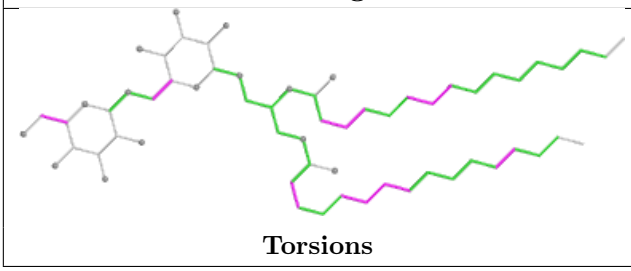
Ligand DGD cD 518



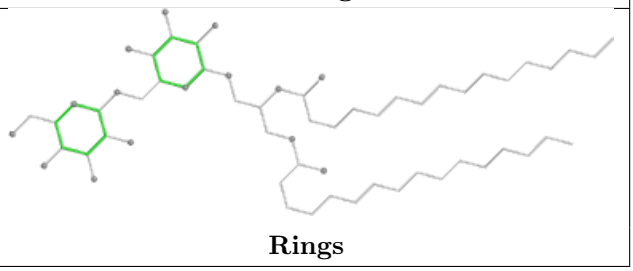
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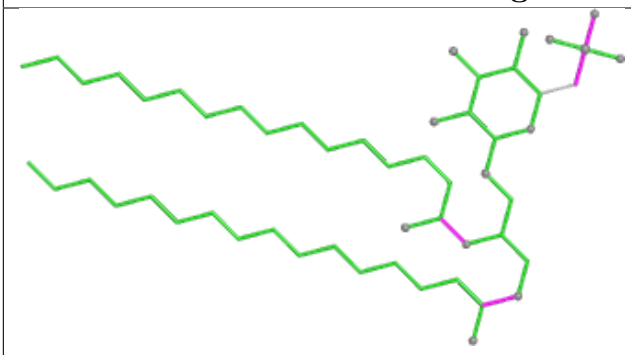


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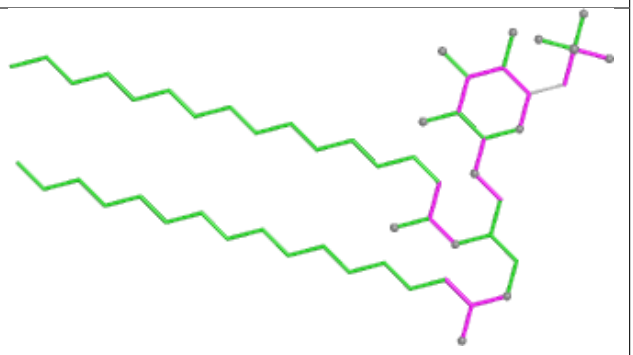


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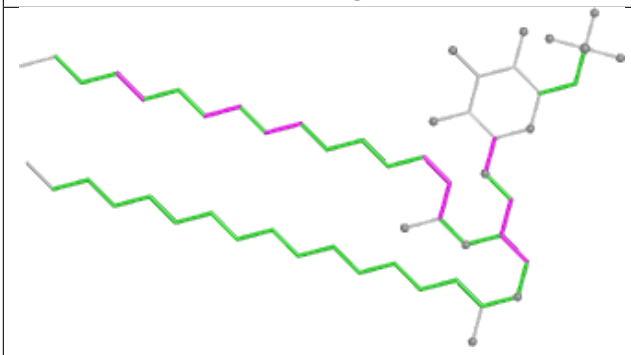
Ligand SQD CD 501



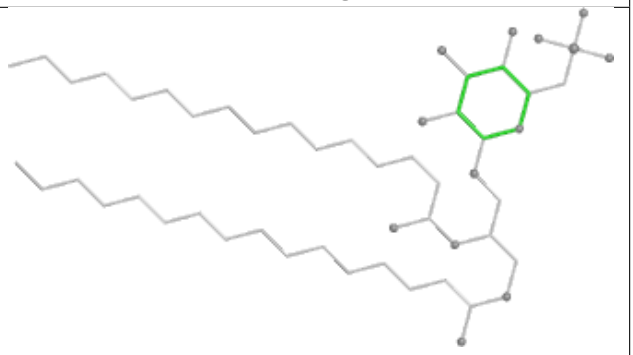
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Bond angles

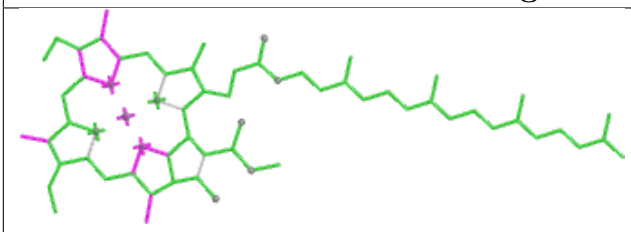


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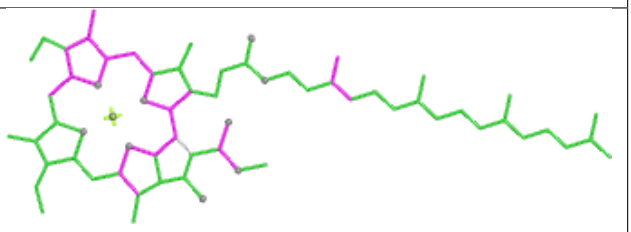


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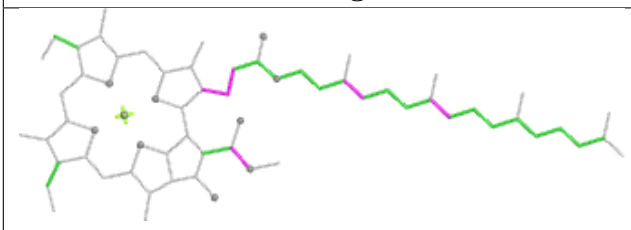
Ligand CLA c1 508



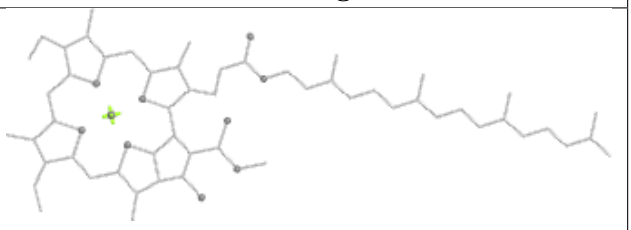
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Bond angles

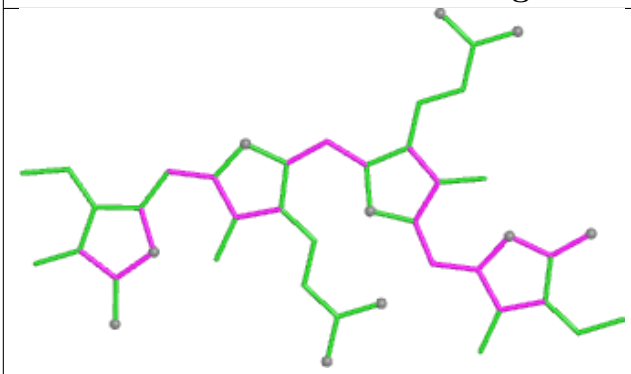


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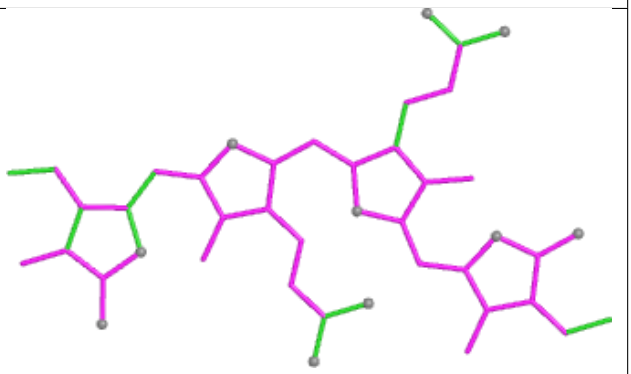


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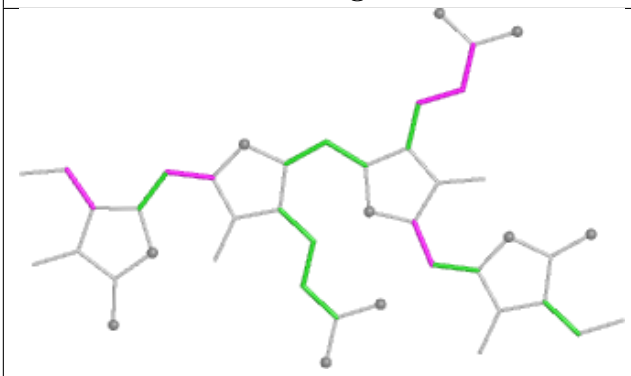
Ligand CYC 2G 201



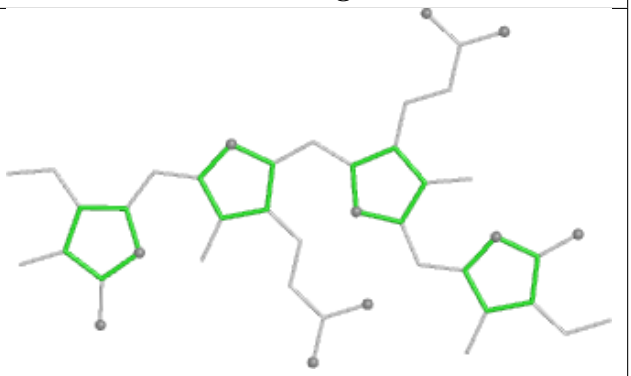
Bond lengths



Bond angles

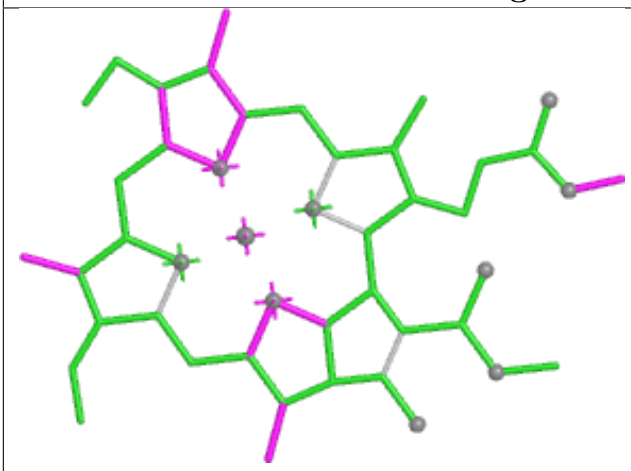


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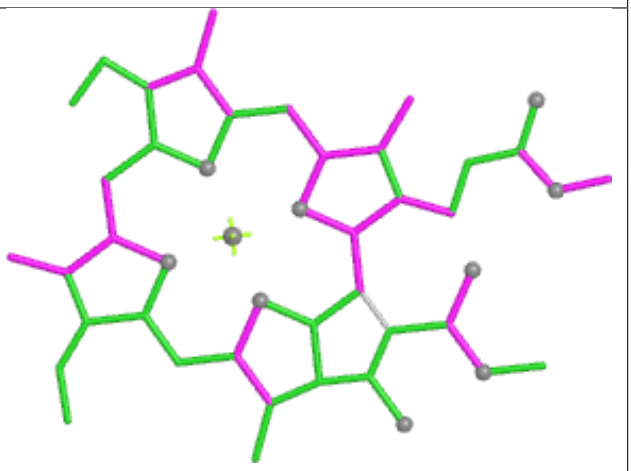


Rings

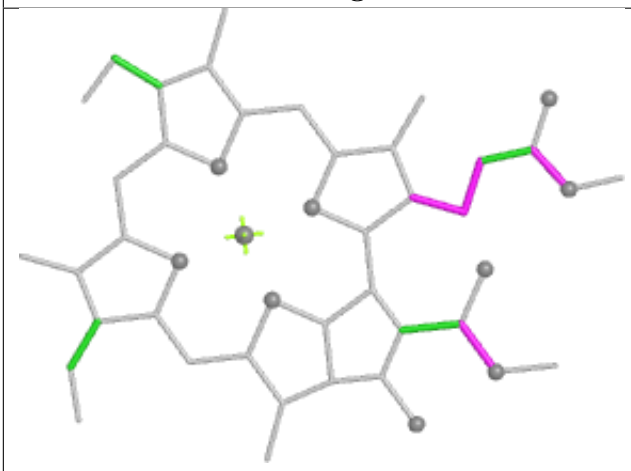
Ligand CLA AD 404



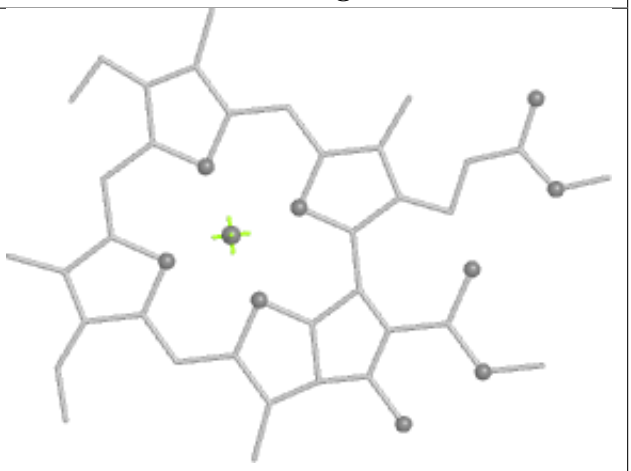
Bond lengths



Bond angles

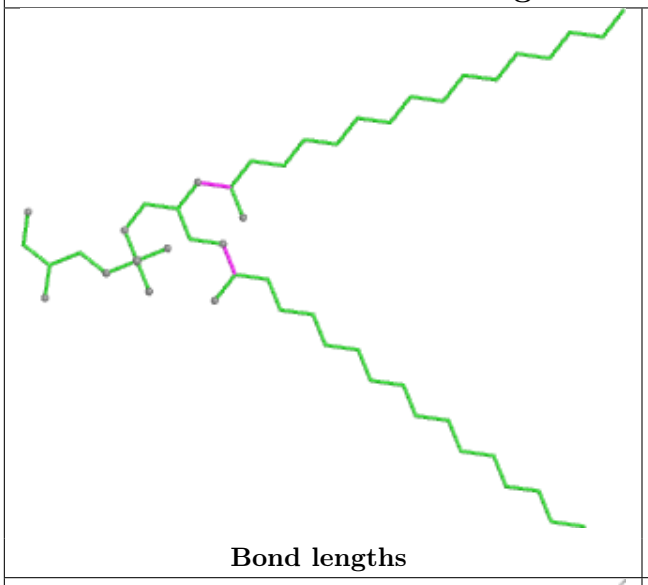


Torsions

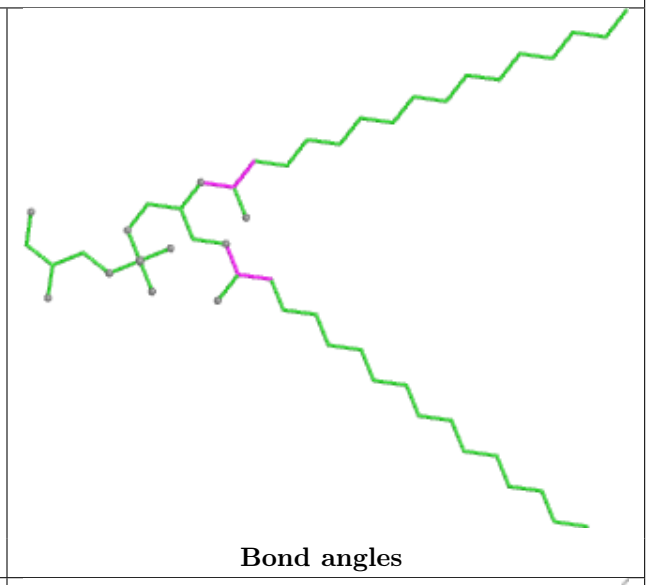


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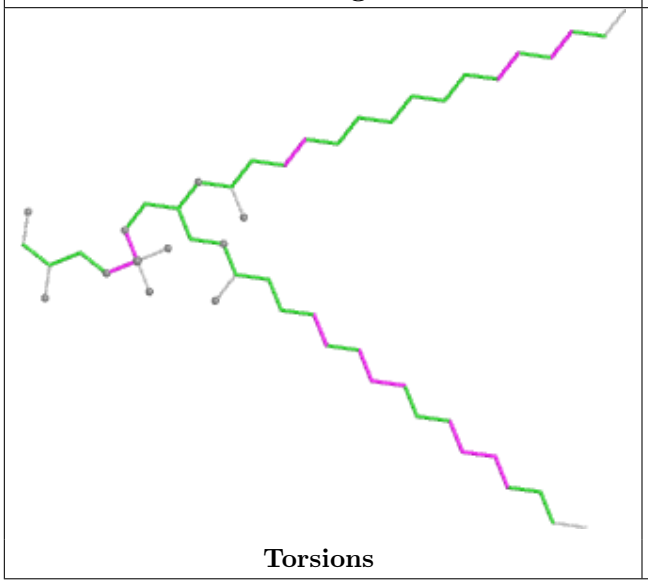
Ligand LHG D1 408



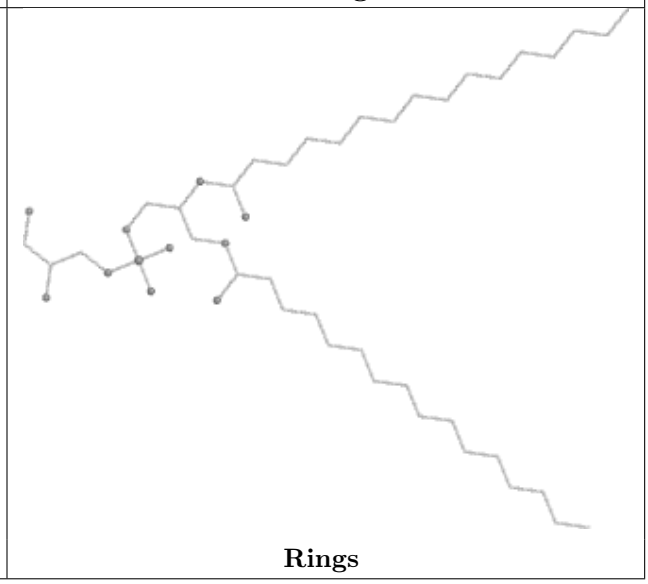
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Bond angles

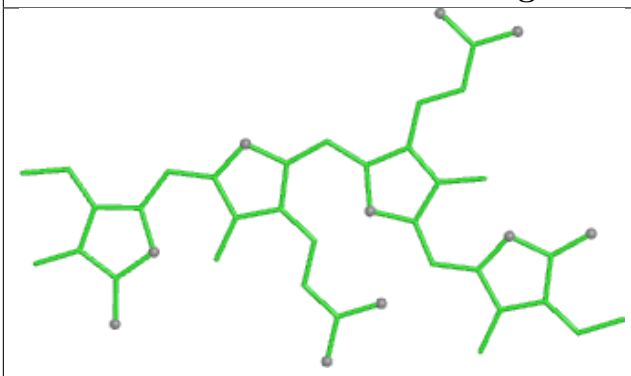


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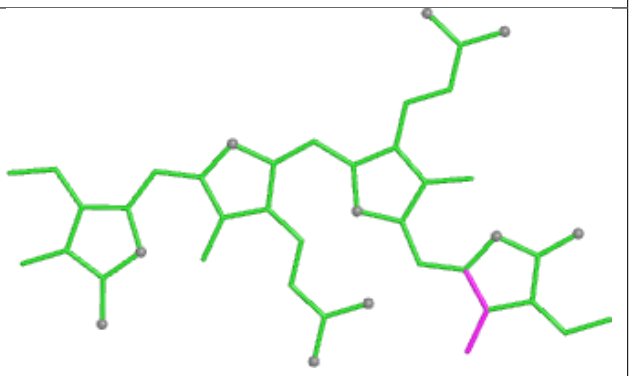


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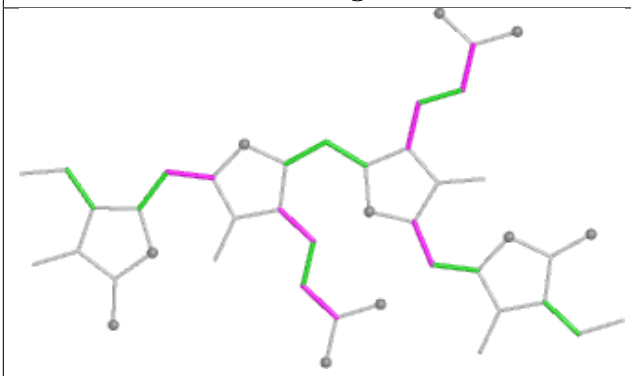
Ligand CYC c2 202



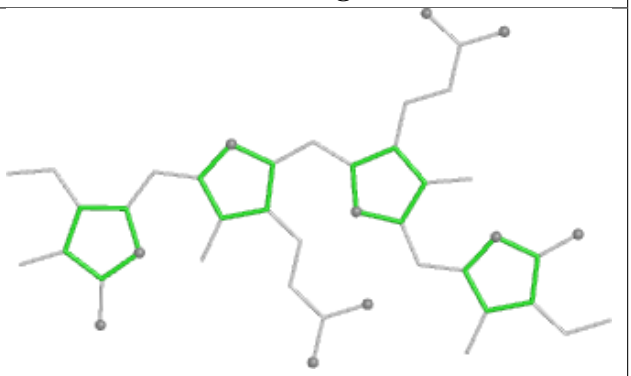
Bond lengths



Bond angles

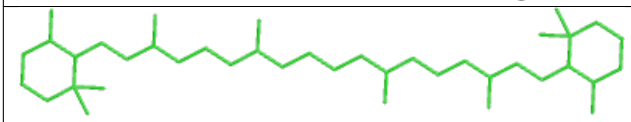


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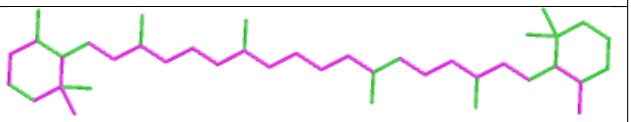


Rings

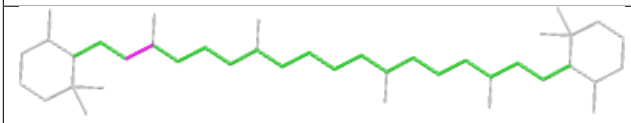
Ligand BCR ZE 102



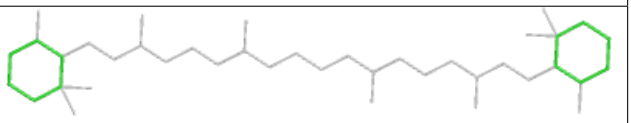
Bond lengths



Bond angles

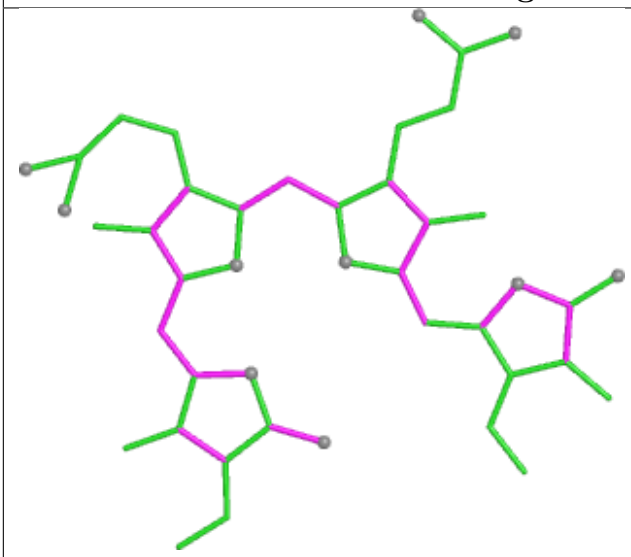


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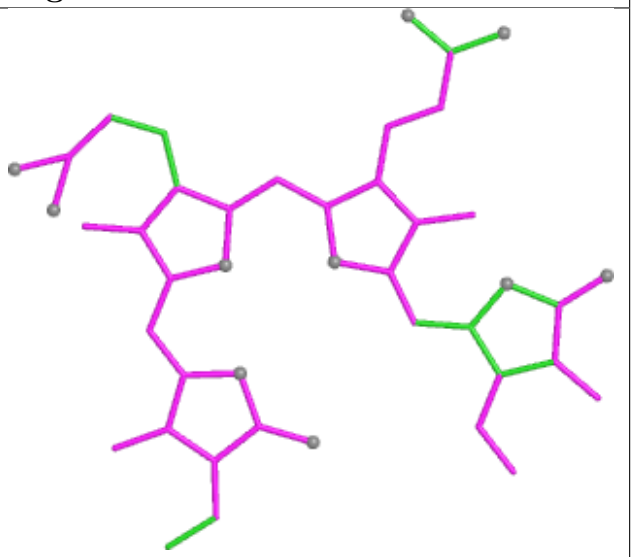


Rings

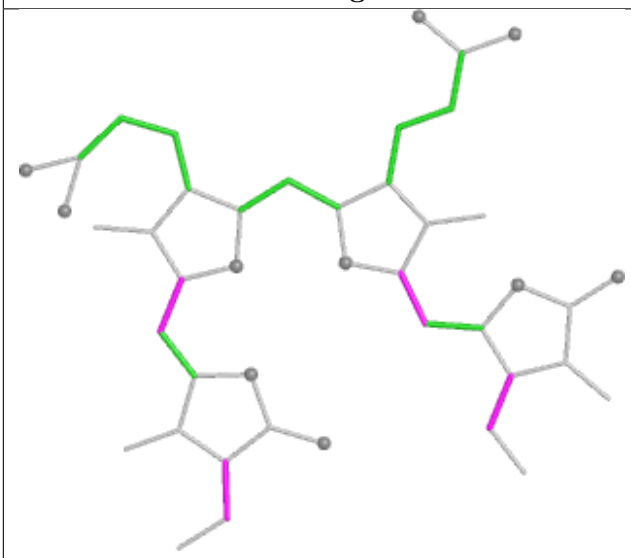
Ligand CYC g2 202



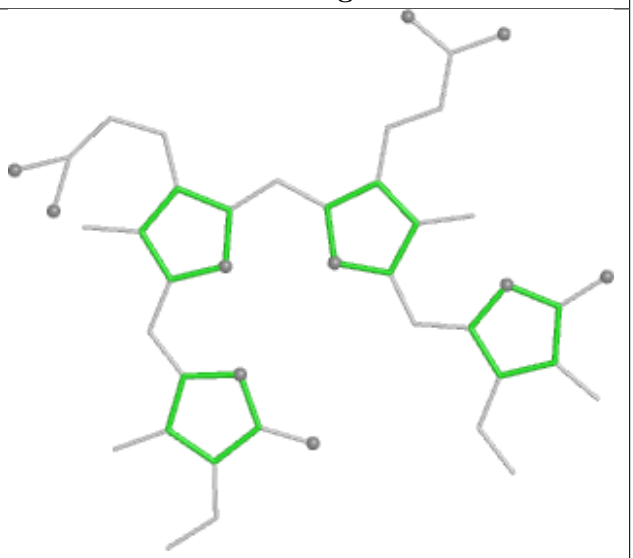
Bond lengths



Bond angles

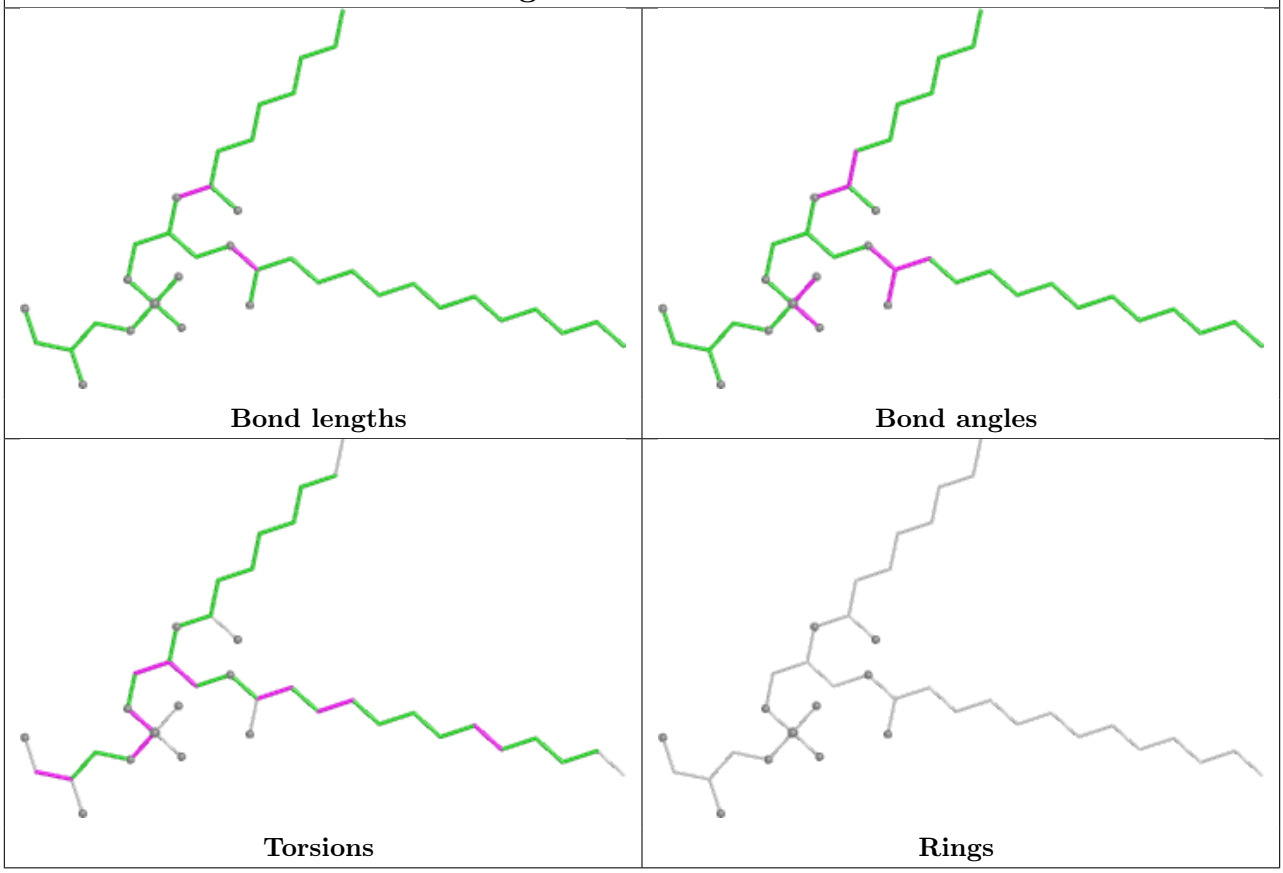


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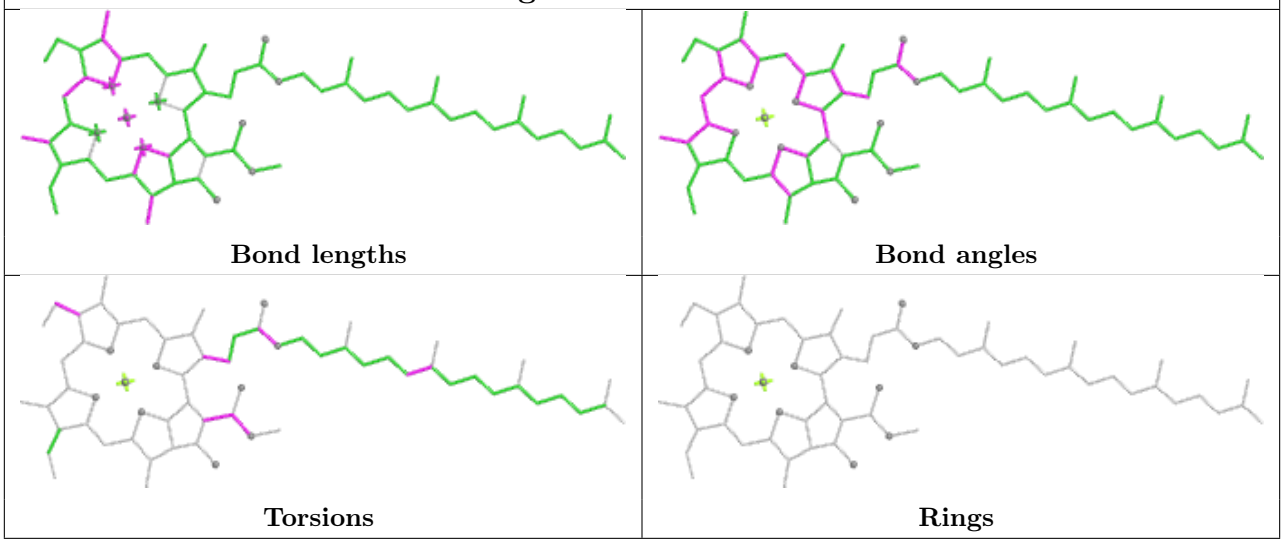


Rings

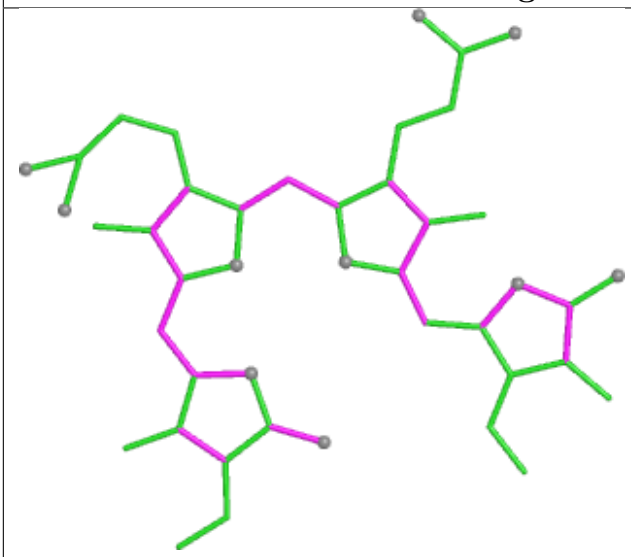
Ligand LHG a1 412



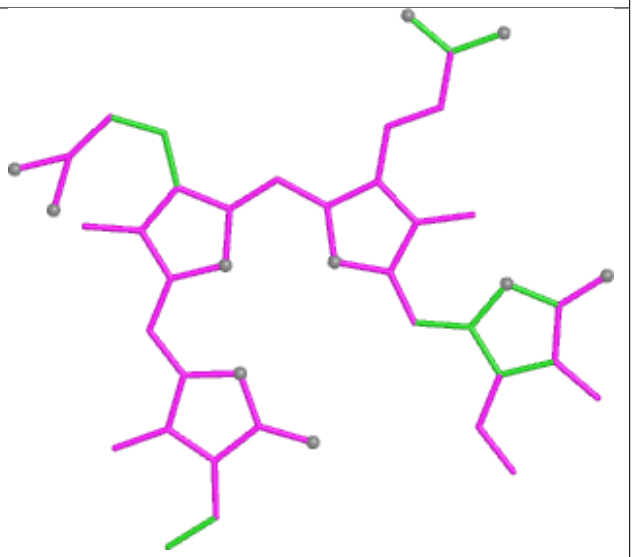
Ligand CLA cE 504



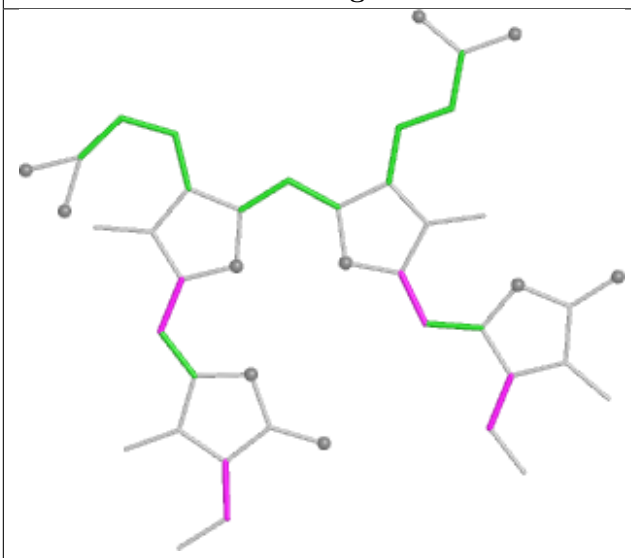
Ligand CYC c8 201



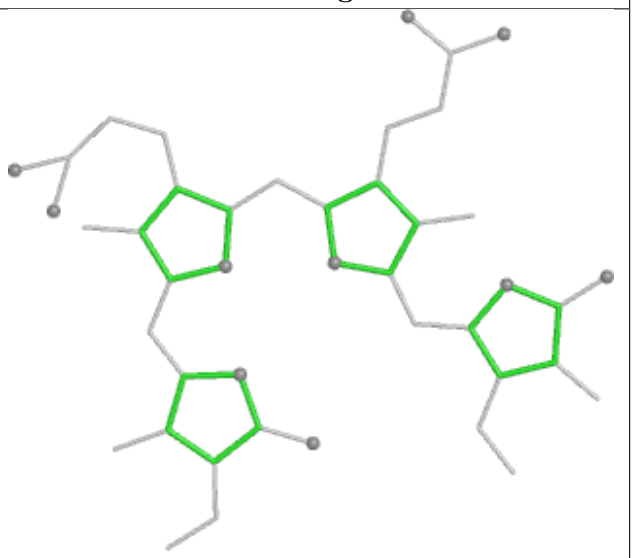
Bond lengths



Bond angles

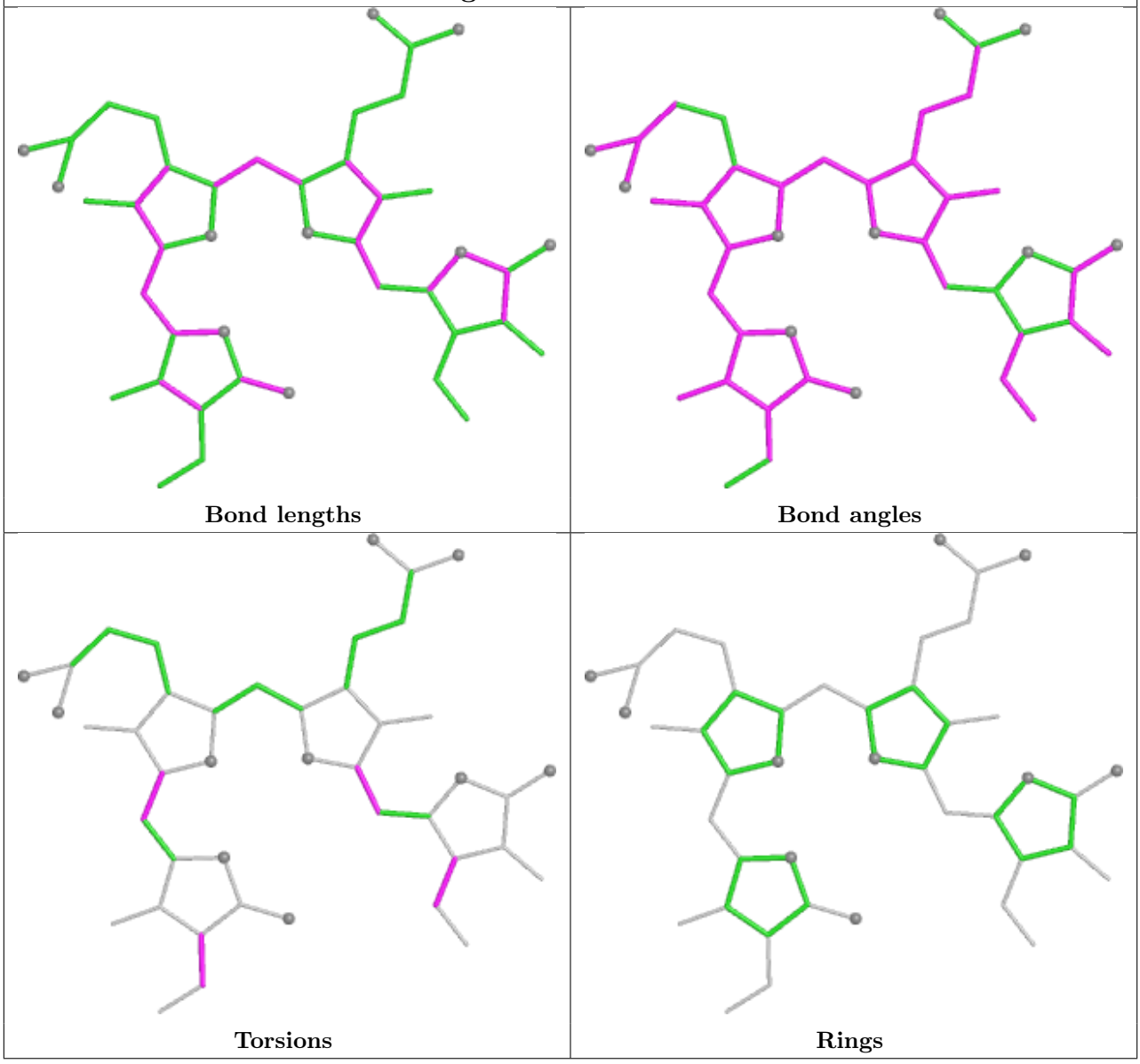


Torsions



Rings

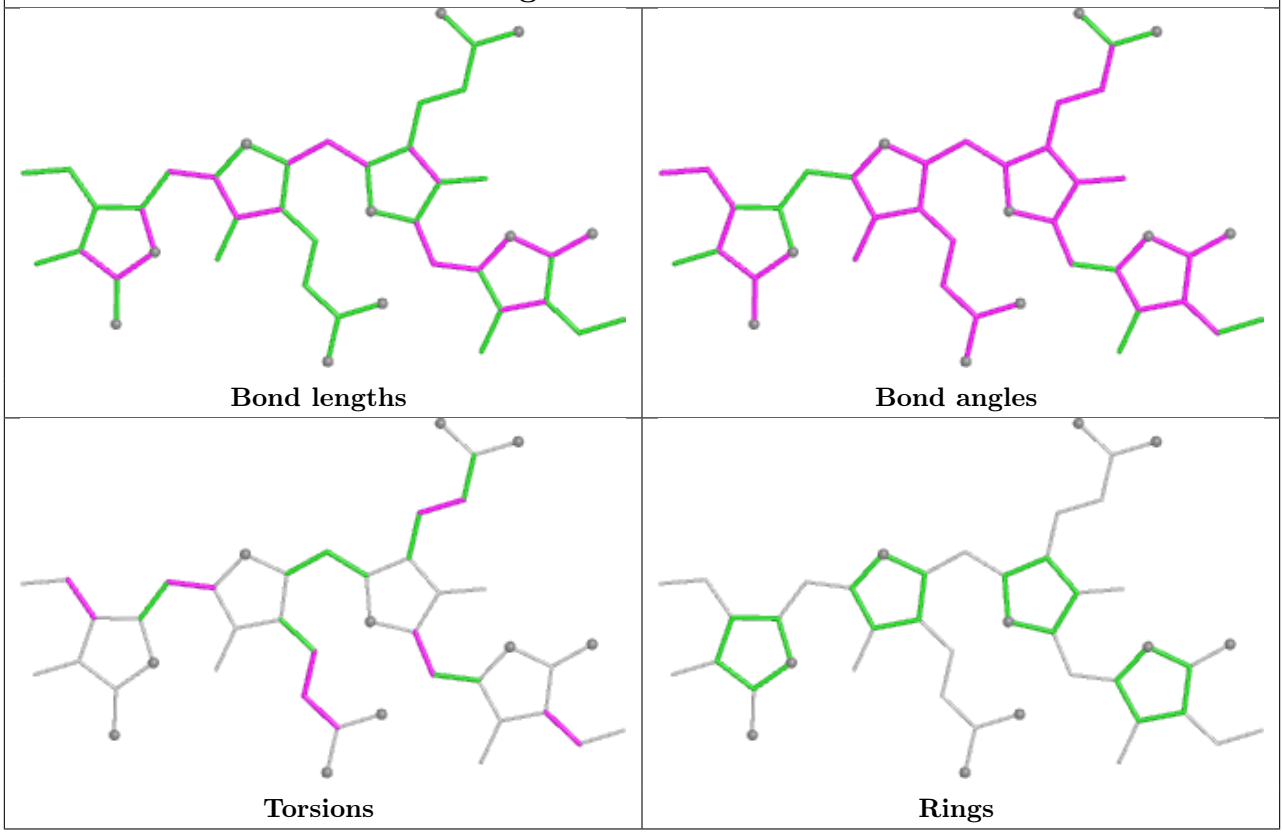
Ligand CYC cJ 201



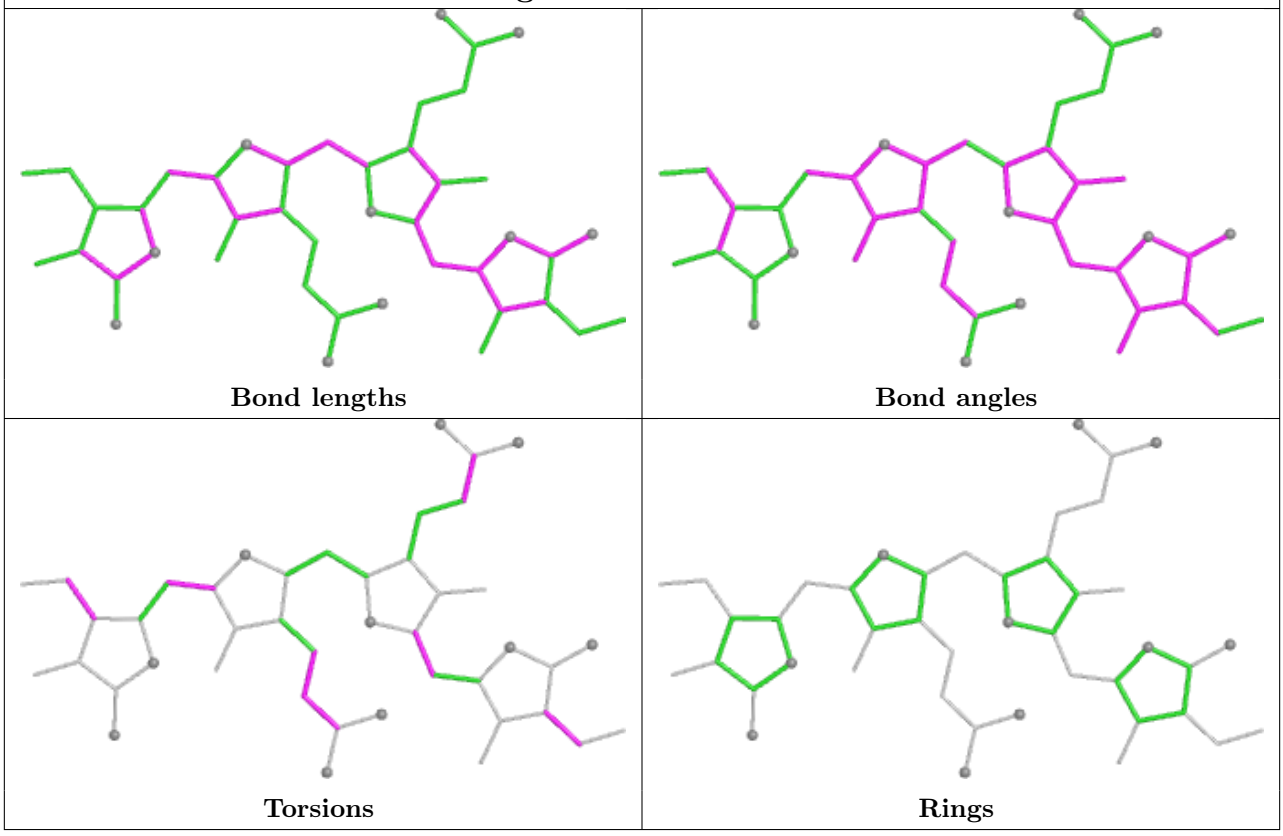
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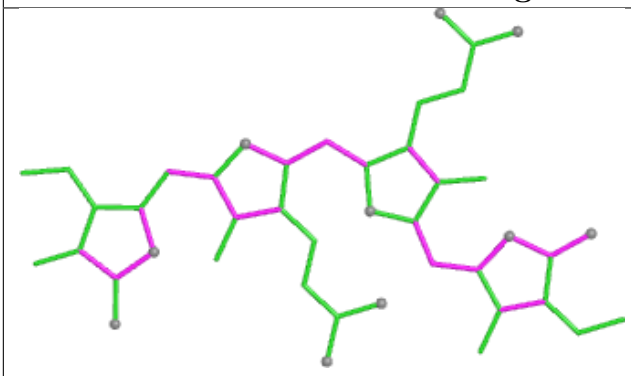
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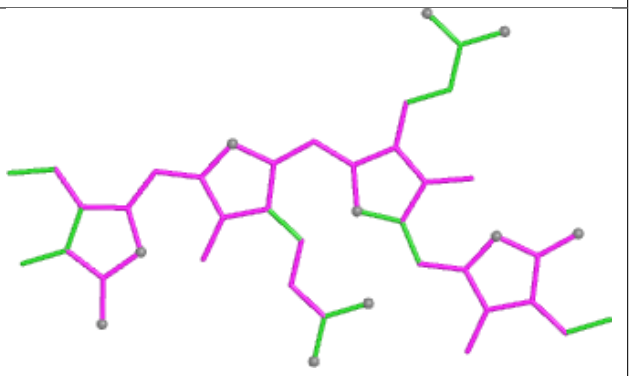
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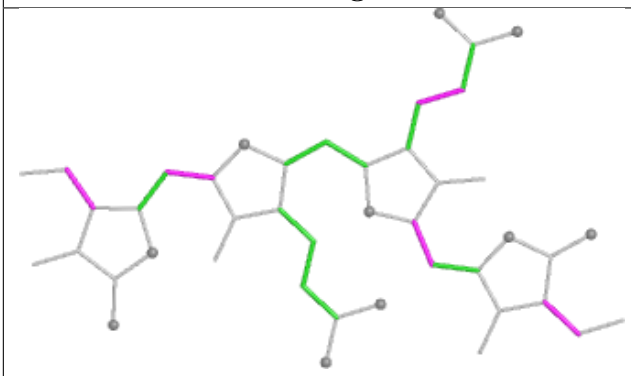
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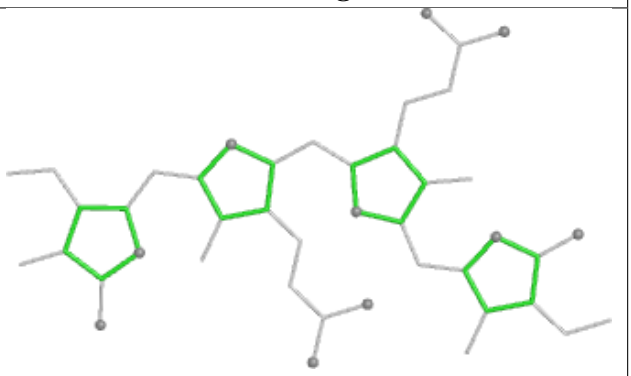
Bond lengths



Bond angles

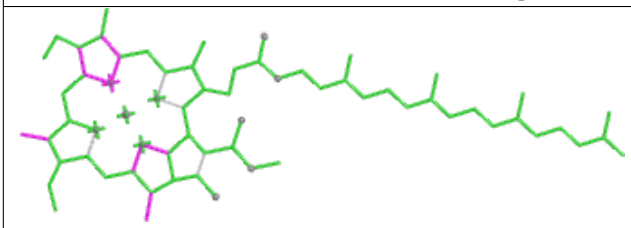


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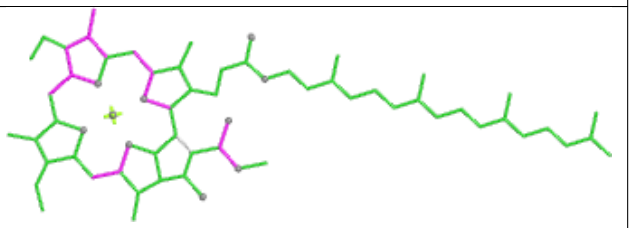


Rings

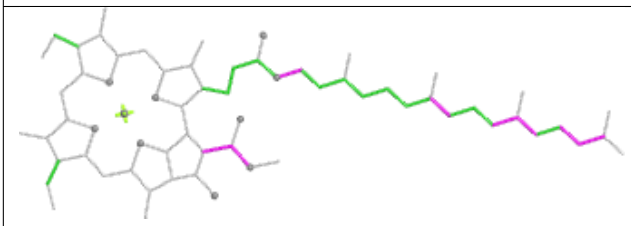
Ligand CLA BE 608



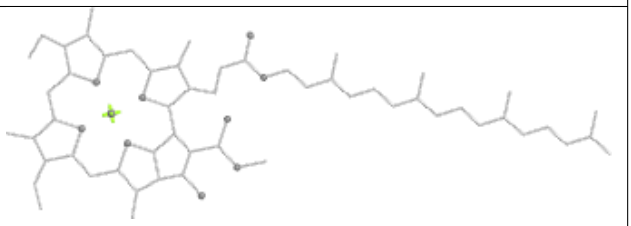
Bond lengths



Bond angles

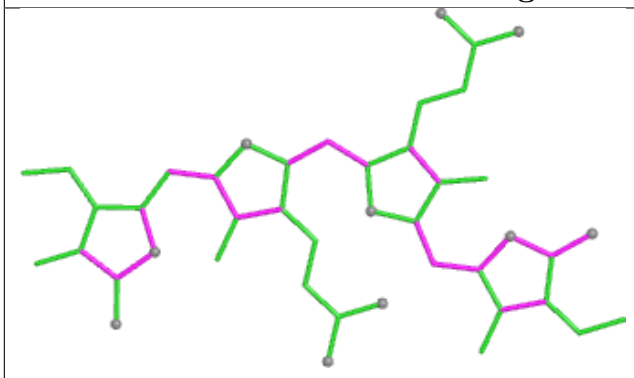


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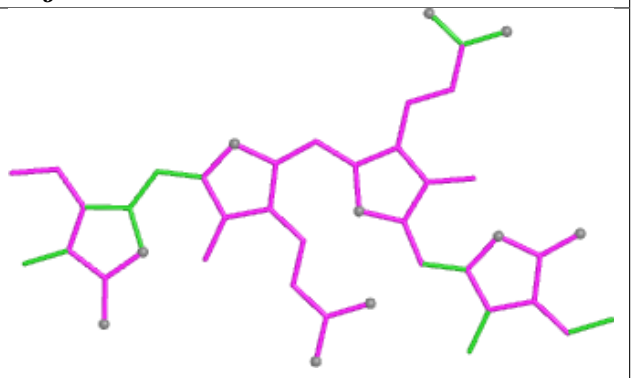


Rings

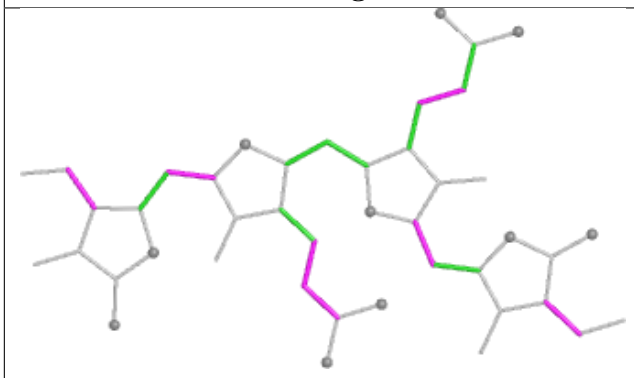
Ligand CYC jC 201



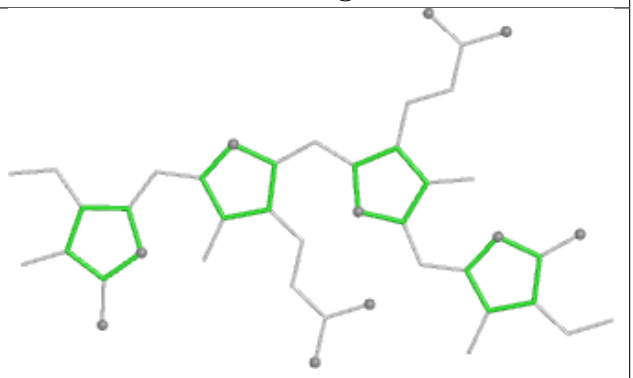
Bond lengths



Bond angles

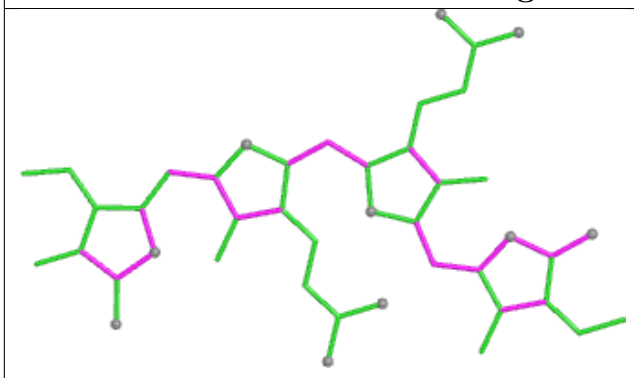


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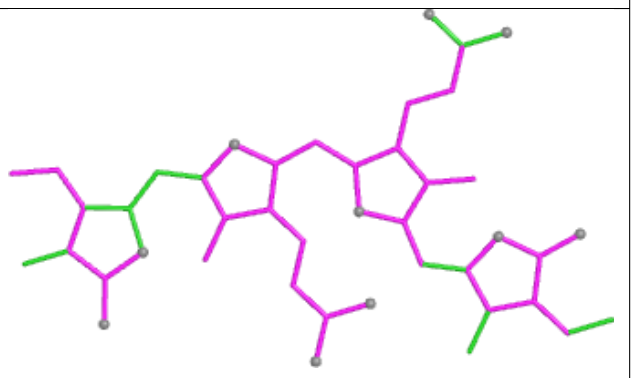


Rings

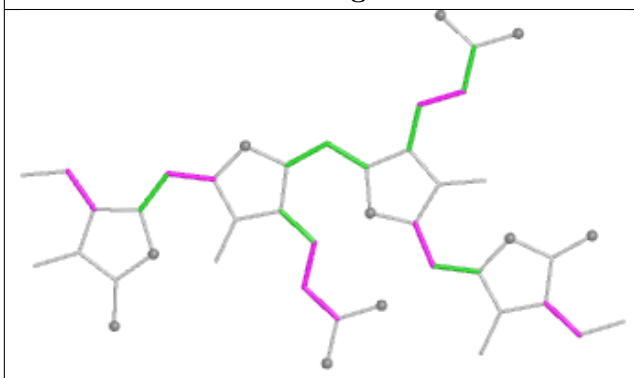
Ligand CYC b9 201



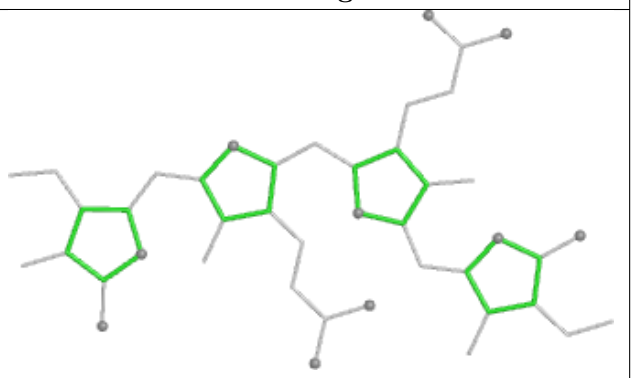
Bond lengths



Bond angles

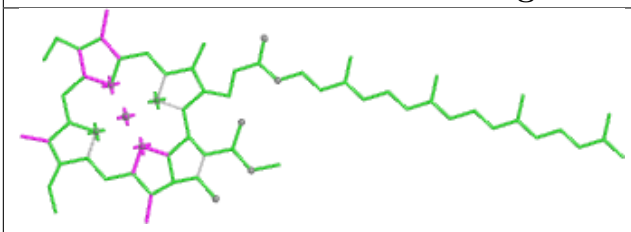


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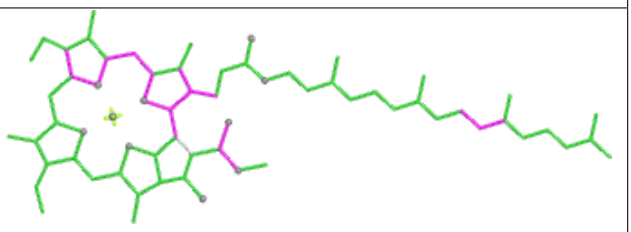


Rings

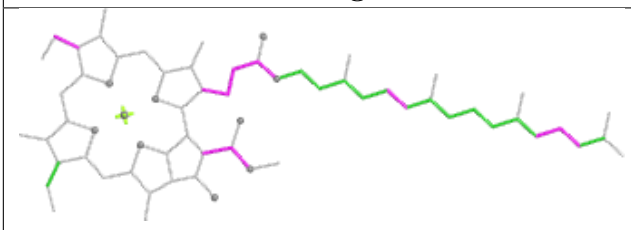
Ligand CLA cE 503



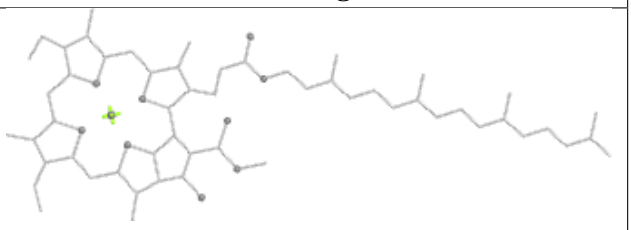
Bond lengths



Bond angles

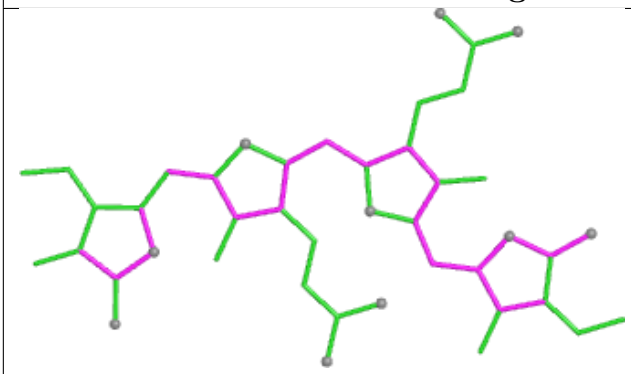


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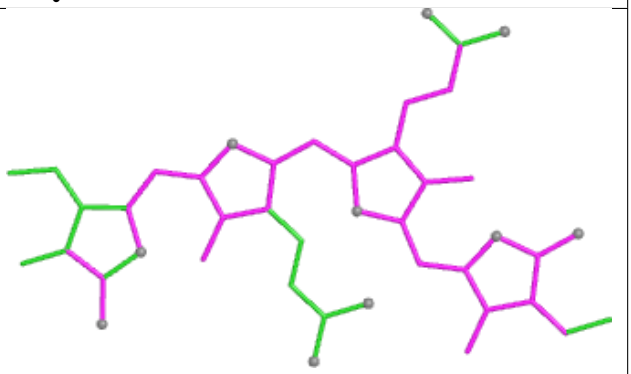


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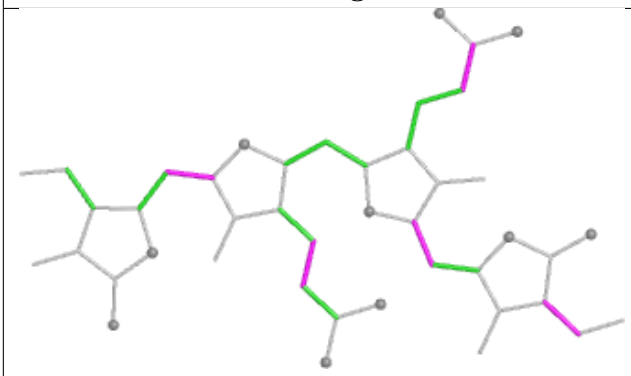
Ligand CYC QB 201



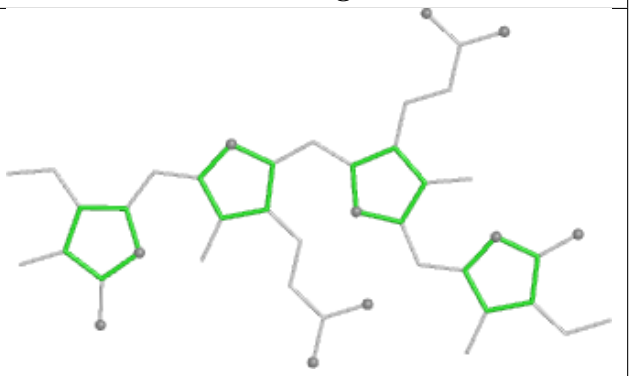
Bond lengths



Bond angles

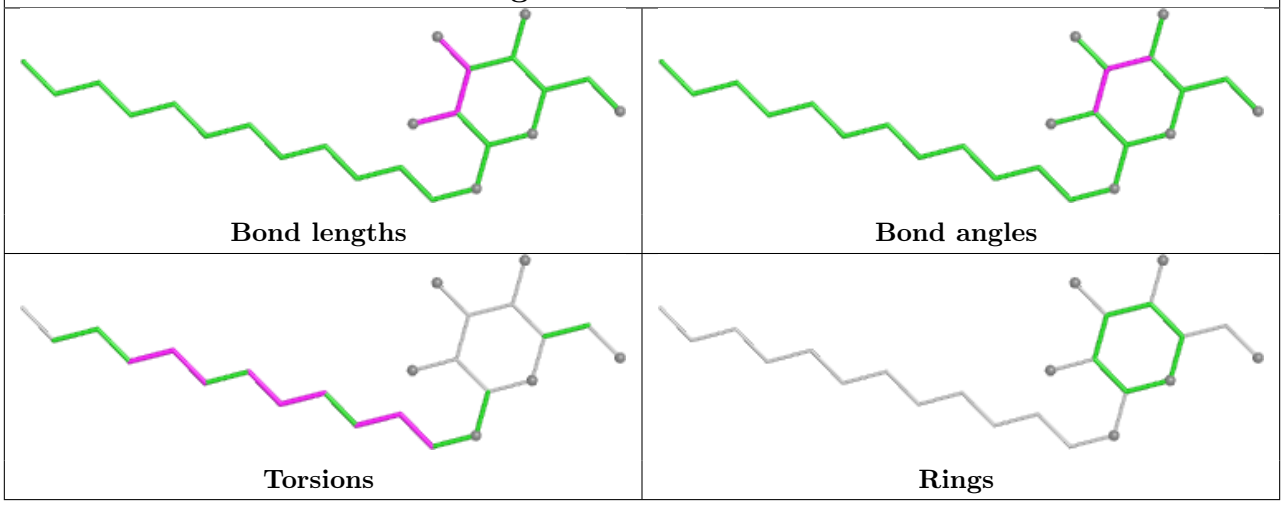


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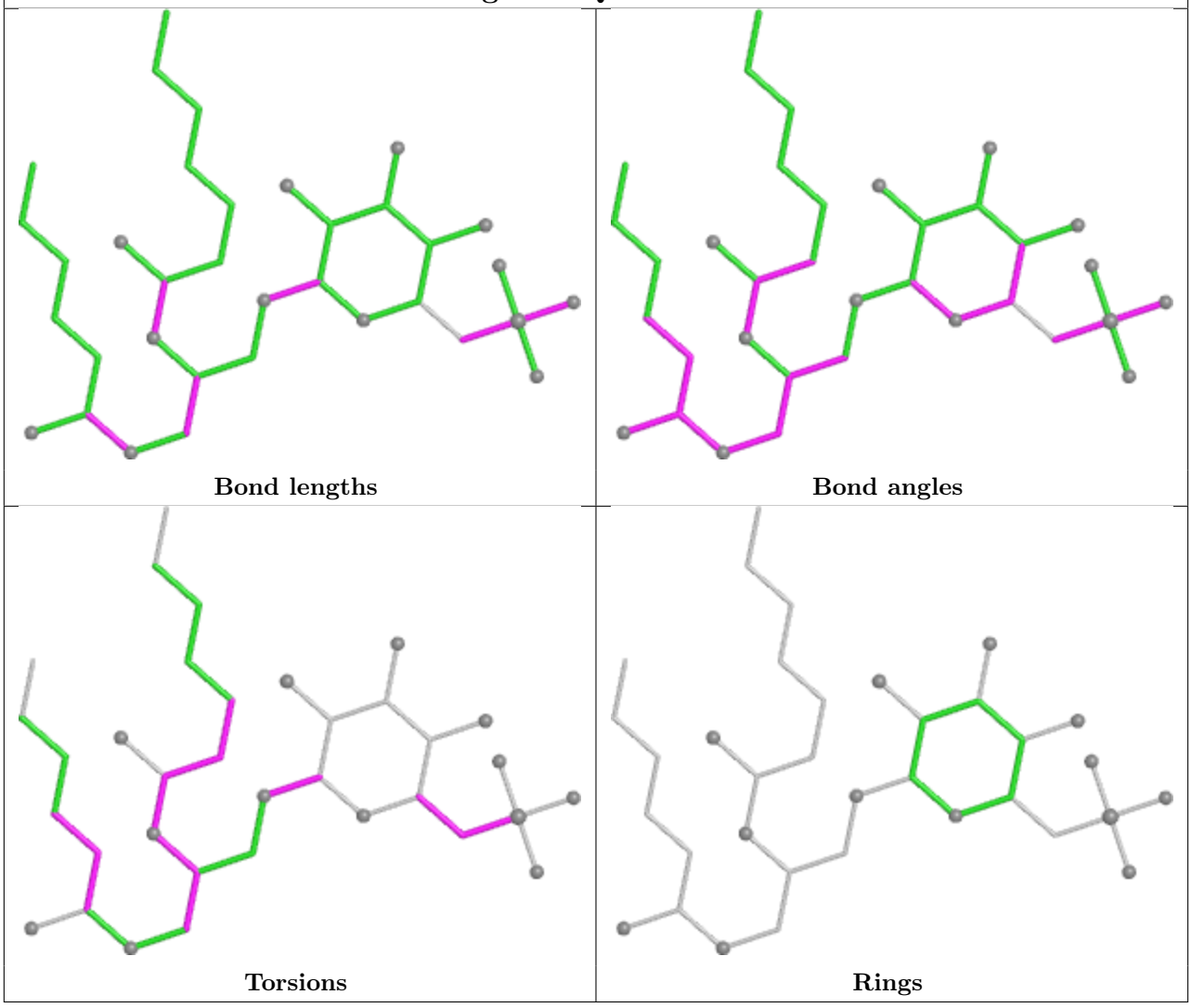


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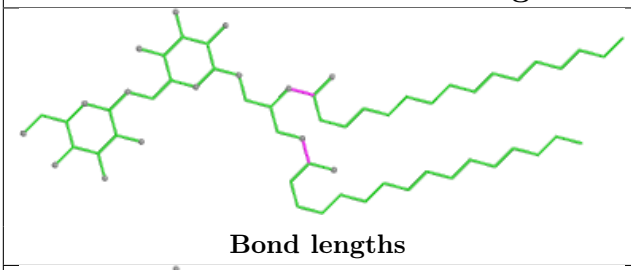
Ligand LMT BE 619



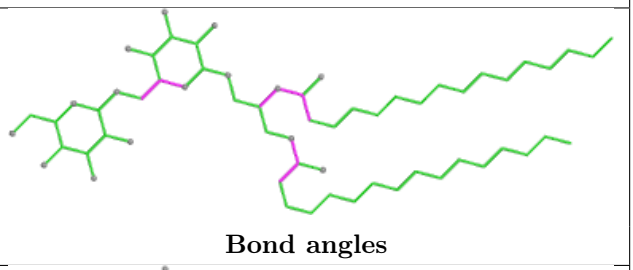
Ligand SQD h1 103



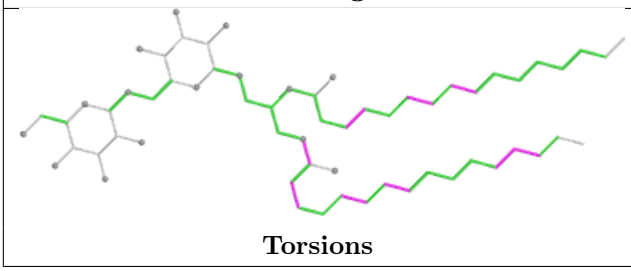
Ligand DGD JE 101



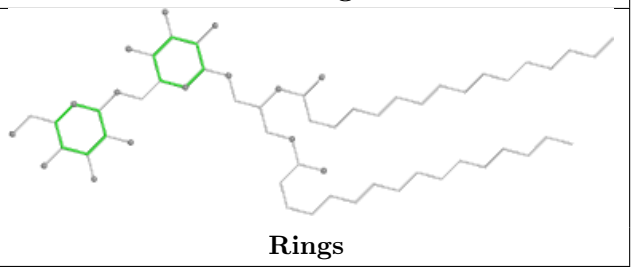
Bond lengths



Bond angles

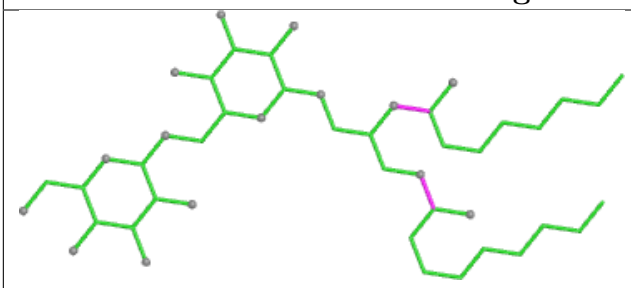


Torsions

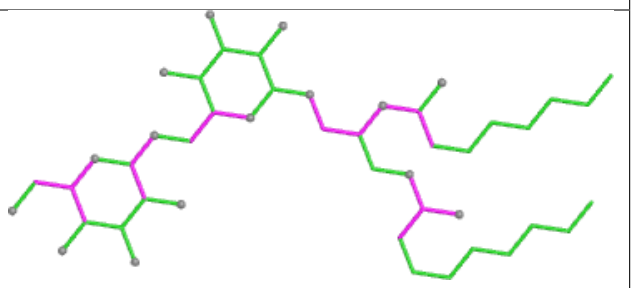


Rings

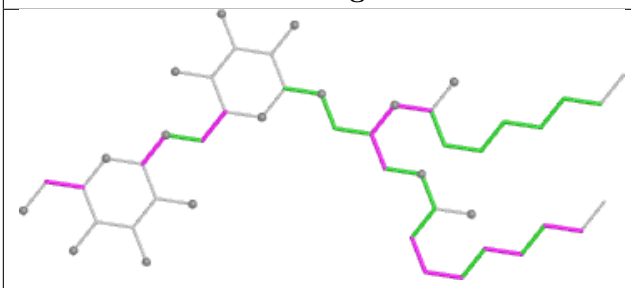
Ligand DGD cE 516



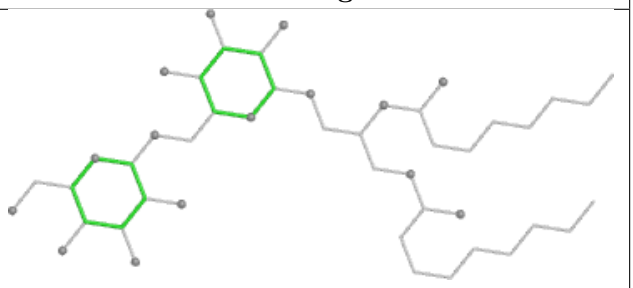
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Bond angles

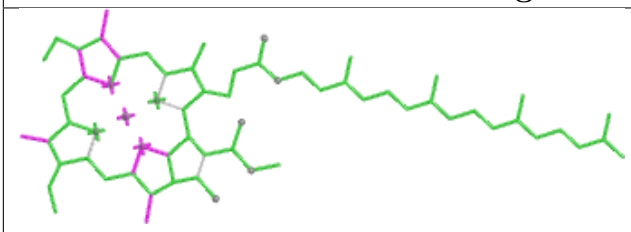


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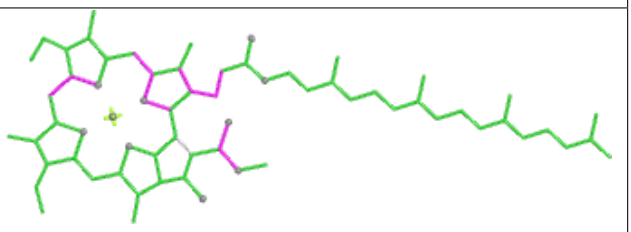


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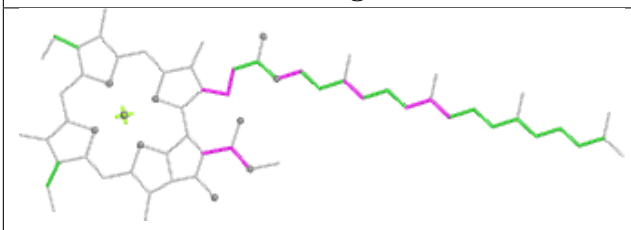
Ligand CLA cD 511



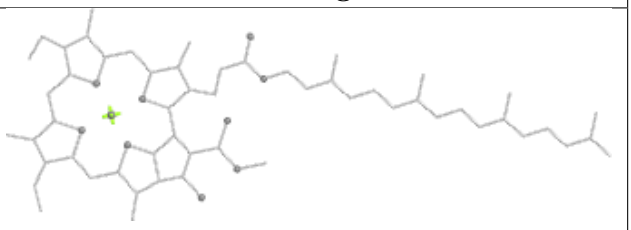
Bond lengths



Bond angles

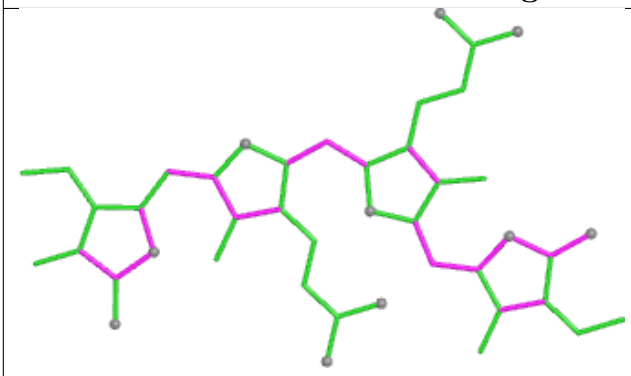


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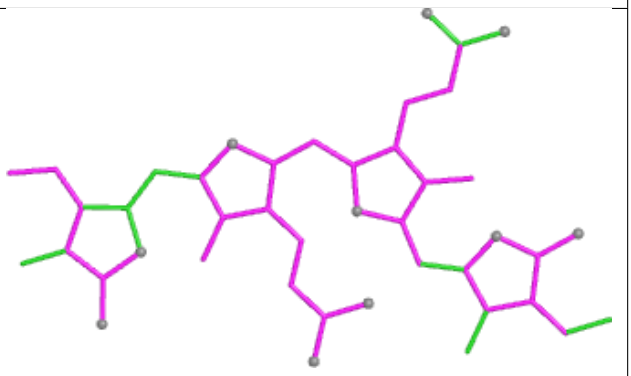


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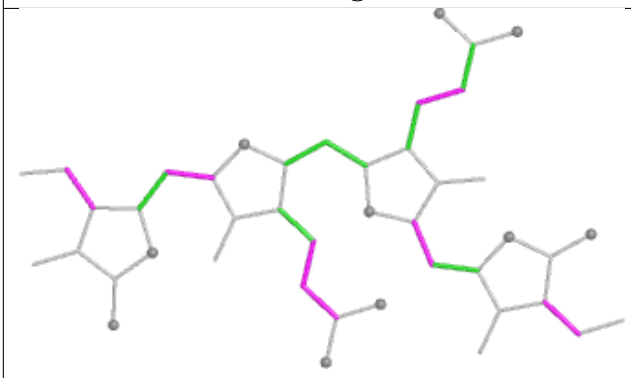
Ligand CYC l9 201



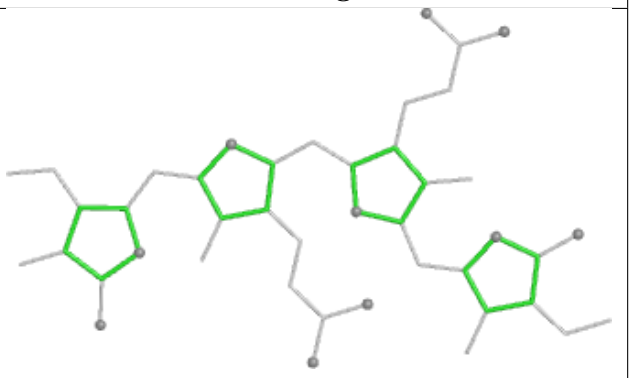
Bond lengths



Bond angles

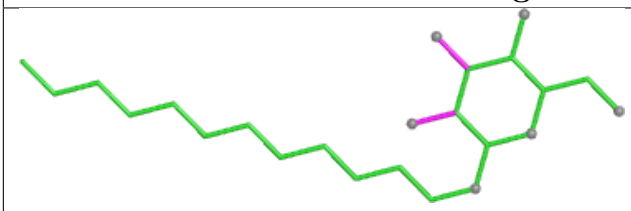


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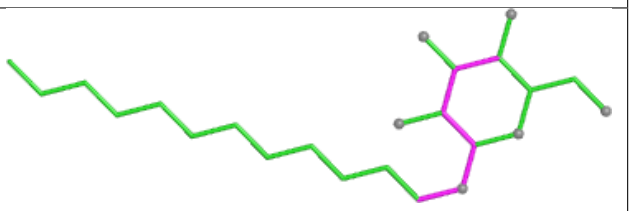


Rings

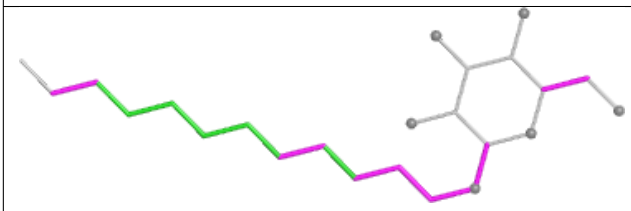
Ligand LMT B1 620



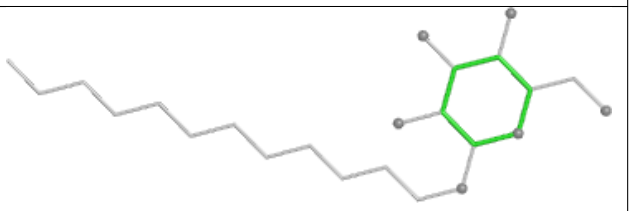
Bond lengths



Bond angles

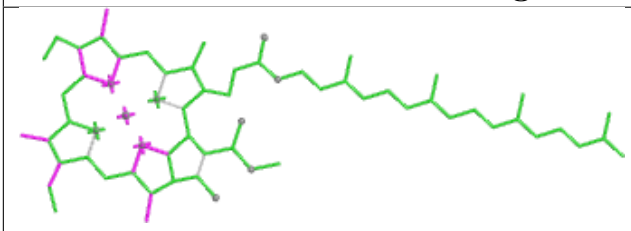


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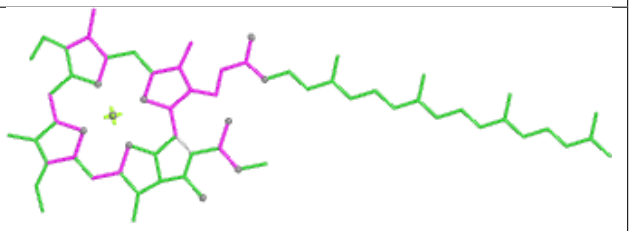


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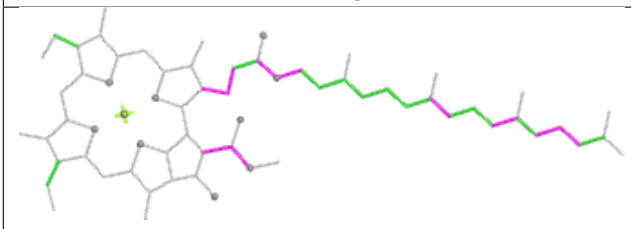
Ligand CLA CE 506



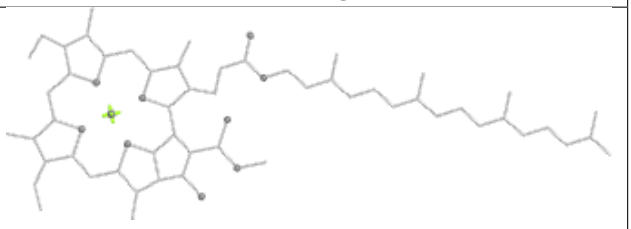
Bond lengths



Bond angles

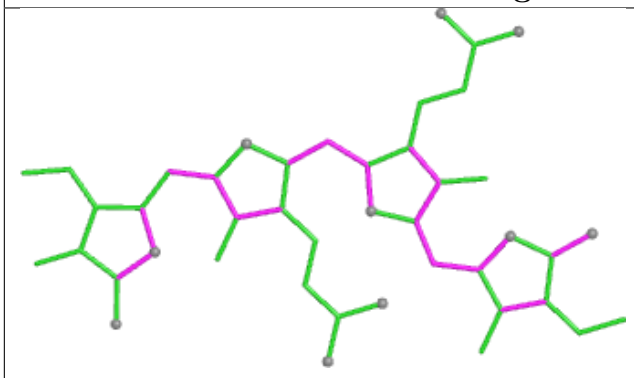


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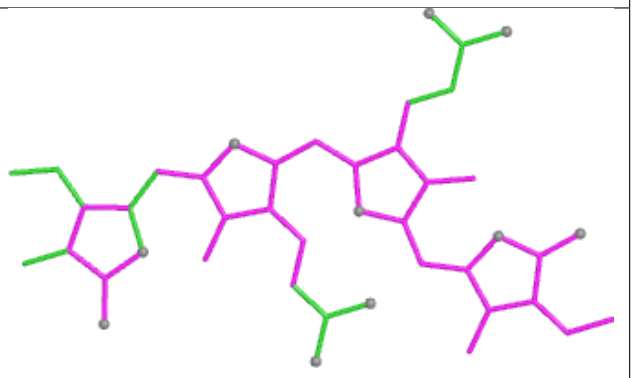


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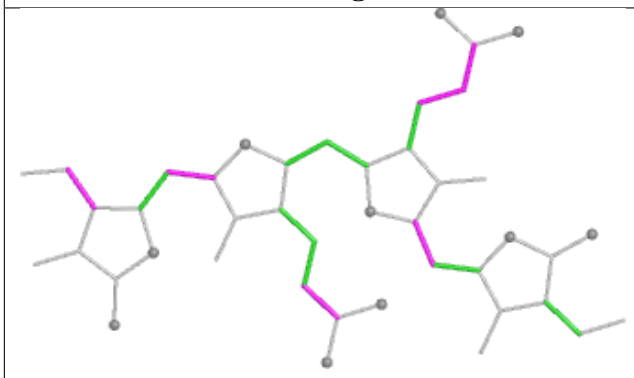
Ligand CYC Y4 201



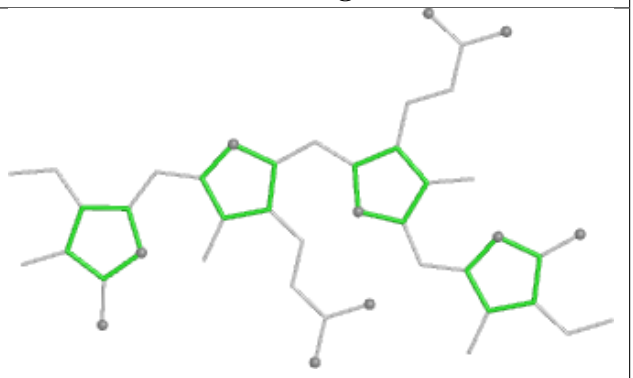
Bond lengths



Bond angles

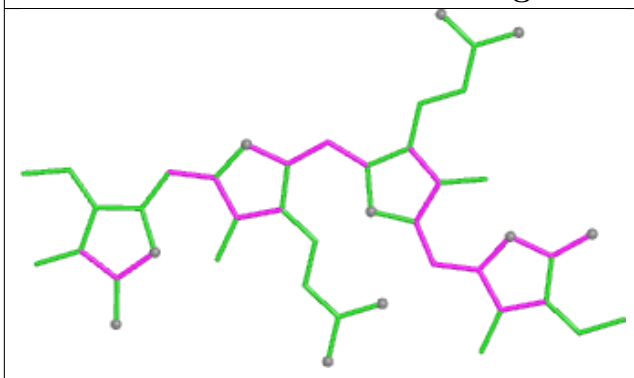


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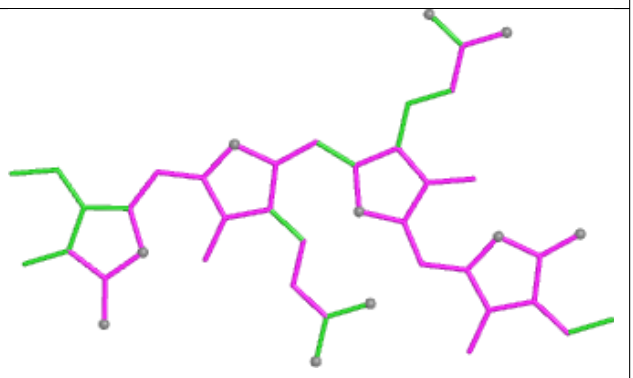


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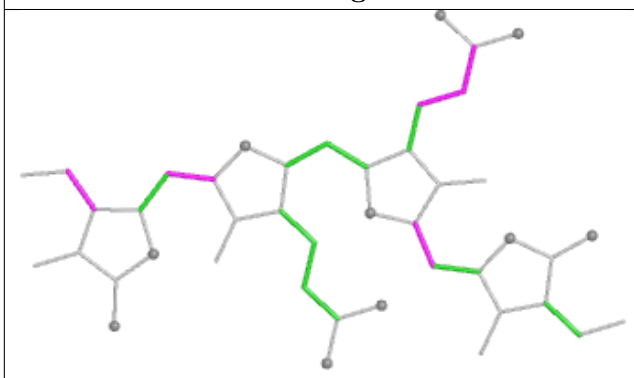
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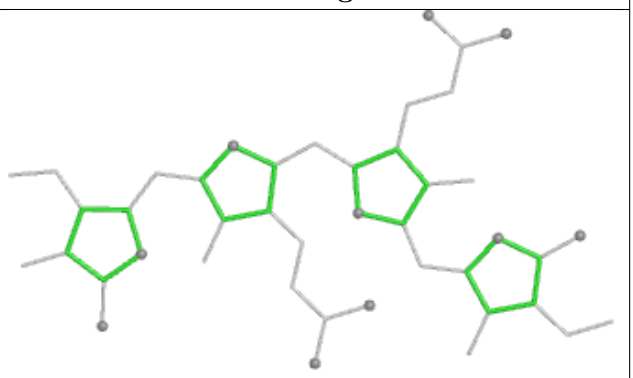
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Bond angles

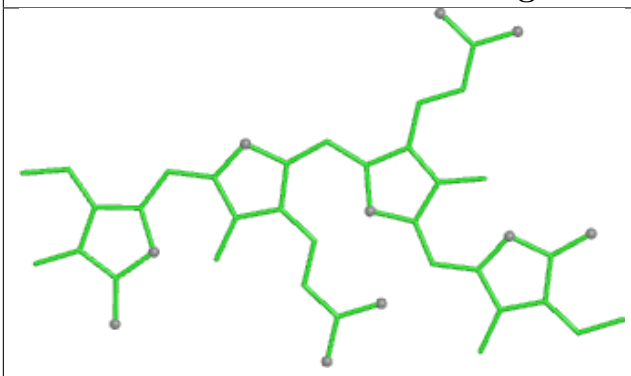


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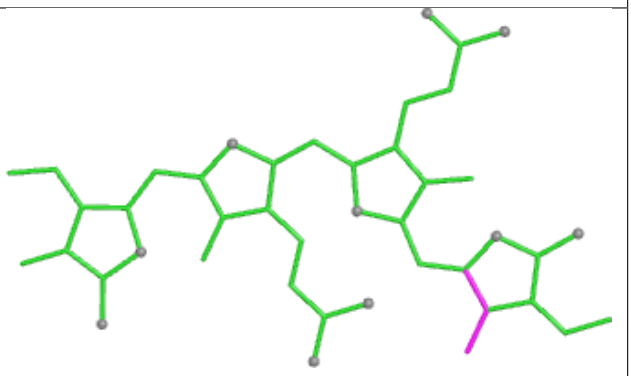


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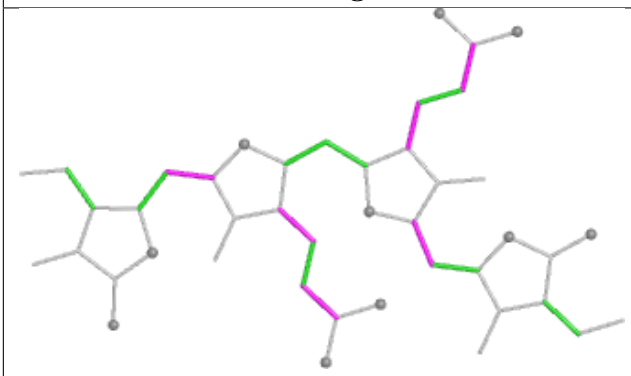
Ligand CYC c9 202



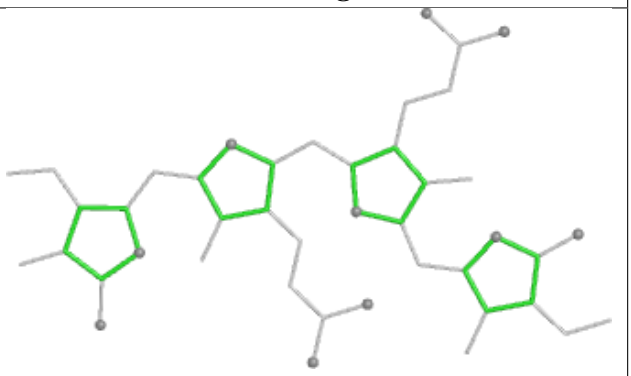
Bond lengths



Bond angles

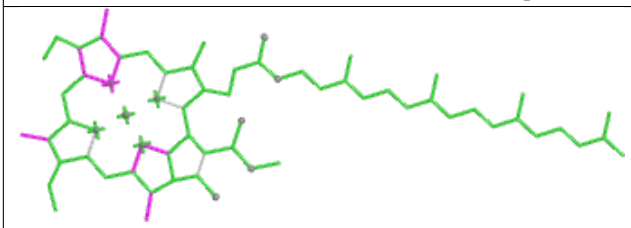


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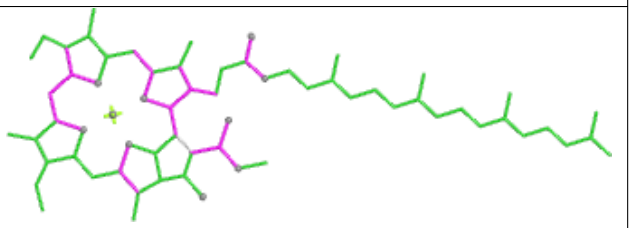


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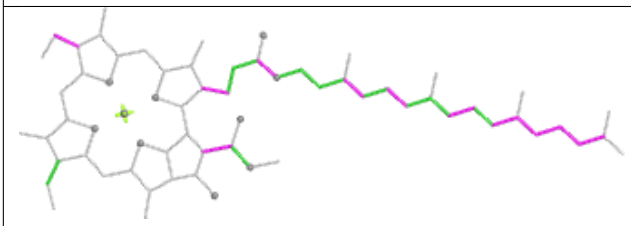
Ligand CLA b1 606



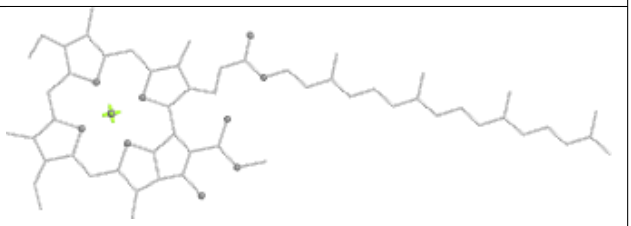
Bond lengths



Bond angles

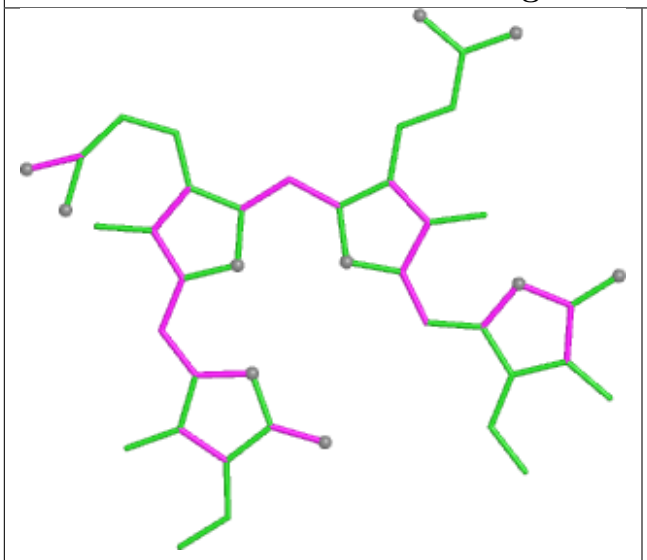


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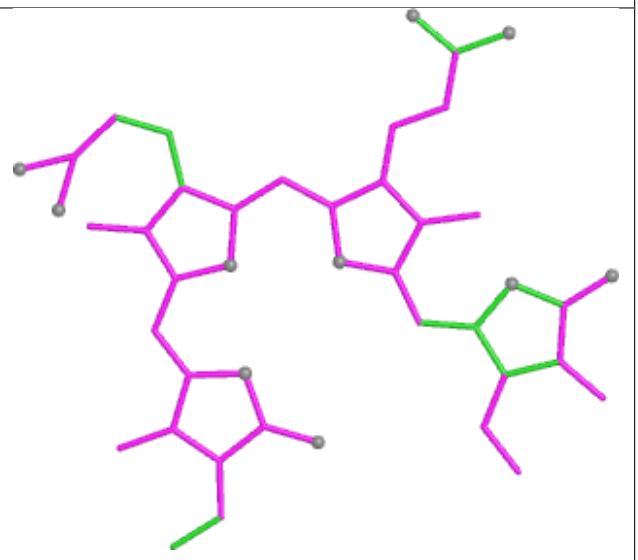


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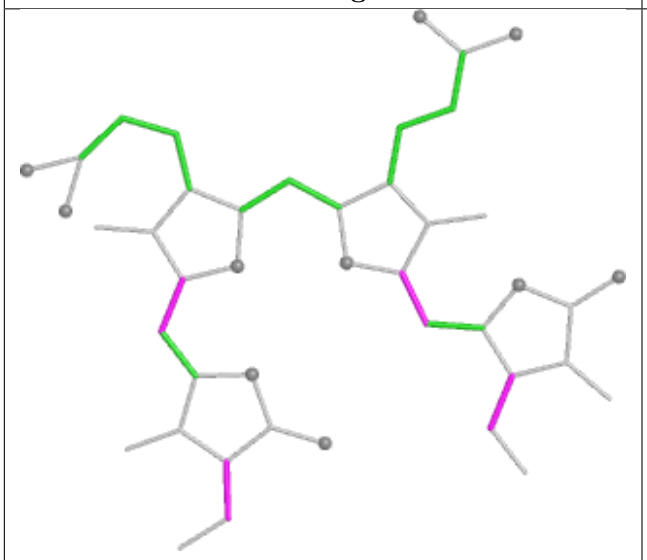
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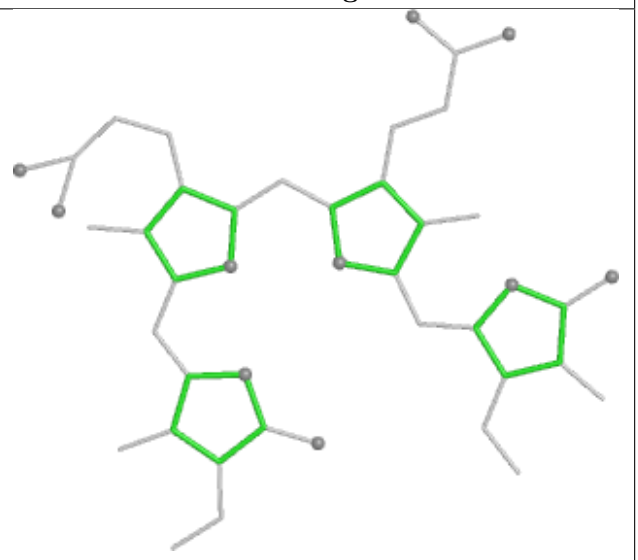
Bond lengths



Bond angles



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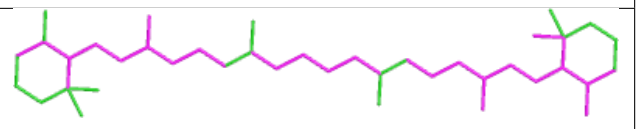


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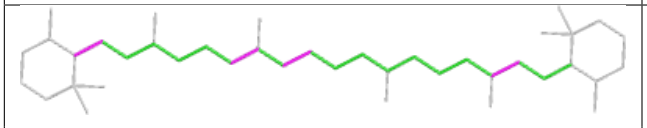
Ligand BCR b1 616



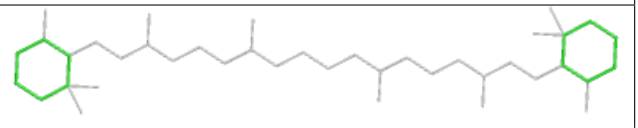
Bond lengths



Bond angles

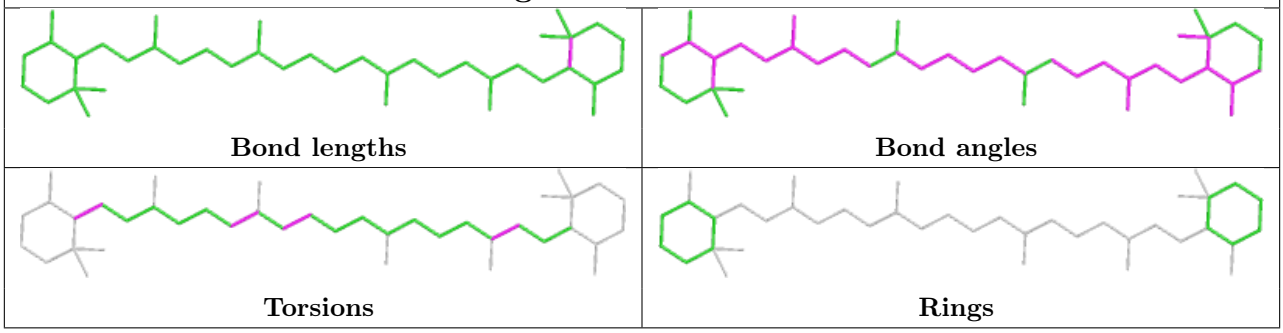


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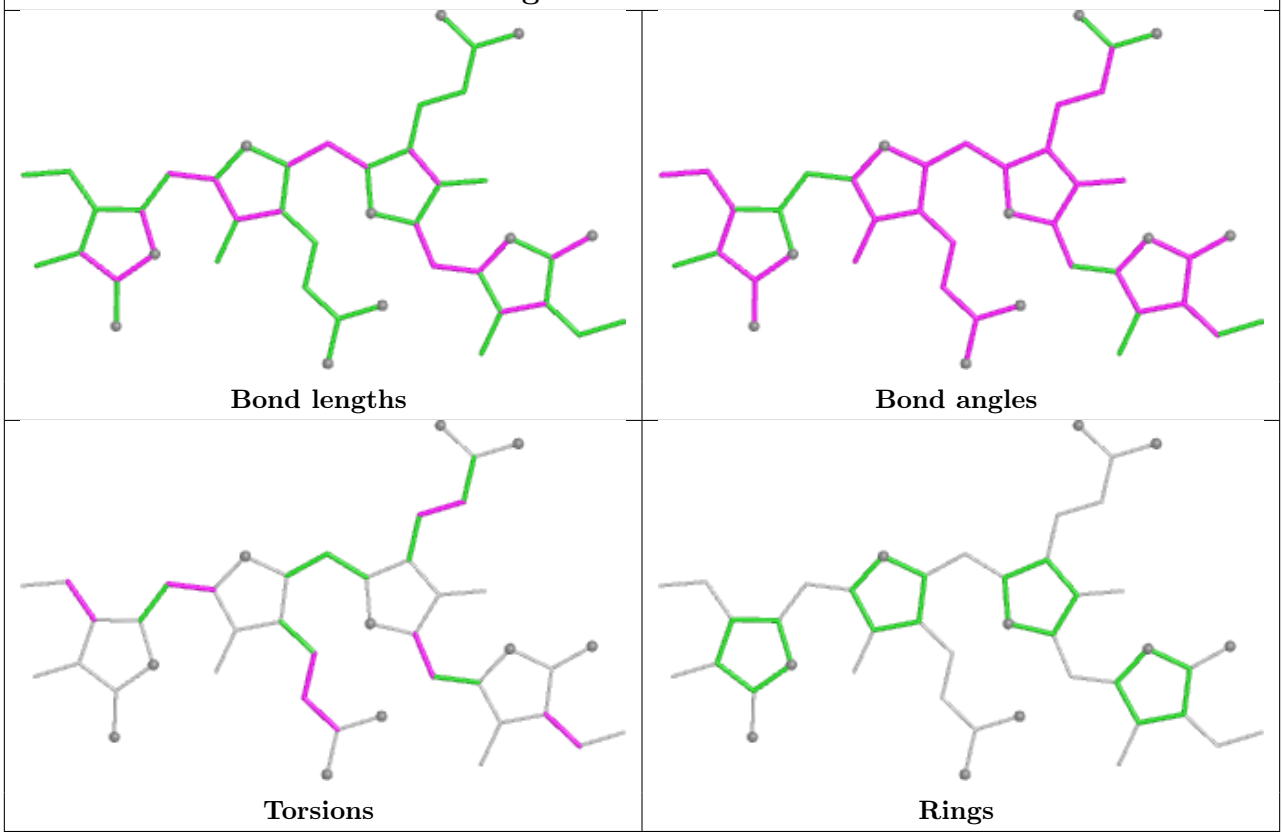


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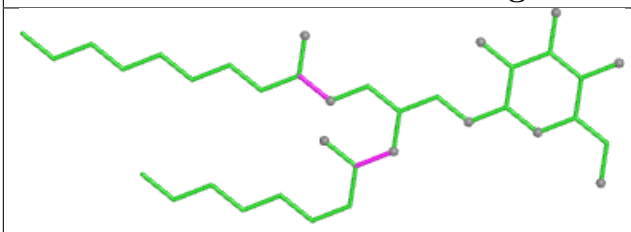
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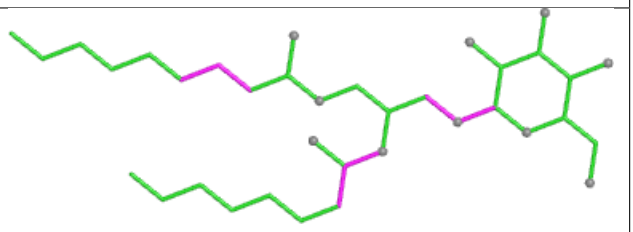
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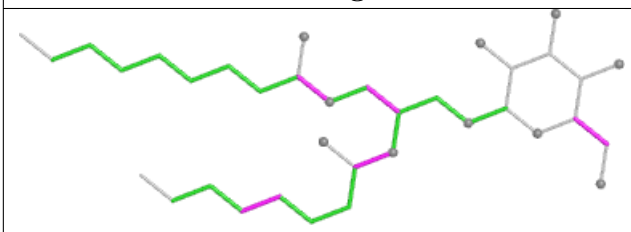
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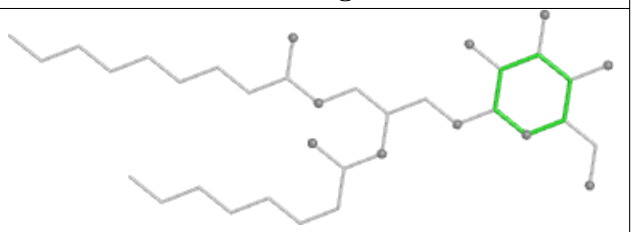
Bond lengths



Bond angles

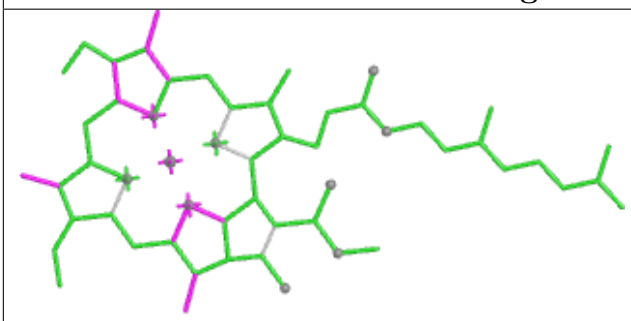


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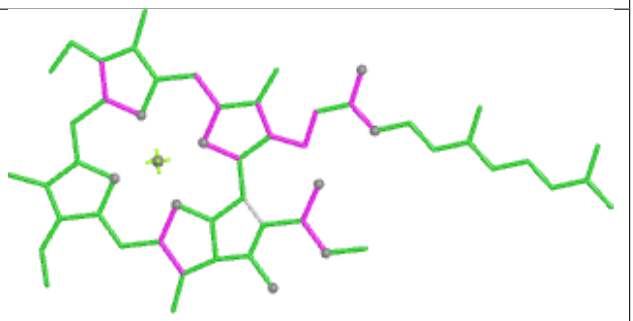


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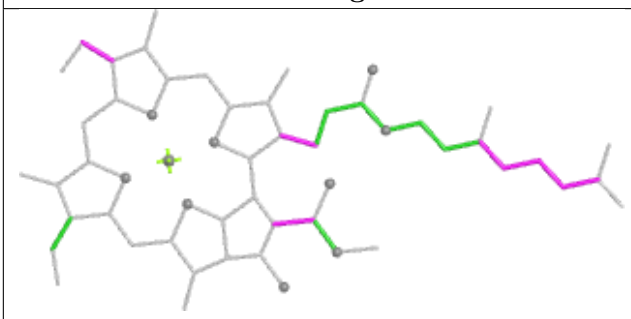
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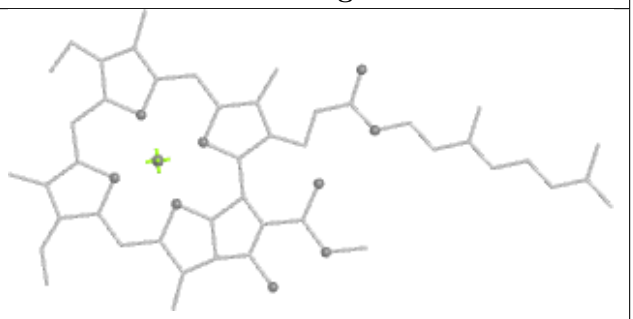
Bond lengths



Bond angles

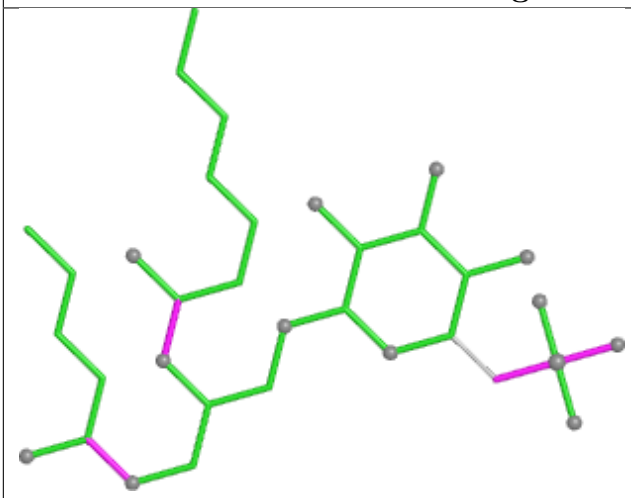


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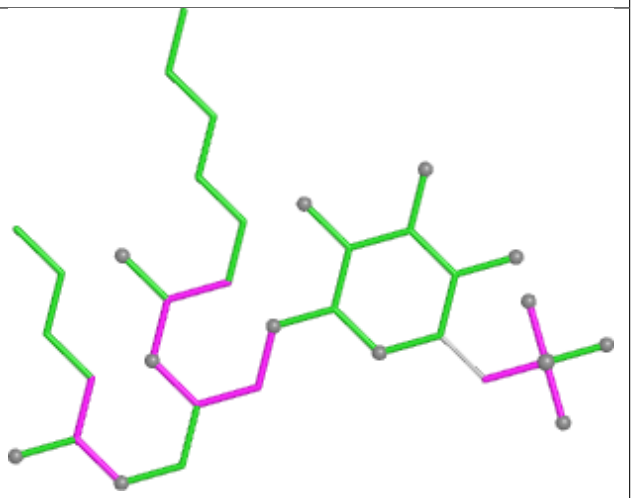


Rings

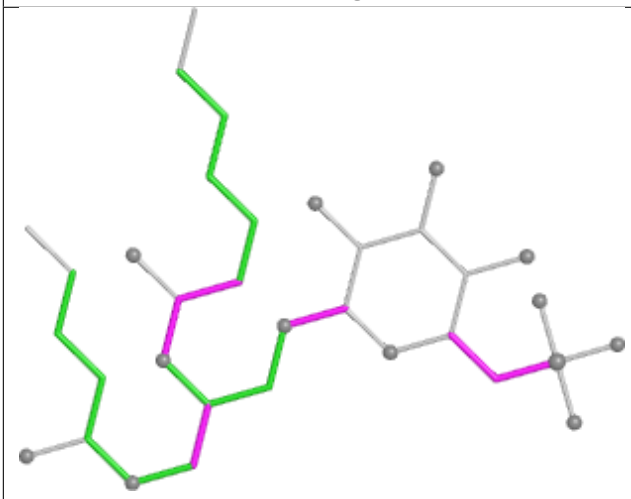
Ligand SQD DE 414



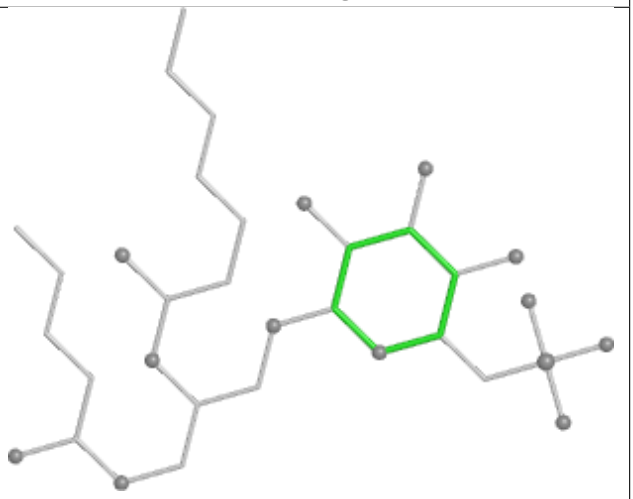
Bond lengths



Bond angles

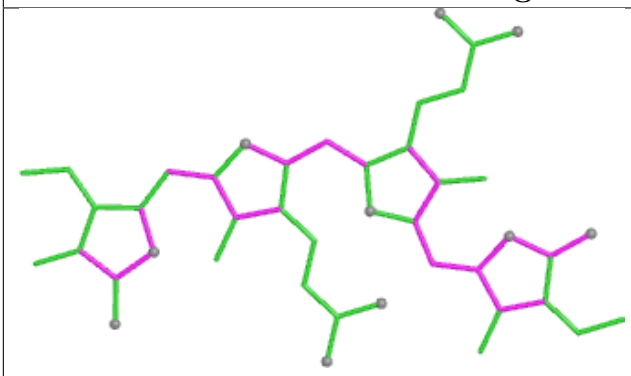


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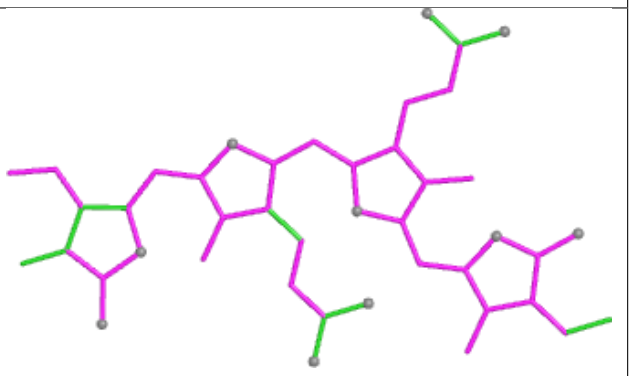


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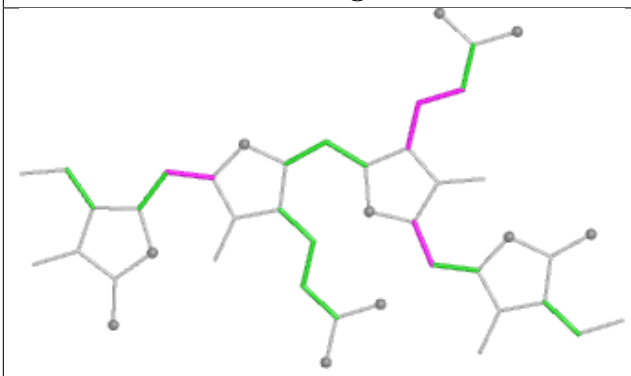
Ligand CYC zB 201



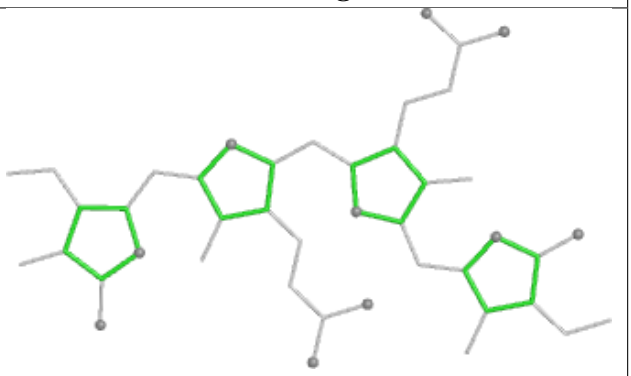
Bond lengths



Bond angles

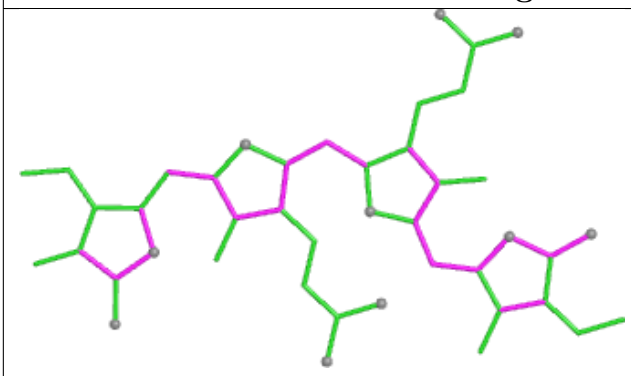


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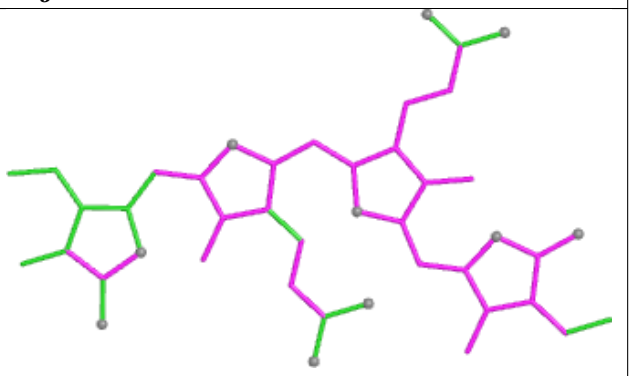


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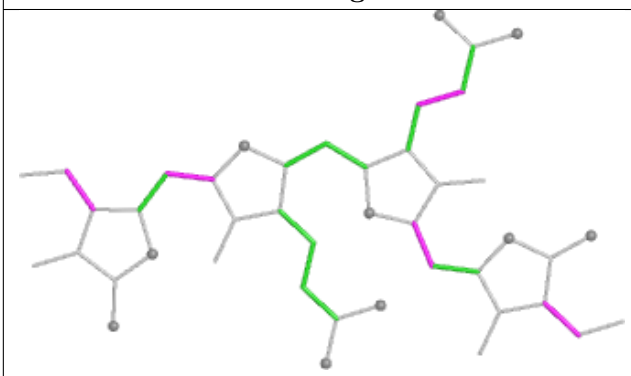
Ligand CYC jK 201



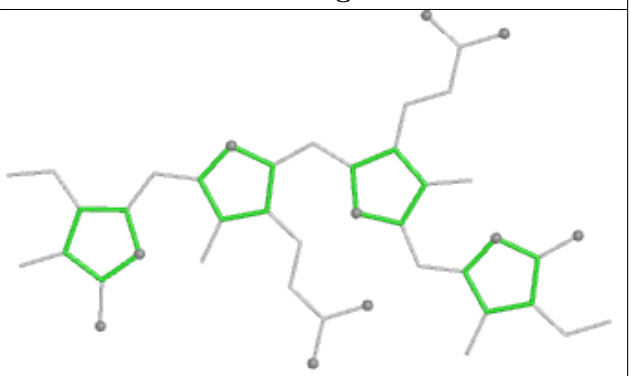
Bond lengths



Bond angles

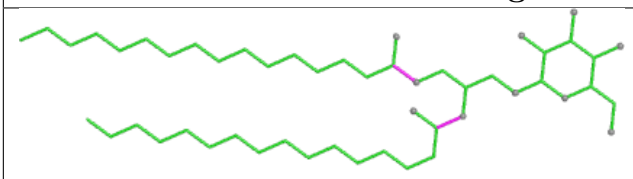


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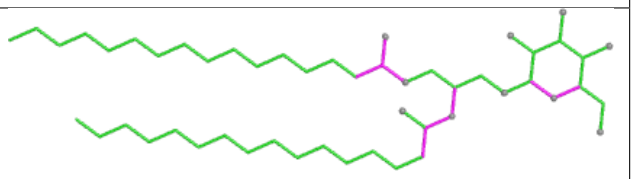


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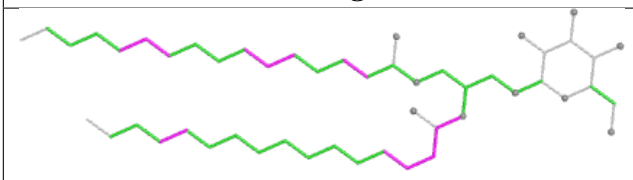
Ligand LMG CE 520



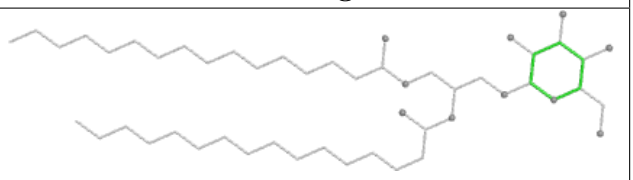
Bond lengths



Bond angles

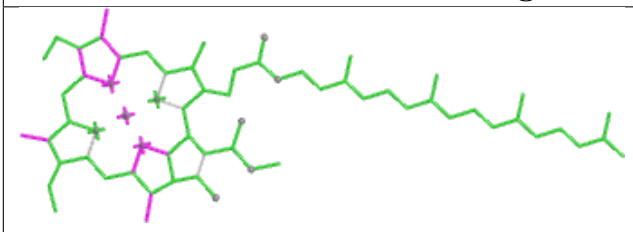


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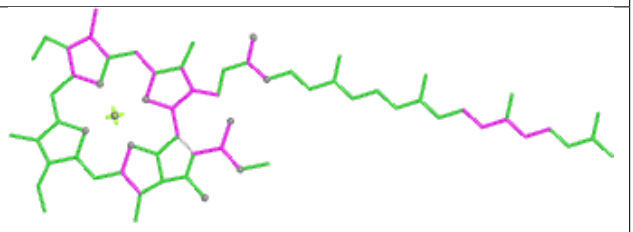


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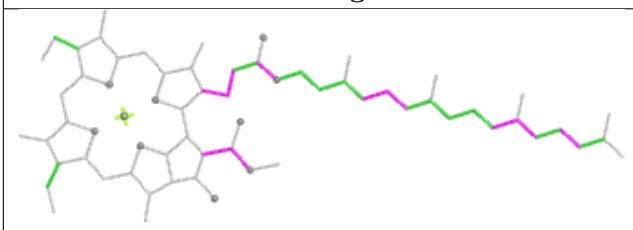
Ligand CLA cE 512



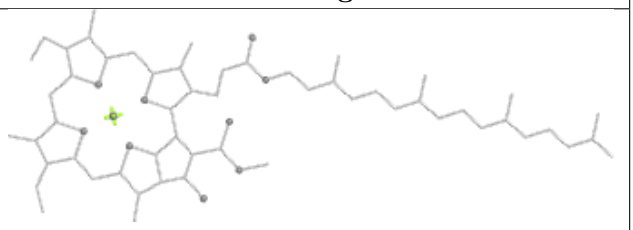
Bond lengths



Bond angles

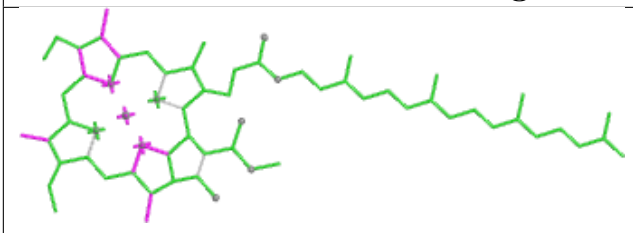


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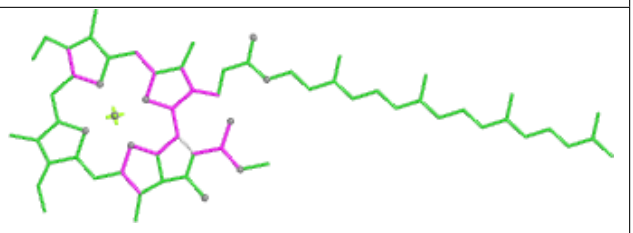


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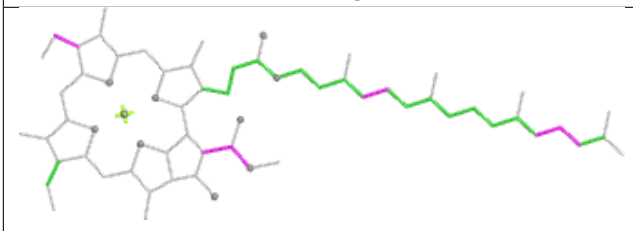
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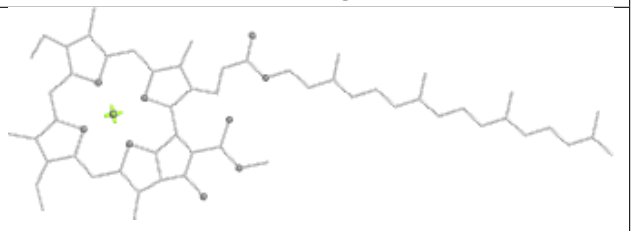
Bond lengths



Bond angles

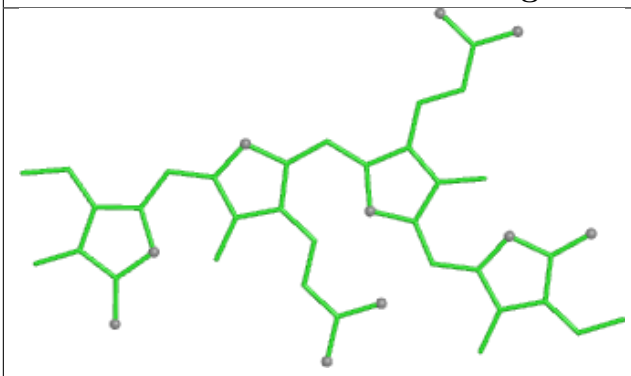


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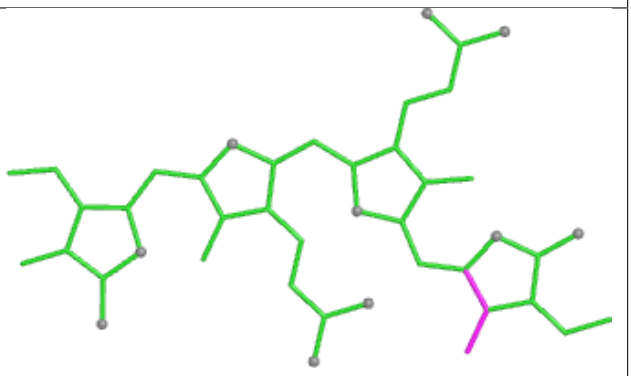


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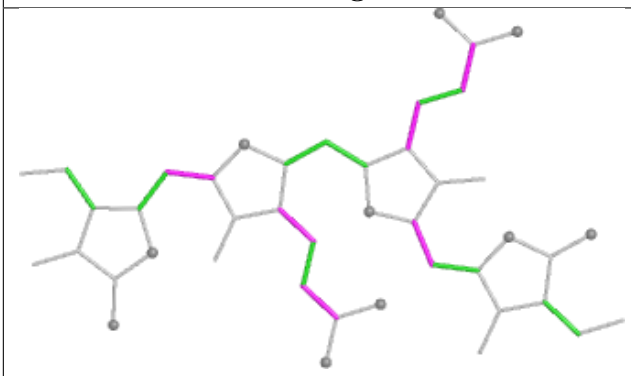
Ligand CYC i6 201



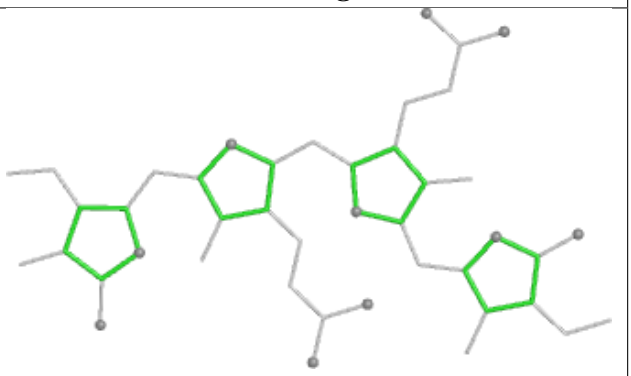
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Bond angles

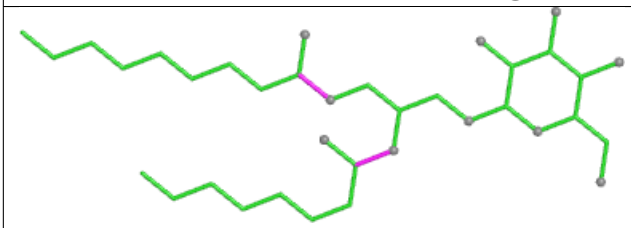


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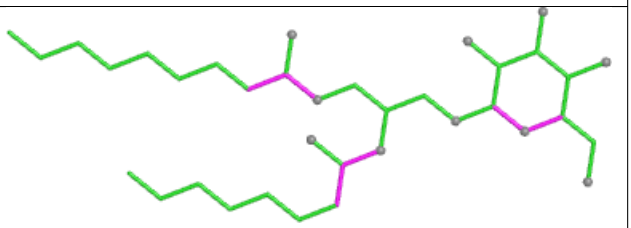


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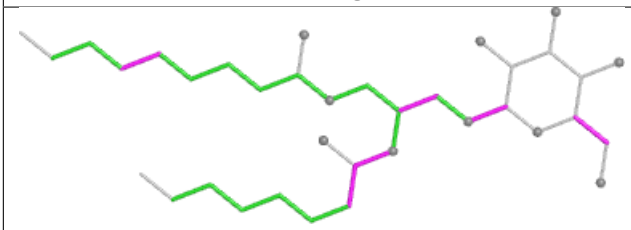
Ligand LMG M1 101



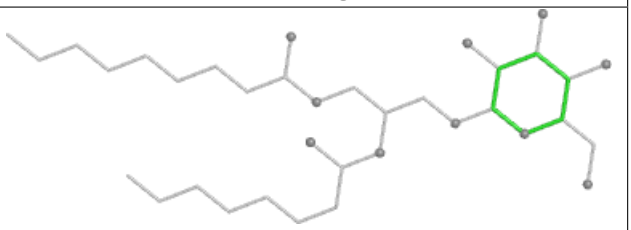
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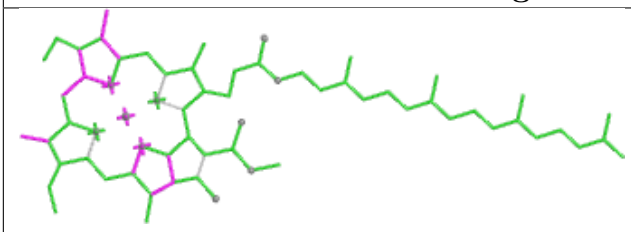


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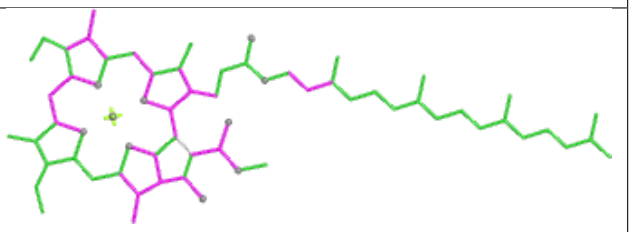


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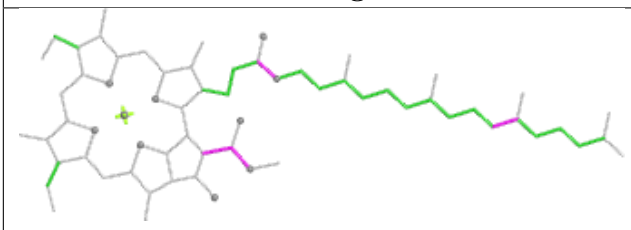
Ligand CLA CE 510



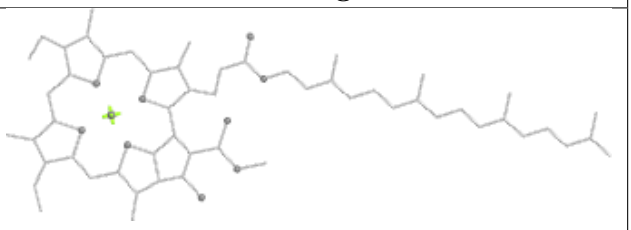
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Bond angles

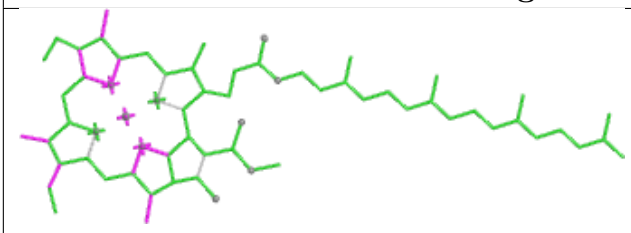


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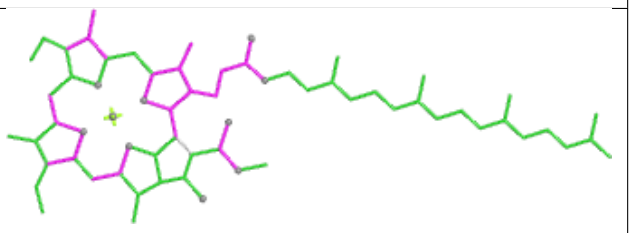


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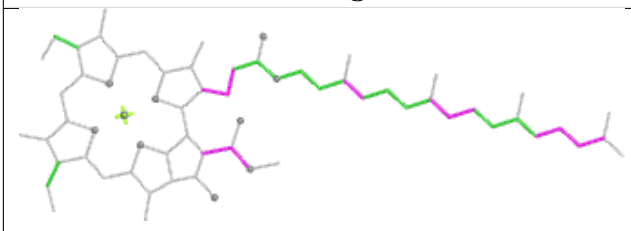
Ligand CLA cE 506



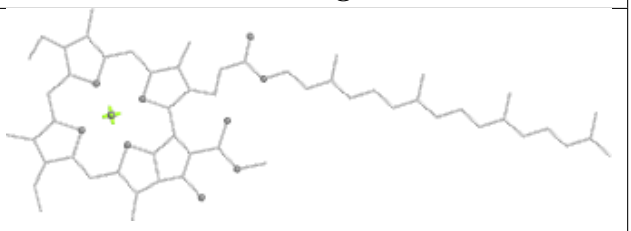
Bond lengths



Bond angles

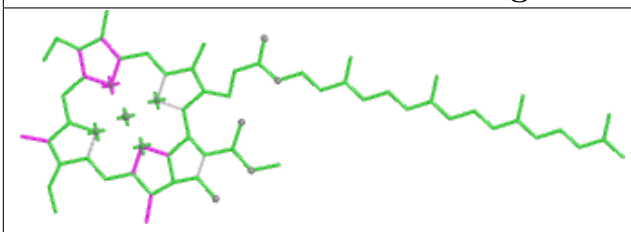


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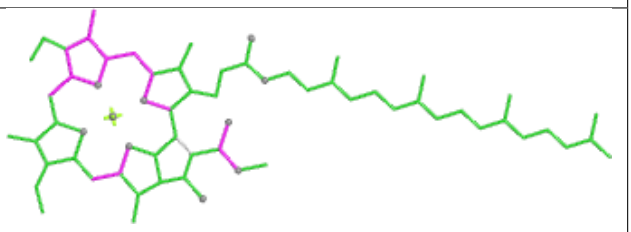


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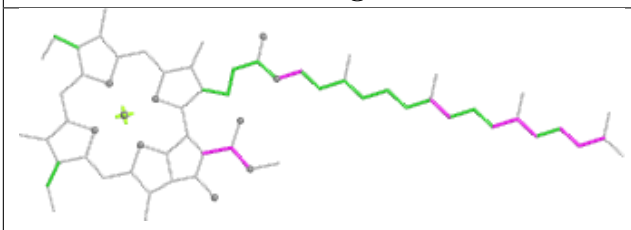
Ligand CLA BD 608



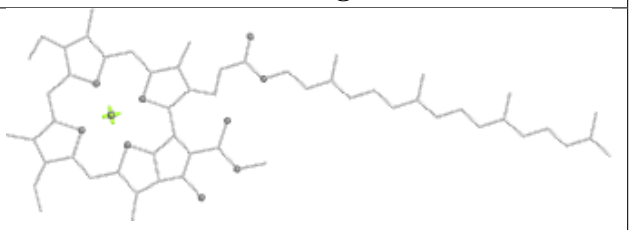
Bond lengths



Bond angles

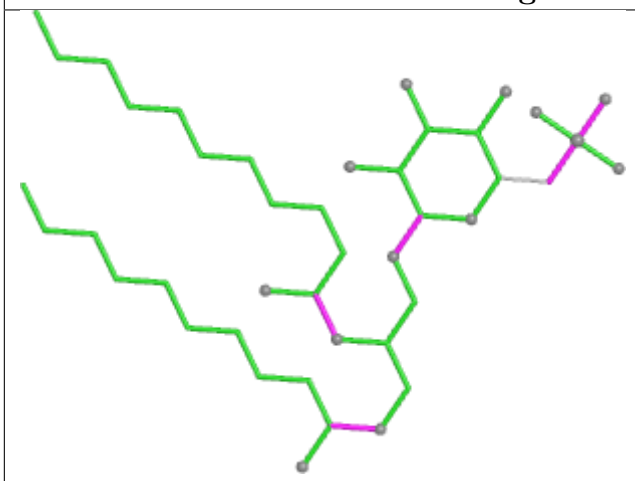


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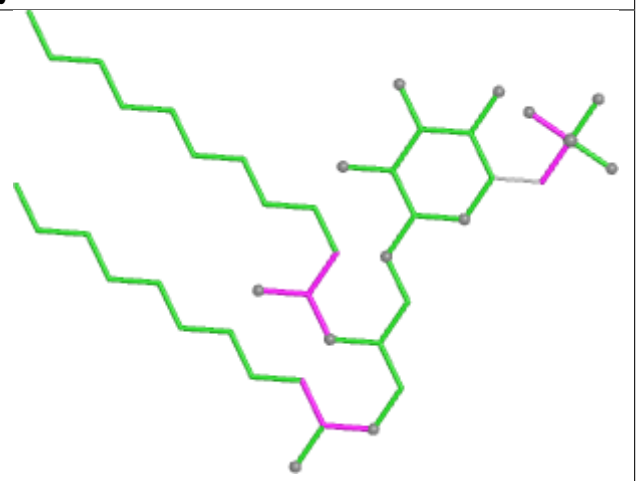


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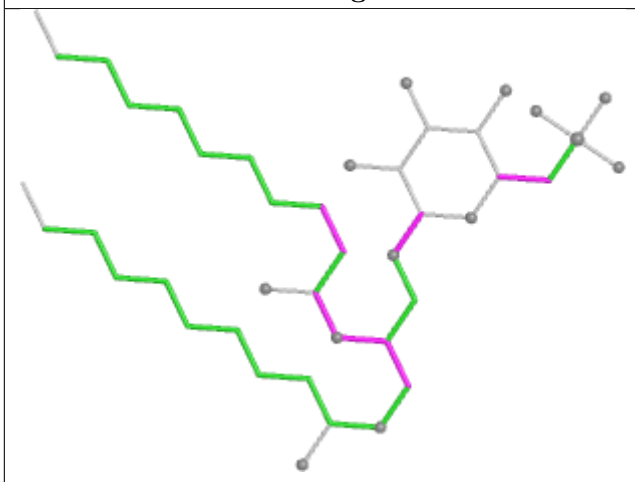
Ligand SQD L1 101



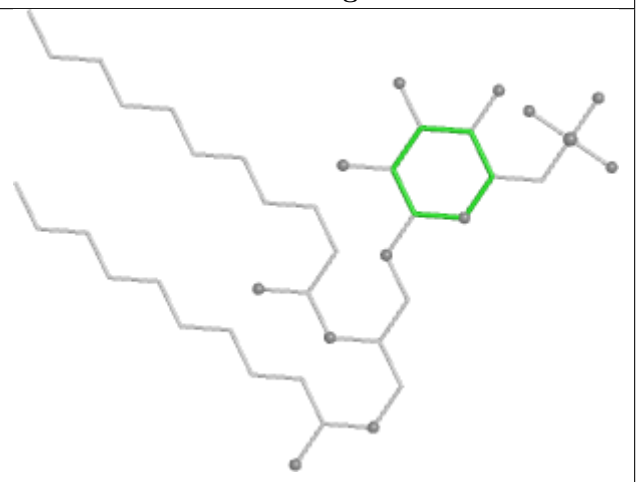
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Bond angles

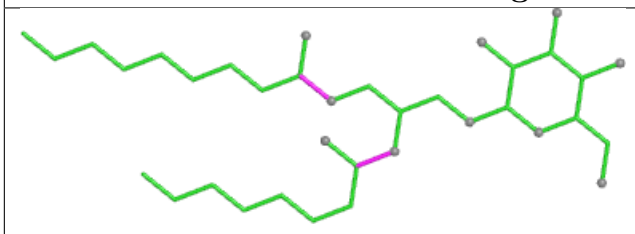


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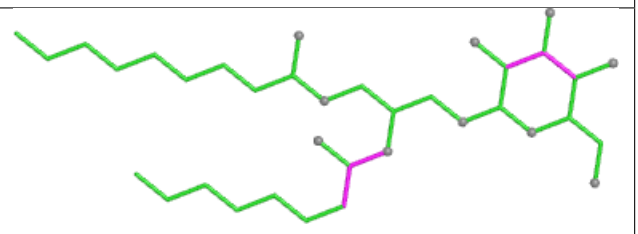


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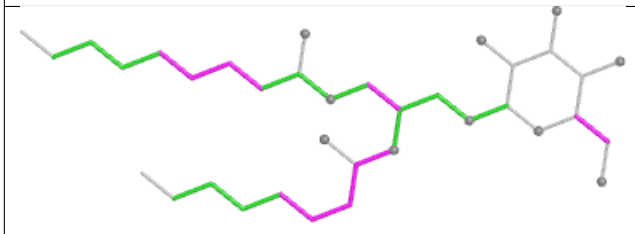
Ligand LMG aD 409



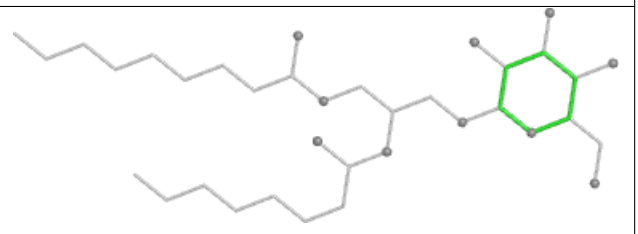
Bond lengths



Bond angles

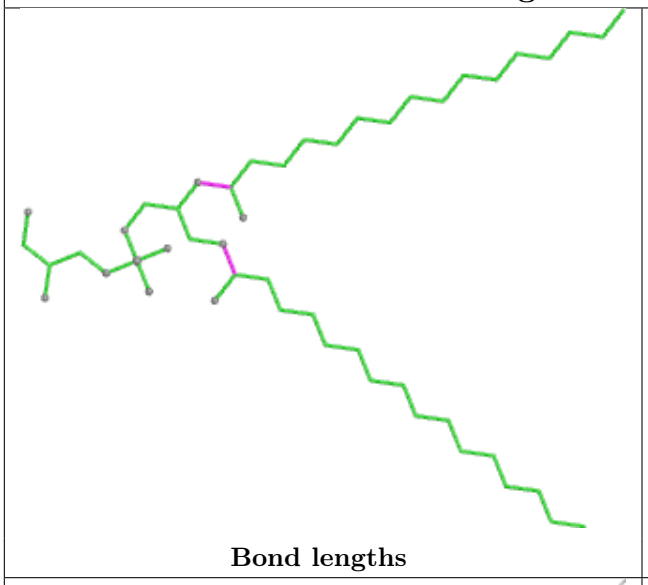


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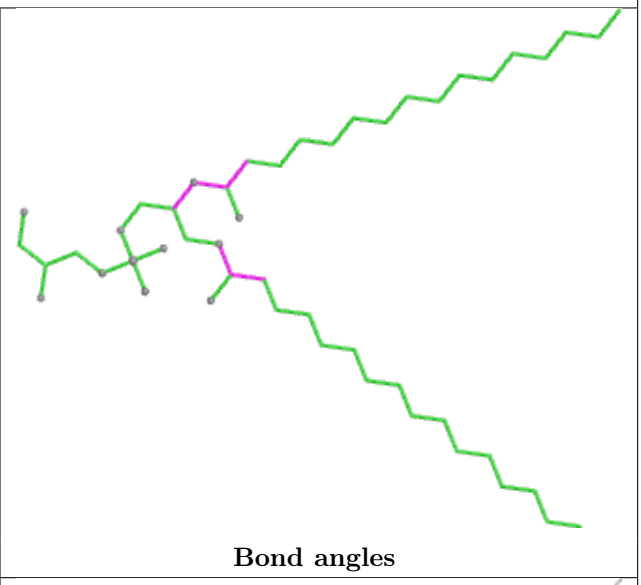


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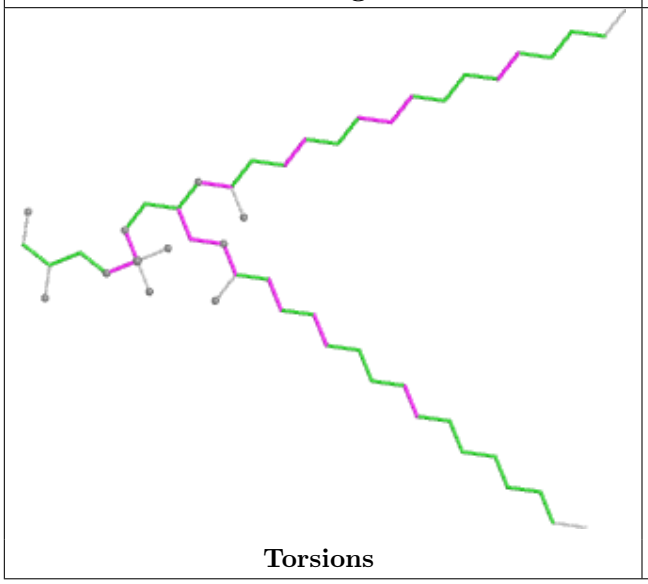
Ligand LHG lD 101



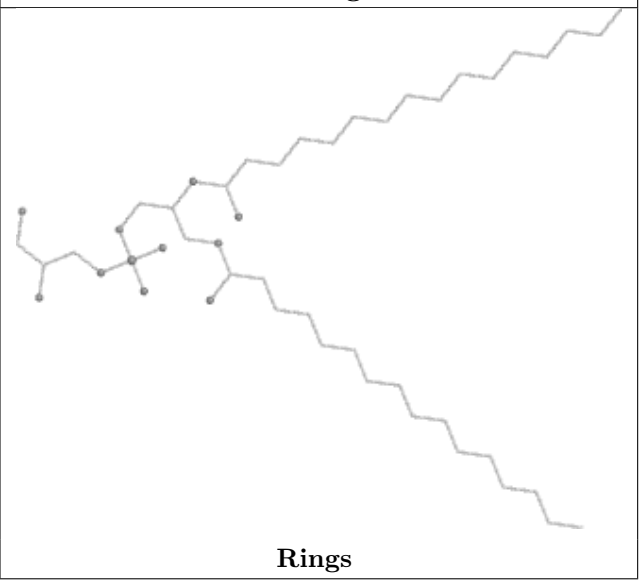
Bond lengths



Bond angles

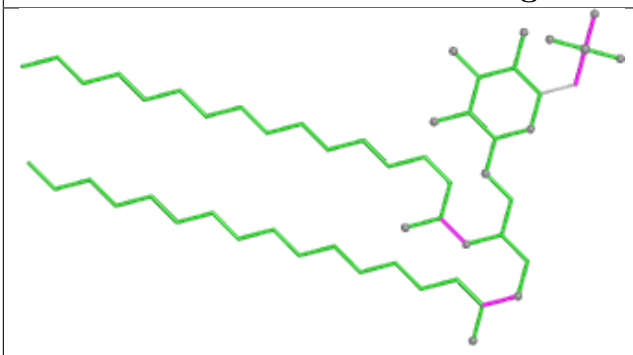


Torsions

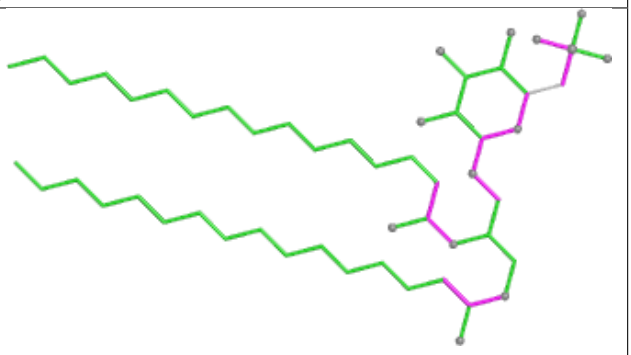


Rings

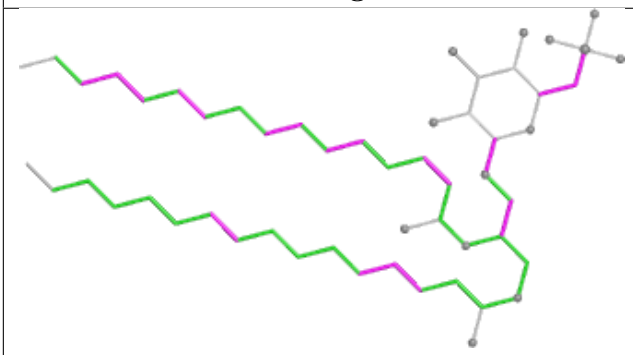
Ligand SQD c1 501



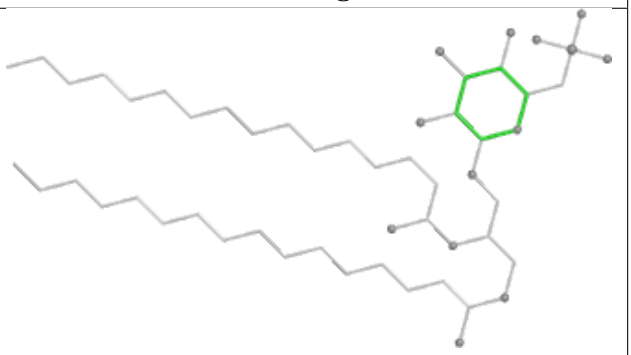
Bond lengths



Bond angles

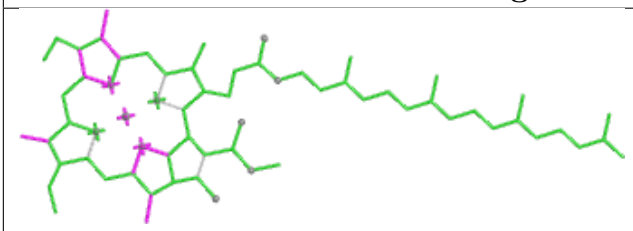


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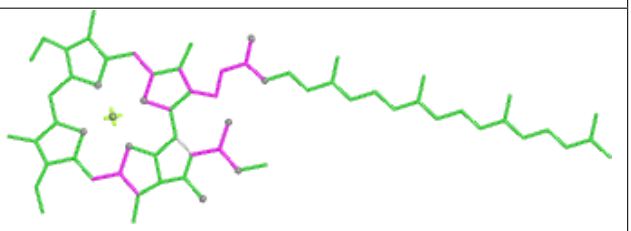


Rings

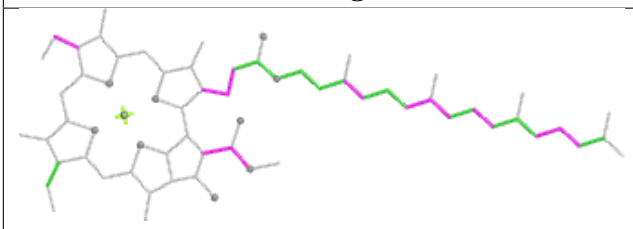
Ligand CLA CD 512



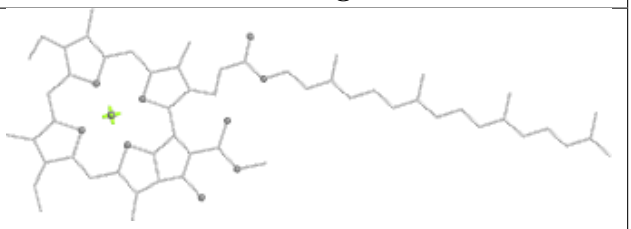
Bond lengths



Bond angles

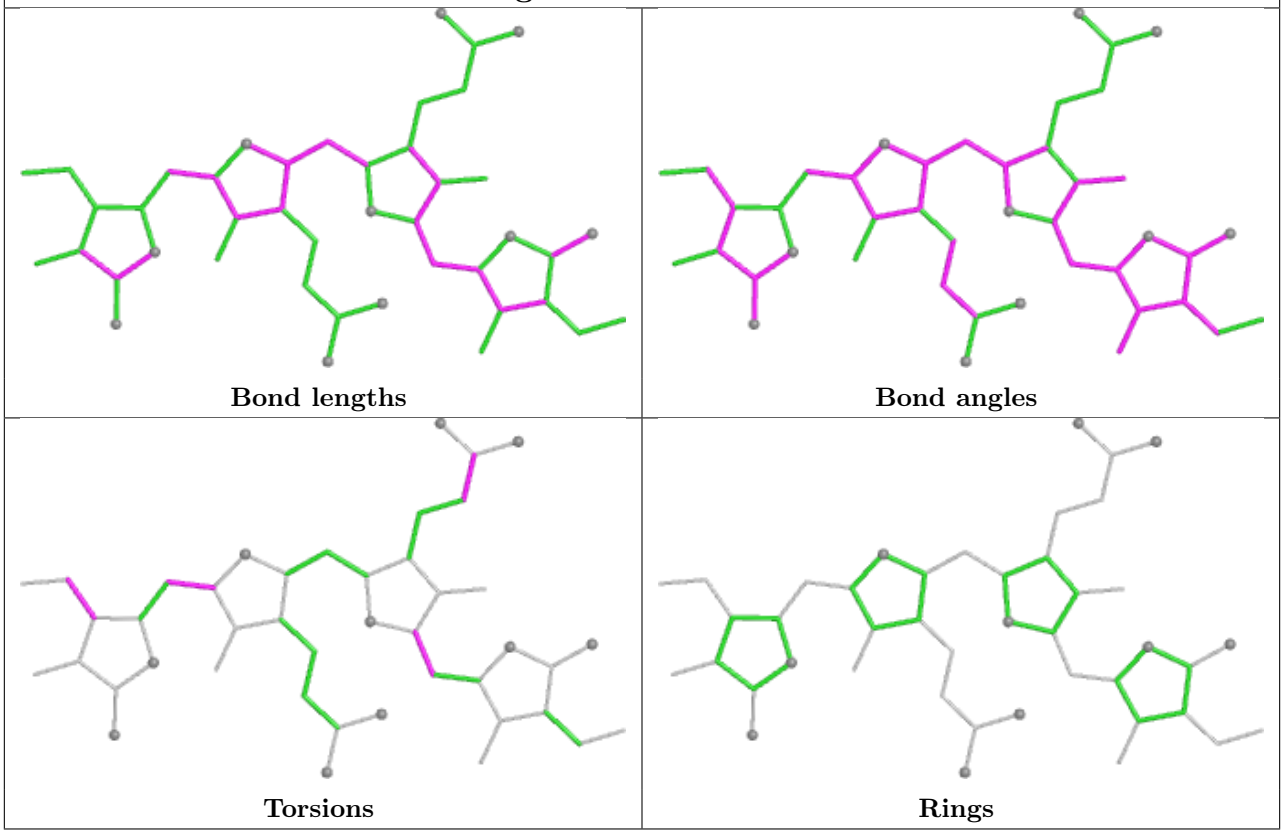


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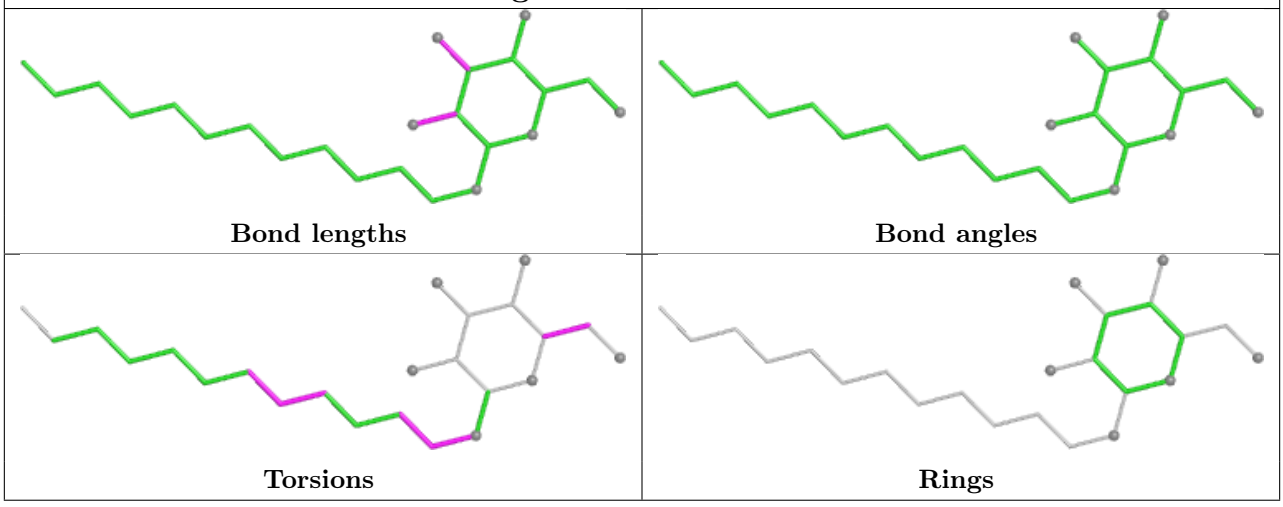


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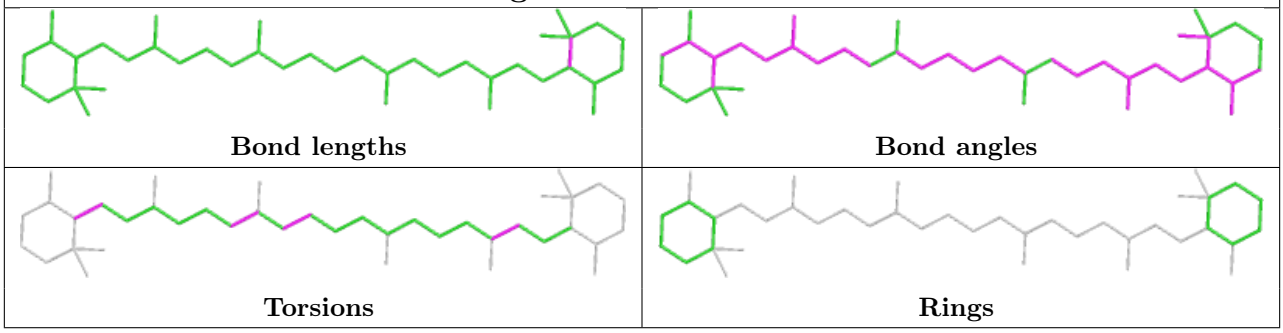
Ligand CYC JF 201



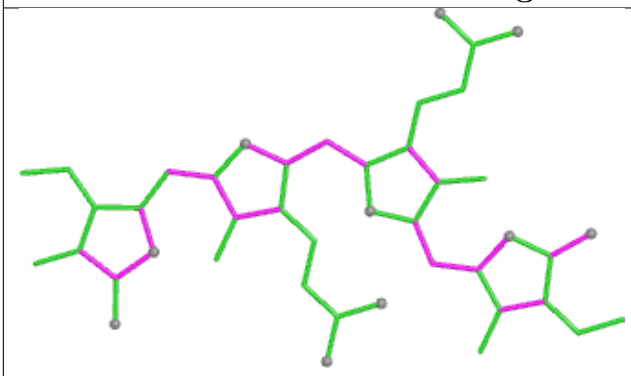
Ligand LMT bD 602



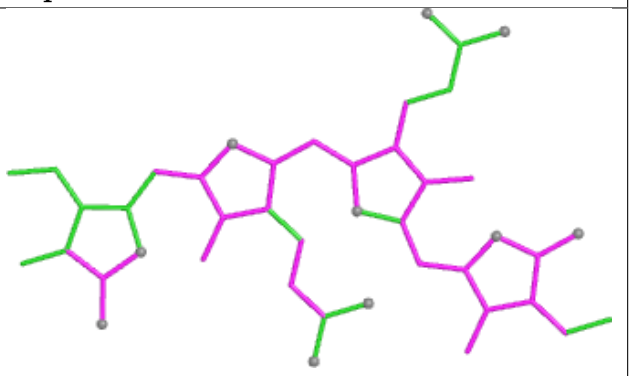
Ligand BCR BD 615



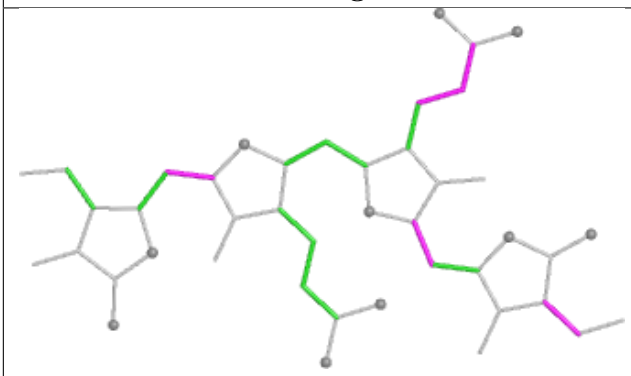
Ligand CYC p4 201



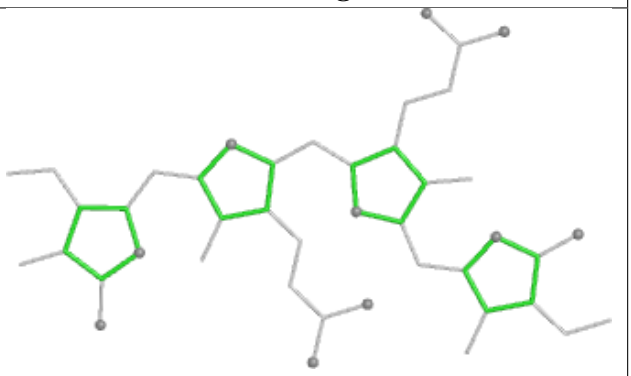
Bond lengths



Bond angles

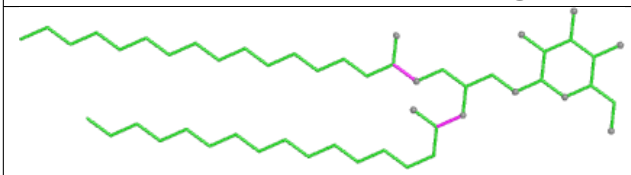


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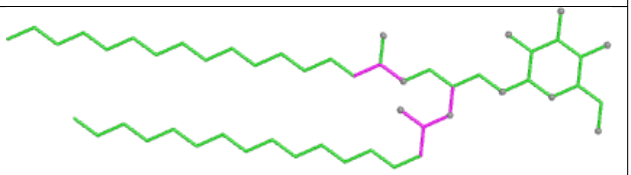


Rings

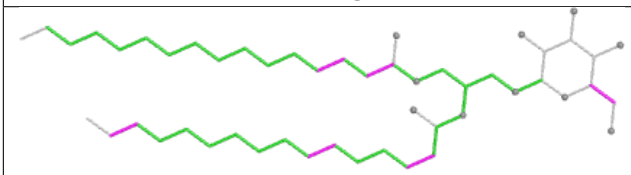
Ligand LMG B1 618



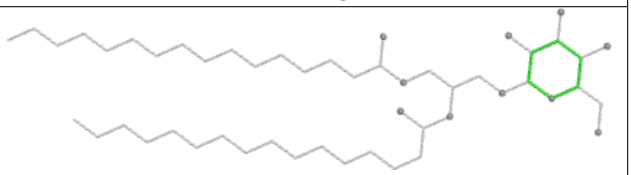
Bond lengths



Bond angles



Torsions



Rings

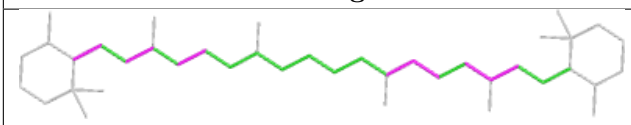
Ligand BCR z1 101



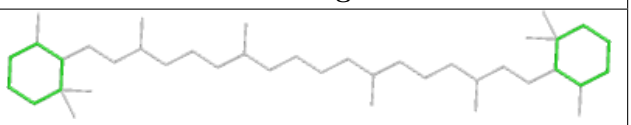
Bond lengths



Bond angles

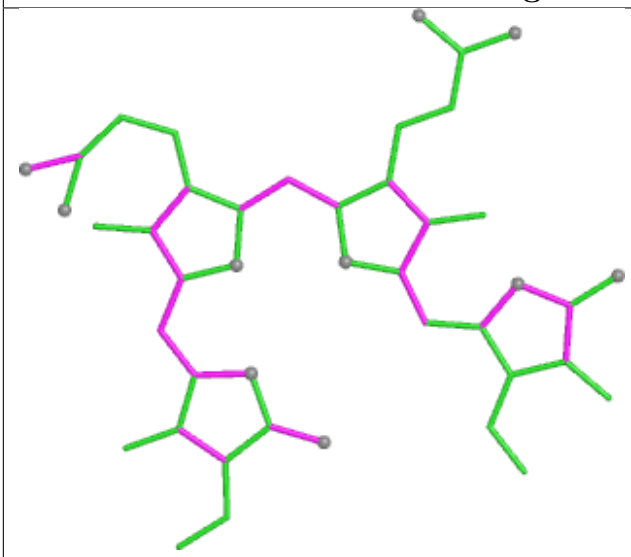


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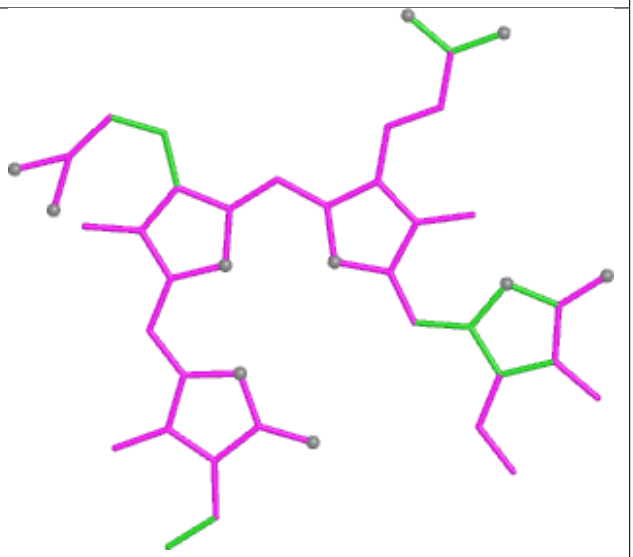


Rings

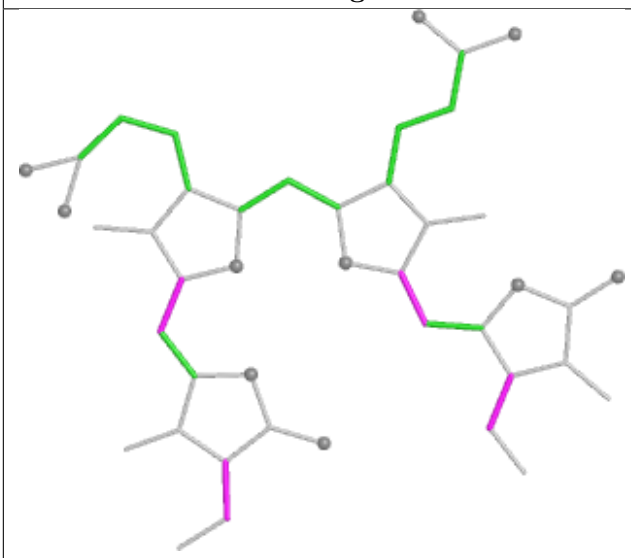
Ligand CYC iI 202



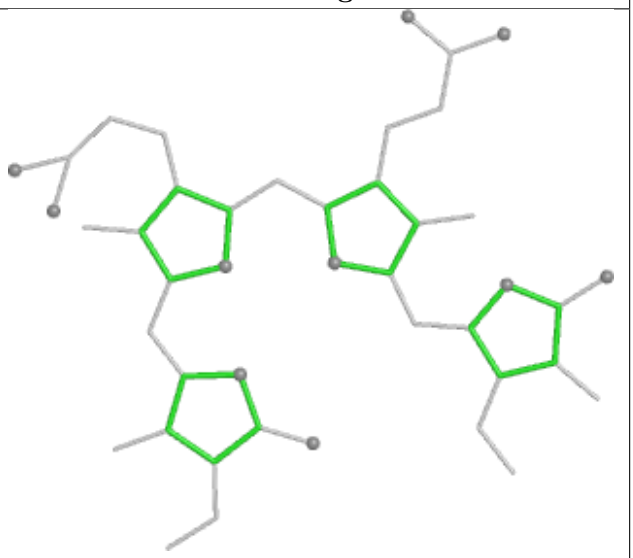
Bond lengths



Bond angles

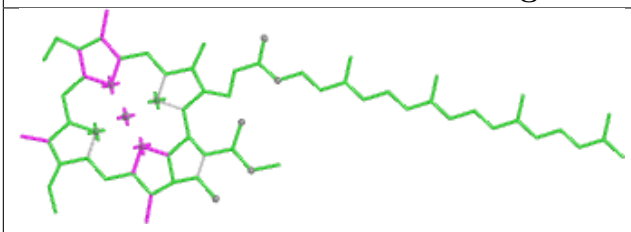


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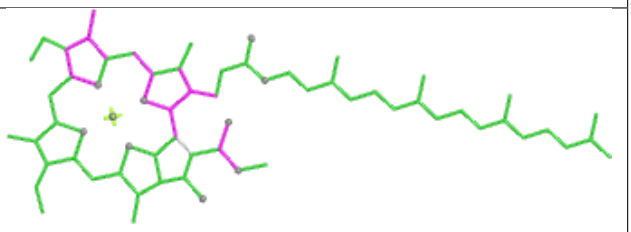


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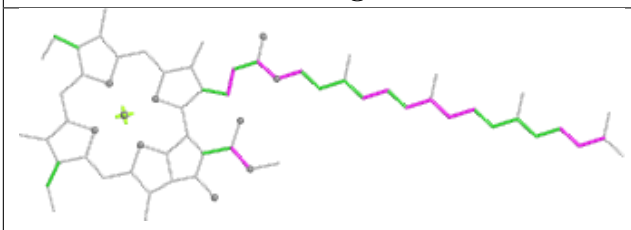
Ligand CLA c1 514



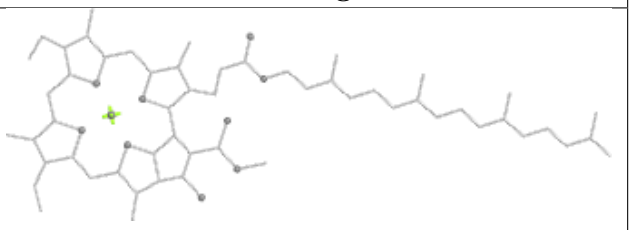
Bond lengths



Bond angles

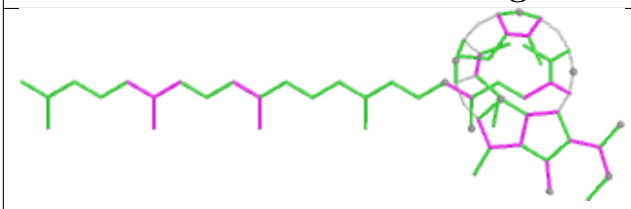


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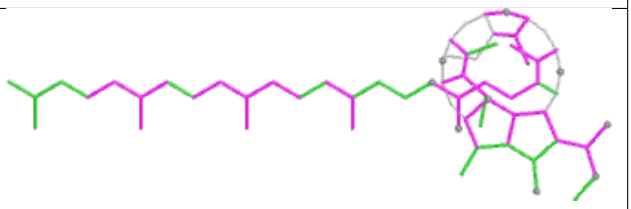


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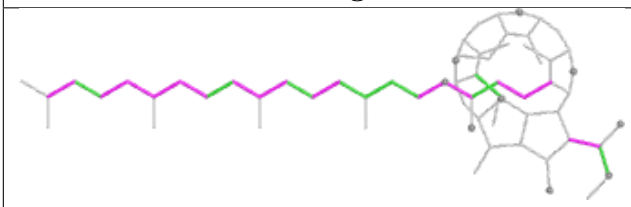
Ligand PHO DE 401



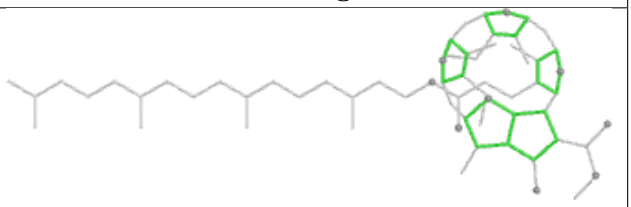
Bond lengths



Bond angles

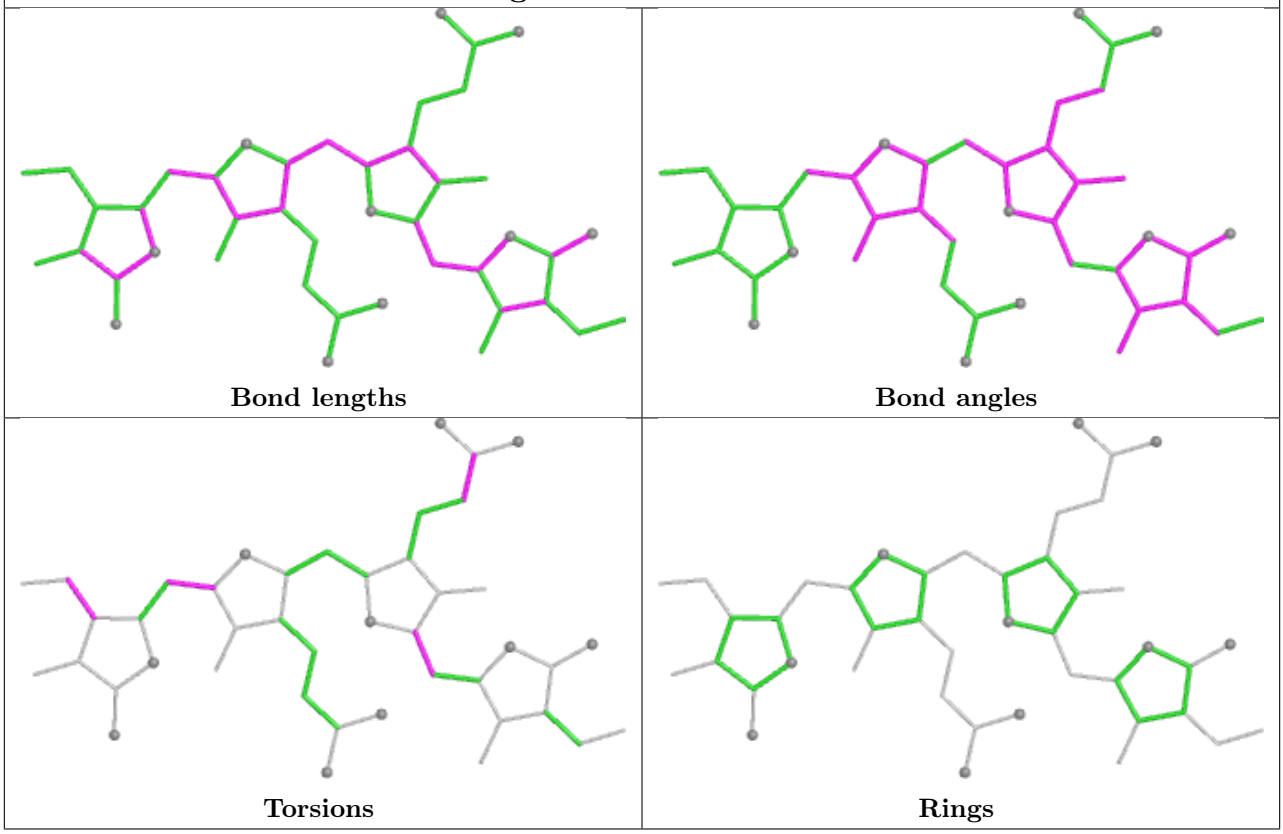


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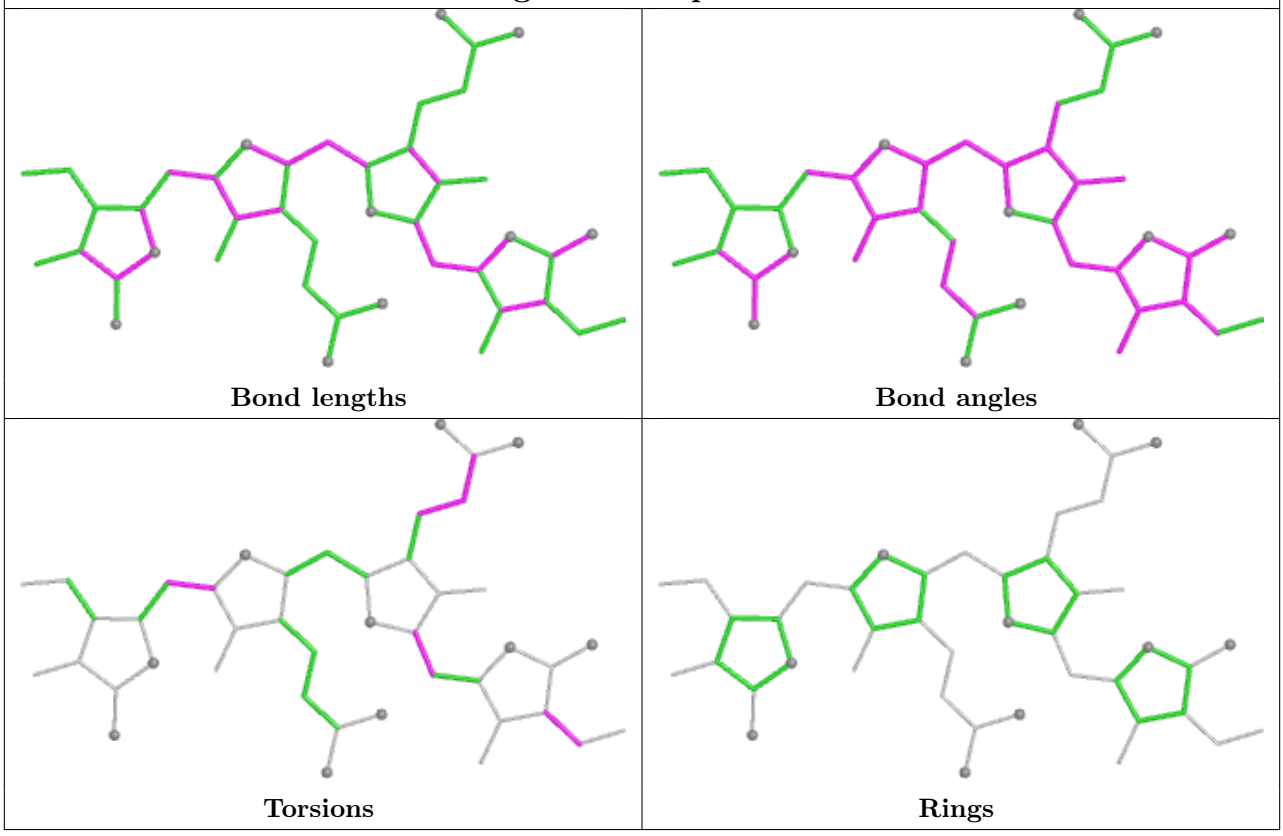


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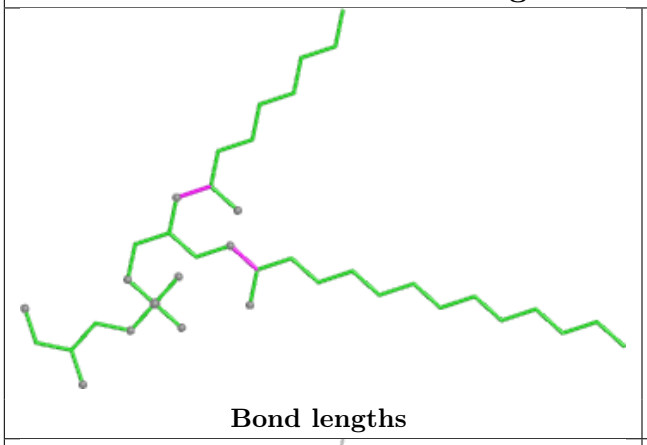
Ligand CYC XB 201



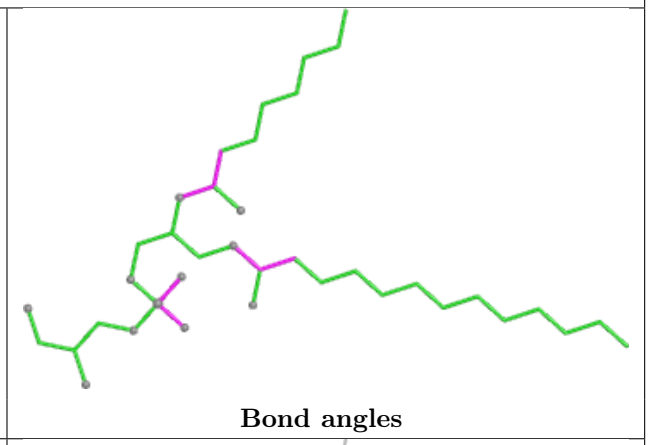
Ligand CYC pB 201



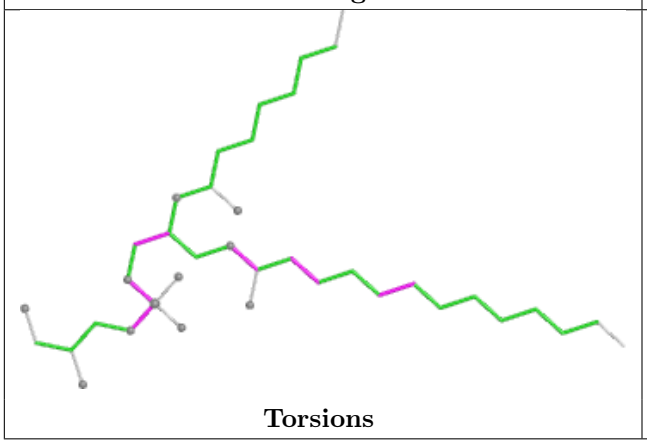
Ligand LHG AD 411



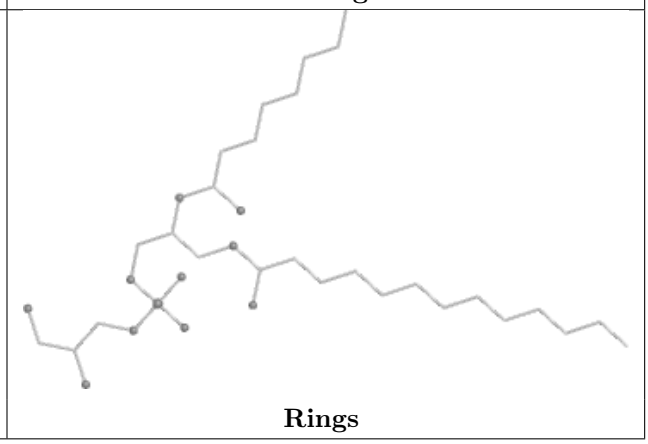
Bond lengths



Bond angles

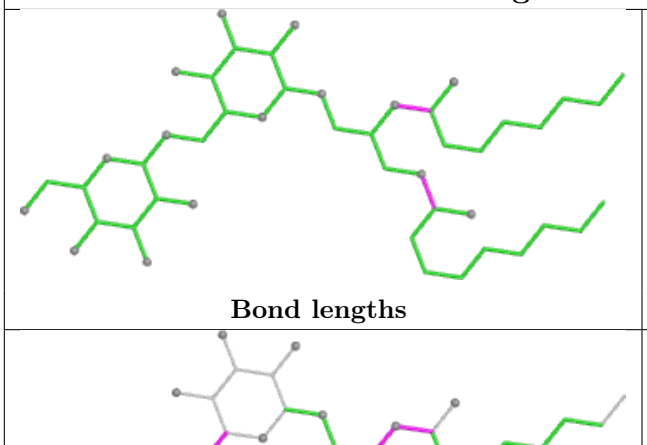


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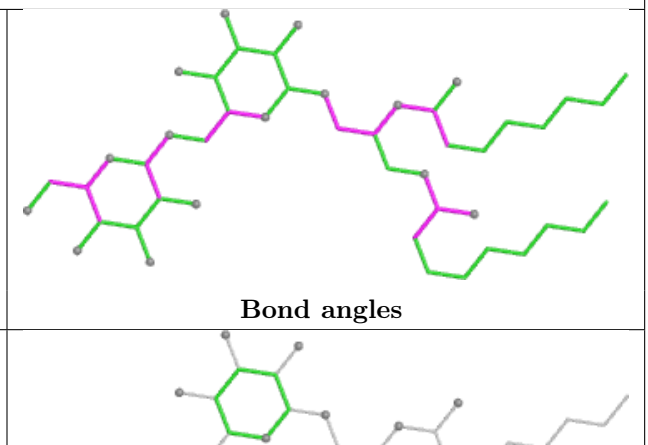


Rings

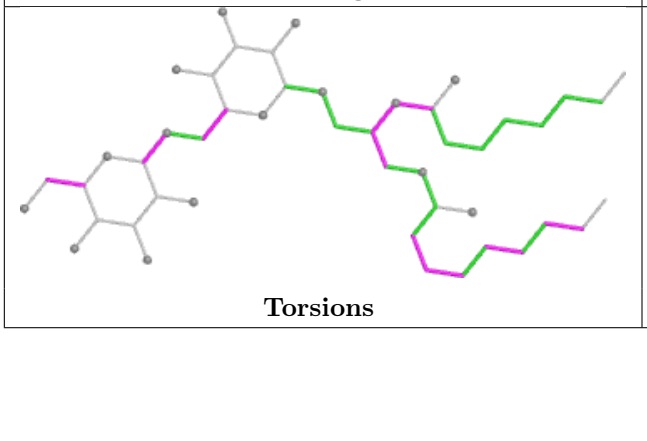
Ligand DGD cD 516



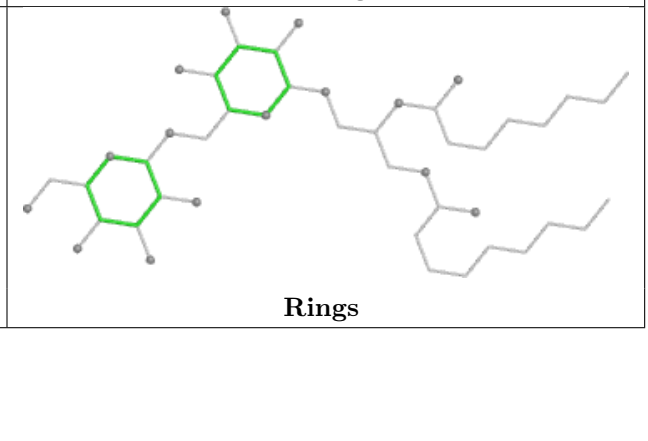
Bond lengths



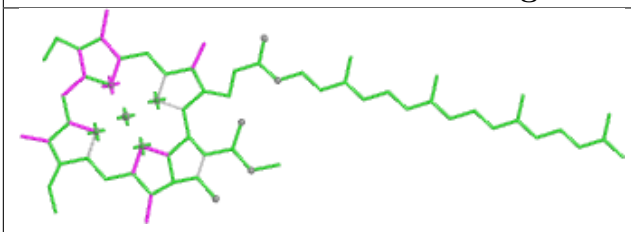
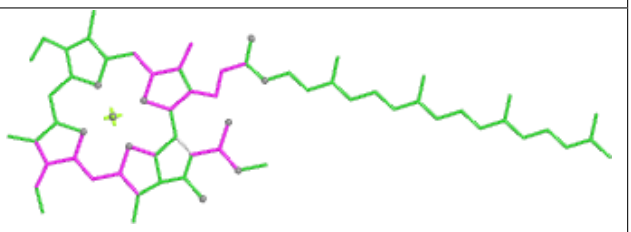
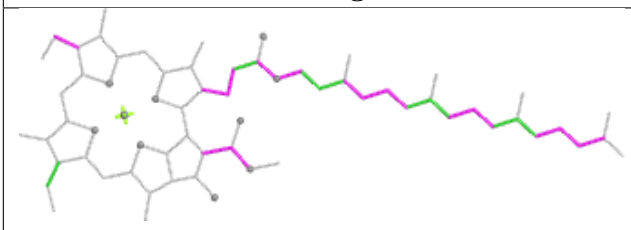
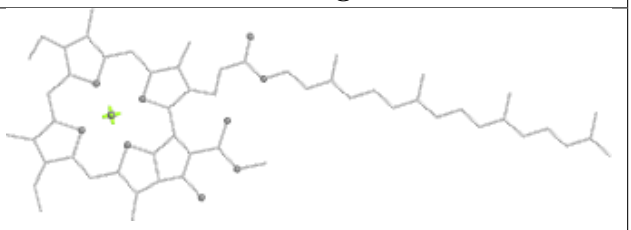
Bond angles

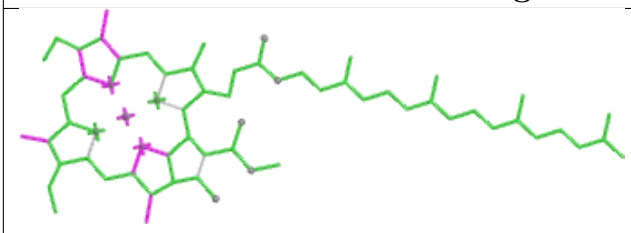
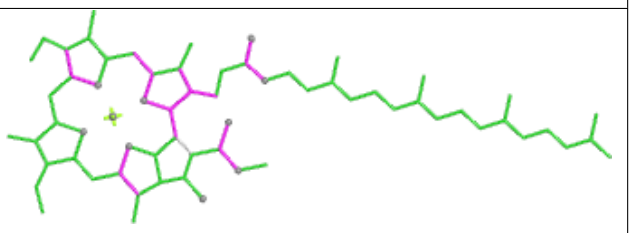
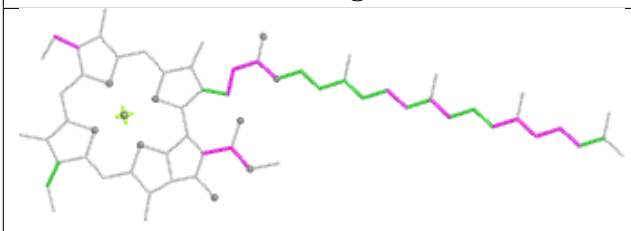
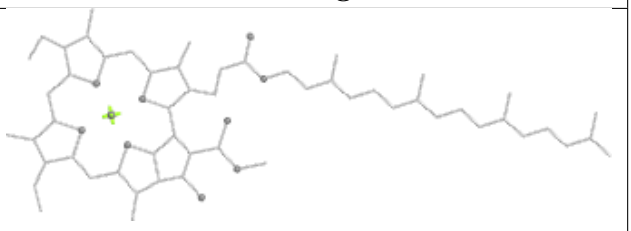


Torsions

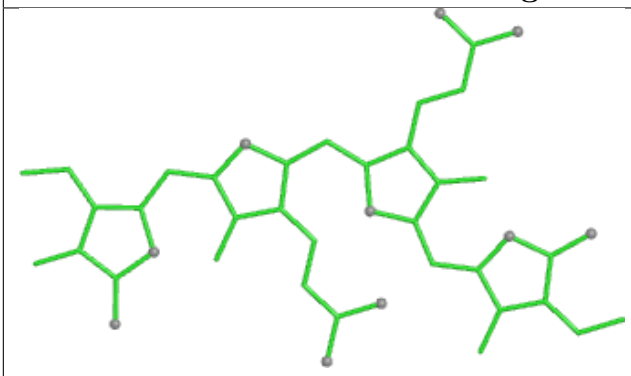


Rings

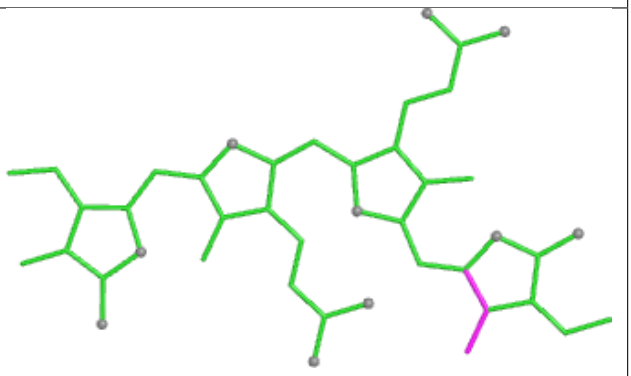
Ligand CLA c1 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bD 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

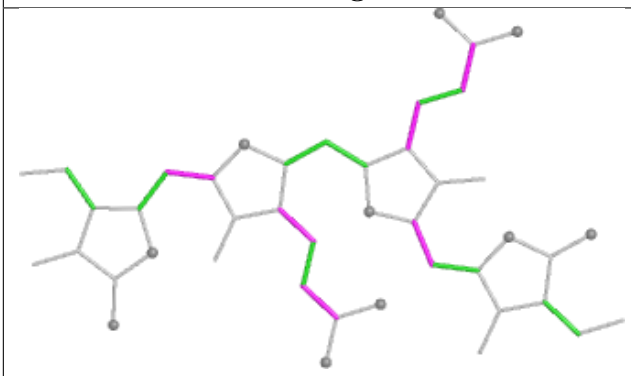
Ligand CYC i5 201



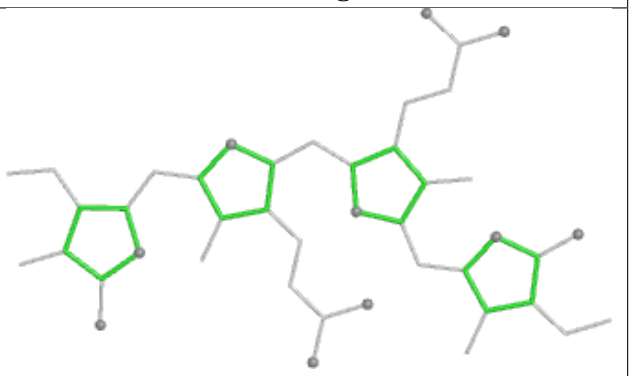
Bond lengths



Bond angles

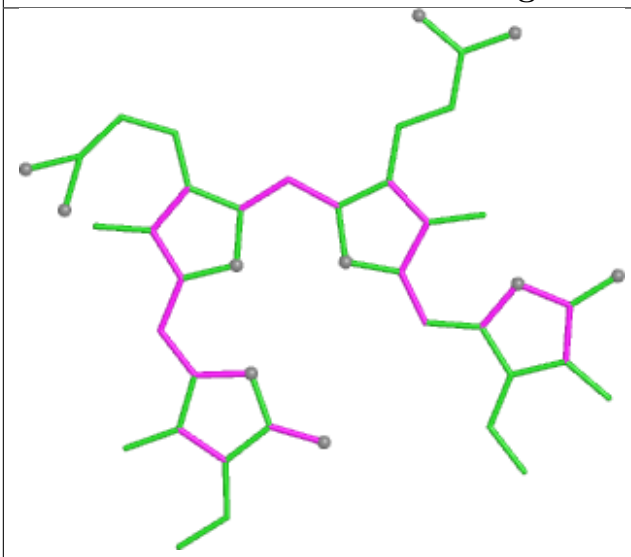


Torsions

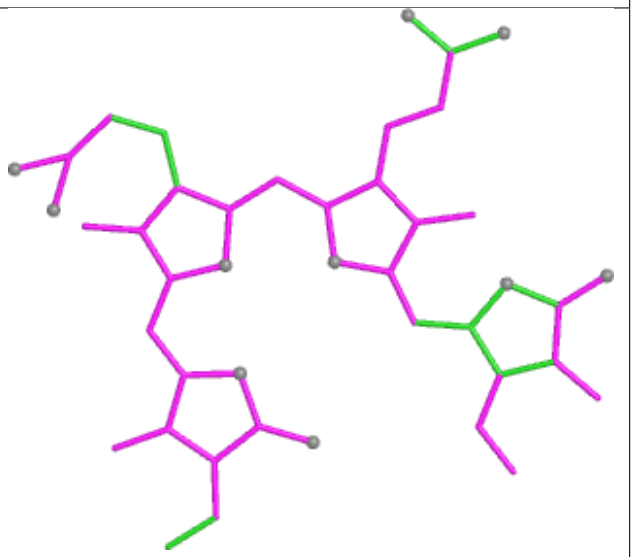


Rings

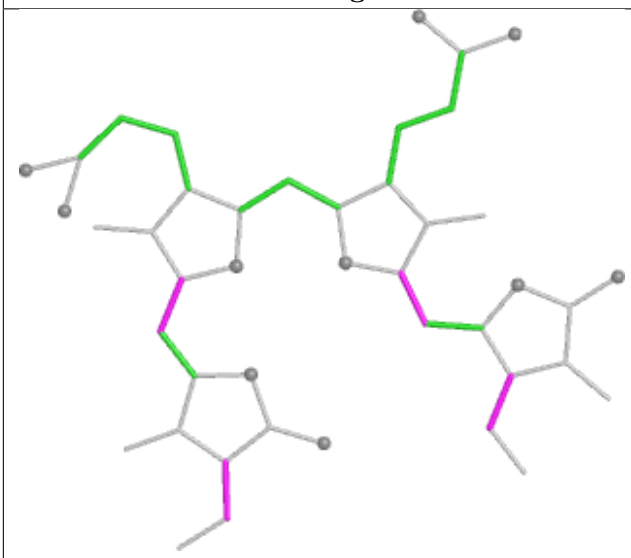
Ligand CYC c7 201



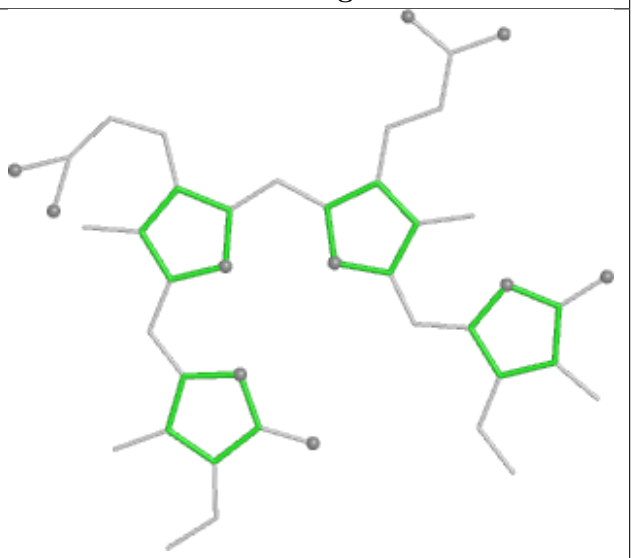
Bond lengths



Bond angles

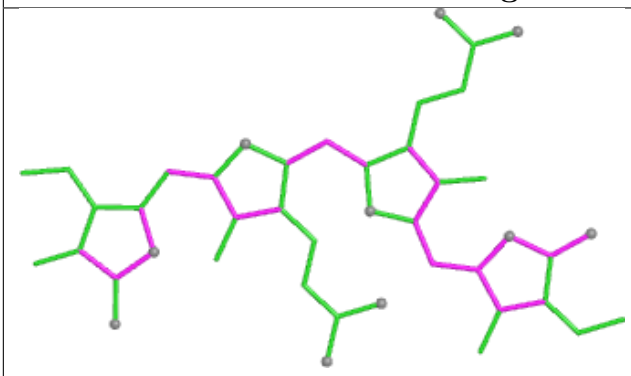


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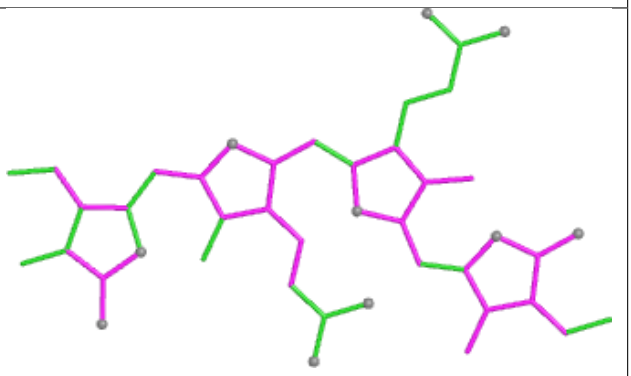


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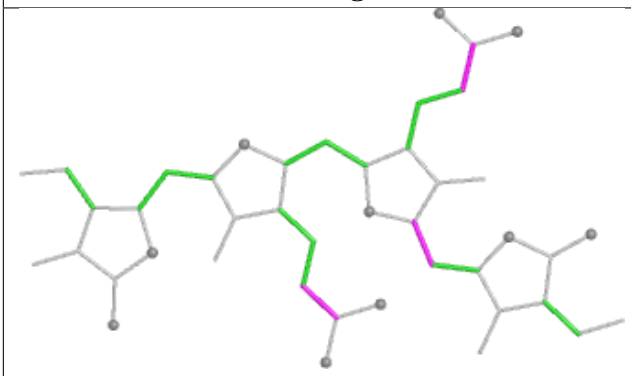
Ligand CYC BB 1002



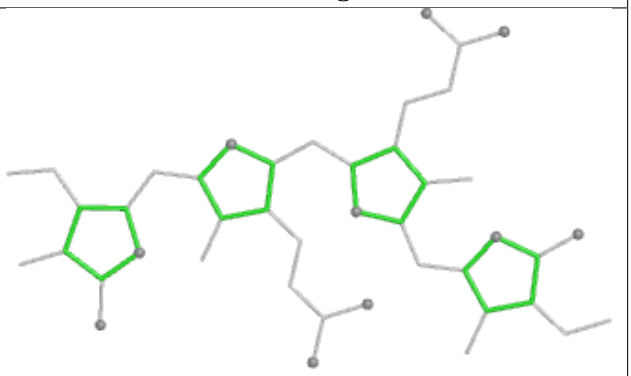
Bond lengths



Bond angles

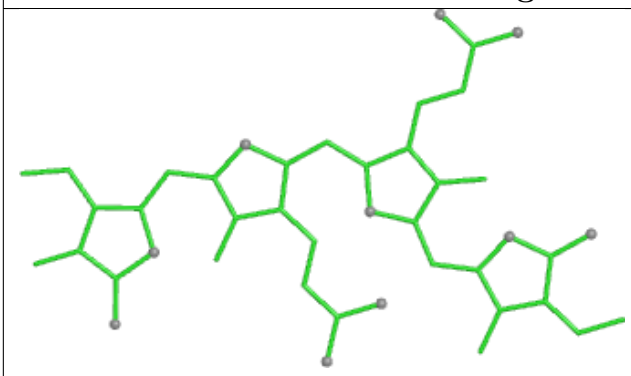


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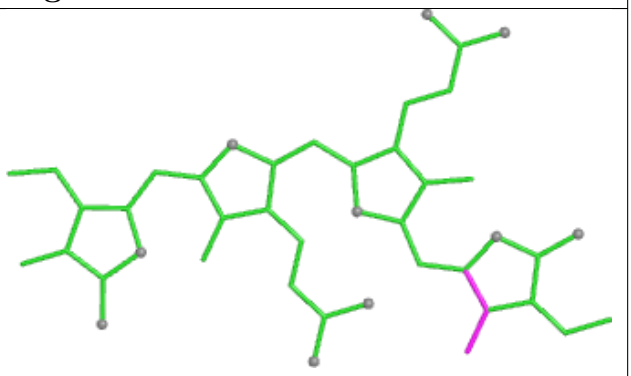


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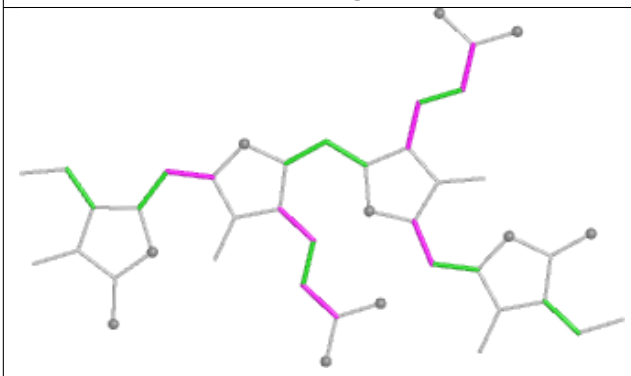
Ligand CYC g3 201



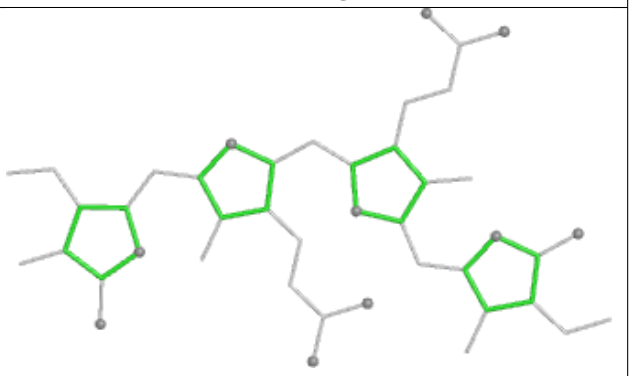
Bond lengths



Bond angles

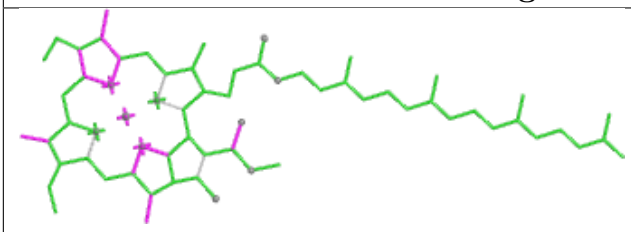


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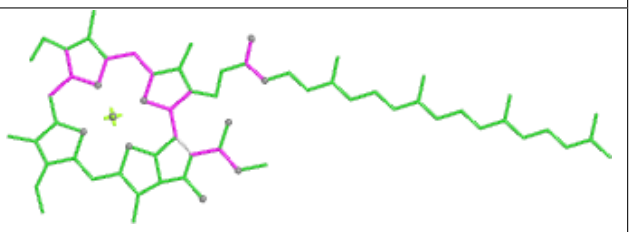


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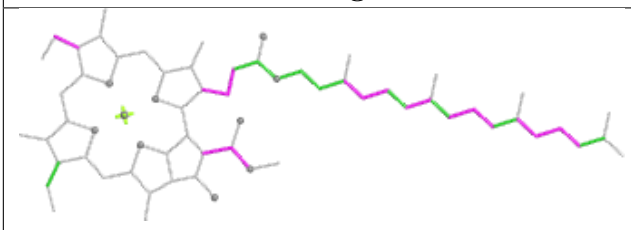
Ligand CLA b1 605



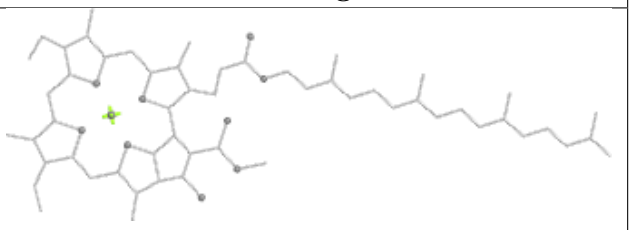
Bond lengths



Bond angles

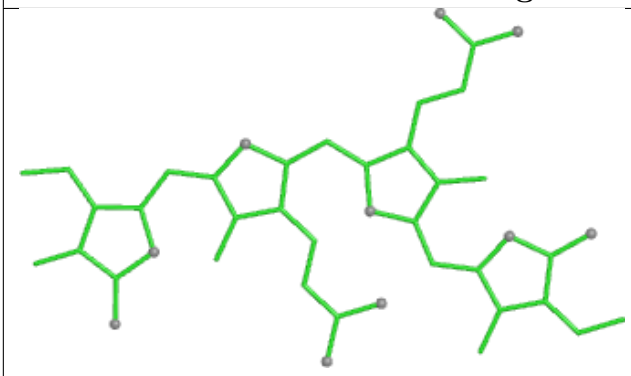


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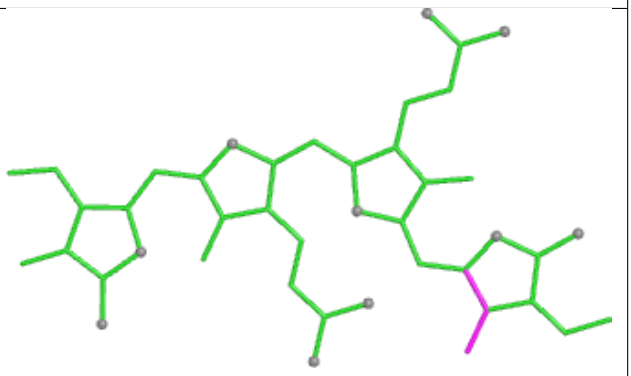


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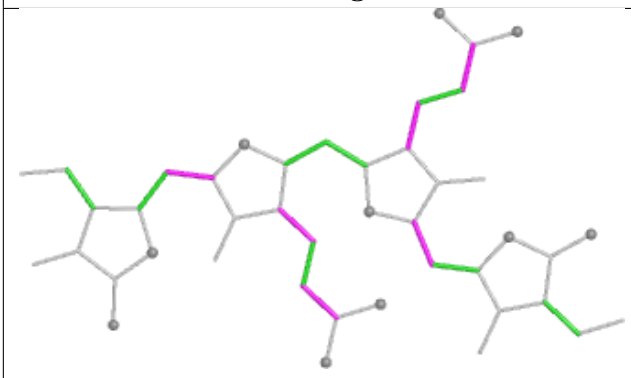
Ligand CYC iH 201



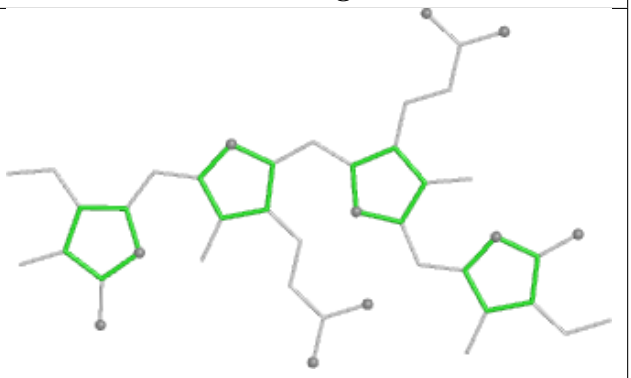
Bond lengths



Bond angles

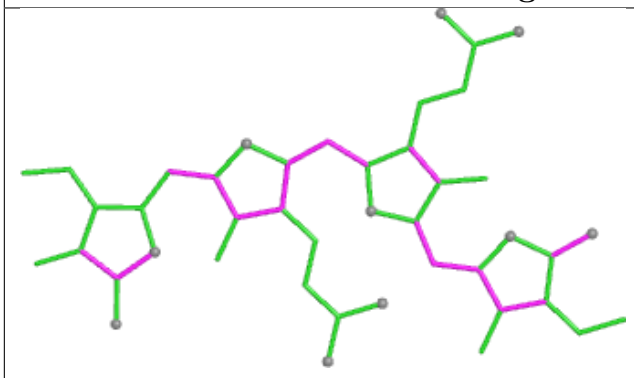


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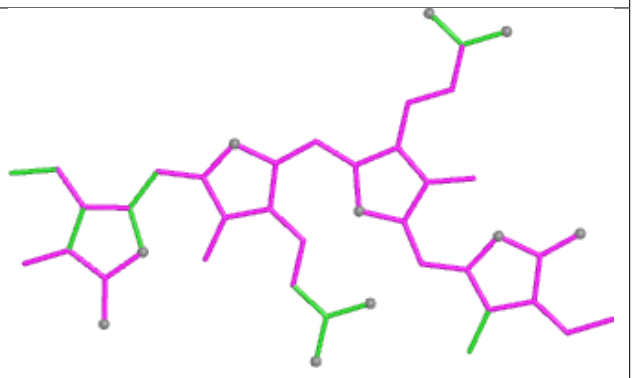


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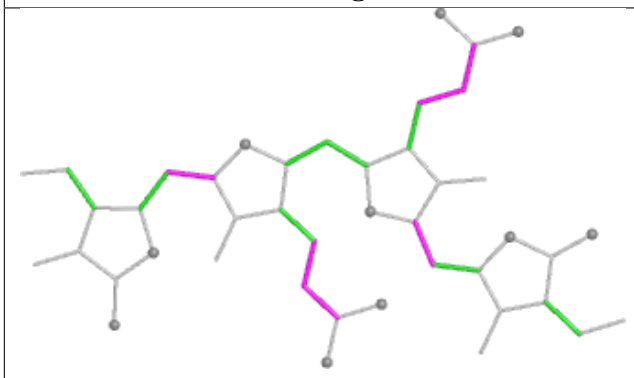
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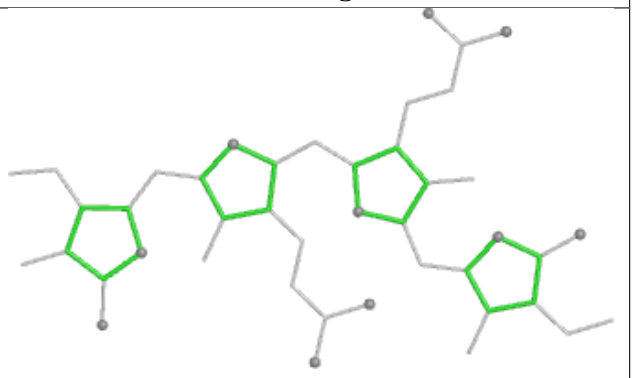
Bond lengths



Bond angles

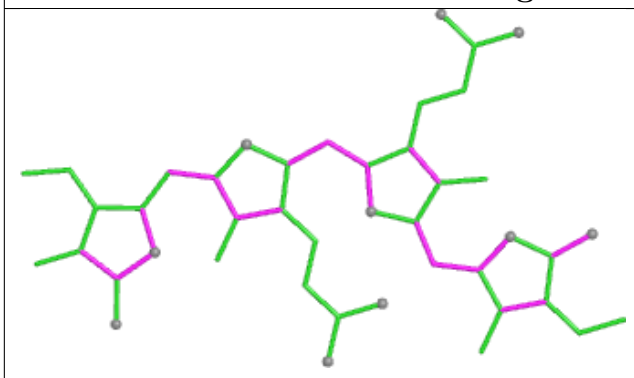


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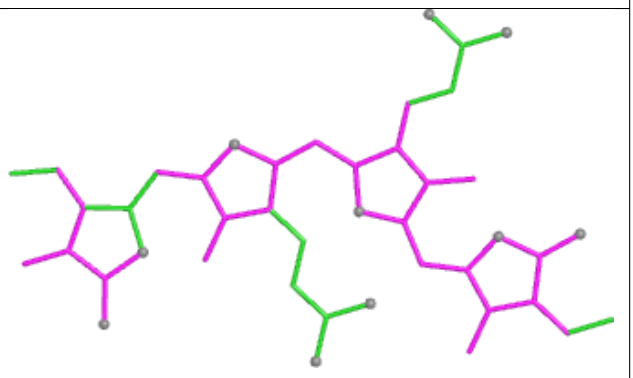


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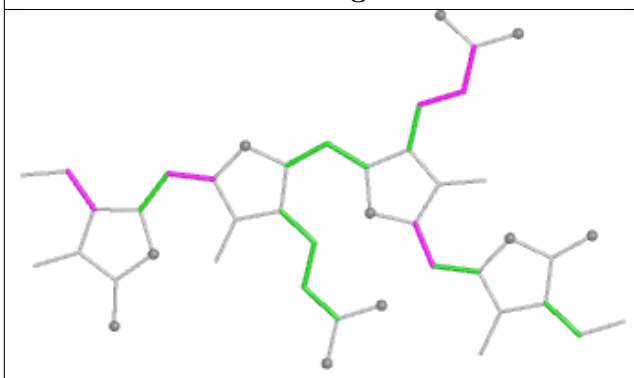
Ligand CYC sB 201



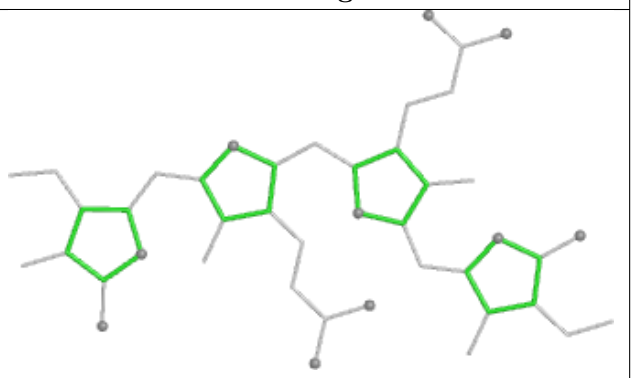
Bond lengths



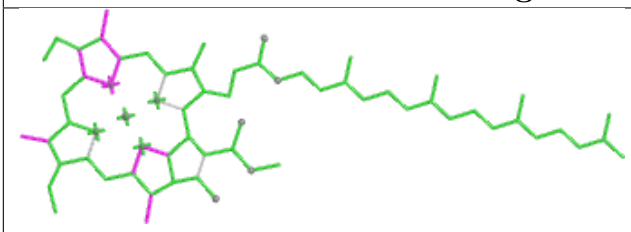
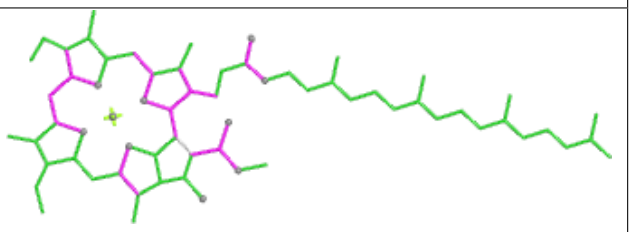
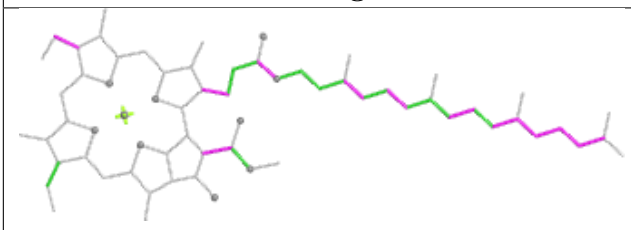
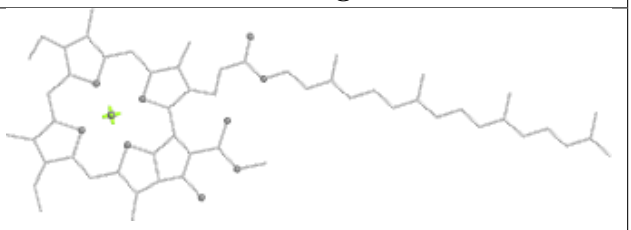
Bond angles

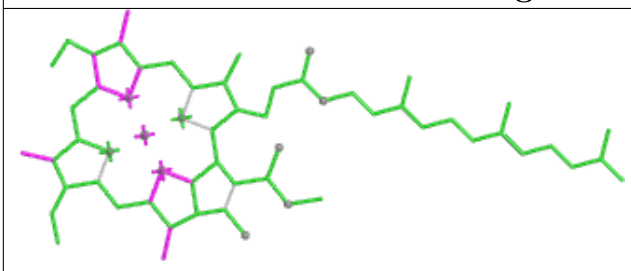
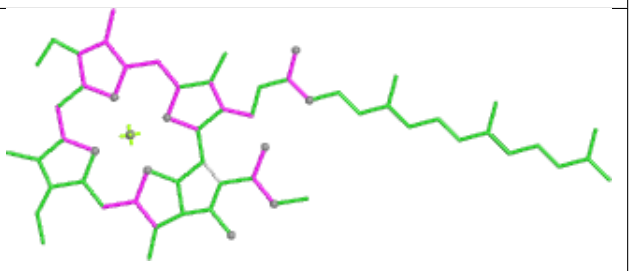
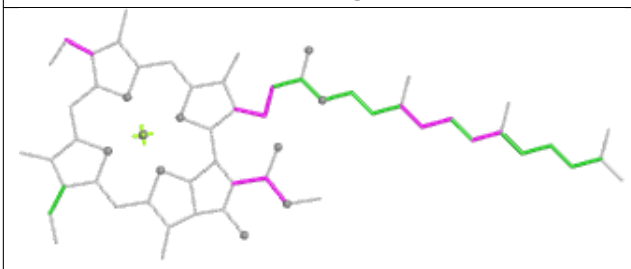
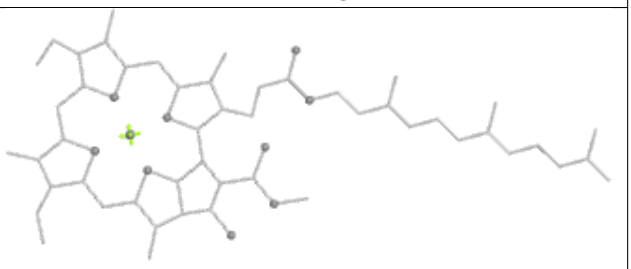


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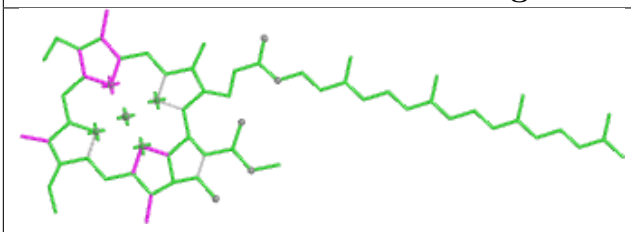


Rings

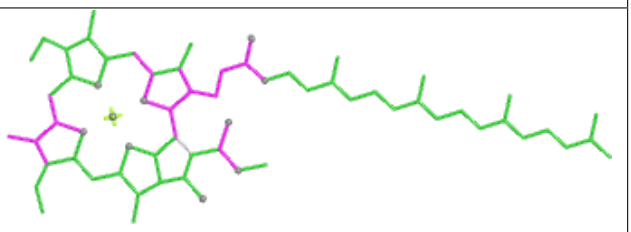
Ligand CLA B1 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B1 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

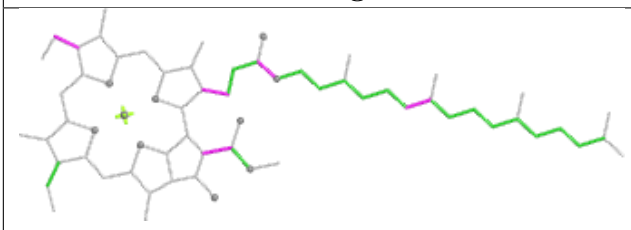
Ligand CLA CD 504



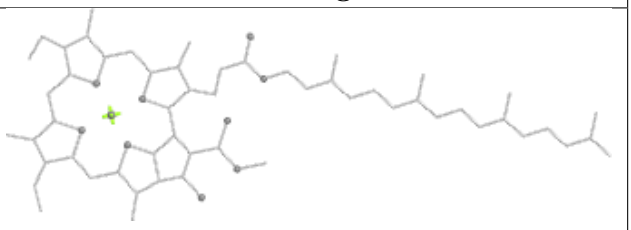
Bond lengths



Bond angles

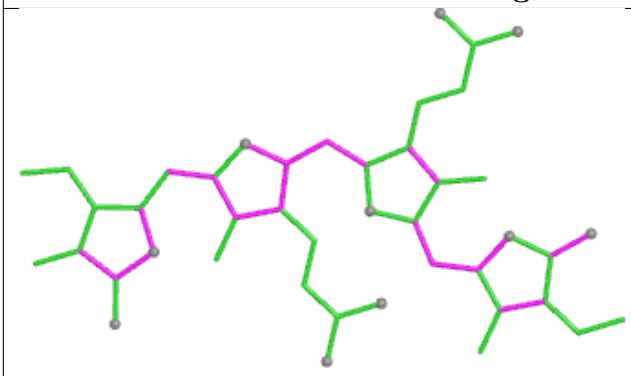


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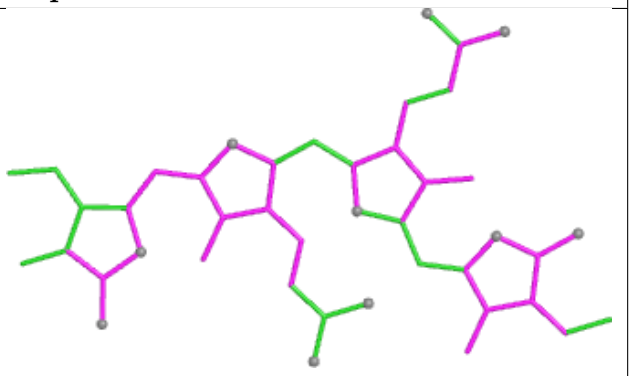


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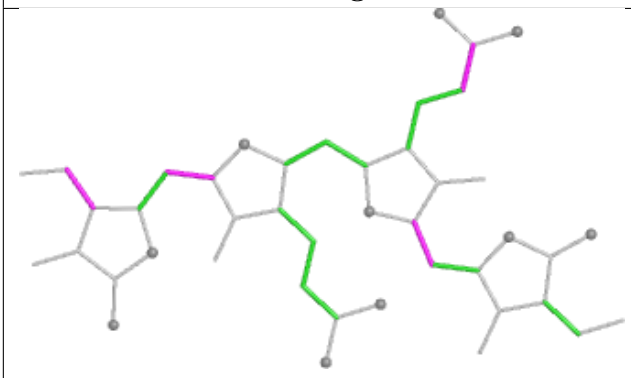
Ligand CYC qB 201



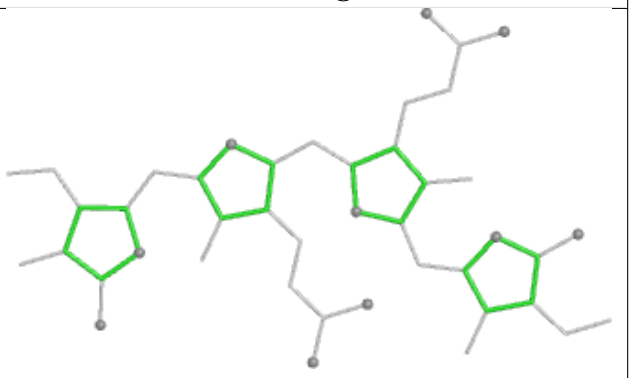
Bond lengths



Bond angles

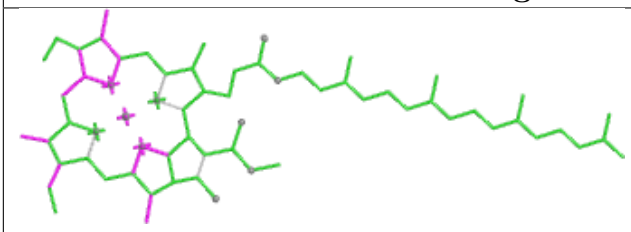


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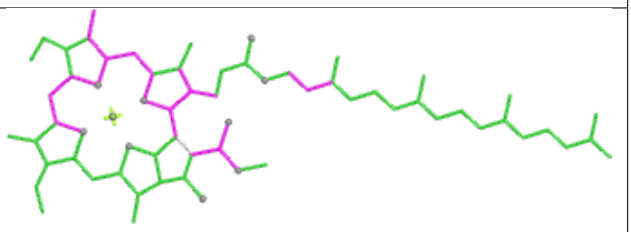


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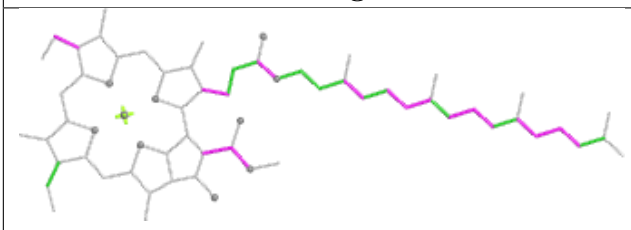
Ligand CLA bD 611



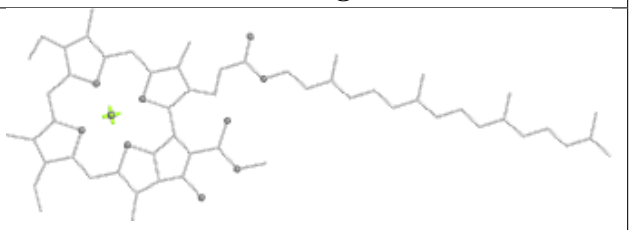
Bond lengths



Bond angles

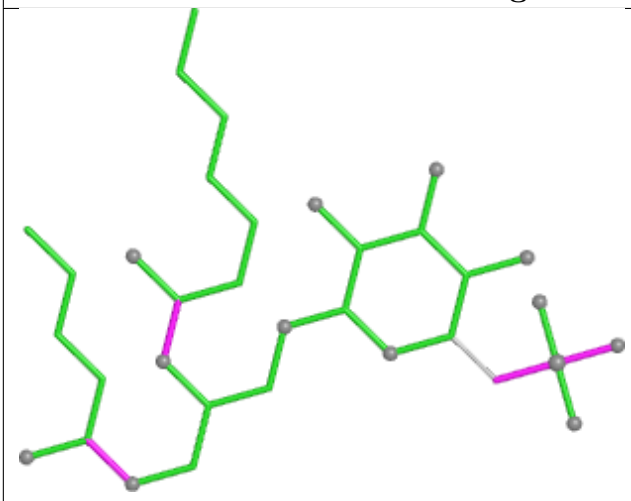


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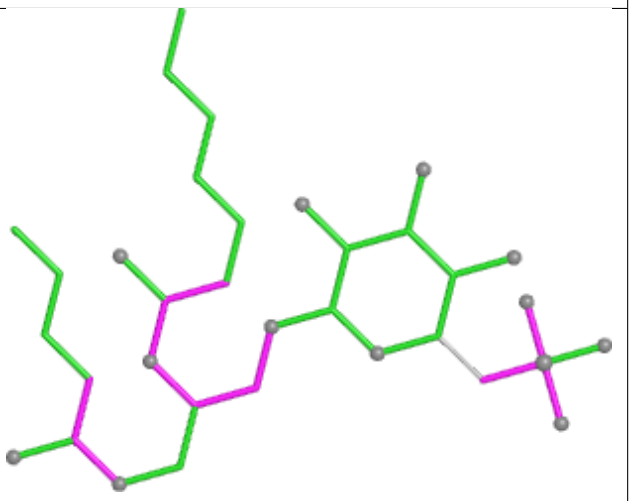


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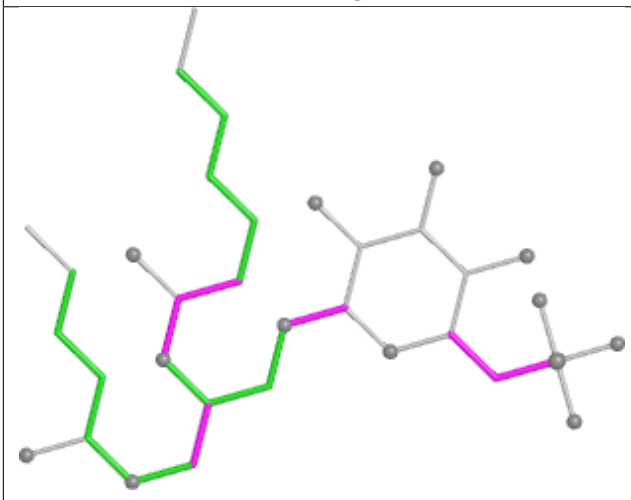
Ligand SQD DD 414



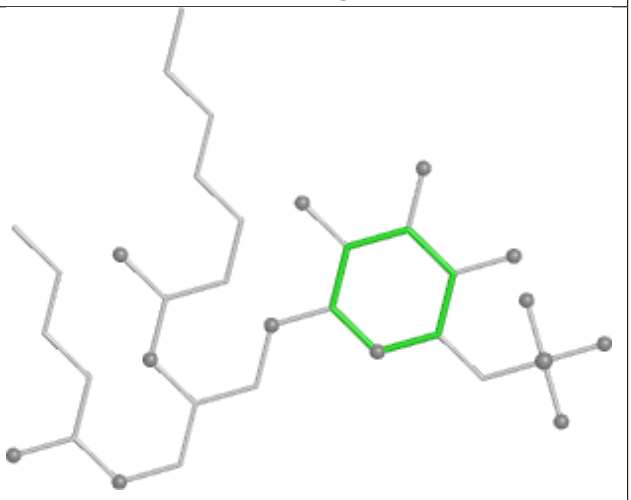
Bond lengths



Bond angles

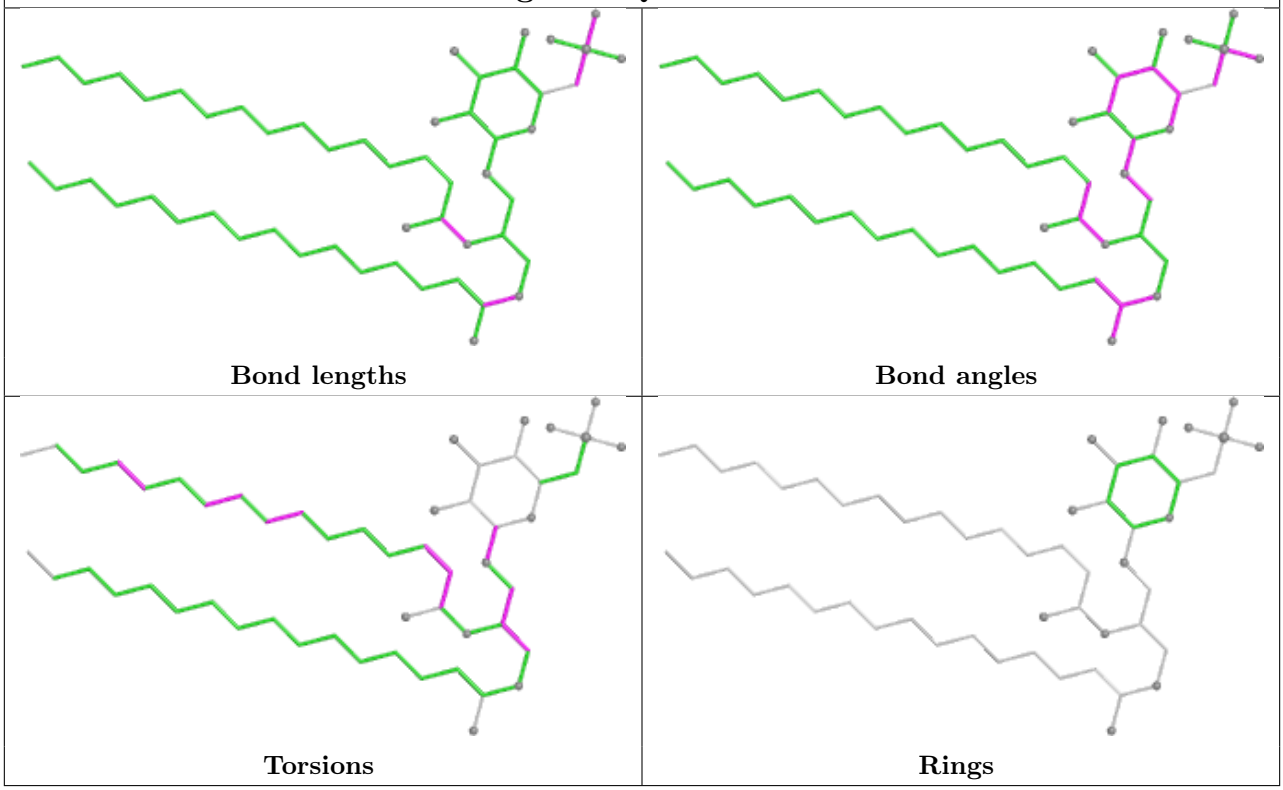


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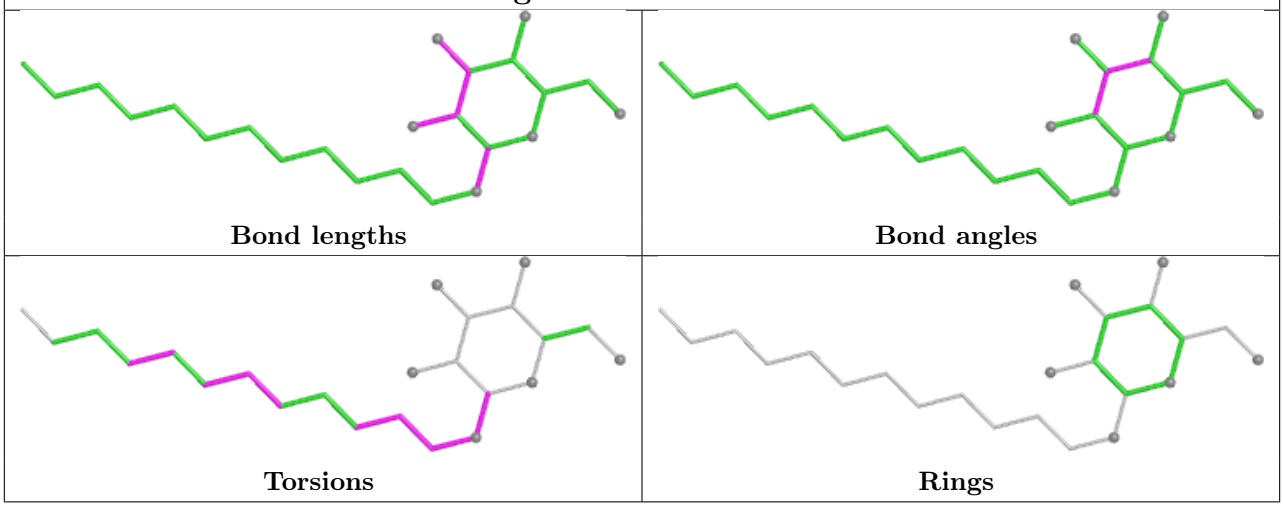


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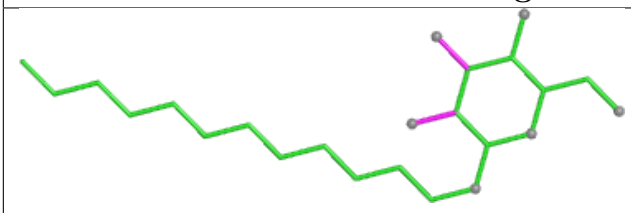
Ligand SQD C1 501



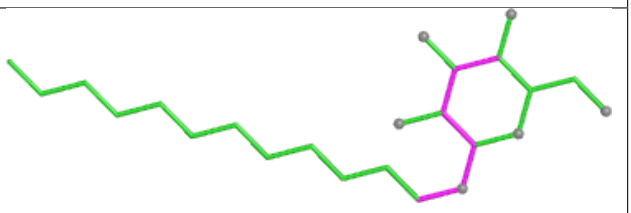
Ligand LMT B1 623



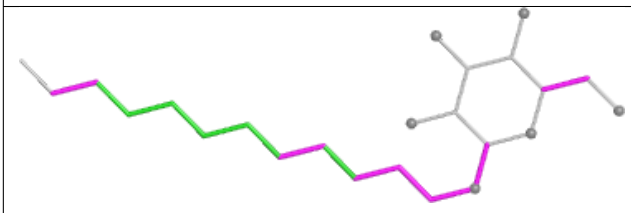
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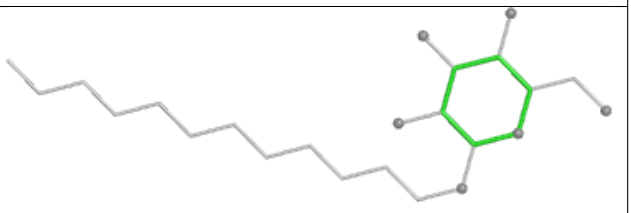
Bond lengths



Bond angles

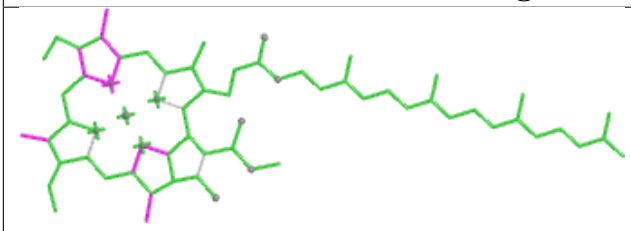


Torsions

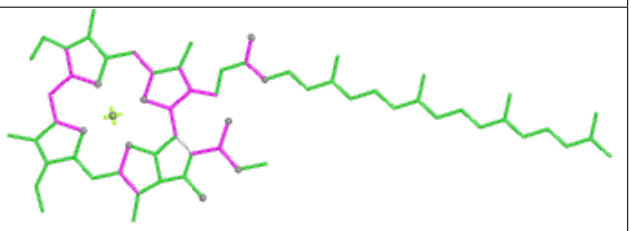


Rings

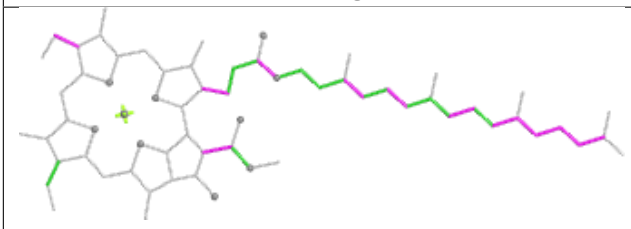
Ligand CLA bE 606



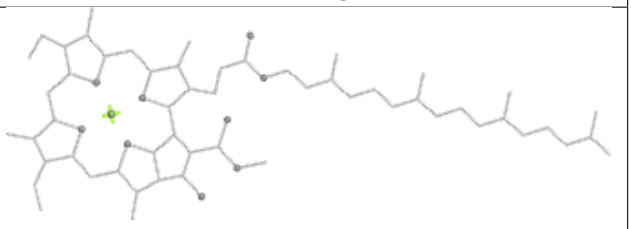
Bond lengths



Bond angles

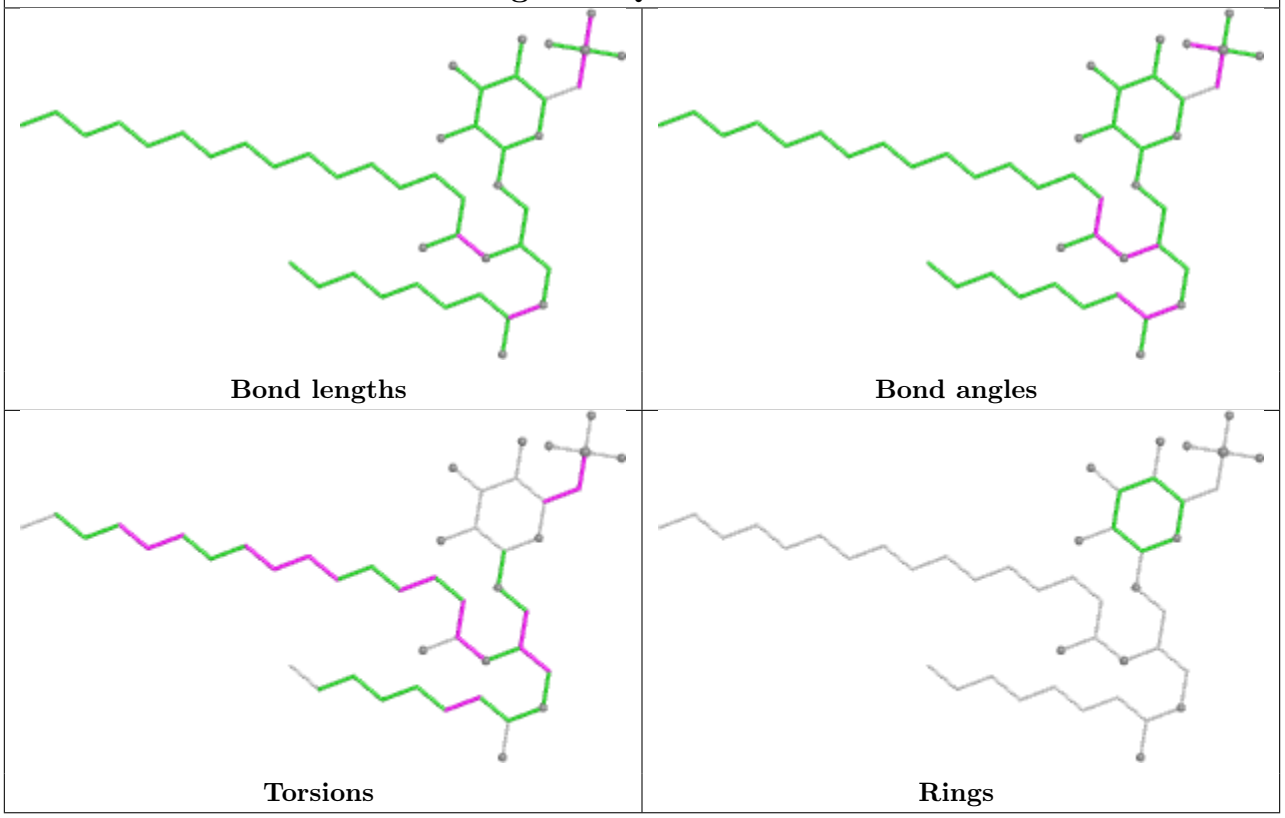


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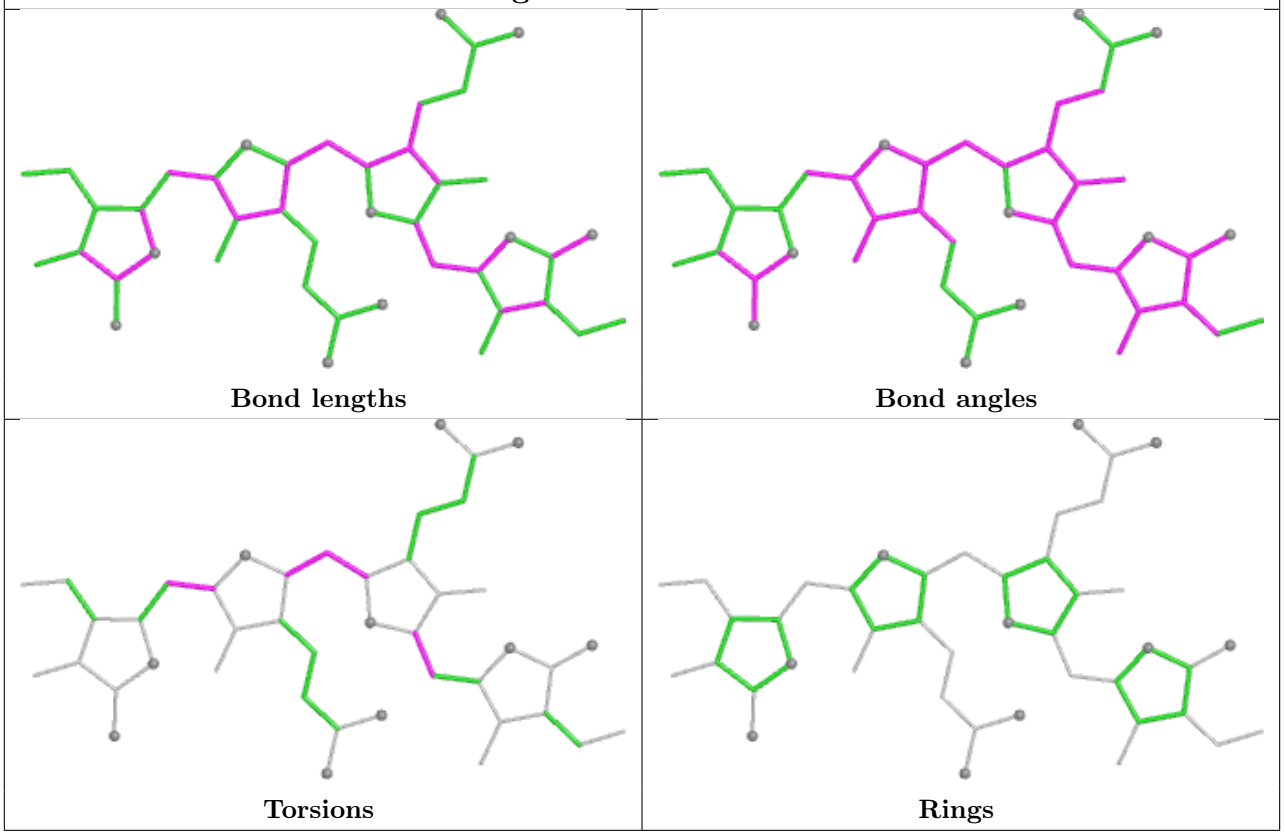


Rings

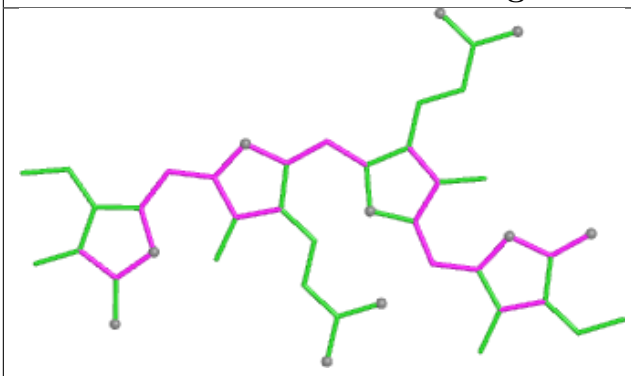
Ligand SQD AD 407



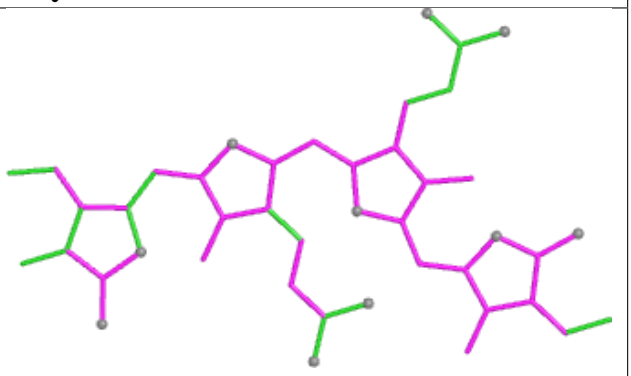
Ligand CYC nK 201



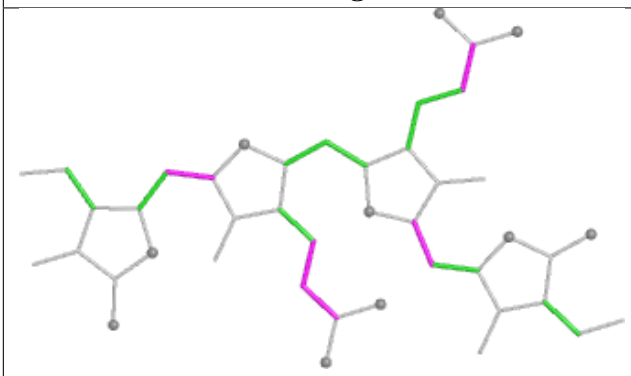
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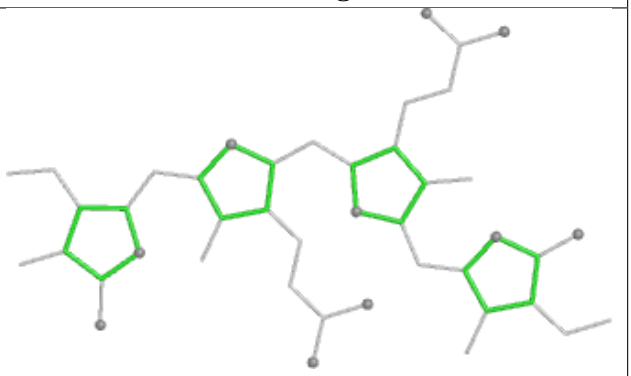
Bond lengths



Bond angles

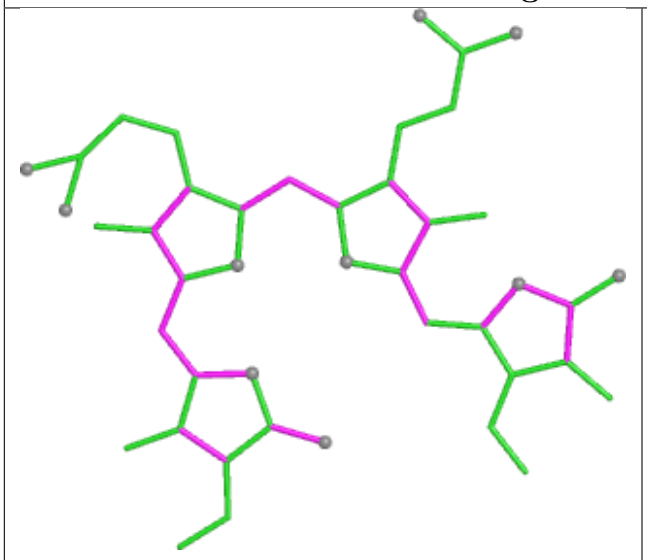


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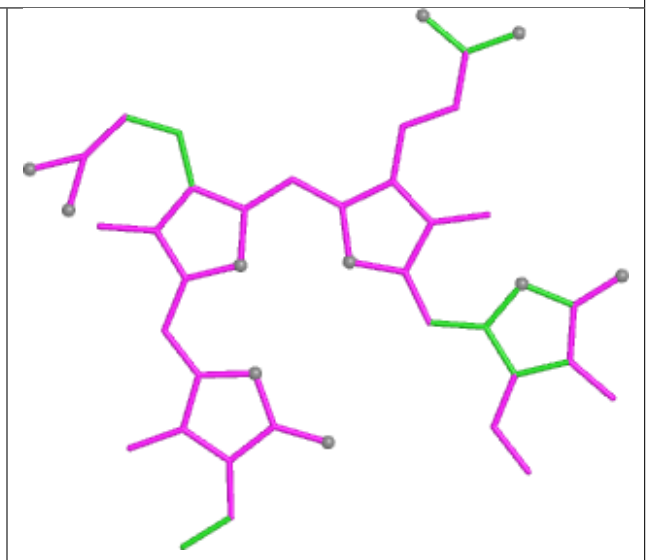


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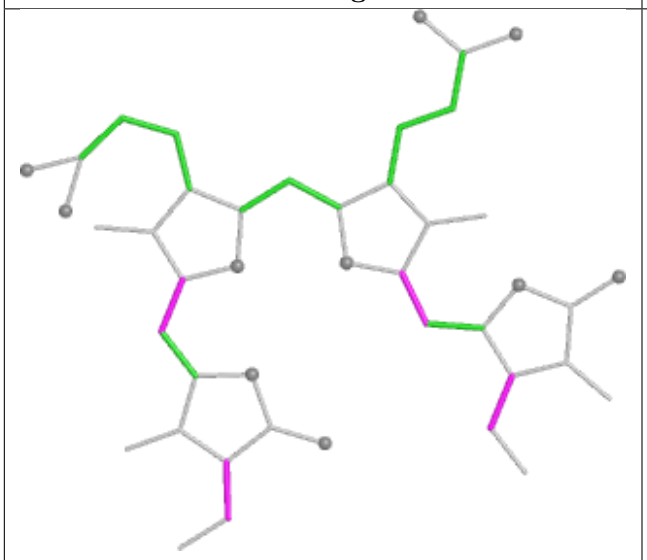
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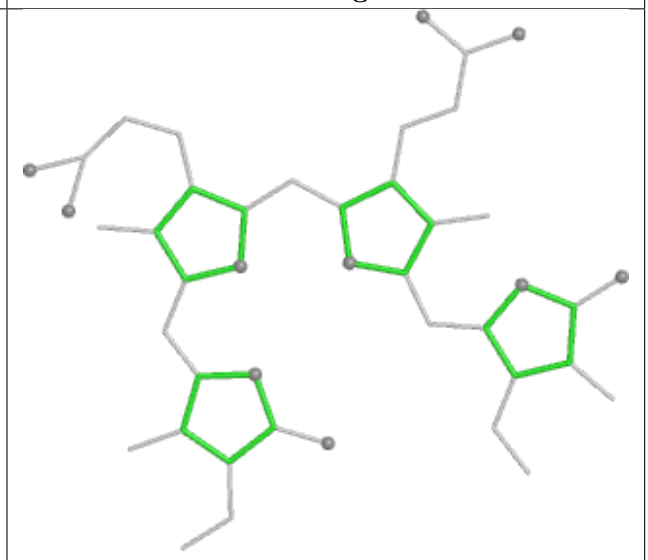
Bond lengths



Bond angles

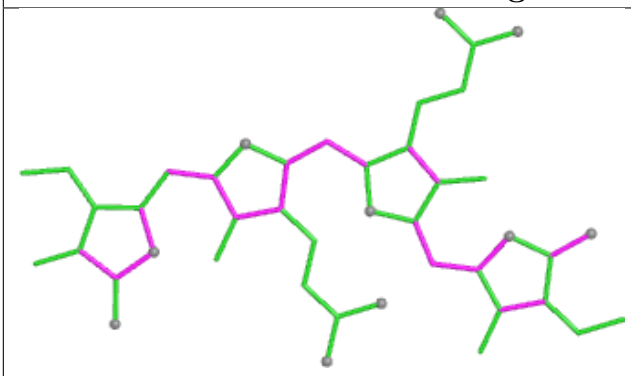


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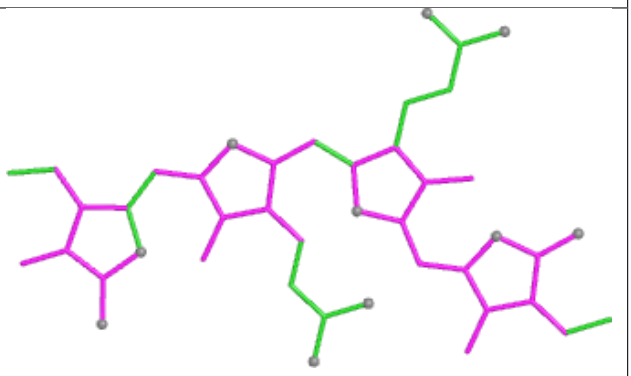


Rings

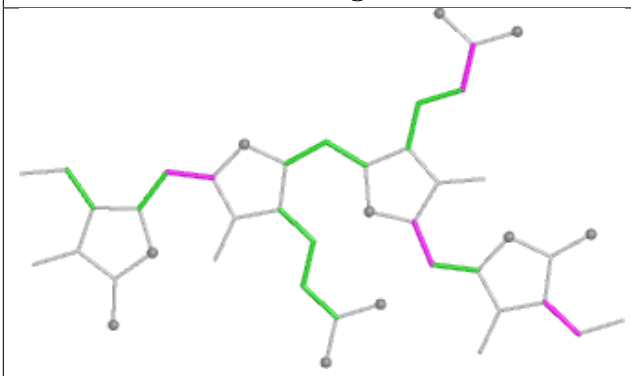
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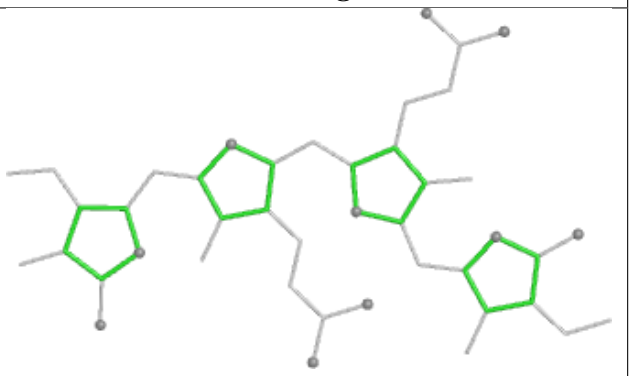
Bond lengths



Bond angles

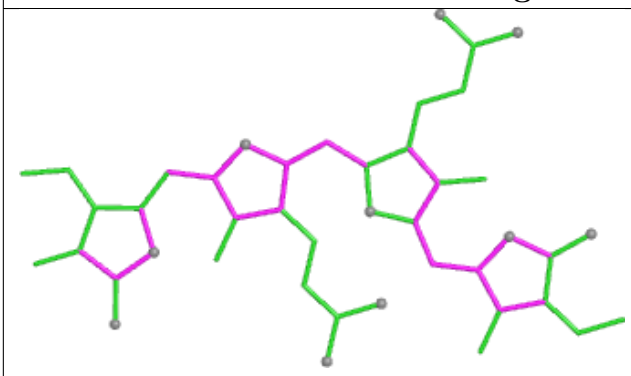


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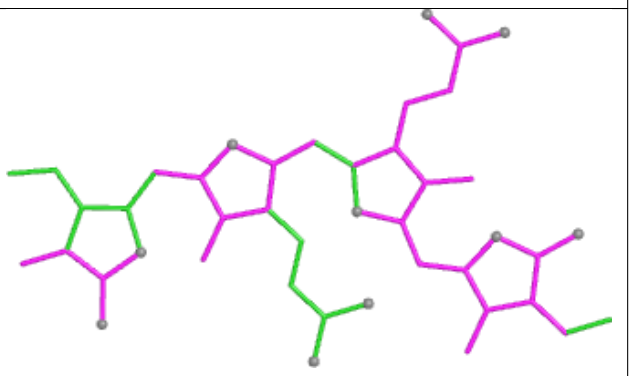


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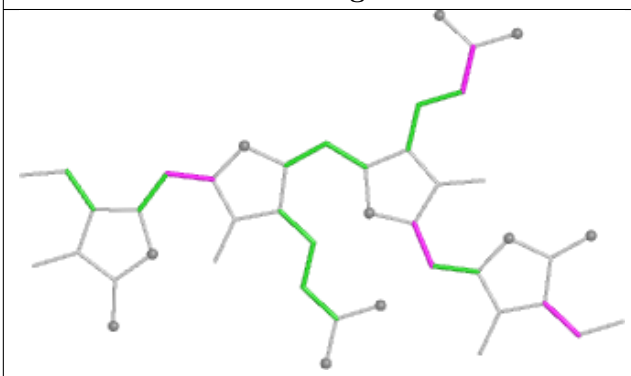
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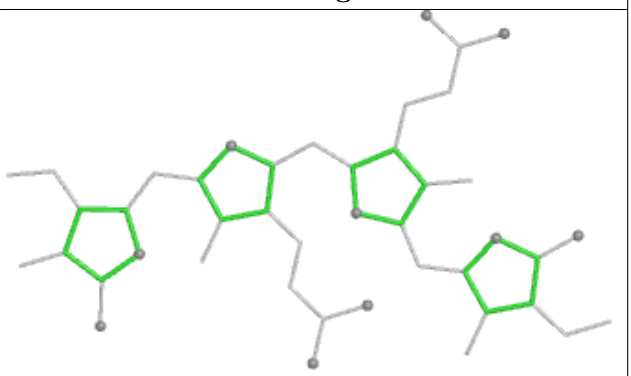
Bond lengths



Bond angles

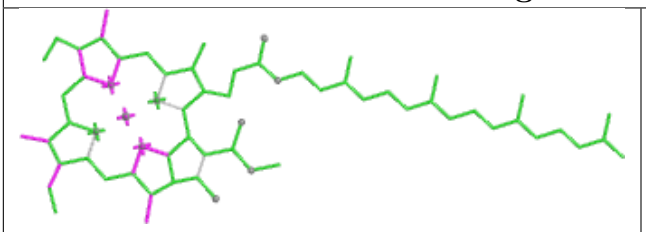


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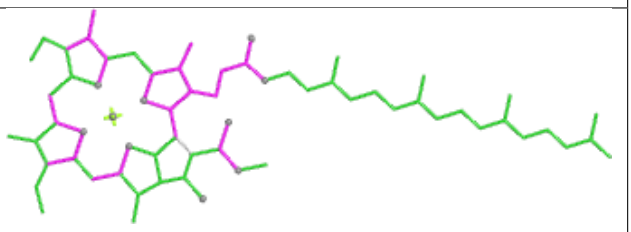


Rings

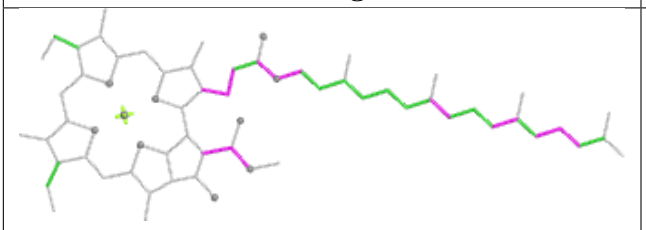
Ligand CLA C1 506



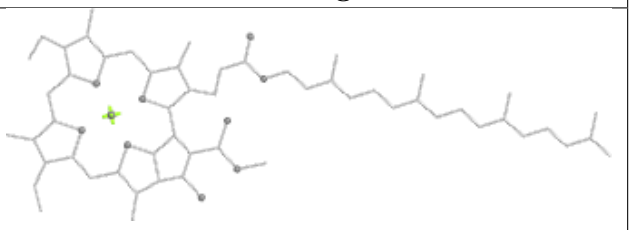
Bond lengths



Bond angles

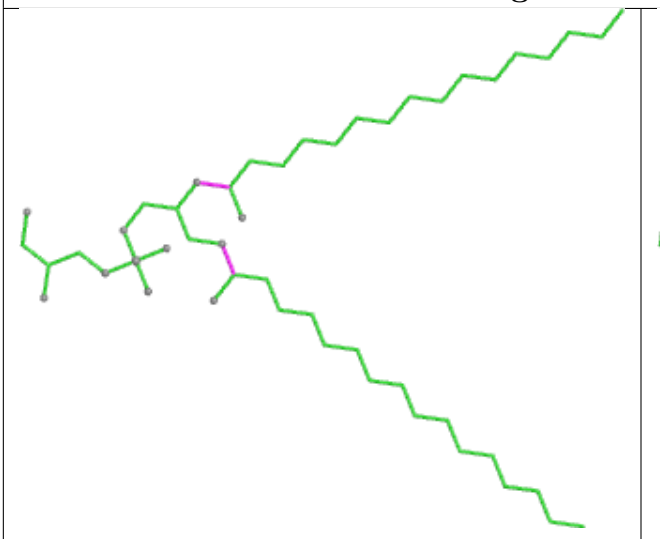


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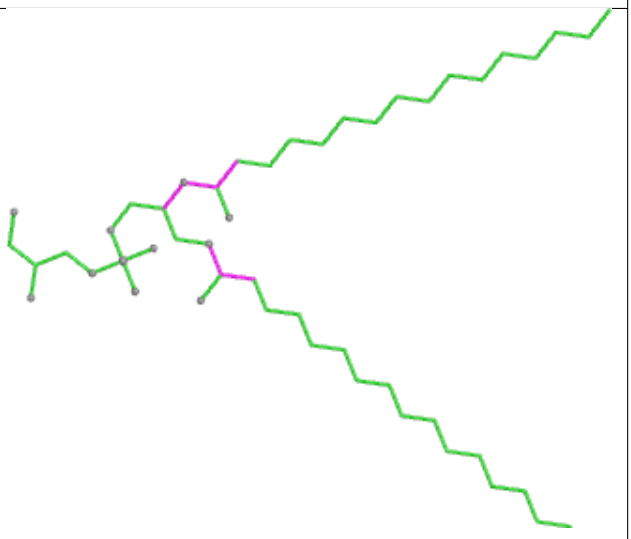


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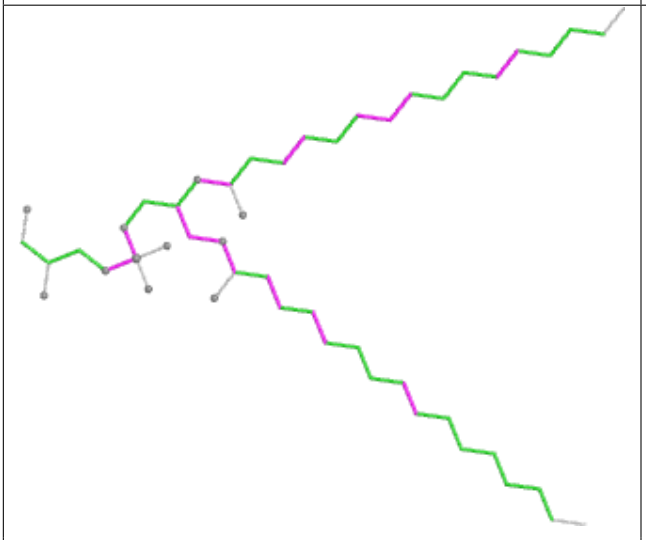
Ligand LHG BE 620



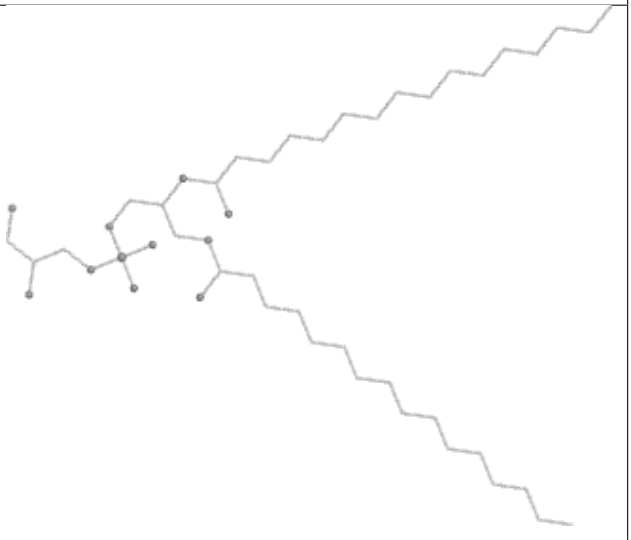
Bond lengths



Bond angles

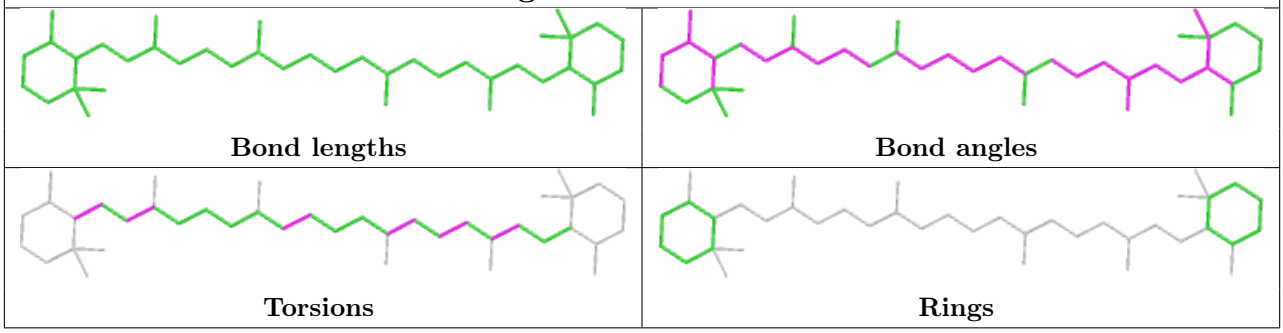


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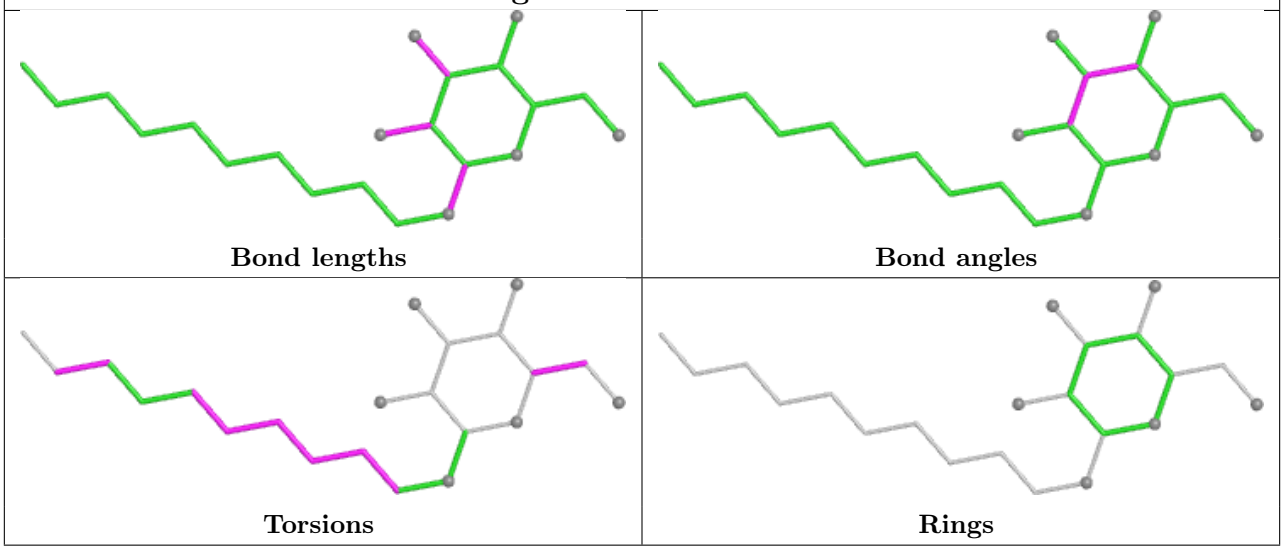


Rings

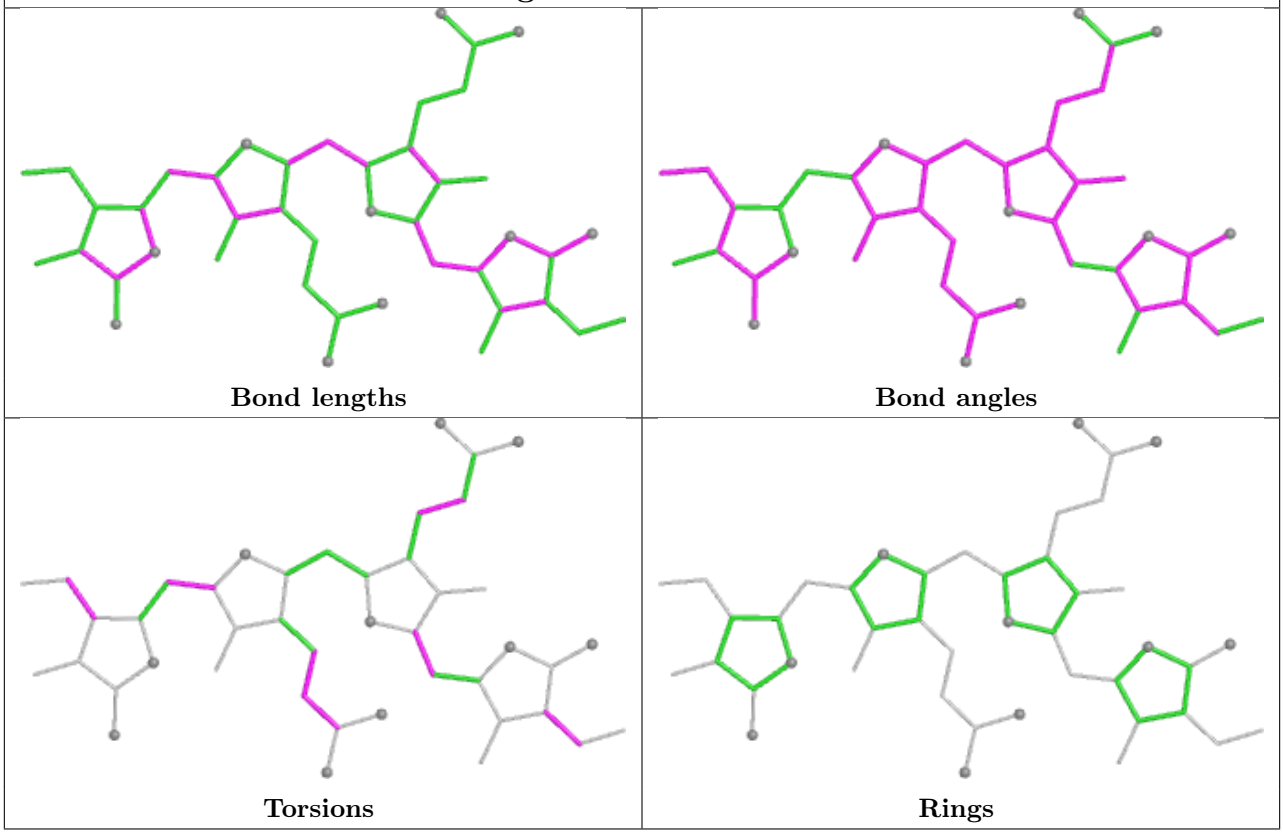
Ligand BCR IE 102



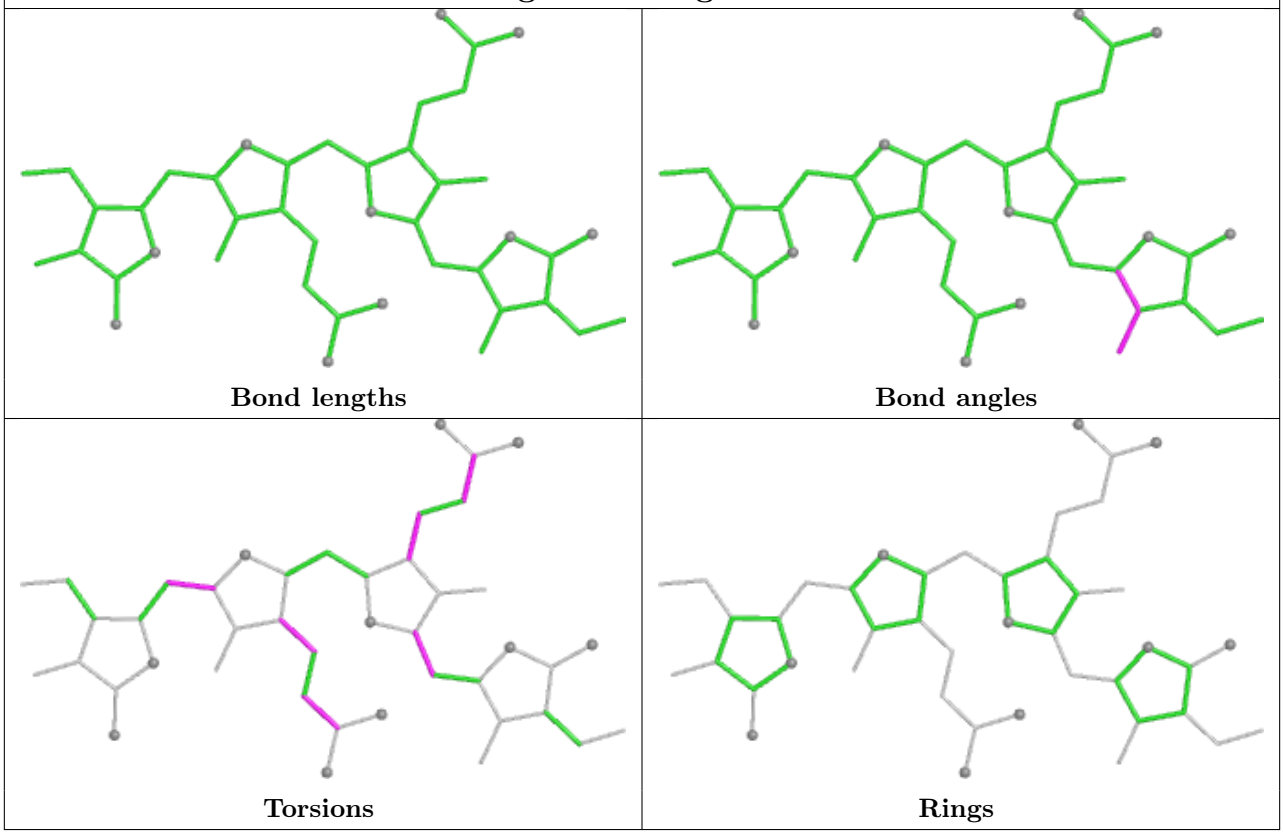
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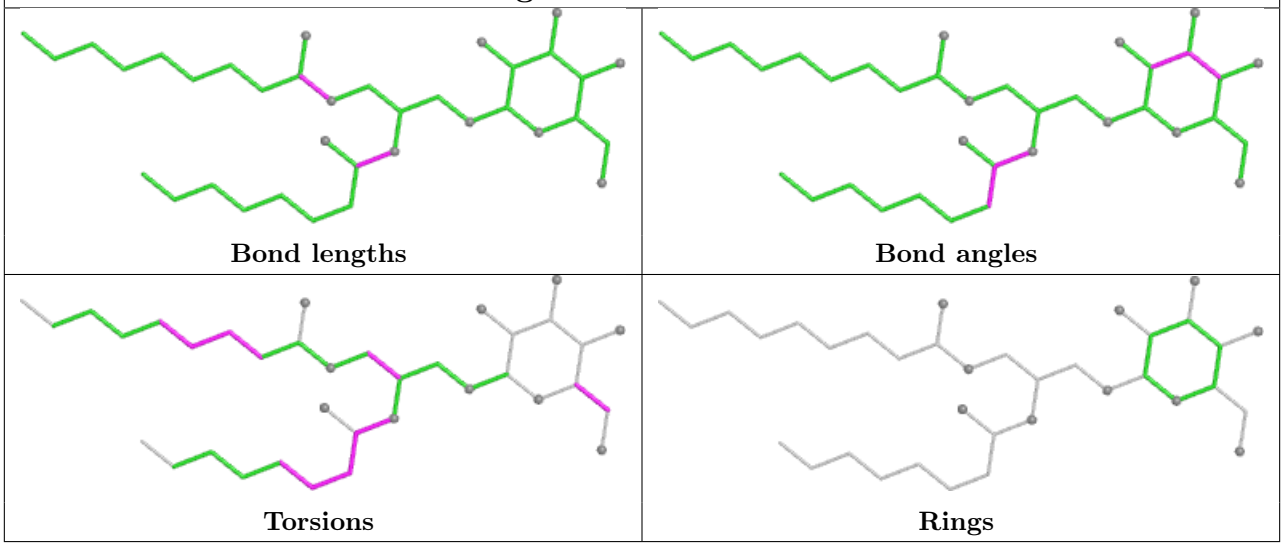
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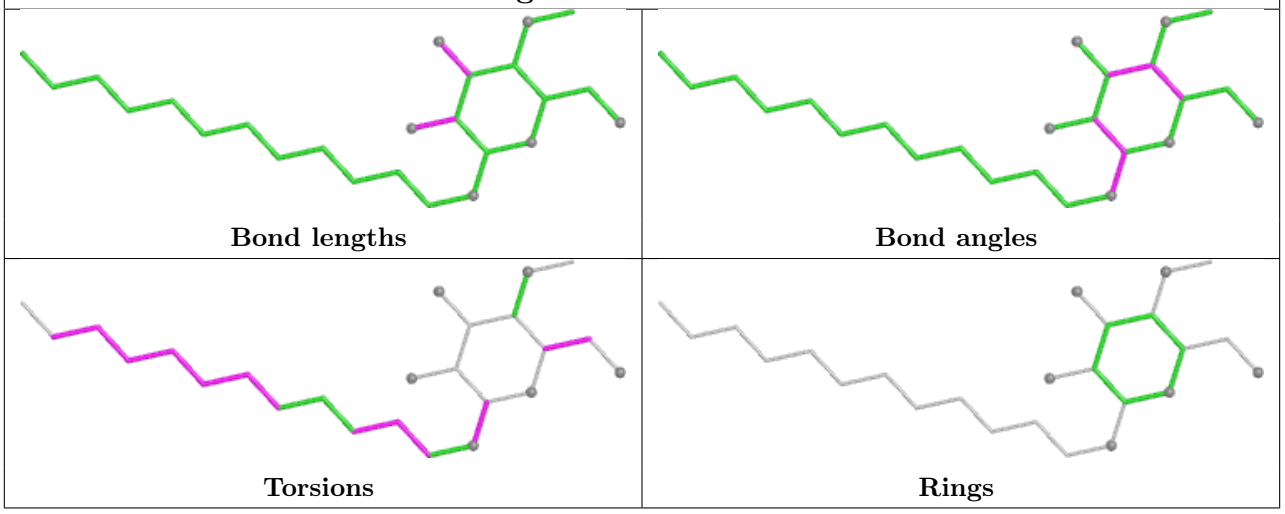
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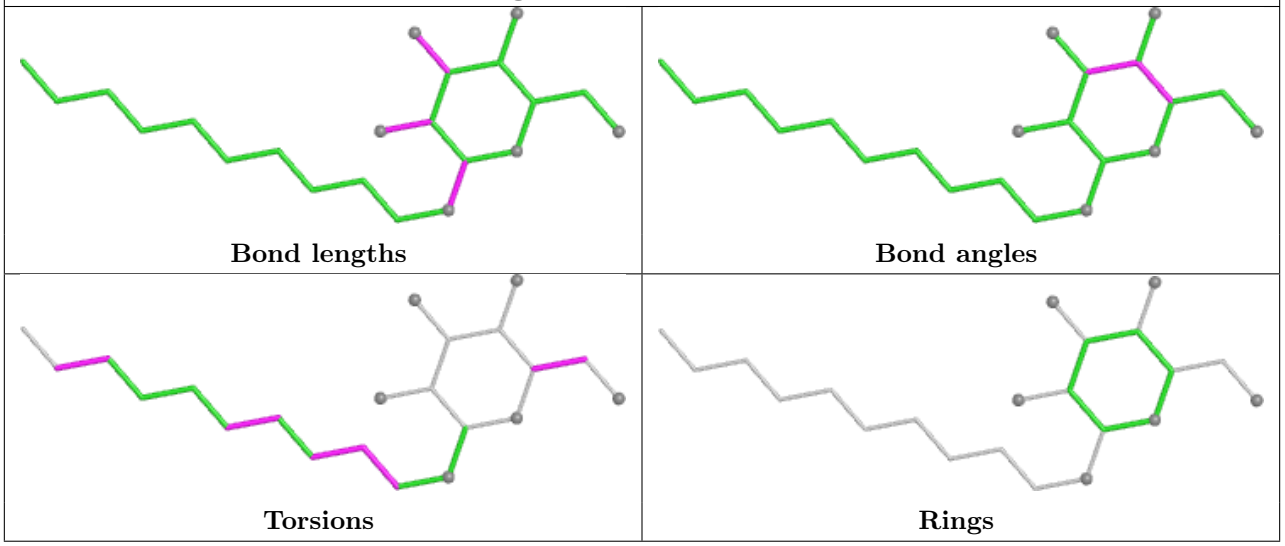
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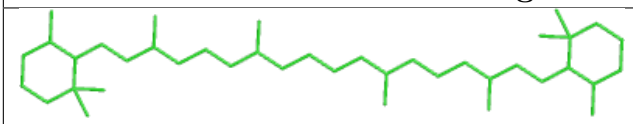
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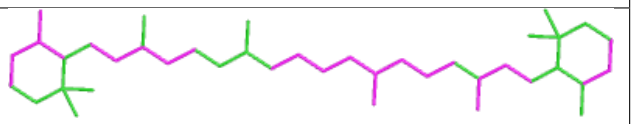
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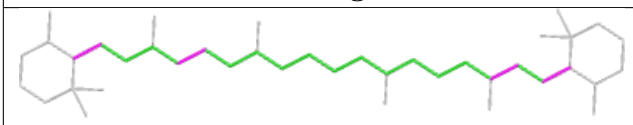
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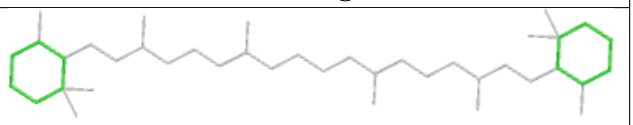
Bond lengths



Bond angles

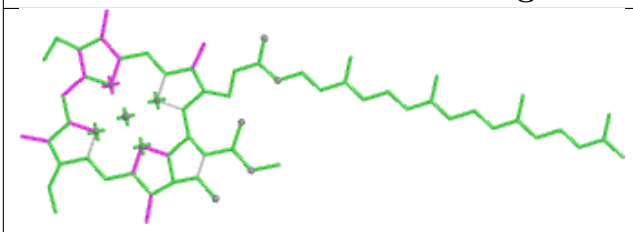


Torsions

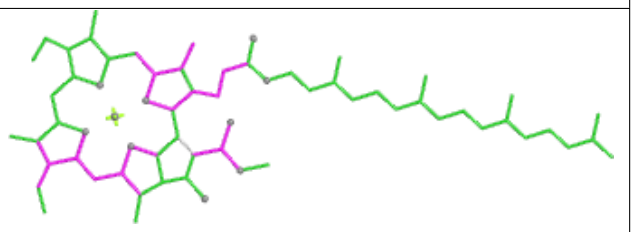


Rings

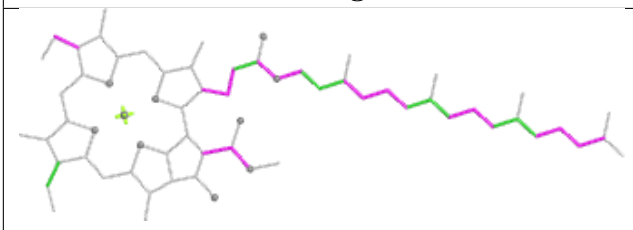
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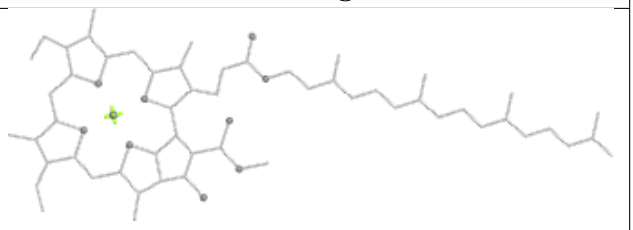
Bond lengths



Bond angles

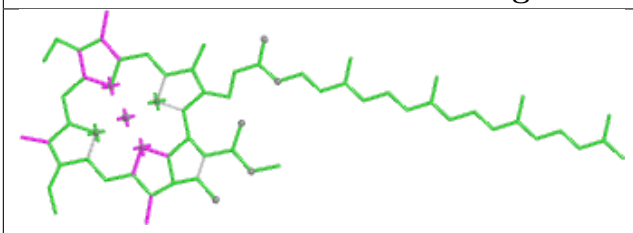


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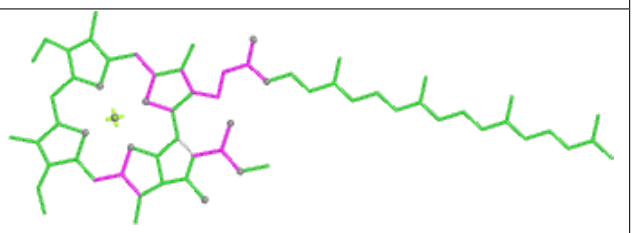


Rings

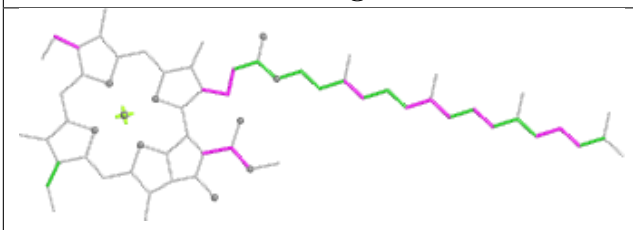
Ligand CLA CE 512



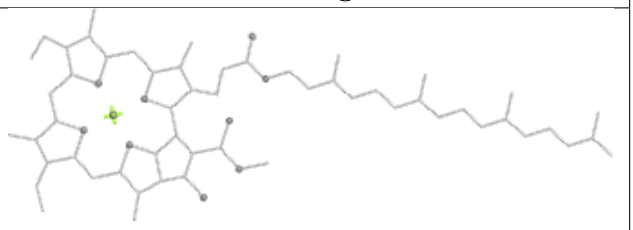
Bond lengths



Bond angles

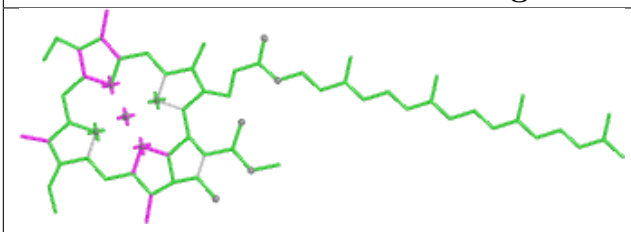


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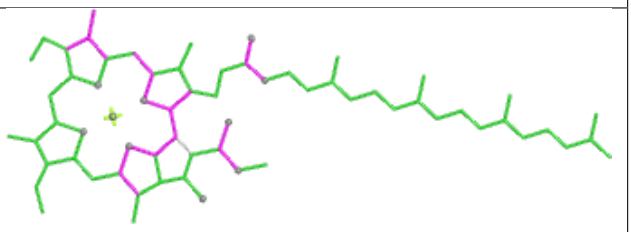


Rings

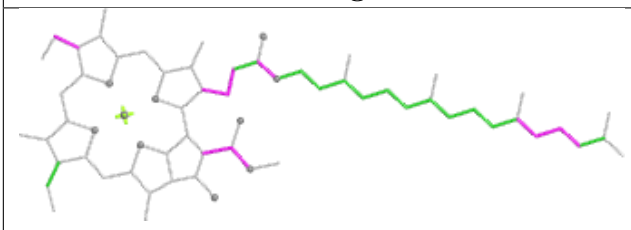
Ligand CLA BD 607



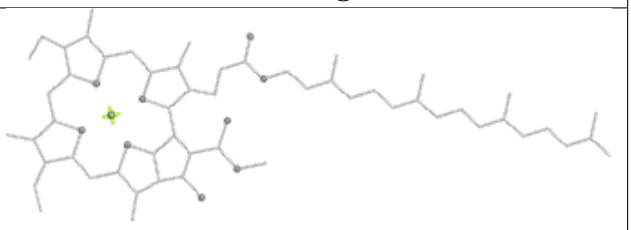
Bond lengths



Bond angles

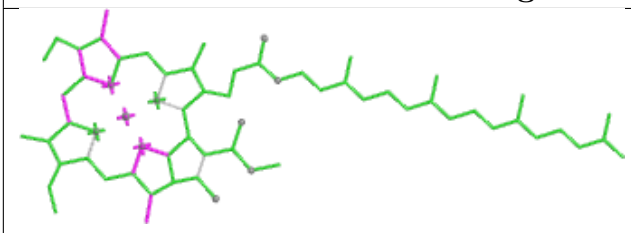


Torsions

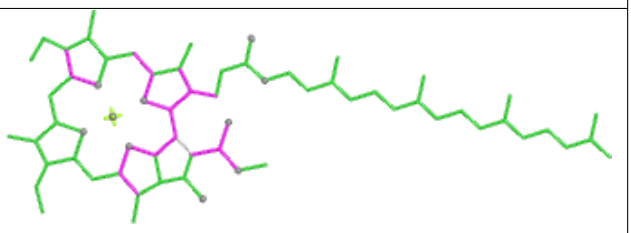


Rings

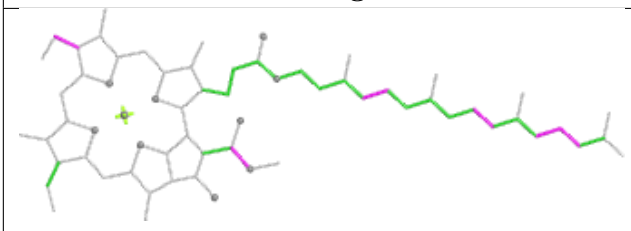
Ligand CLA cE 505



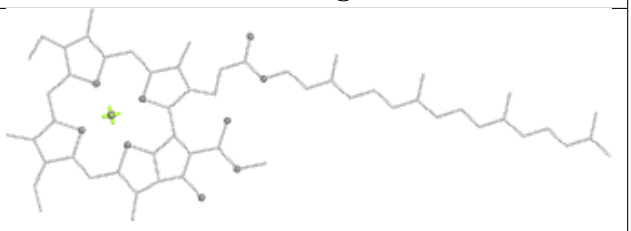
Bond lengths



Bond angles

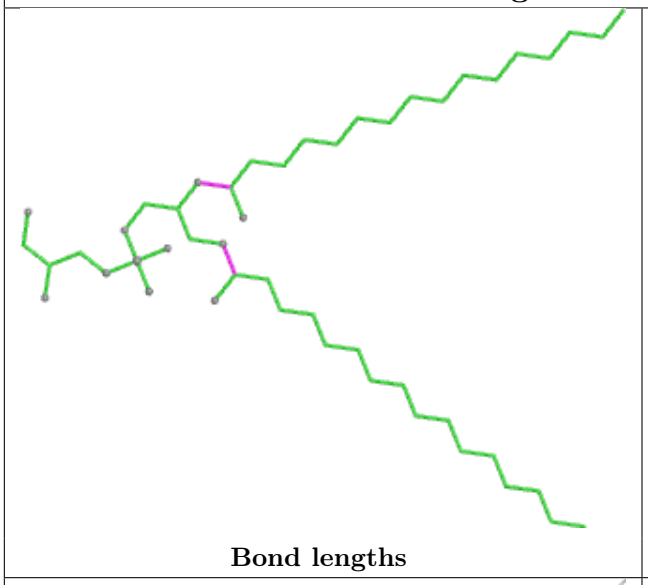


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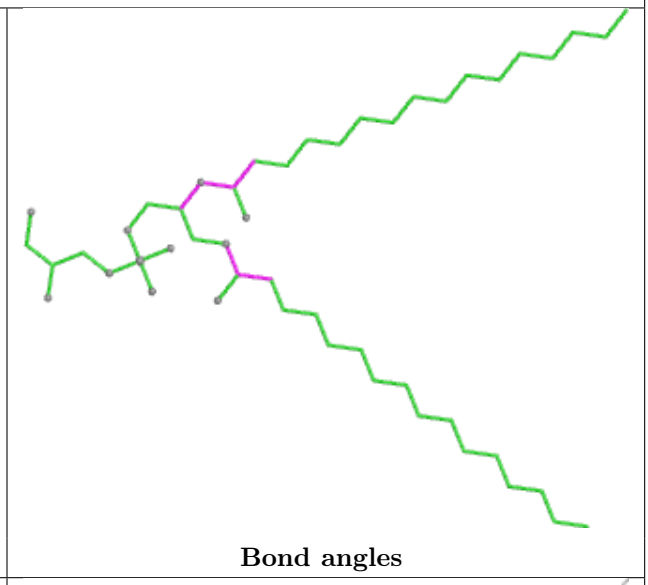


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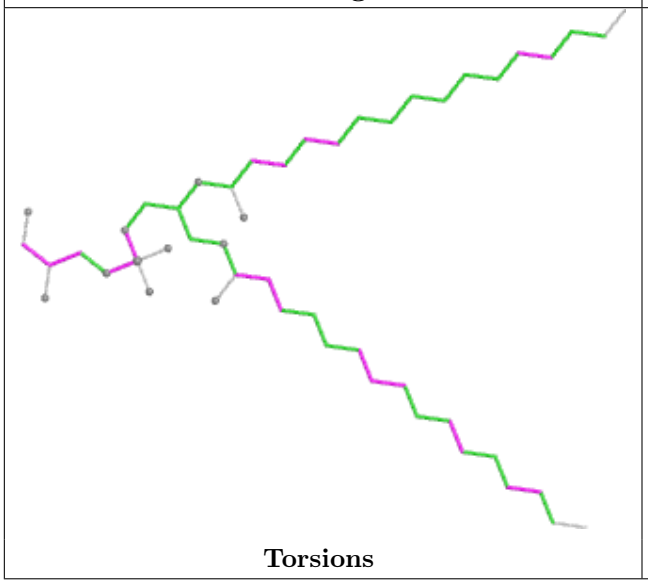
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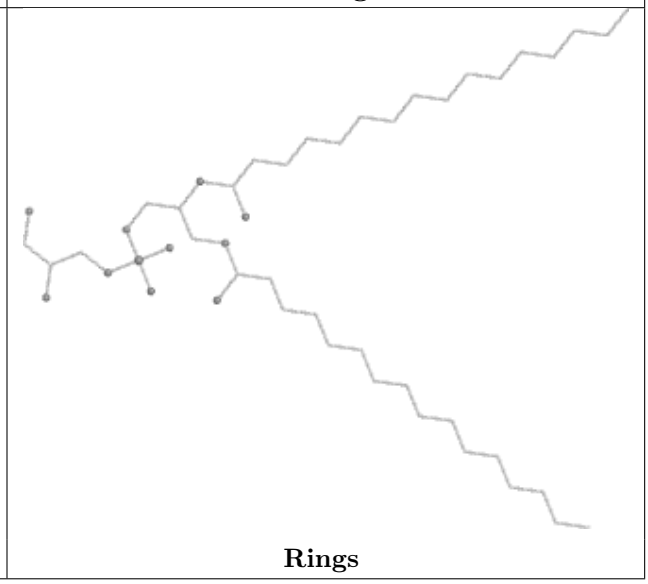
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Bond angles

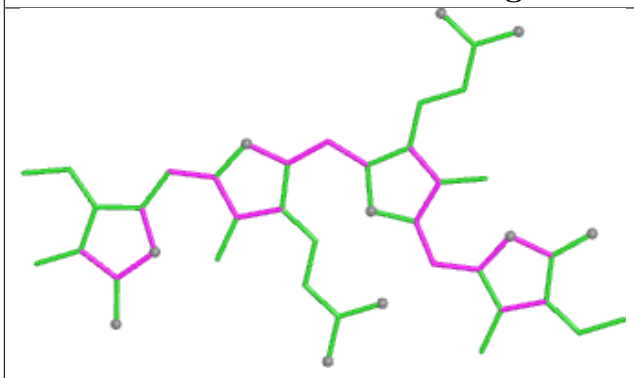


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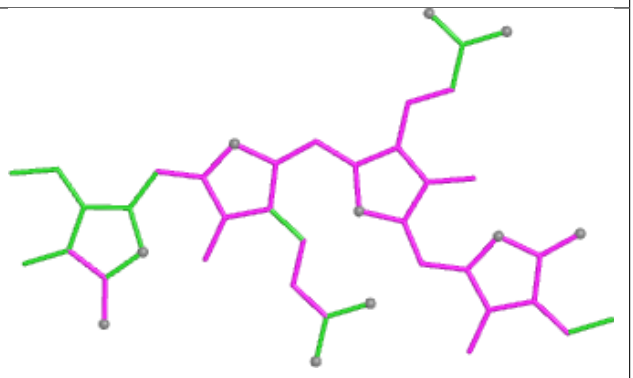


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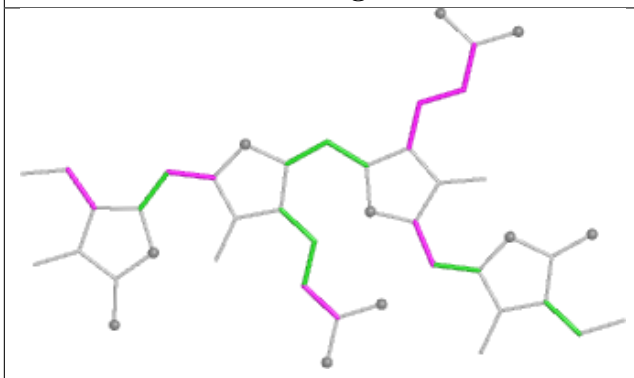
Ligand CYC MG 201



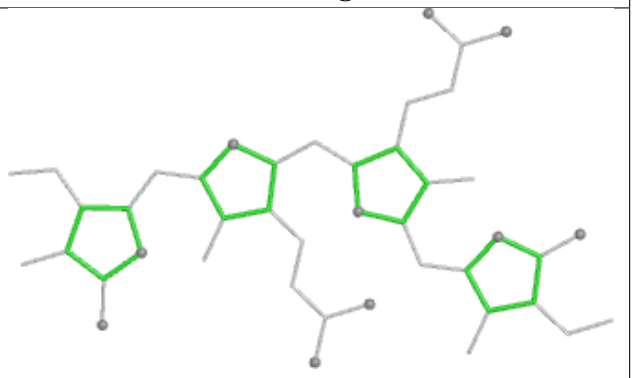
Bond lengths



Bond angles

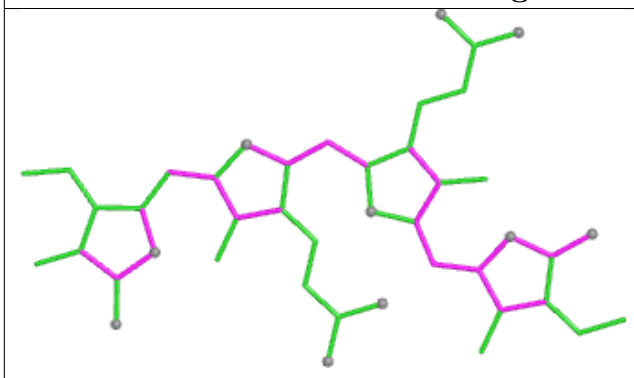


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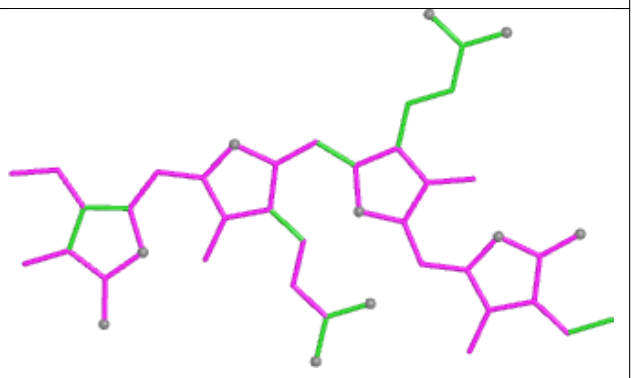


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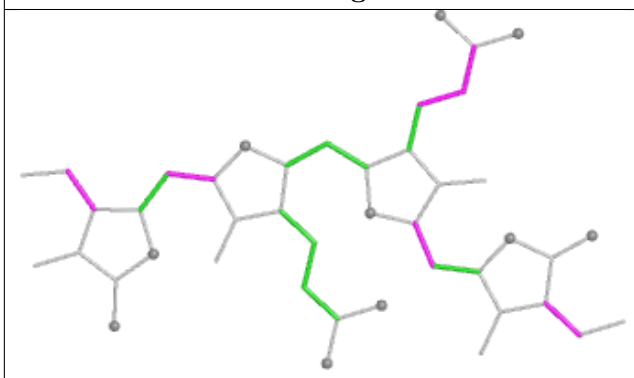
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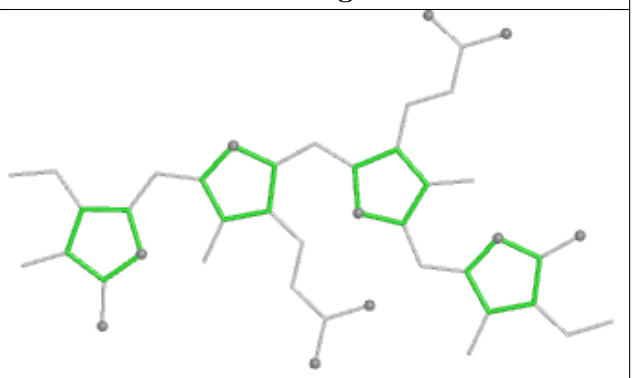
Bond lengths



Bond angles

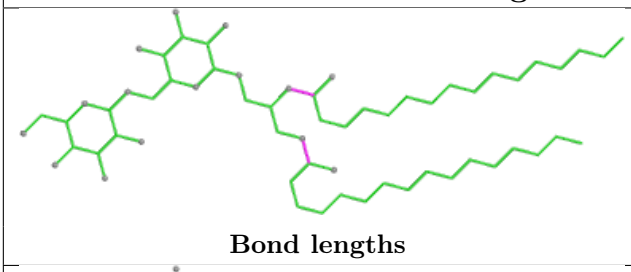


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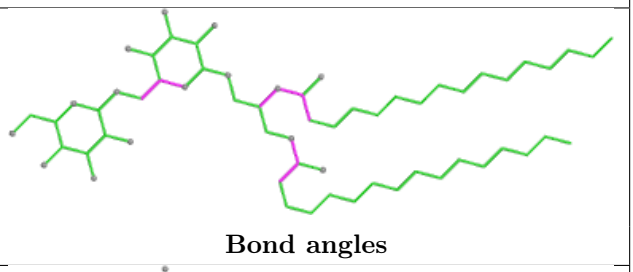


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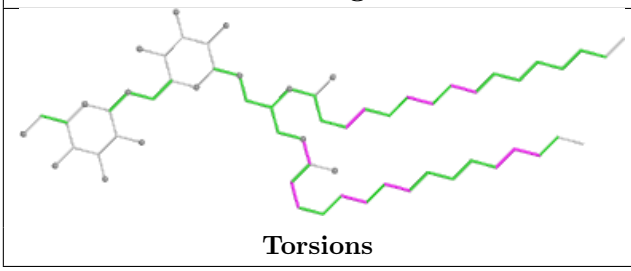
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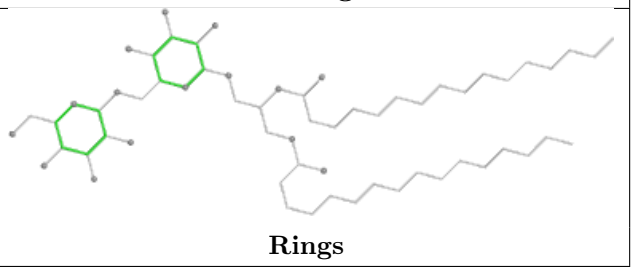
Bond lengths



Bond angles

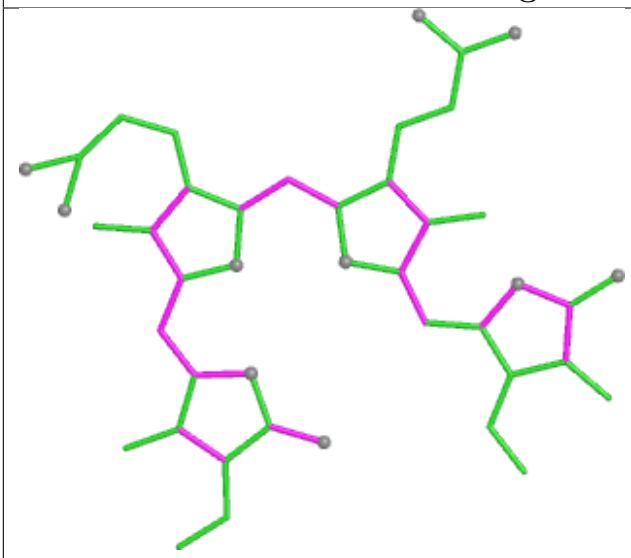


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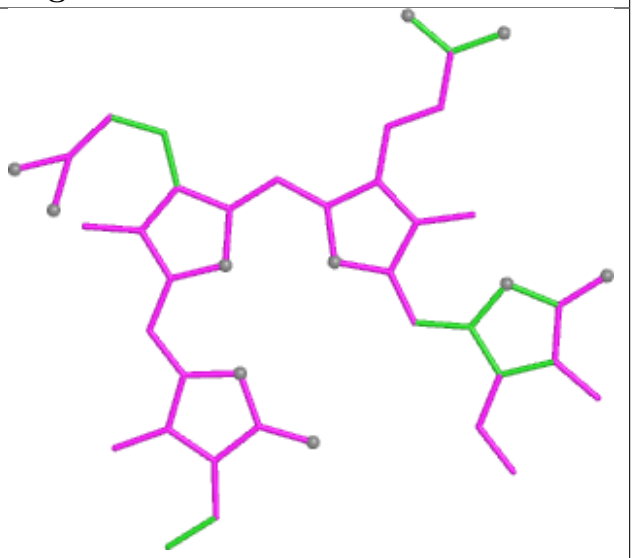


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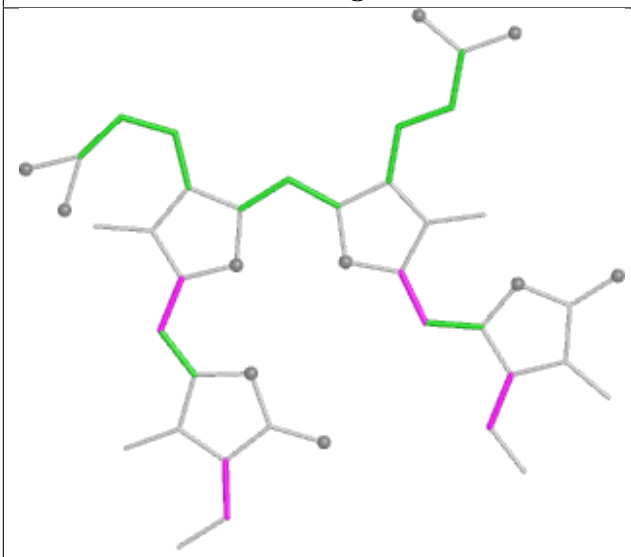
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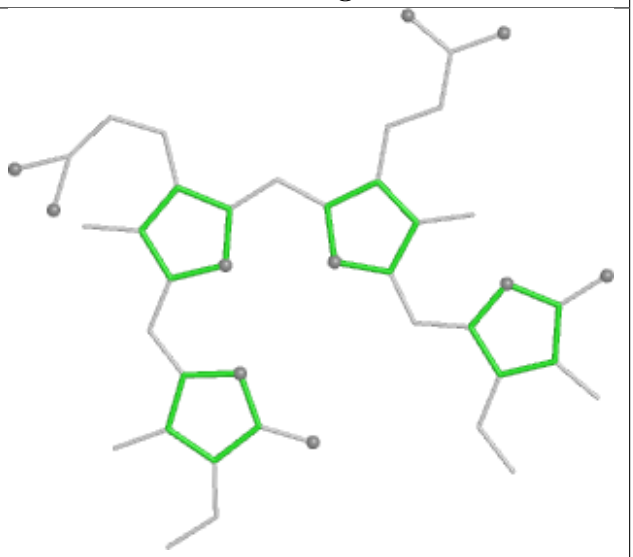
Bond lengths



Bond angles

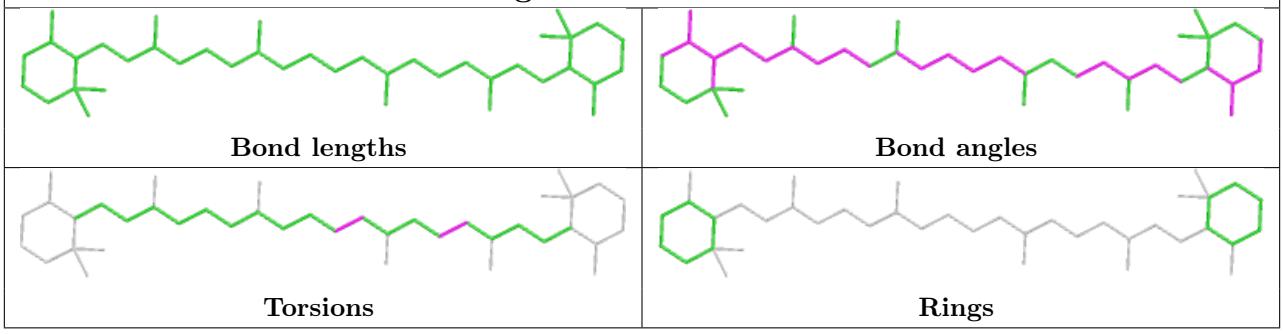


Torsions



Rings

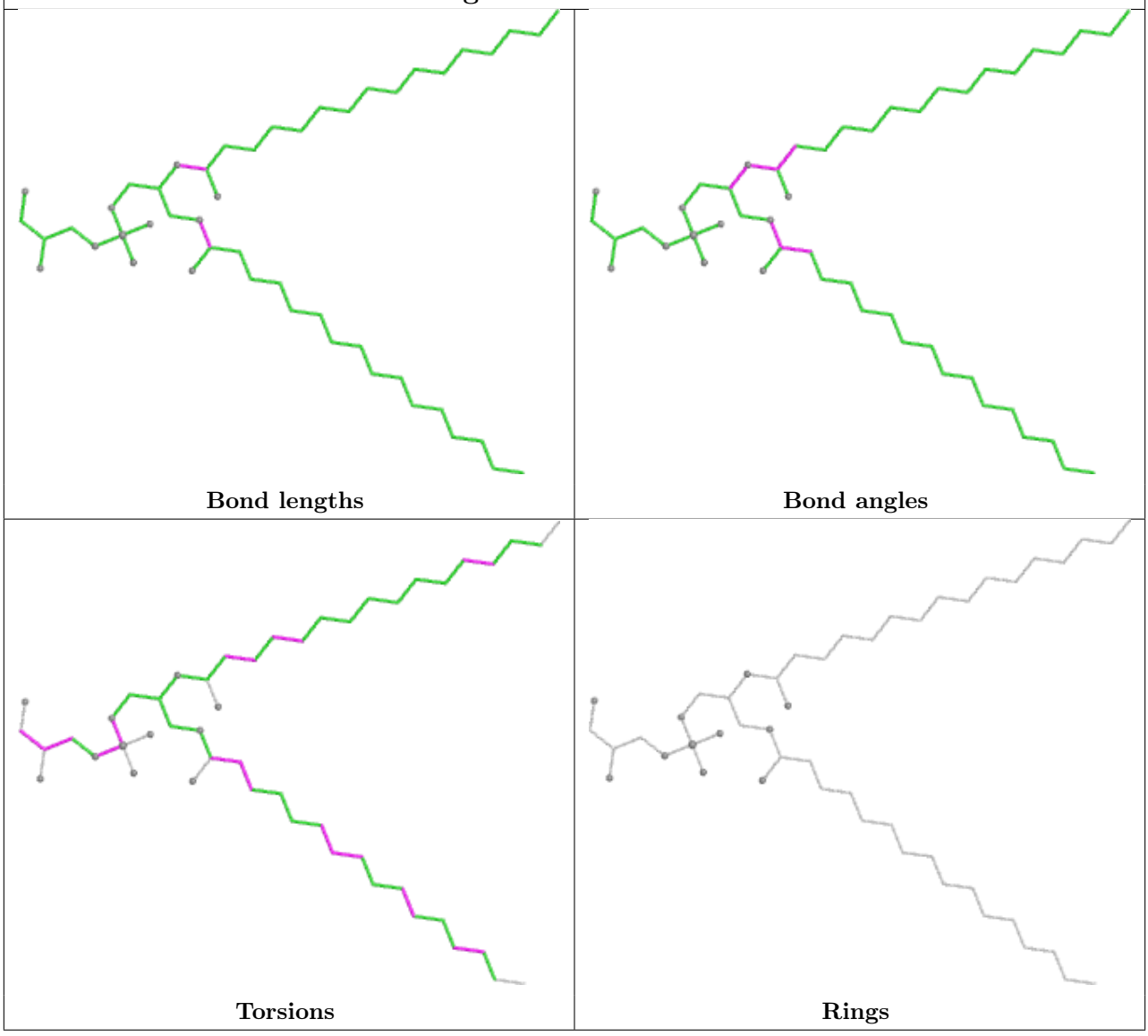
Ligand BCR B1 616



Bond lengths | Bond angles

Torsions | Rings

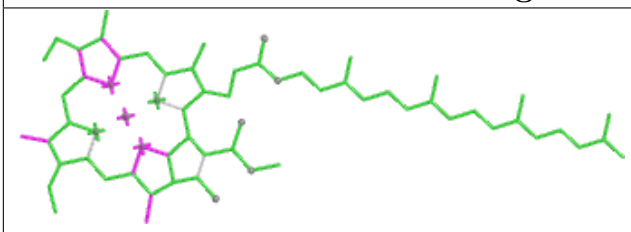
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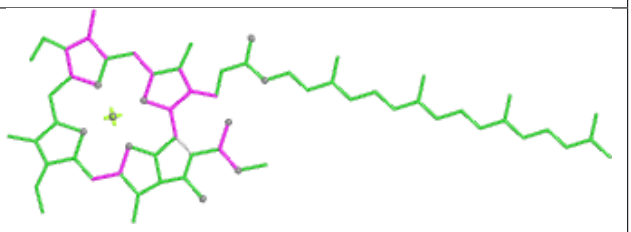
Bond lengths | Bond angles

Torsions | Rings

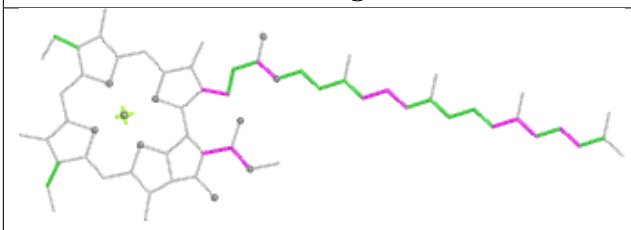
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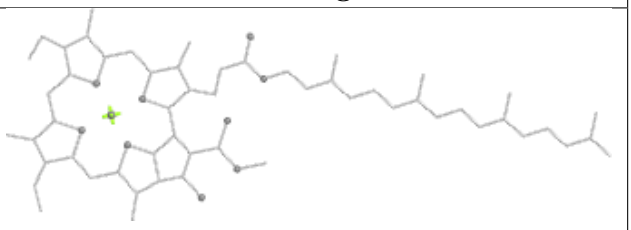
Bond lengths



Bond angles

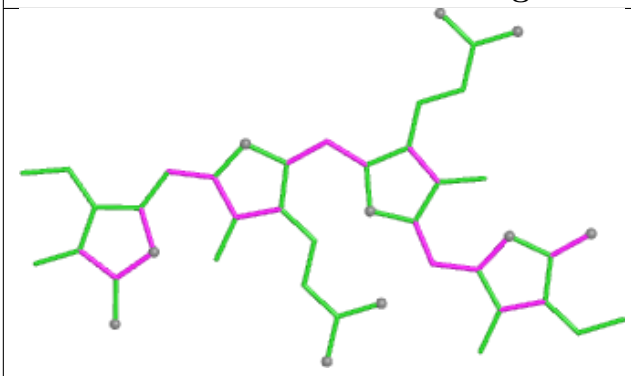


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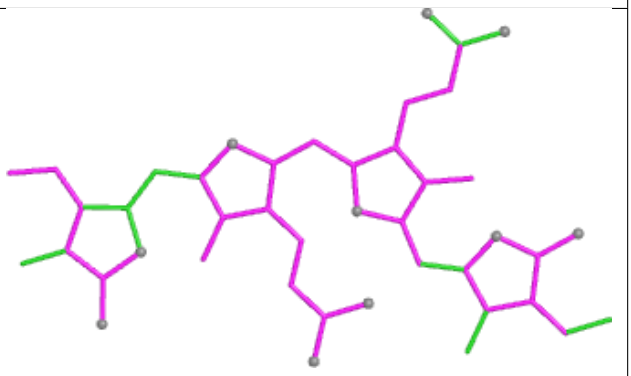


Rings

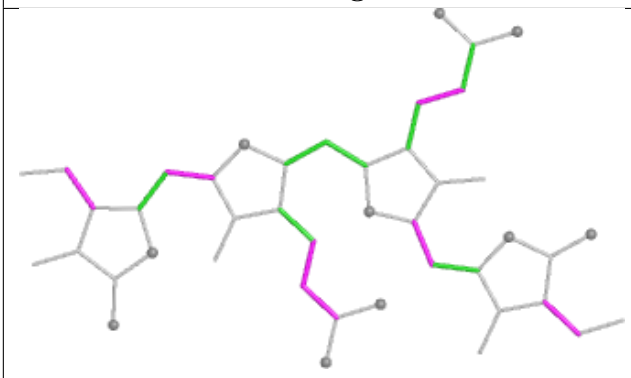
Ligand CYC dC 201



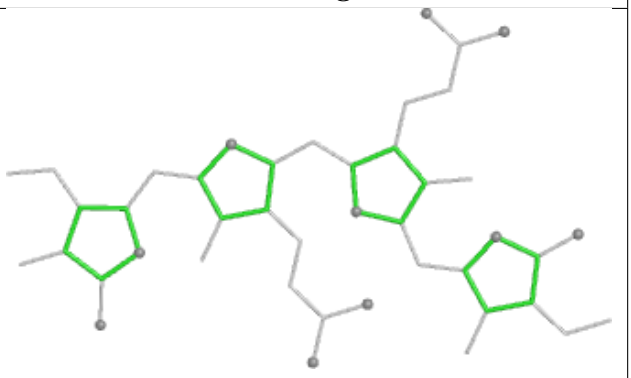
Bond lengths



Bond angles

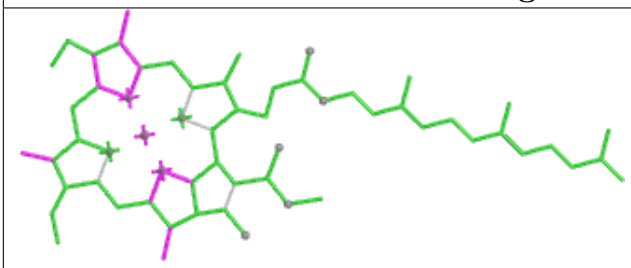


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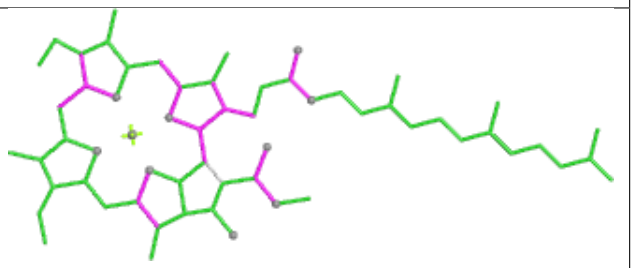


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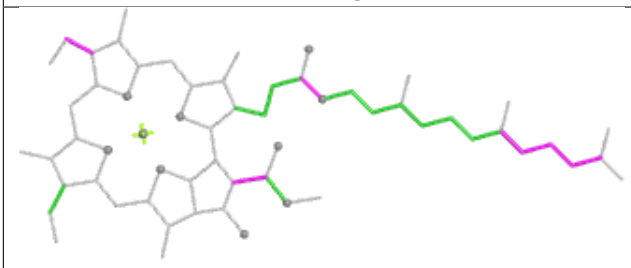
Ligand CLA h1 102



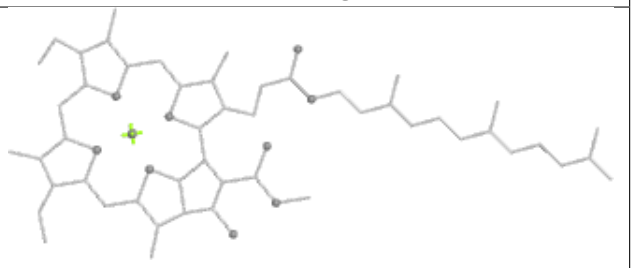
Bond lengths



Bond angles

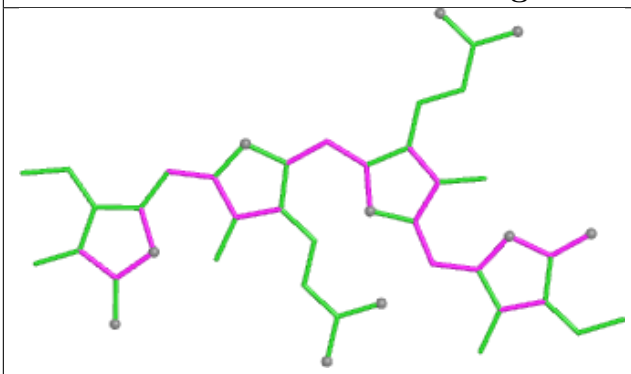


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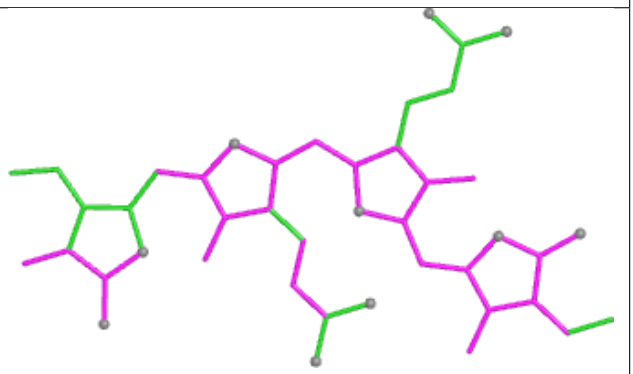


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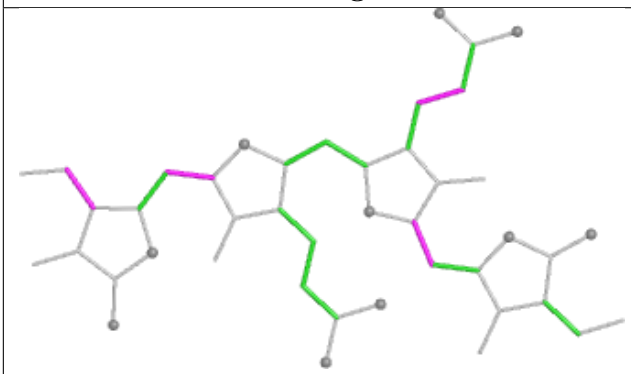
Ligand CYC OL 201



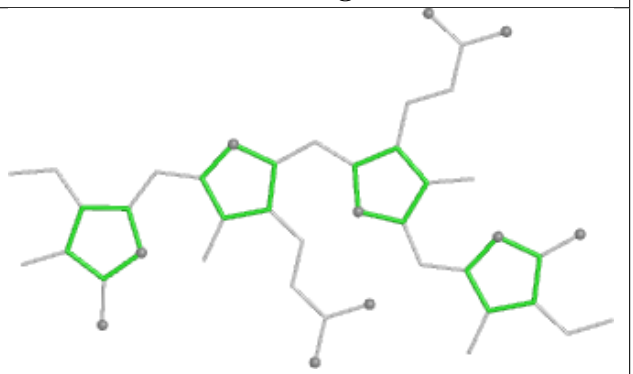
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Bond angles

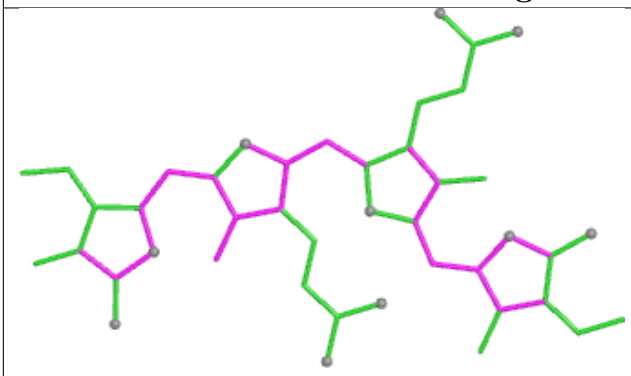


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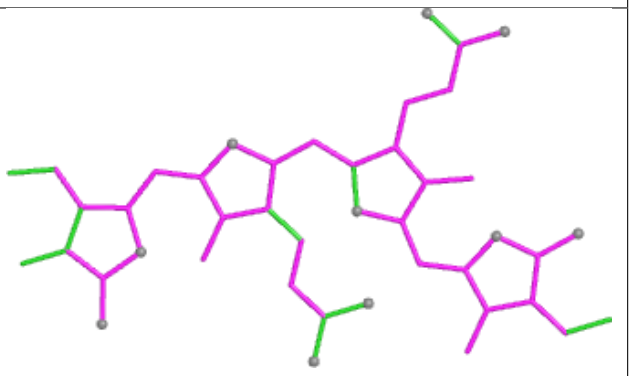


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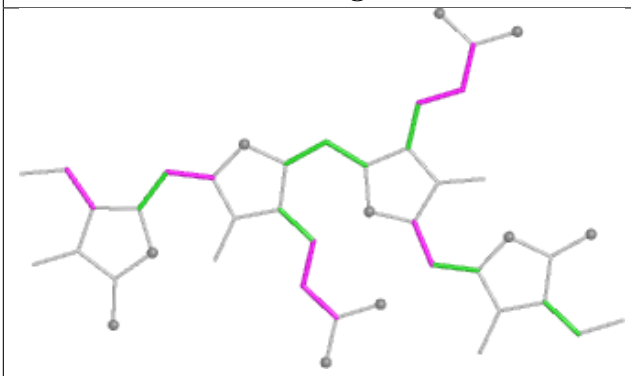
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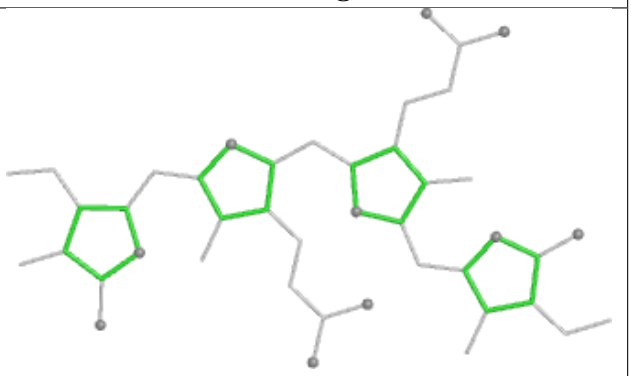
Bond lengths



Bond angles

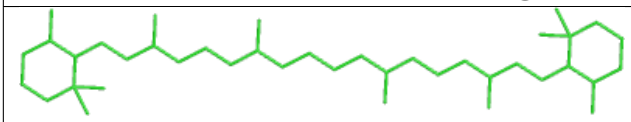


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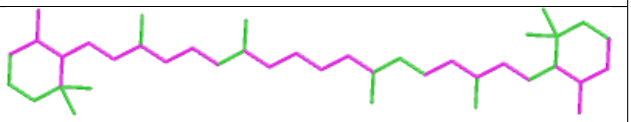


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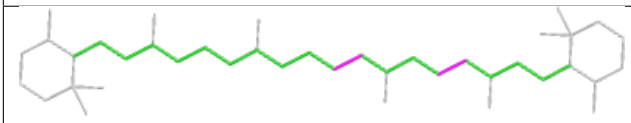
Ligand BCR b1 617



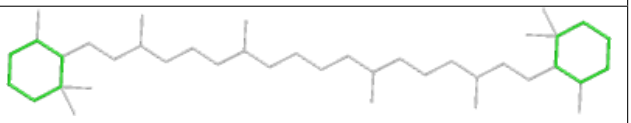
Bond lengths



Bond angles

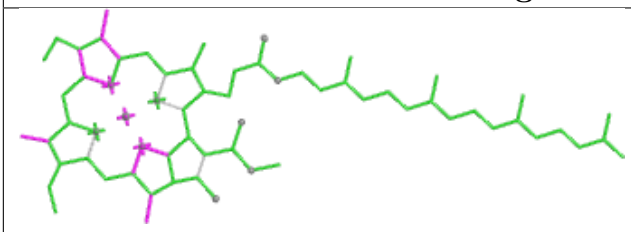


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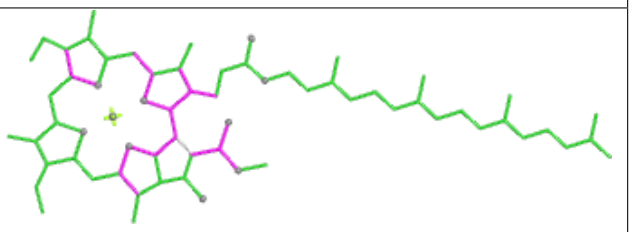


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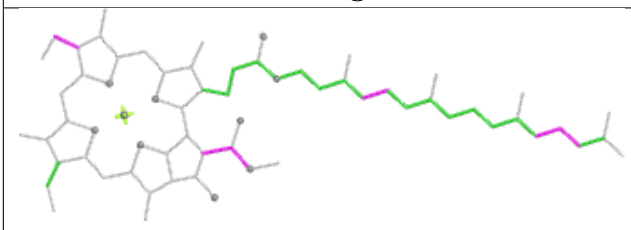
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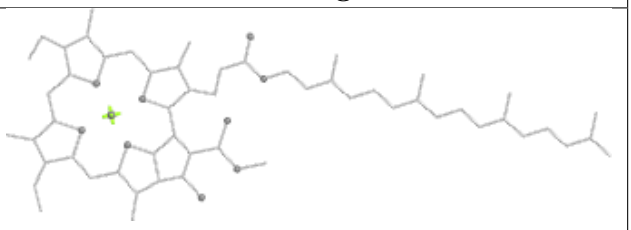
Bond lengths



Bond angles



Torsions



Rings

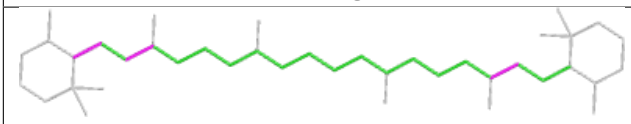
Ligand BCR i1 101



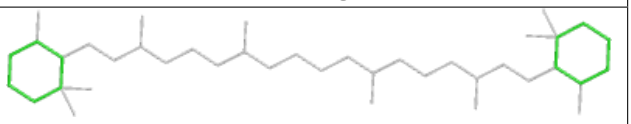
Bond lengths



Bond angles

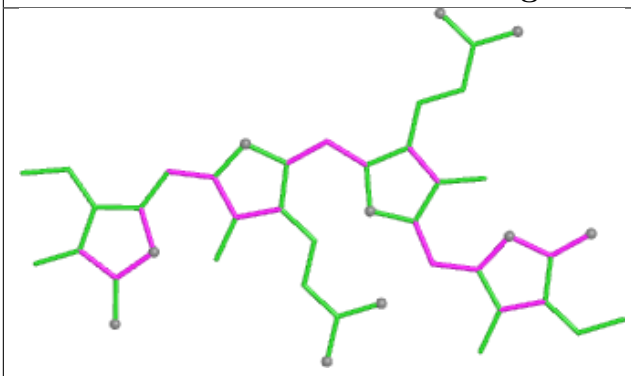


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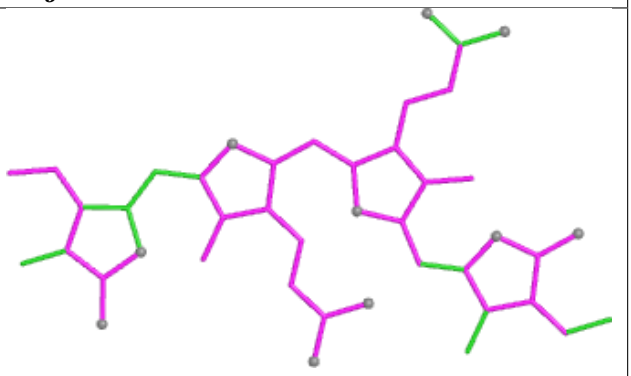


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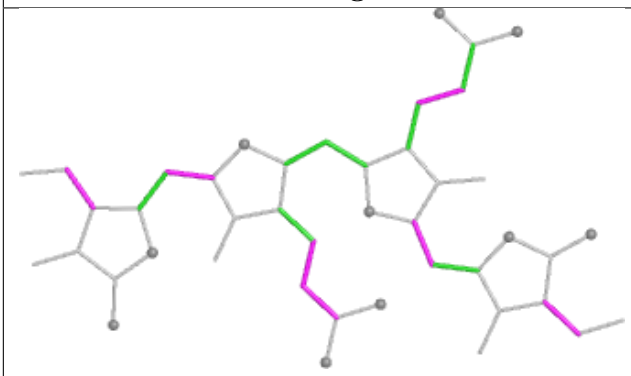
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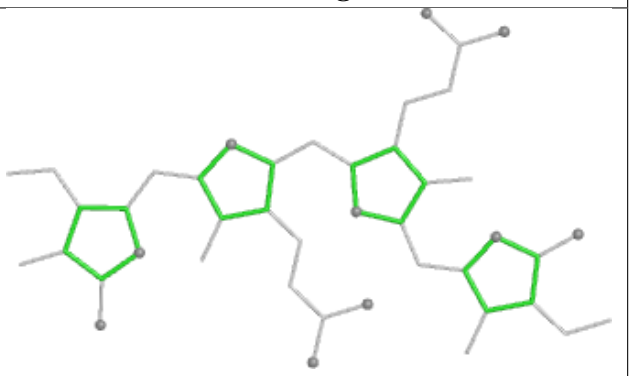
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Bond angles

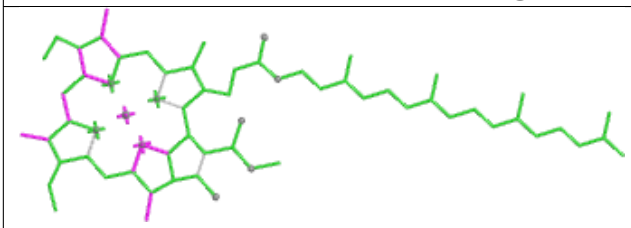


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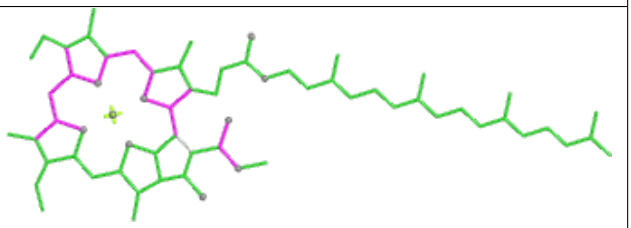


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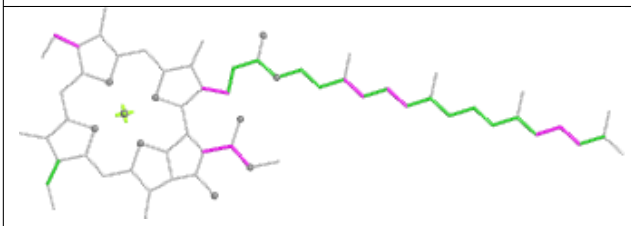
Ligand CLA HE 103



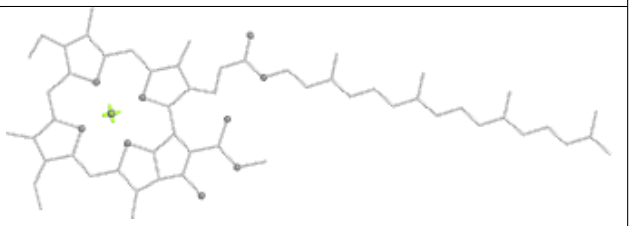
Bond lengths



Bond angles

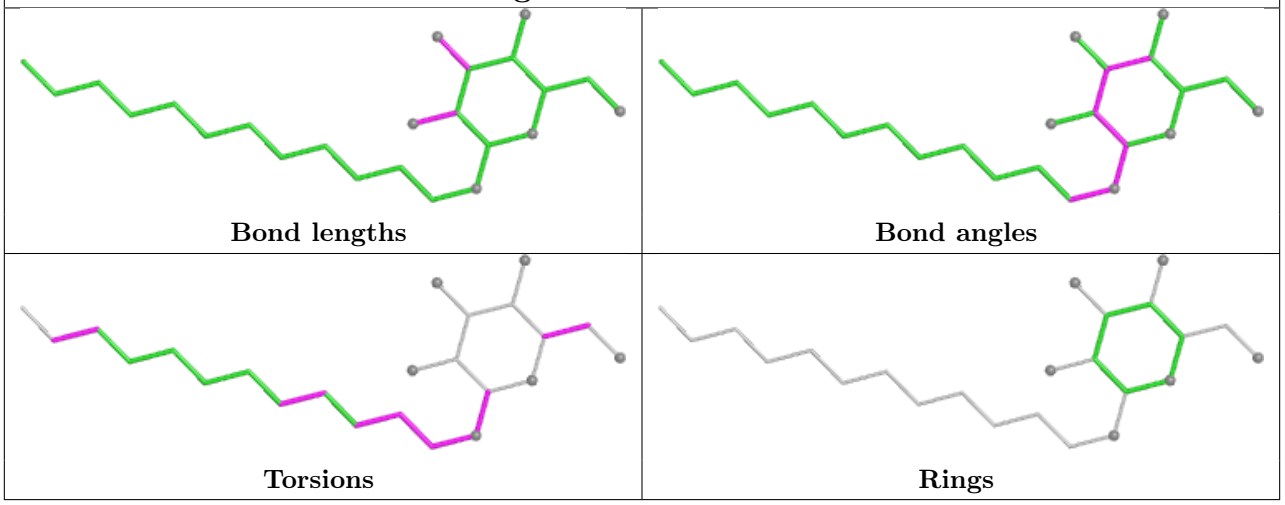


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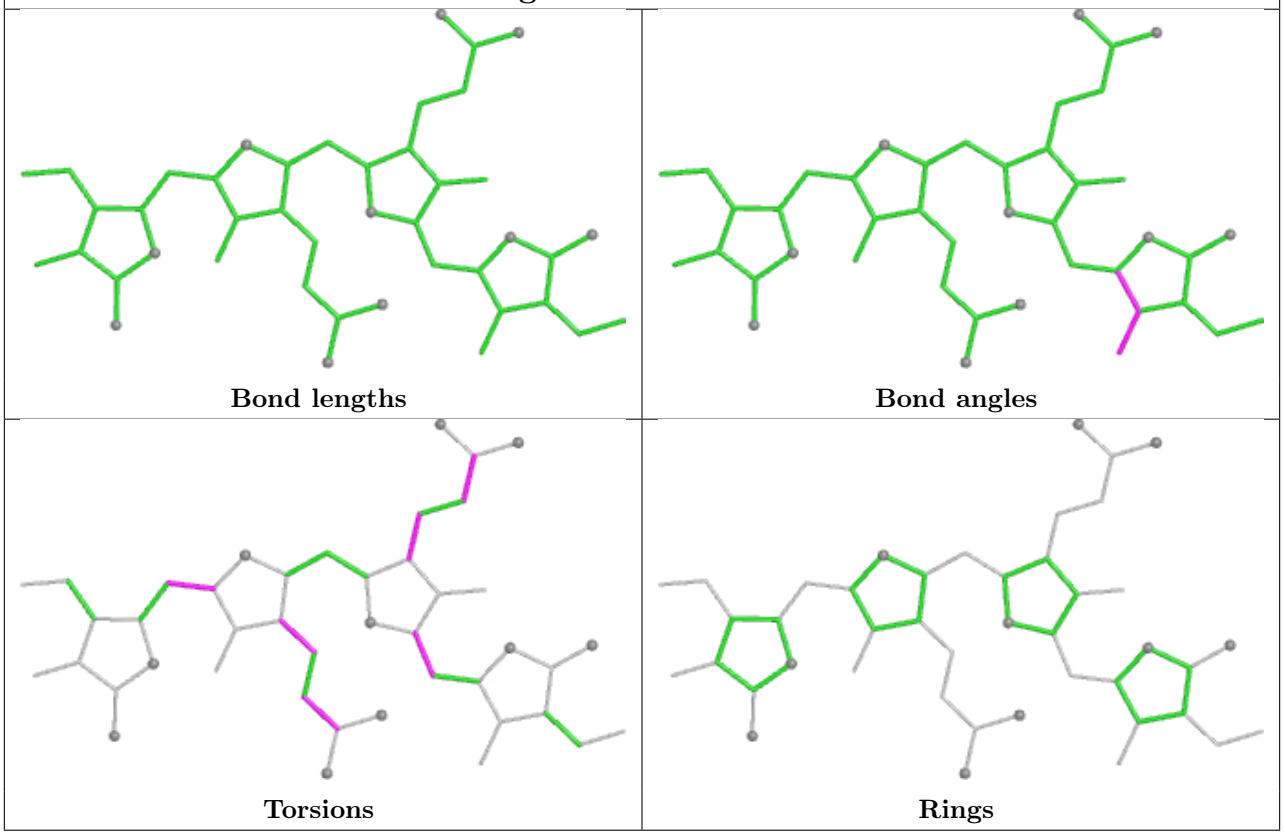


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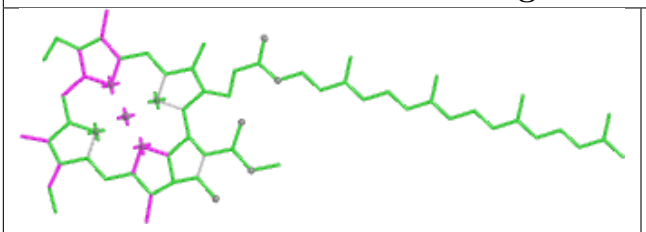
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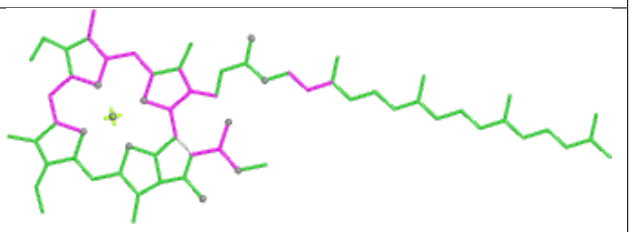
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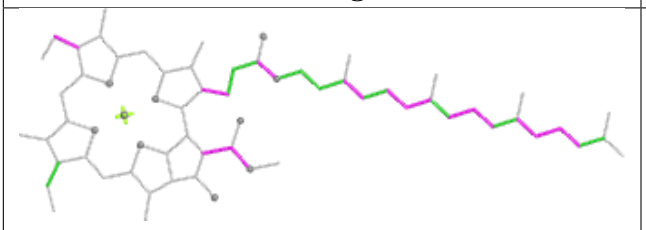
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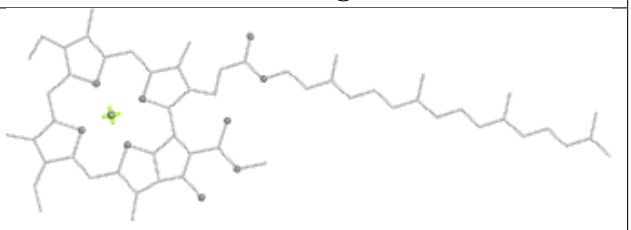
Bond lengths



Bond angles

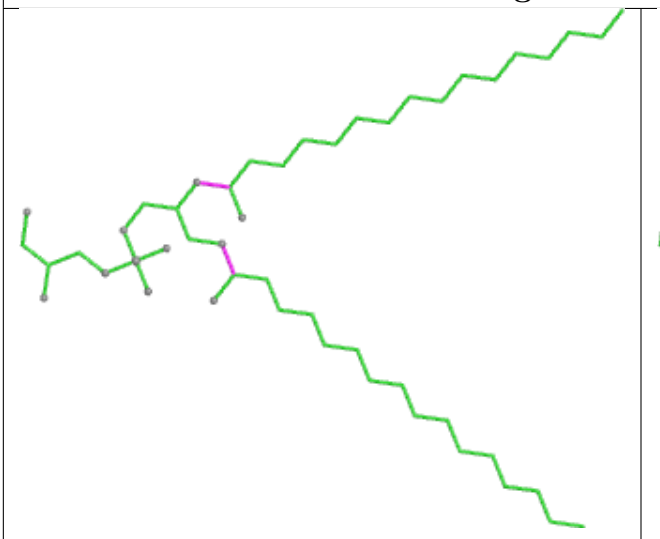


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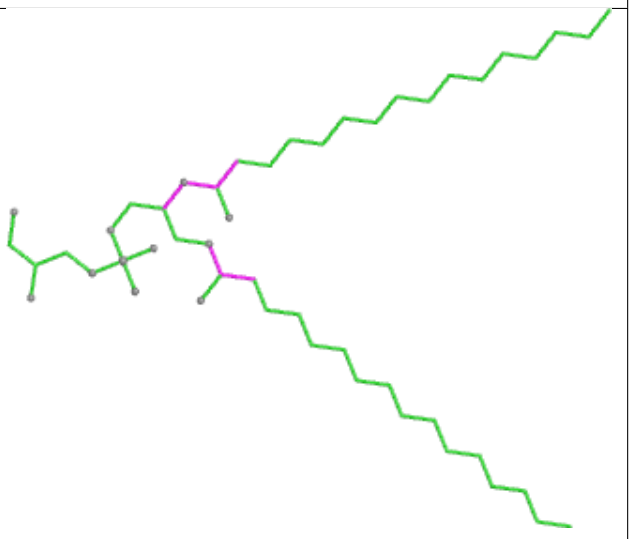


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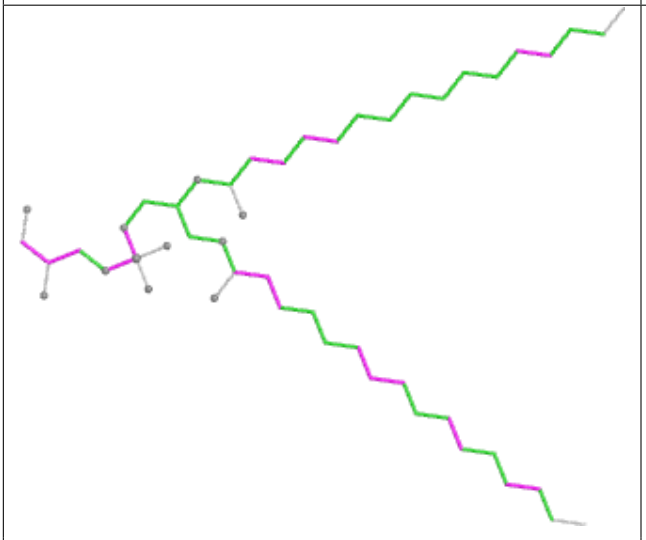
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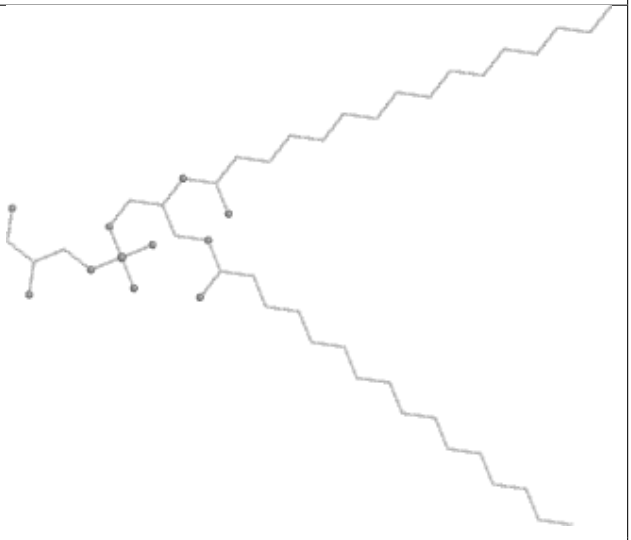
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Bond angles

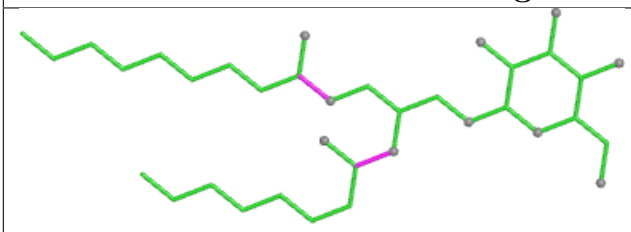


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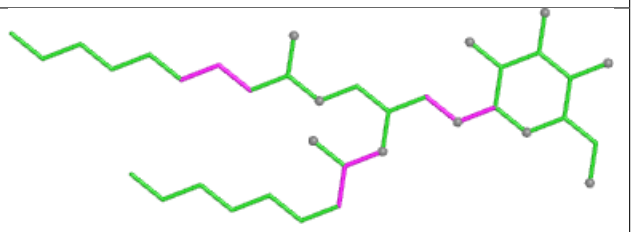


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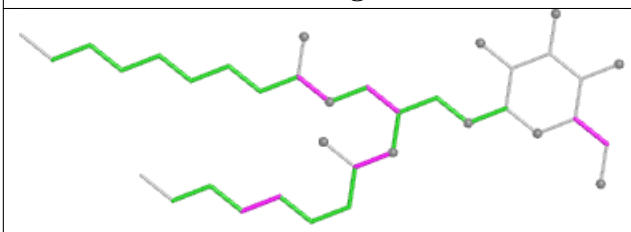
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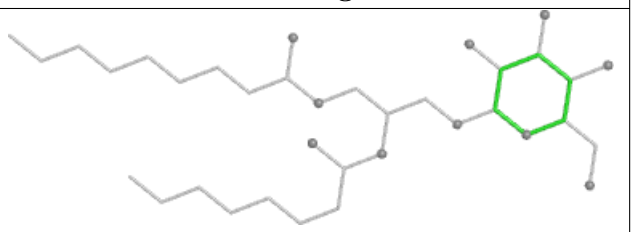
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Bond angles

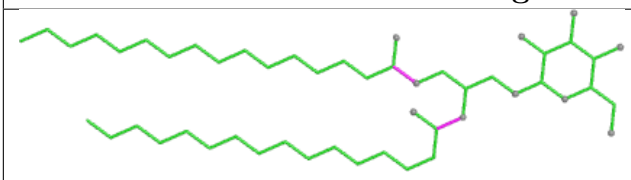


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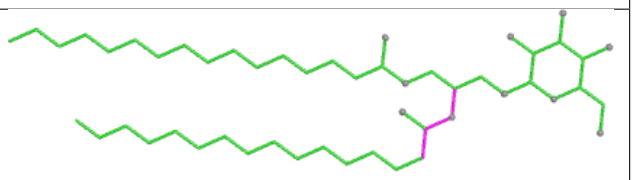


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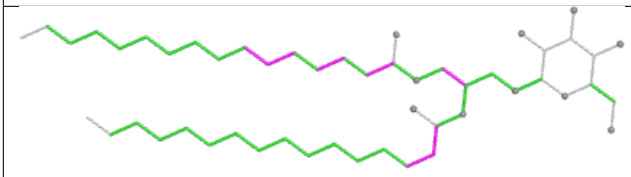
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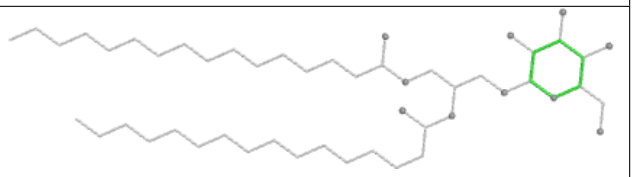
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Bond angles

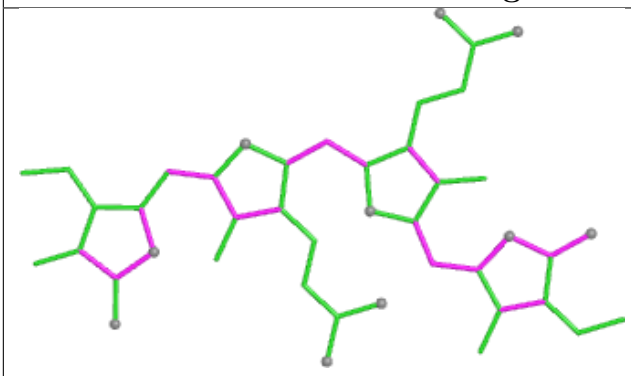


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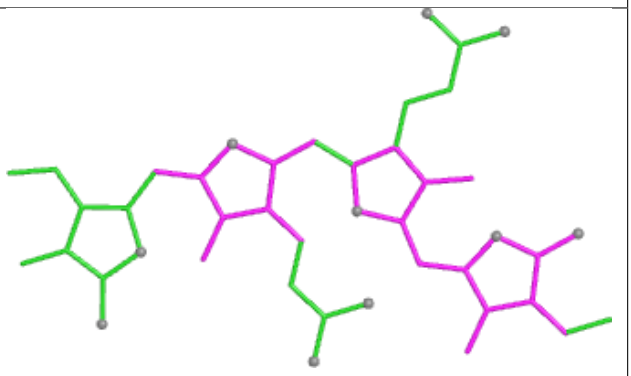


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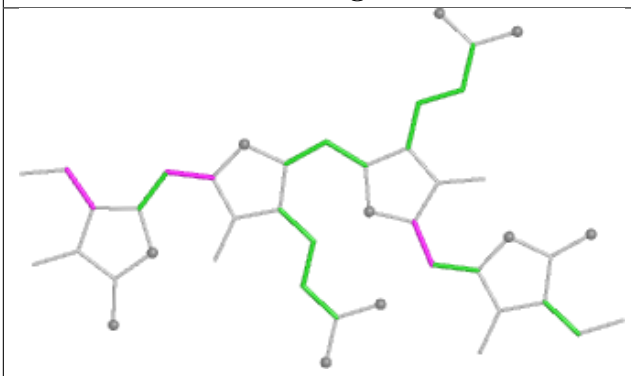
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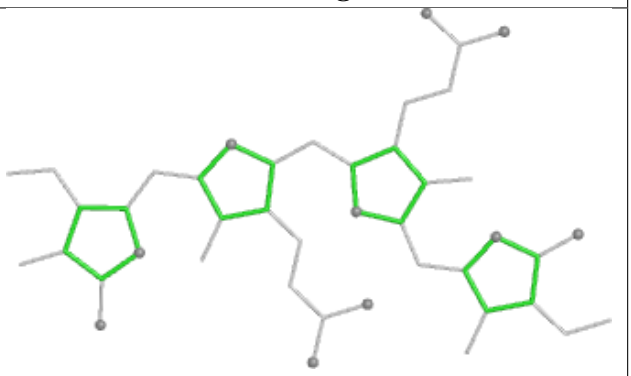
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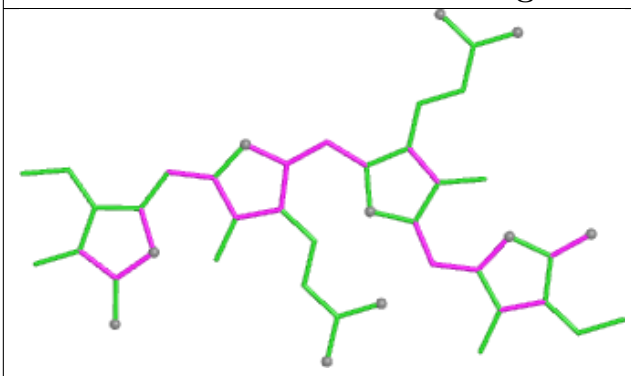


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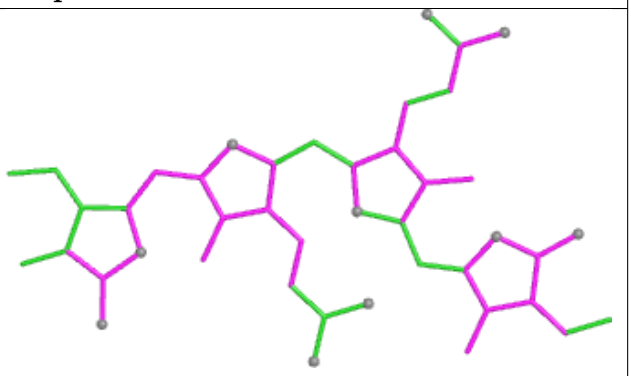


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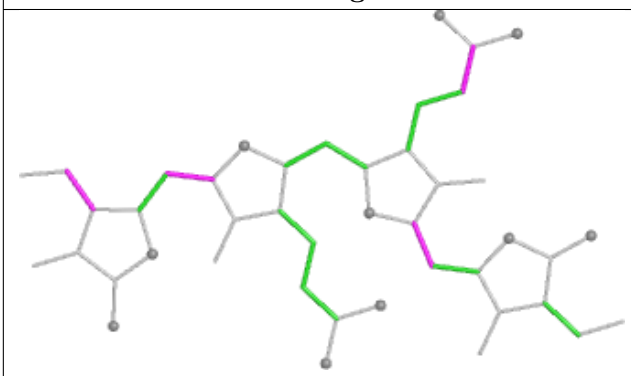
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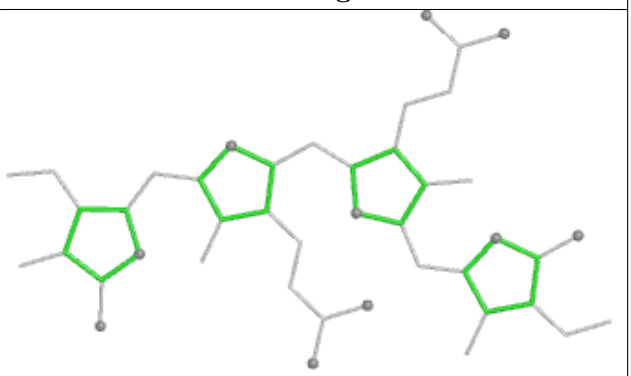
Bond lengths



Bond angles

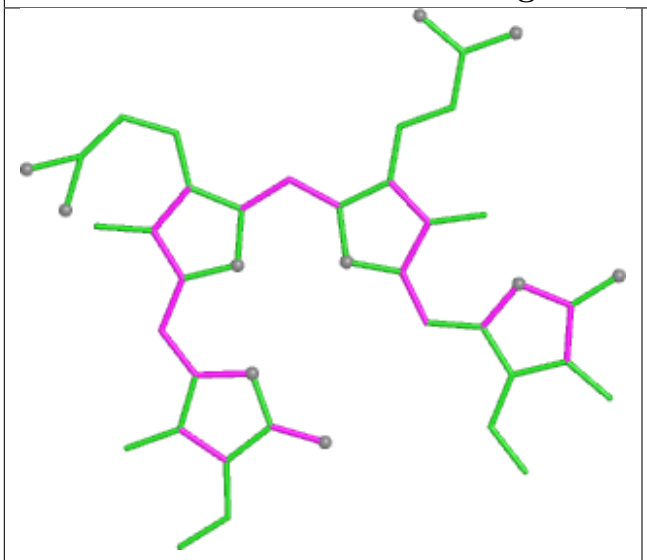


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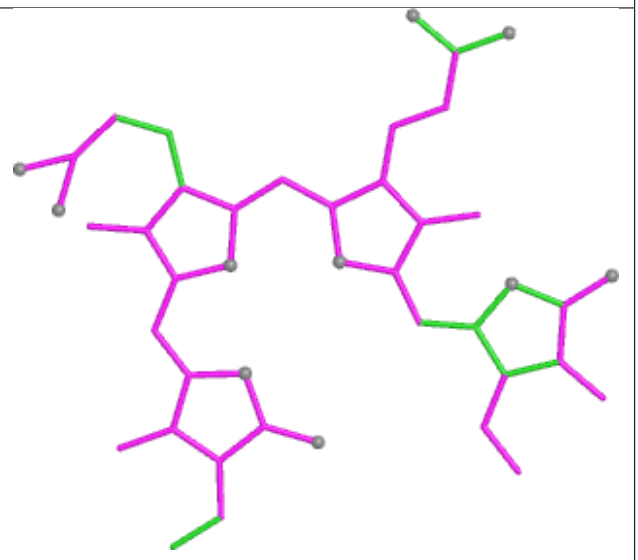


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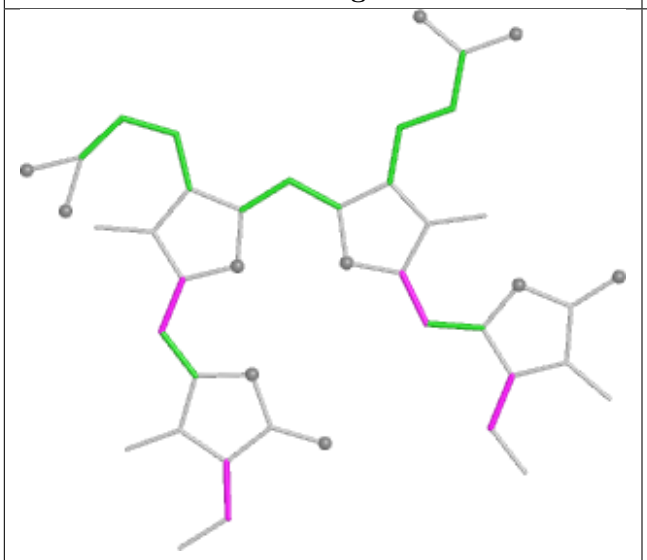
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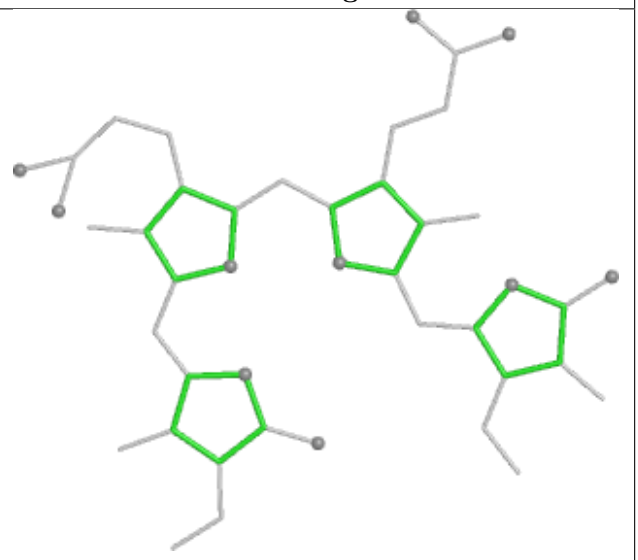
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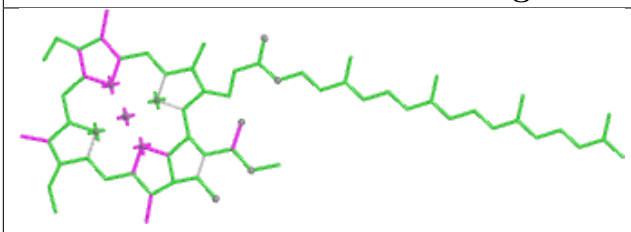


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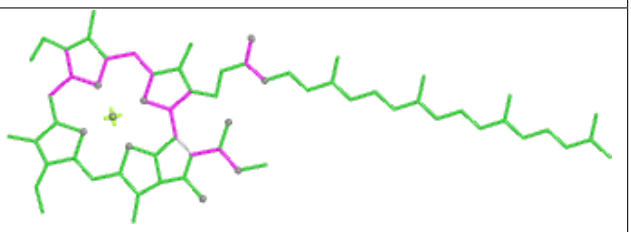


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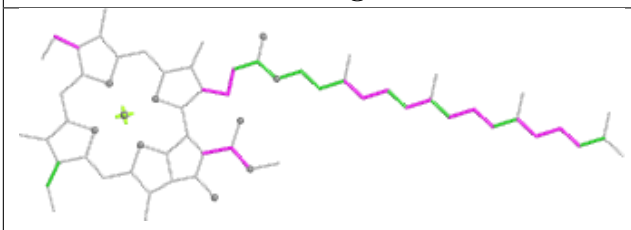
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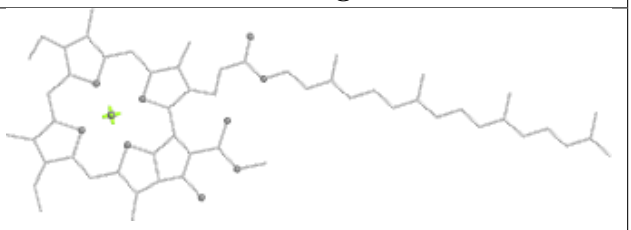
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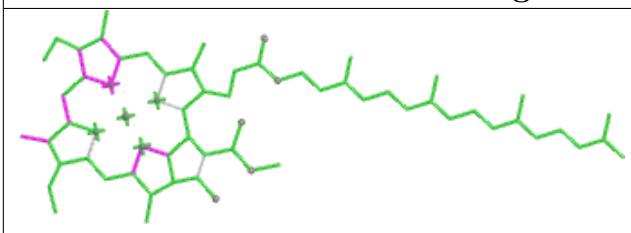


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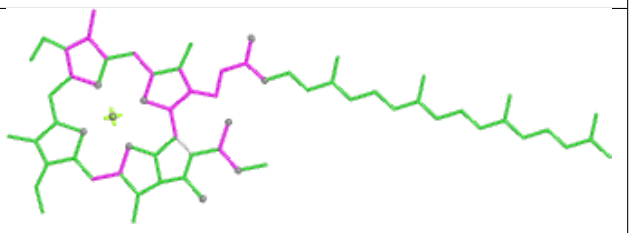


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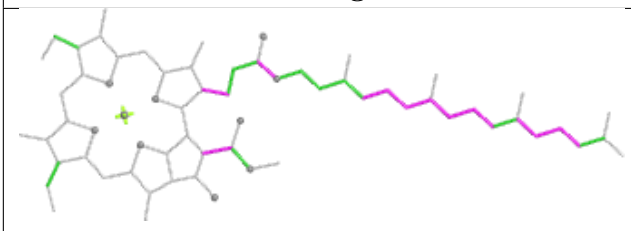
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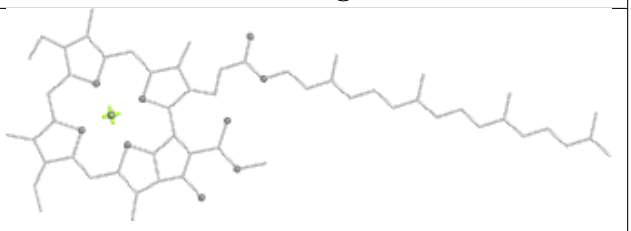
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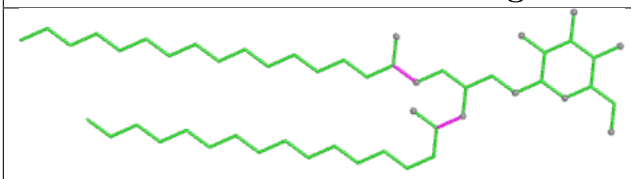


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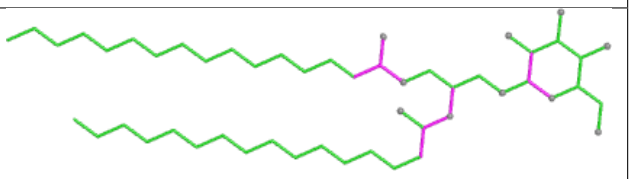


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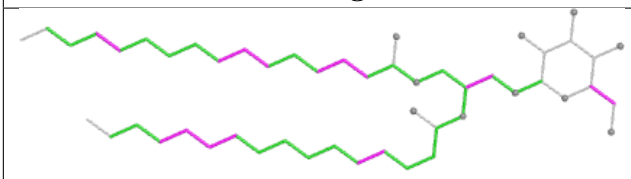
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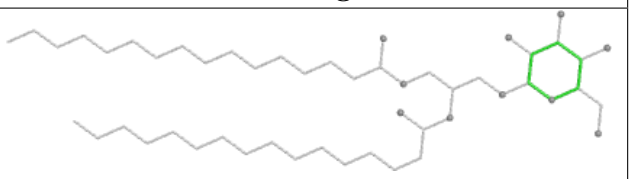
Bond lengths



Bond angles

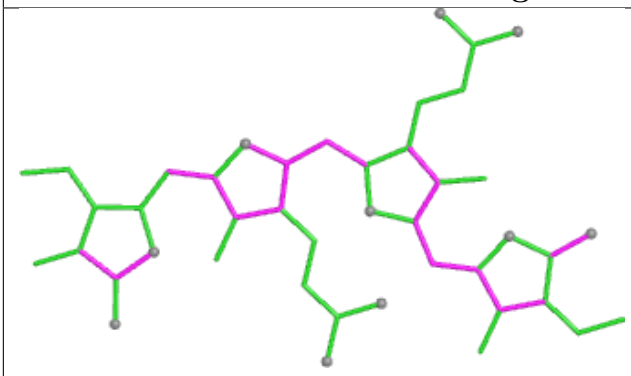


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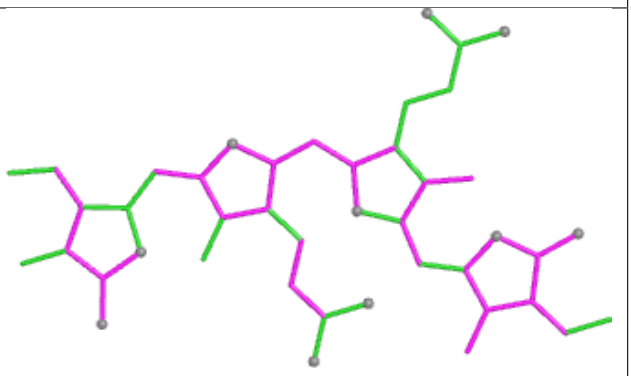


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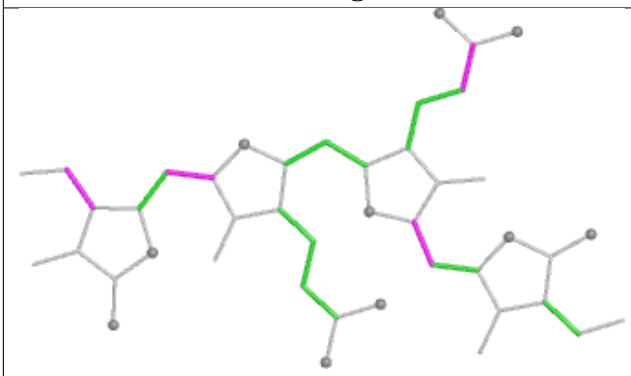
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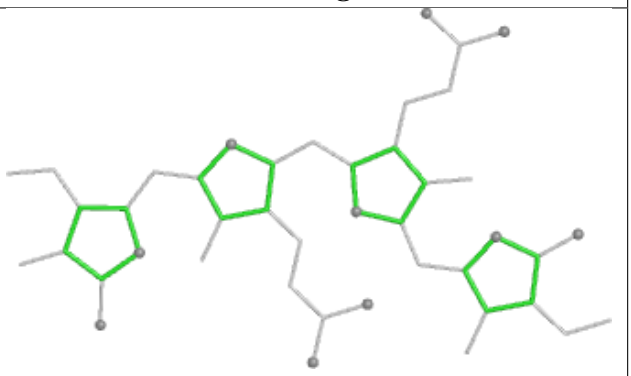
Bond lengths



Bond angles

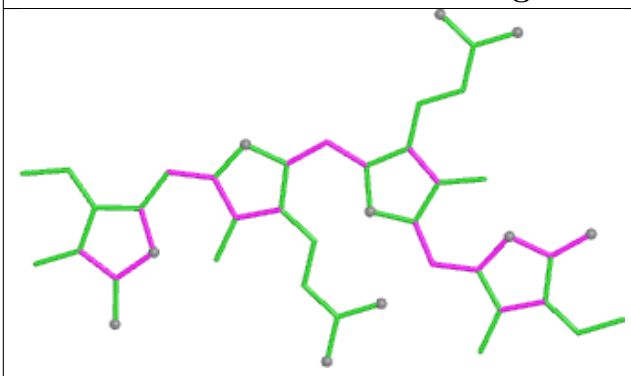


Torsions

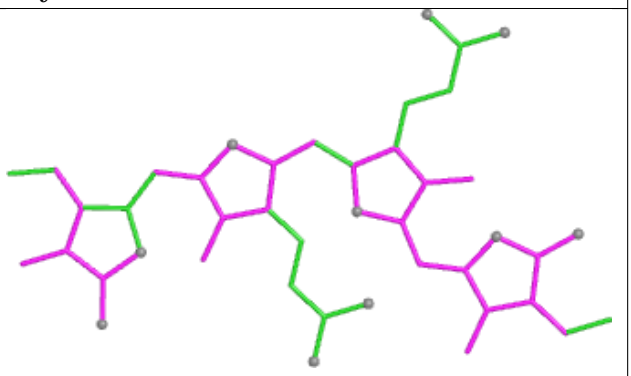


Rings

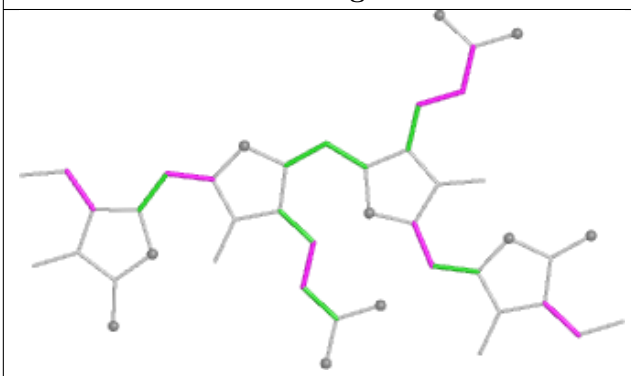
Ligand CYC yB 201



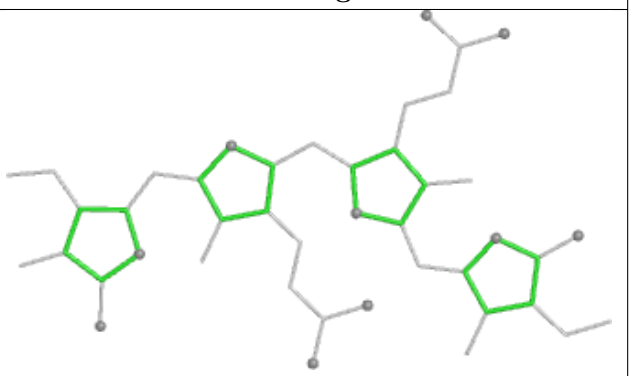
Bond lengths



Bond angles

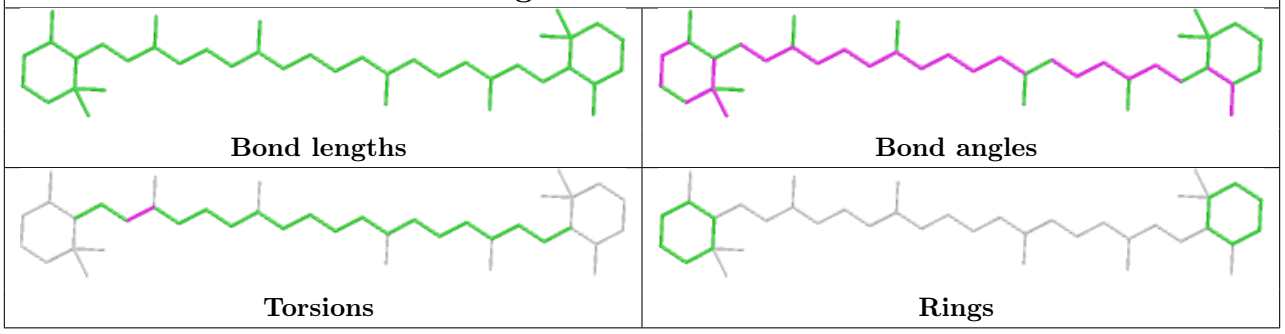


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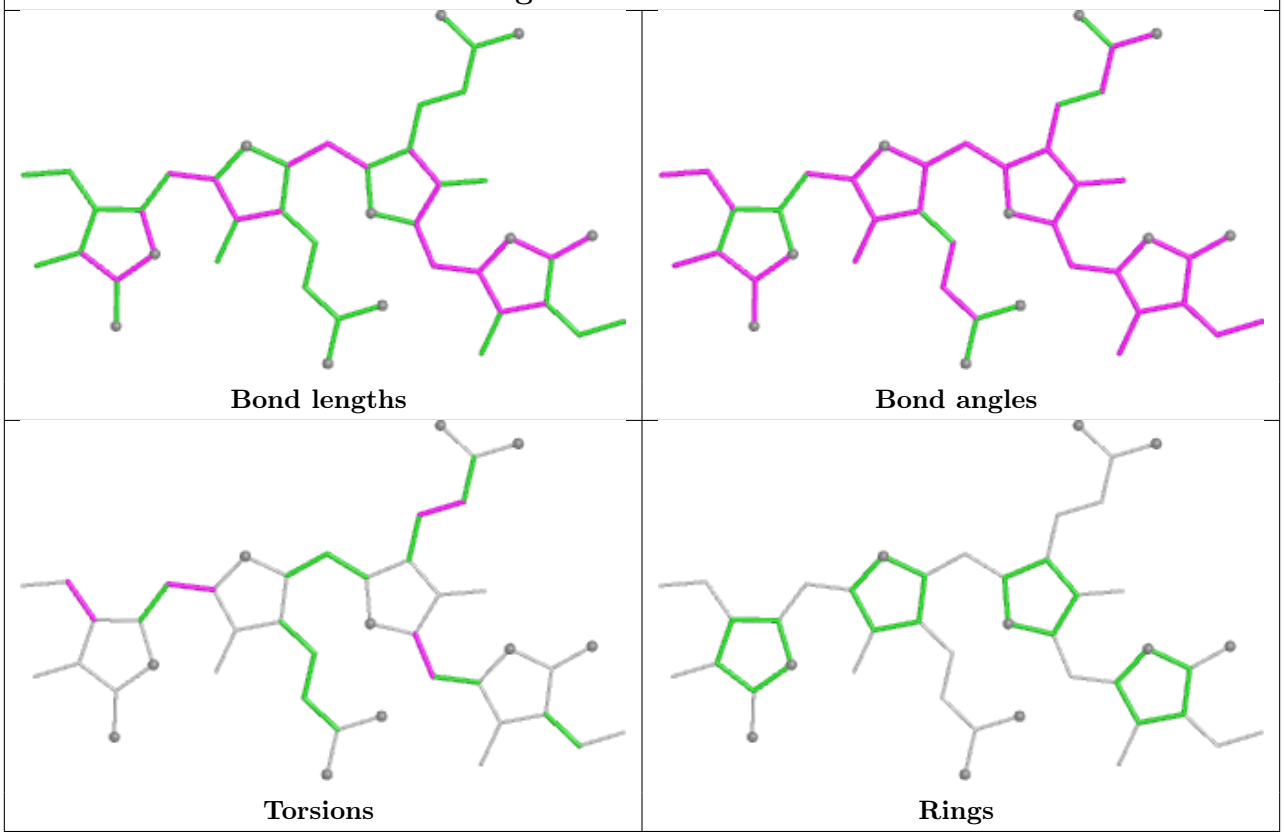


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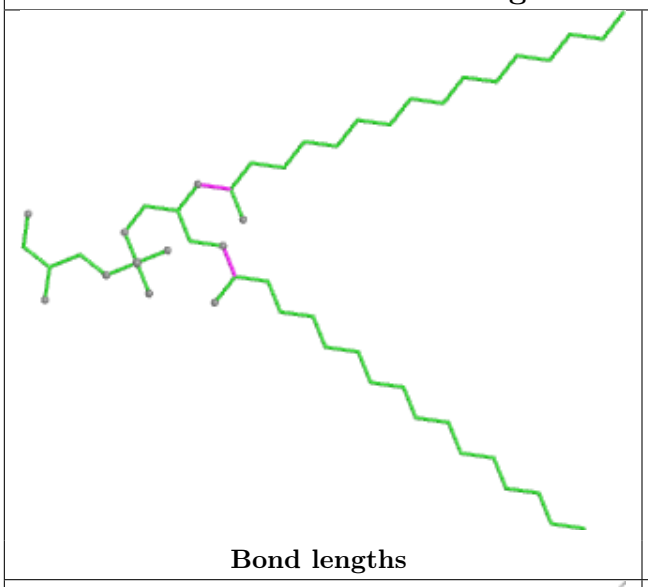
Ligand BCR kE 102



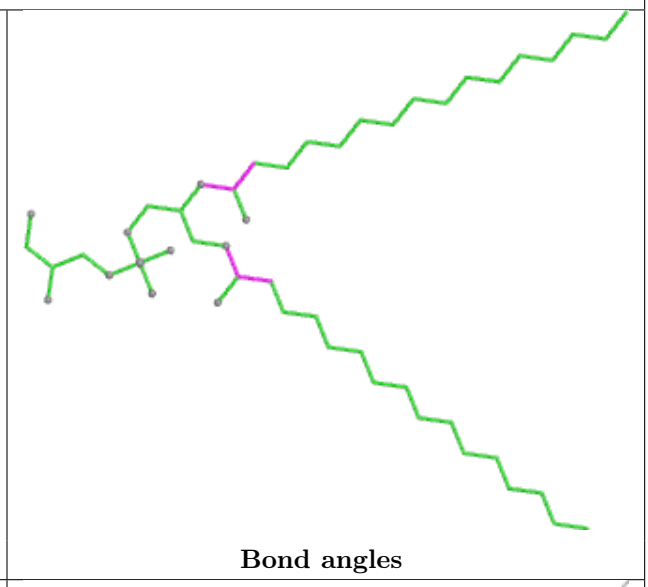
Ligand CYC IG 201



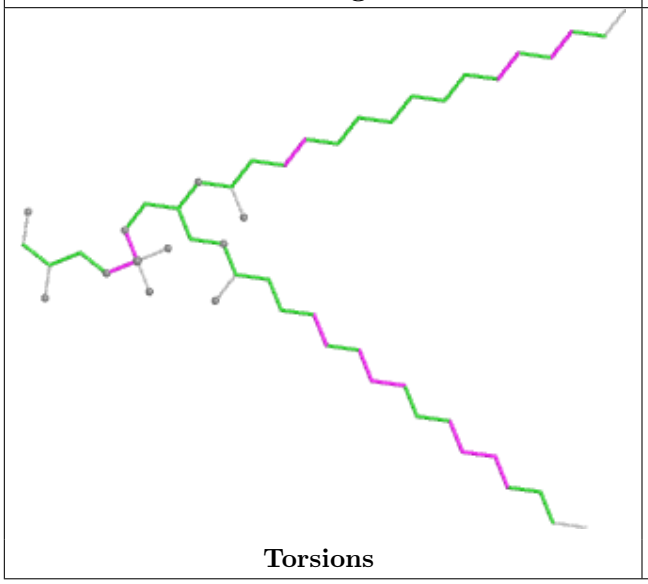
Ligand LHG DD 409



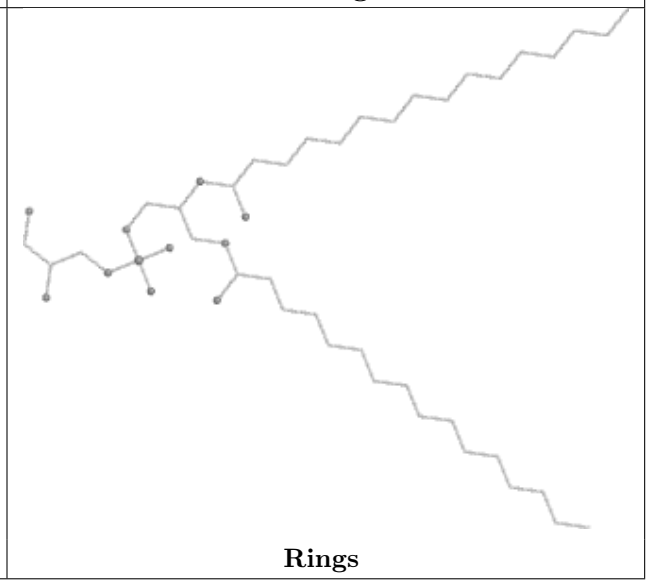
Bond lengths



Bond angles

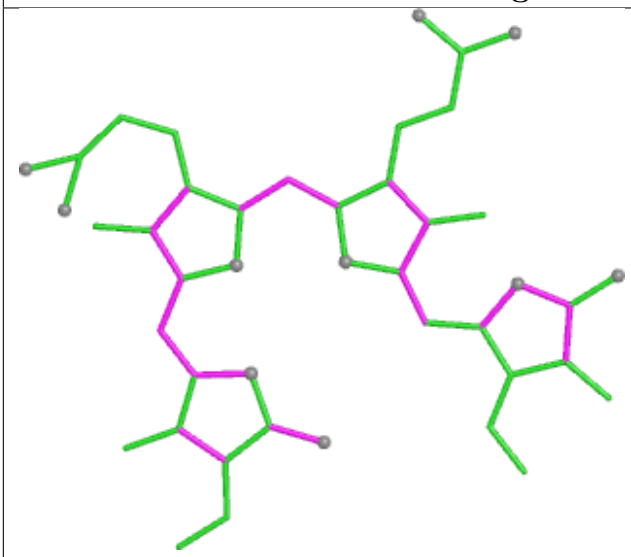


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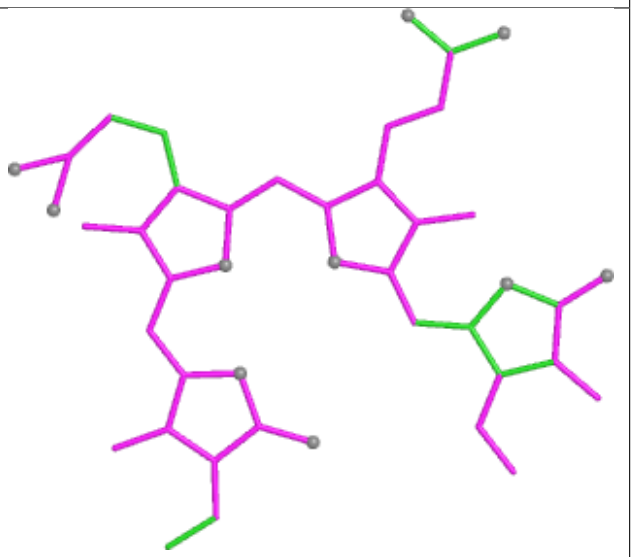


Rings

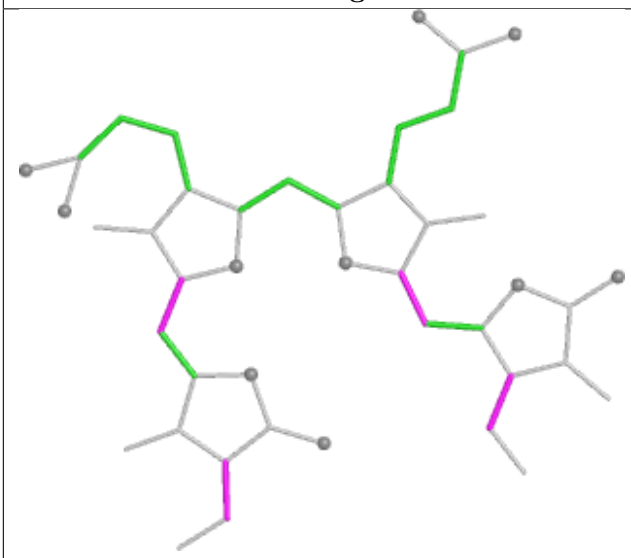
Ligand CYC kH 201



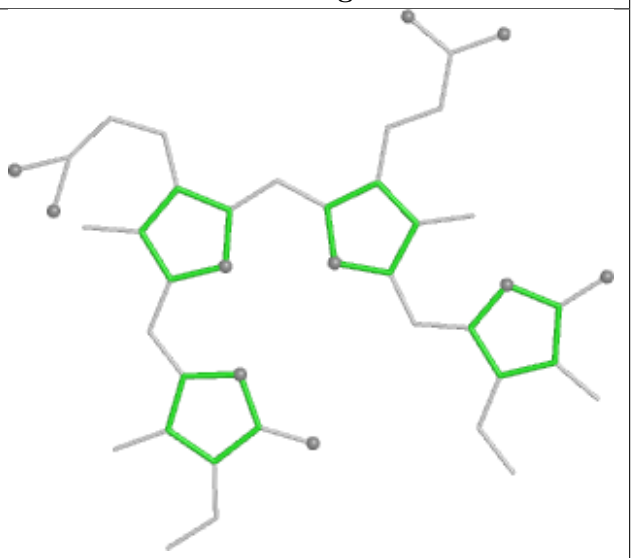
Bond lengths



Bond angles

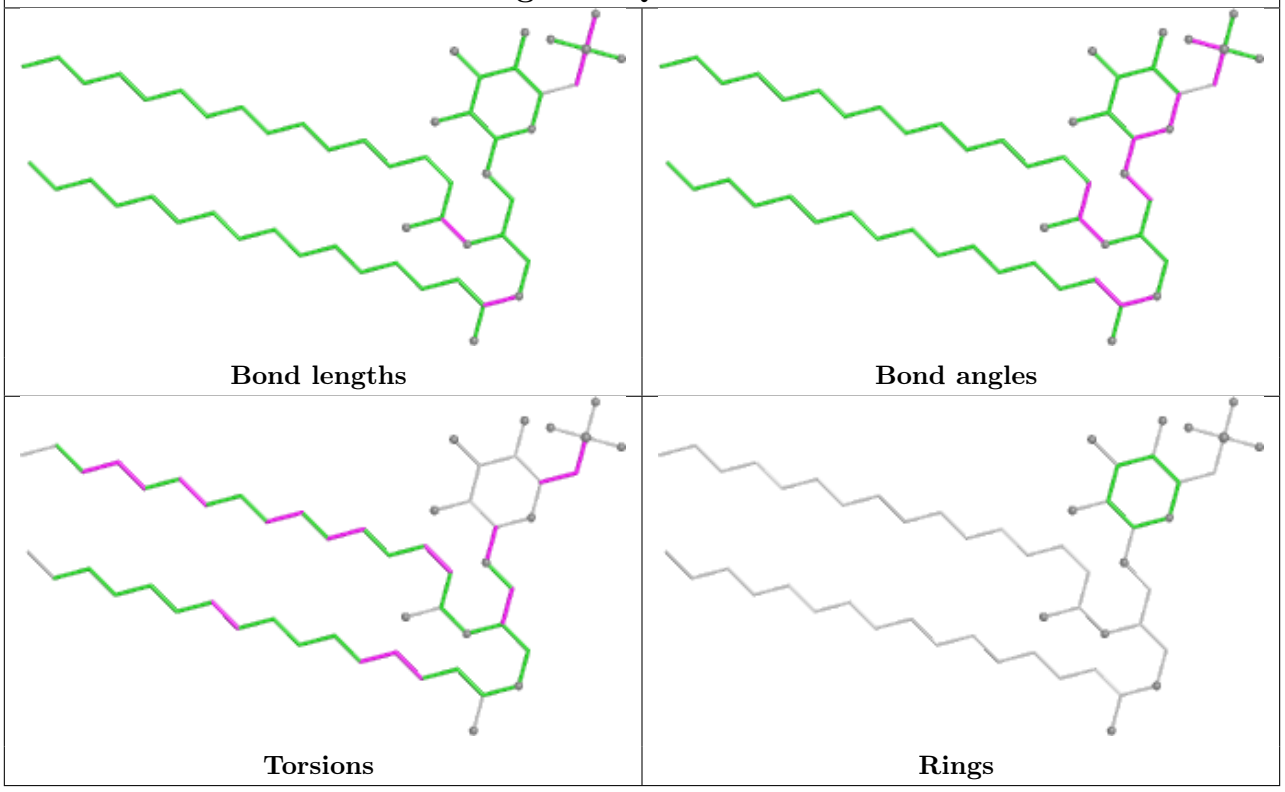


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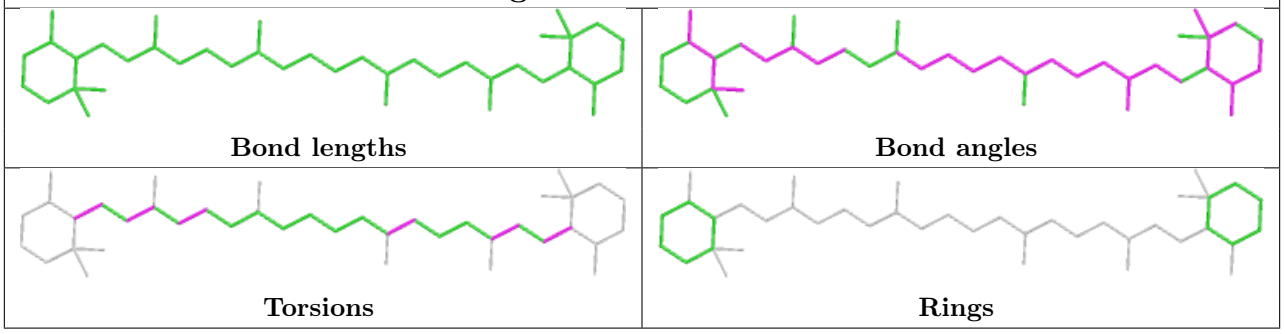


Rings

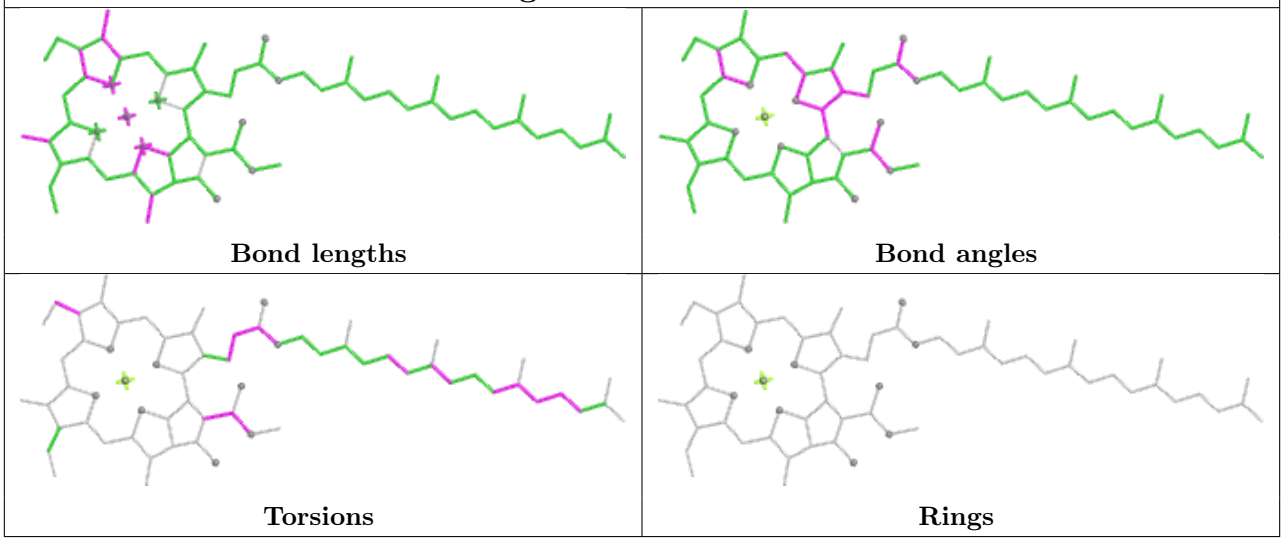
Ligand SQD cD 502



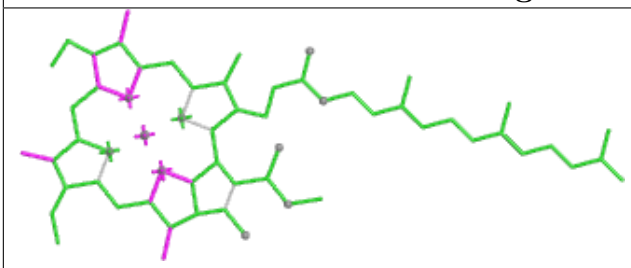
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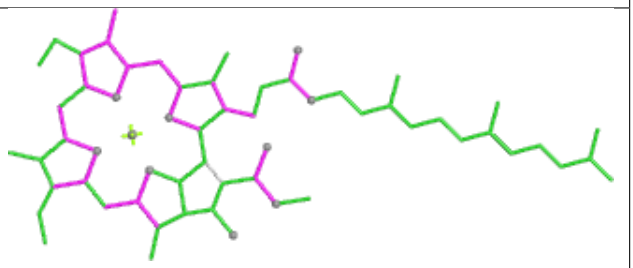
Ligand CLA b1 610



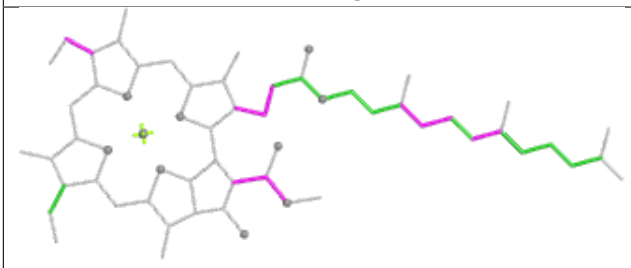
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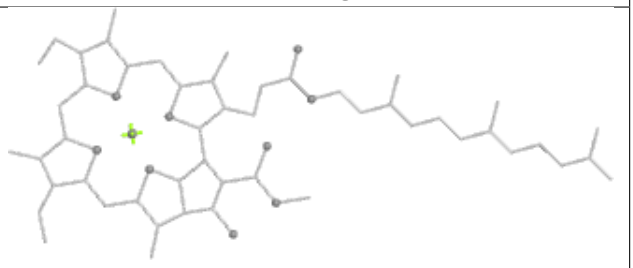
Bond lengths



Bond angles

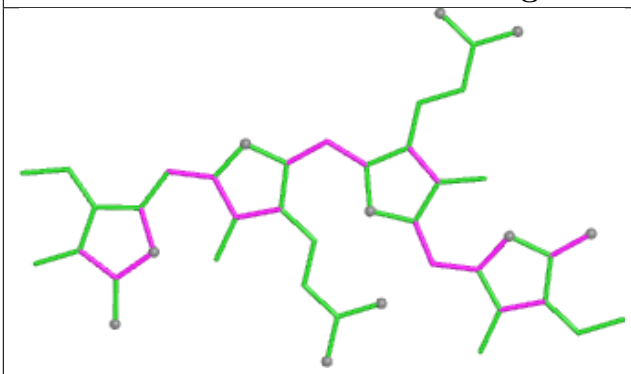


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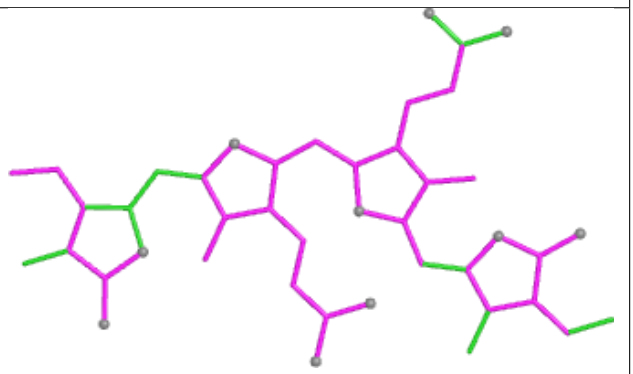


Rings

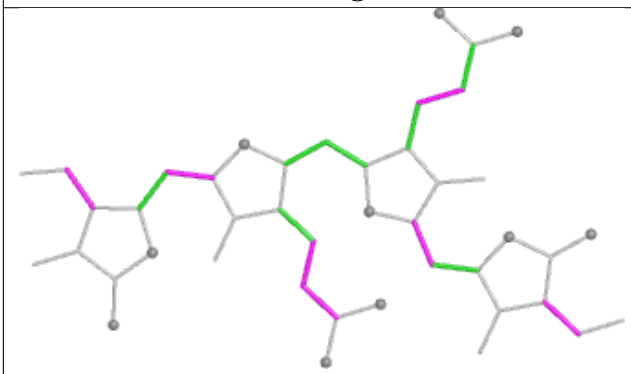
Ligand CYC l2 201



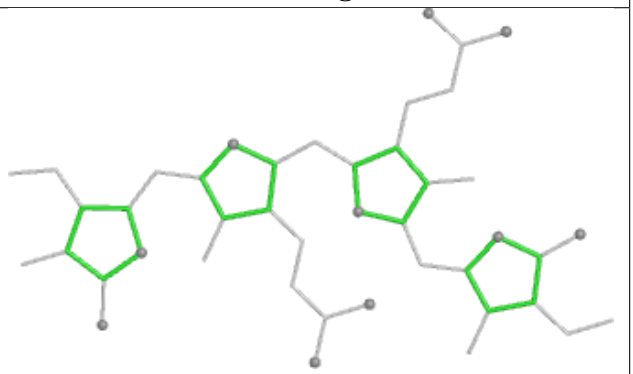
Bond lengths



Bond angles

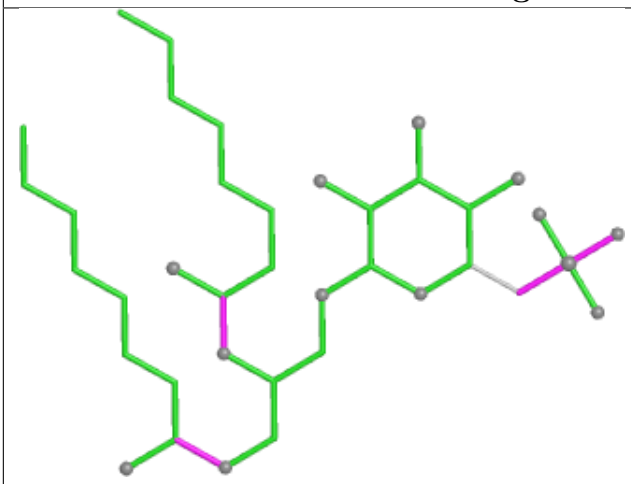


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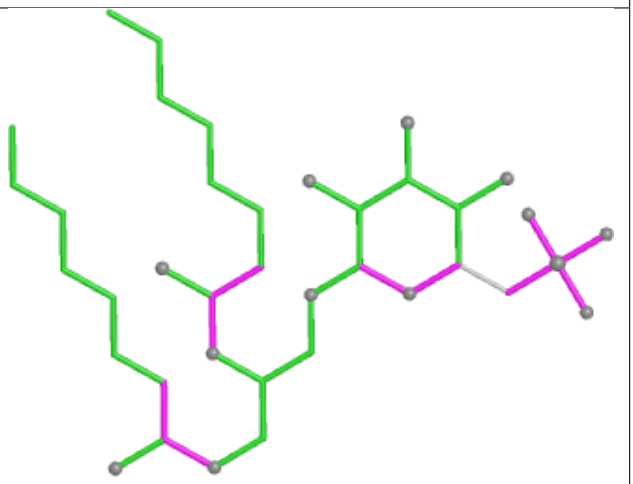


Rings

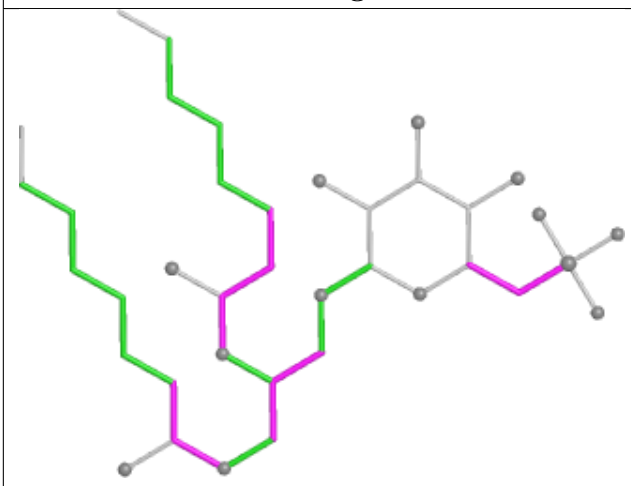
Ligand SQD BE 621



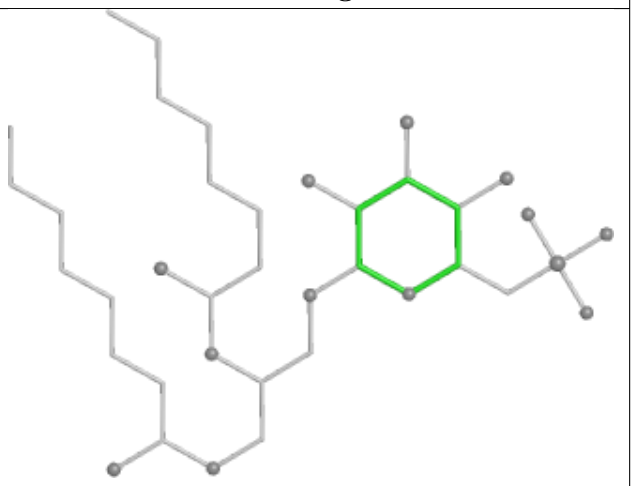
Bond lengths



Bond angles

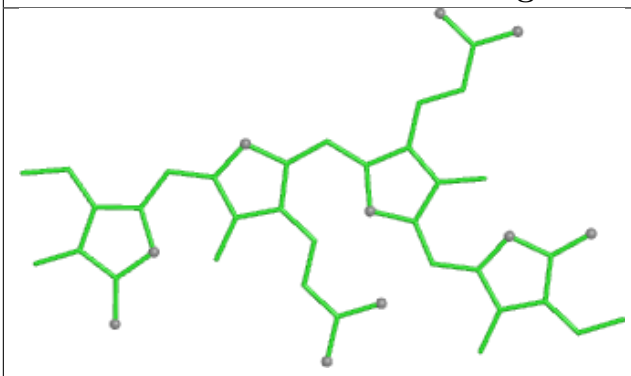


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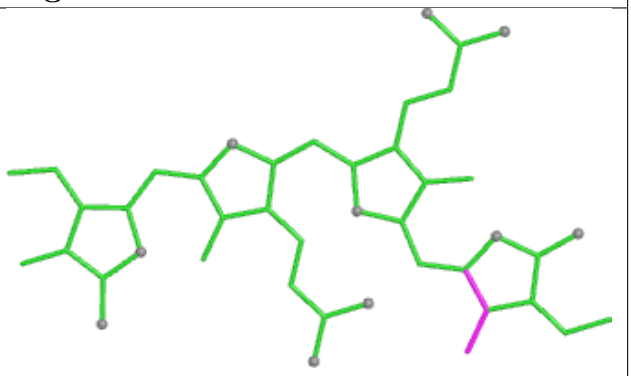


Rings

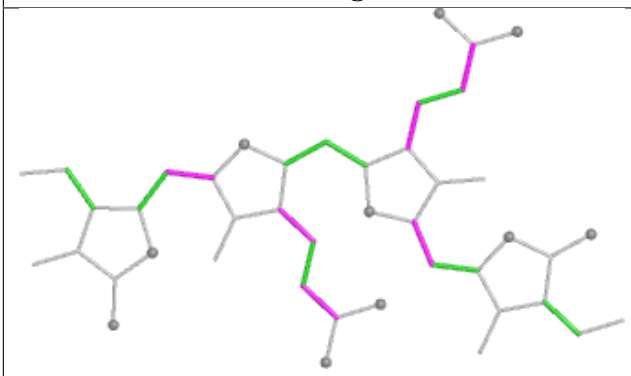
Ligand CYC g9 201



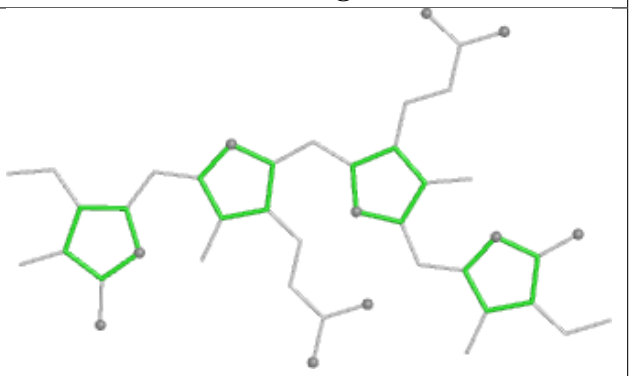
Bond lengths



Bond angles

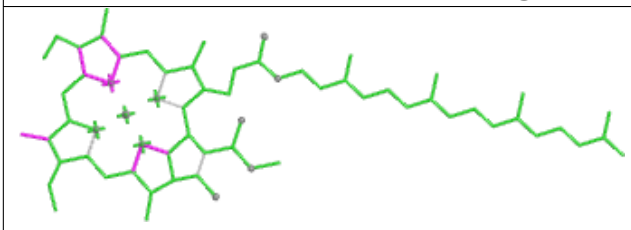


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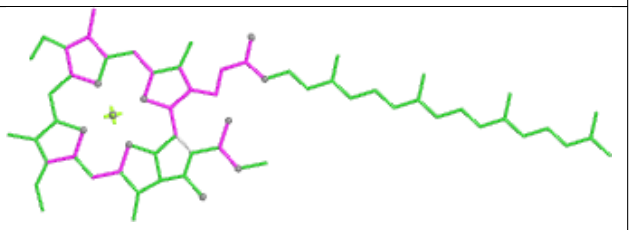


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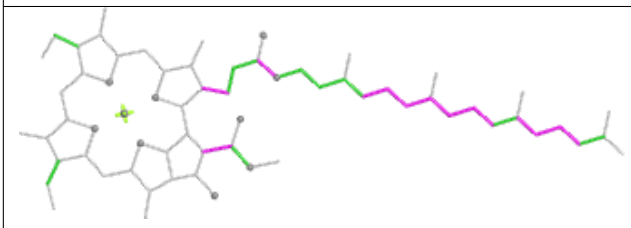
Ligand CLA bE 612



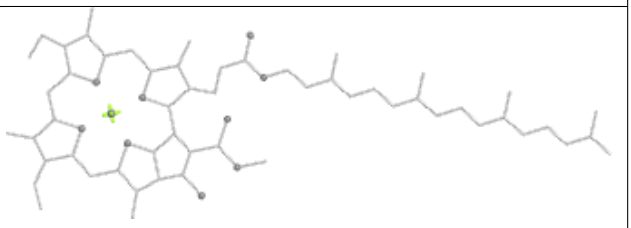
Bond lengths



Bond angles

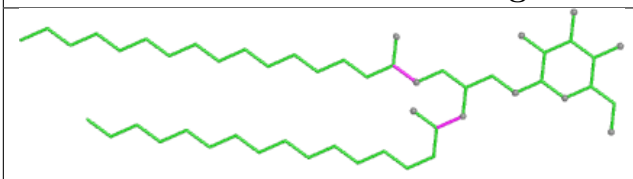


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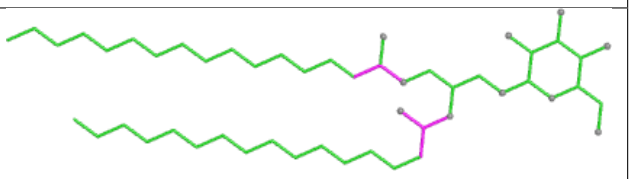


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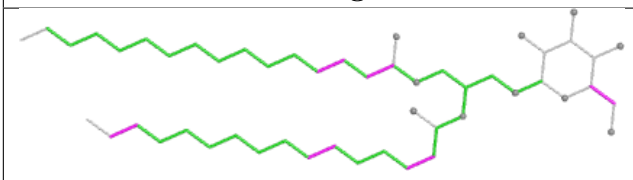
Ligand LMG bD 619



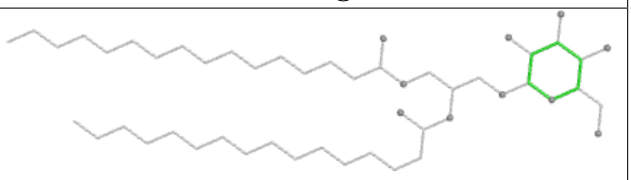
Bond lengths



Bond angles

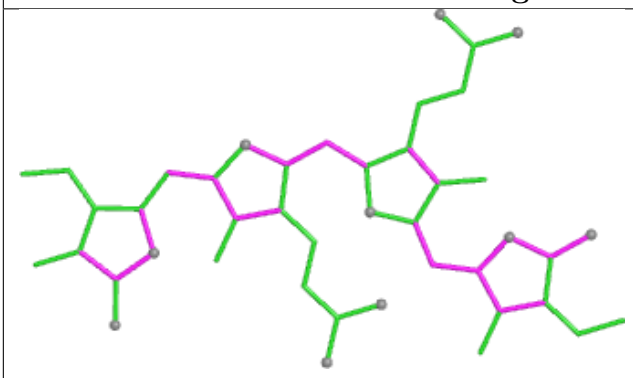


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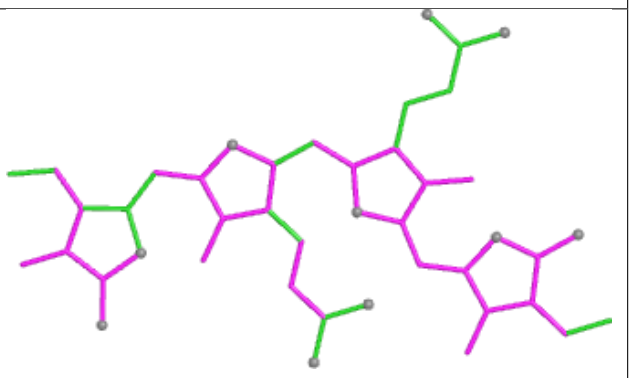


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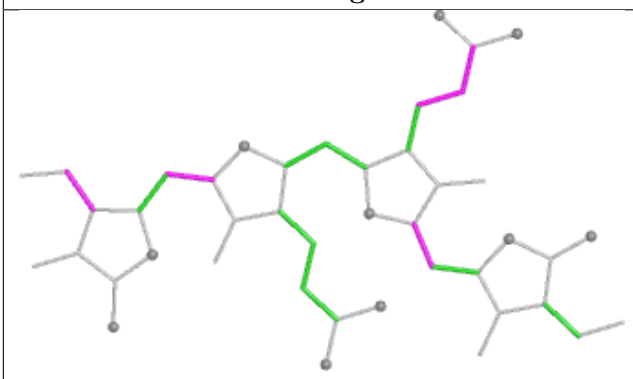
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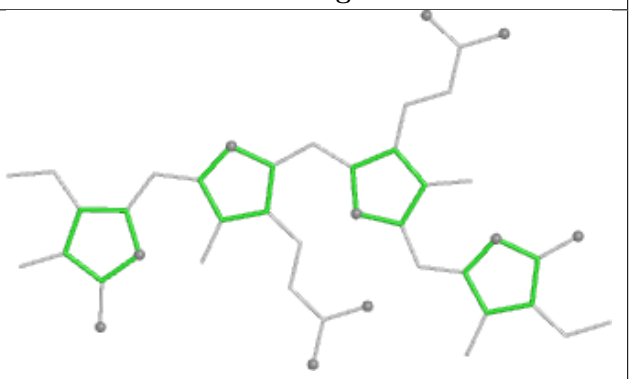
Bond lengths



Bond angles

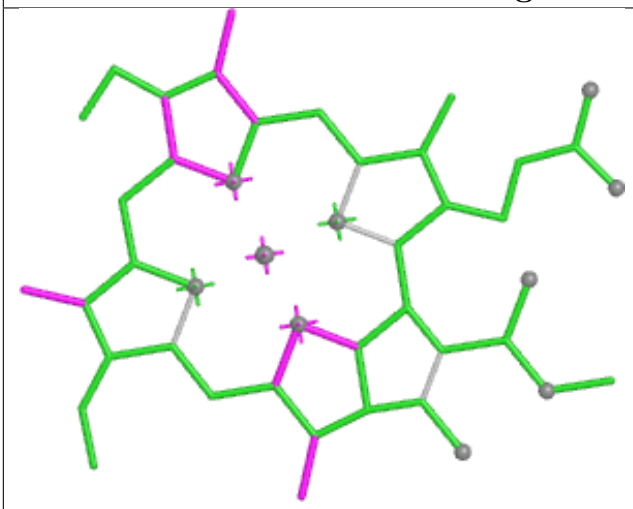


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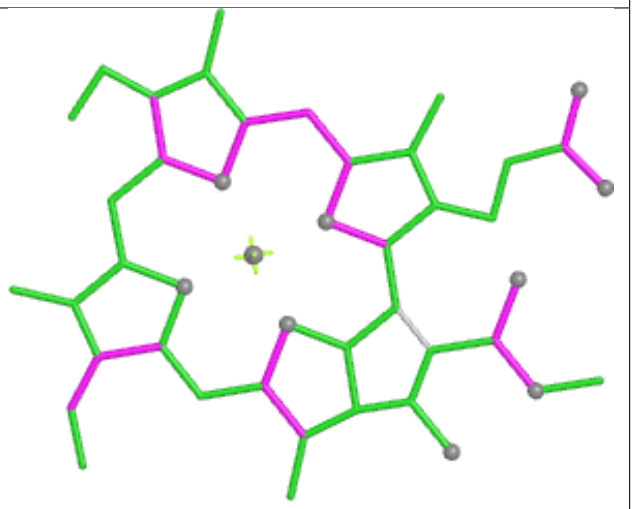


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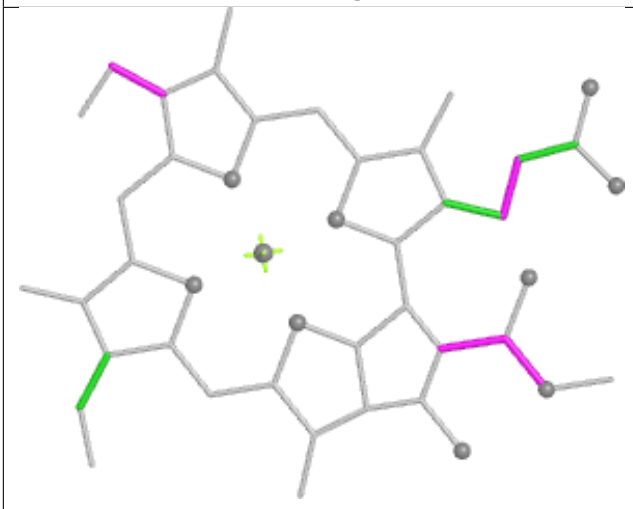
Ligand CLA B1 601



Bond lengths



Bond angles

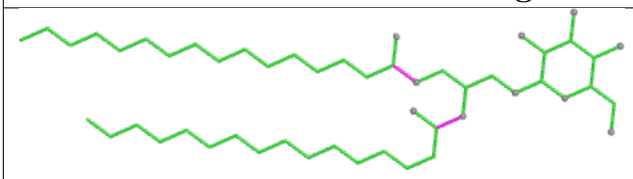


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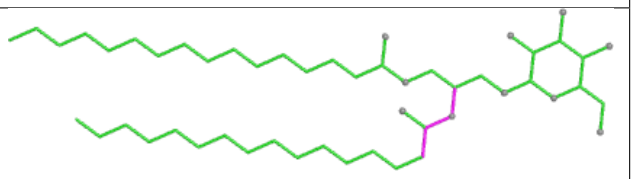


Rings

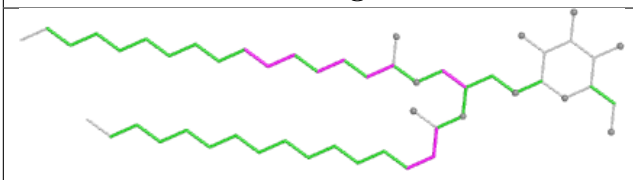
Ligand LMG a1 408



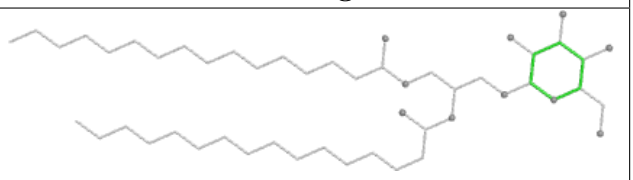
Bond lengths



Bond angles

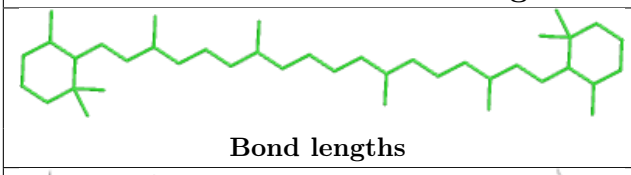


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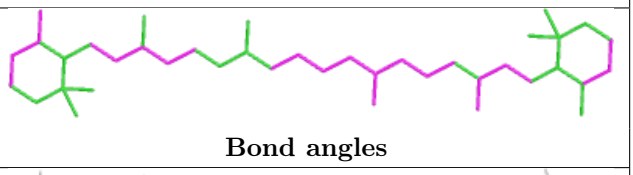


Rings

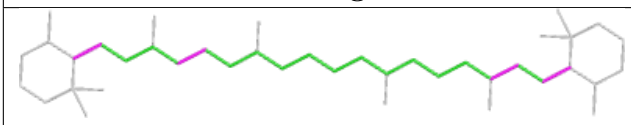
Ligand BCR DE 407



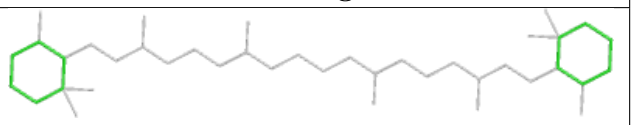
Bond lengths



Bond angles

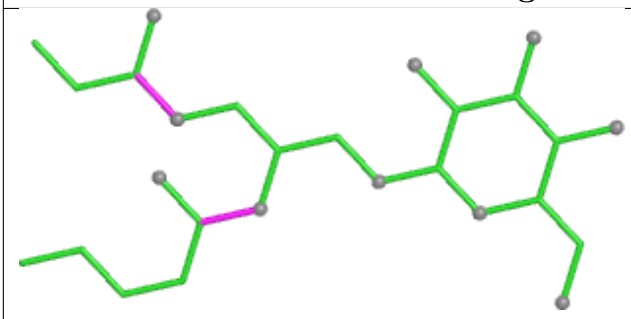


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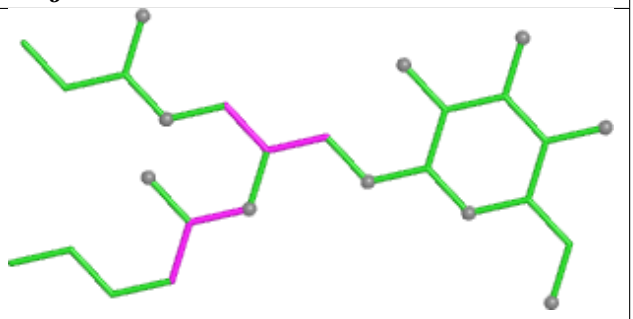


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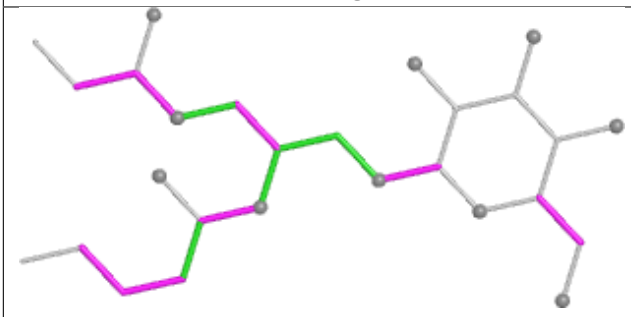
Ligand LMG j1 102



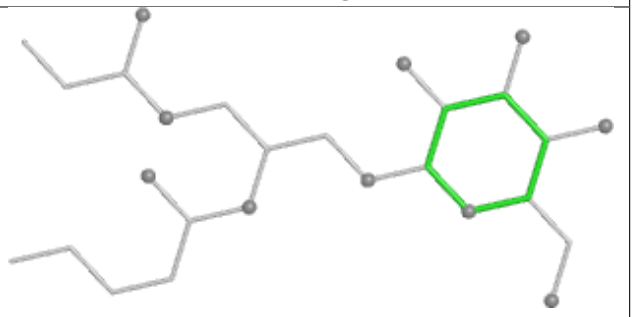
Bond lengths



Bond angles



Torsions

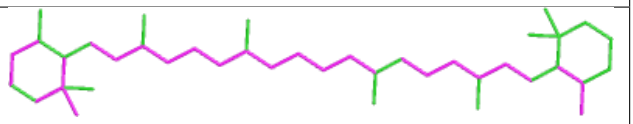


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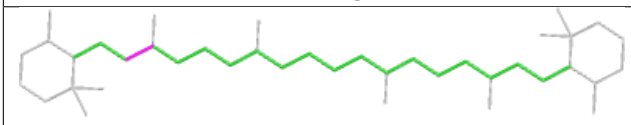
Ligand BCR kD 102



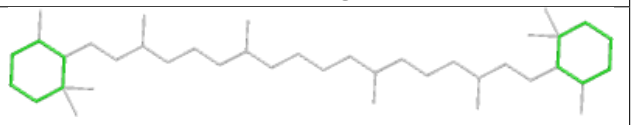
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Bond angles

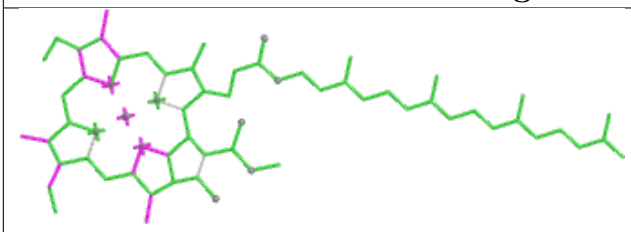


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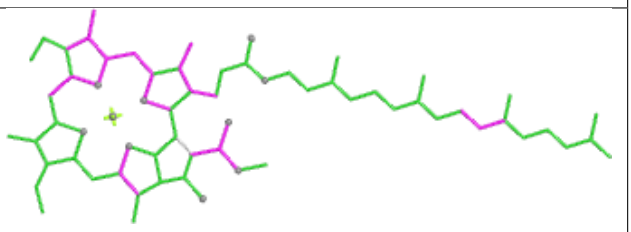


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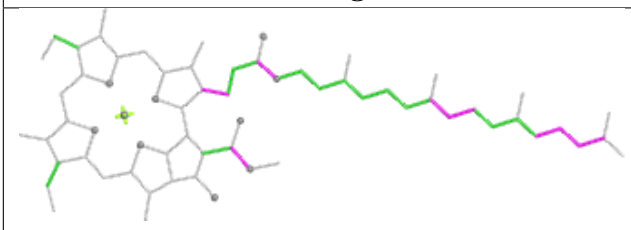
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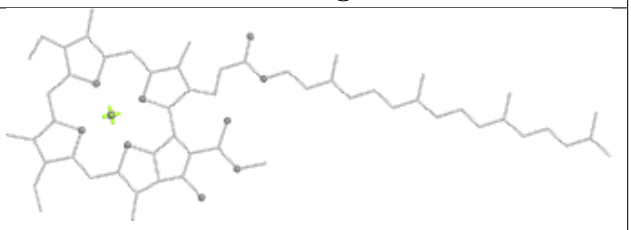
Bond lengths



Bond angles

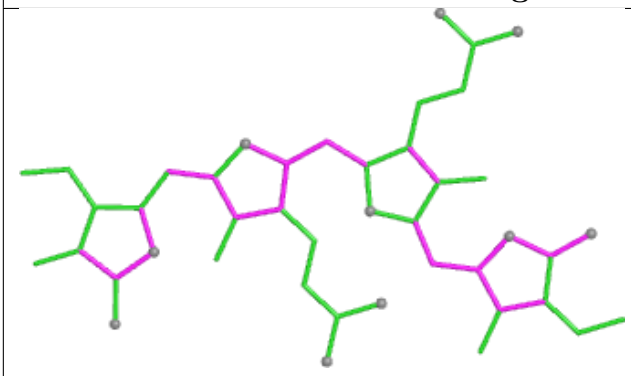


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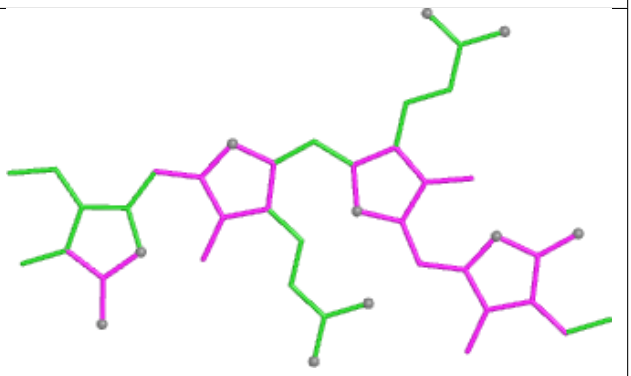


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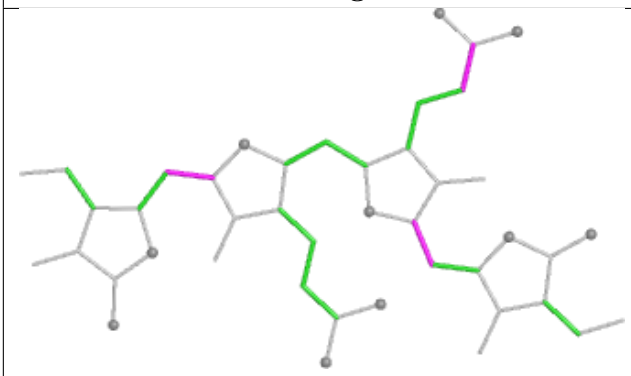
Ligand CYC ZB 201



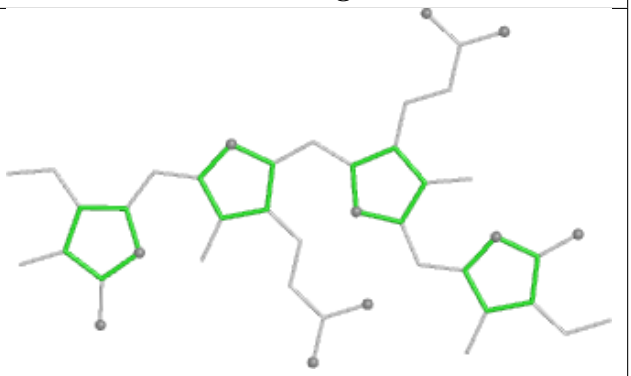
Bond lengths



Bond angles

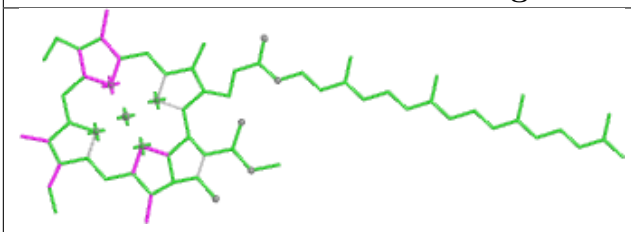


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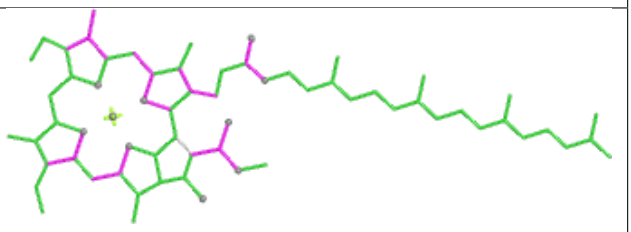


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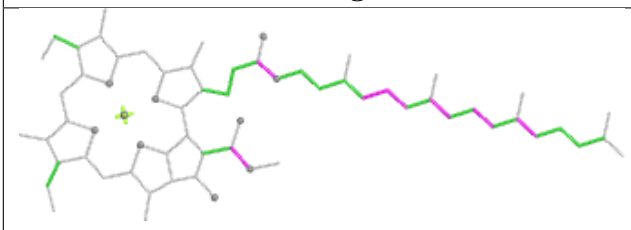
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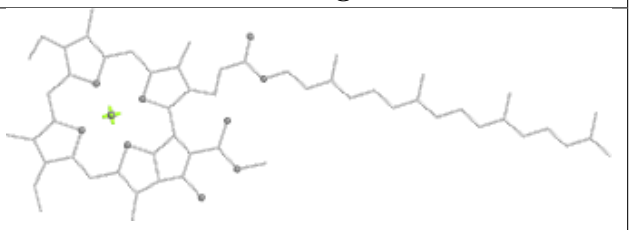
Bond lengths



Bond angles

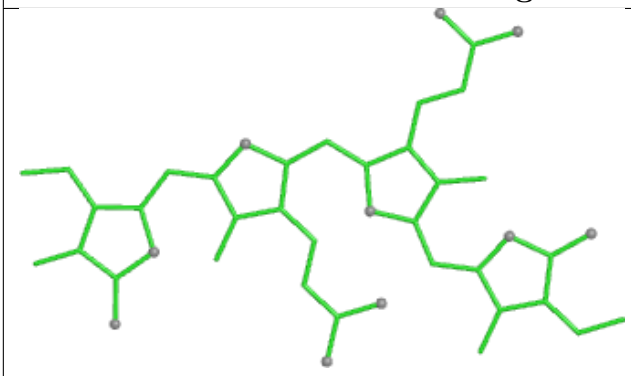


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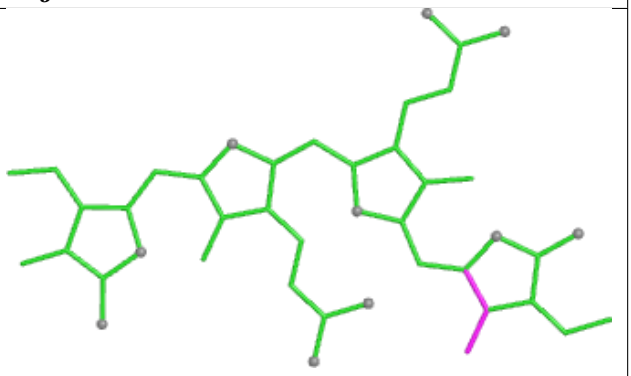


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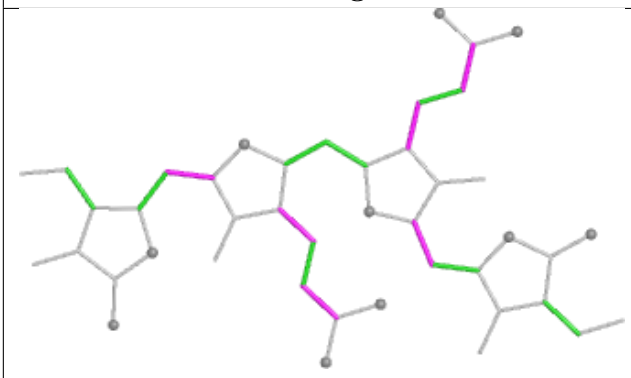
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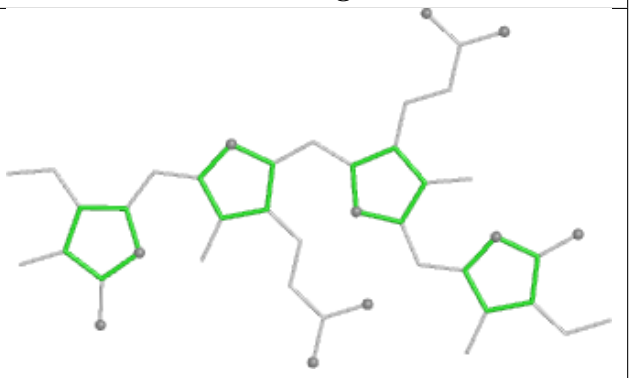
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Bond angles

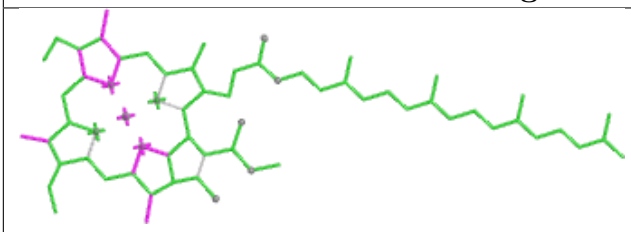


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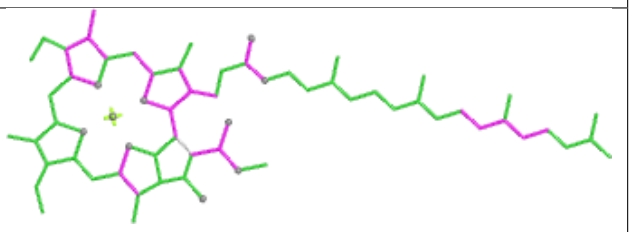


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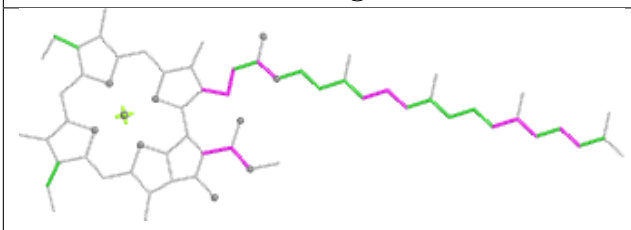
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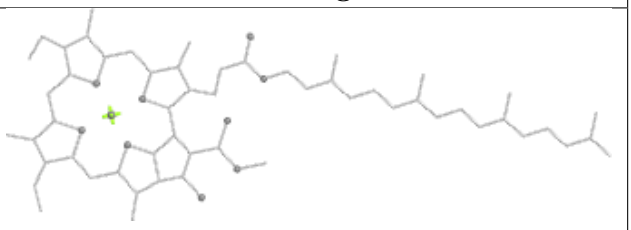
Bond lengths



Bond angles

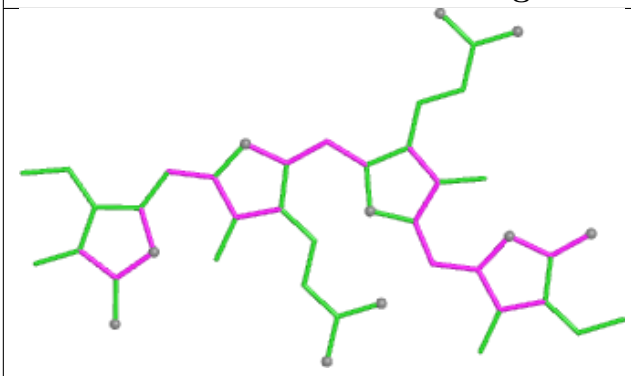


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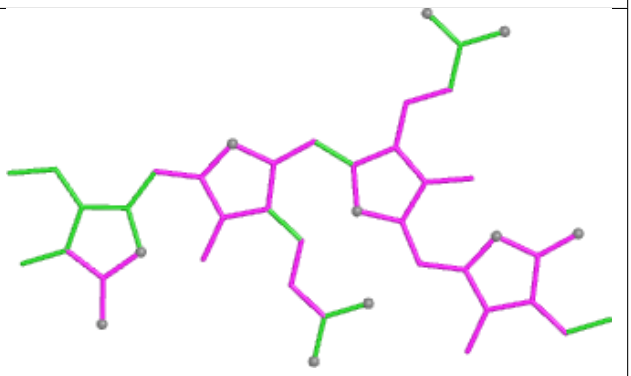


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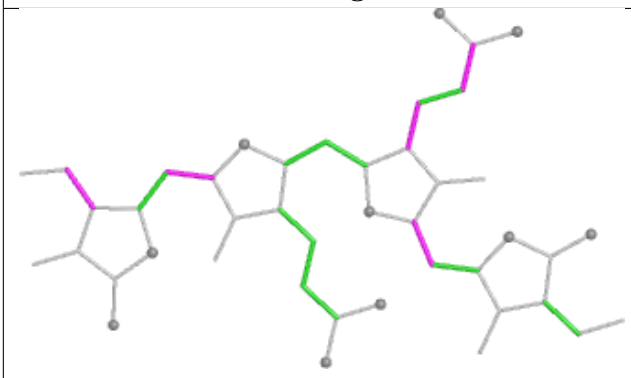
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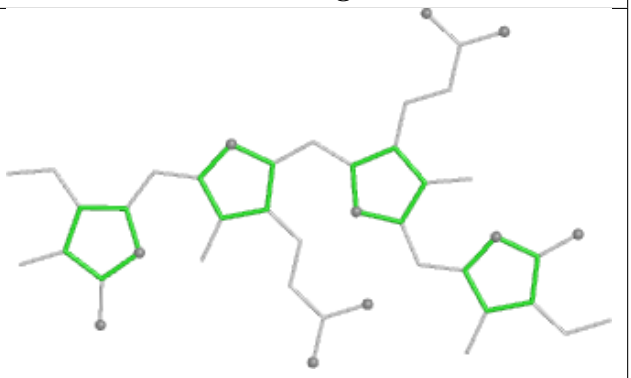
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Bond angles

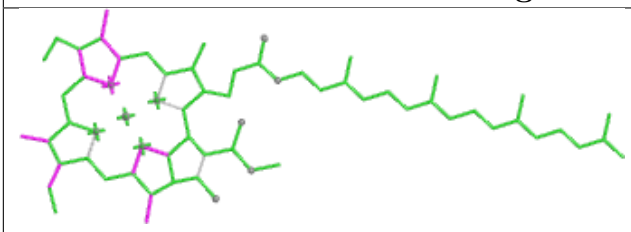


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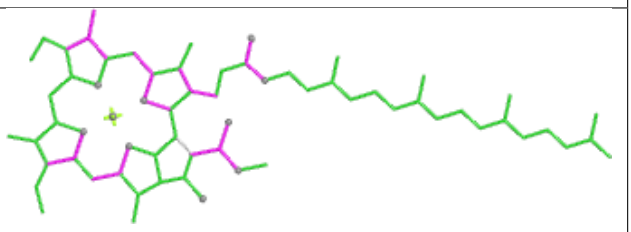


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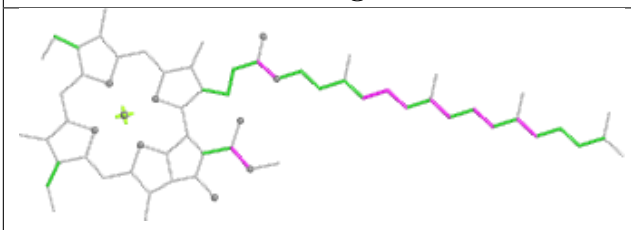
Ligand CLA B1 605



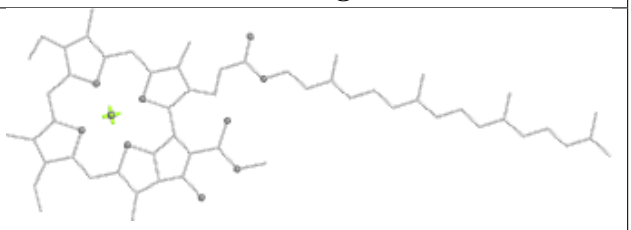
Bond lengths



Bond angles



Torsions

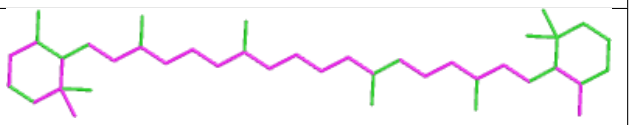


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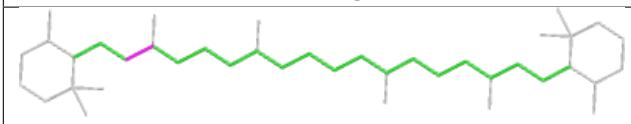
Ligand BCR Z1 102



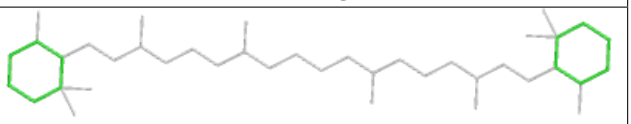
Bond lengths



Bond angles

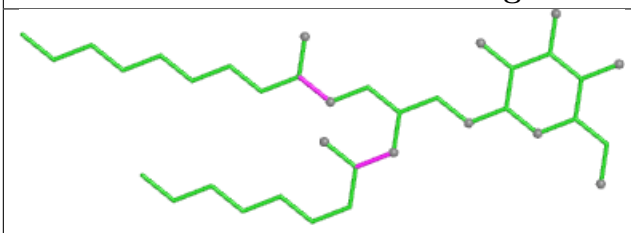


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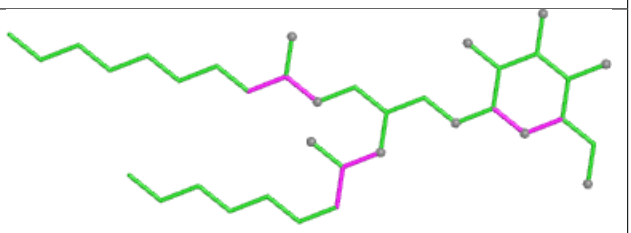


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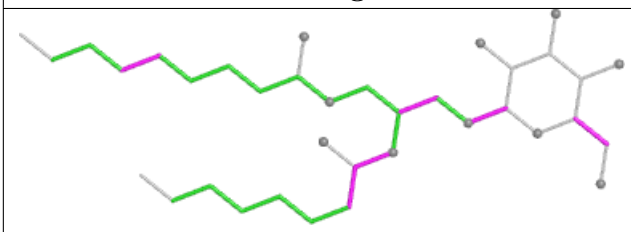
Ligand LMG ME 101



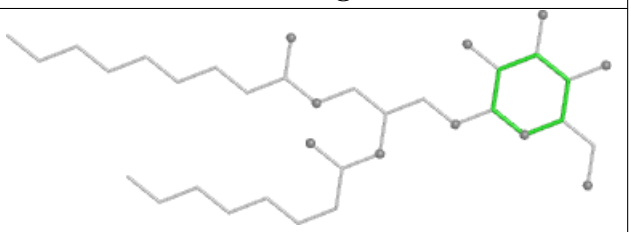
Bond lengths



Bond angles

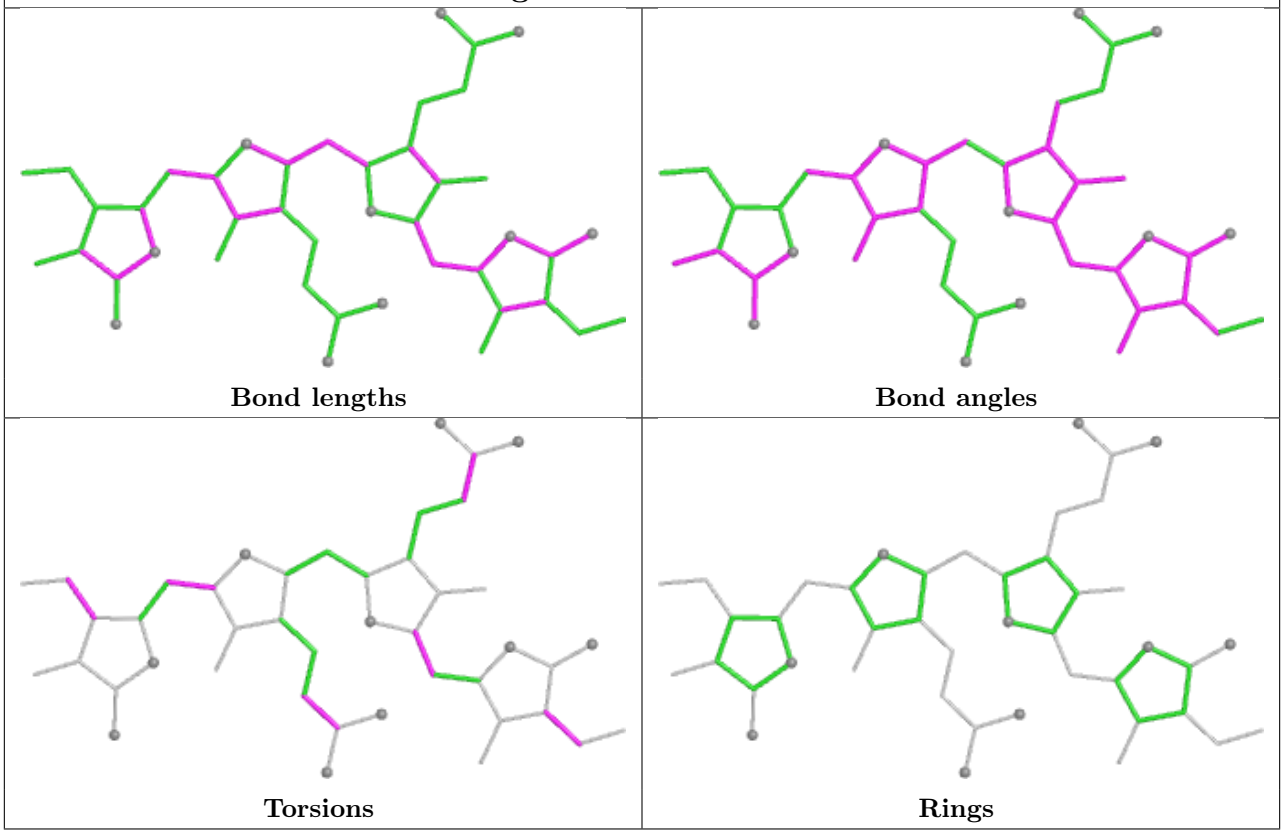


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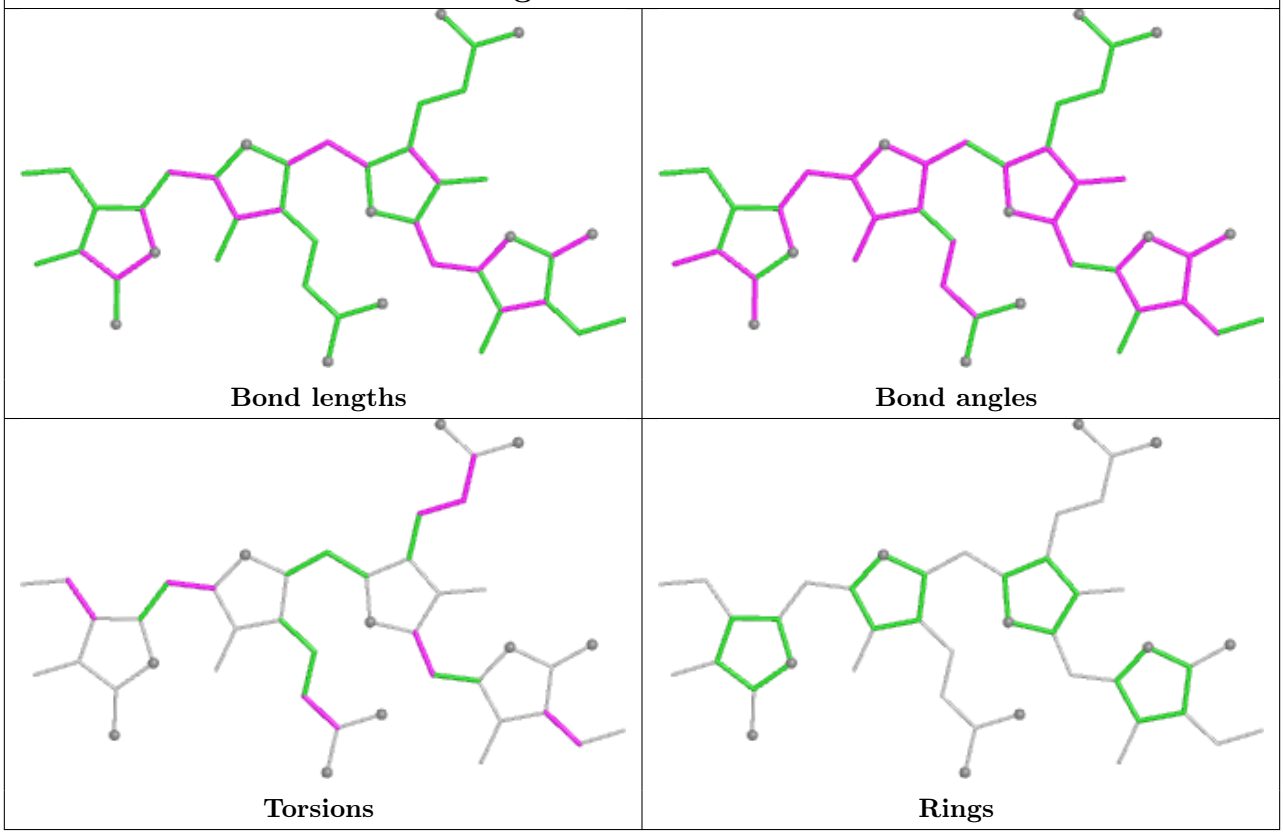


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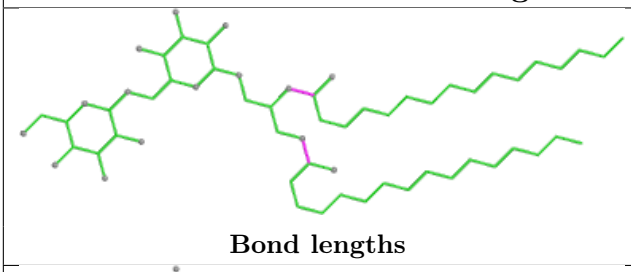
Ligand CYC XF 201



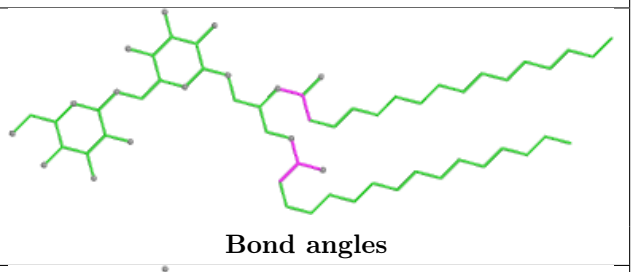
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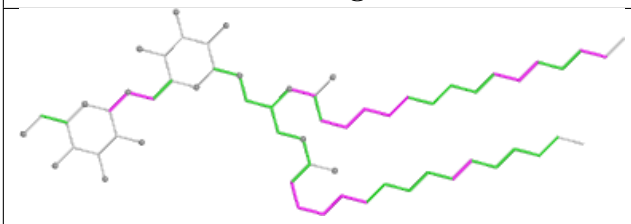
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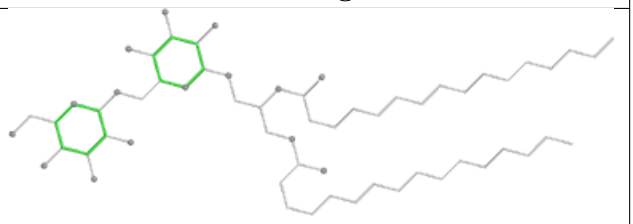
Bond lengths



Bond angles

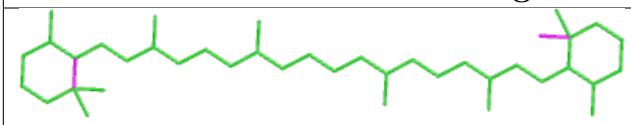


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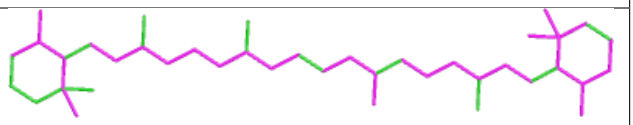


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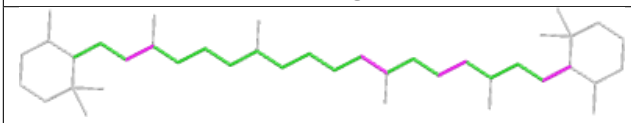
Ligand BCR X1 102



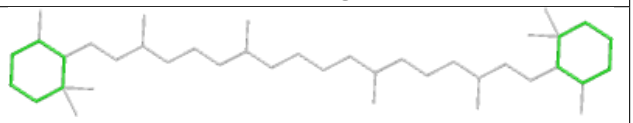
Bond lengths



Bond angles

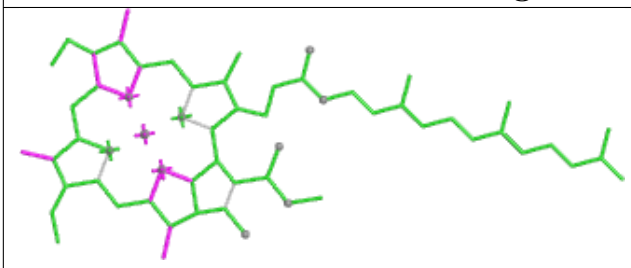


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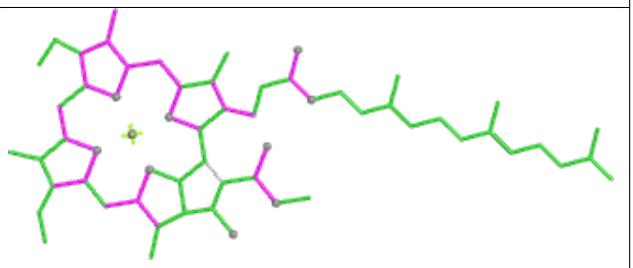


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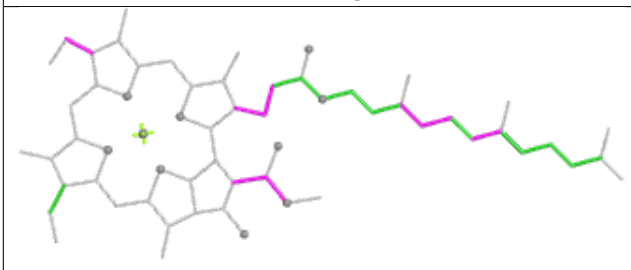
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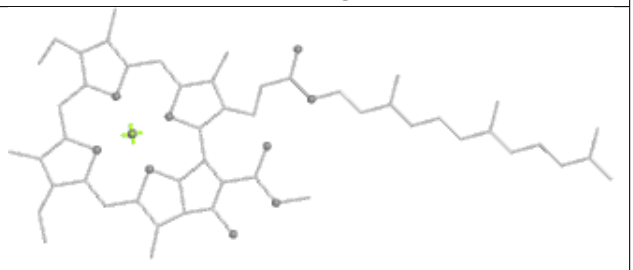
Bond lengths



Bond angles

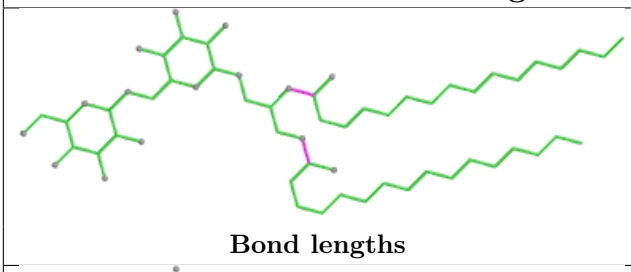


Torsions

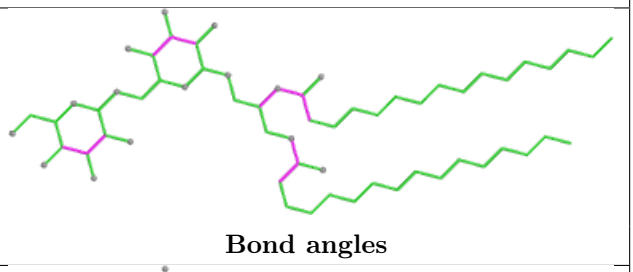


Rings

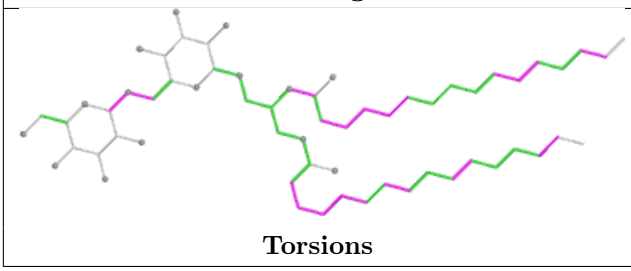
Ligand DGD CE 518



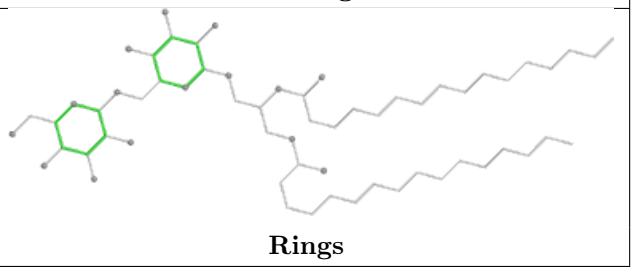
Bond lengths



Bond angles

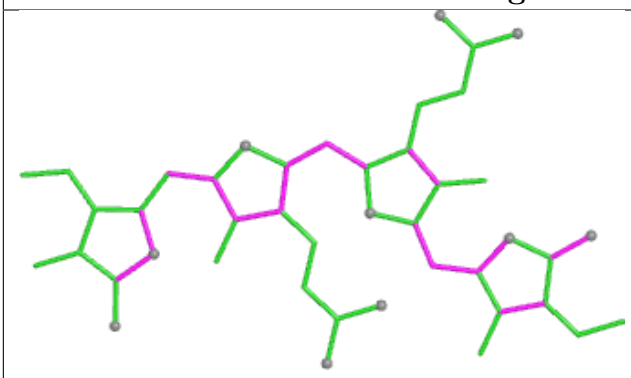


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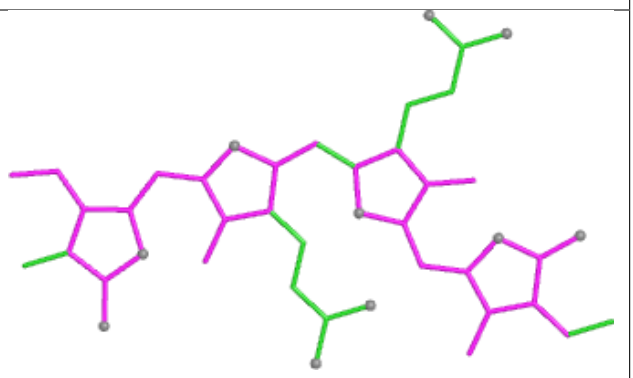


Rings

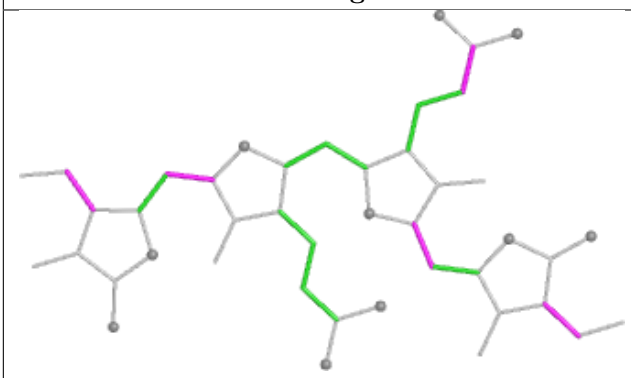
Ligand CYC RG 201



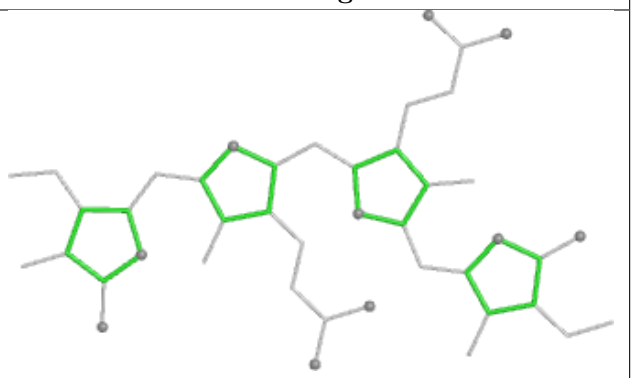
Bond lengths



Bond angles

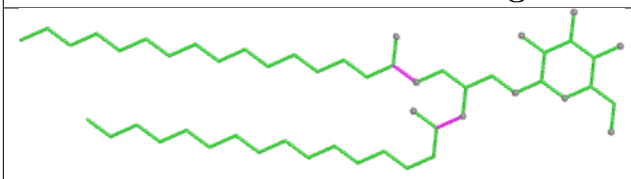


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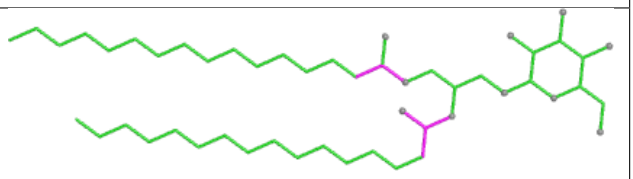


Rings

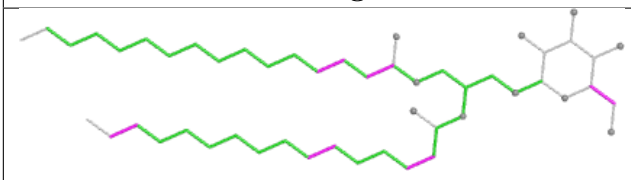
Ligand LMG BE 618



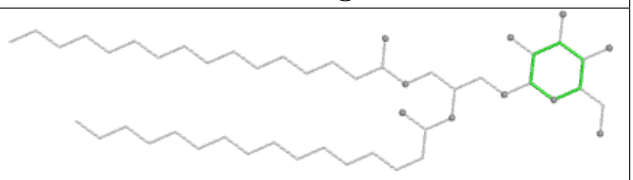
Bond lengths



Bond angles

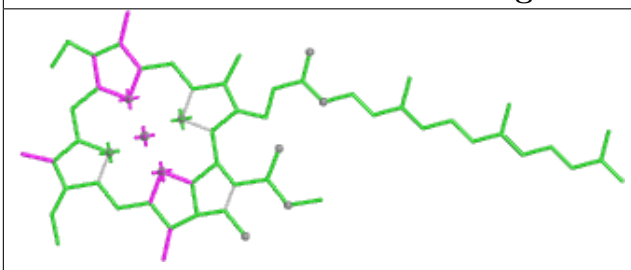


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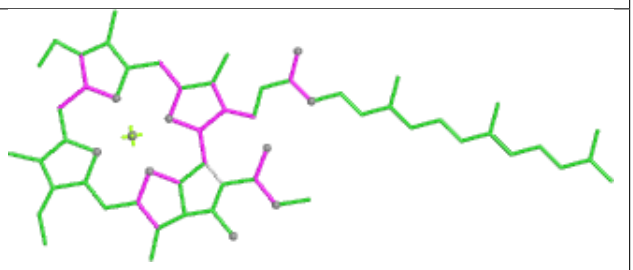


Rings

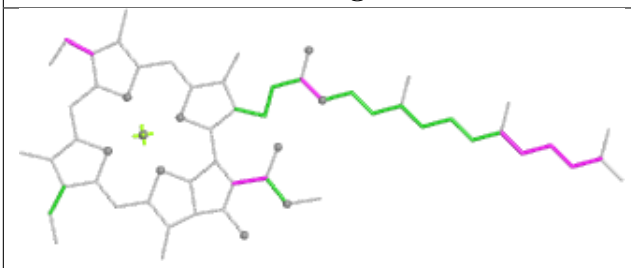
Ligand CLA hE 102



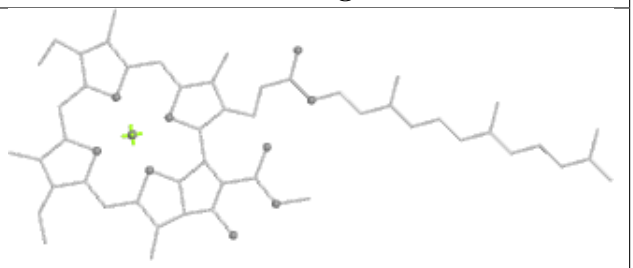
Bond lengths



Bond angles

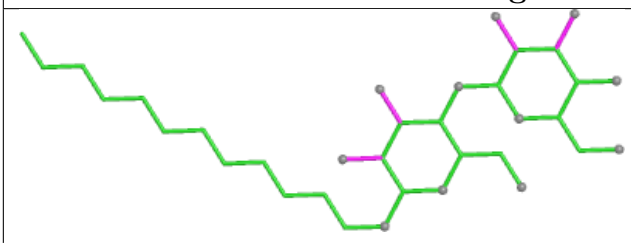


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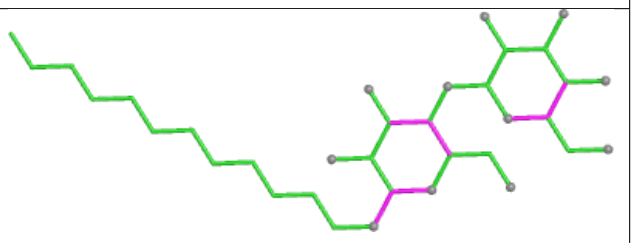


Rings

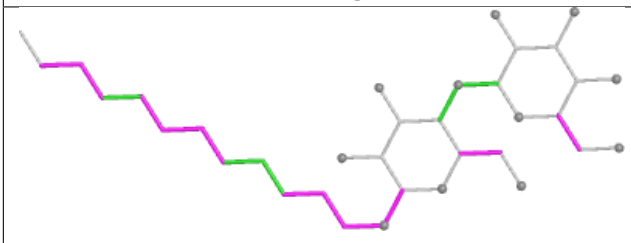
Ligand LMT AE 412



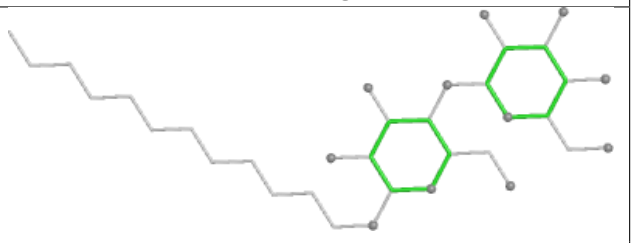
Bond lengths



Bond angles

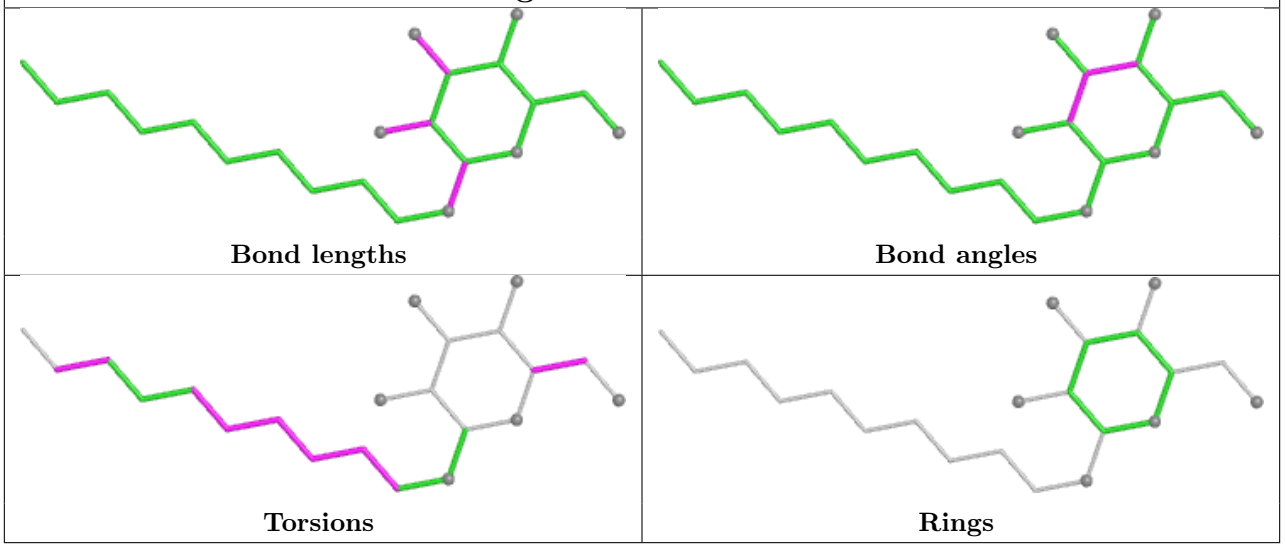


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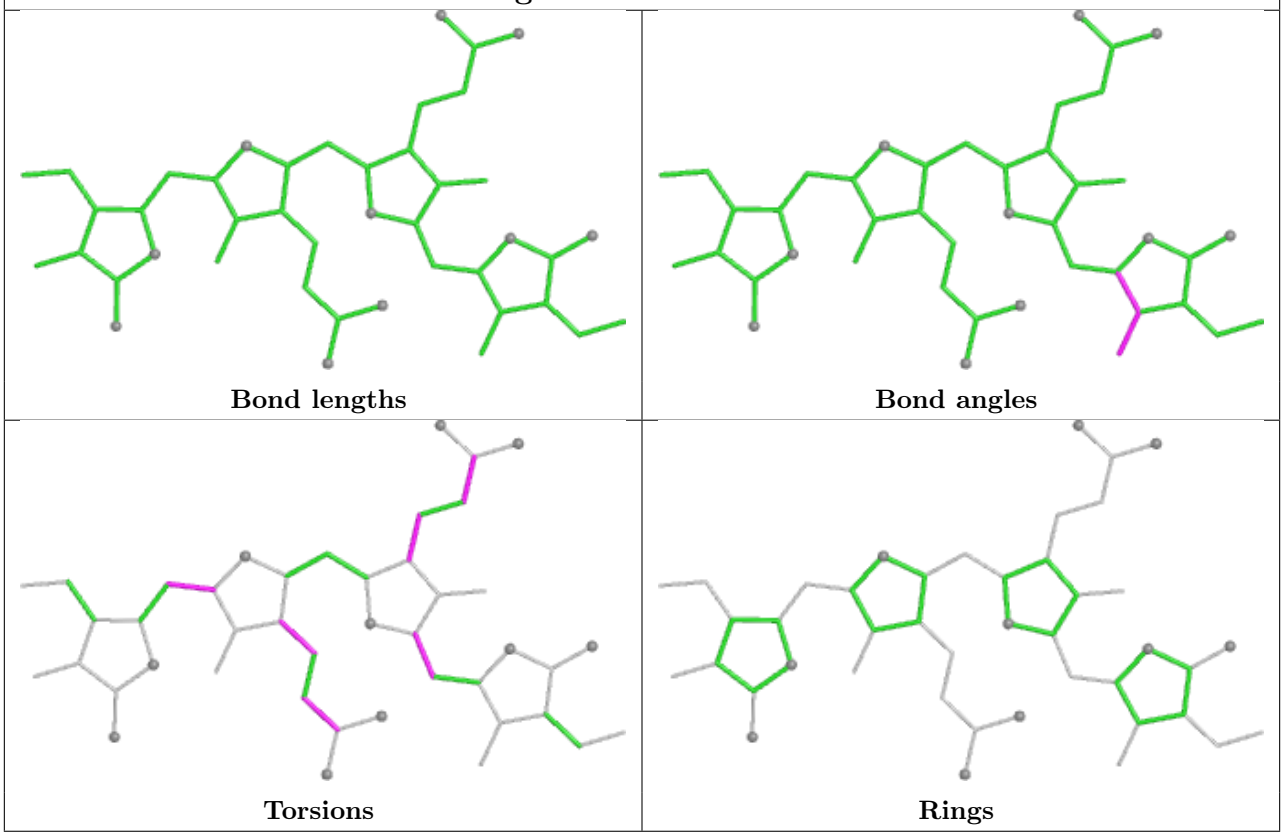


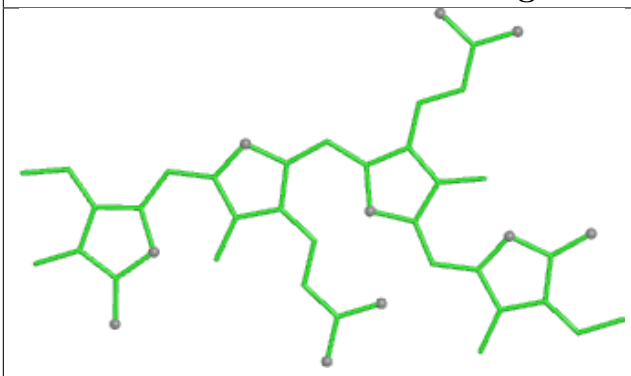
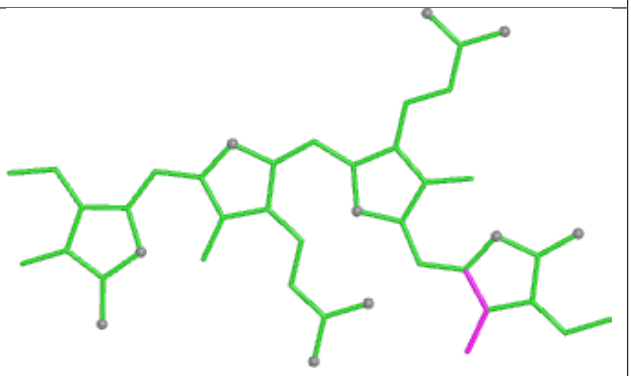
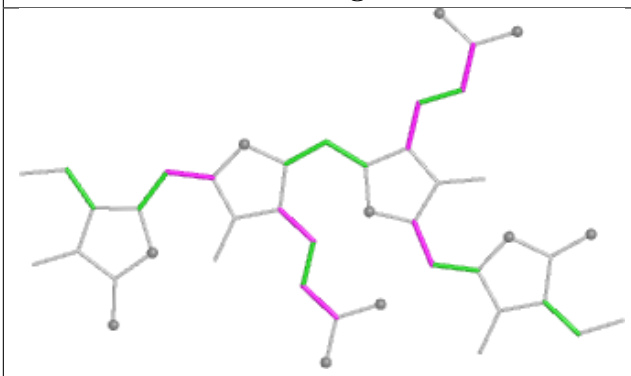
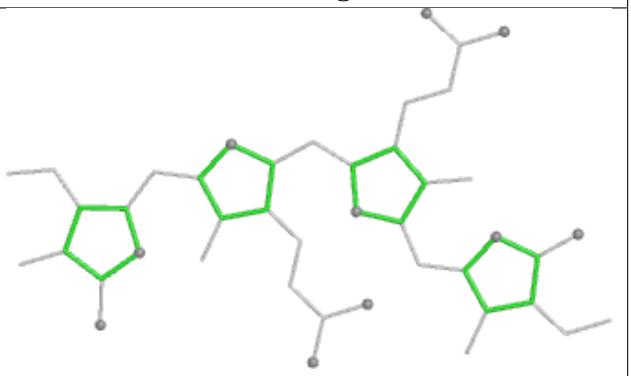
Rings

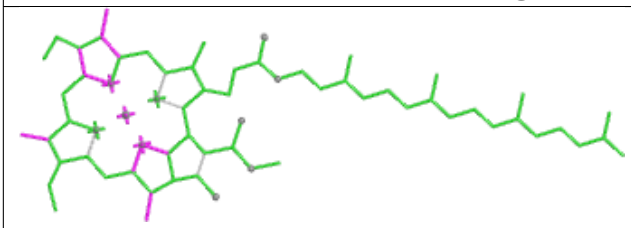
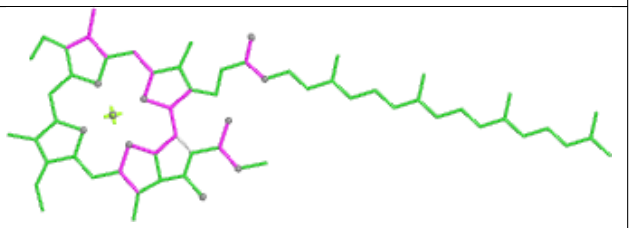
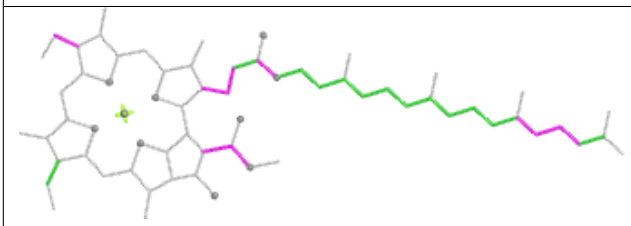
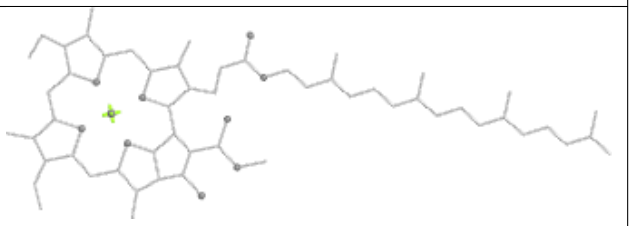
Ligand LMT d1 413



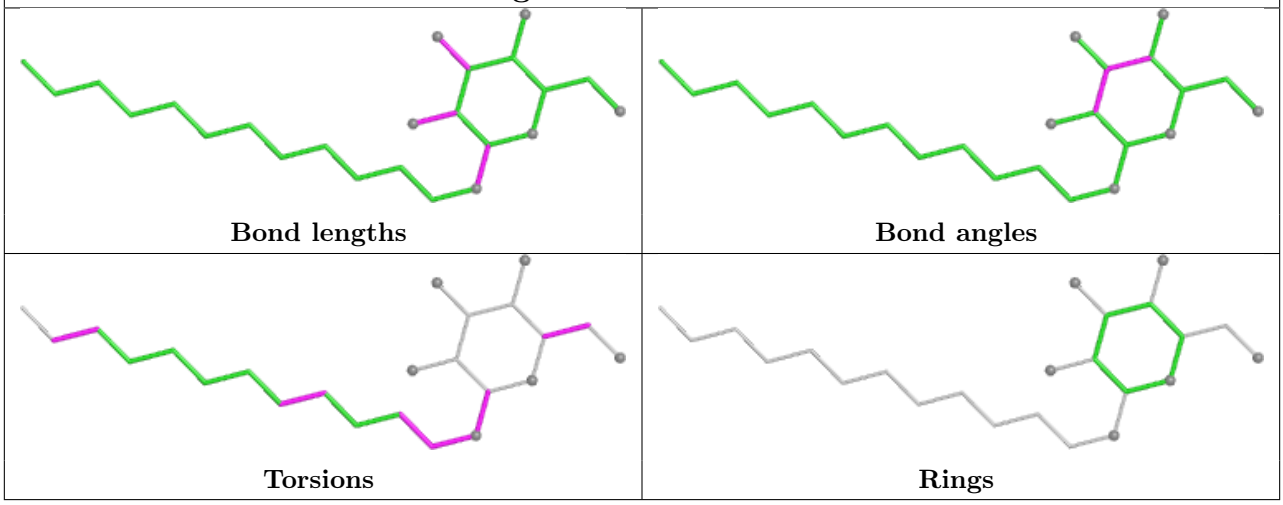
Ligand CYC eC 202



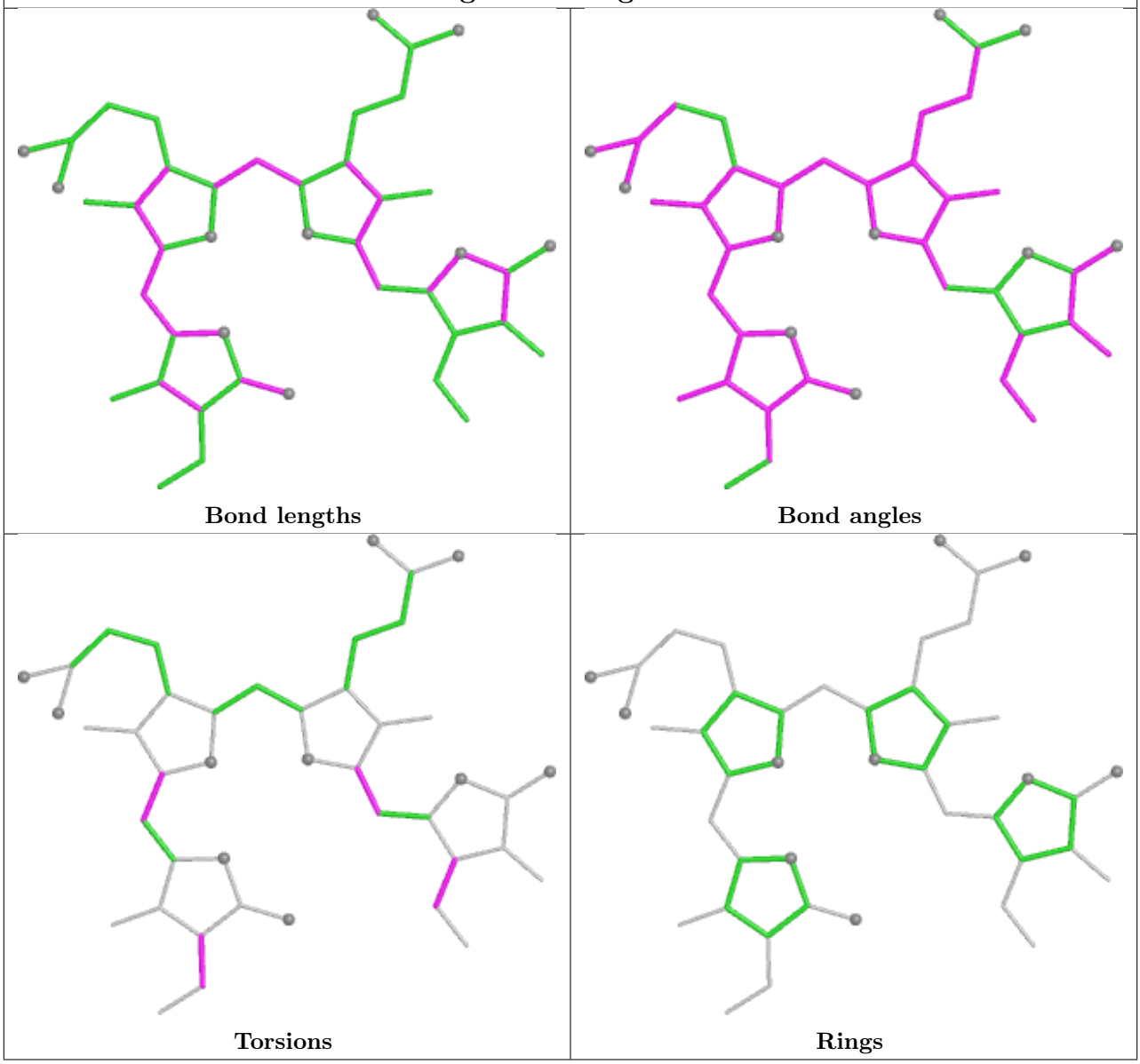
Ligand CYC c7 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BE 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

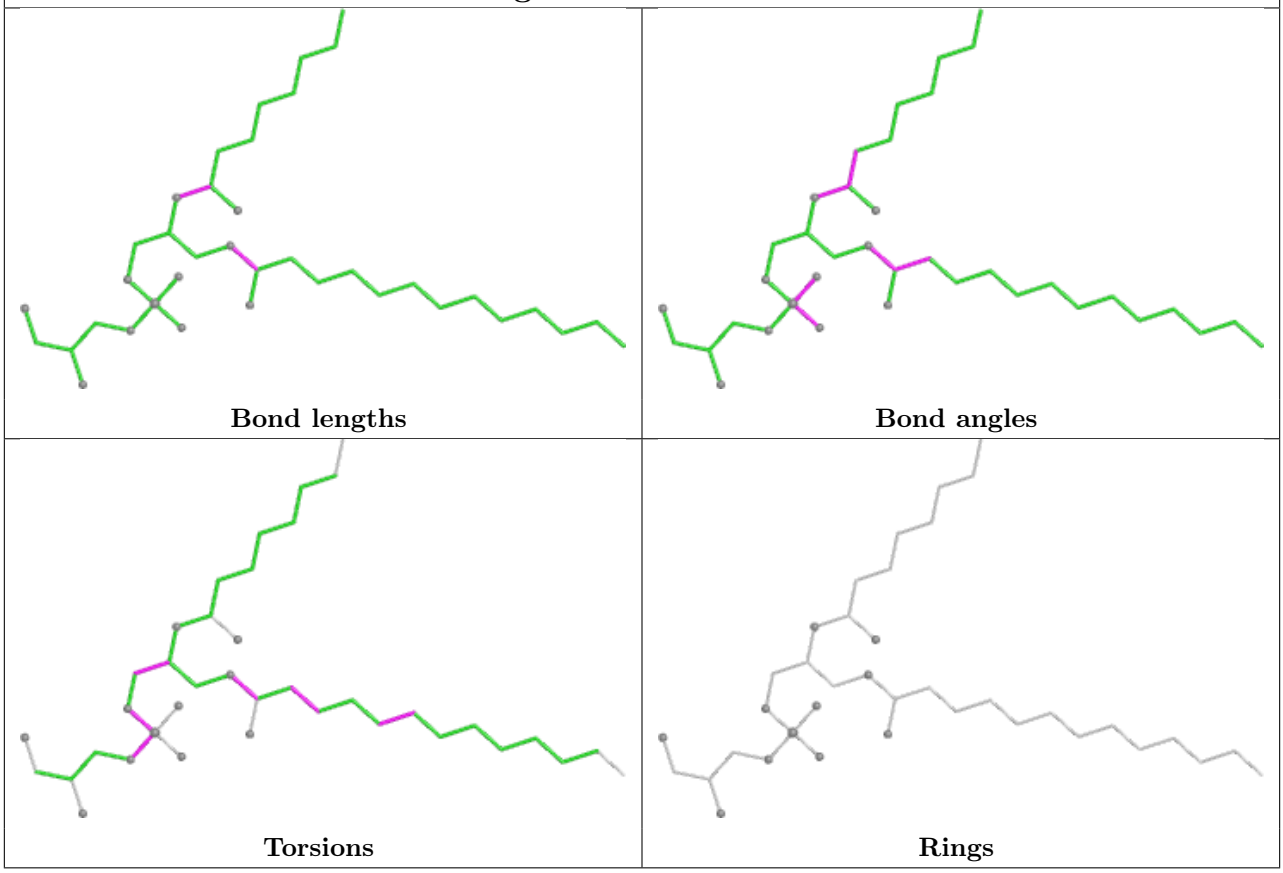
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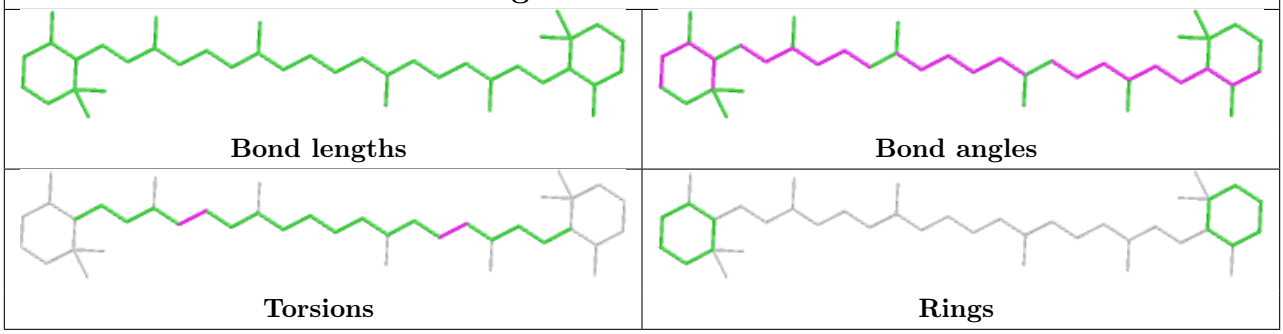
Ligand CYC gJ 202



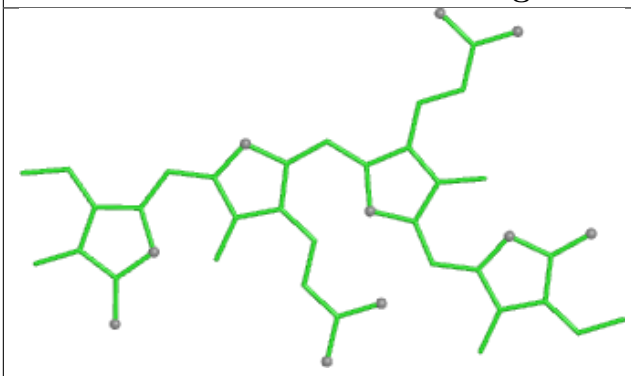
Ligand LHG A1 411



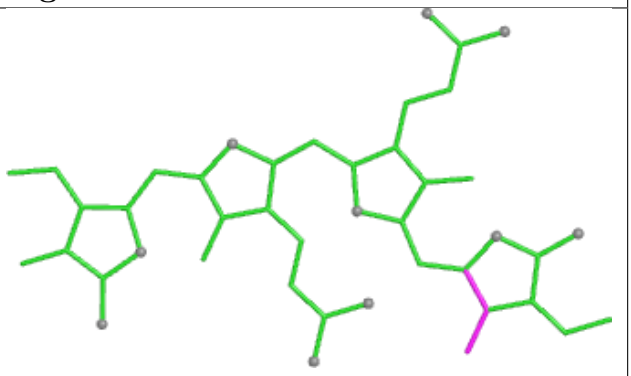
Ligand BCR CE 519



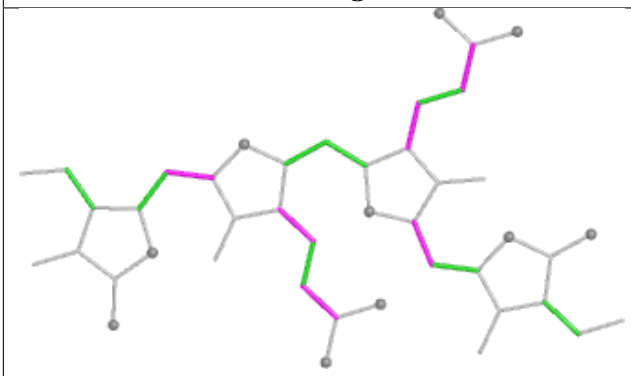
Ligand CYC gA 302



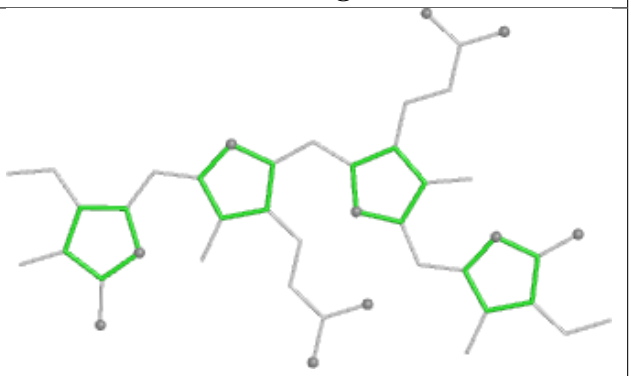
Bond lengths



Bond angles

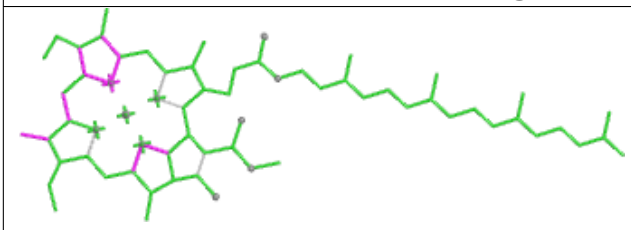


Torsions

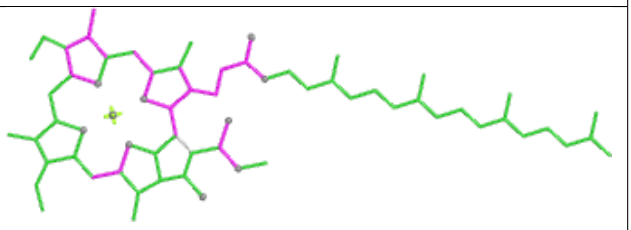


Rings

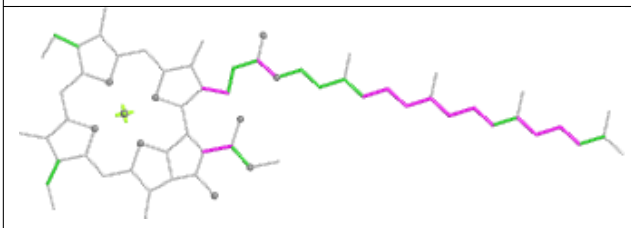
Ligand CLA BD 611



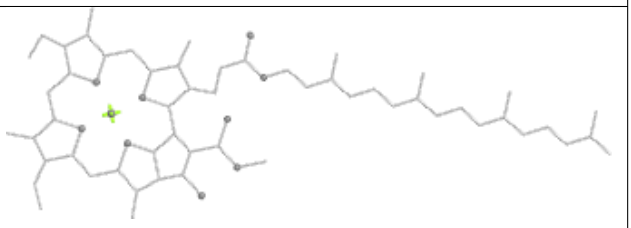
Bond lengths



Bond angles

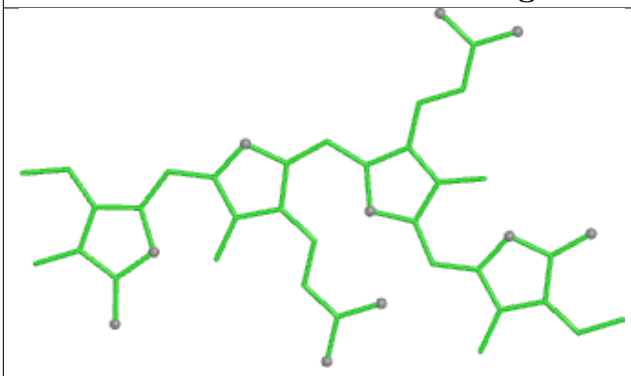


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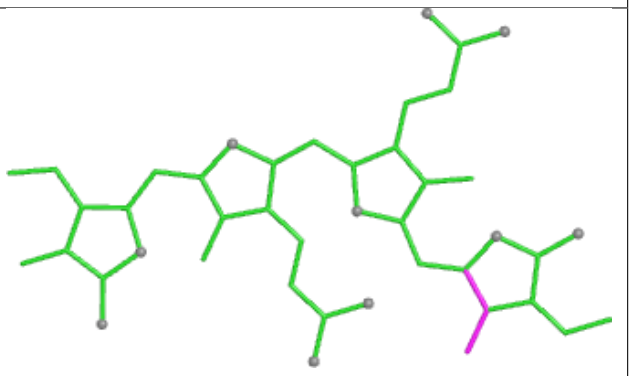


Rings

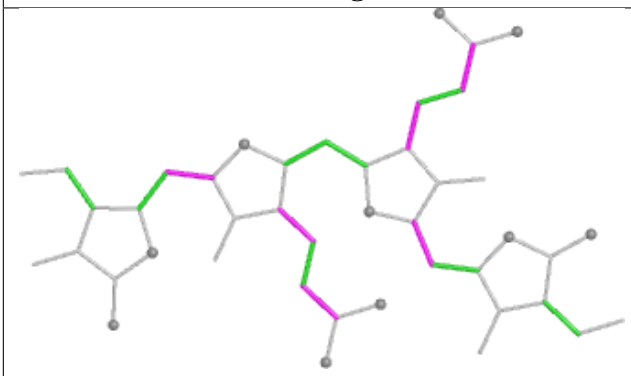
Ligand CYC e8 202



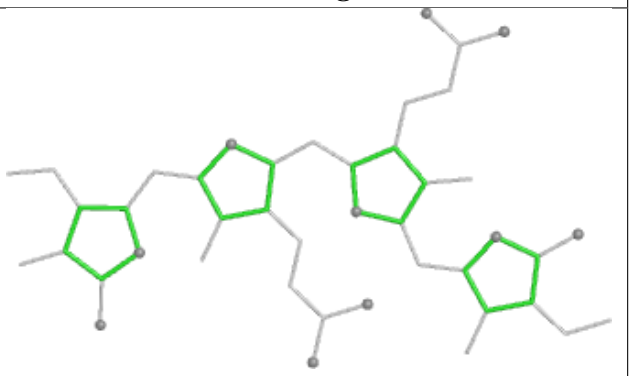
Bond lengths



Bond angles

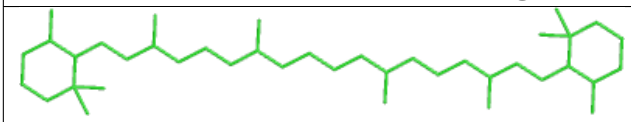


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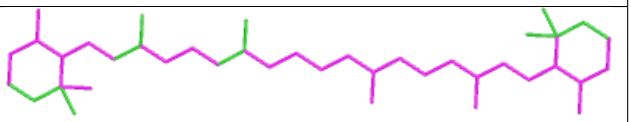


Rings

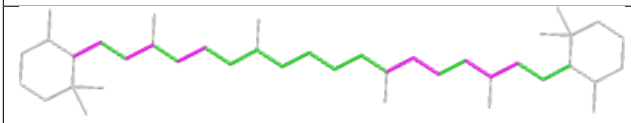
Ligand BCR zD 101



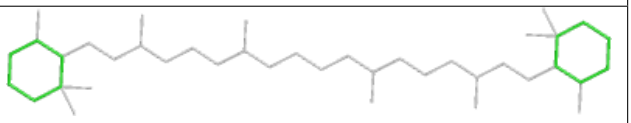
Bond lengths



Bond angles

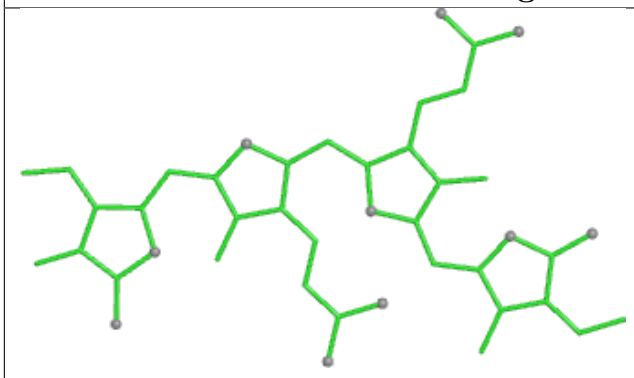


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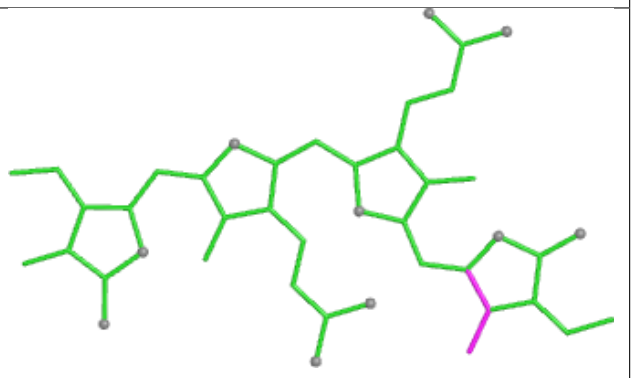


Rings

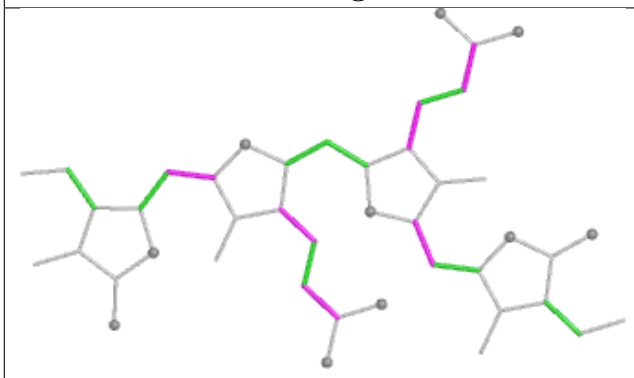
Ligand CYC iA 201



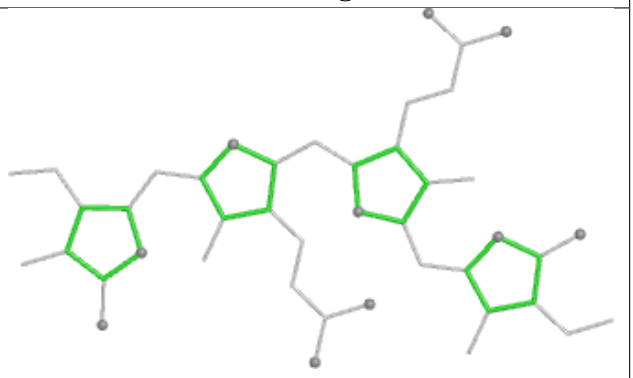
Bond lengths



Bond angles

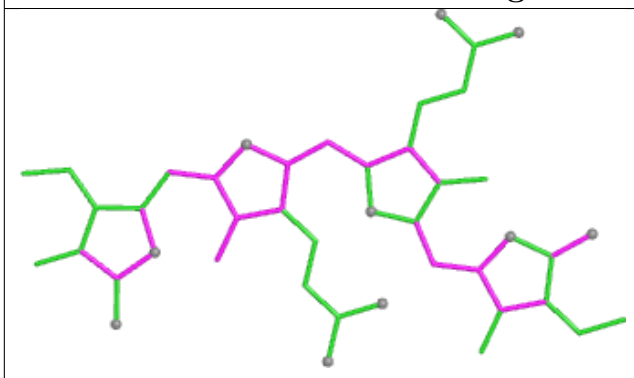


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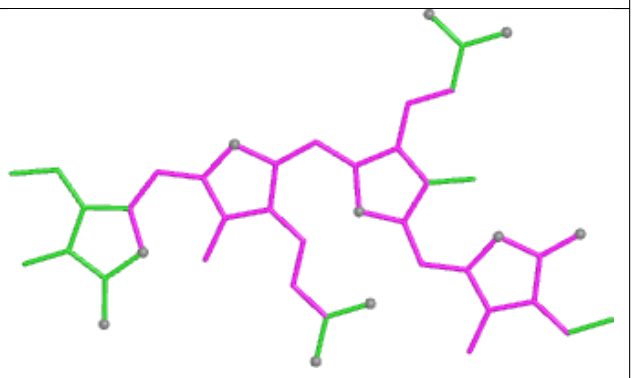


Rings

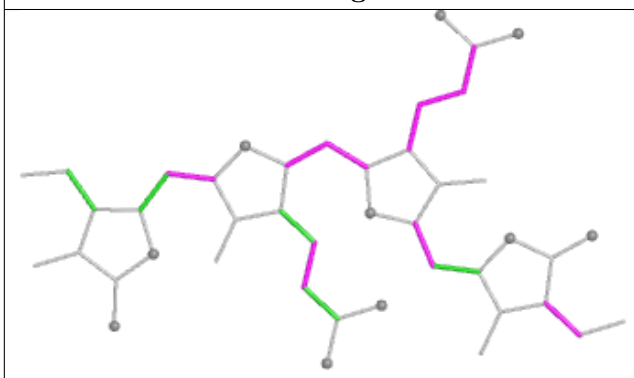
Ligand CYC tB 1001



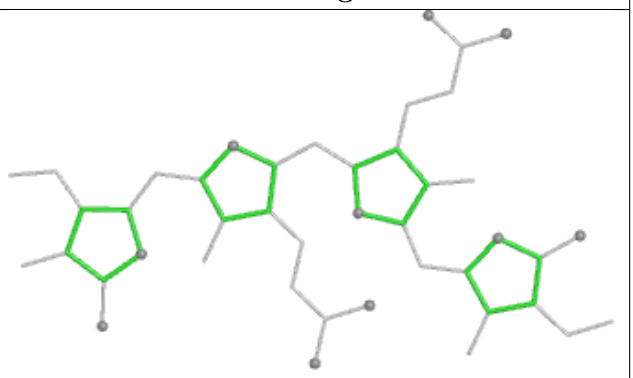
Bond lengths



Bond angles

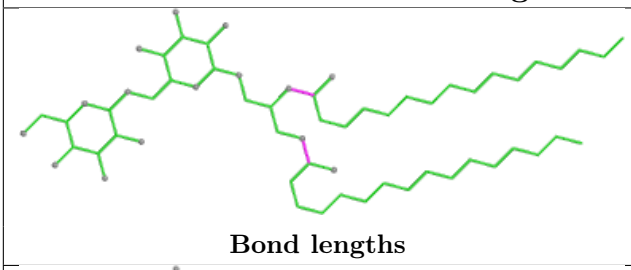


Torsions

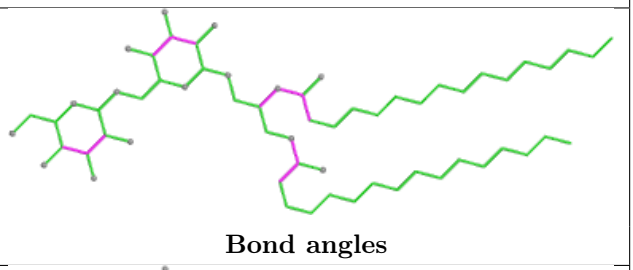


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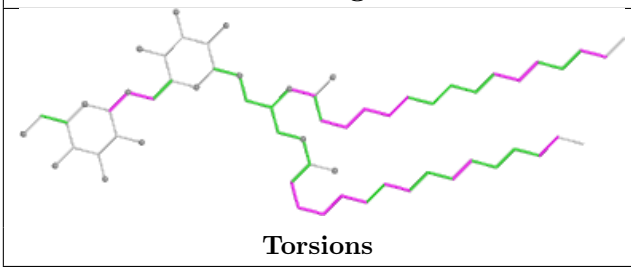
Ligand DGD C1 518



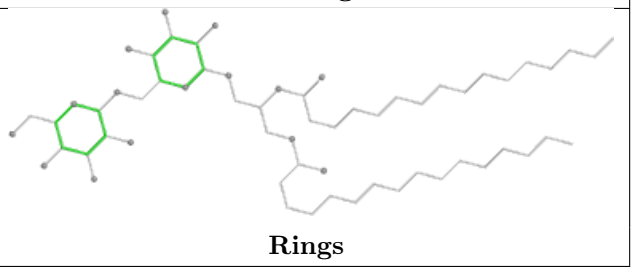
Bond lengths



Bond angles

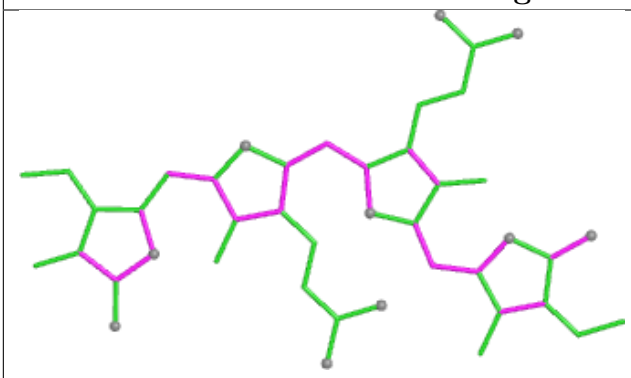


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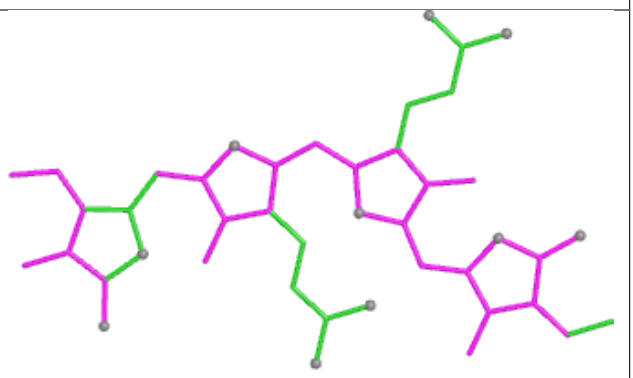


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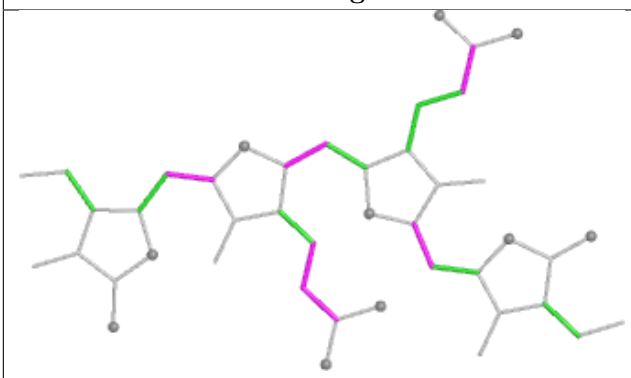
Ligand CYC P4 201



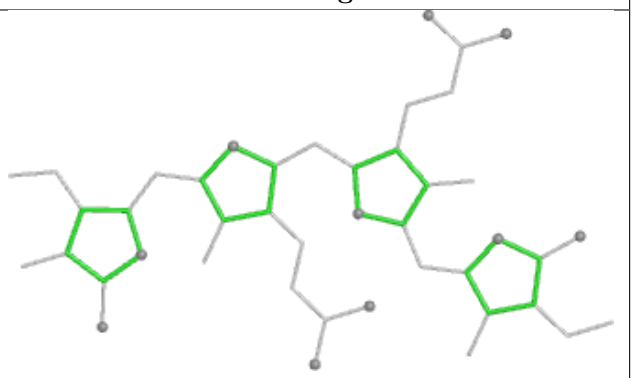
Bond lengths



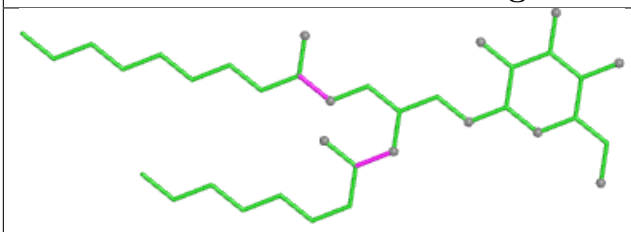
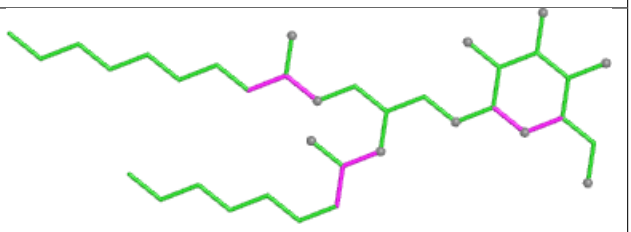
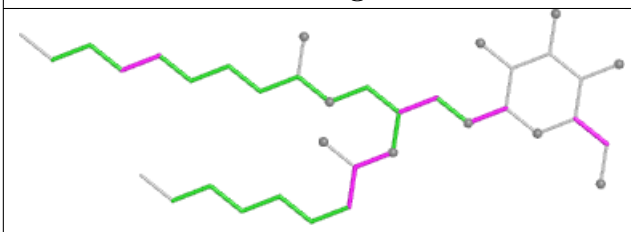
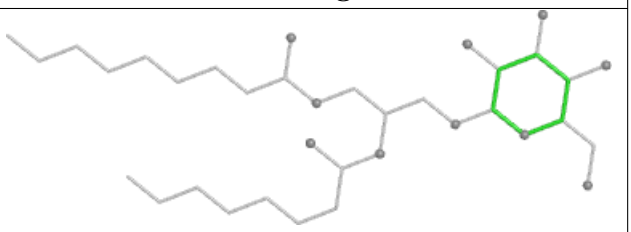
Bond angles



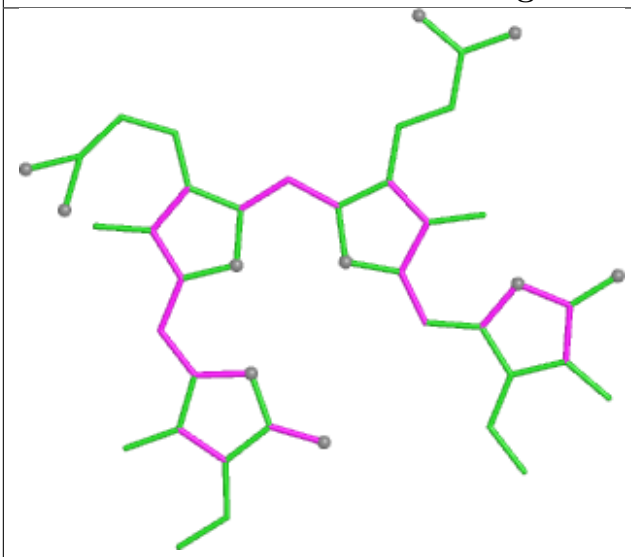
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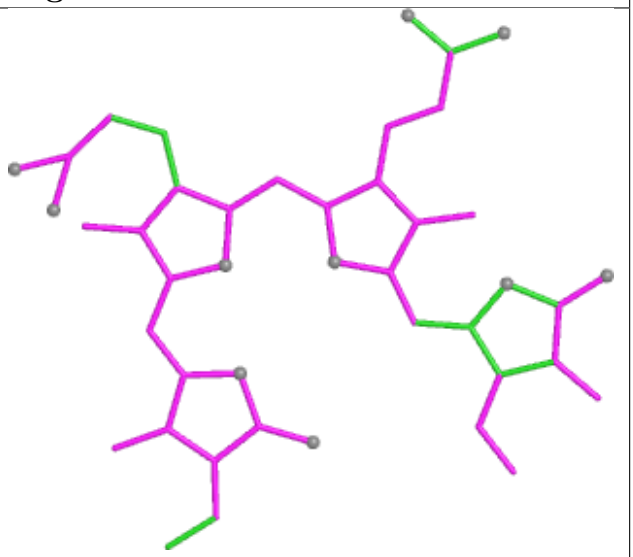
Rings

Ligand LMG m1 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

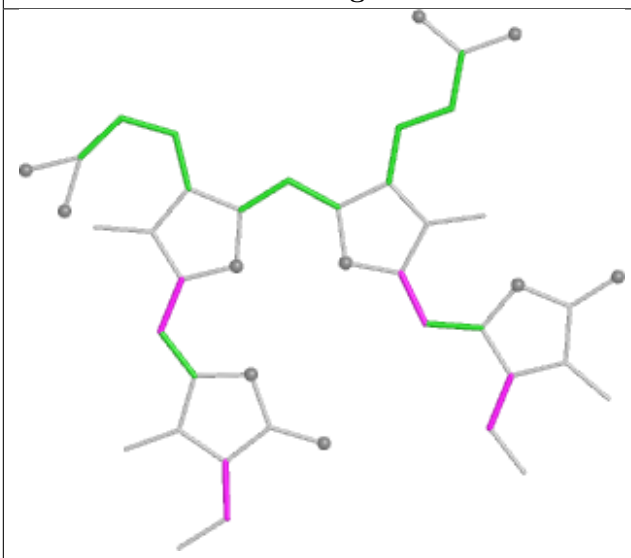
Ligand CYC g9 202



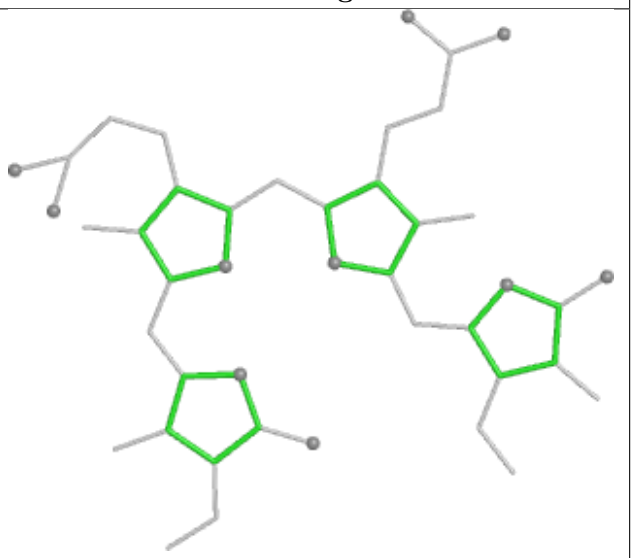
Bond lengths



Bond angles

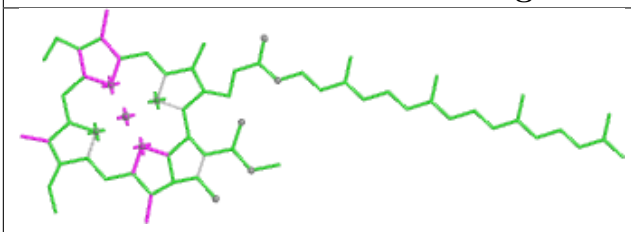


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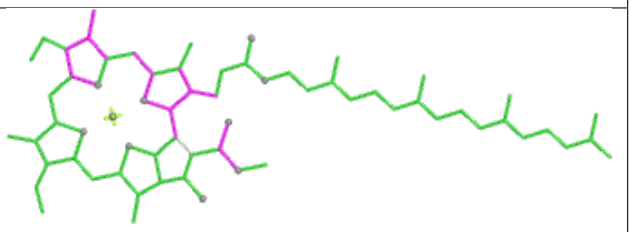


Rings

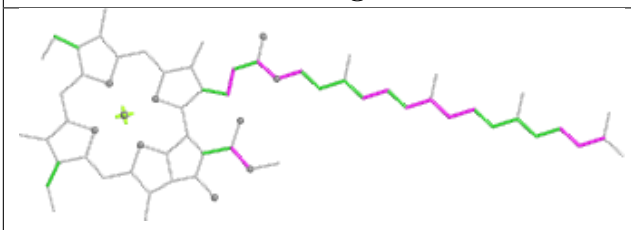
Ligand CLA cD 514



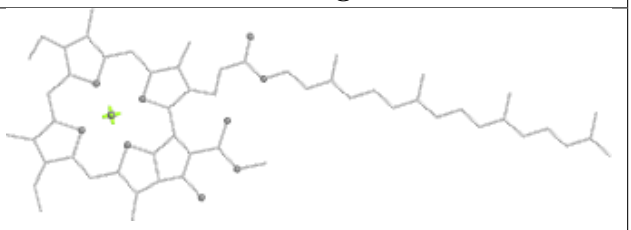
Bond lengths



Bond angles

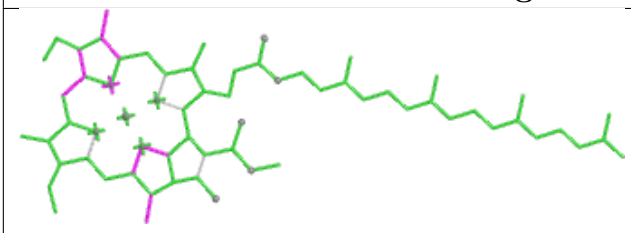


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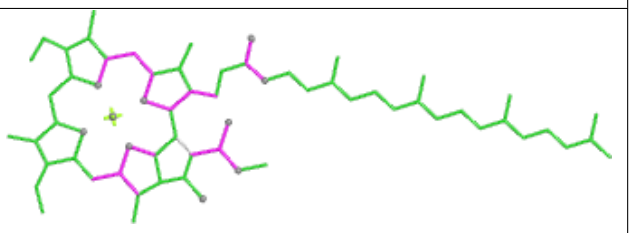


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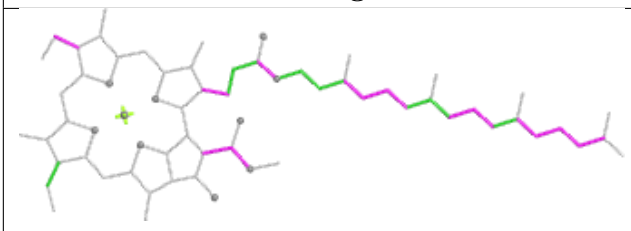
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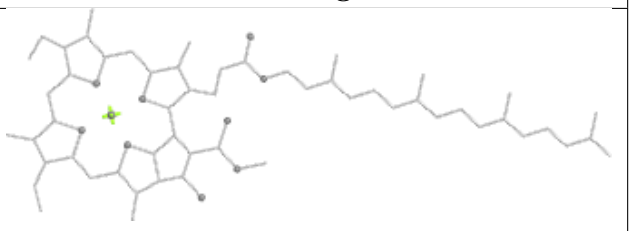
Bond lengths



Bond angles

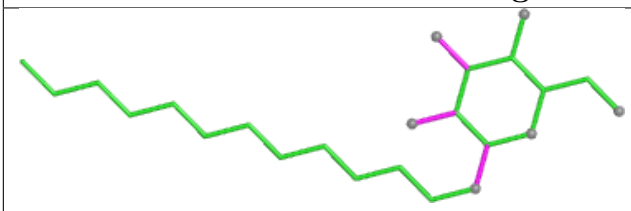


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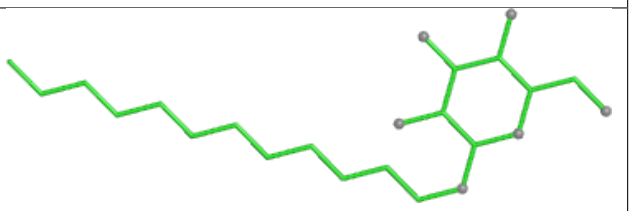


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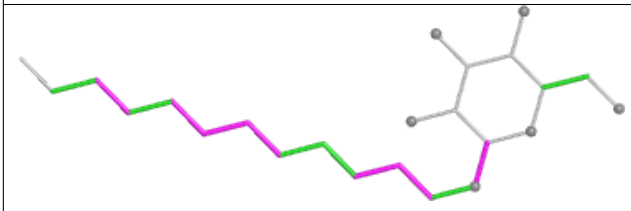
Ligand LMT D1 403



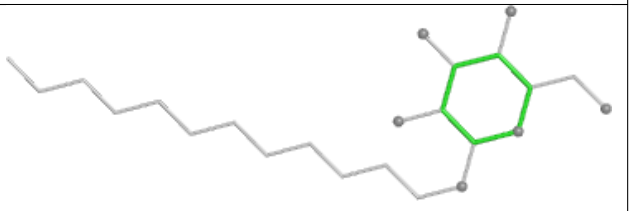
Bond lengths



Bond angles

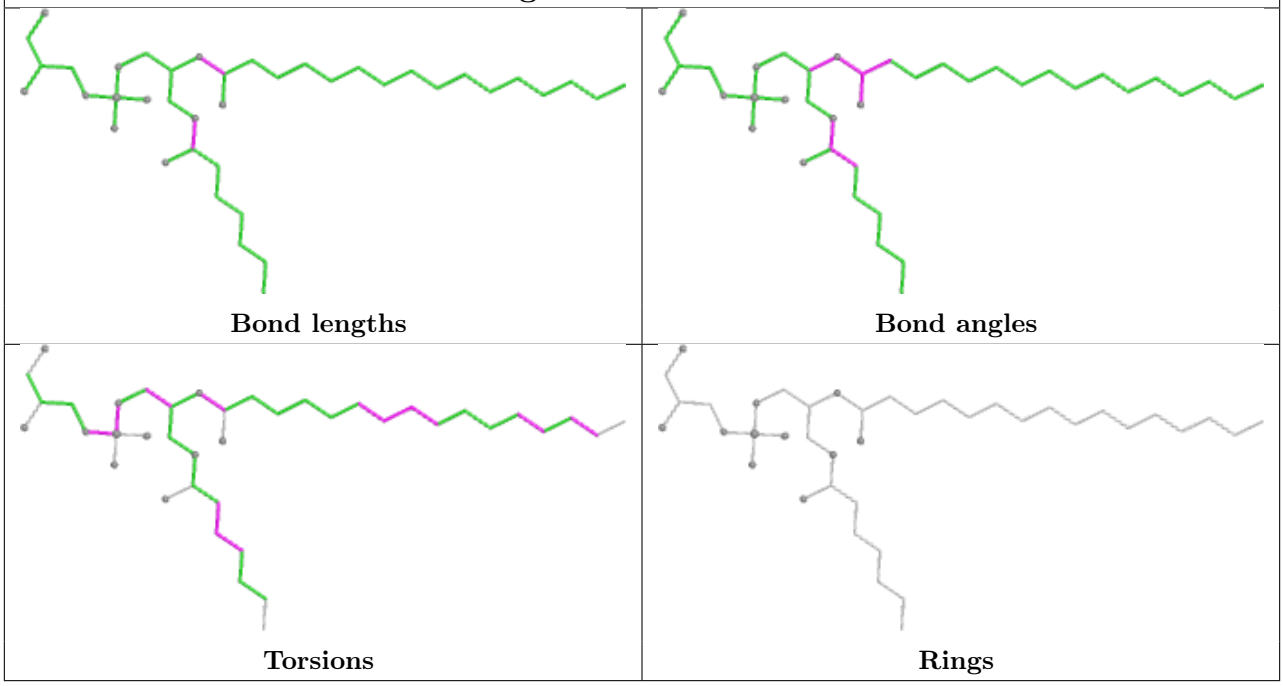


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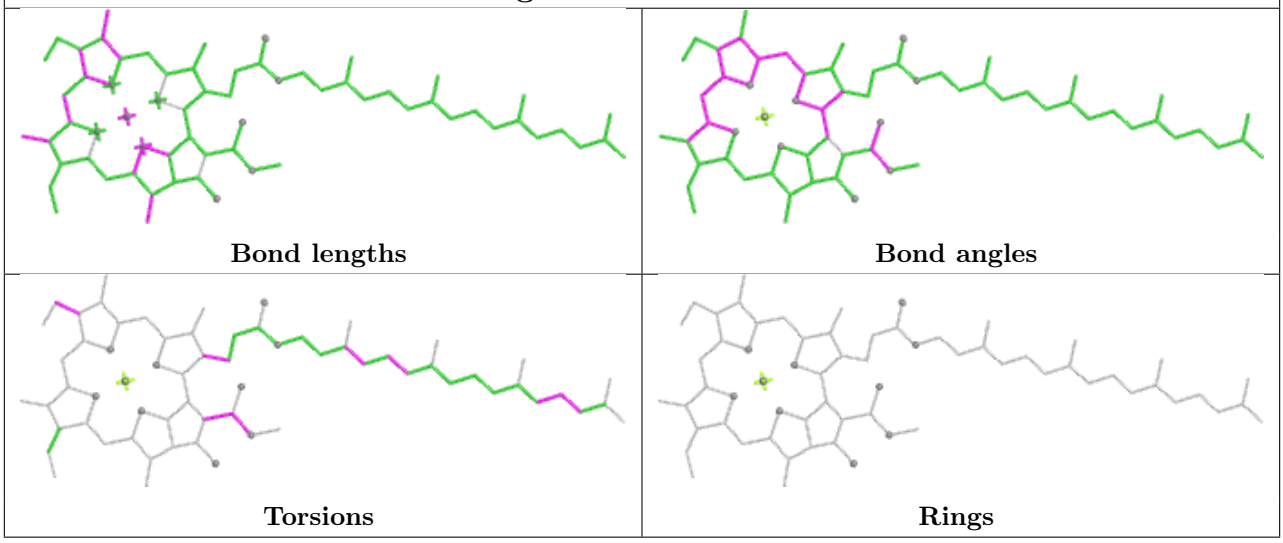


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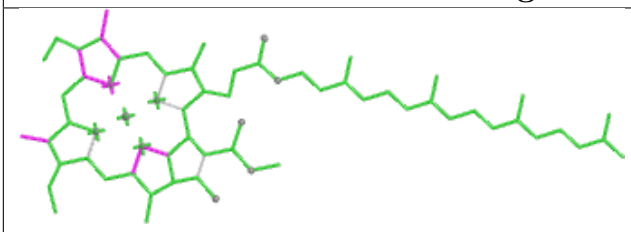
Ligand LHG e1 101



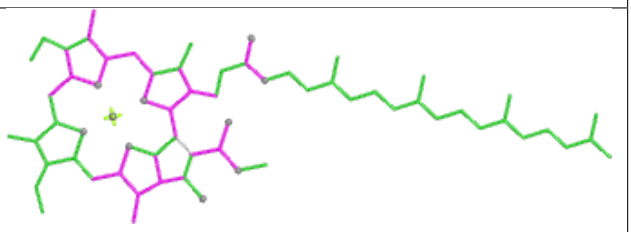
Ligand CLA hE 101



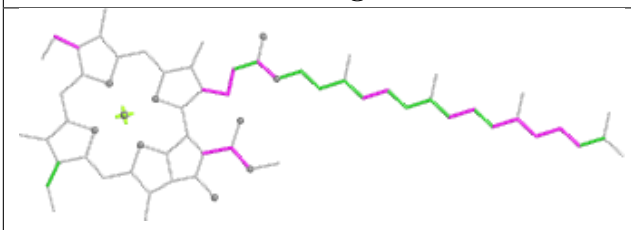
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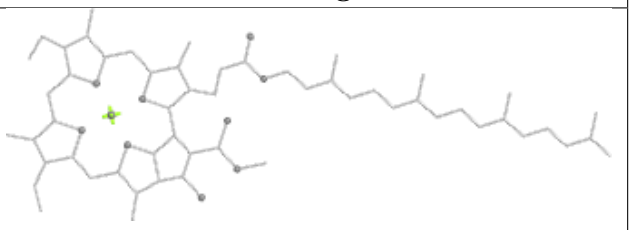
Bond lengths



Bond angles

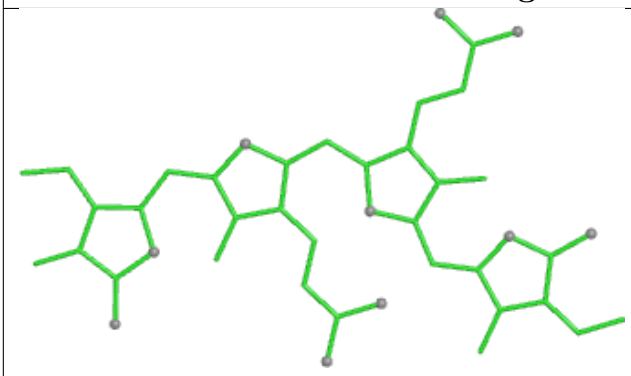


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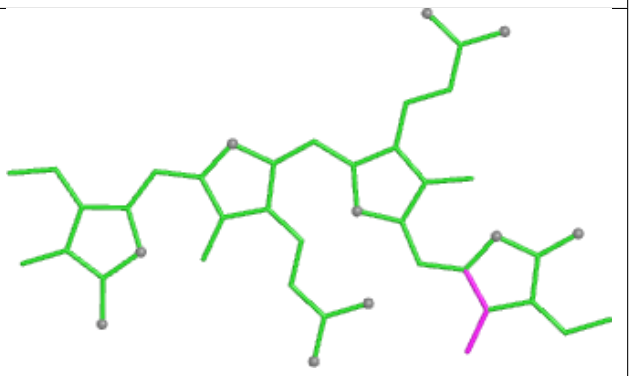


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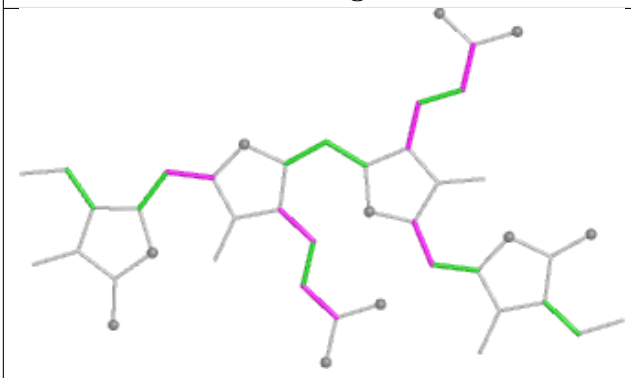
Ligand CYC e5 202



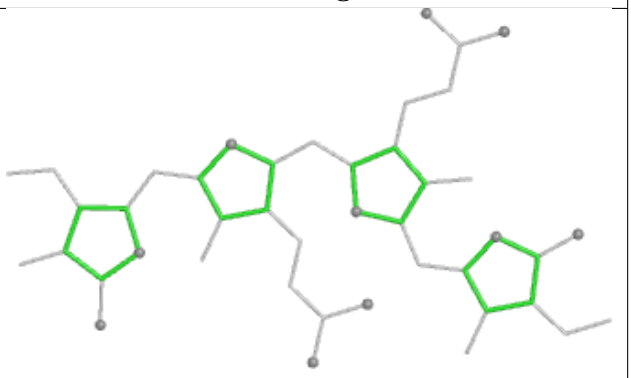
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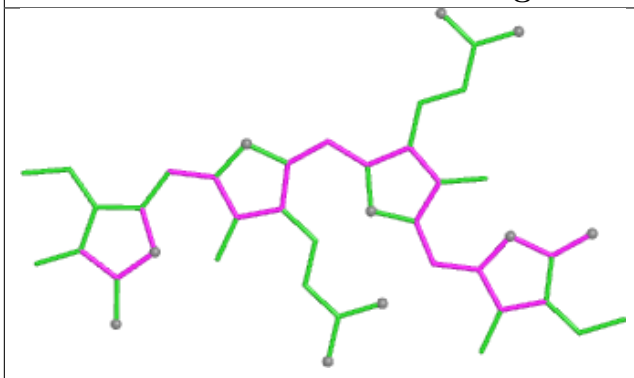


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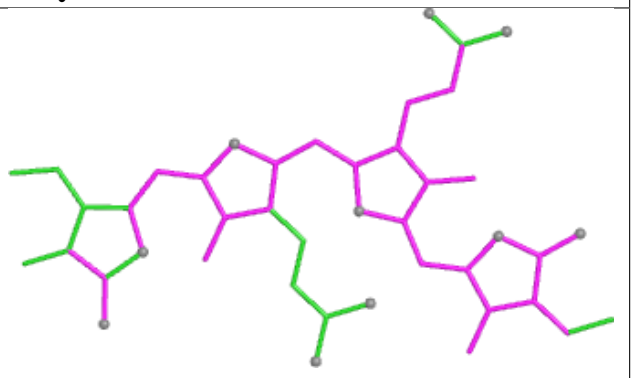


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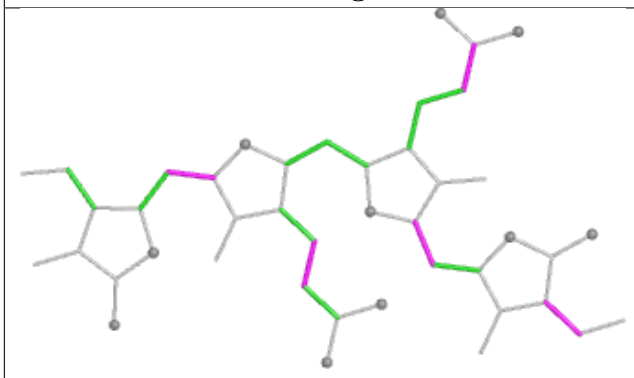
Ligand CYC Q4 201



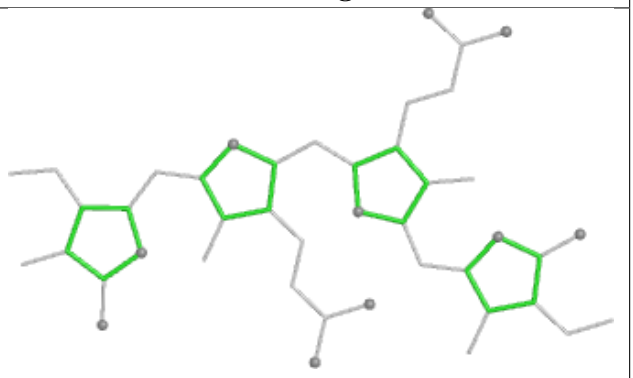
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Bond angles

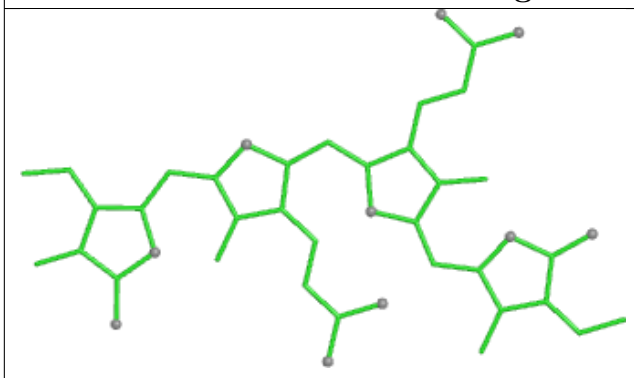


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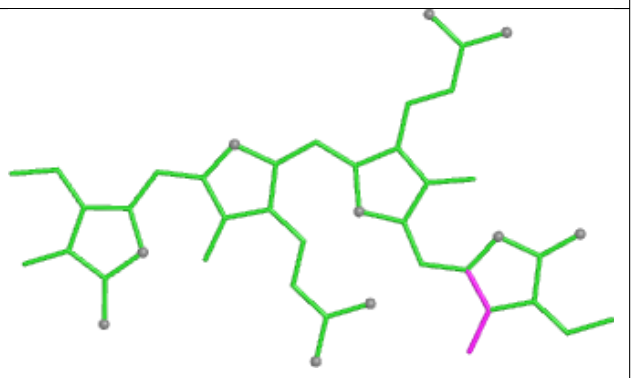


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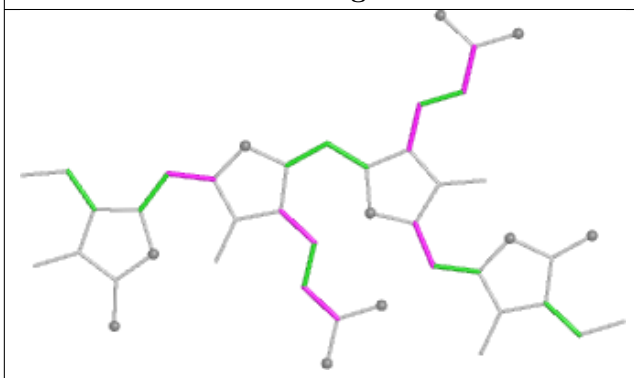
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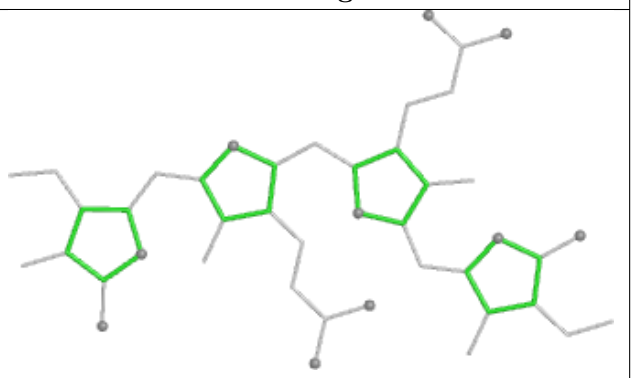
Bond lengths



Bond angles

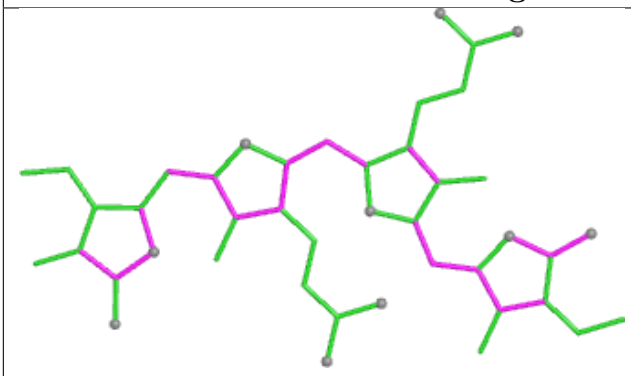


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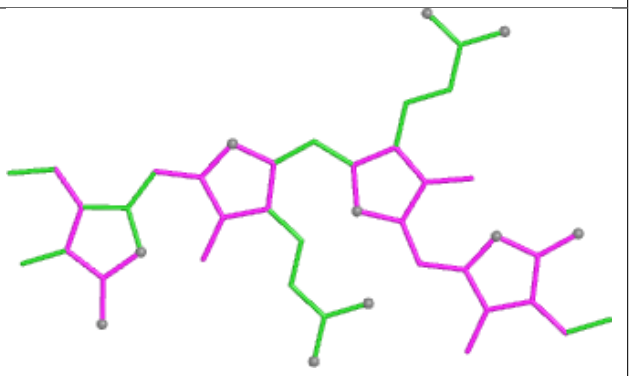


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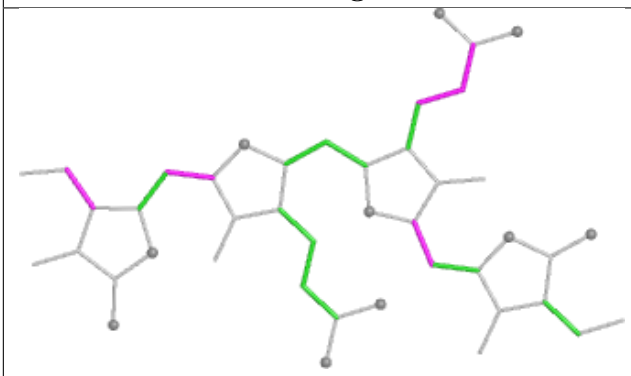
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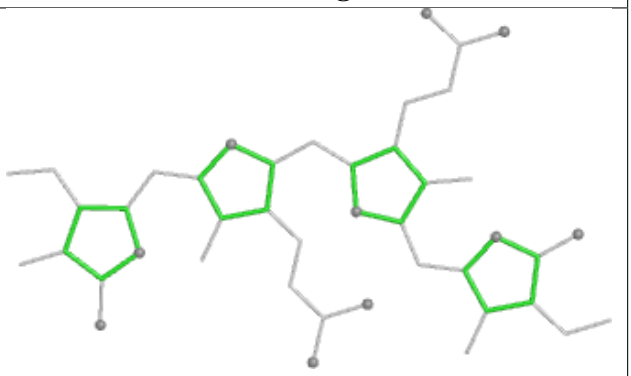
Bond lengths



Bond angles

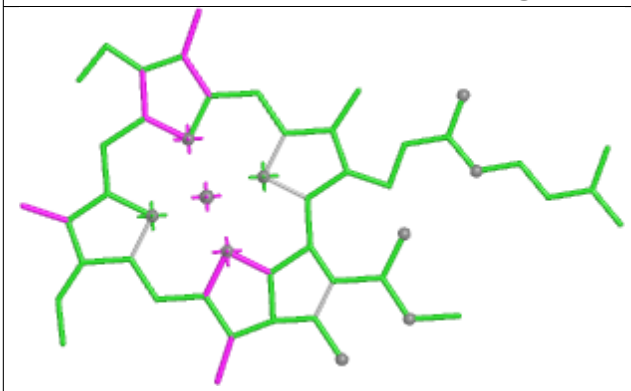


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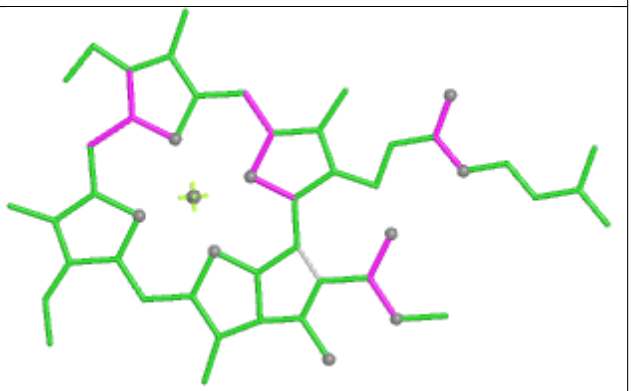


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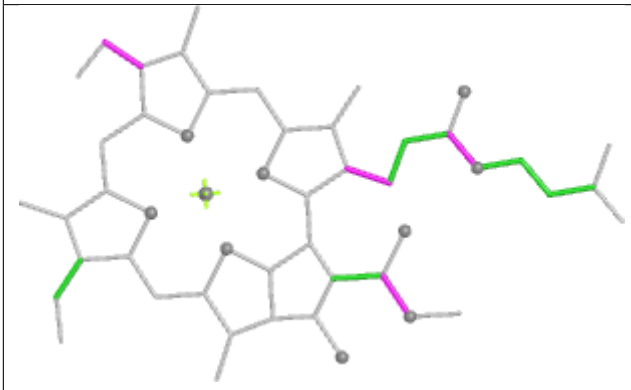
Ligand CLA C1 514



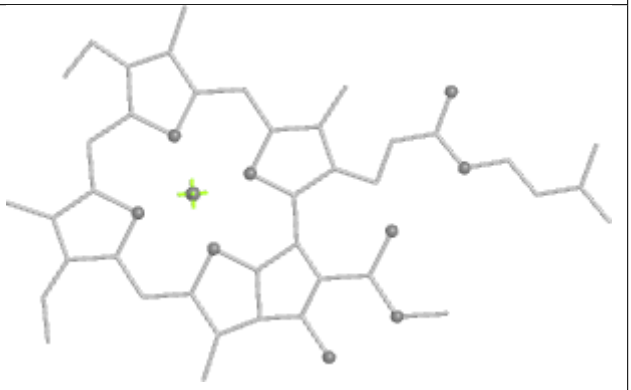
Bond lengths



Bond angles

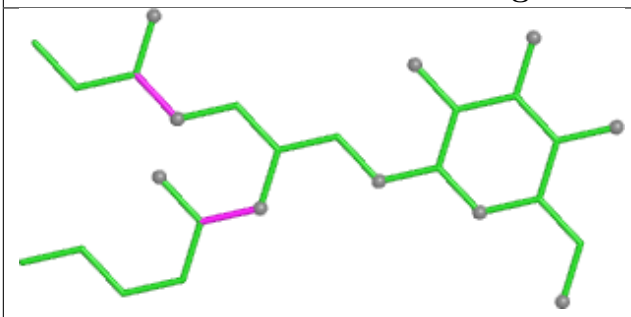


Torsions

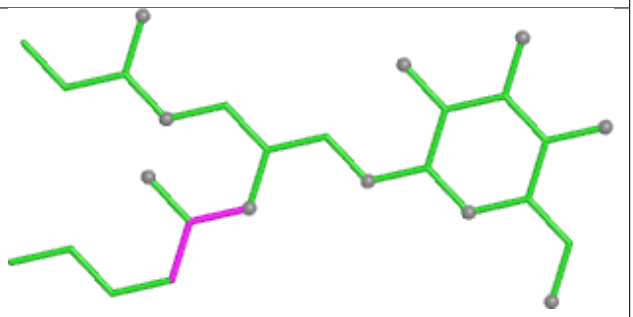


Rings

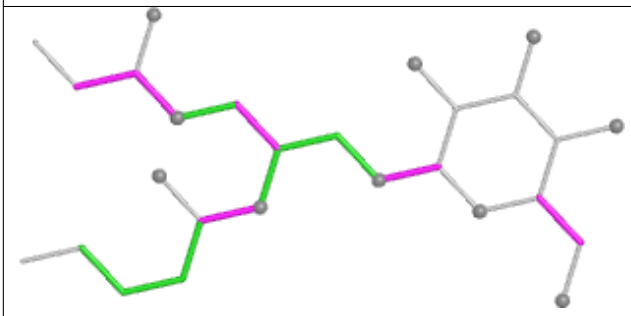
Ligand LMG JE 102



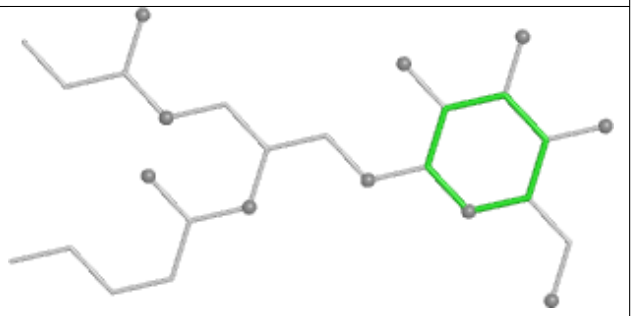
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Bond angles

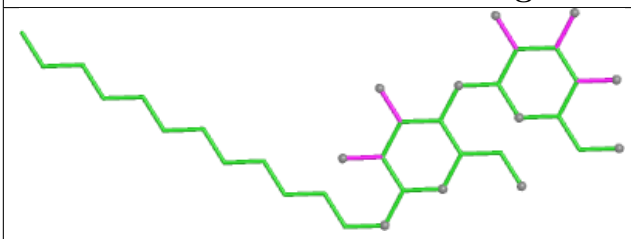


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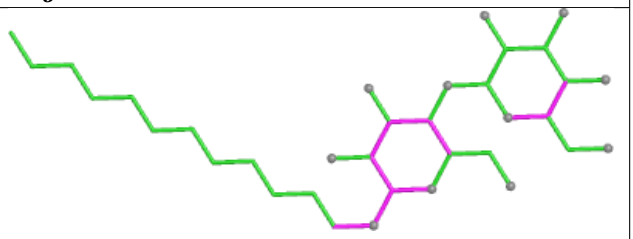


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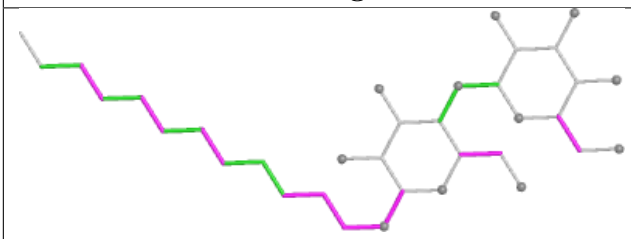
Ligand LMT jD 101



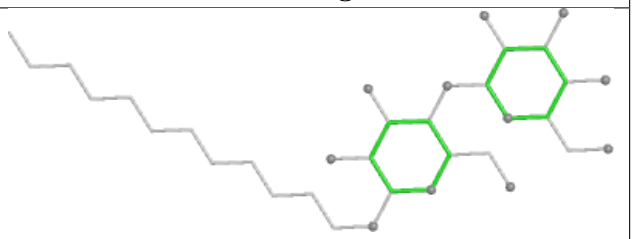
Bond lengths



Bond angles

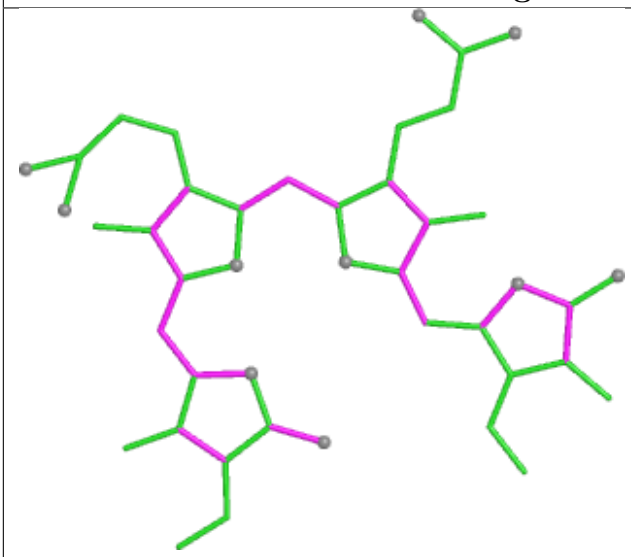


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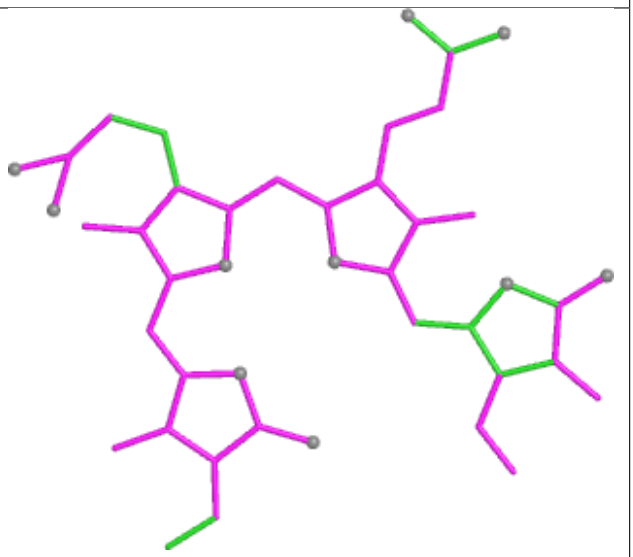


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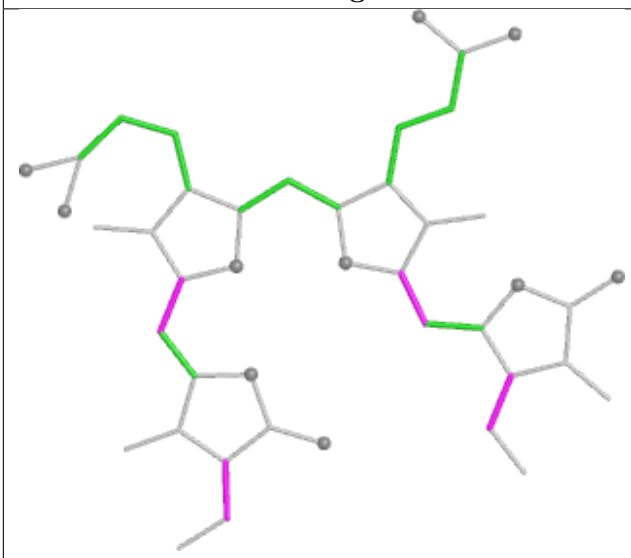
Ligand CYC cA 201



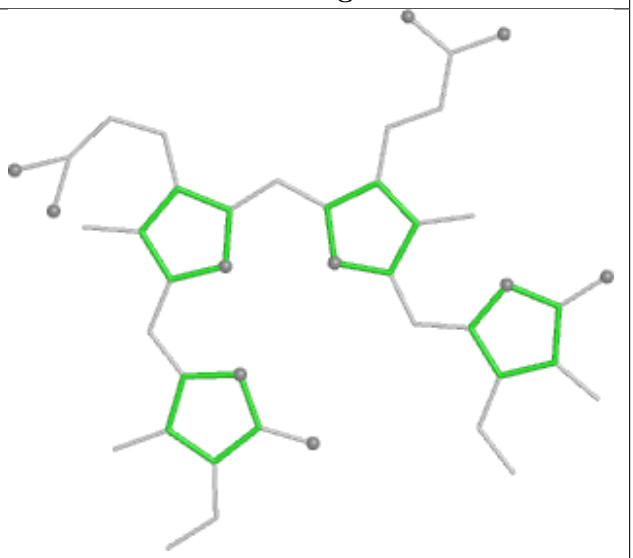
Bond lengths



Bond angles

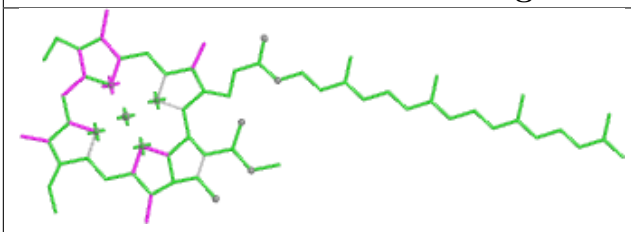


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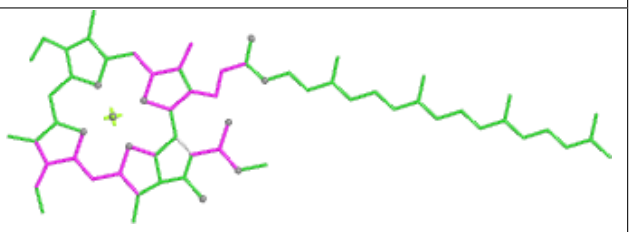


Rings

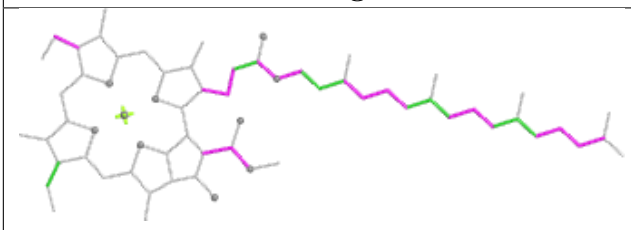
Ligand CLA cD 510



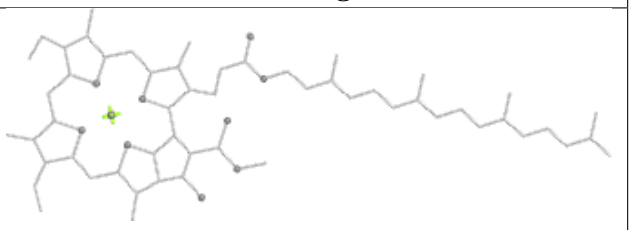
Bond lengths



Bond angles

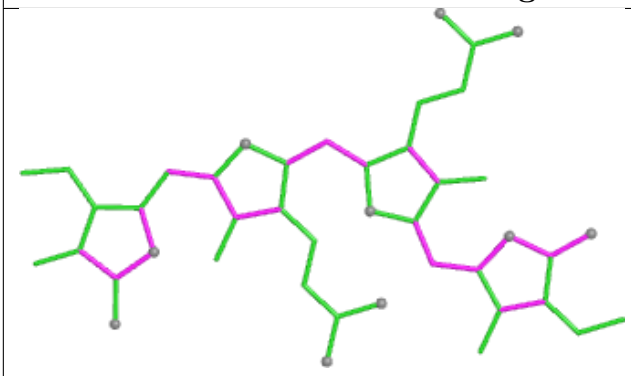


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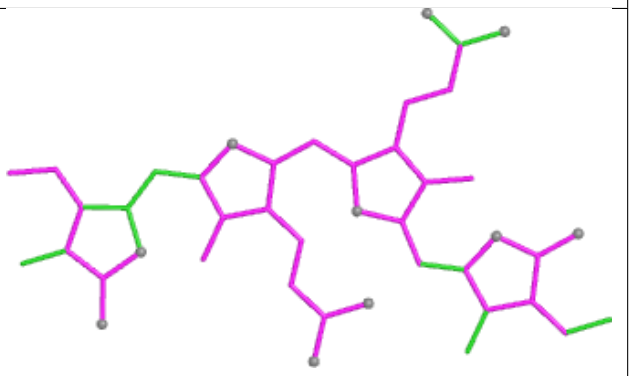


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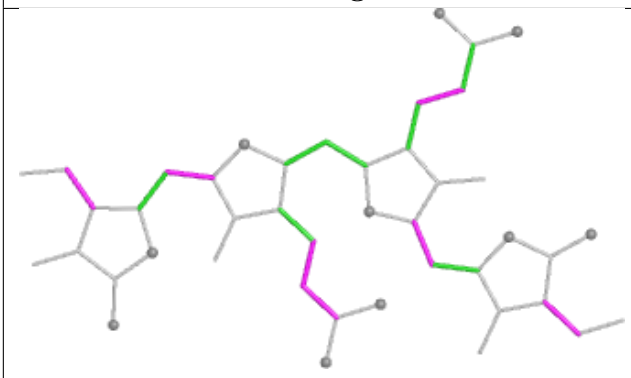
Ligand CYC hI 201



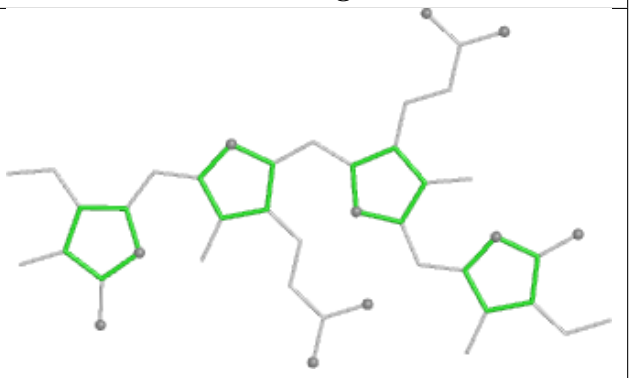
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Bond angles

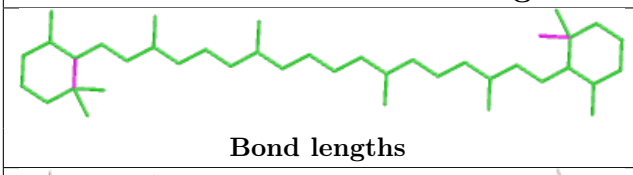


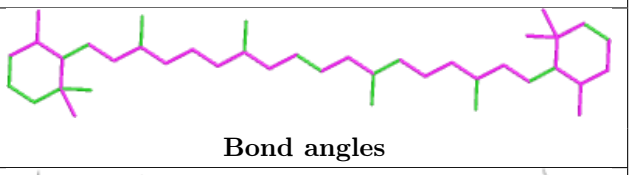
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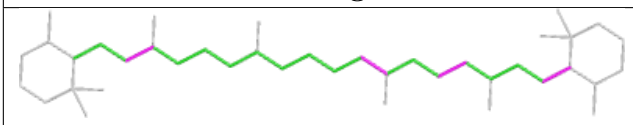


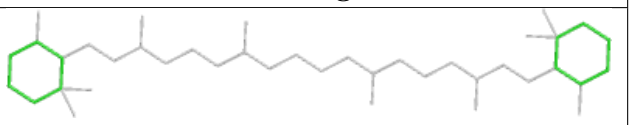
Rings

Ligand BCR hE 105

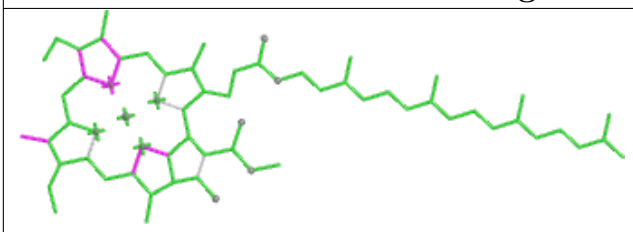

Bond lengths

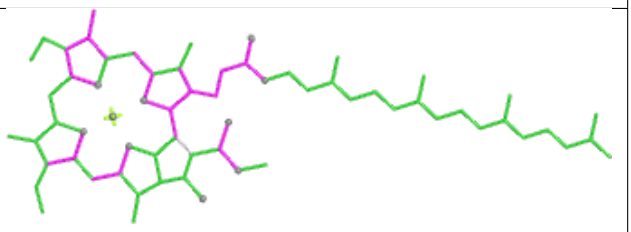

Bond angles

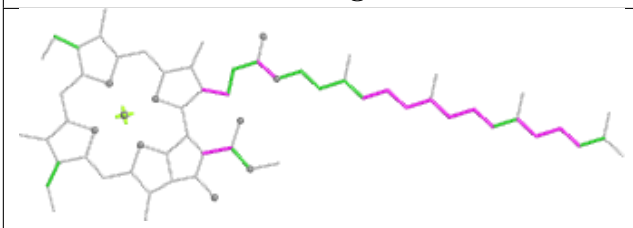

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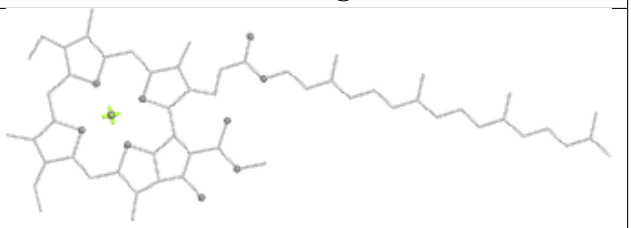

Rings

Ligand CLA b1 612

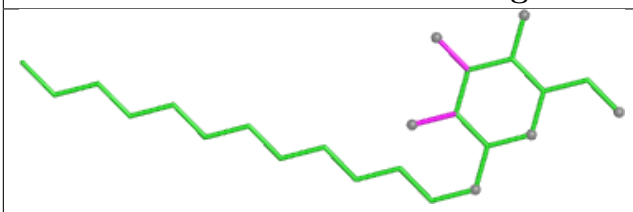

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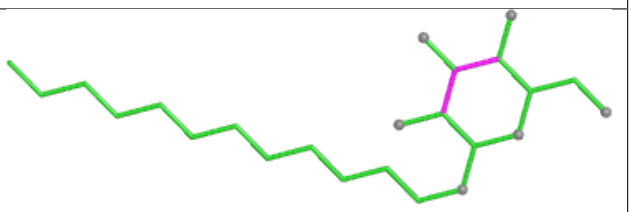

Bond angles

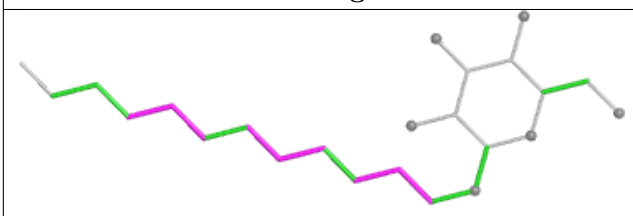

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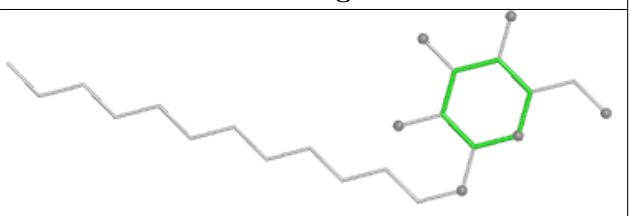

Rings

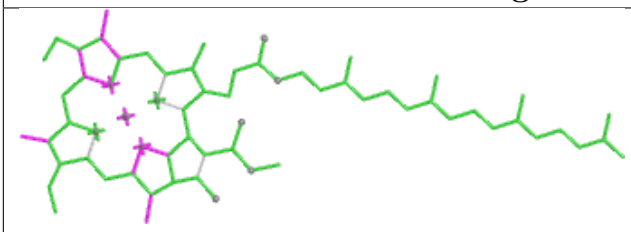
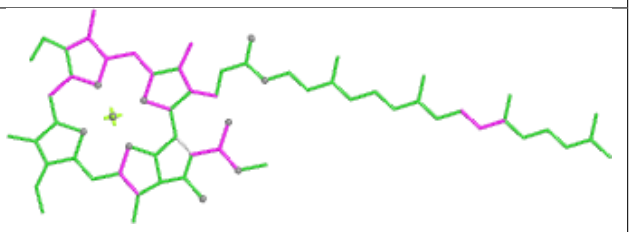
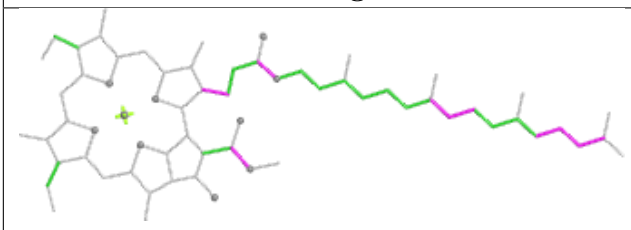
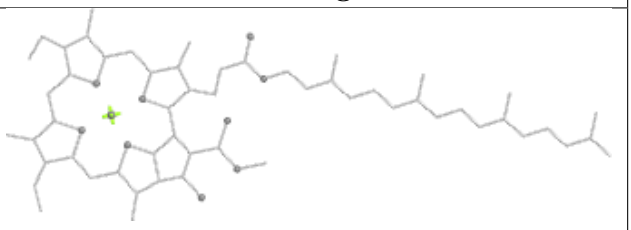
Ligand LMT bD 620

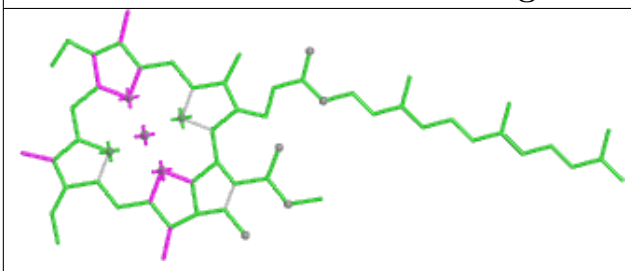
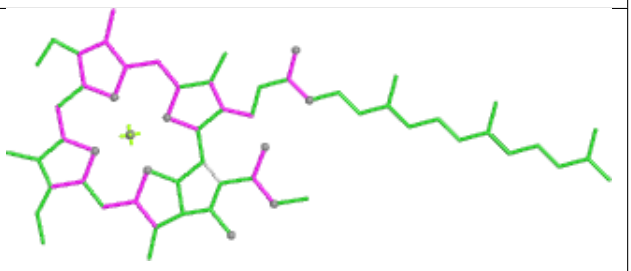
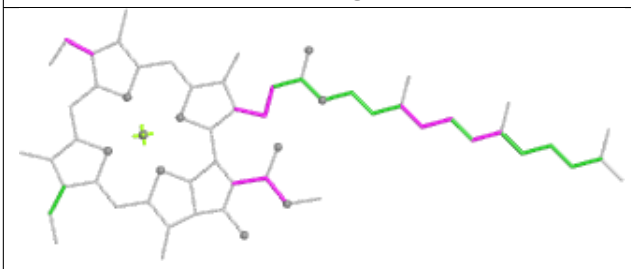
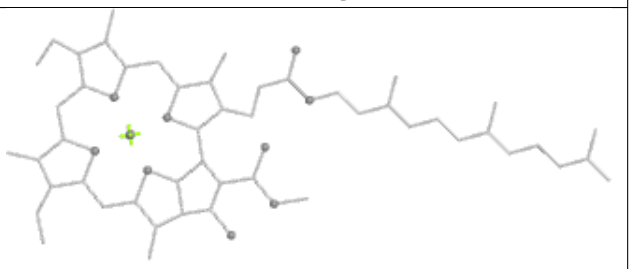

Bond lengths


Bond angles

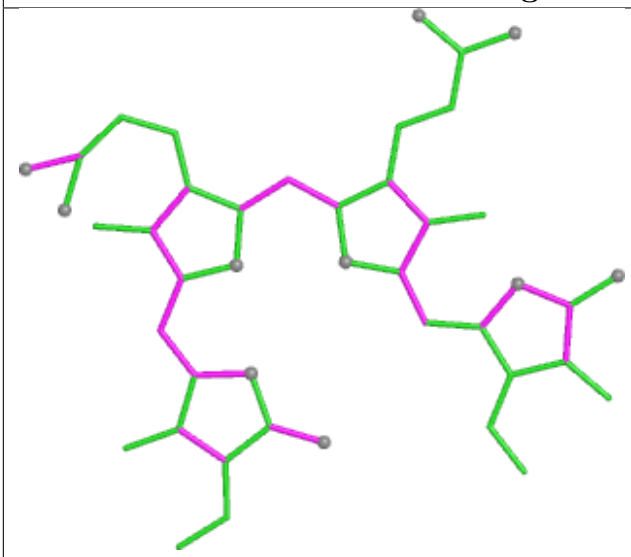

Torsions


Rings

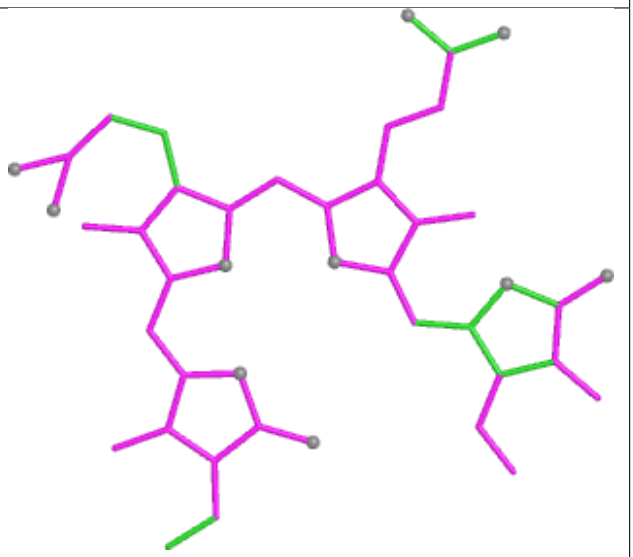
Ligand CLA DE 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b1 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

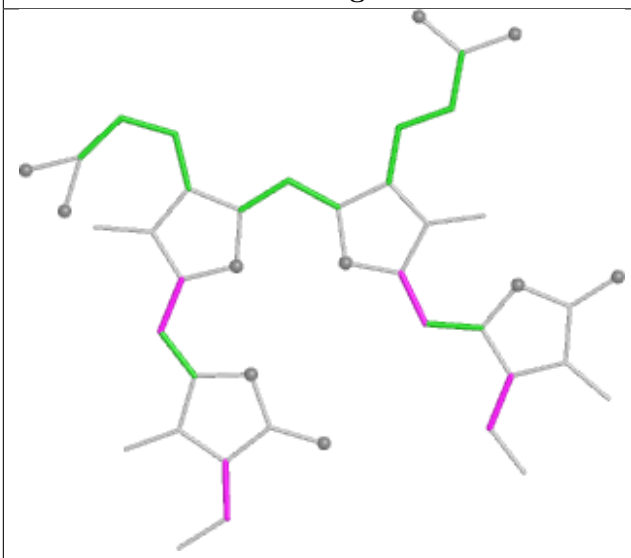
Ligand CYC i5 202



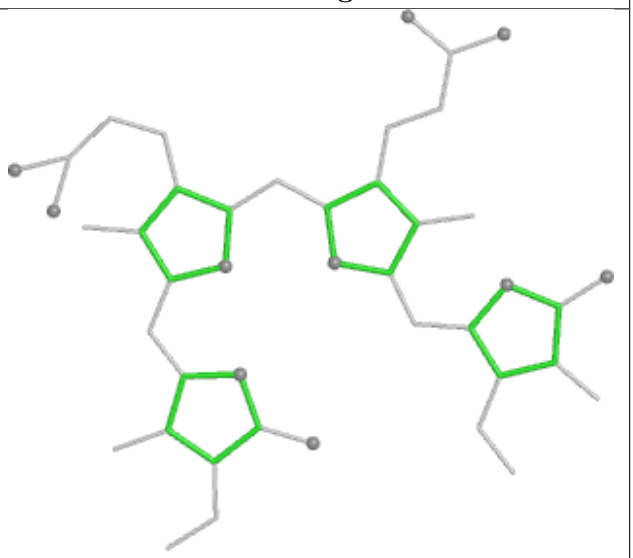
Bond lengths



Bond angles

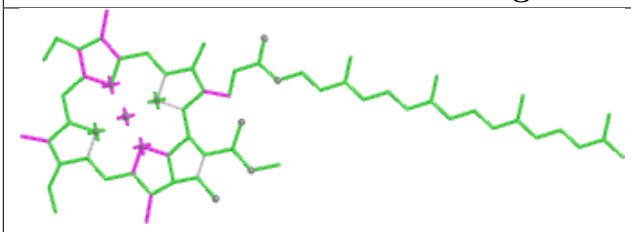


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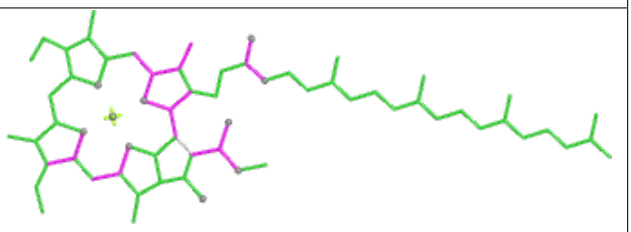


Rings

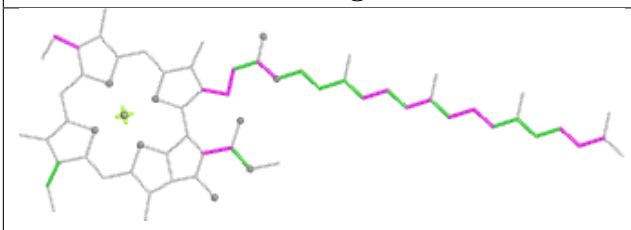
Ligand CLA BE 602



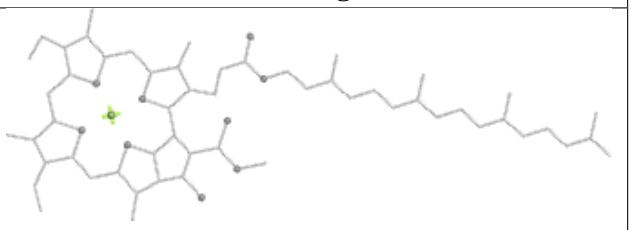
Bond lengths



Bond angles

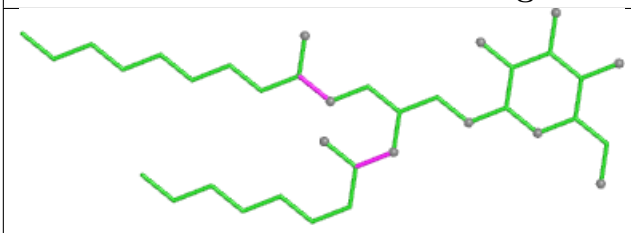


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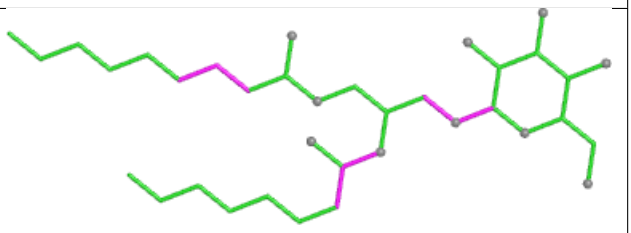


Rings

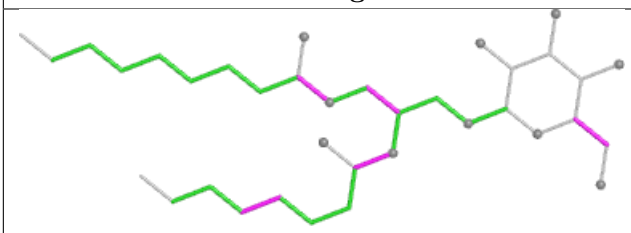
Ligand LMG t1 101



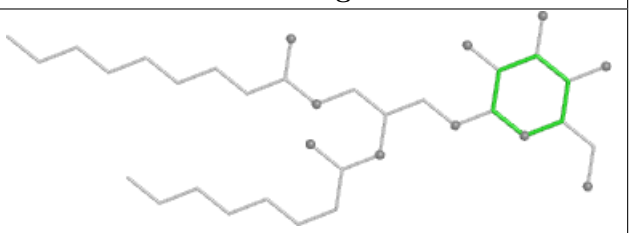
Bond lengths



Bond angles

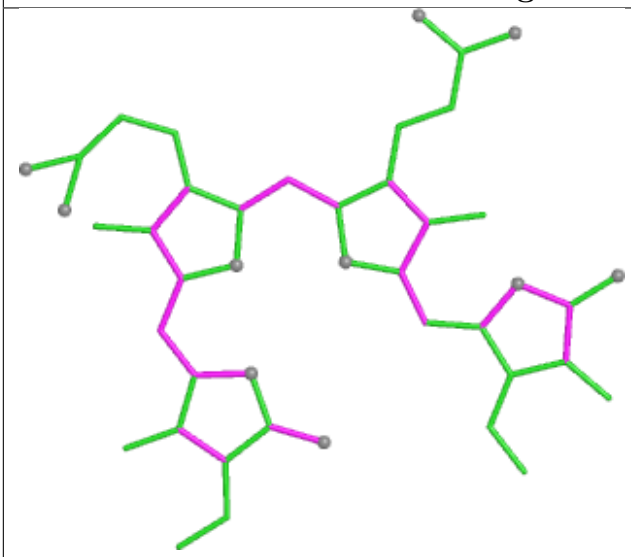


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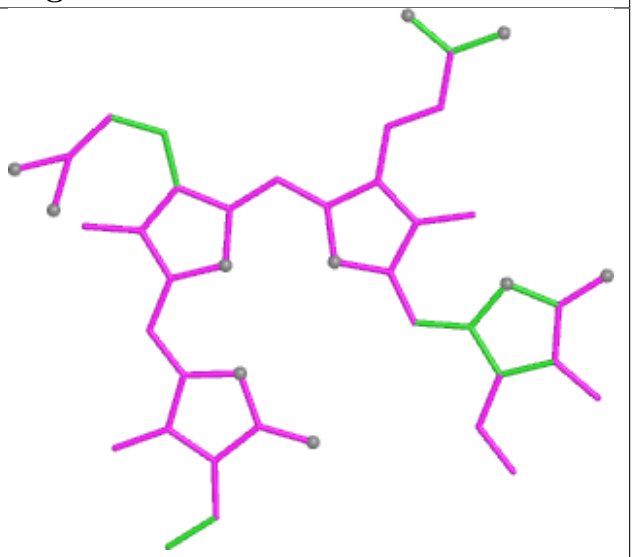


Rings

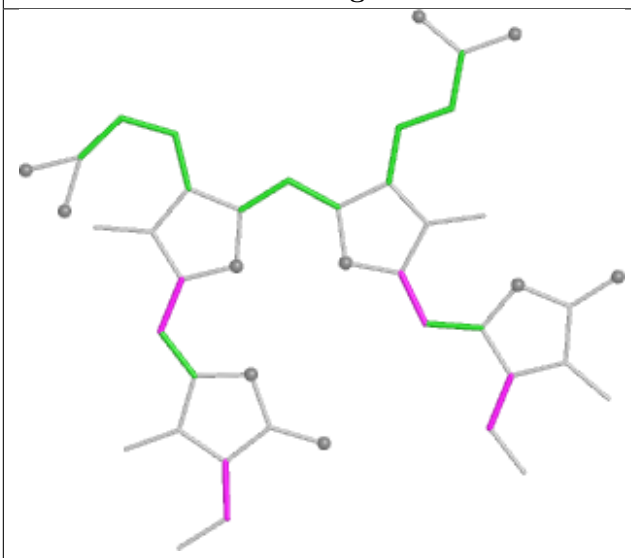
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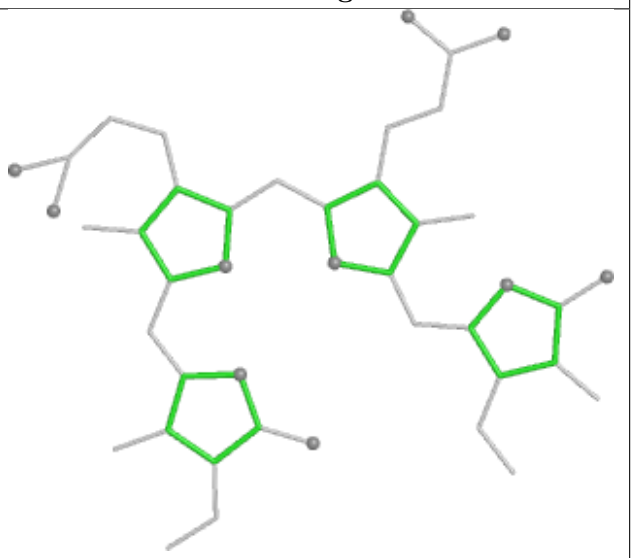
Bond lengths



Bond angles

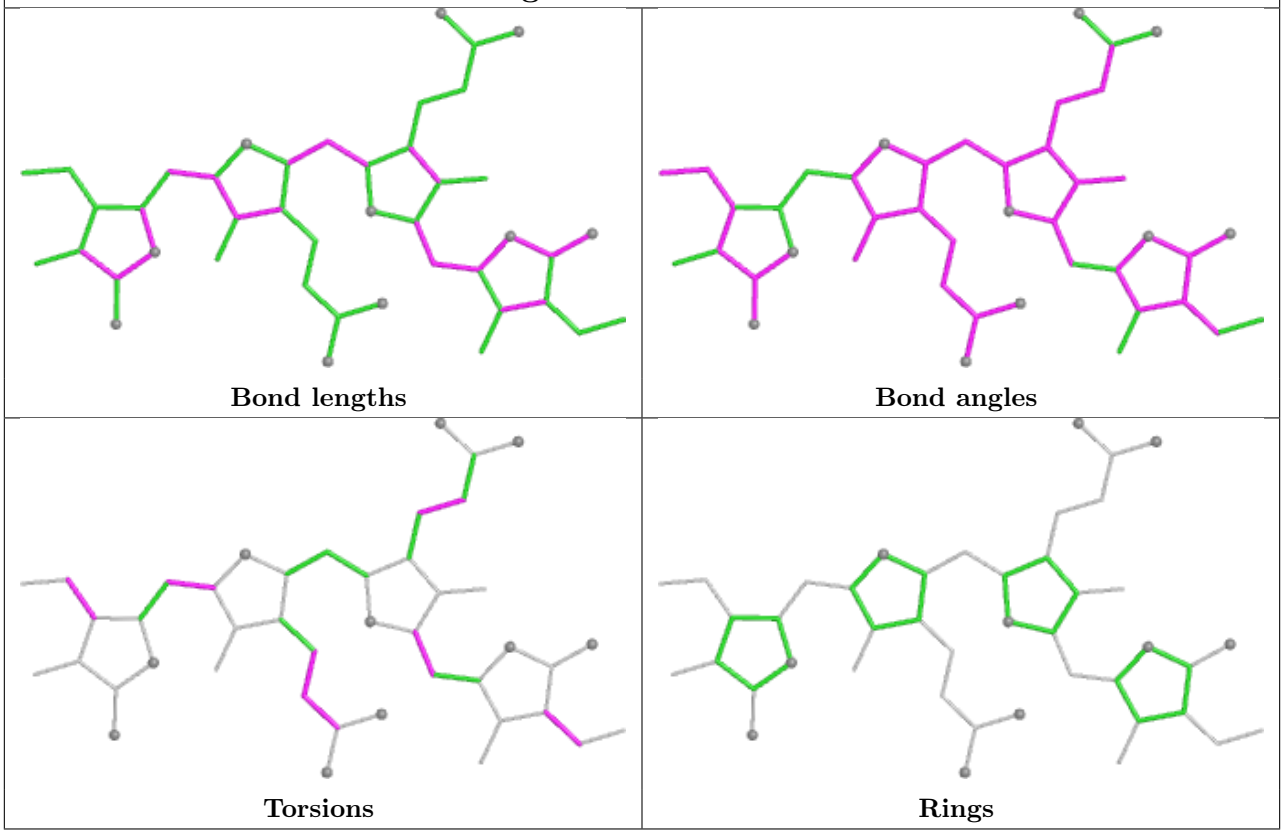


Torsions

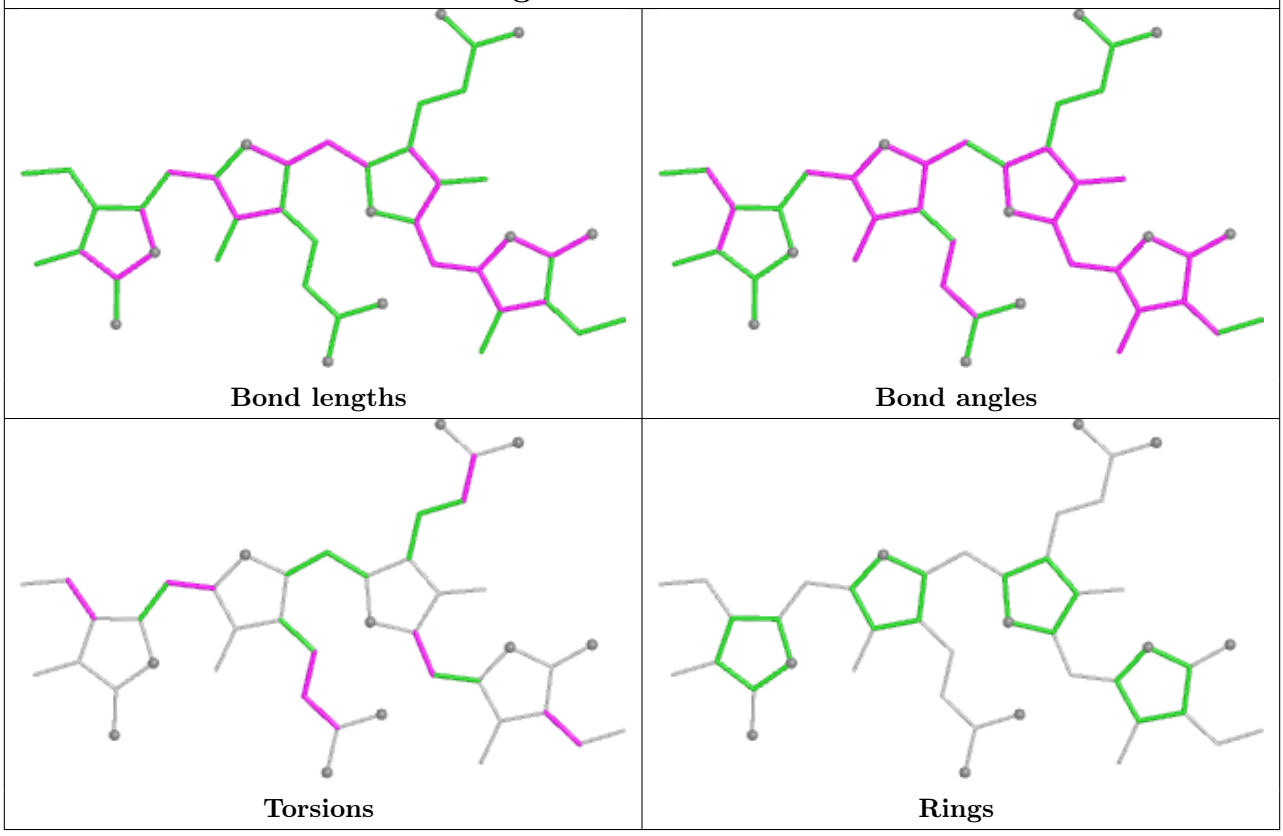


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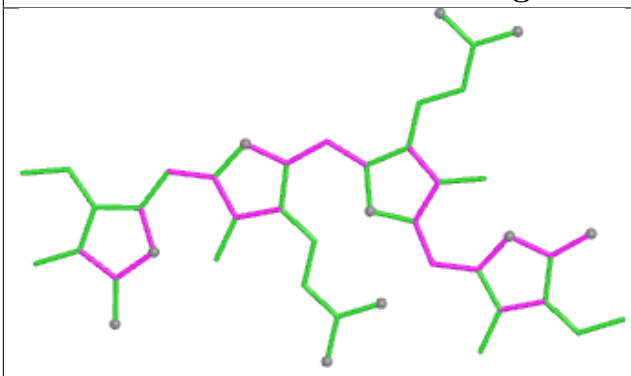
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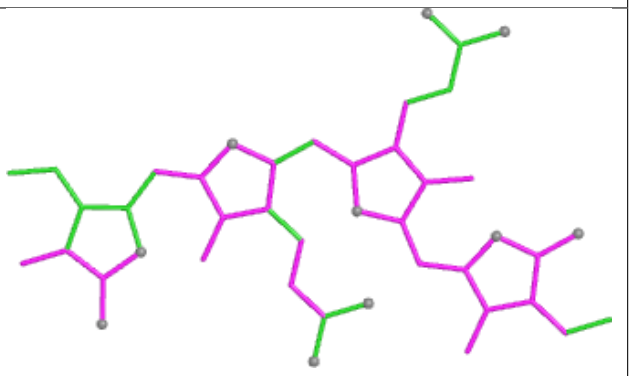
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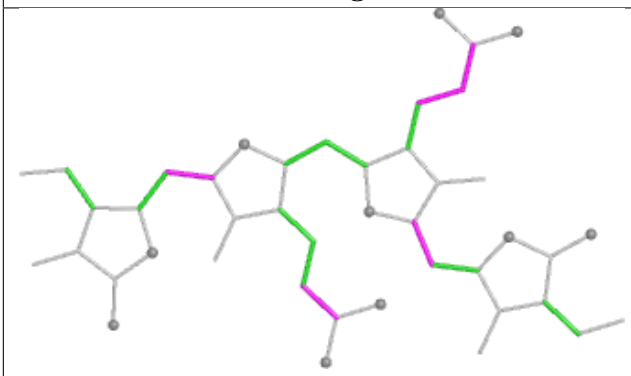
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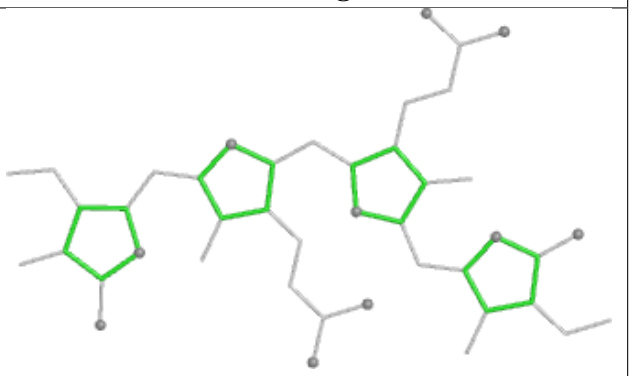
Bond lengths



Bond angles

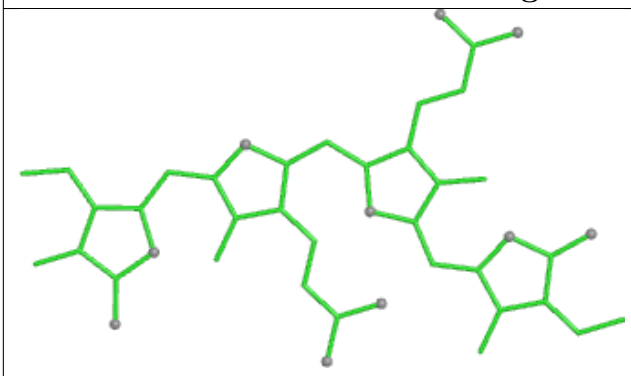


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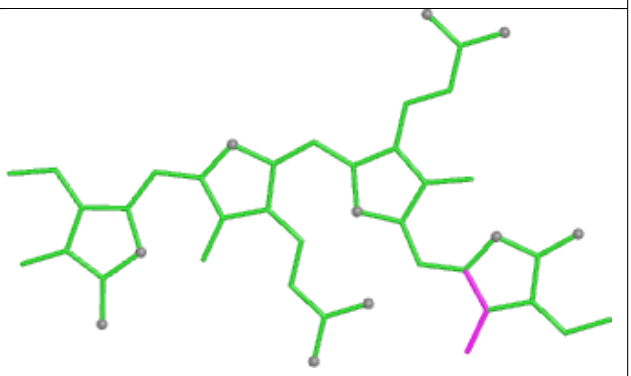


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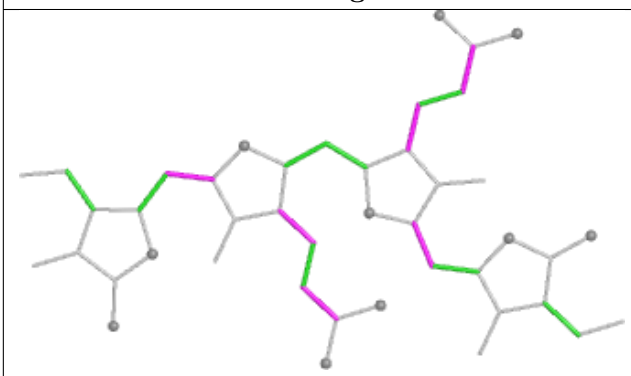
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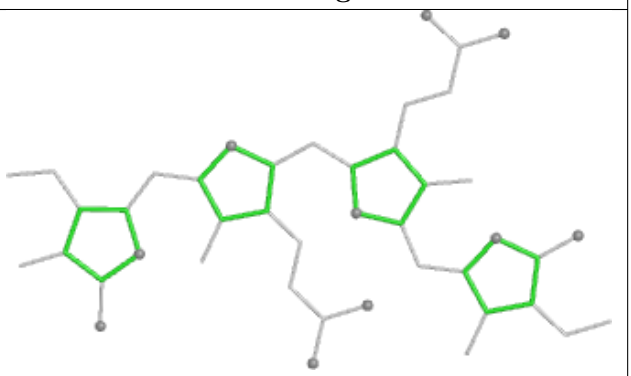
Bond lengths



Bond angles

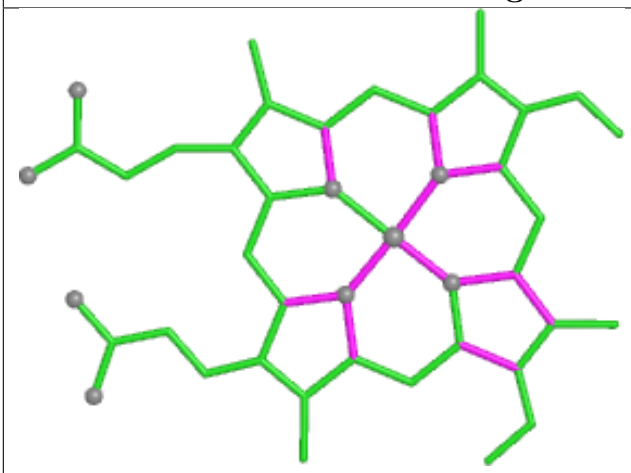


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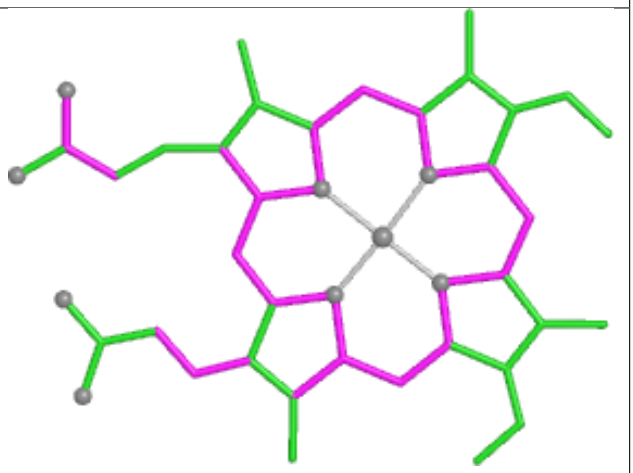


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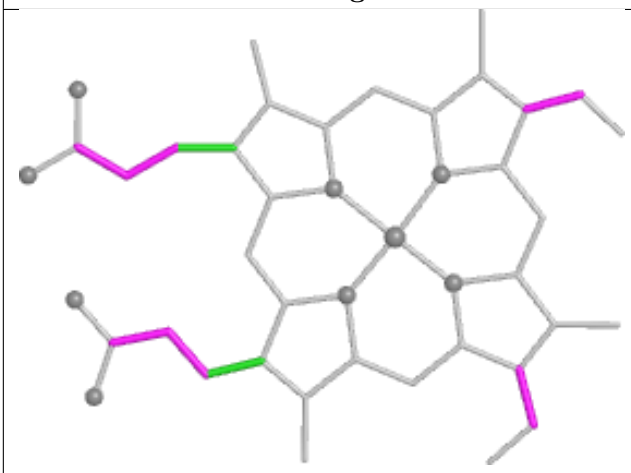
Ligand HEM ED 101



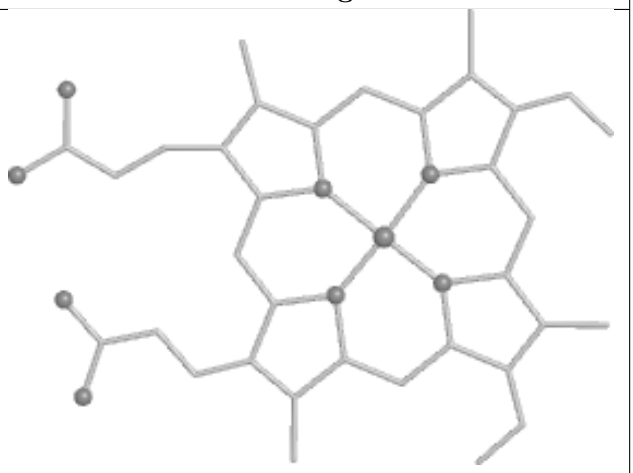
Bond lengths



Bond angles

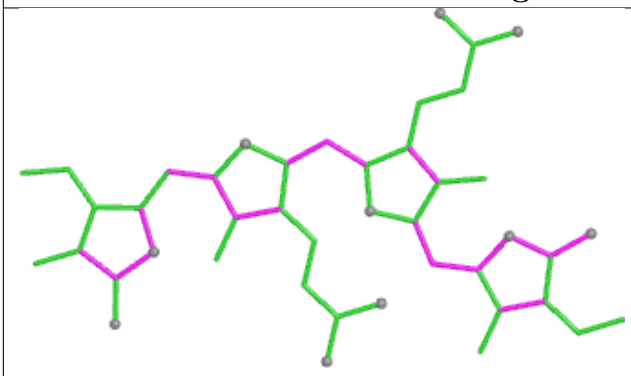


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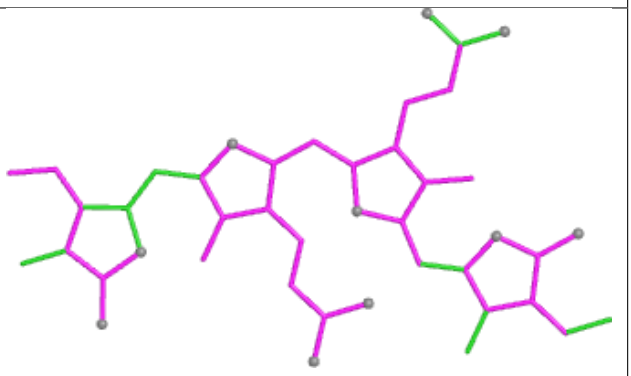


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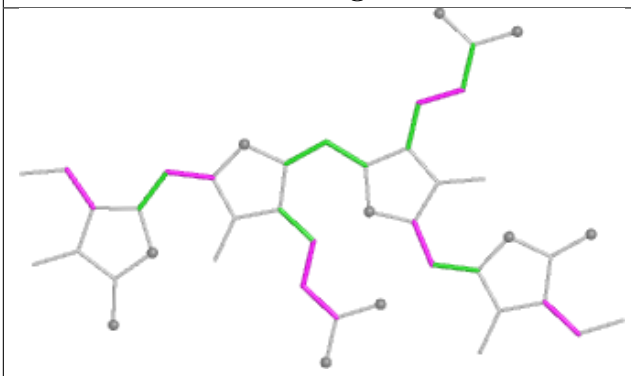
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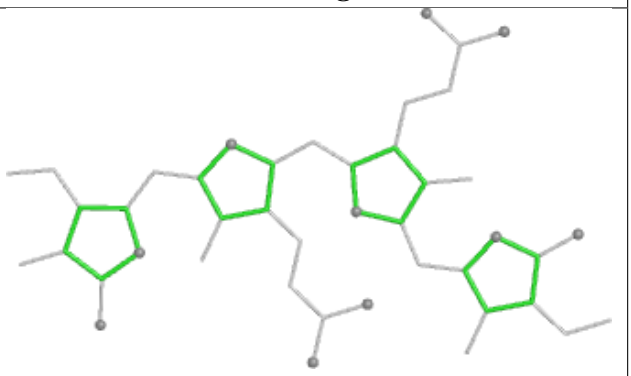
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Bond angles

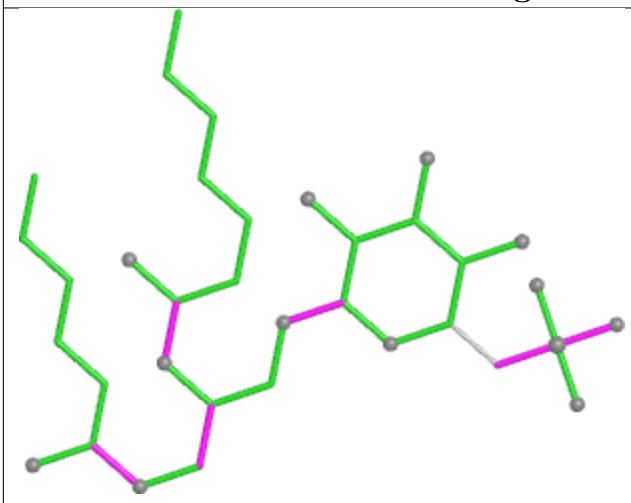


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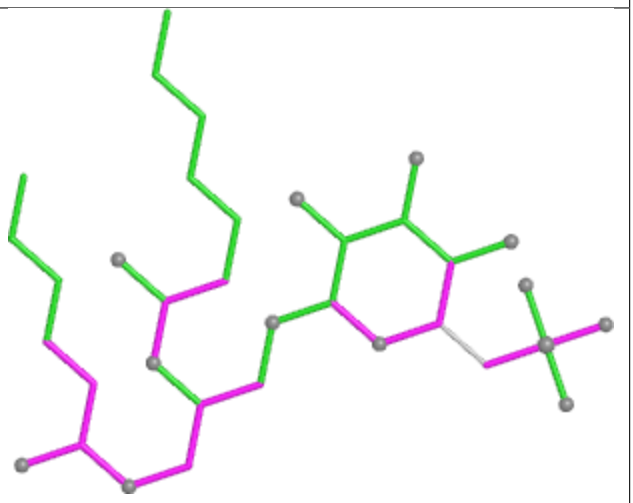


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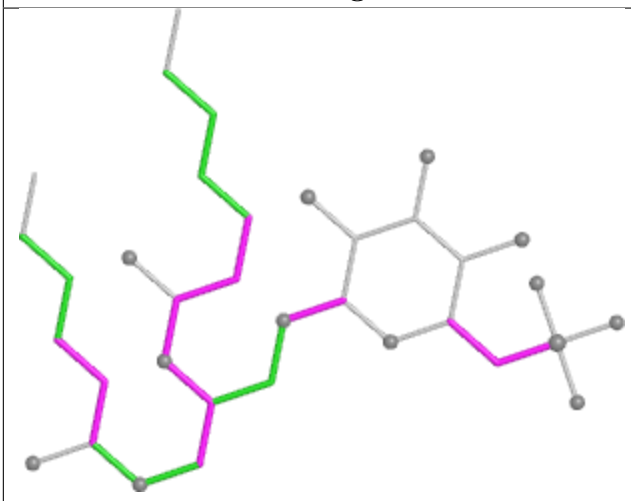
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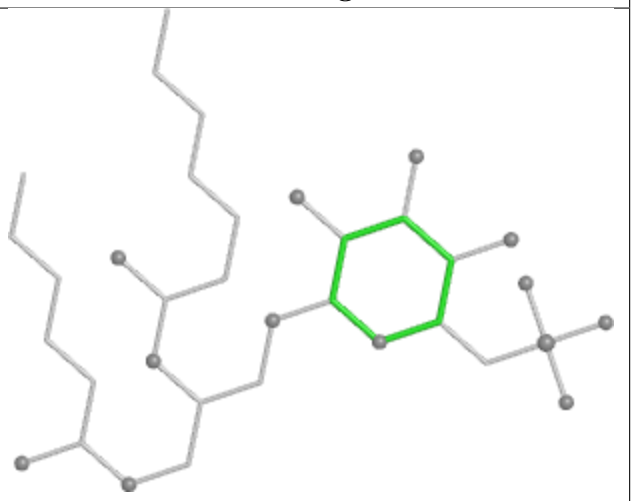
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Bond angles

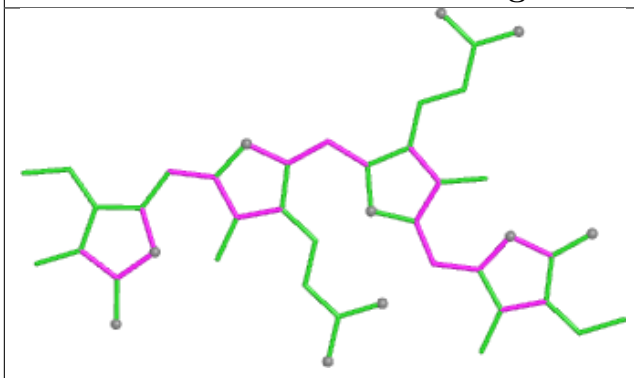


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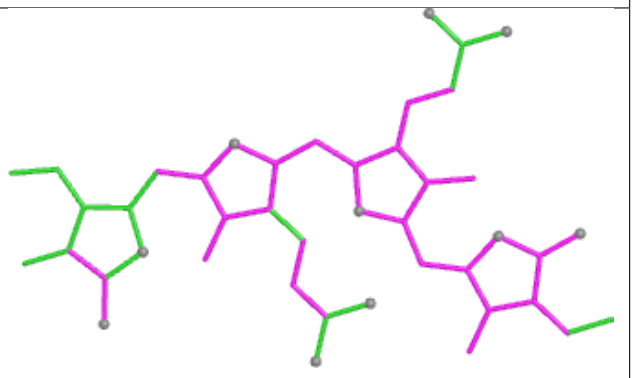


Rings

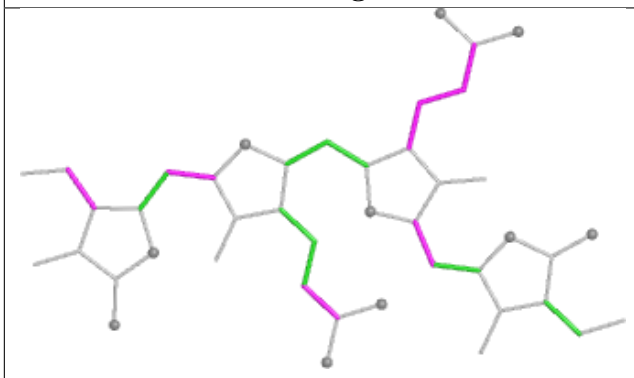
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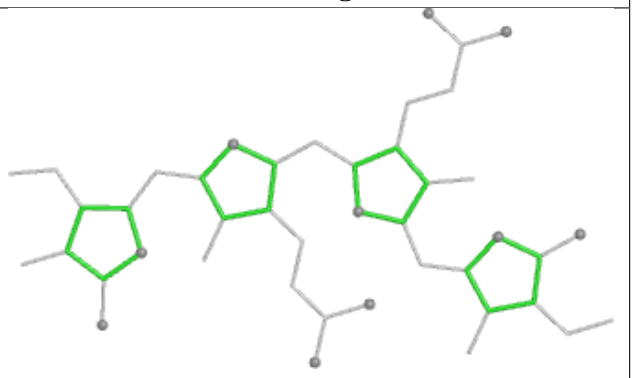
Bond lengths



Bond angles

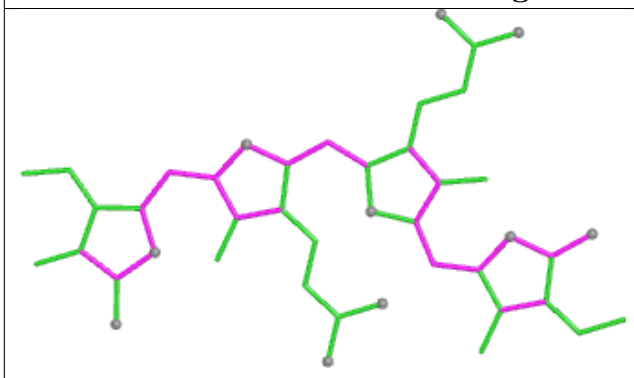


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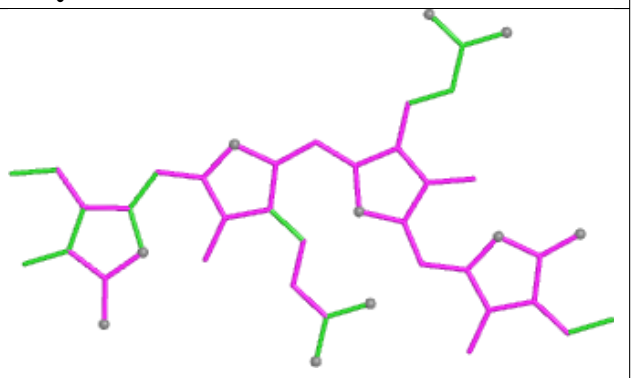


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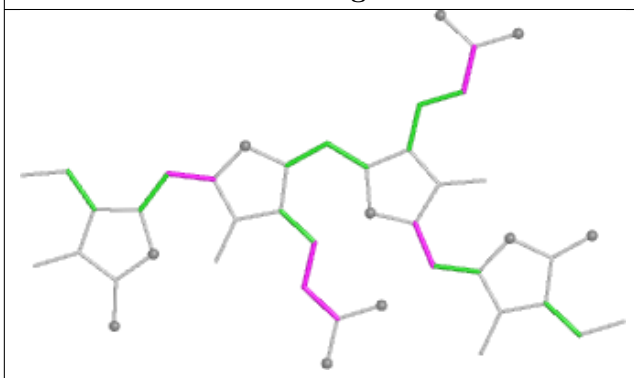
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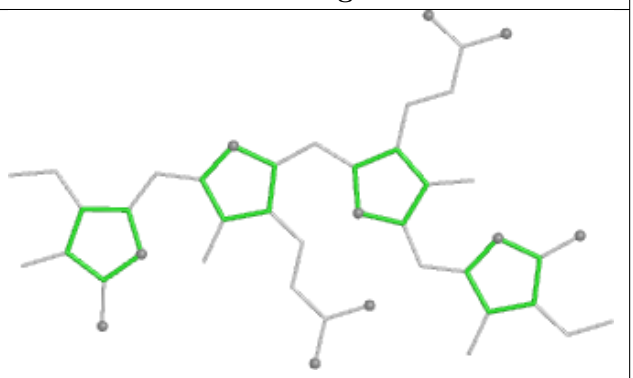
Bond lengths



Bond angles

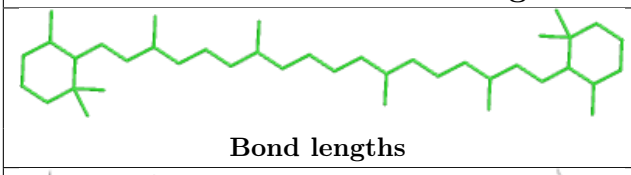


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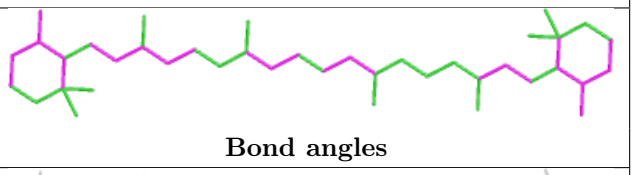


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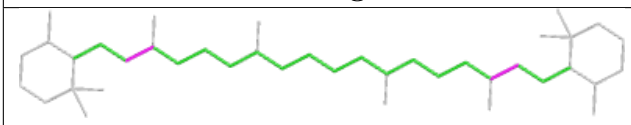
Ligand BCR BD 617



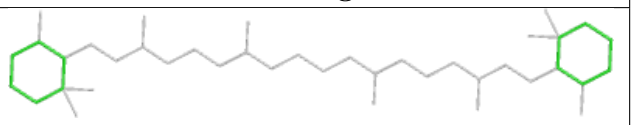
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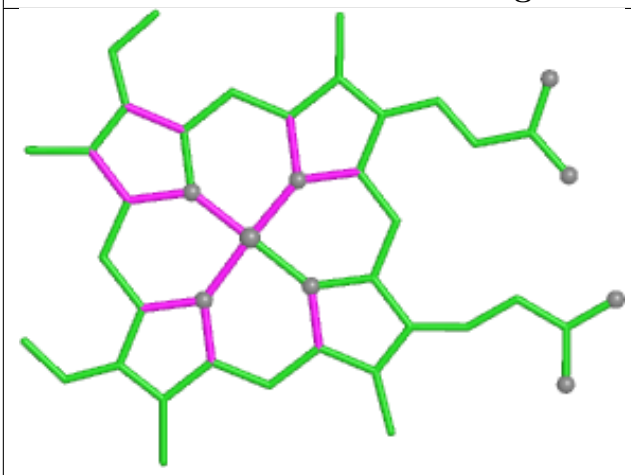


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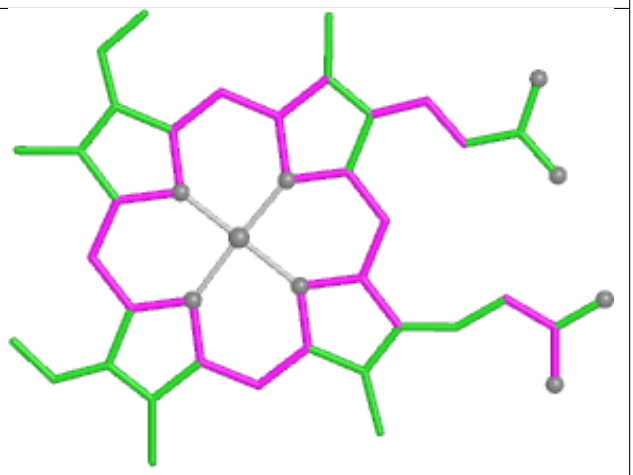


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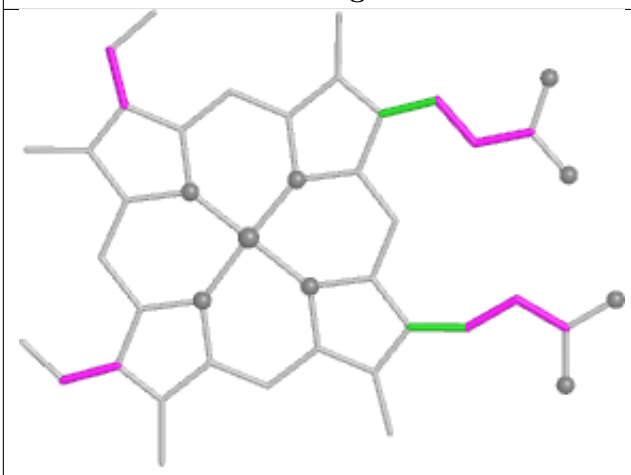
Ligand HEM fE 101



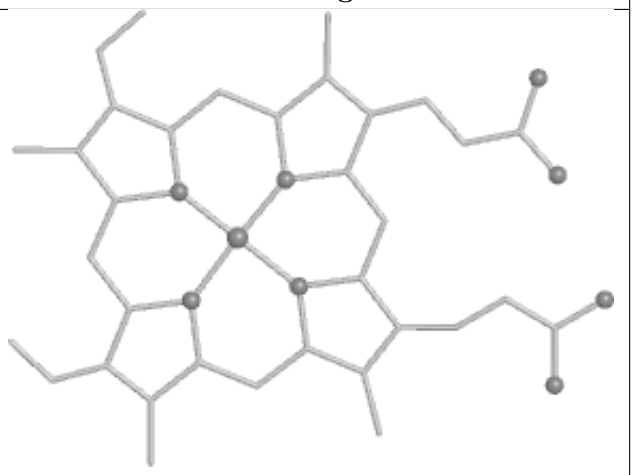
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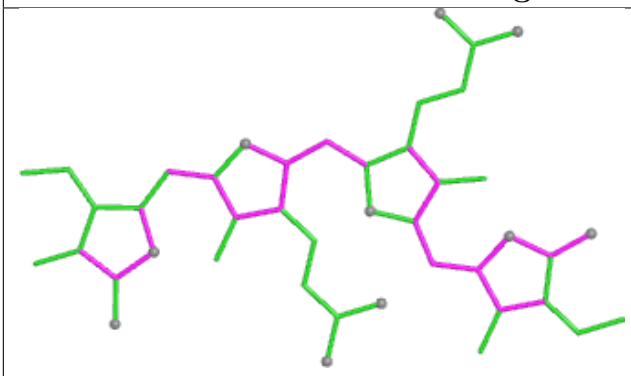


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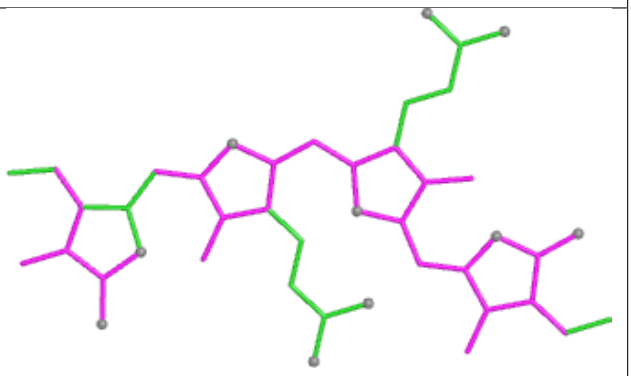


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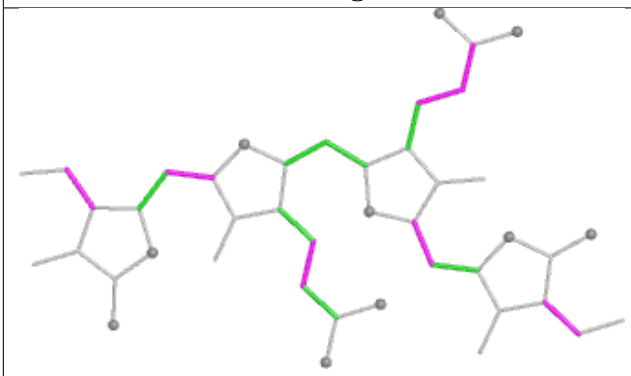
Ligand CYC oB 201



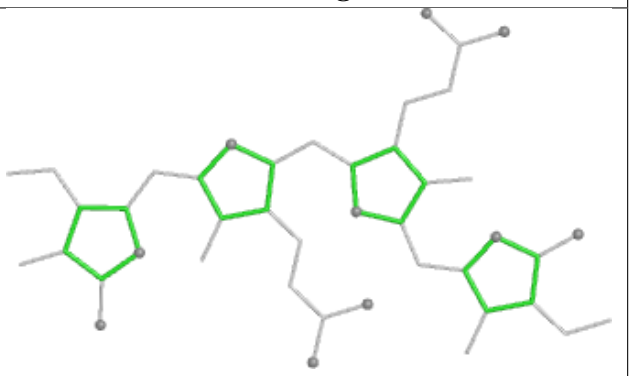
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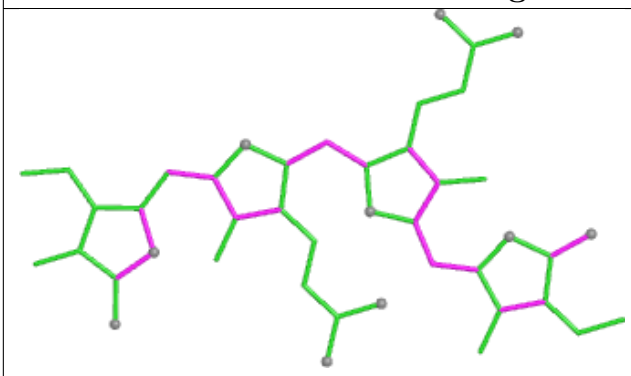


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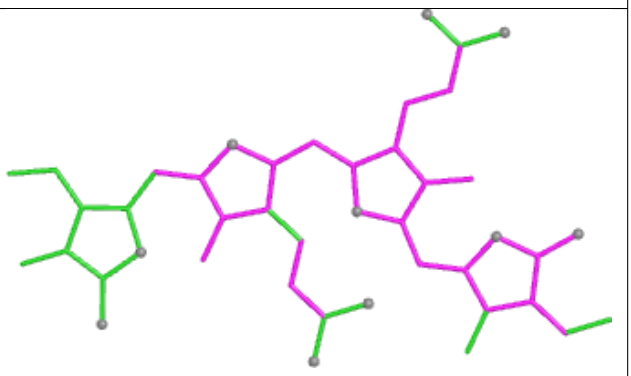


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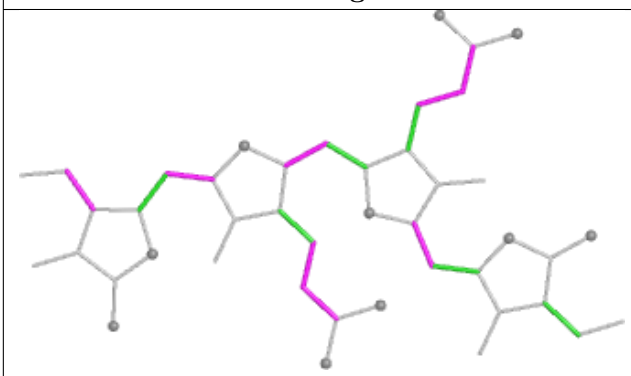
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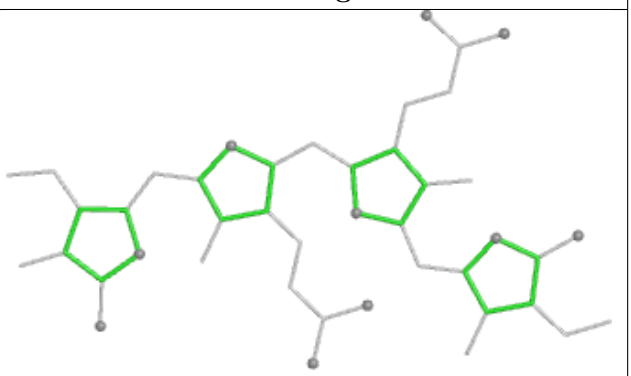
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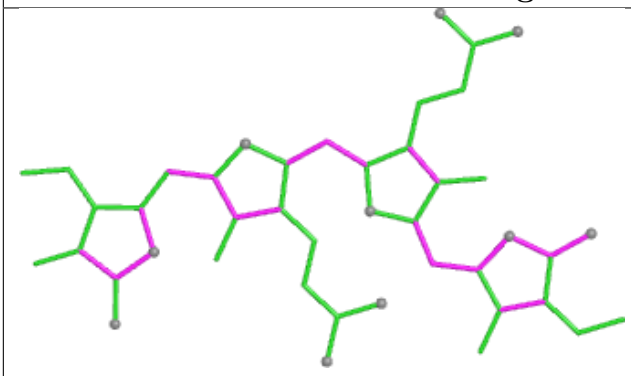


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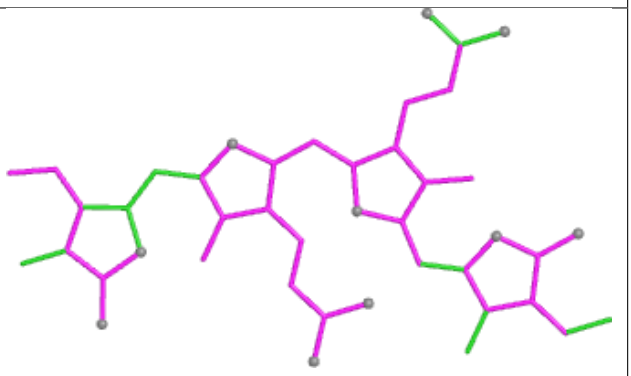


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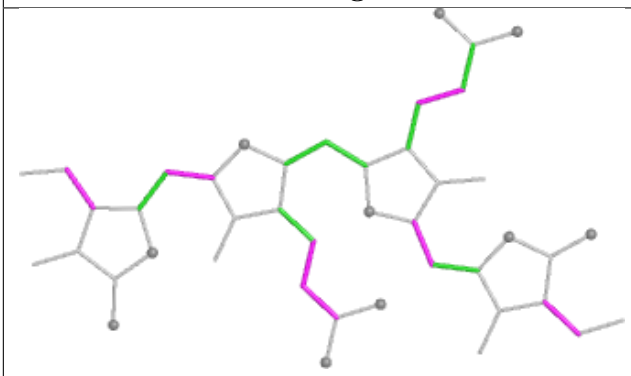
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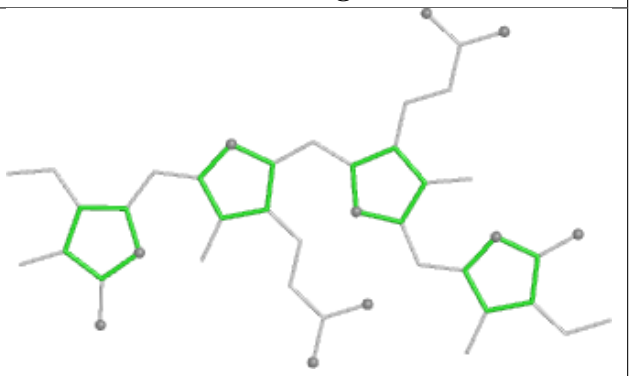
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Bond angles

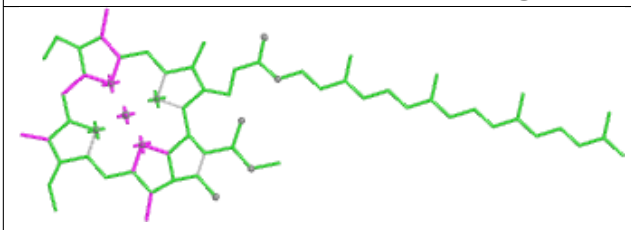


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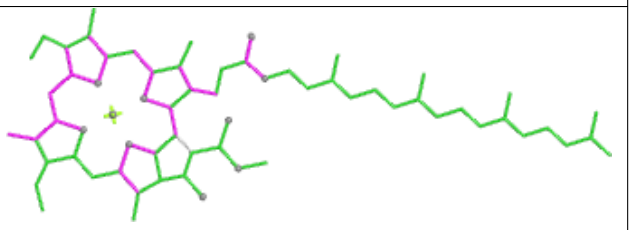


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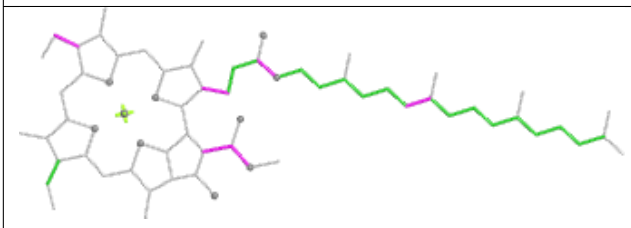
Ligand CLA cD 504



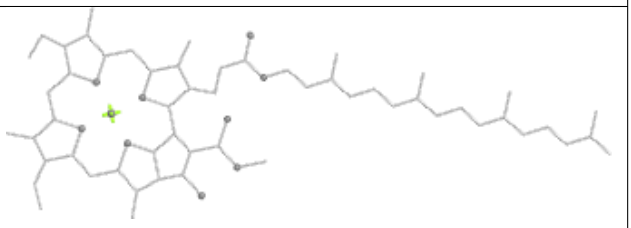
Bond lengths



Bond angles

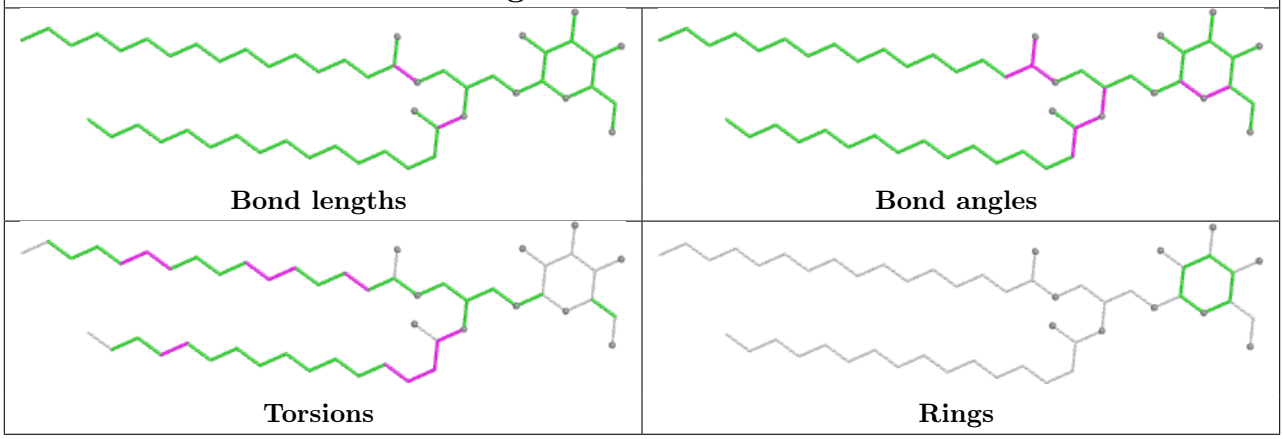


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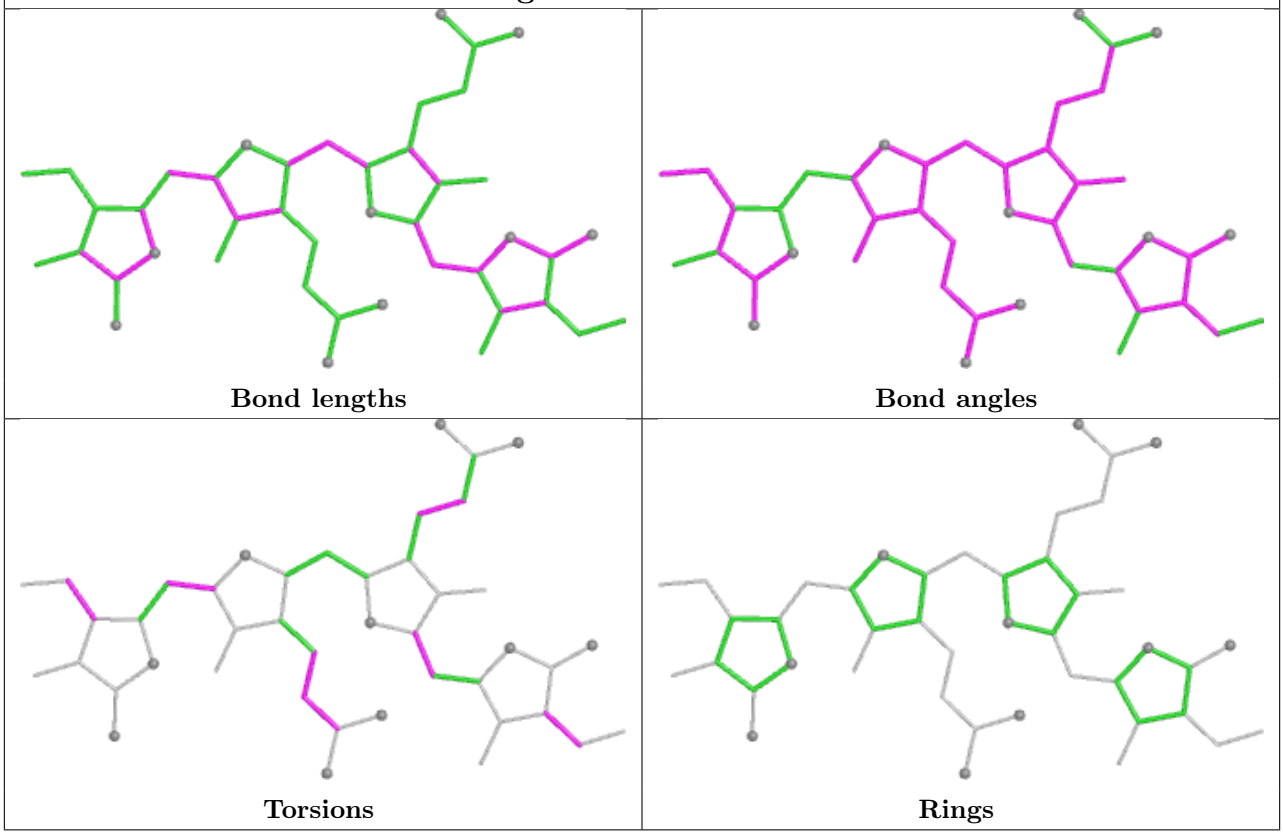


Rings

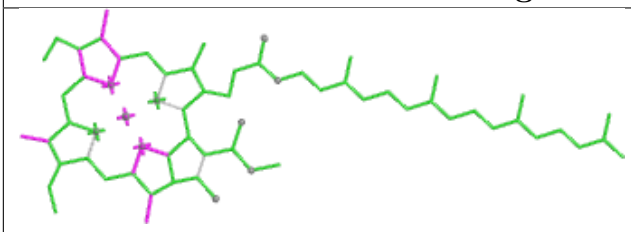
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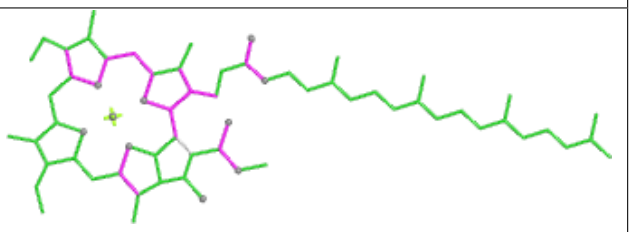
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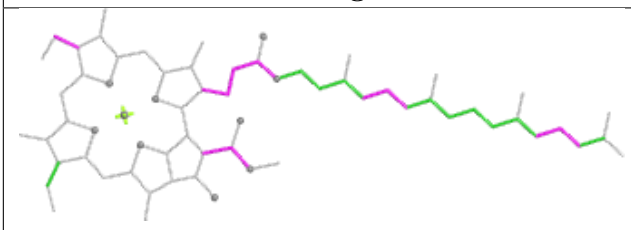
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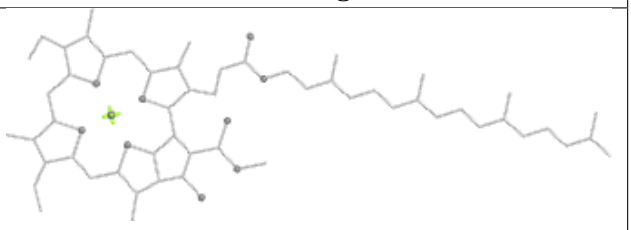
Bond lengths



Bond angles

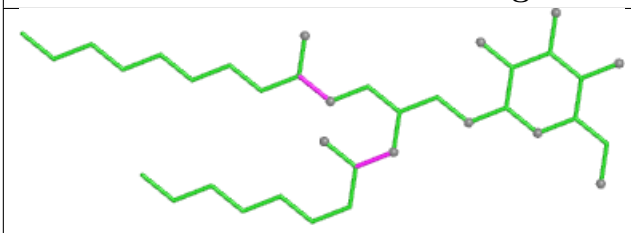


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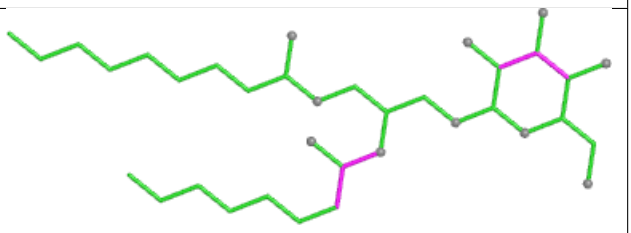


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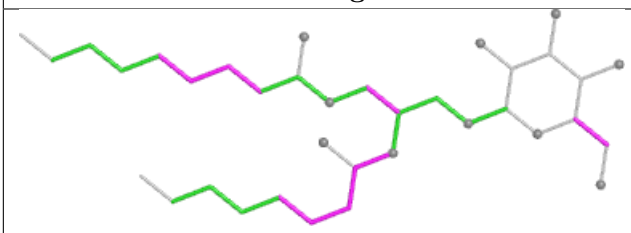
Ligand LMG aE 409



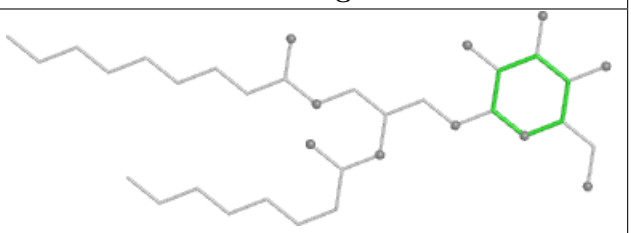
Bond lengths



Bond angles

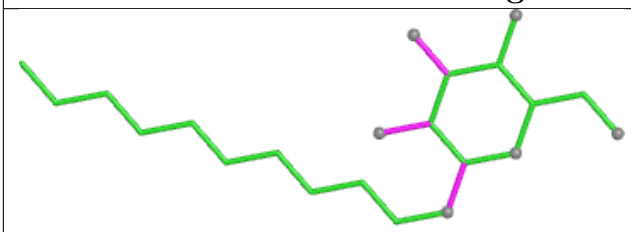


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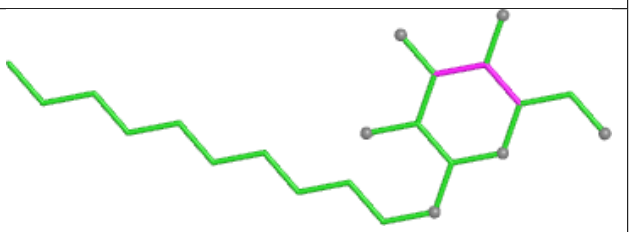


Rings

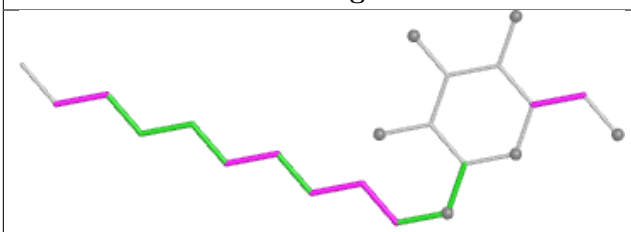
Ligand LMT DD 413



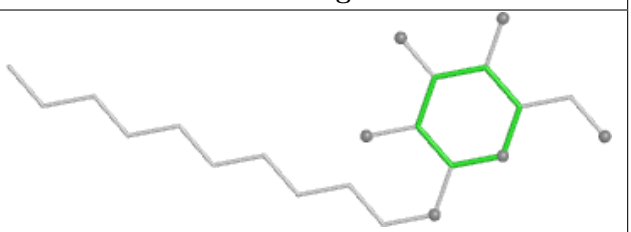
Bond lengths



Bond angles

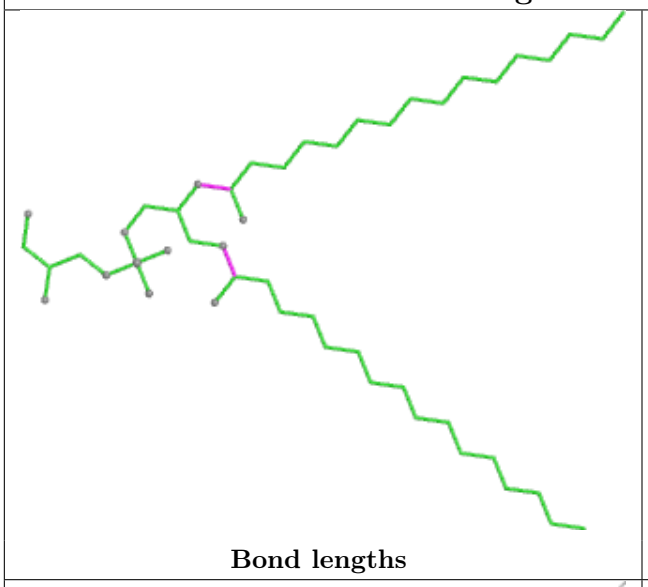


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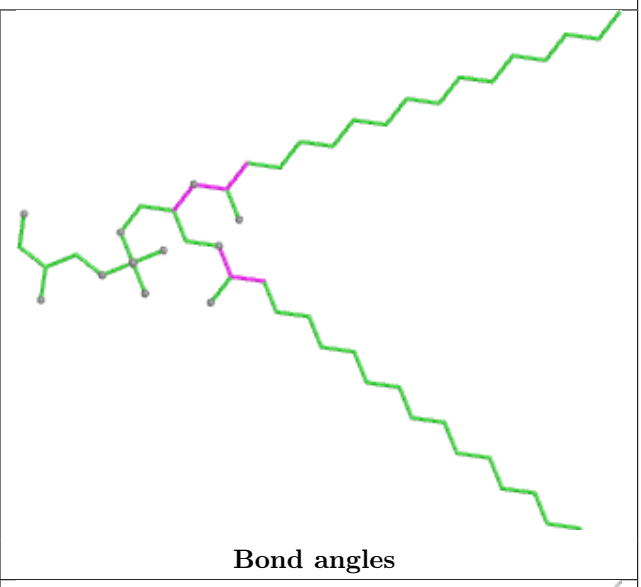


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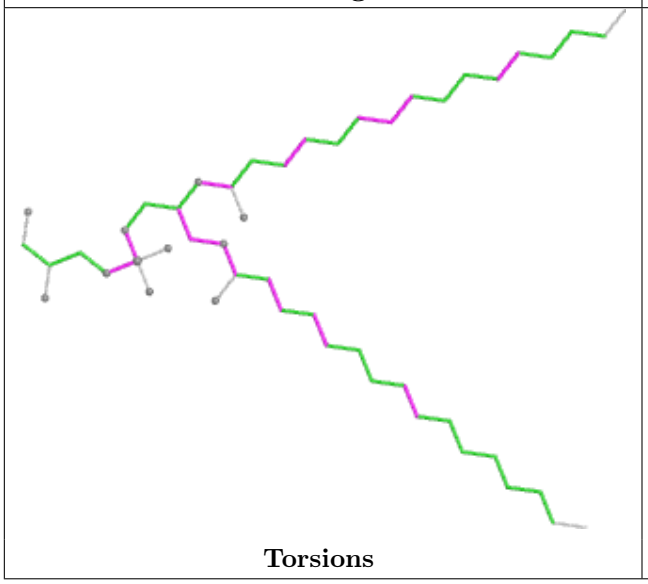
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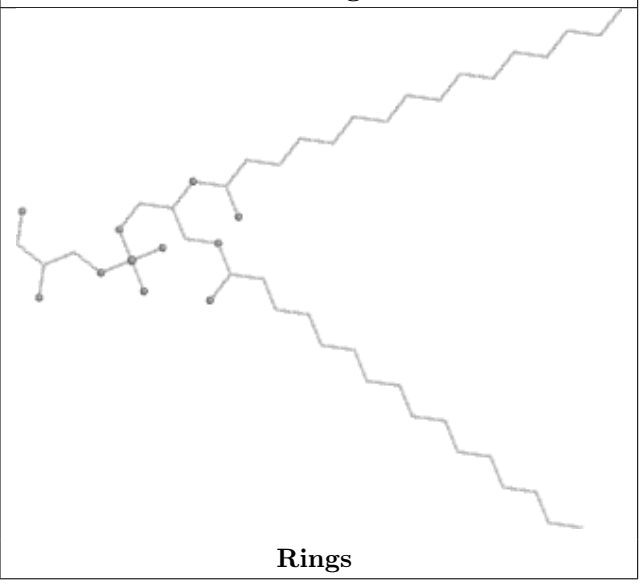
Bond lengths



Bond angles

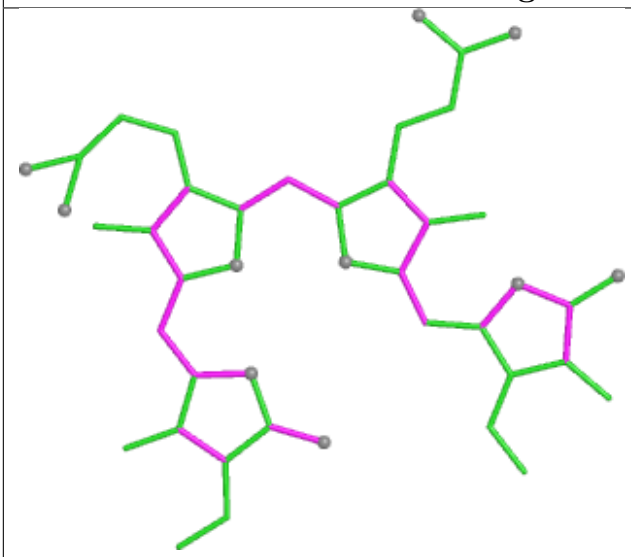


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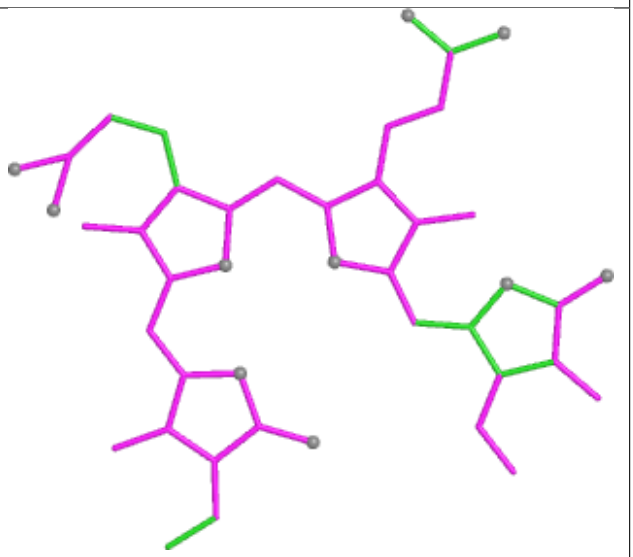


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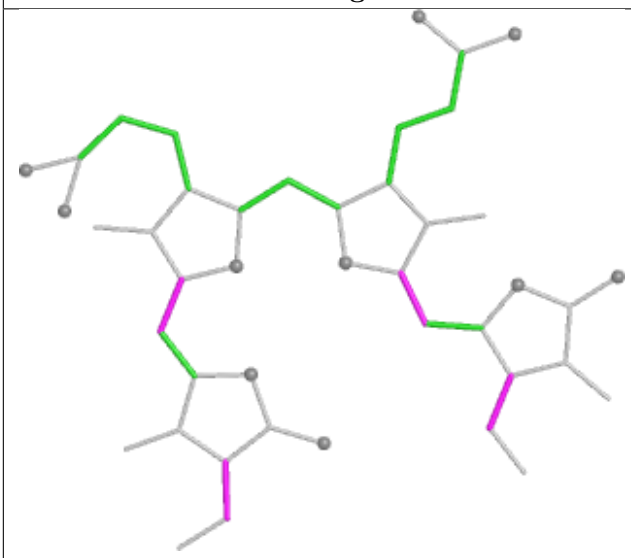
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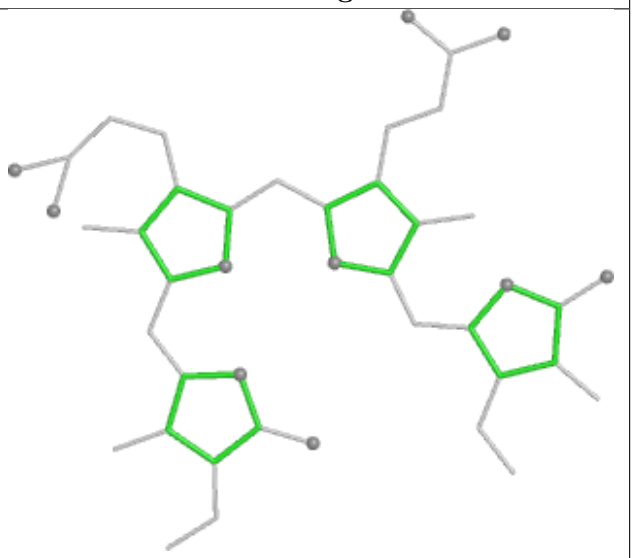
Bond lengths



Bond angles

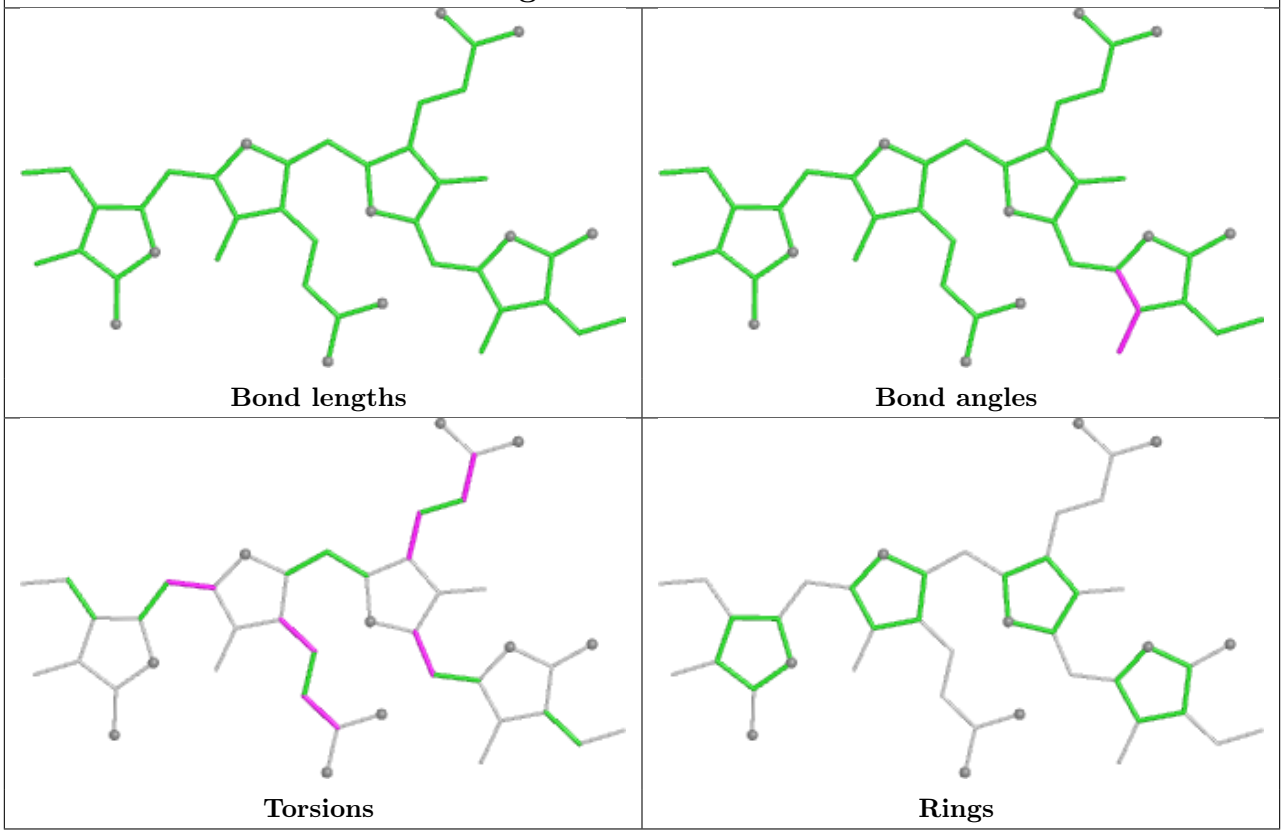


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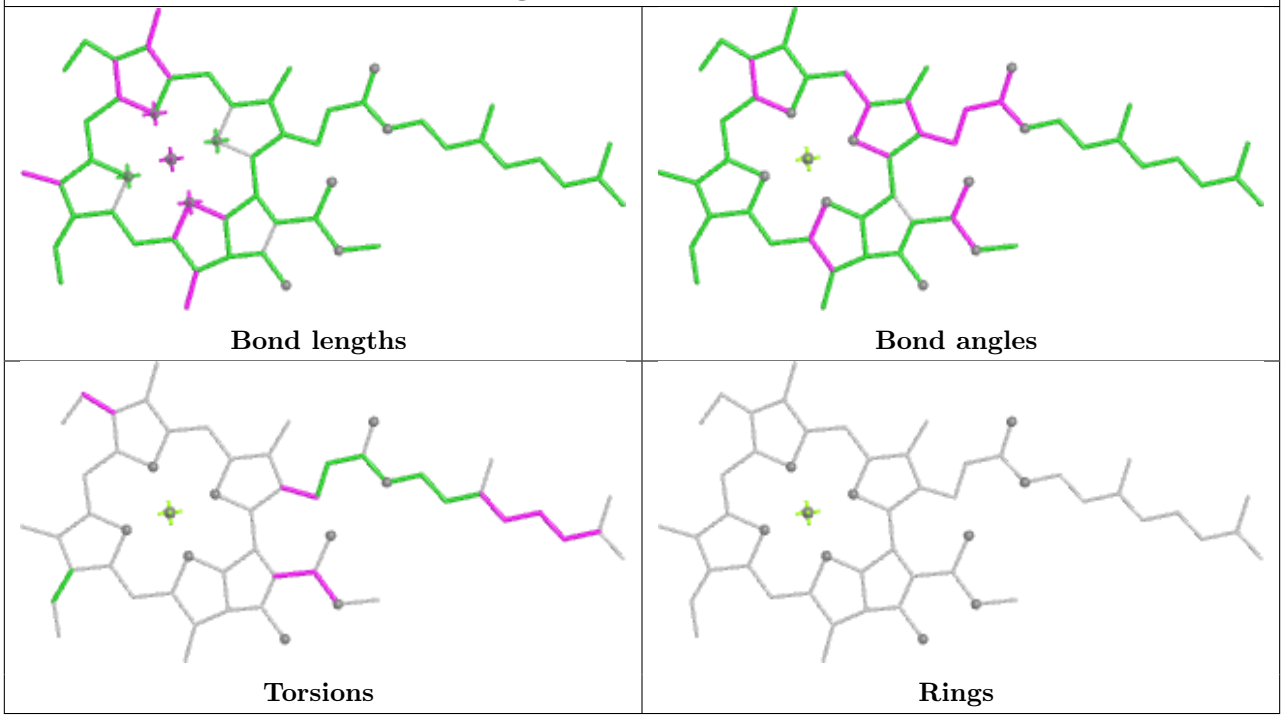


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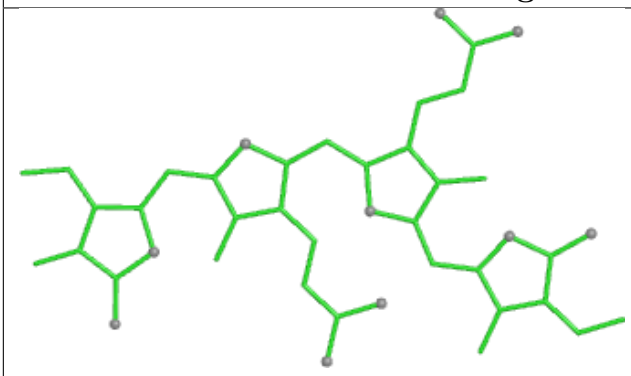
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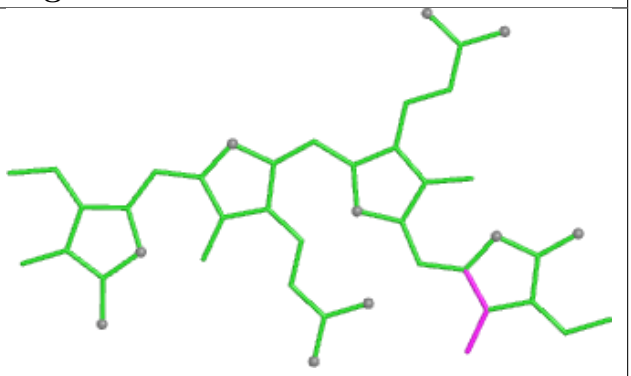
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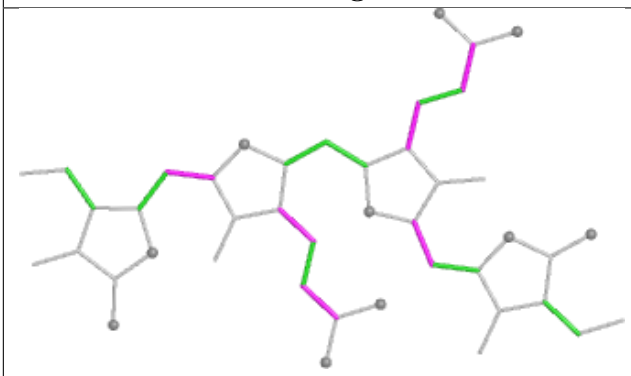
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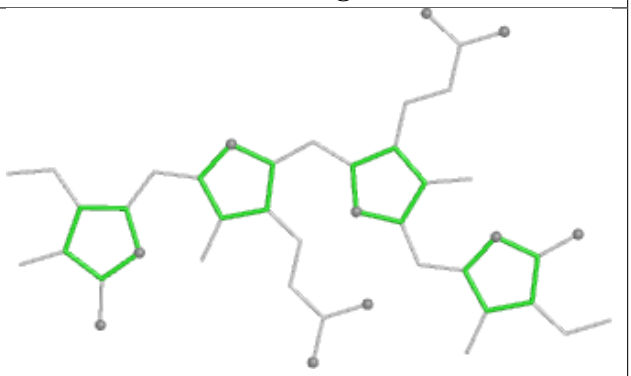
Bond lengths



Bond angles

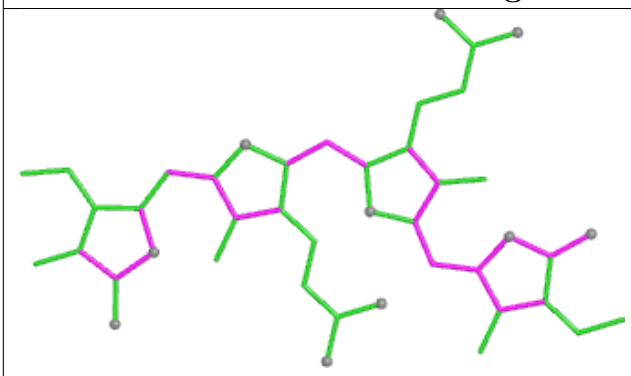


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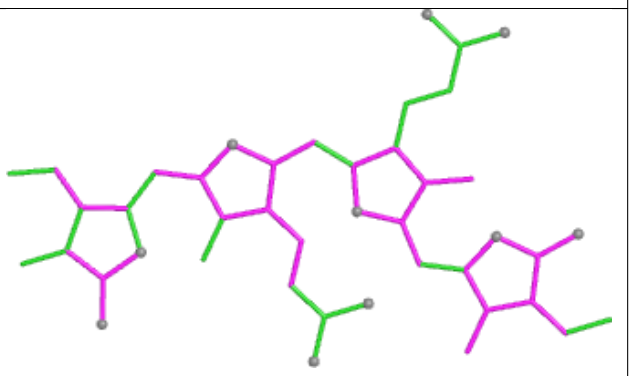


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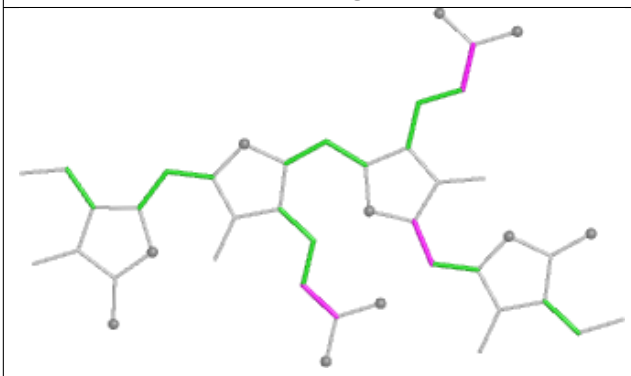
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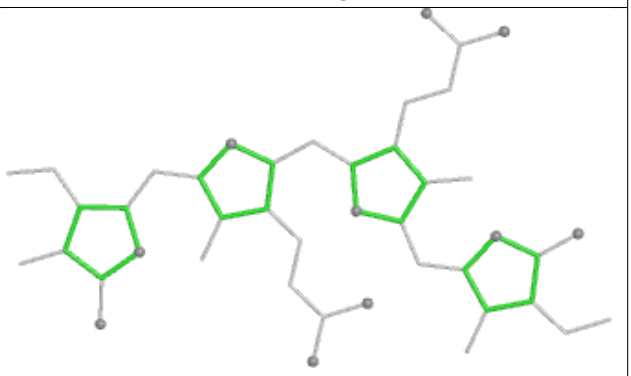
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Bond angles

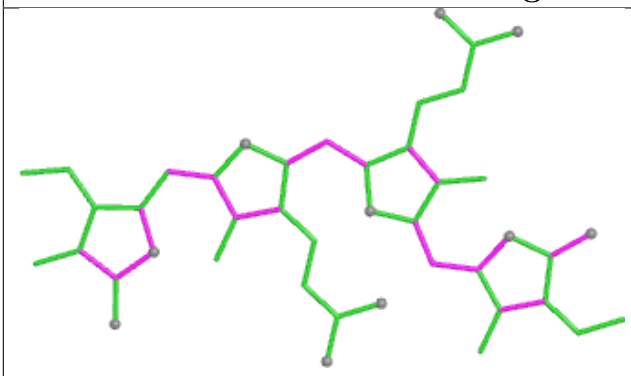


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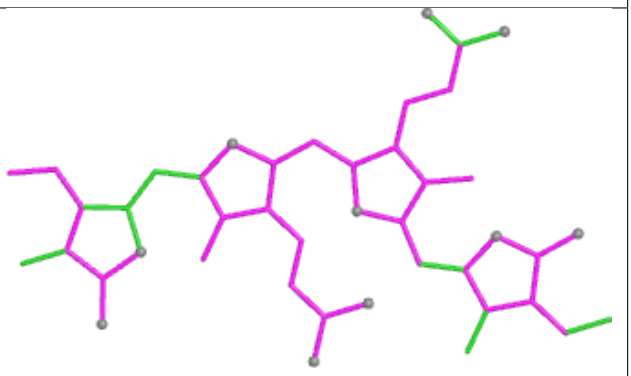


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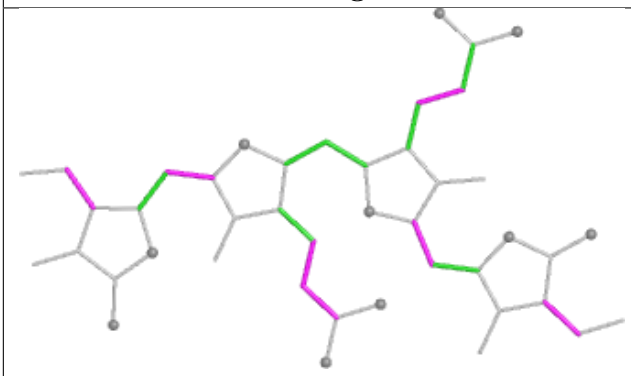
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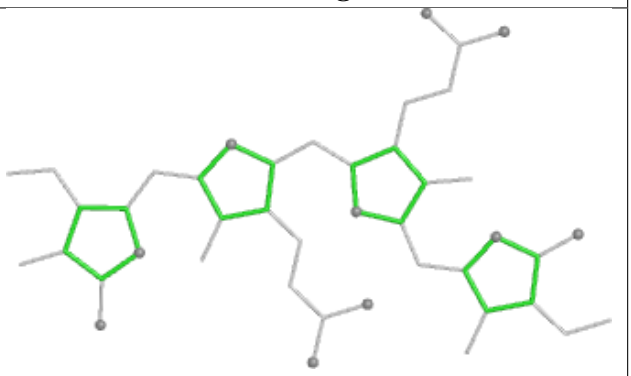
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Bond angles

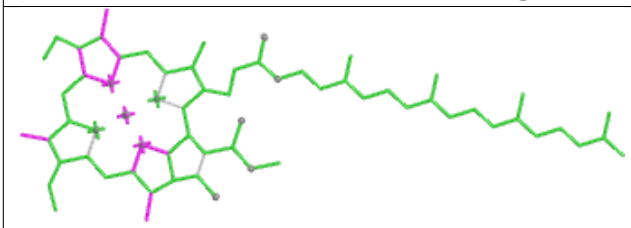


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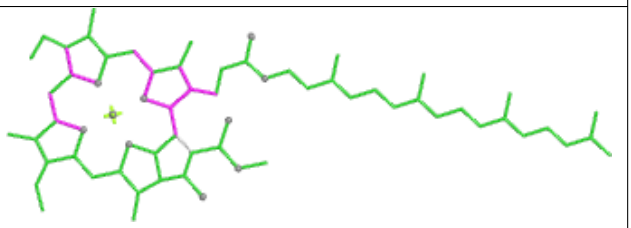


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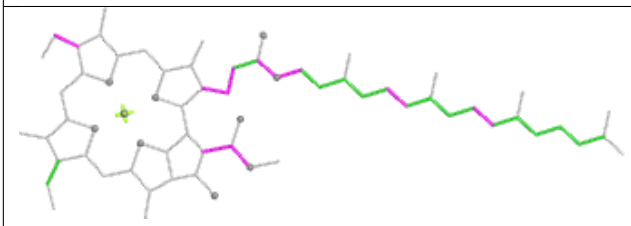
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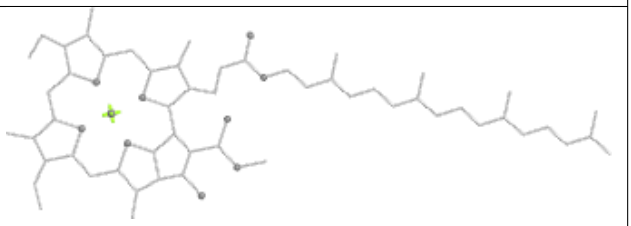
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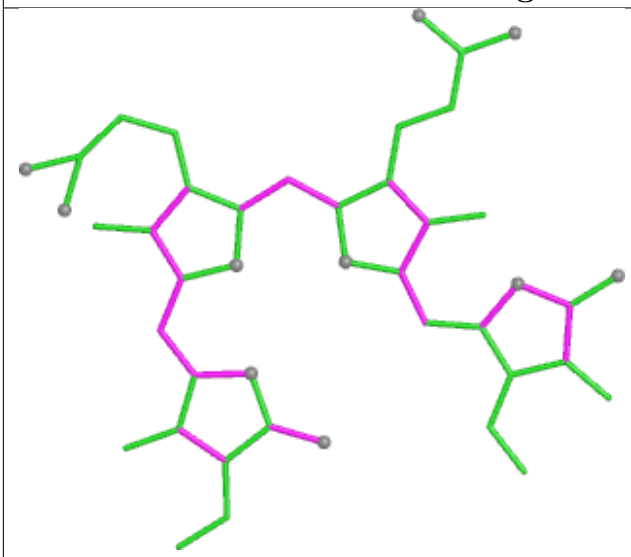


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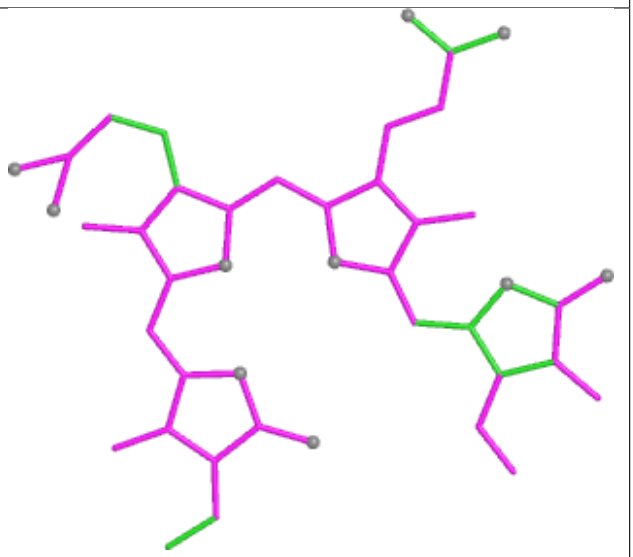


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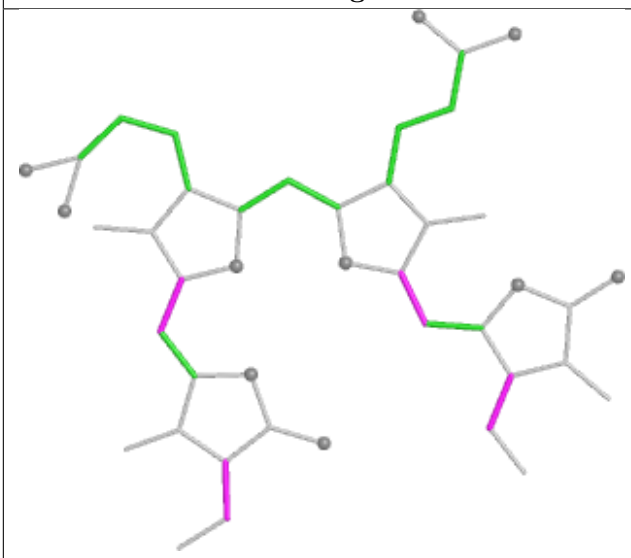
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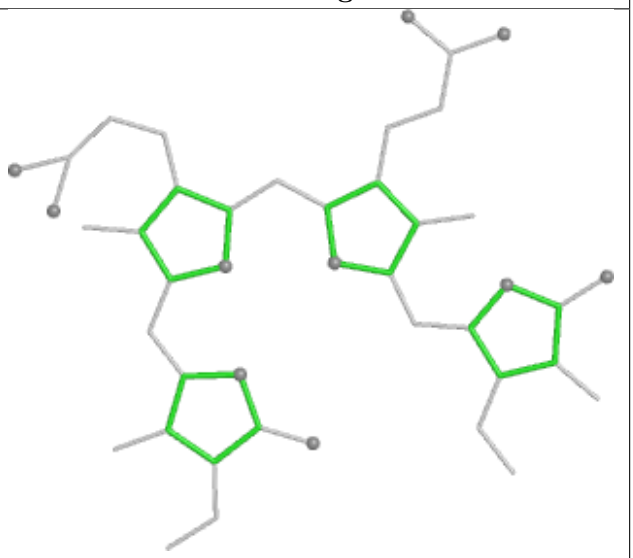
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Bond angles

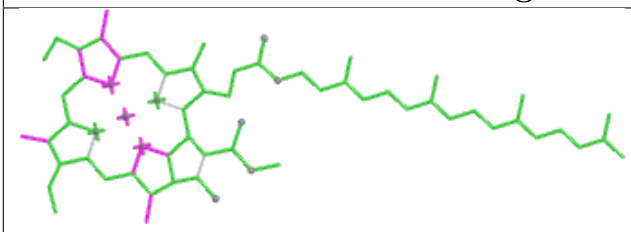


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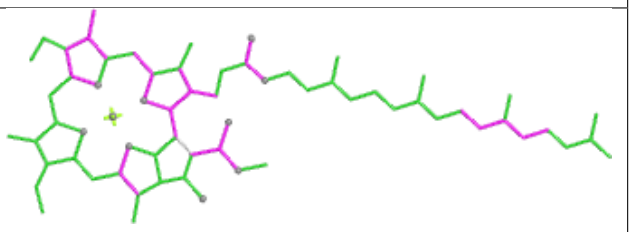


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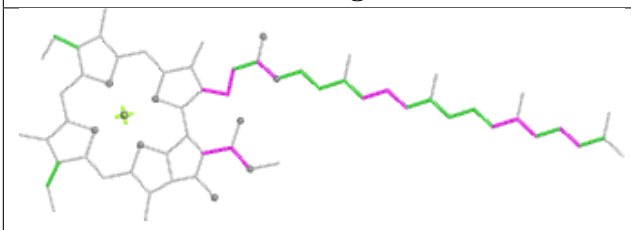
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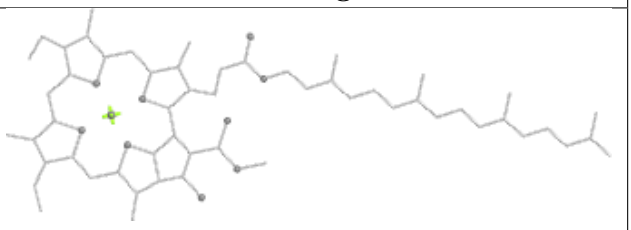
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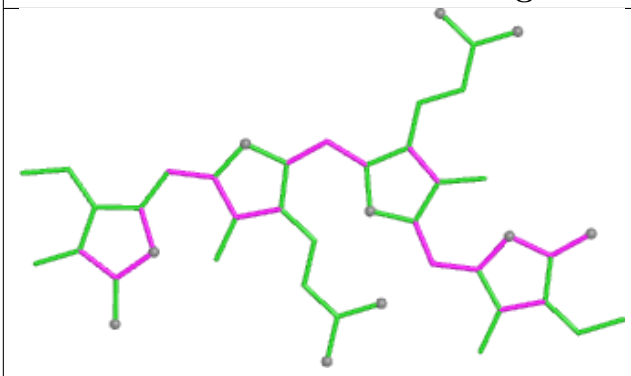


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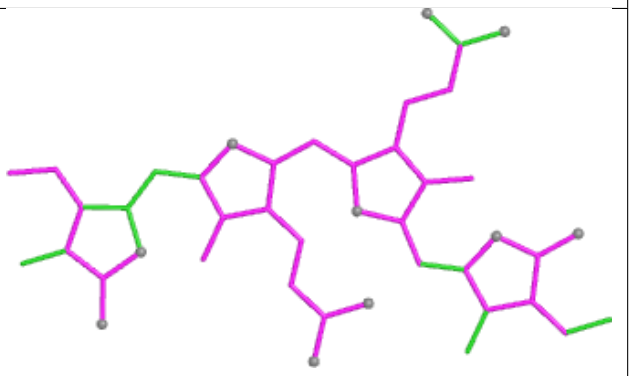


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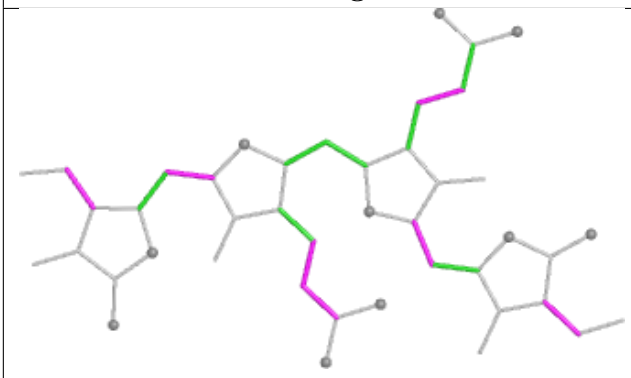
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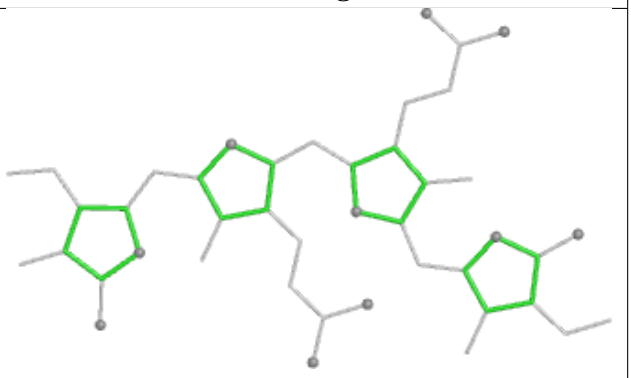
Bond lengths



Bond angles

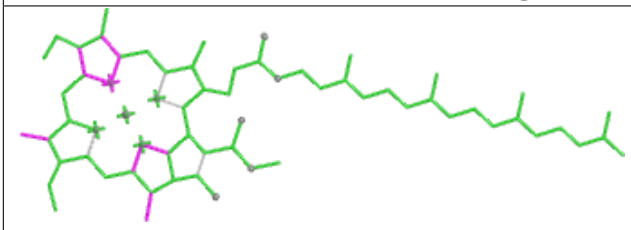


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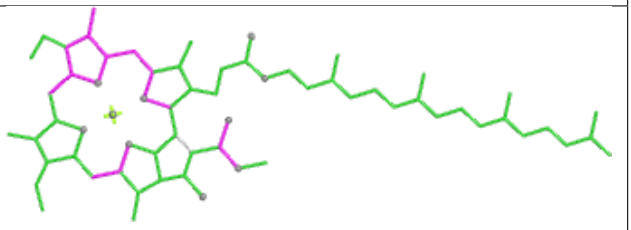


Rings

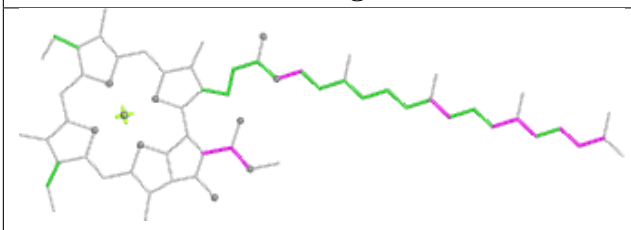
Ligand CLA B1 608



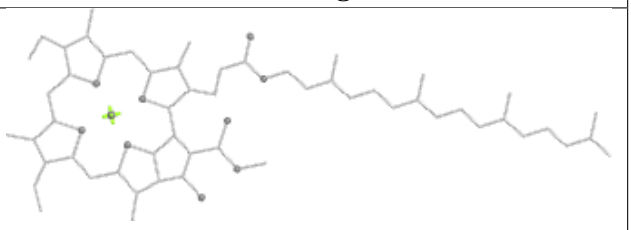
Bond lengths



Bond angles

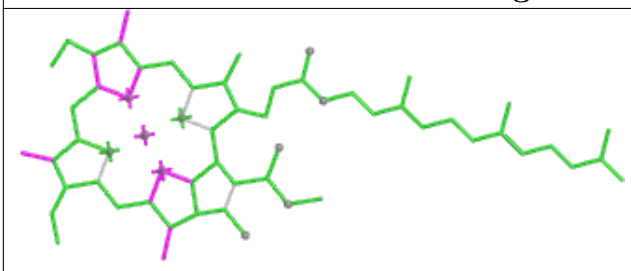


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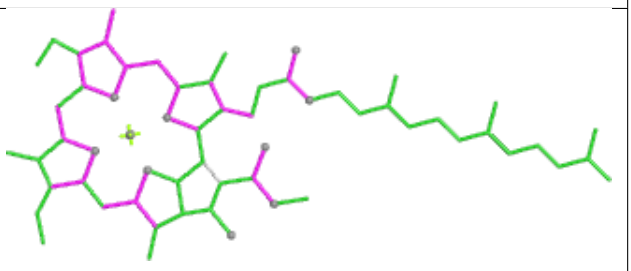


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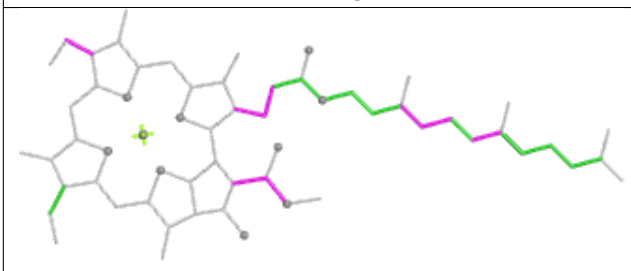
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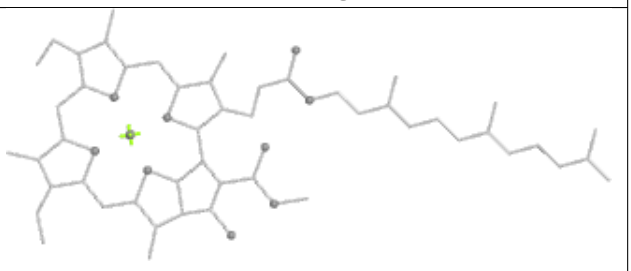
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Bond angles

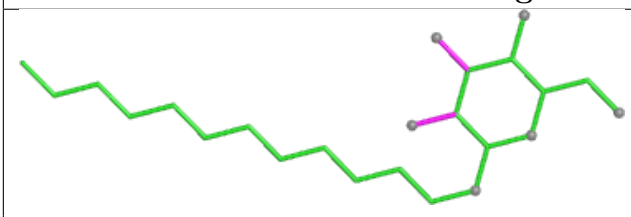


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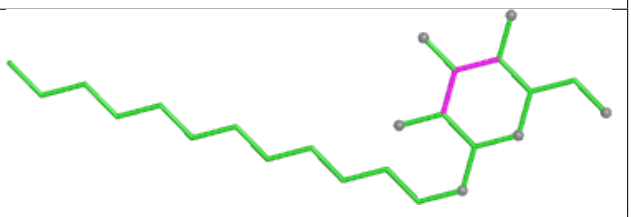


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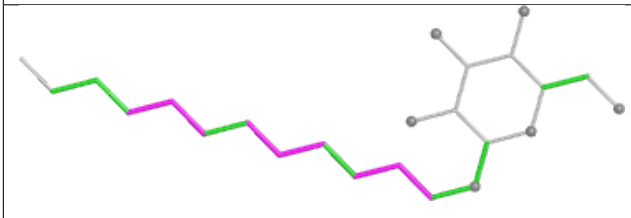
Ligand LMT b1 620



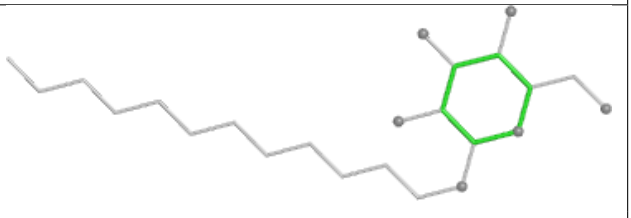
Bond lengths



Bond angles

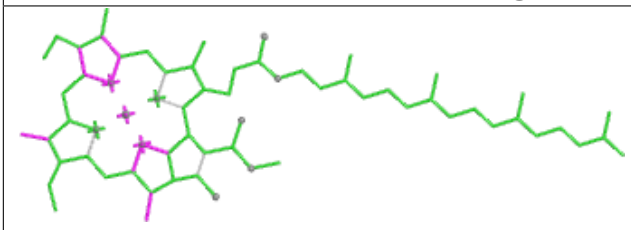


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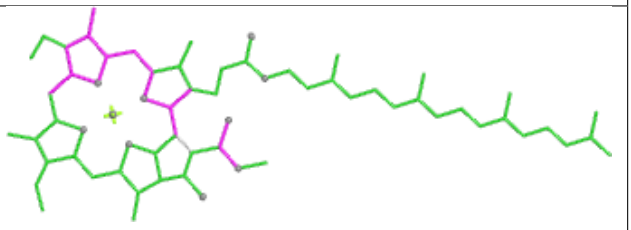


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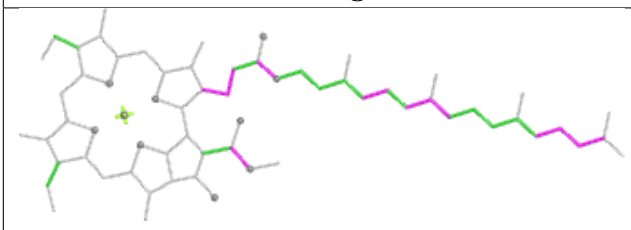
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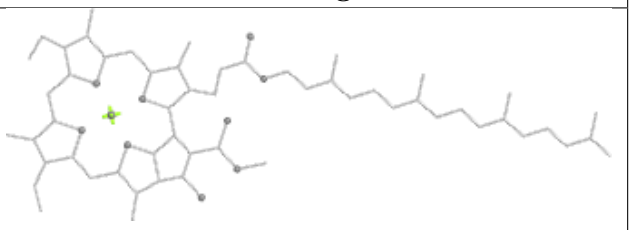
Bond lengths



Bond angles

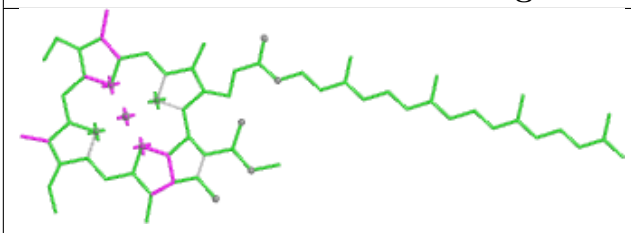


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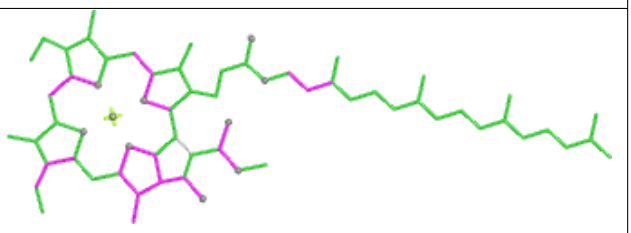


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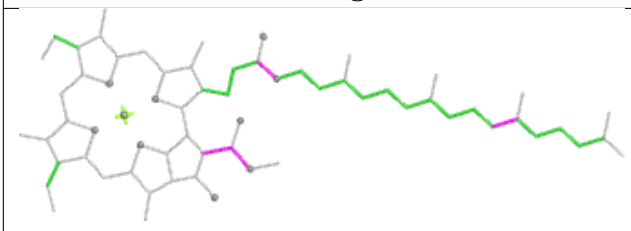
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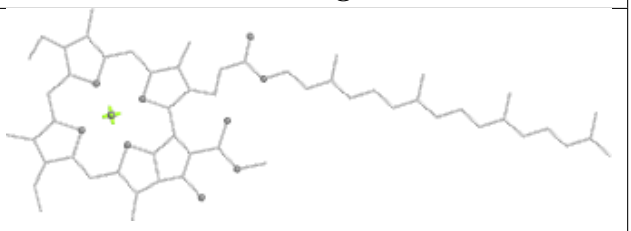
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Bond angles

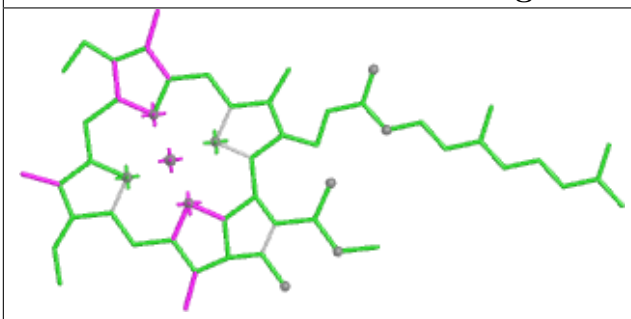


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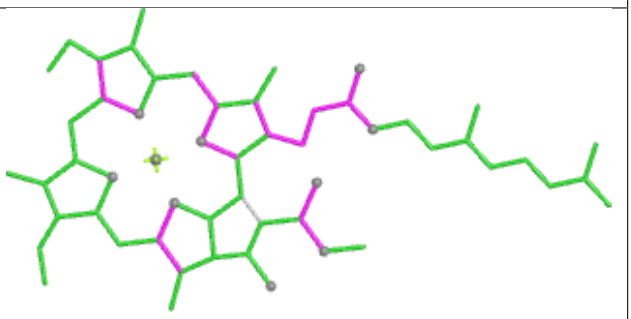


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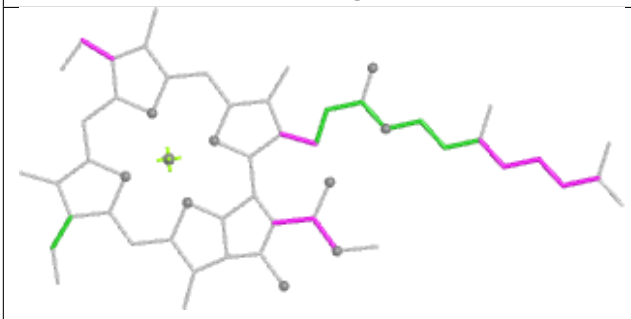
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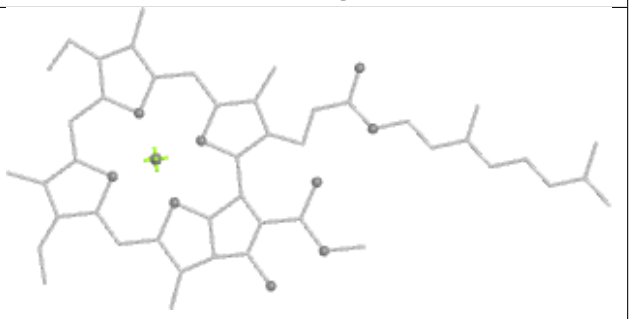
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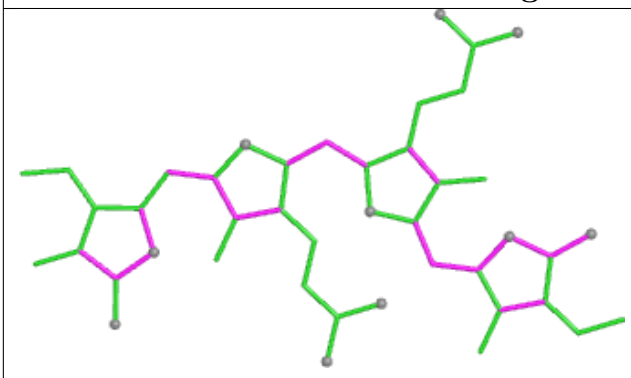


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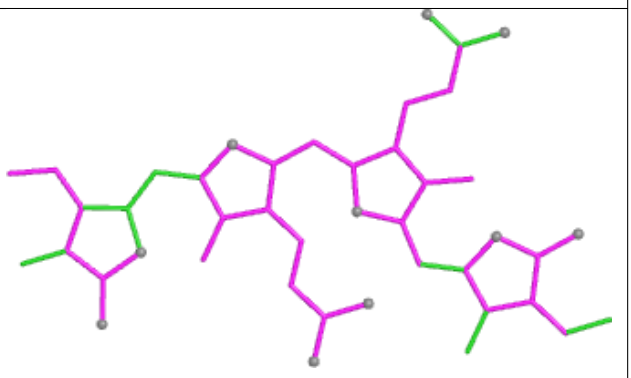


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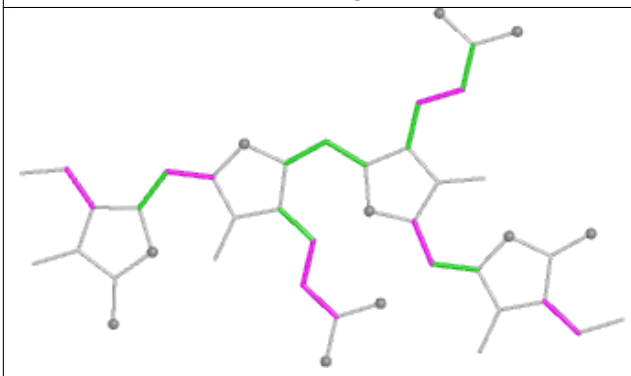
Ligand CYC l6 201



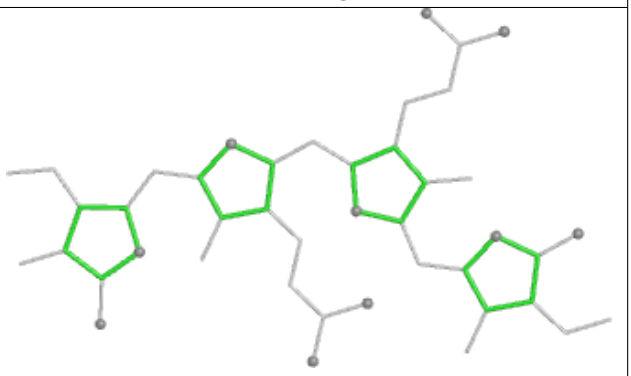
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Bond angles

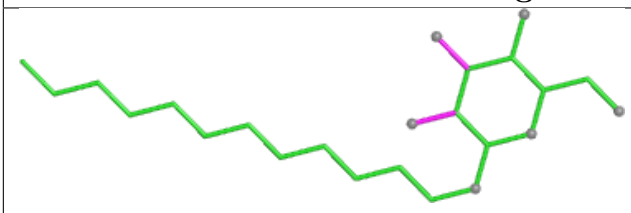


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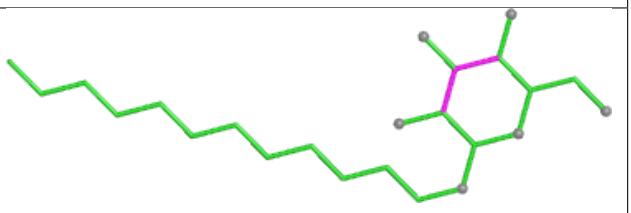


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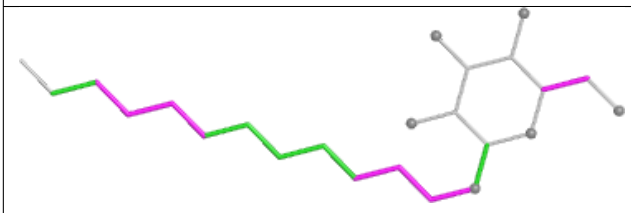
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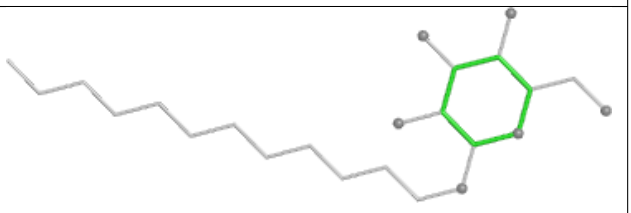
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Bond angles

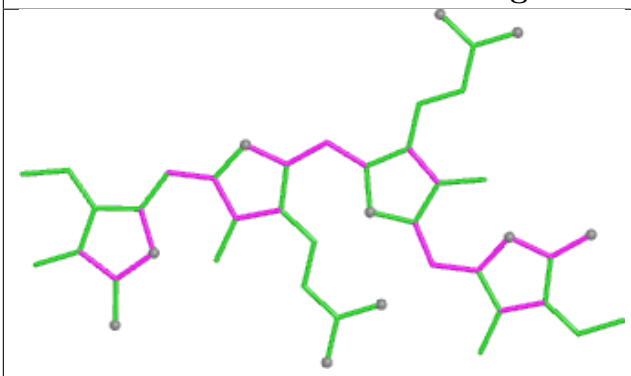


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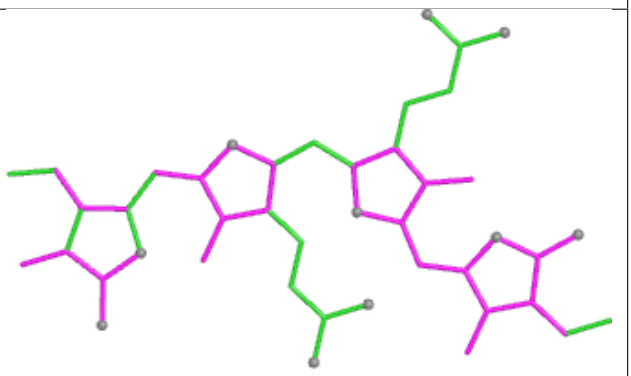


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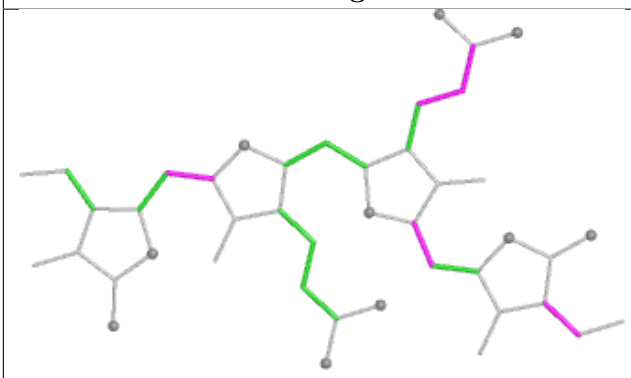
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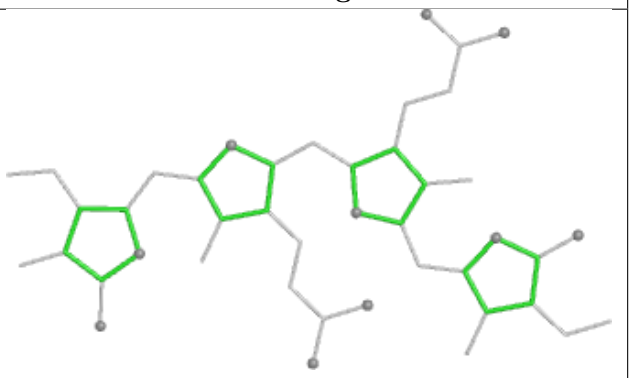
Bond lengths



Bond angles

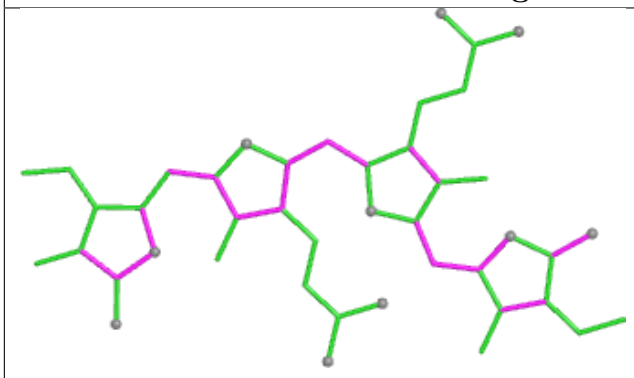


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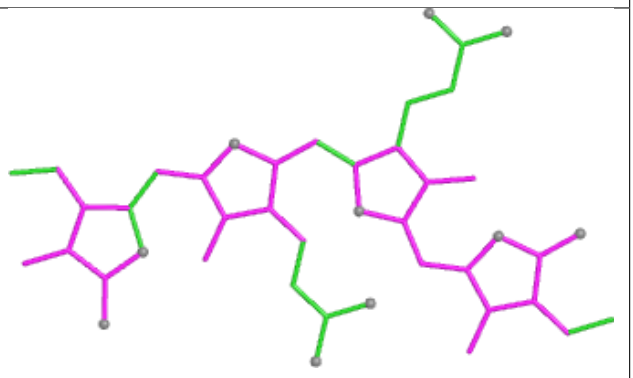


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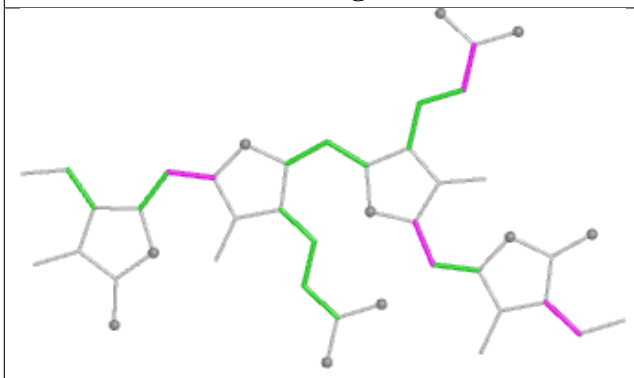
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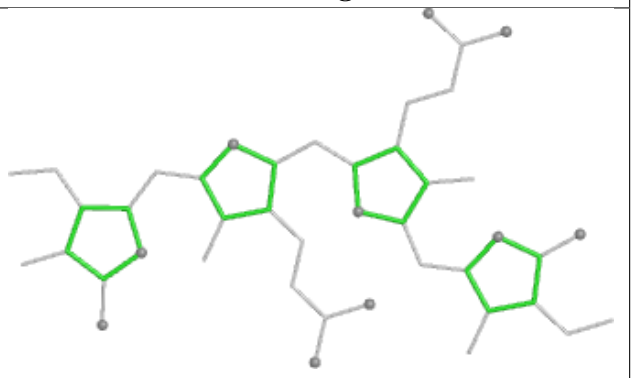
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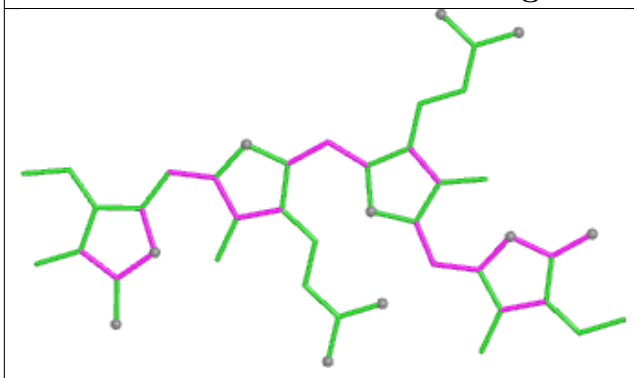


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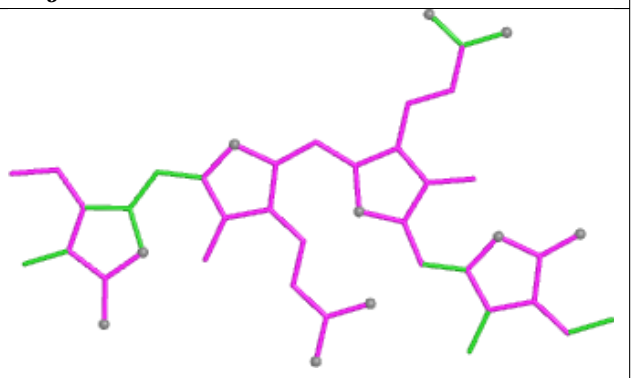


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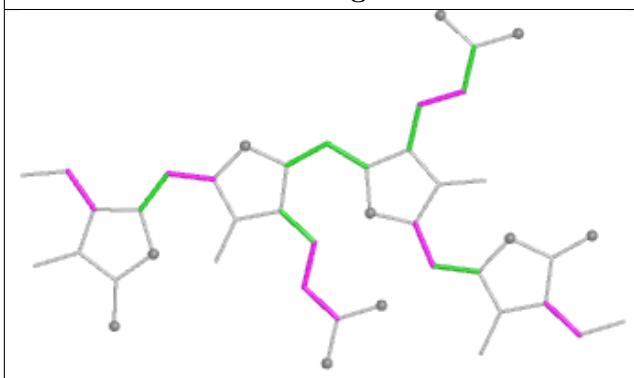
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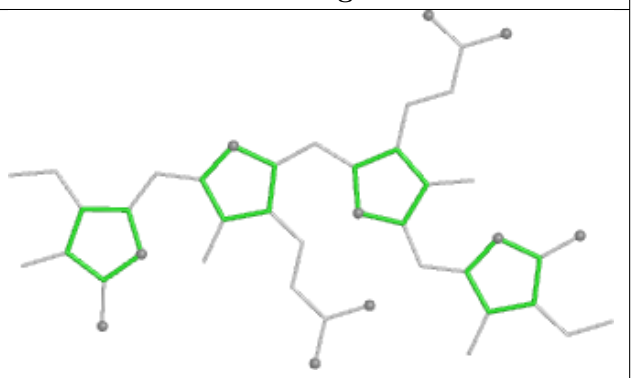
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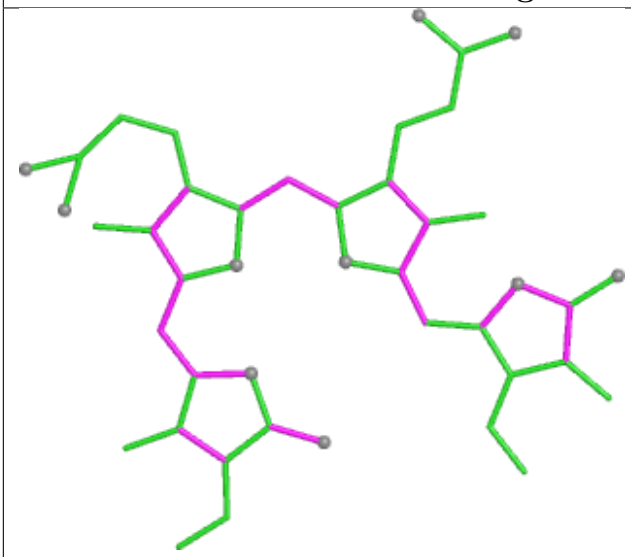


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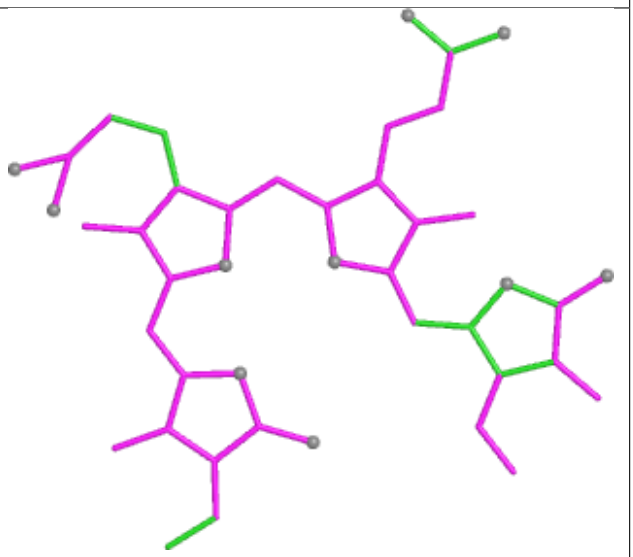


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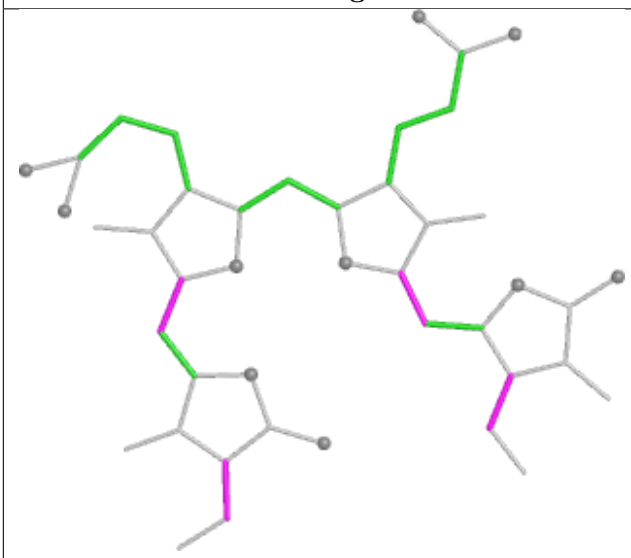
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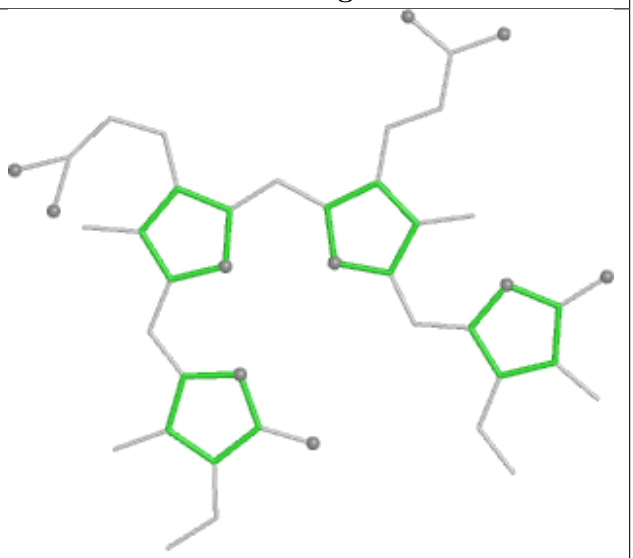
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Bond angles

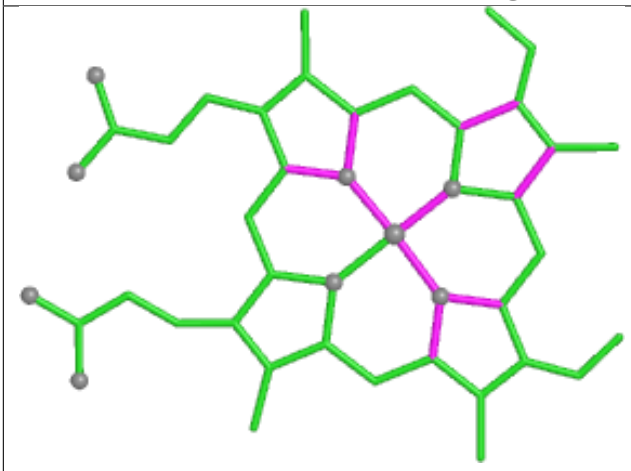


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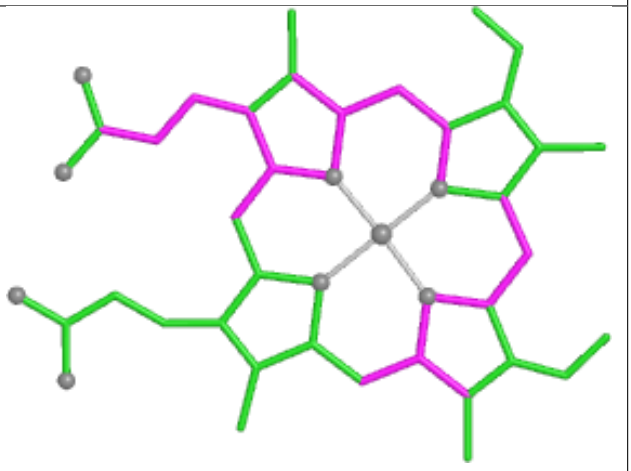


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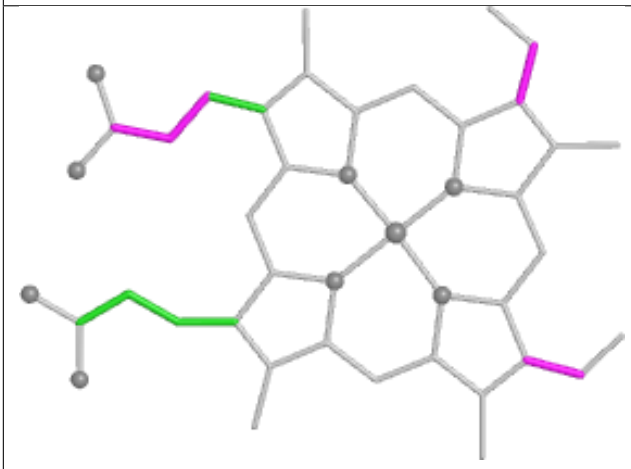
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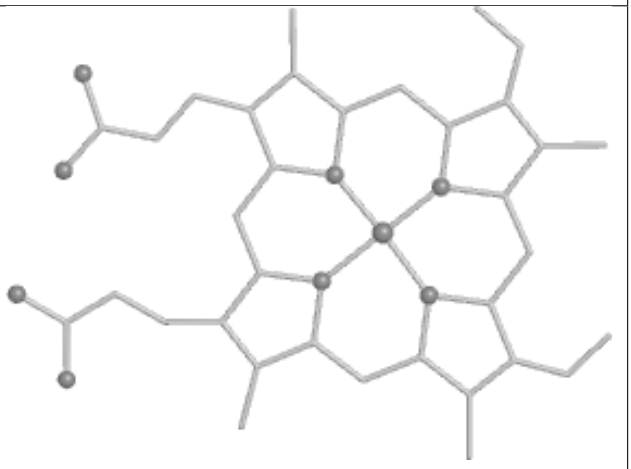
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Bond angles

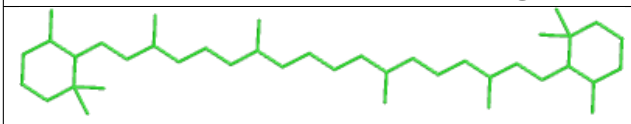


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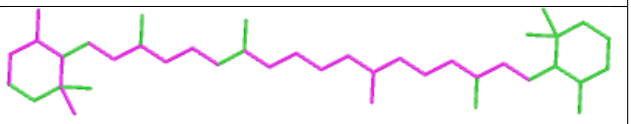


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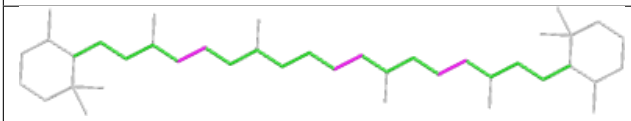
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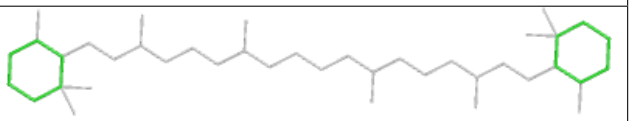
Bond lengths



Bond angles

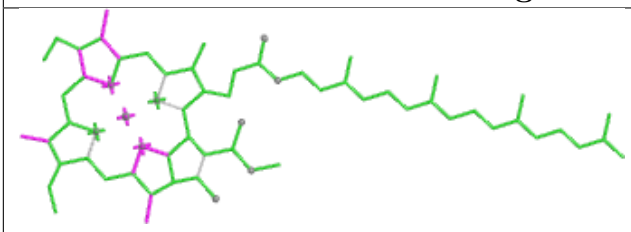


Torsions

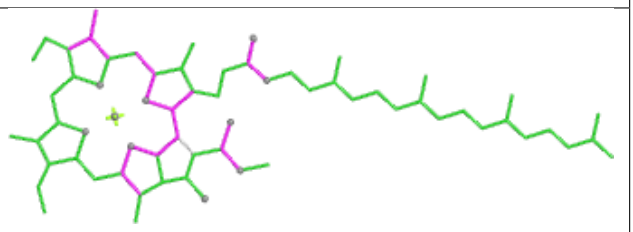


Rings

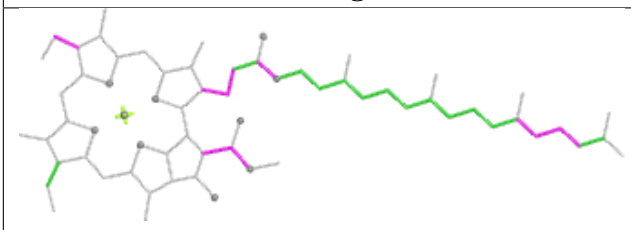
Ligand CLA B1 607



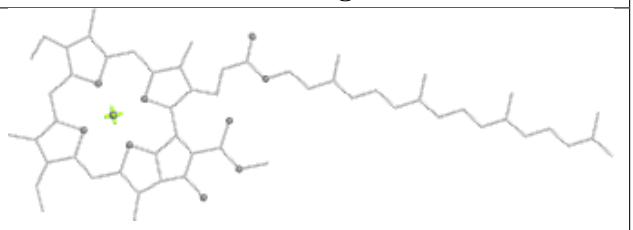
Bond lengths



Bond angles

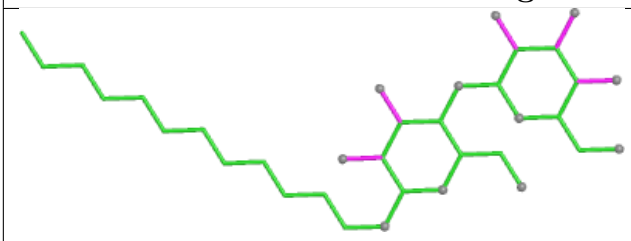


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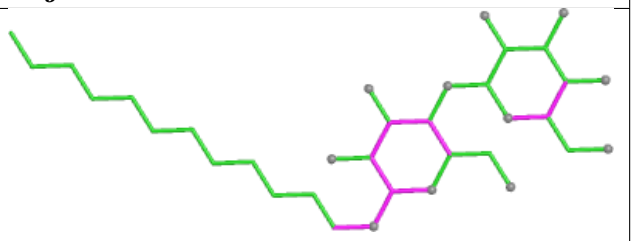


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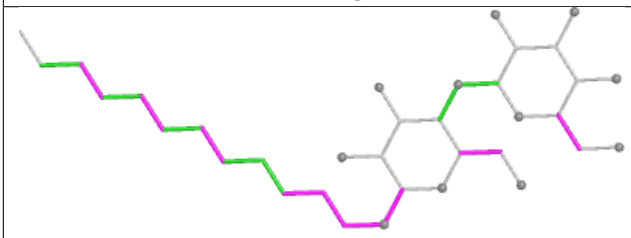
Ligand LMT jE 101



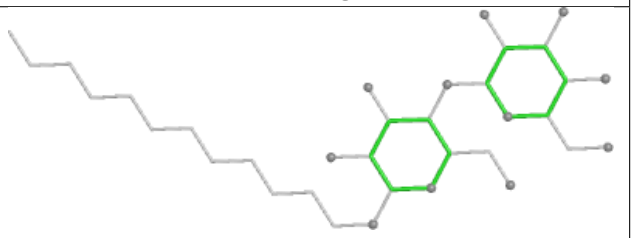
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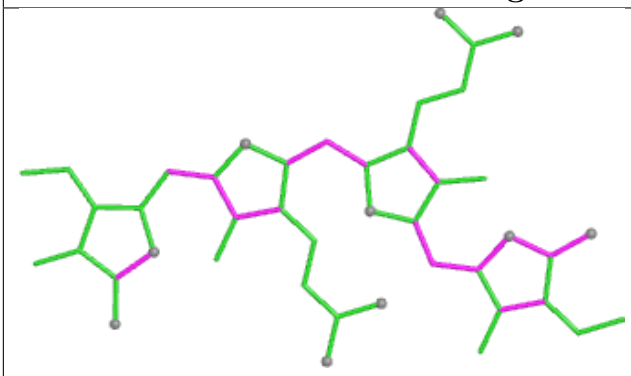


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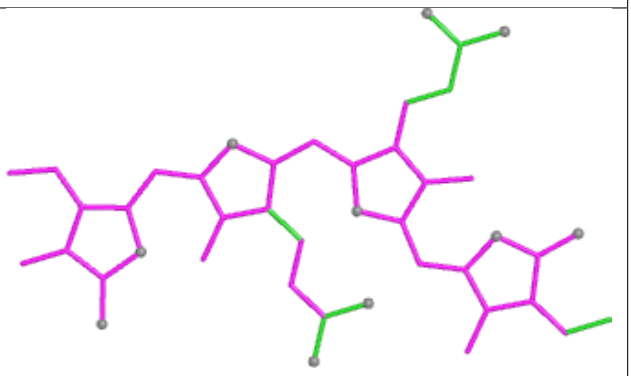


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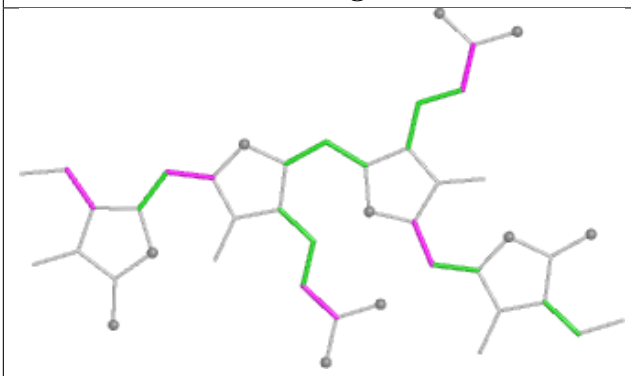
Ligand CYC KK 201



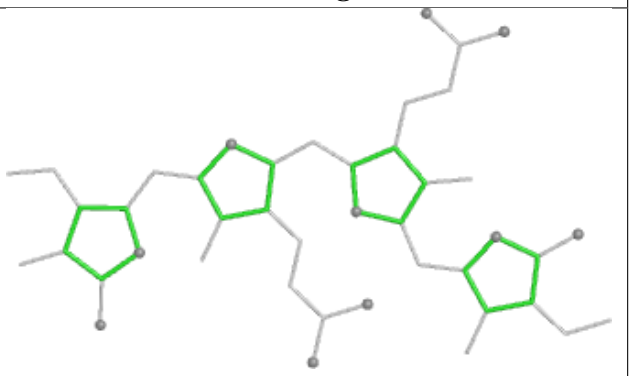
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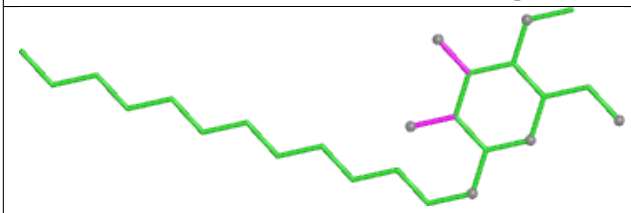


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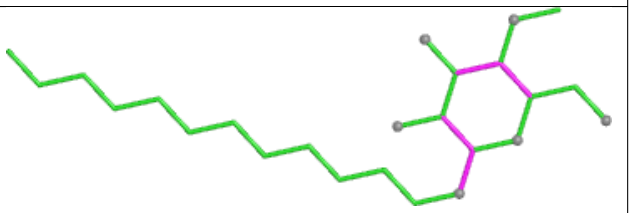


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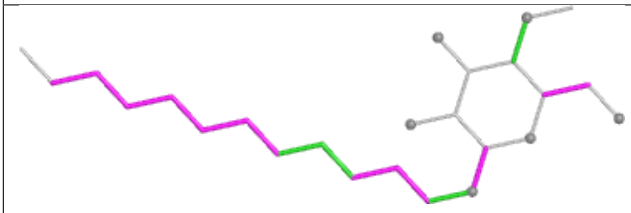
Ligand LMT DE 412



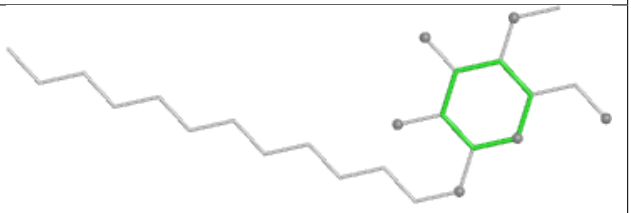
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Bond angles

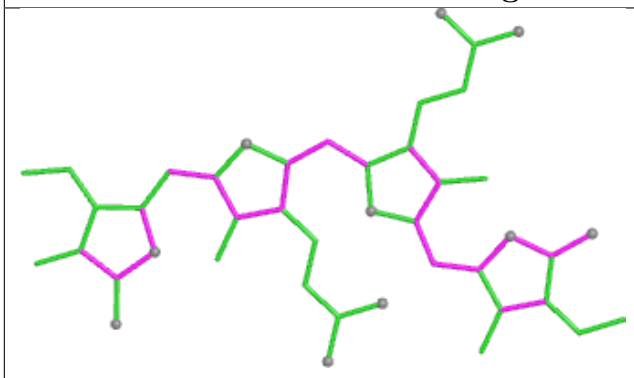


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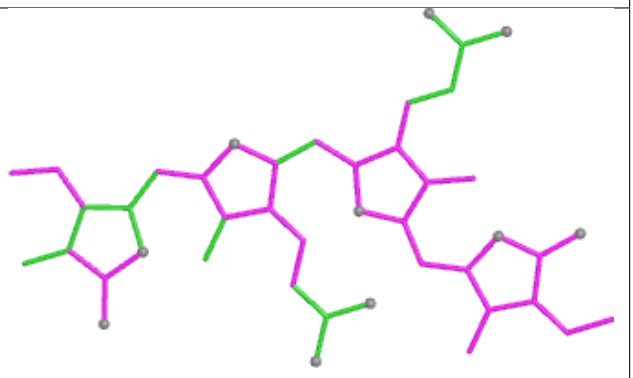


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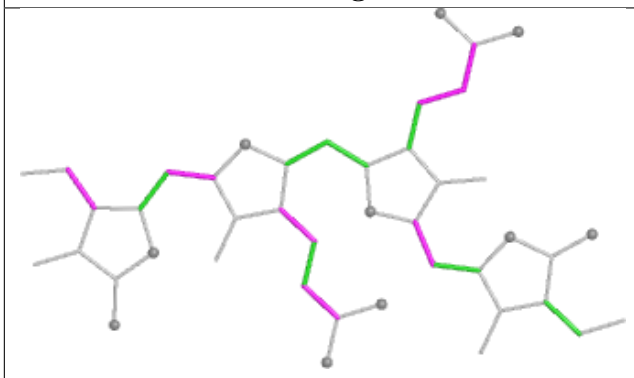
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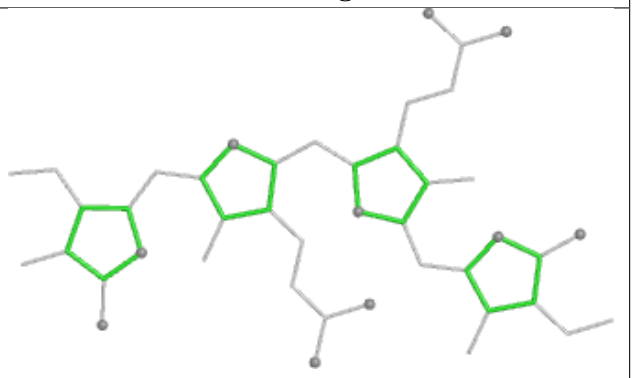
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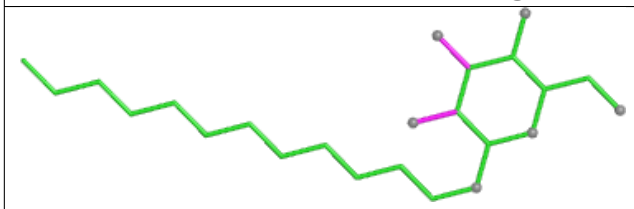


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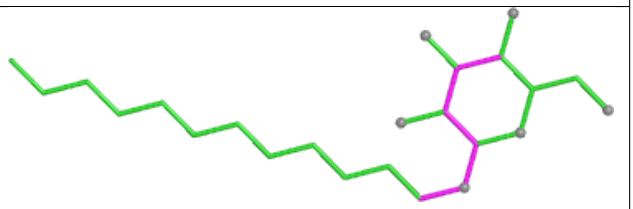


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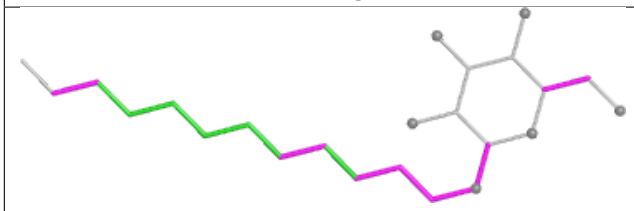
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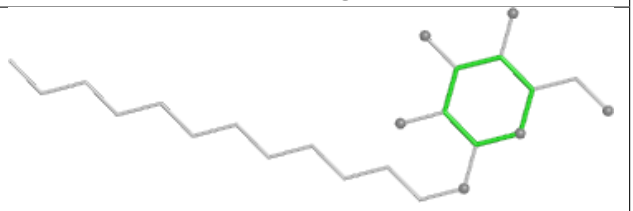
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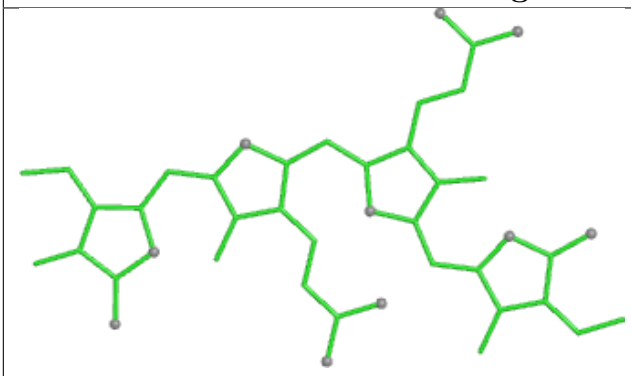


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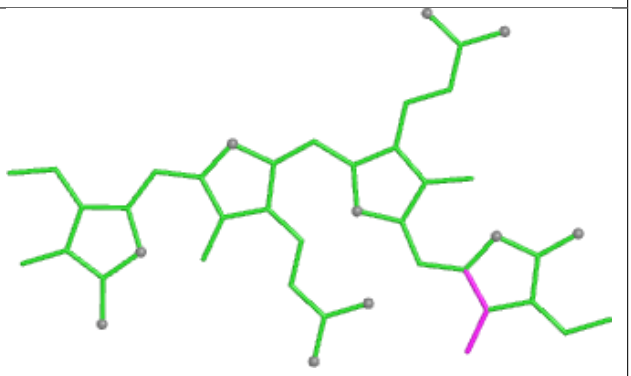


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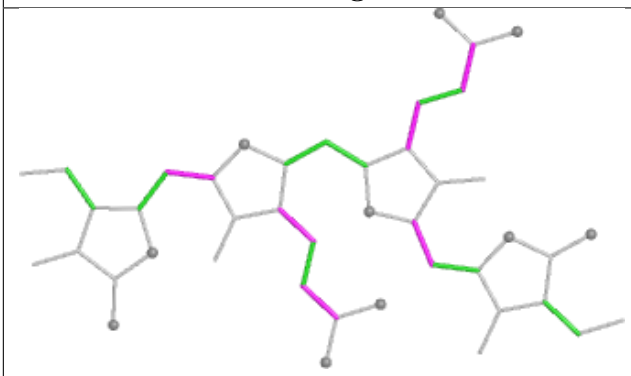
Ligand CYC m2 201



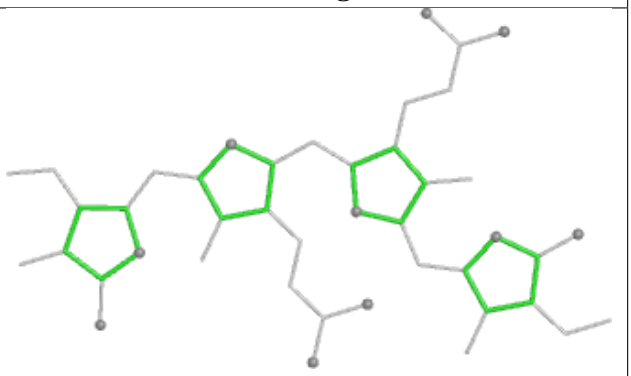
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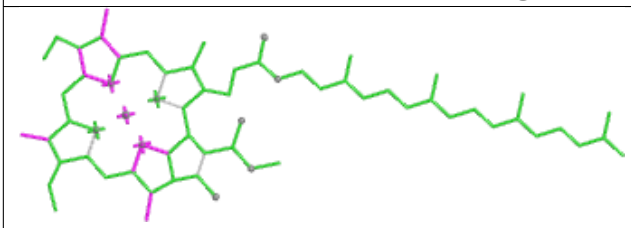


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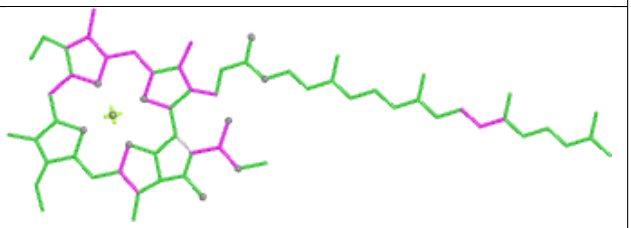


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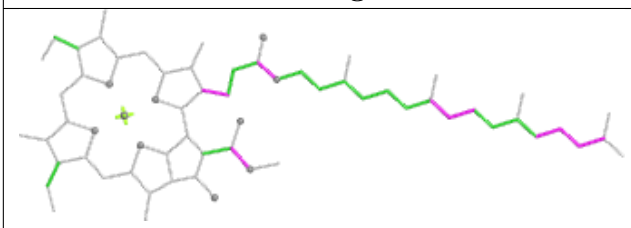
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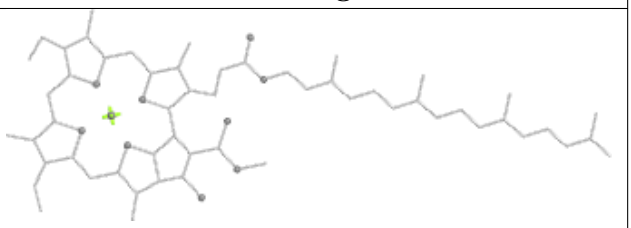
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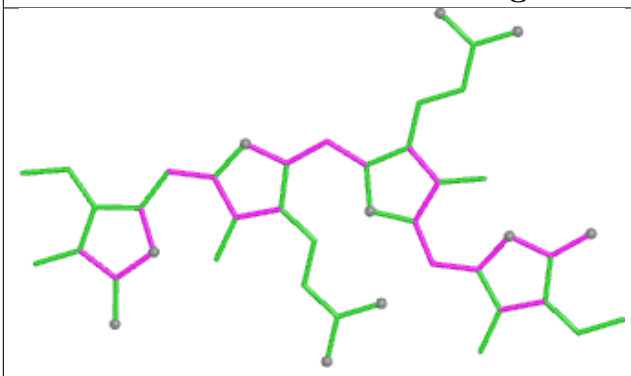


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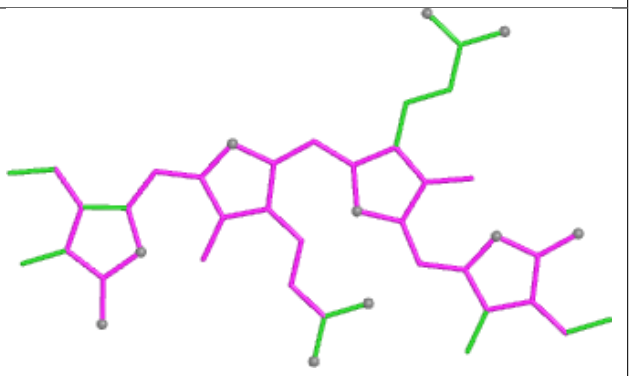


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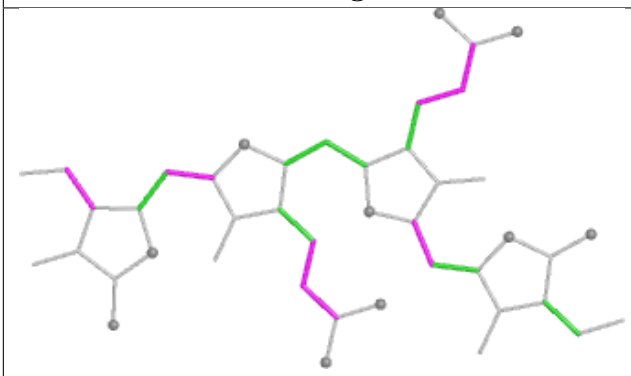
Ligand CYC TB 201



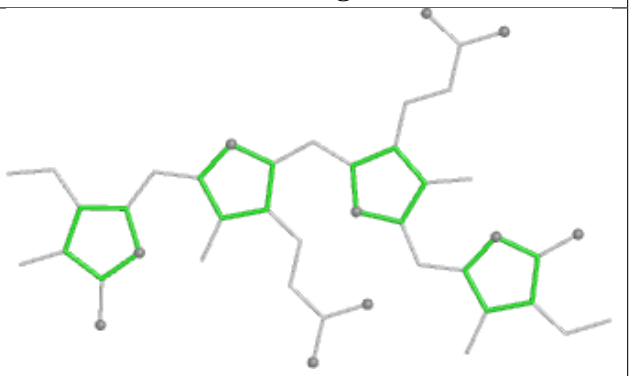
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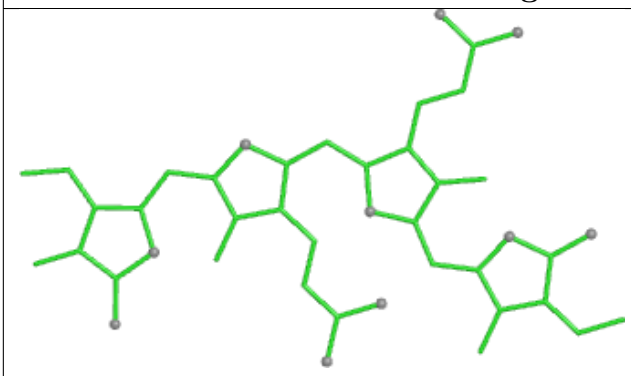


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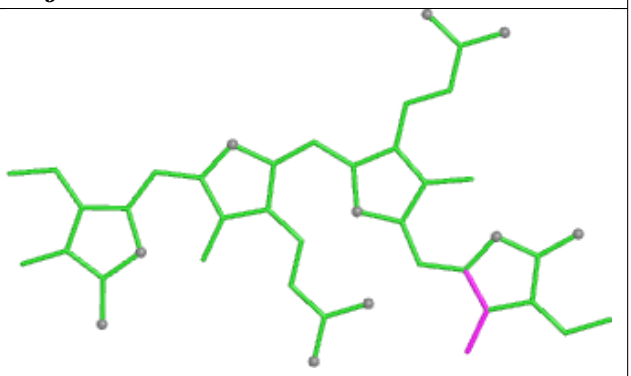


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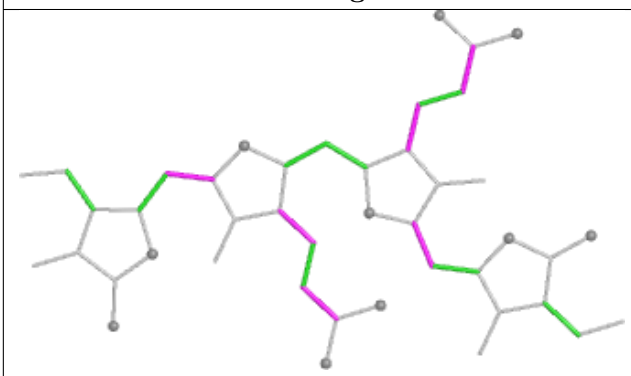
Ligand CYC j6 202



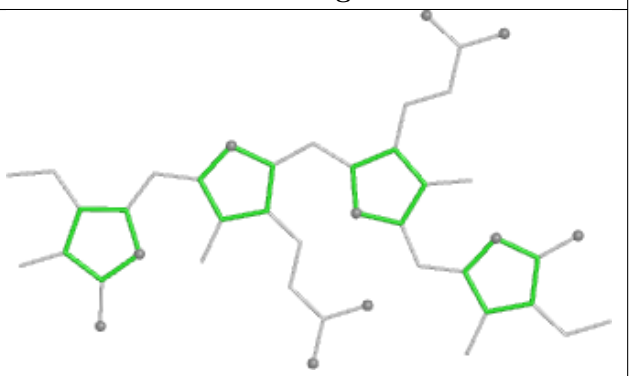
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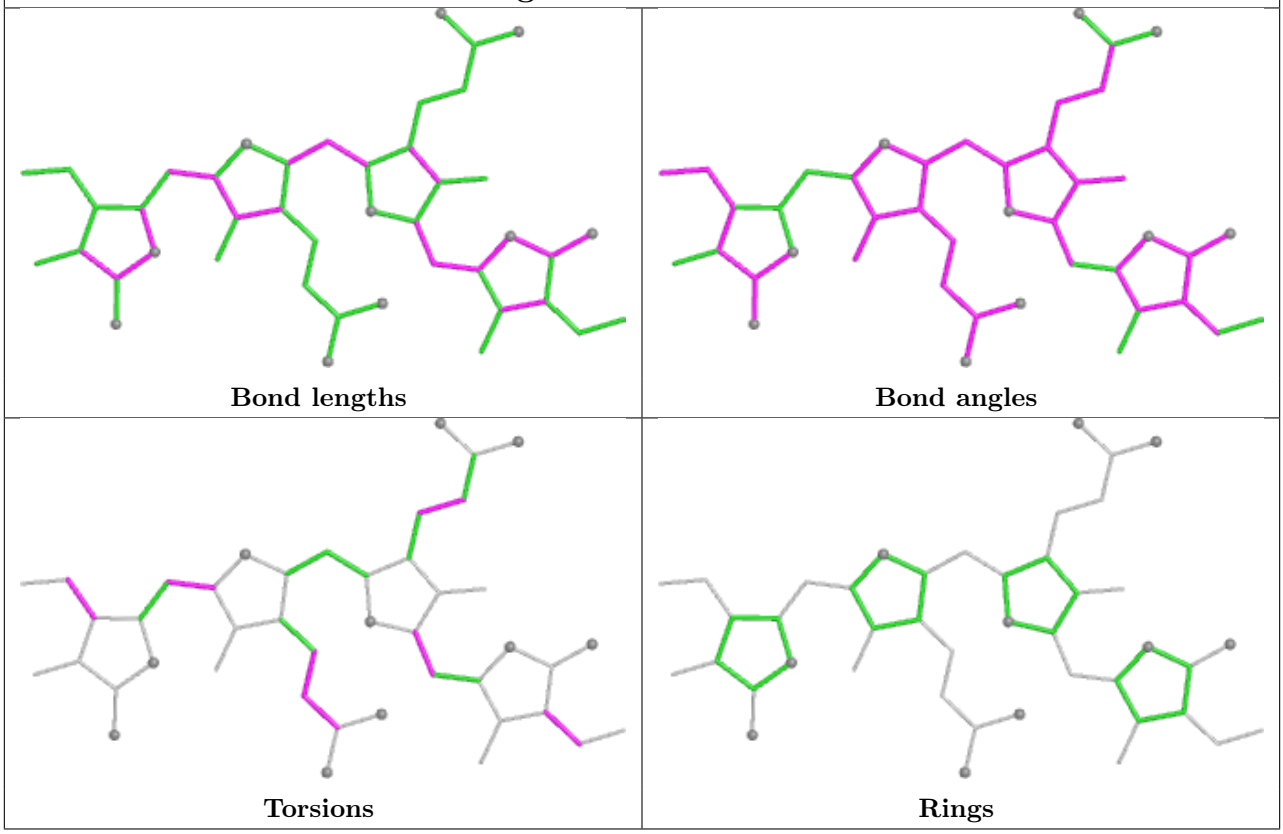


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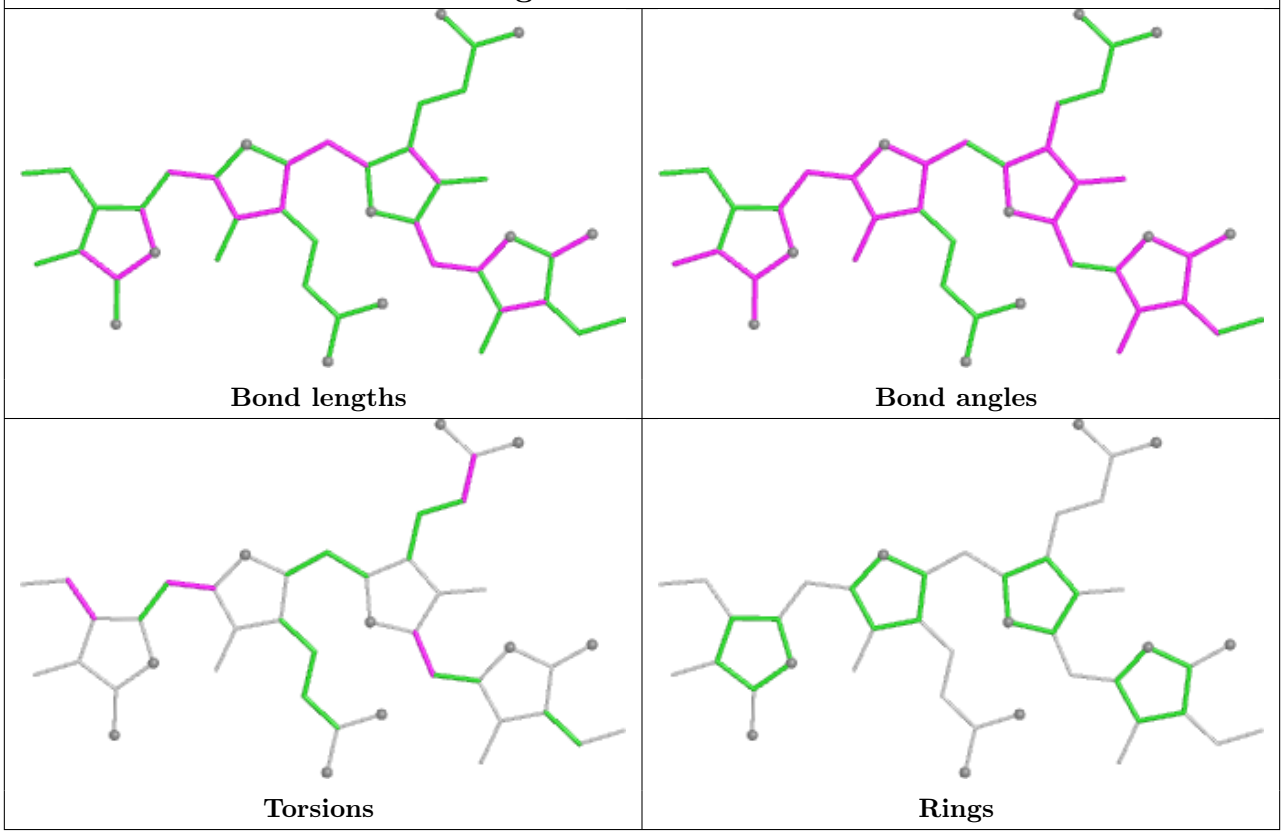


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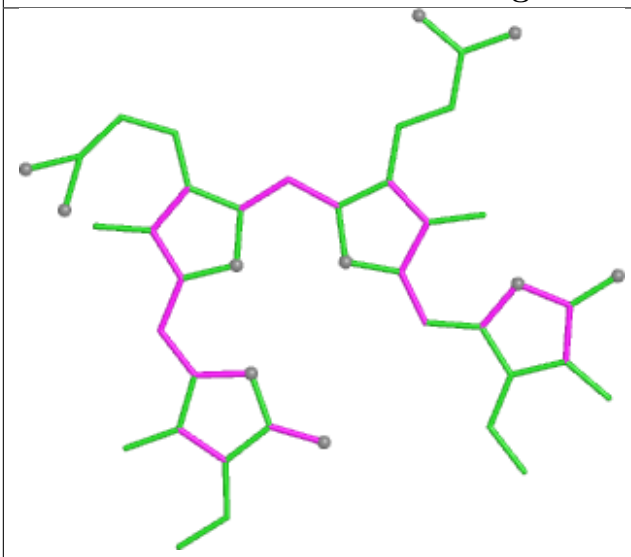
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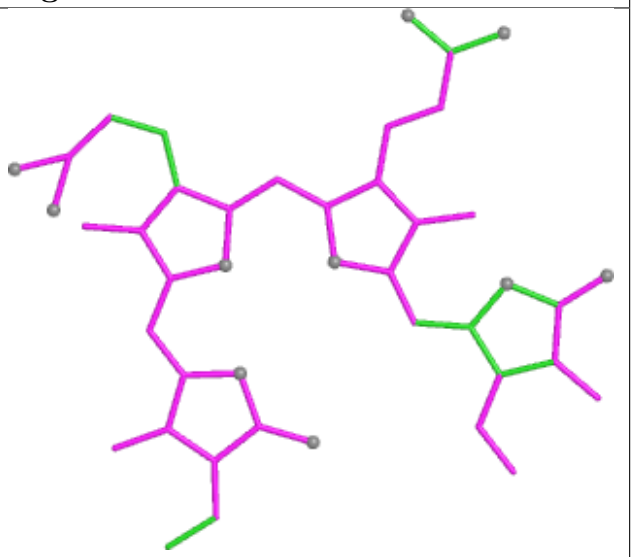
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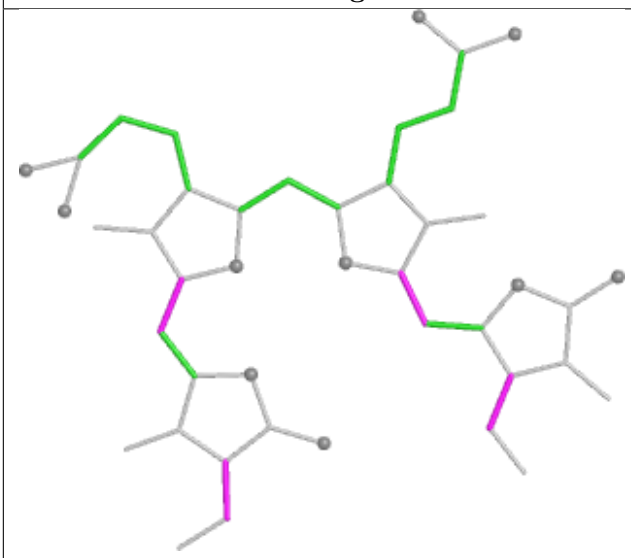
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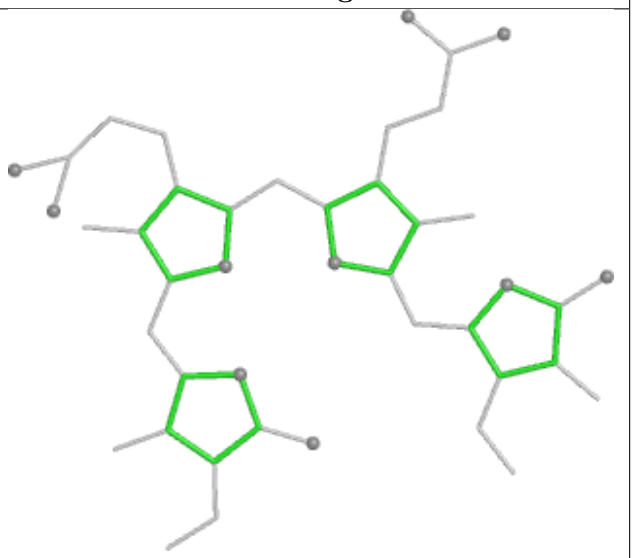
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Bond angles

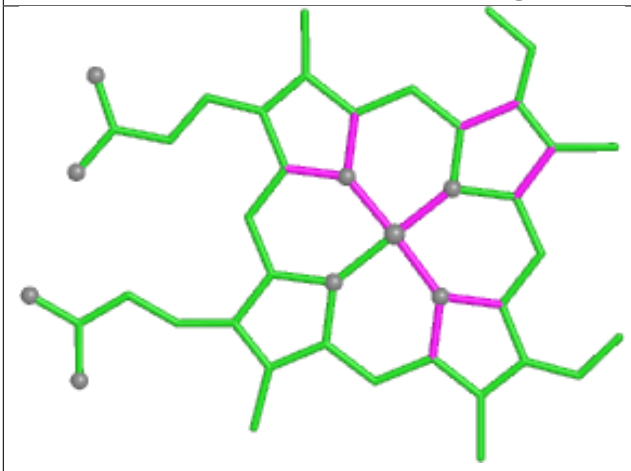


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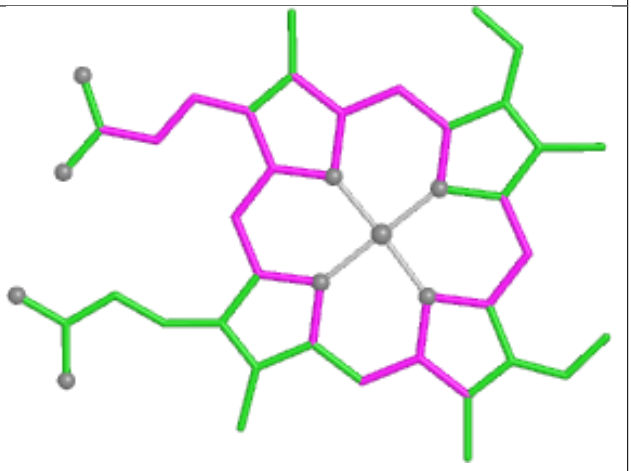


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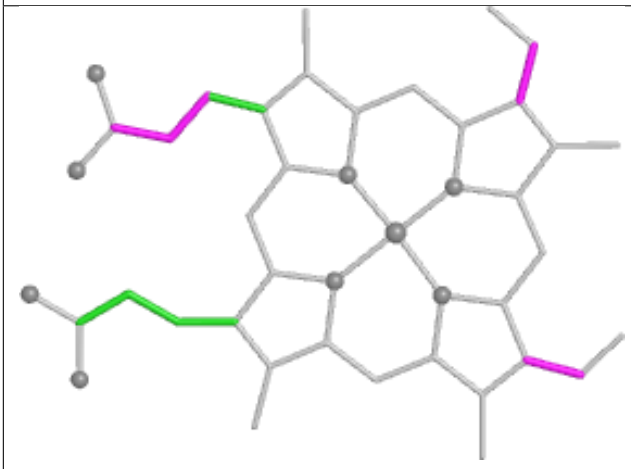
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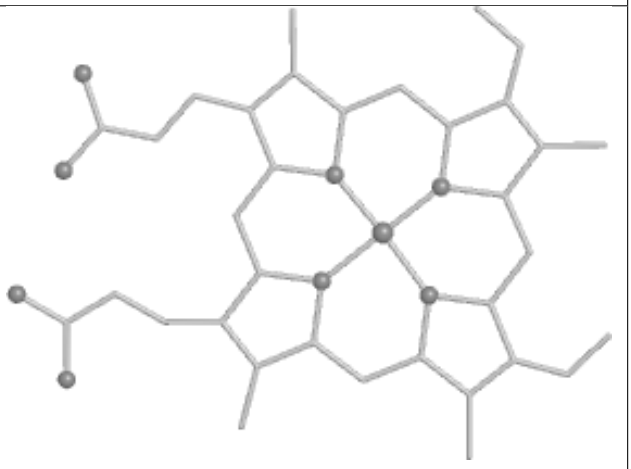
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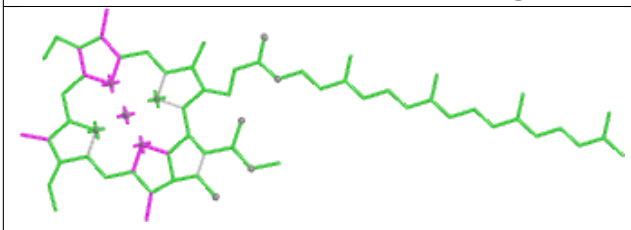


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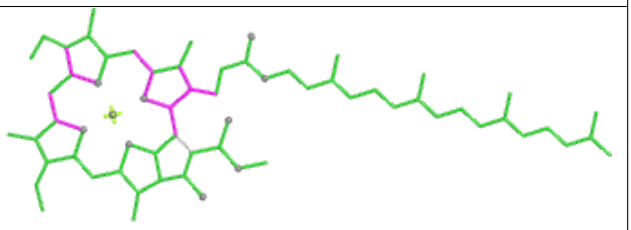


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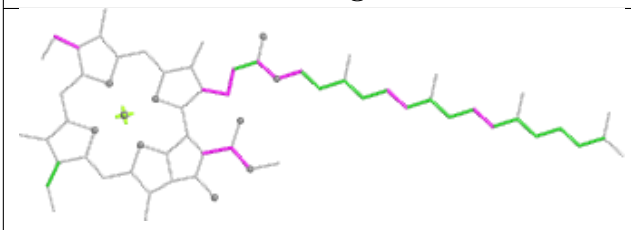
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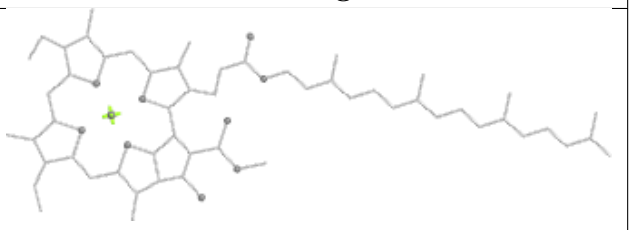
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Bond angles

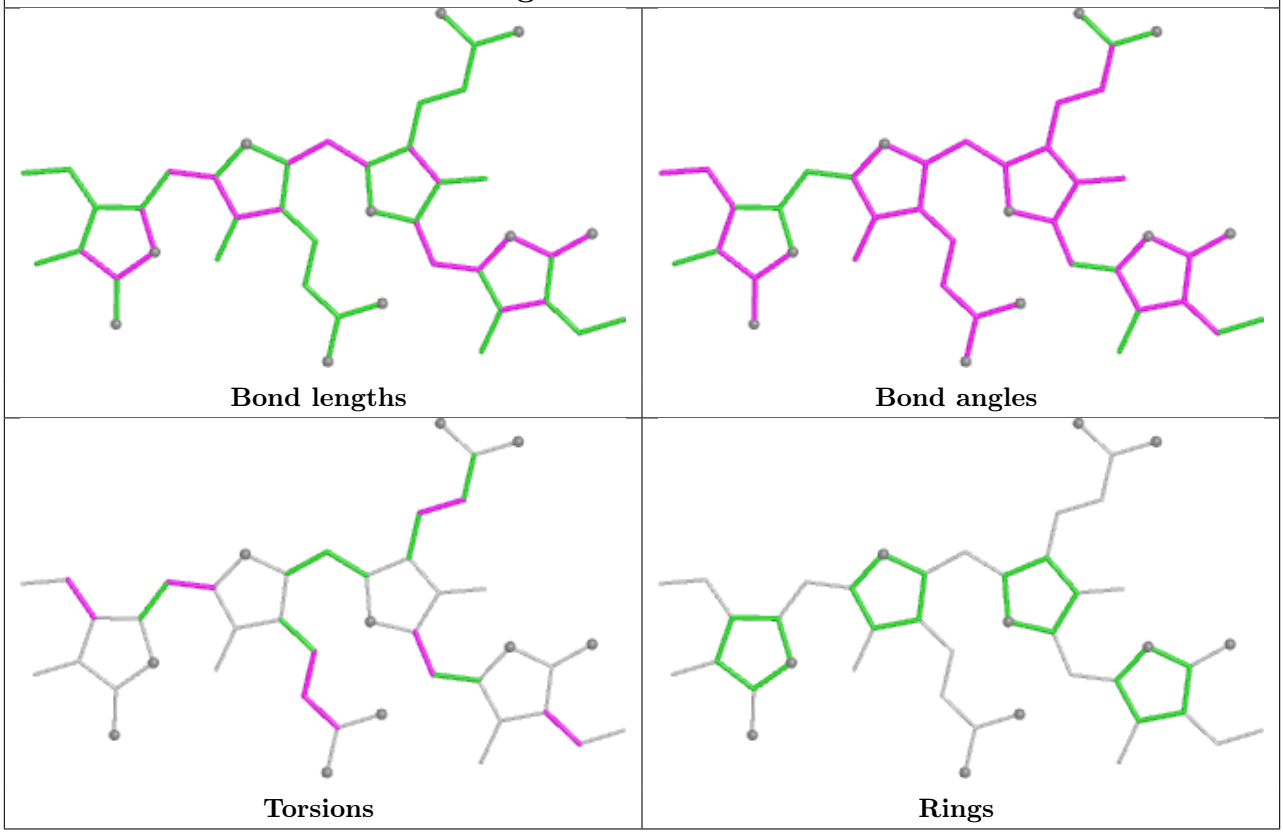


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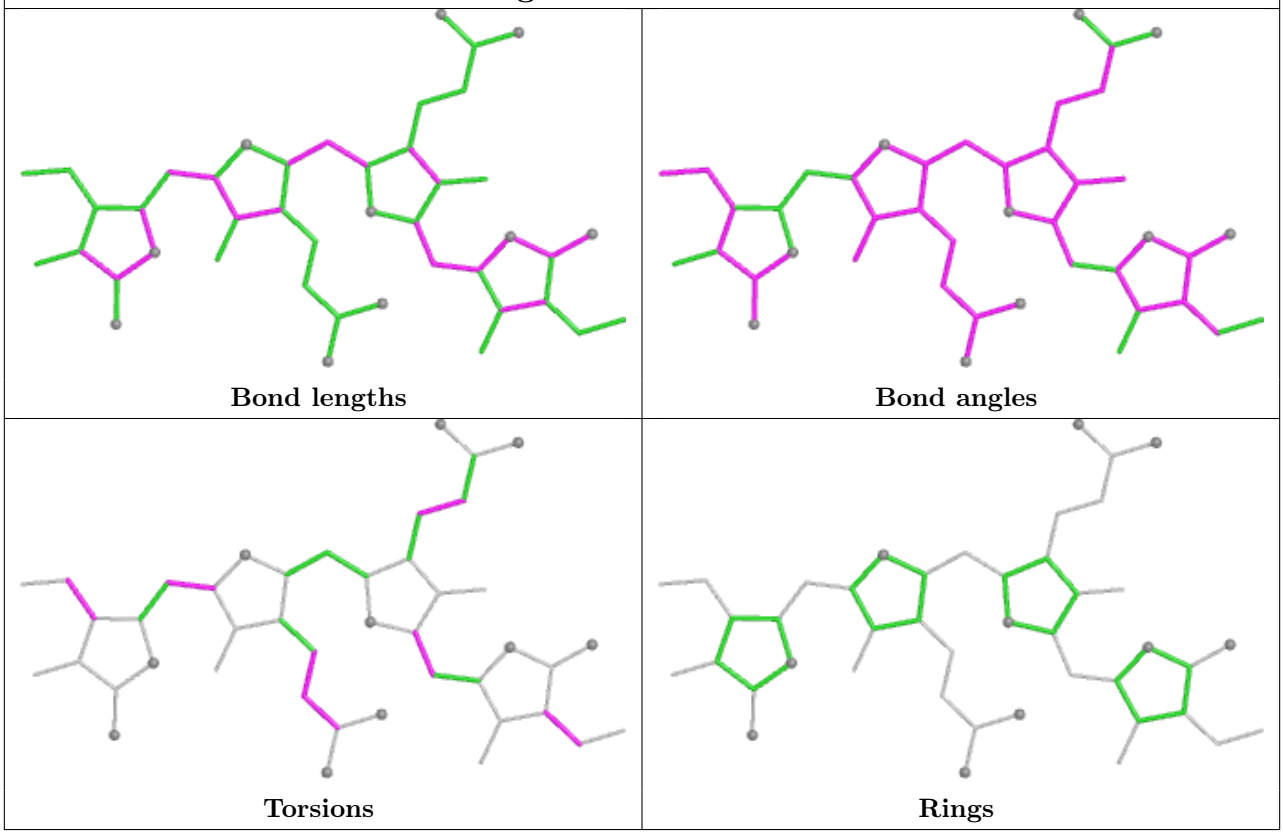


Rings

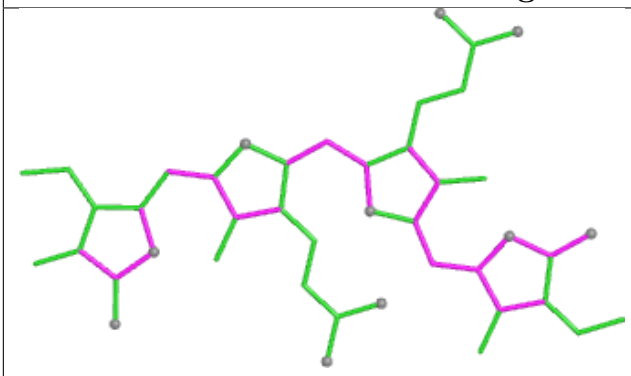
Ligand CYC h9 201



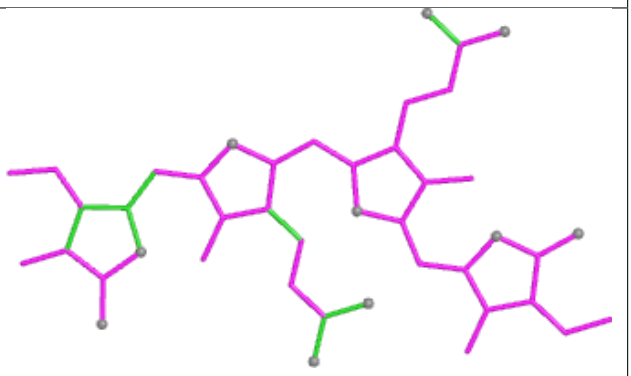
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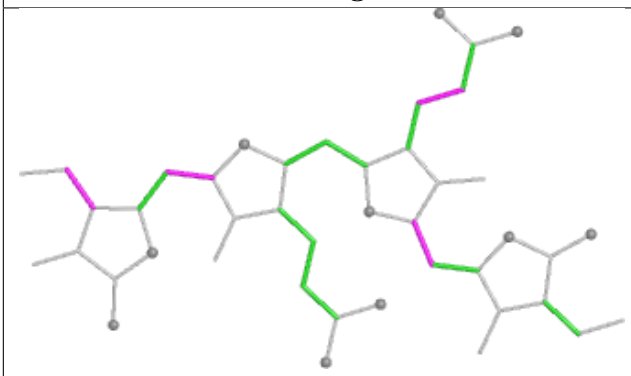
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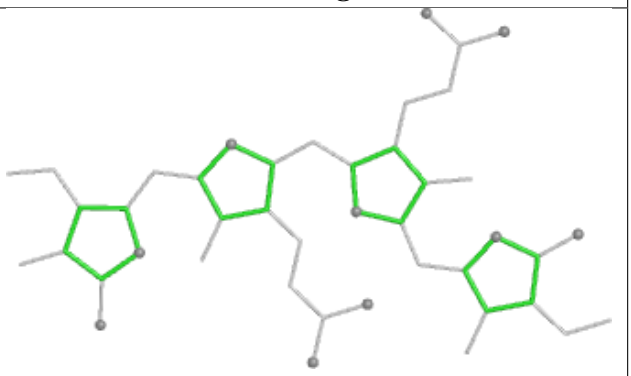
Bond lengths



Bond angles

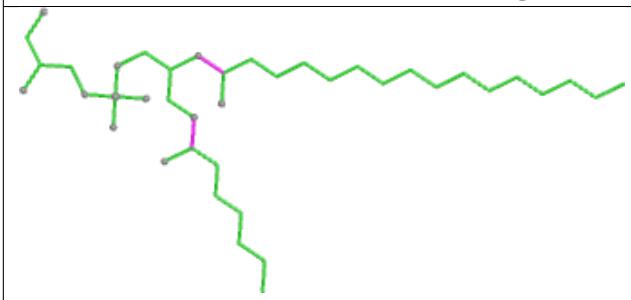


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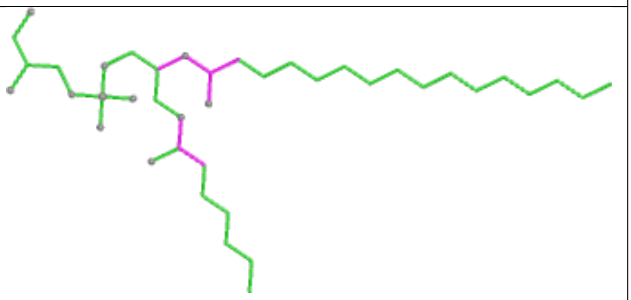


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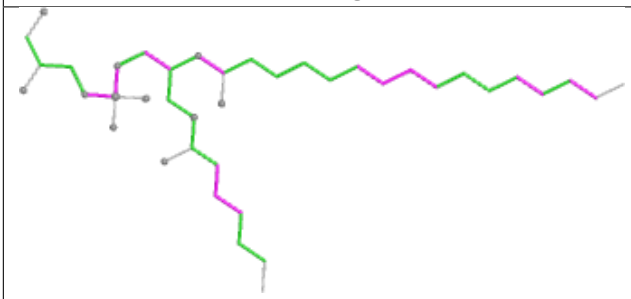
Ligand LHG eD 101



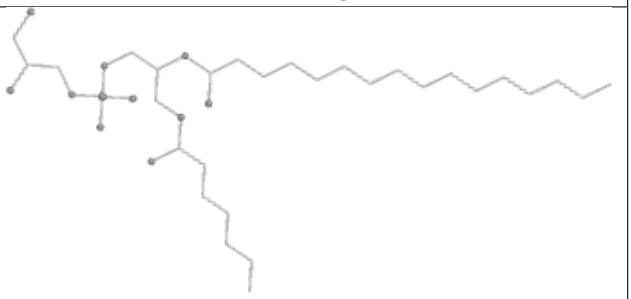
Bond lengths



Bond angles

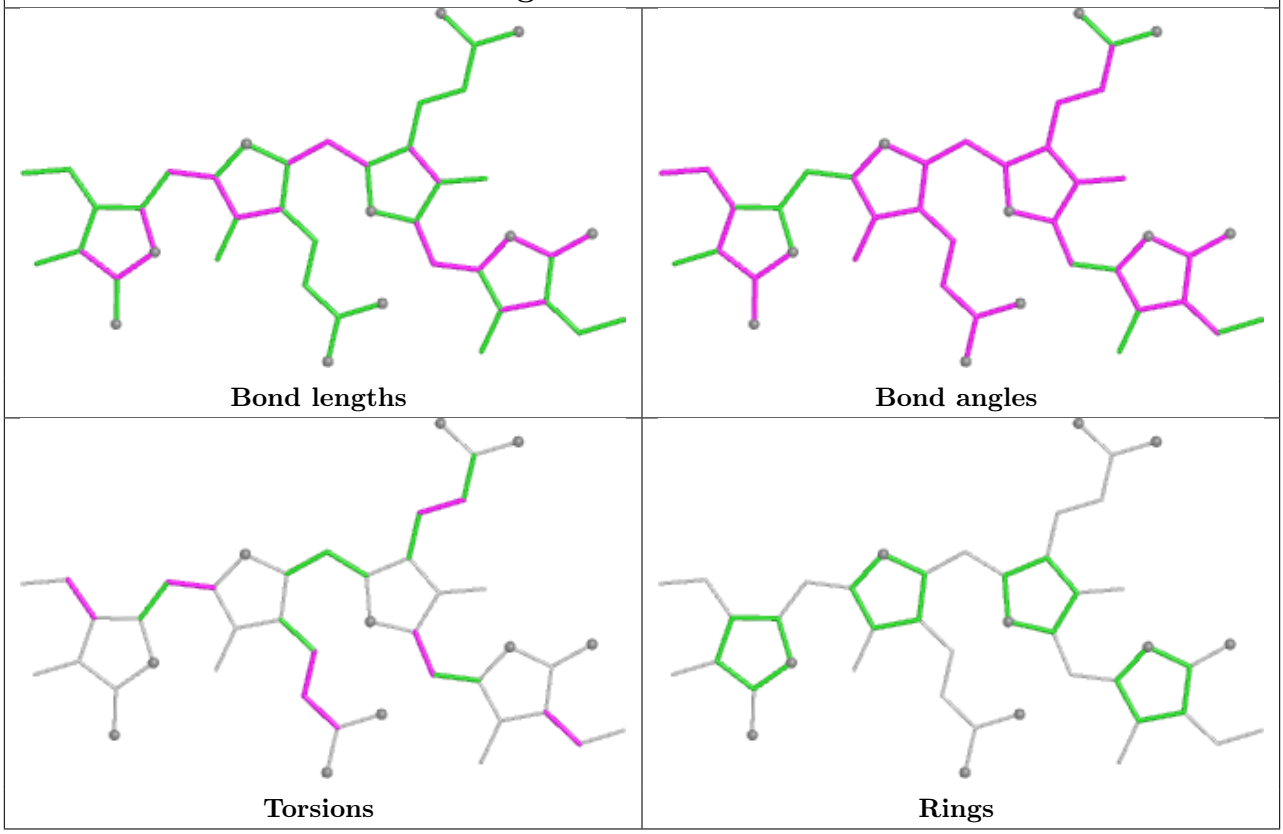


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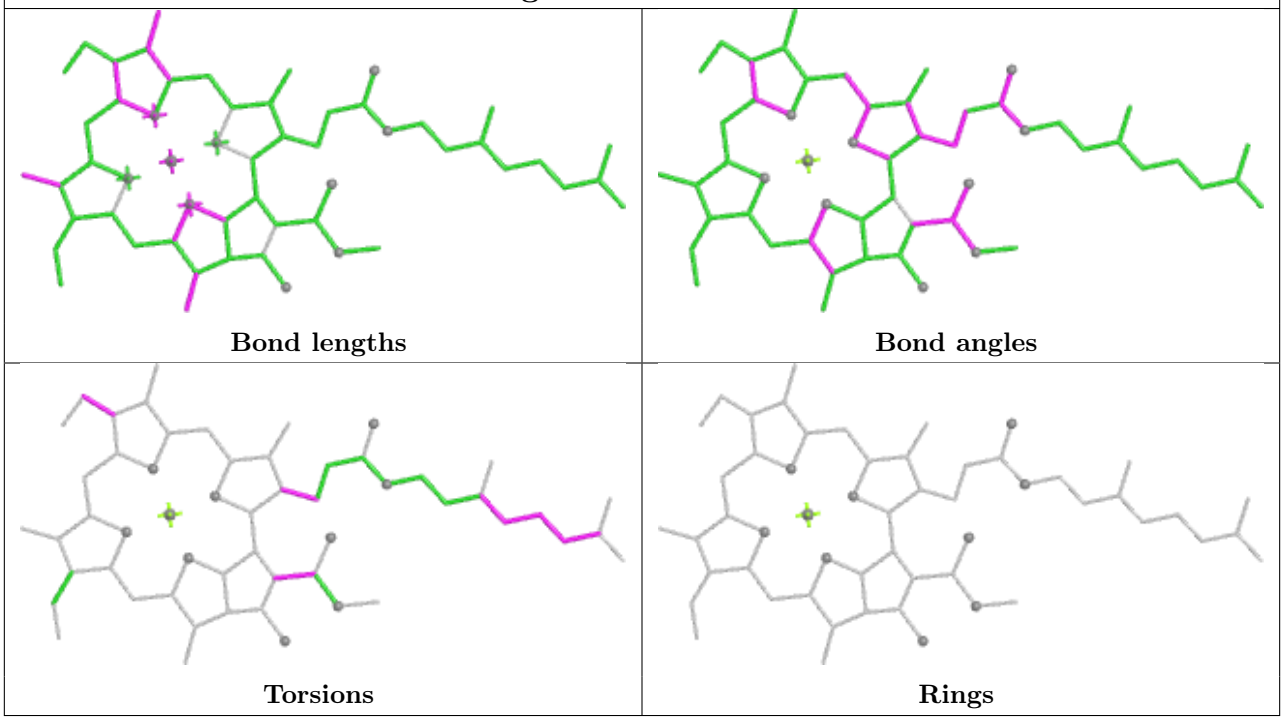


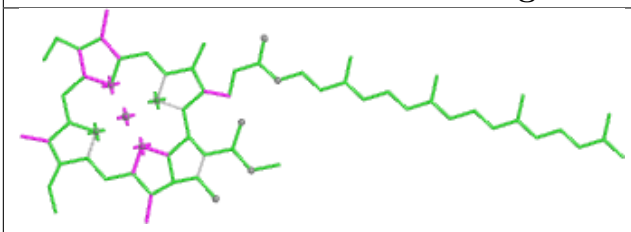
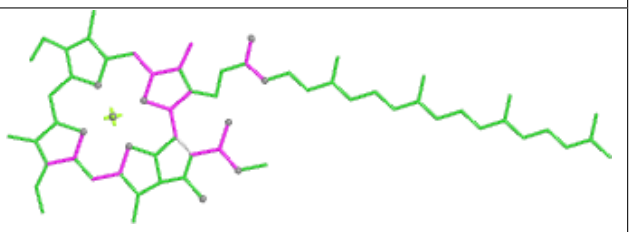
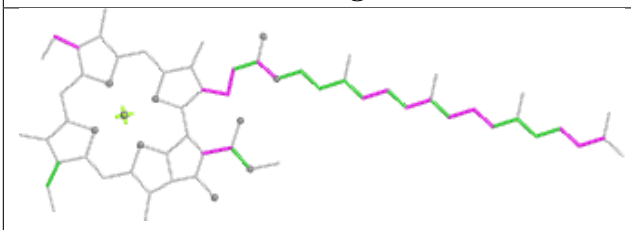
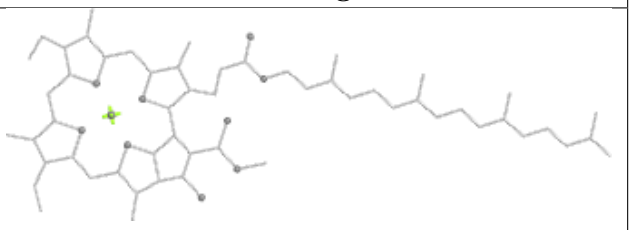
Rings

Ligand CYC h6 201

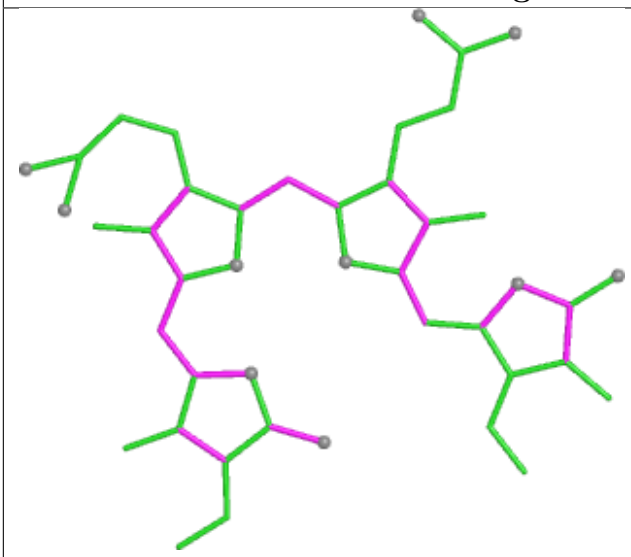


Ligand CLA c1 506

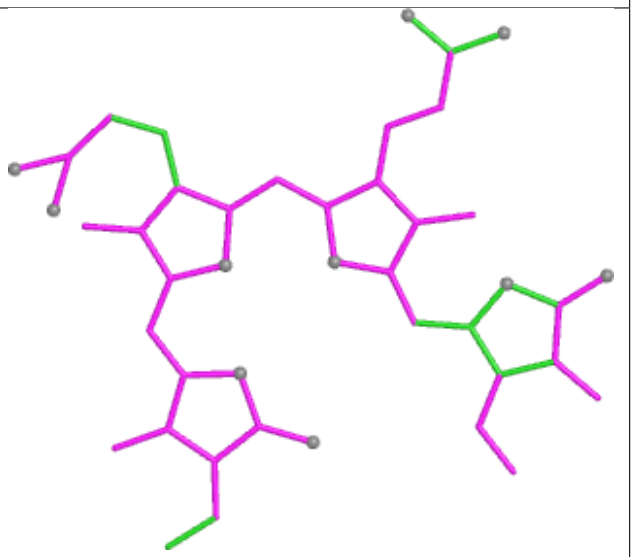


Ligand CLA b1 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

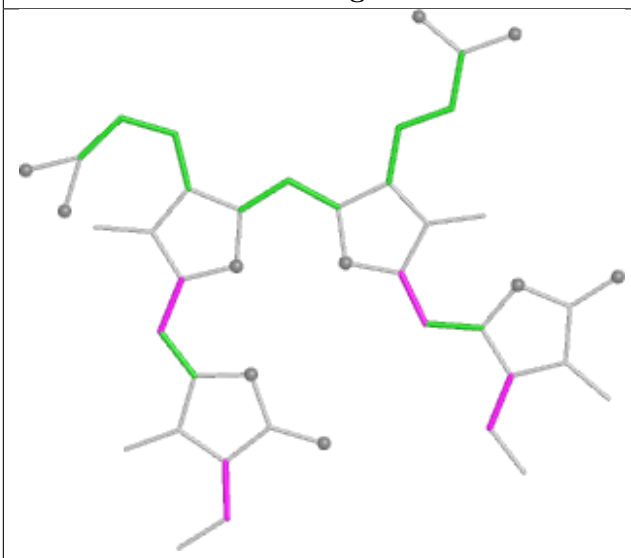
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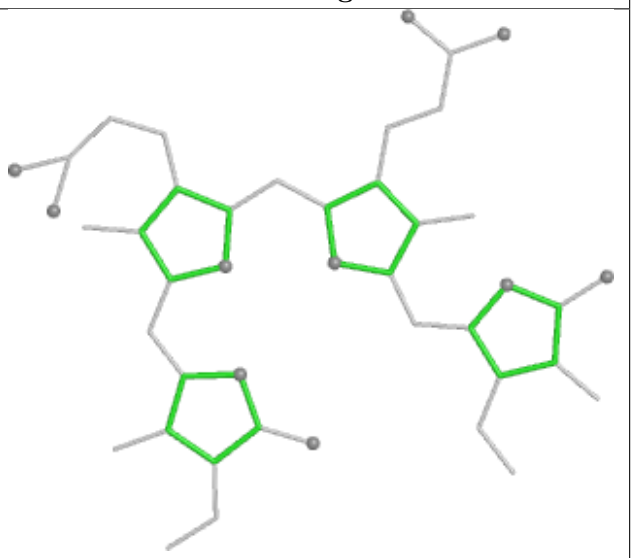
Bond lengths



Bond angles

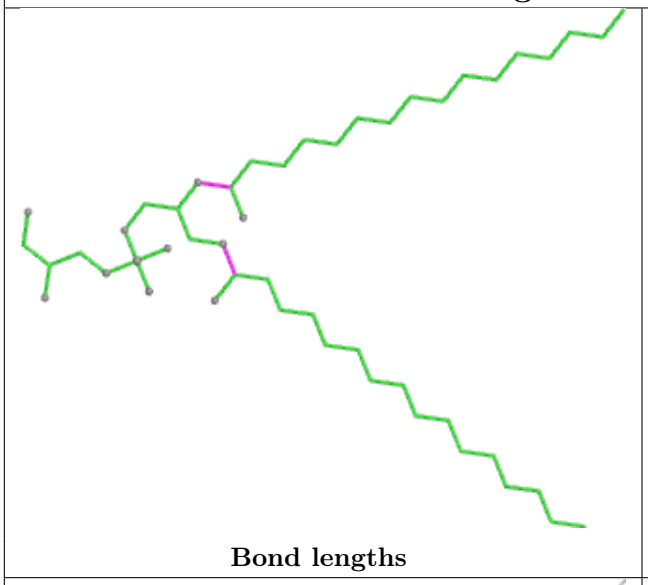


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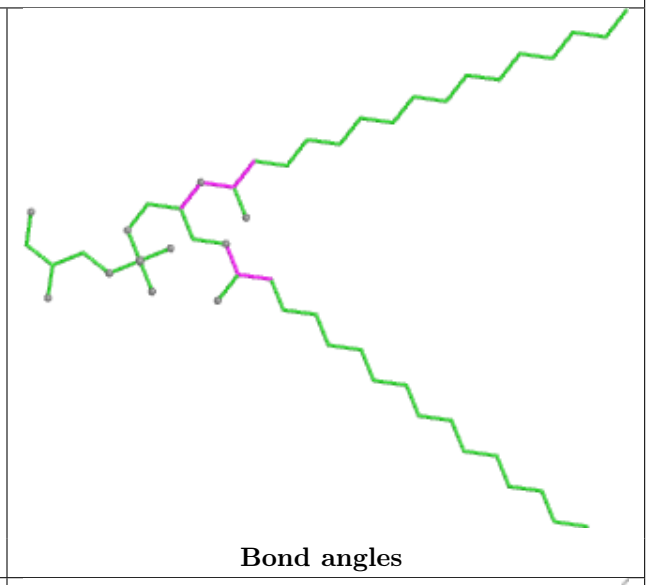


Rings

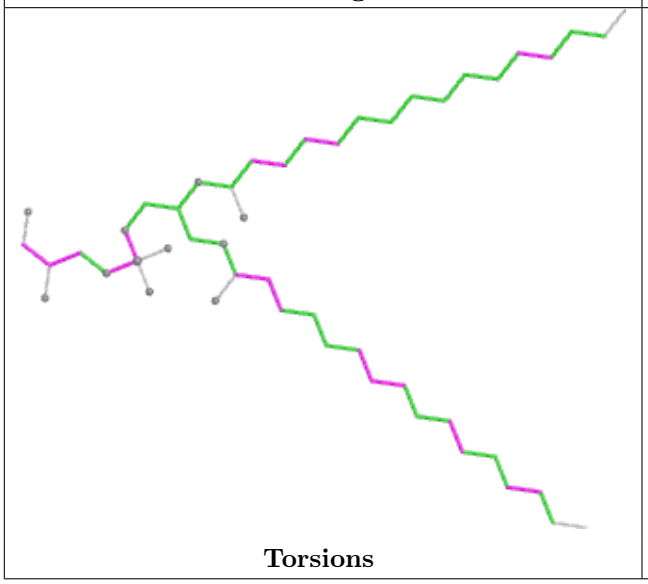
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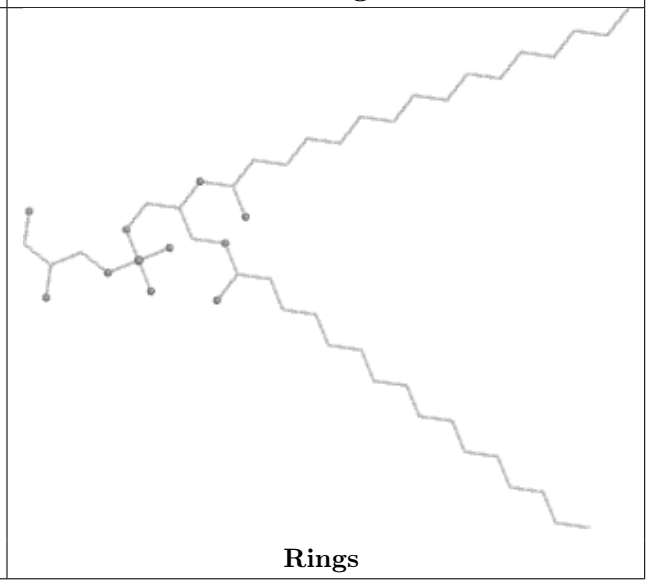
Bond lengths



Bond angles

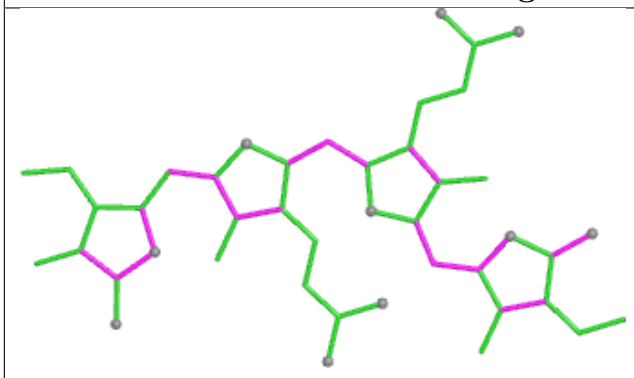


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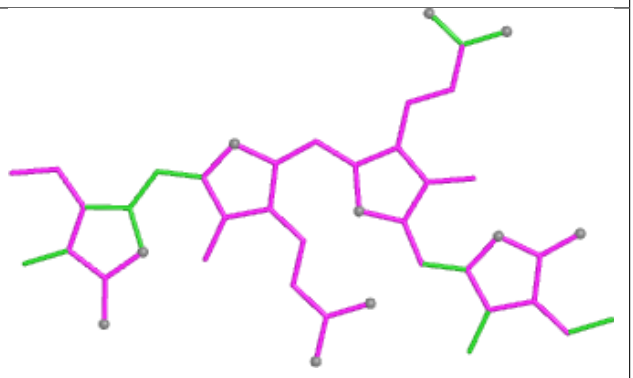


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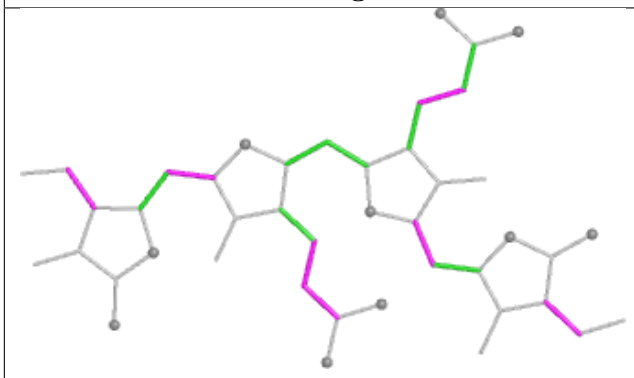
Ligand CYC lC 201



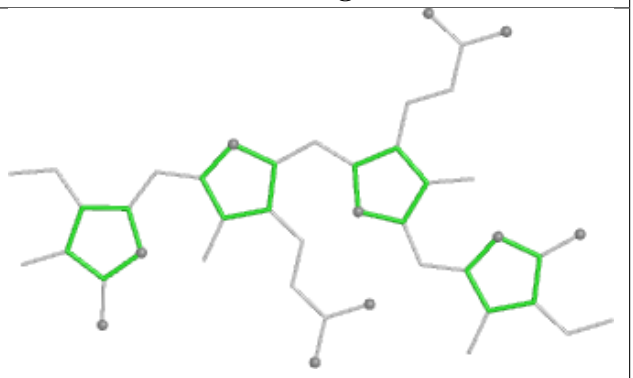
Bond lengths



Bond angles

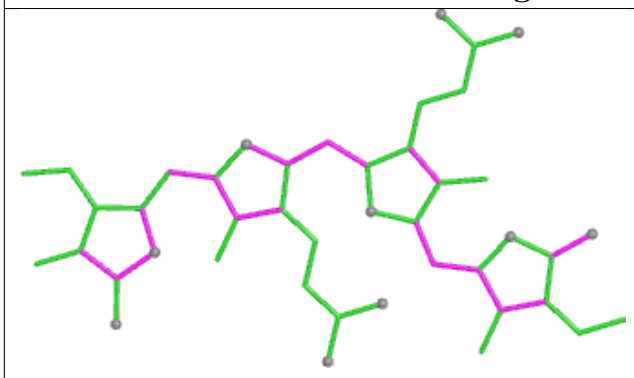


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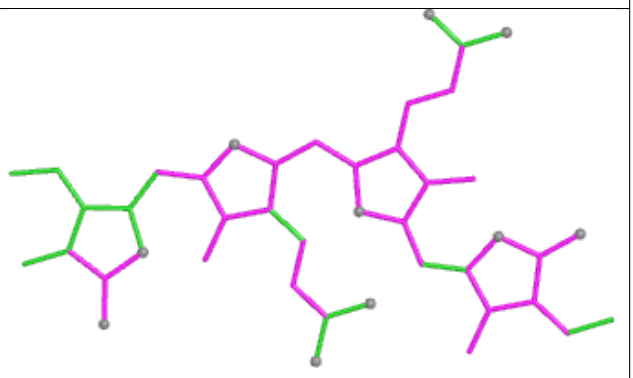


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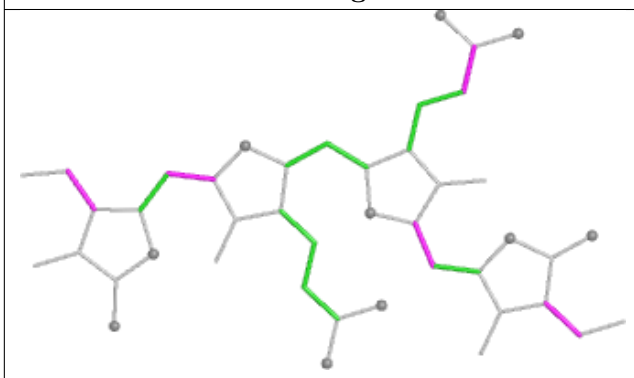
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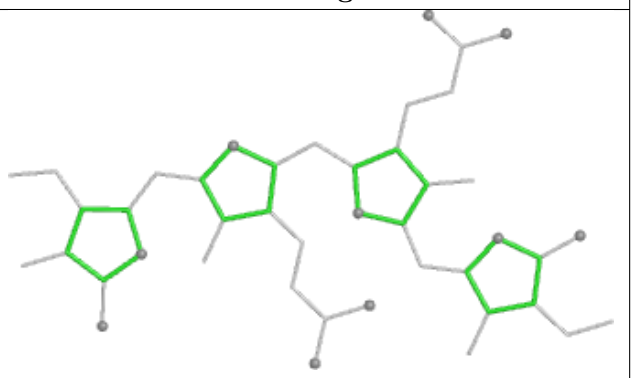
Bond lengths



Bond angles

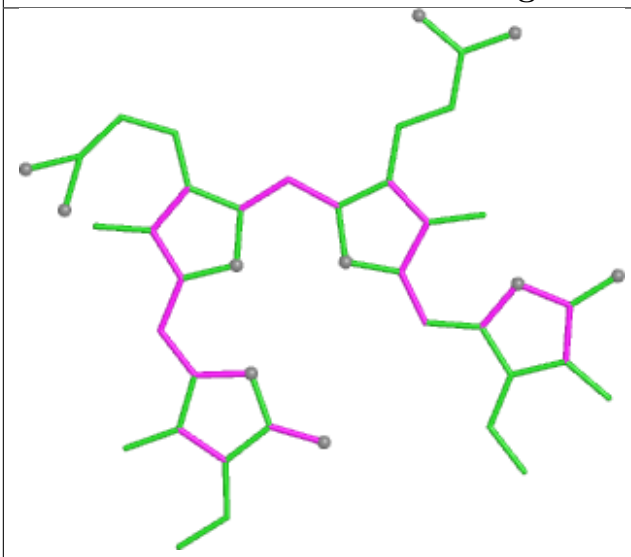


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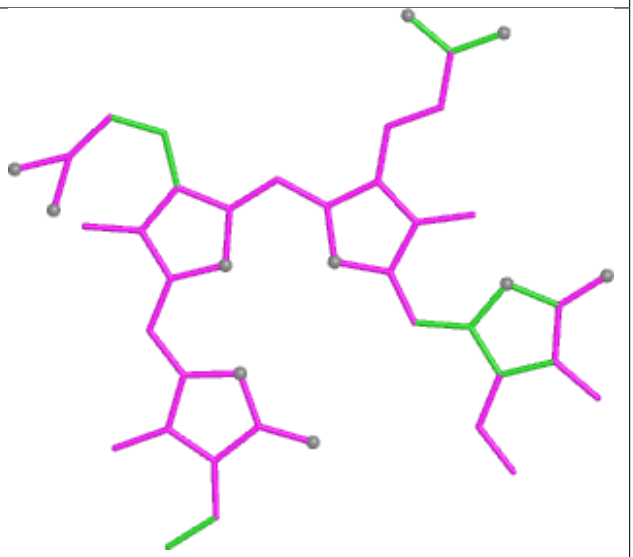


Rings

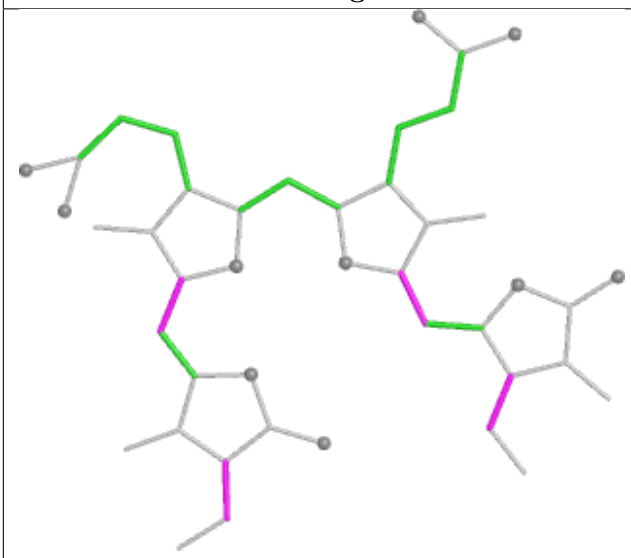
Ligand CYC c2 201



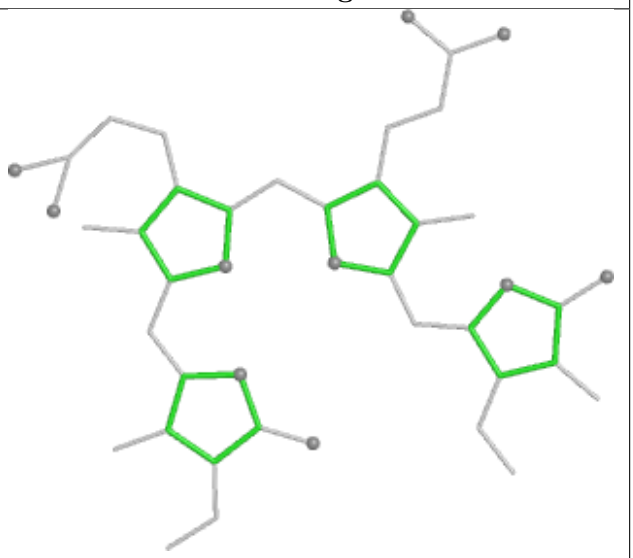
Bond lengths



Bond angles

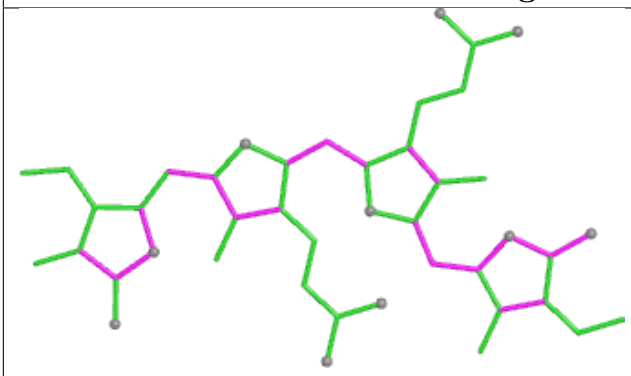


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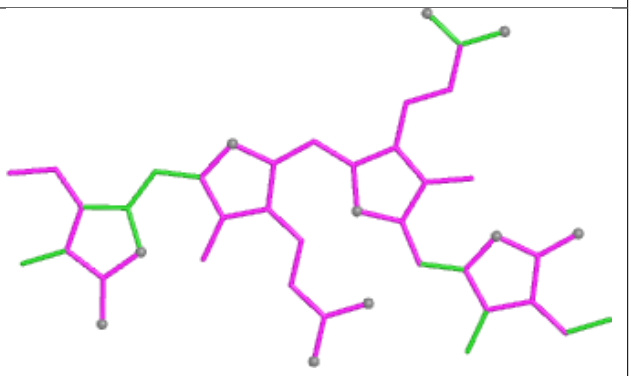


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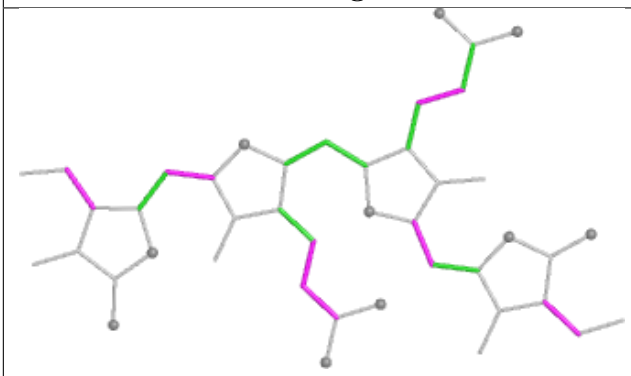
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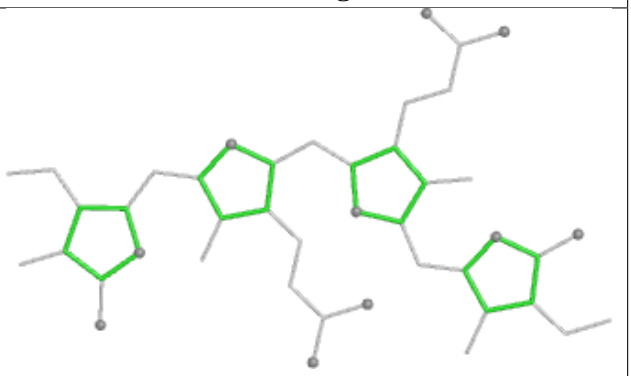
Bond lengths



Bond angles

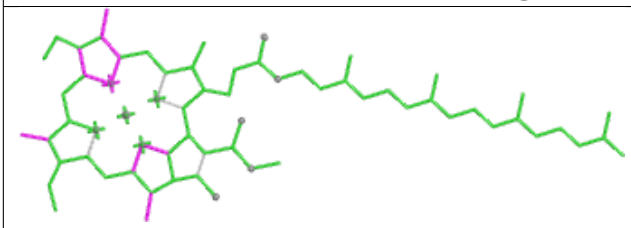


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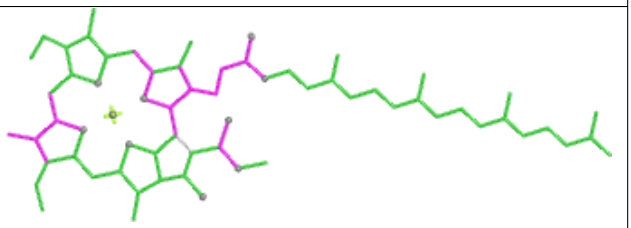


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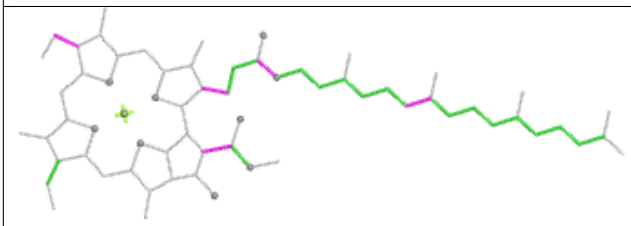
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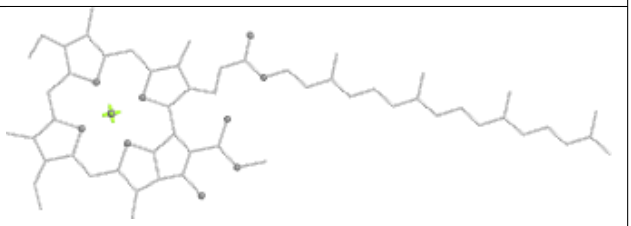
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Bond angles

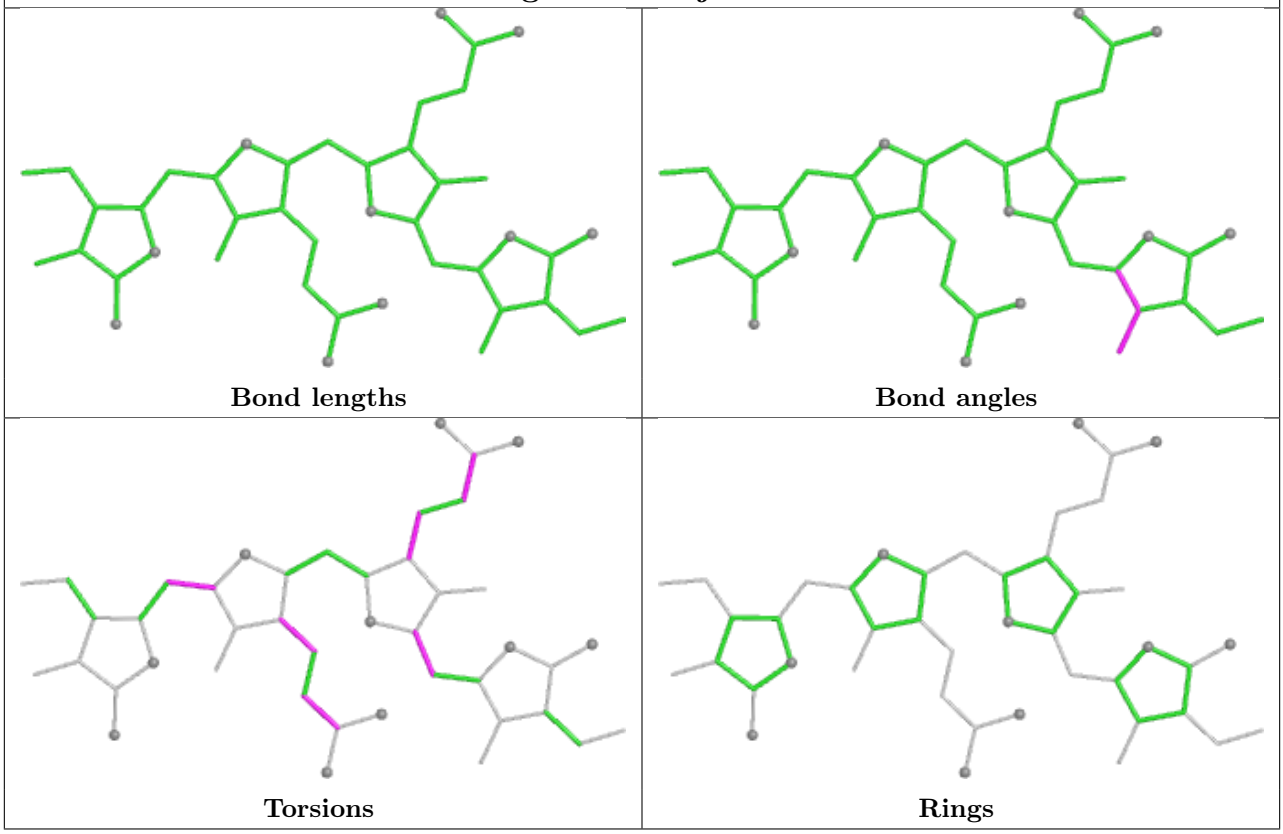


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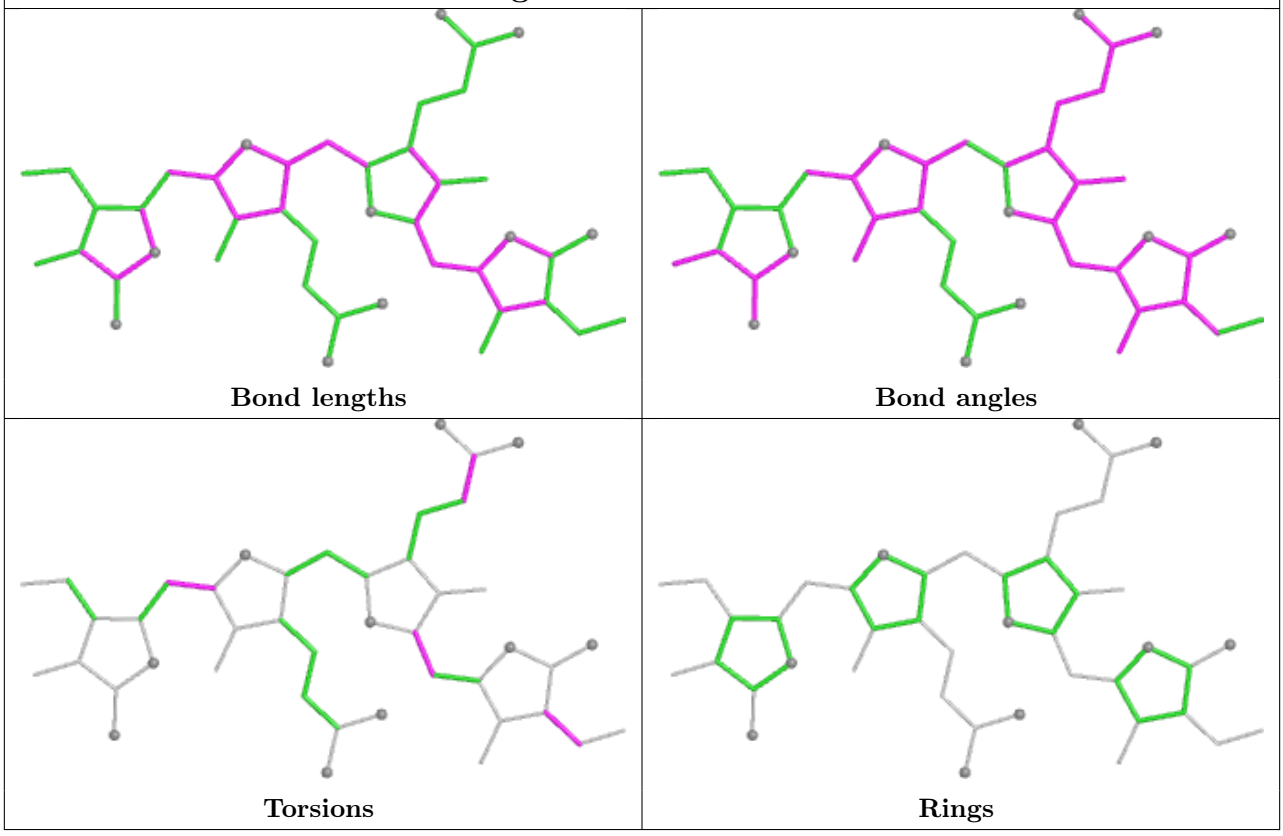


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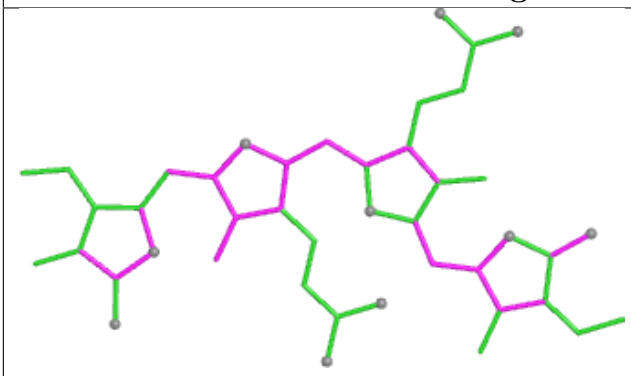
Ligand CYC j3 202



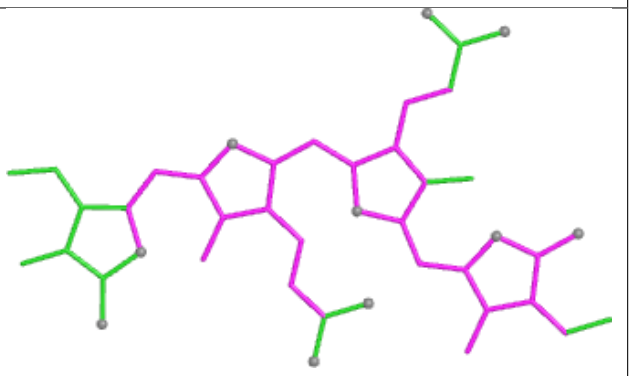
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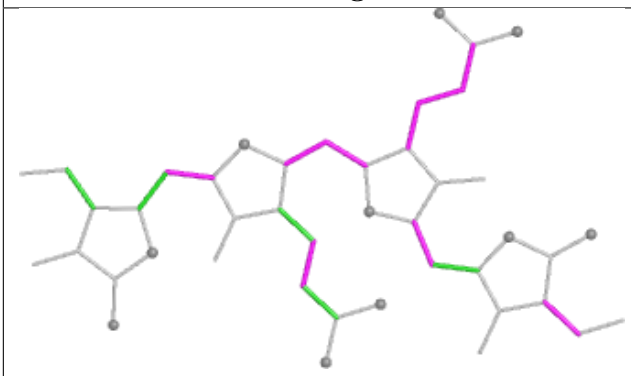
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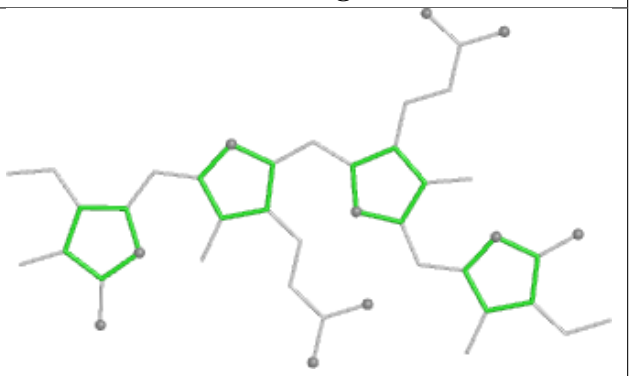
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Bond angles

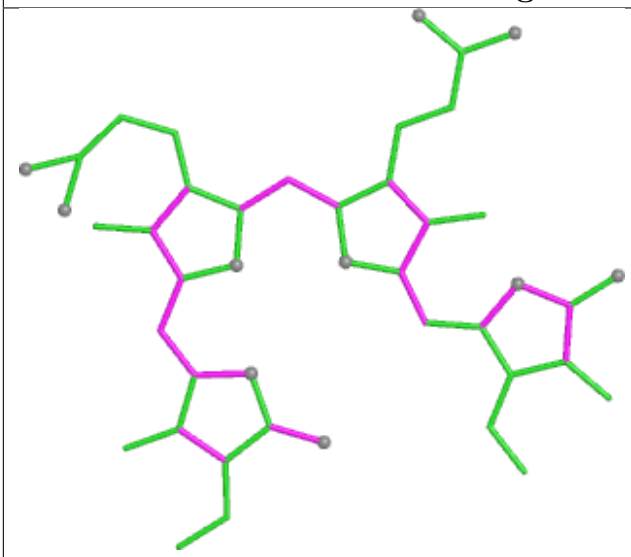


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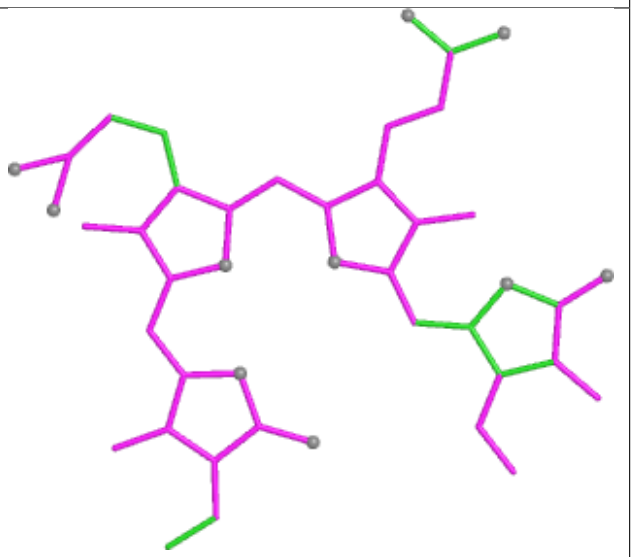


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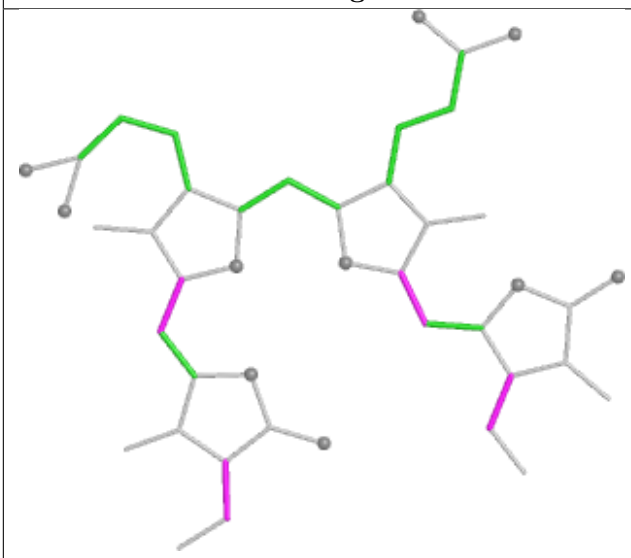
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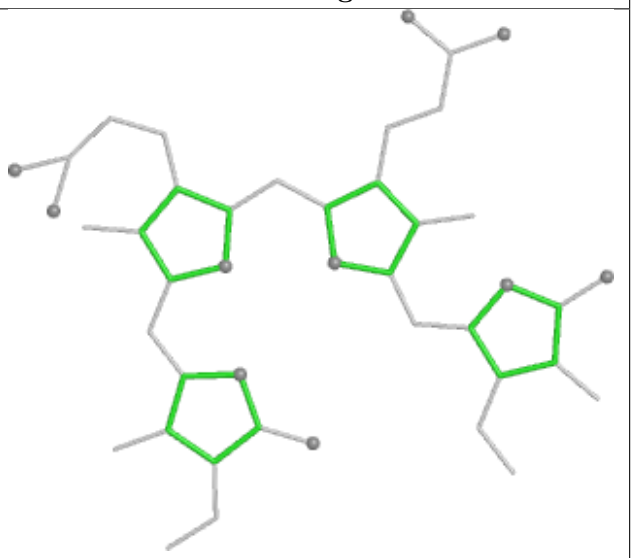
Bond lengths



Bond angles

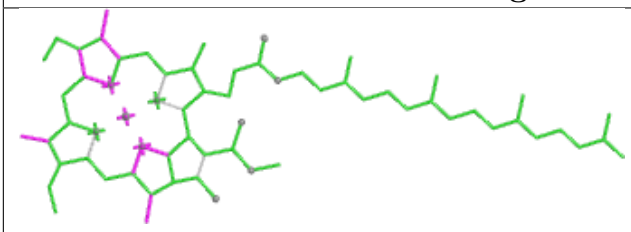


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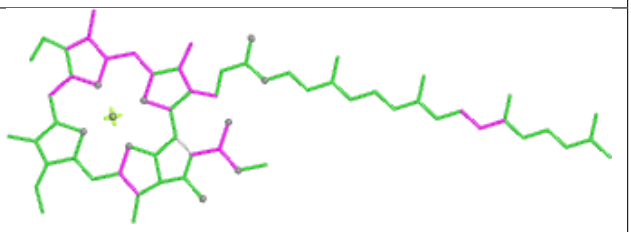


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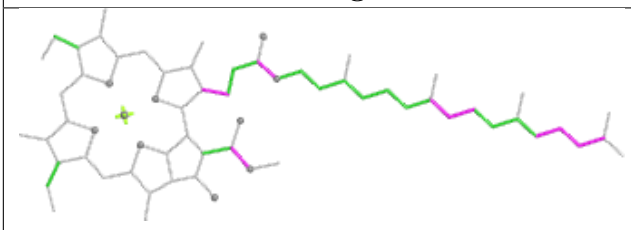
Ligand CLA DD 406



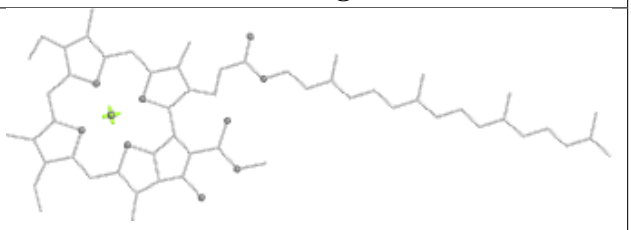
Bond lengths



Bond angles

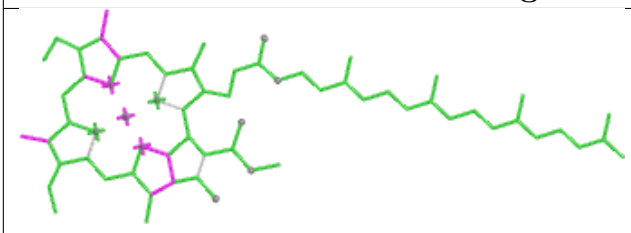


Torsions

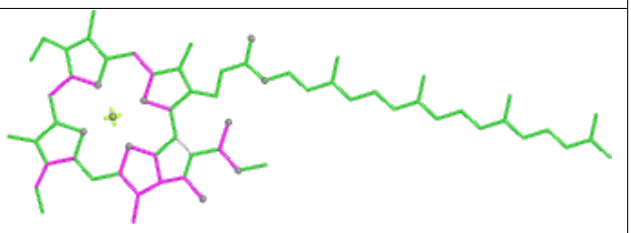


Rings

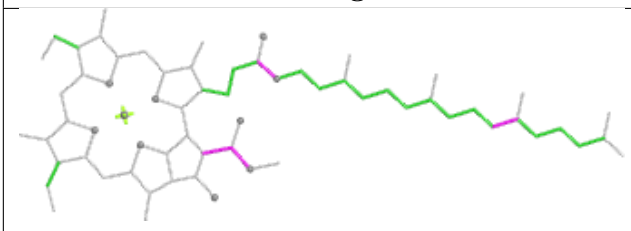
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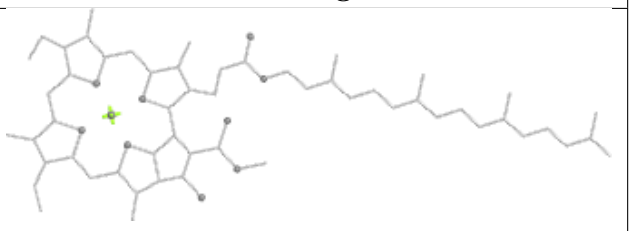
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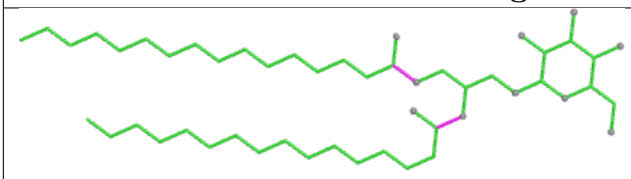


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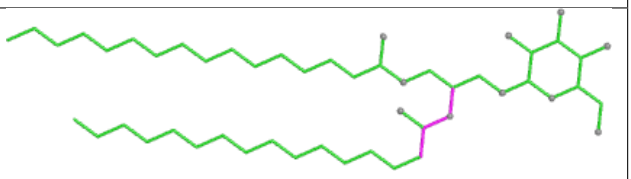


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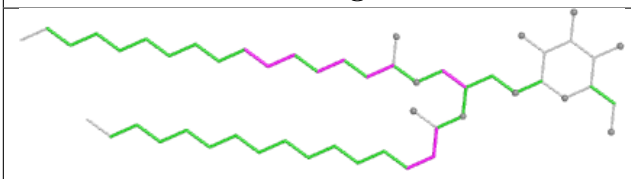
Ligand LMG aD 407



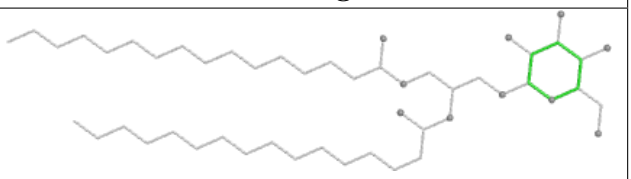
Bond lengths



Bond angles

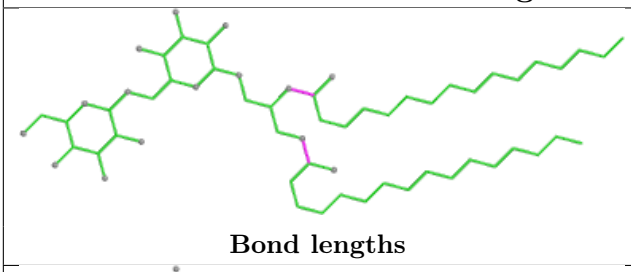


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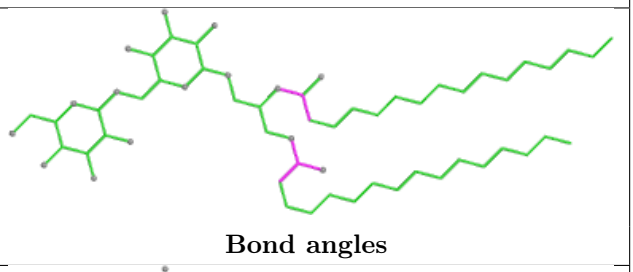


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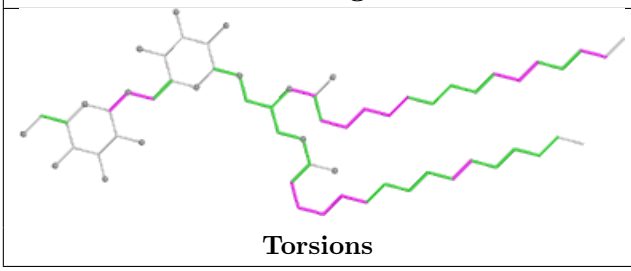
Ligand DGD c1 517



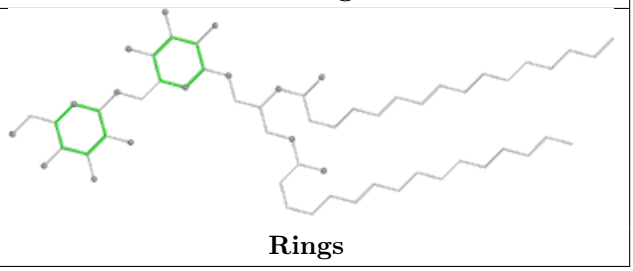
Bond lengths



Bond angles

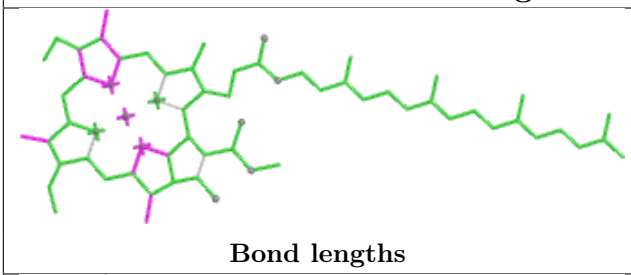


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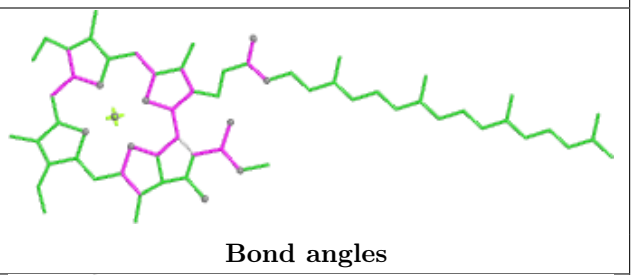


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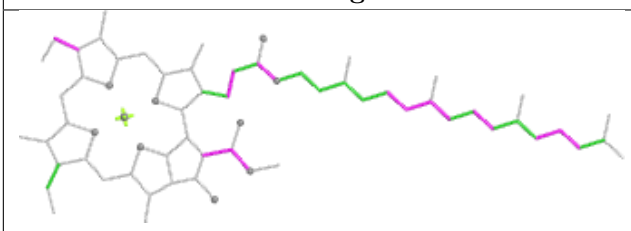
Ligand CLA aD 405



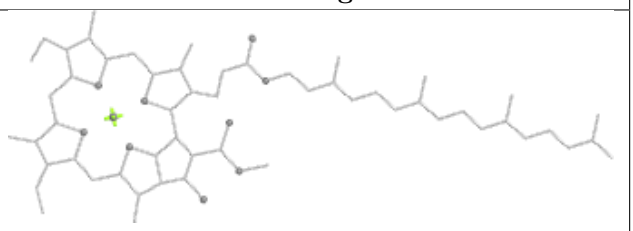
Bond lengths



Bond angles

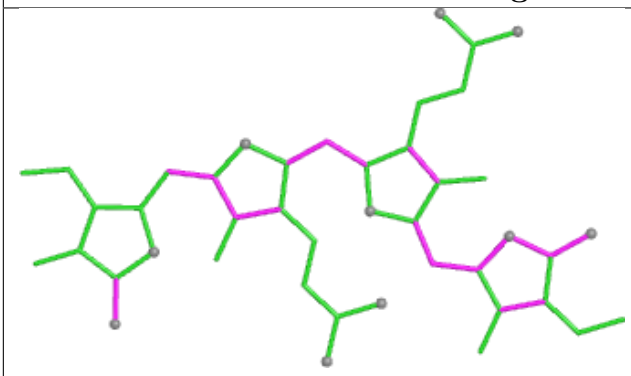


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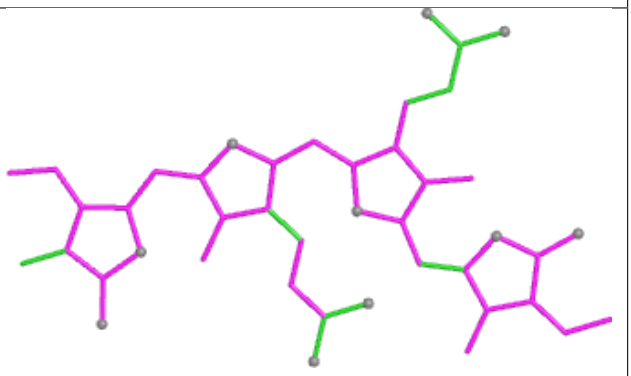


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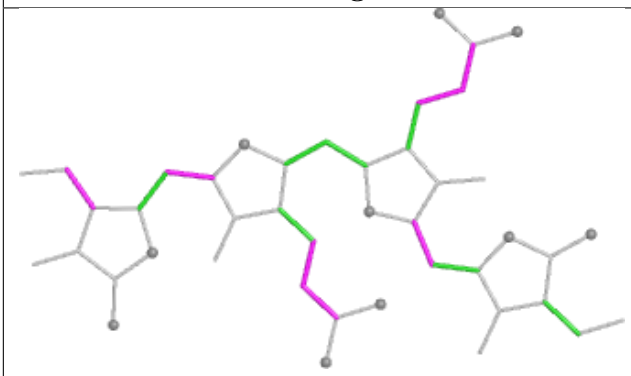
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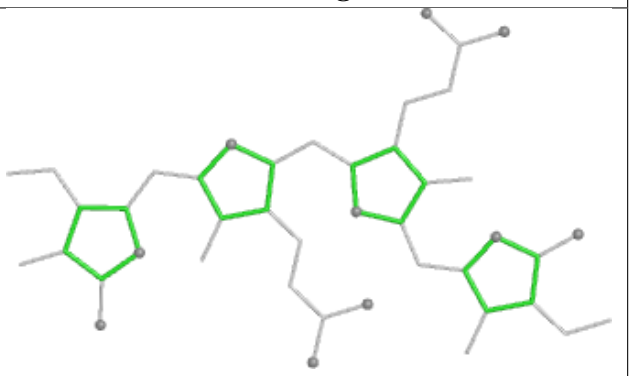
Bond lengths



Bond angles

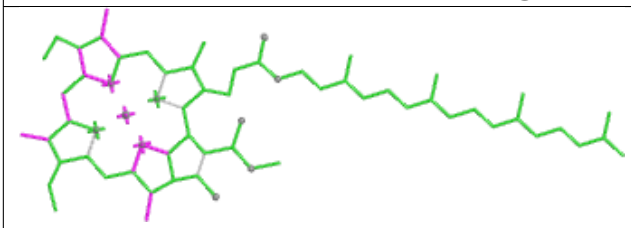


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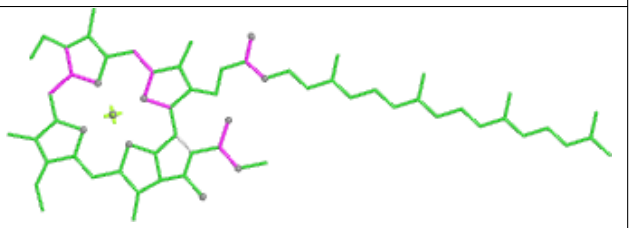


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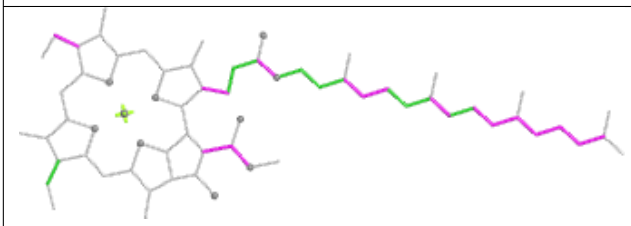
Ligand CLA xE 101



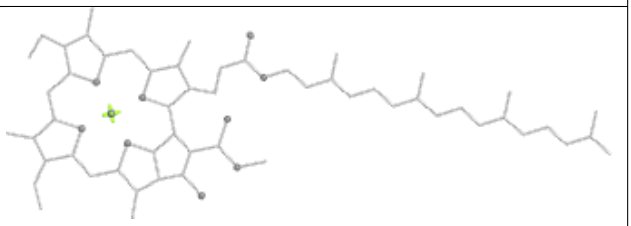
Bond lengths



Bond angles

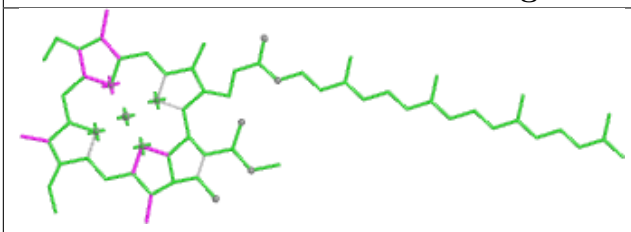


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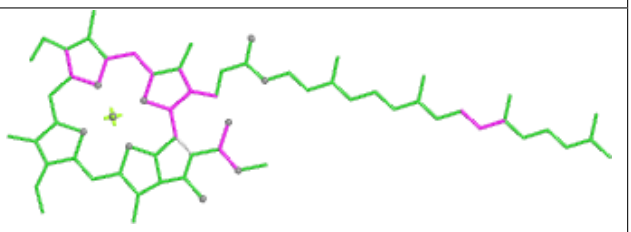


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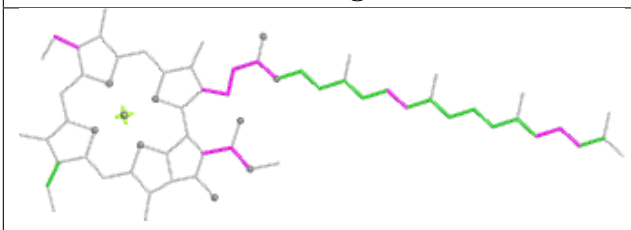
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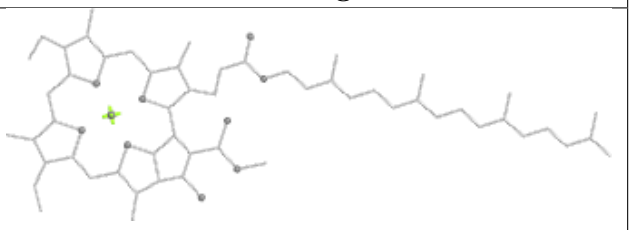
Bond lengths



Bond angles



Torsions



Rings

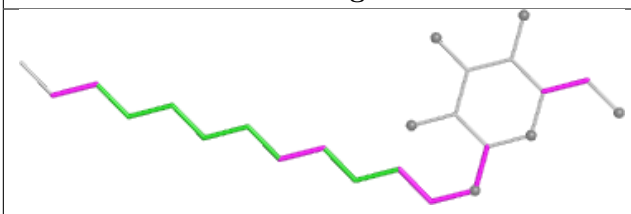
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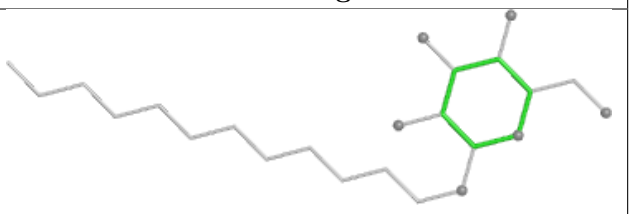
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Bond angles

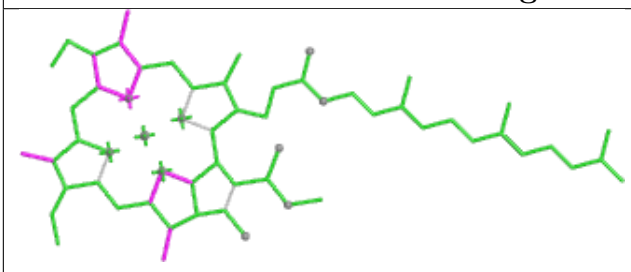


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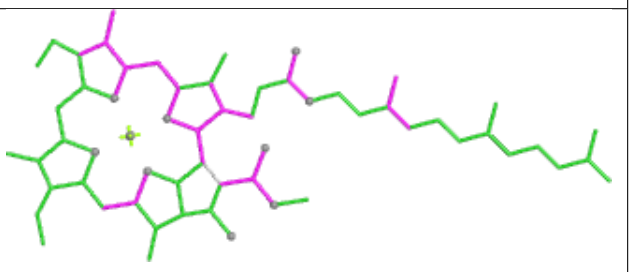


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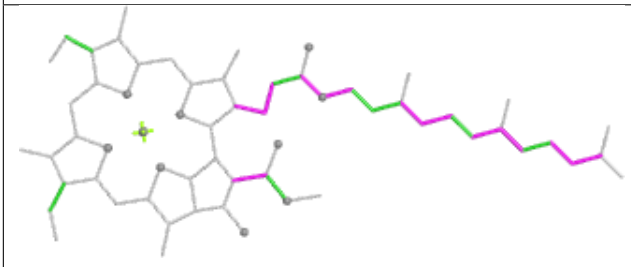
Ligand CLA a1 407



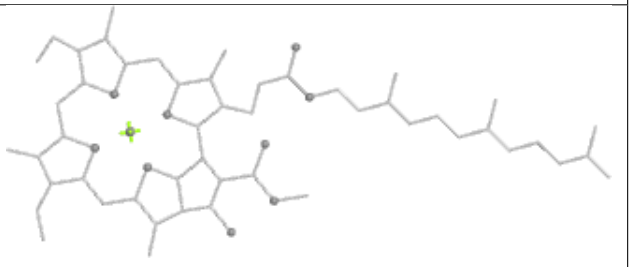
Bond lengths



Bond angles

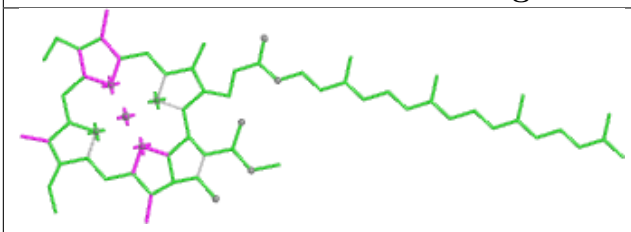


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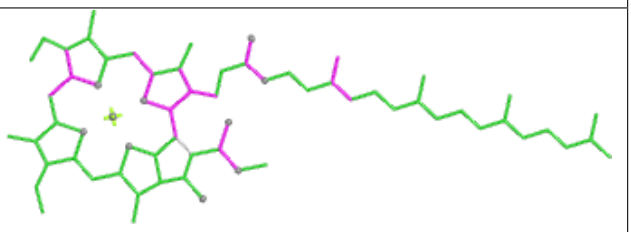


Rings

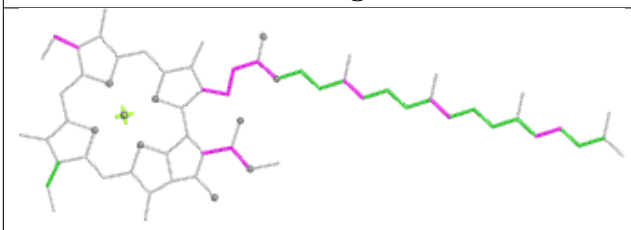
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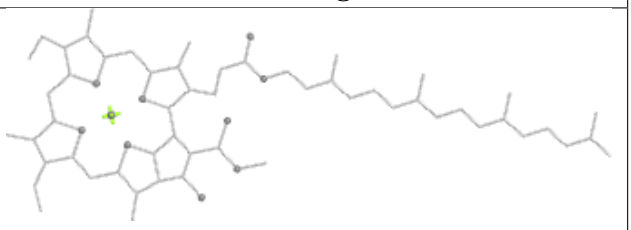
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Bond angles

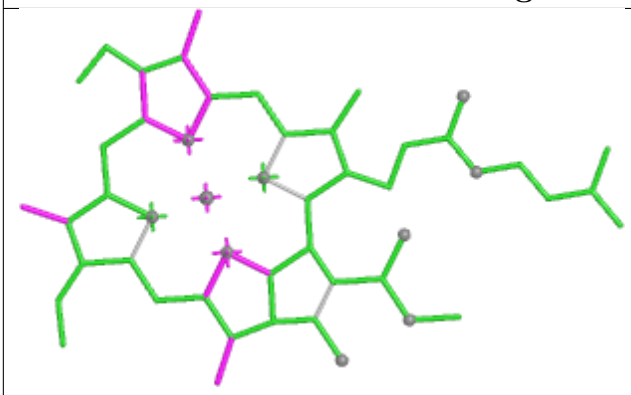


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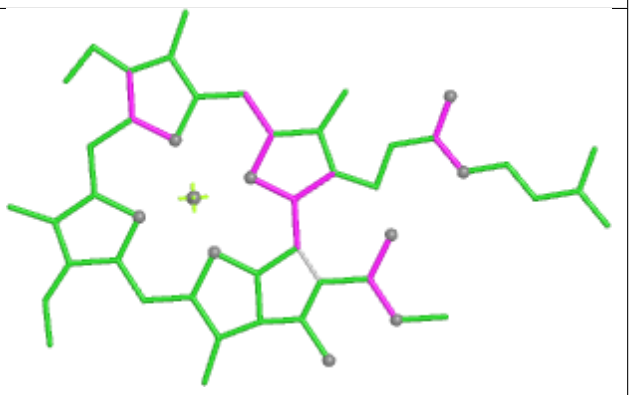


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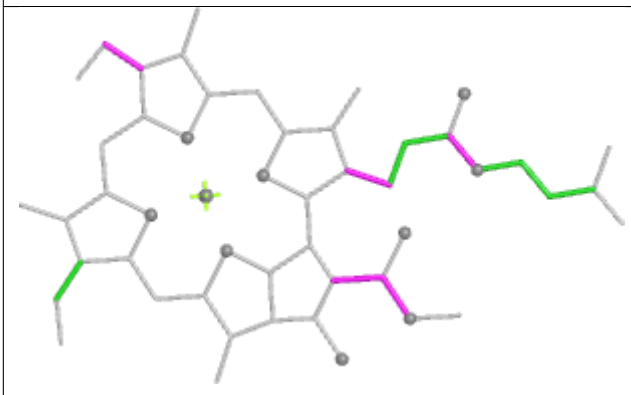
Ligand CLA cD 513



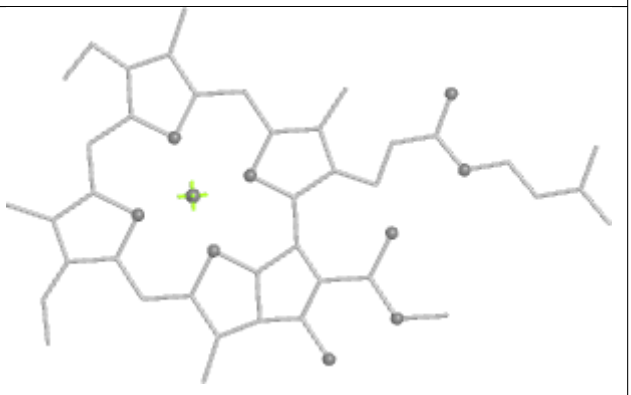
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Bond angles

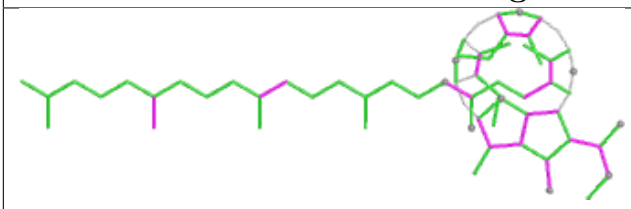


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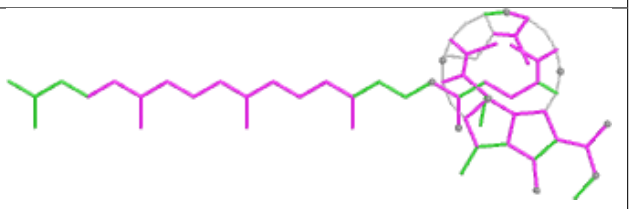


Rings

Ligand PHO DE 403



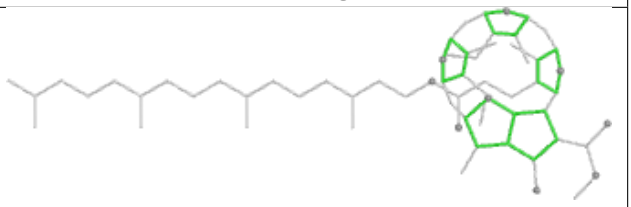
Bond lengths



Bond angles

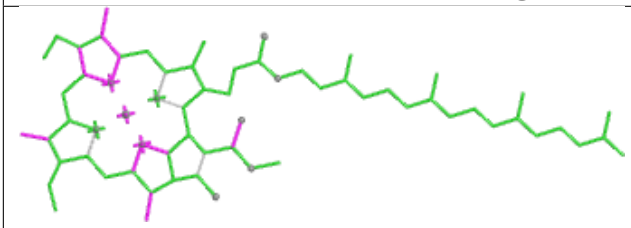


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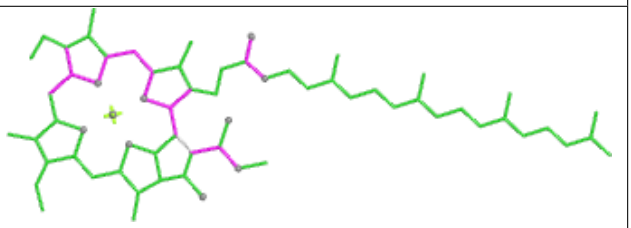


Rings

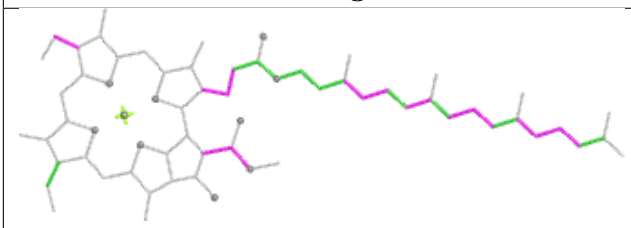
Ligand CLA bD 605



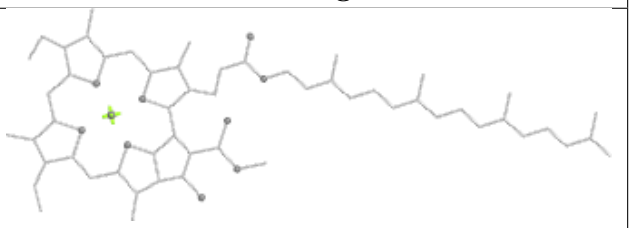
Bond lengths



Bond angles

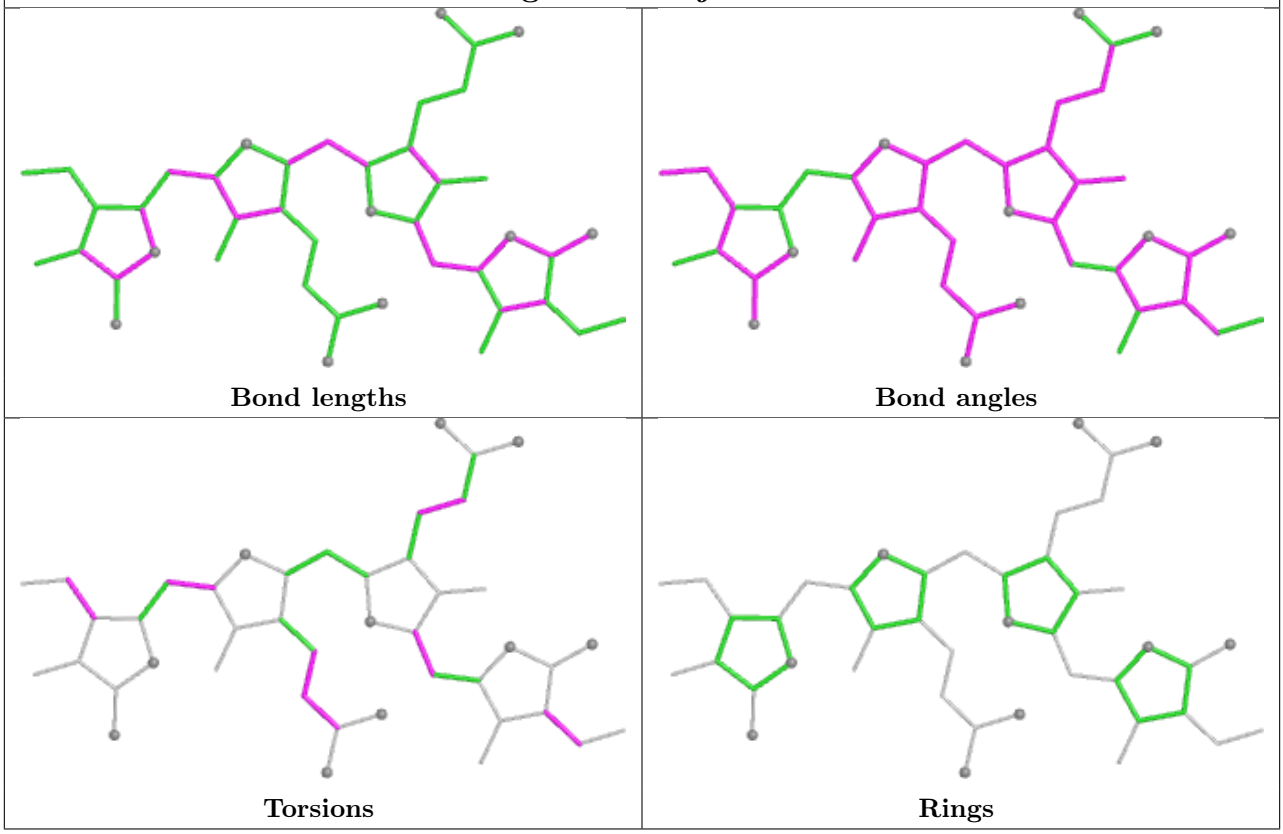


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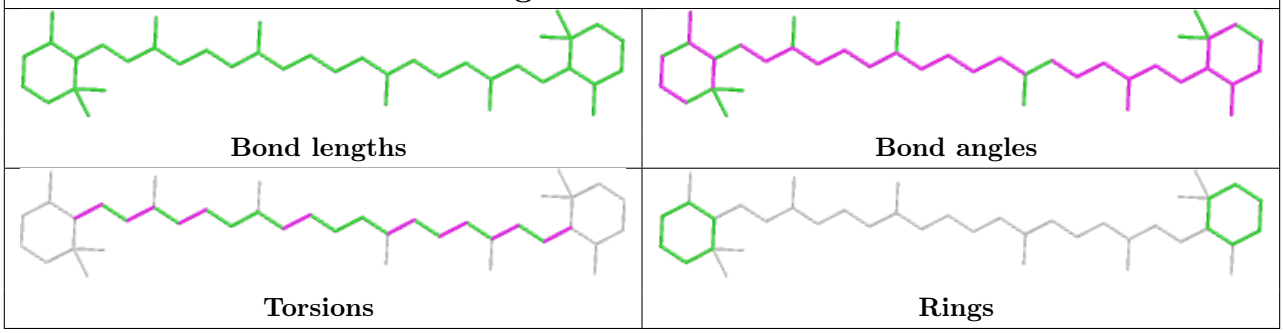


Rings

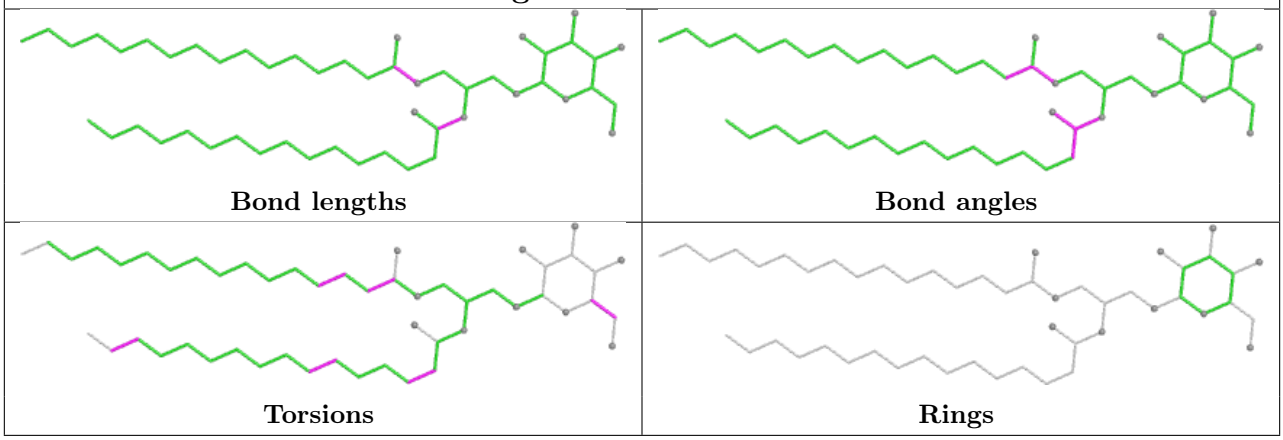
Ligand CYC j2 201



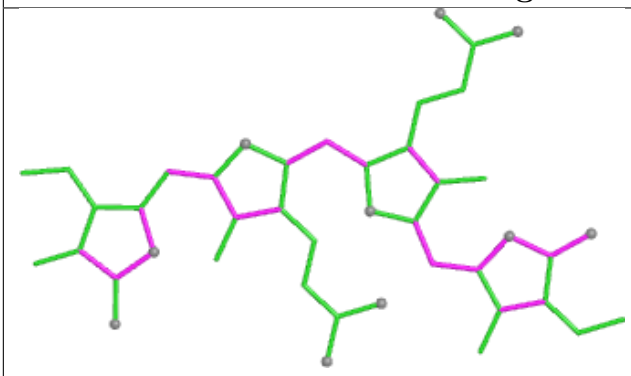
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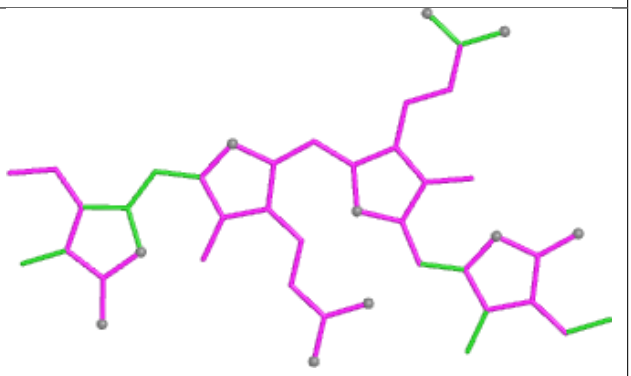
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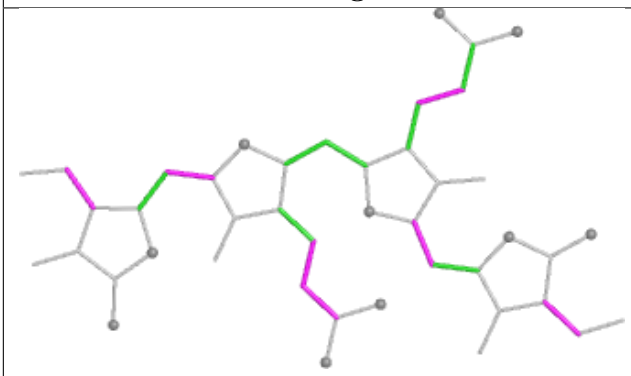
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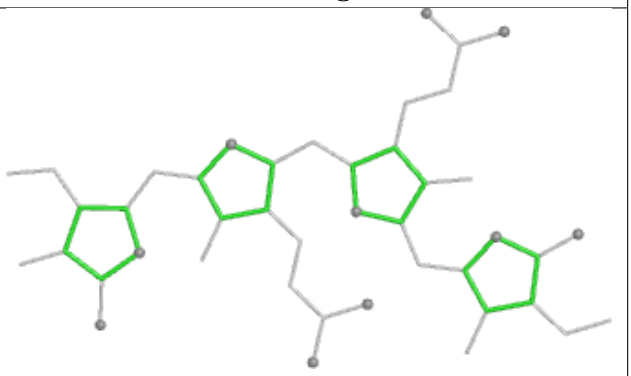
Bond lengths



Bond angles

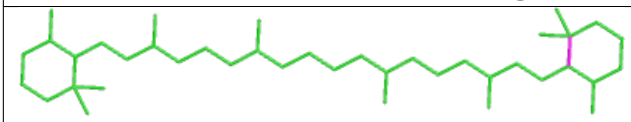


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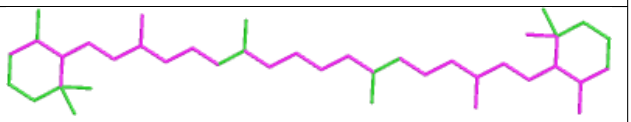


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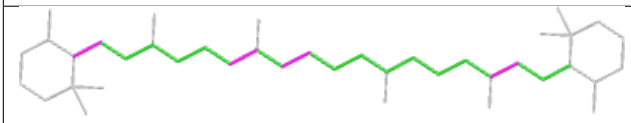
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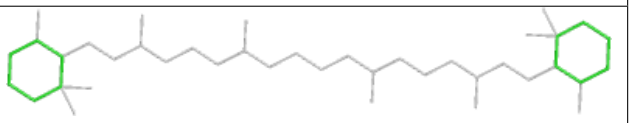
Bond lengths



Bond angles



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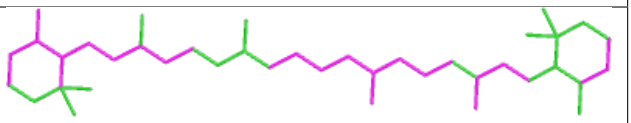


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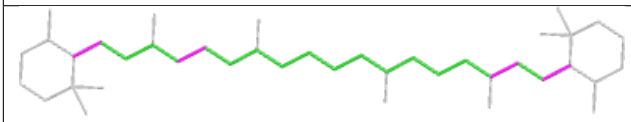
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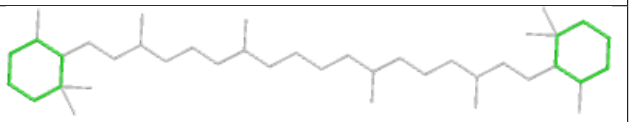
Bond lengths



Bond angles

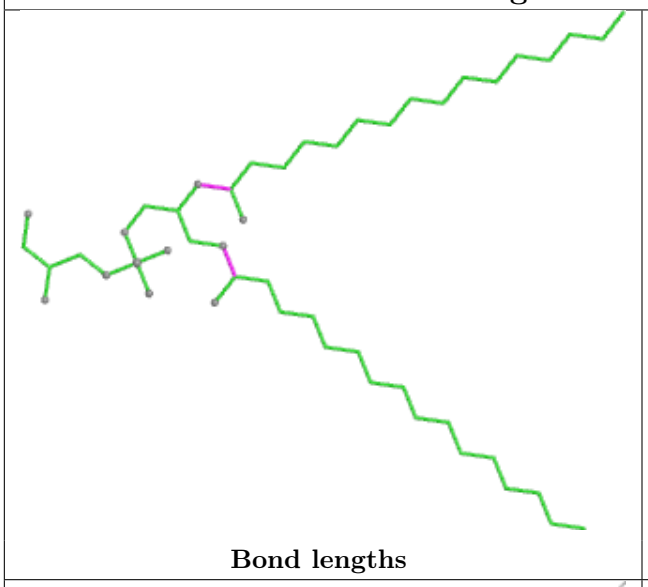


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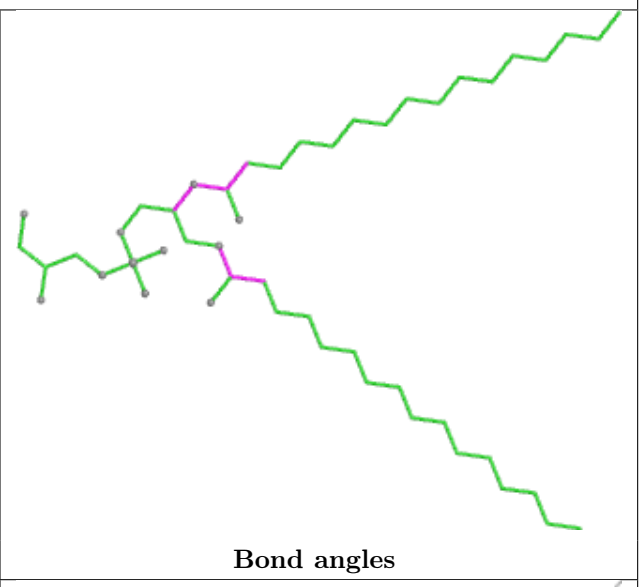


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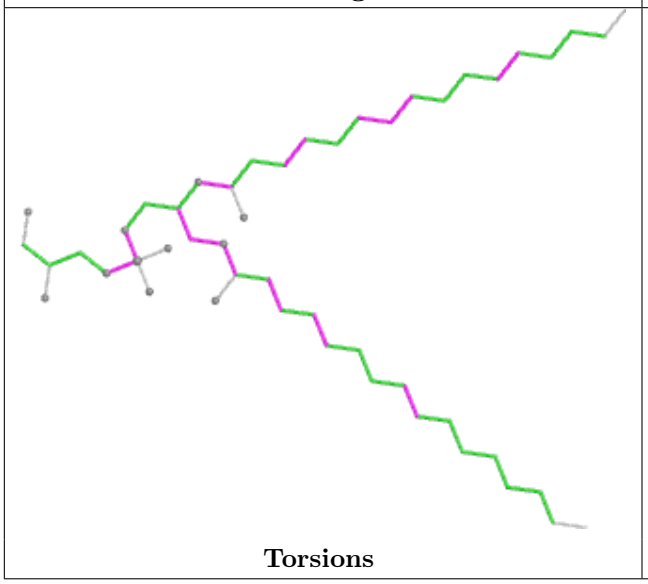
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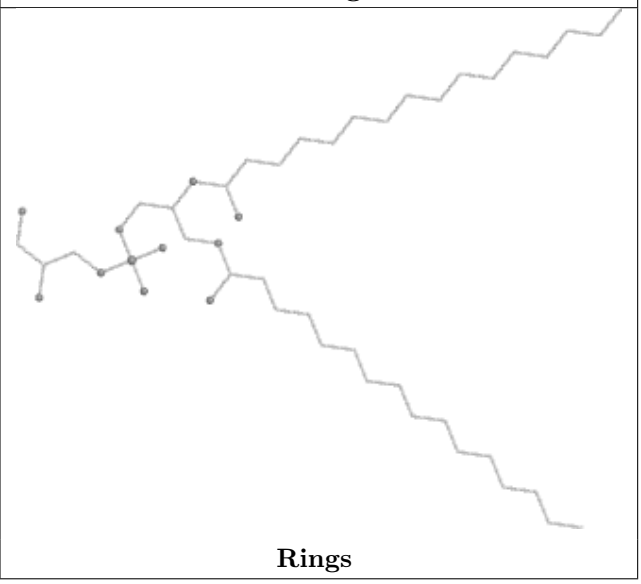
Bond lengths



Bond angles

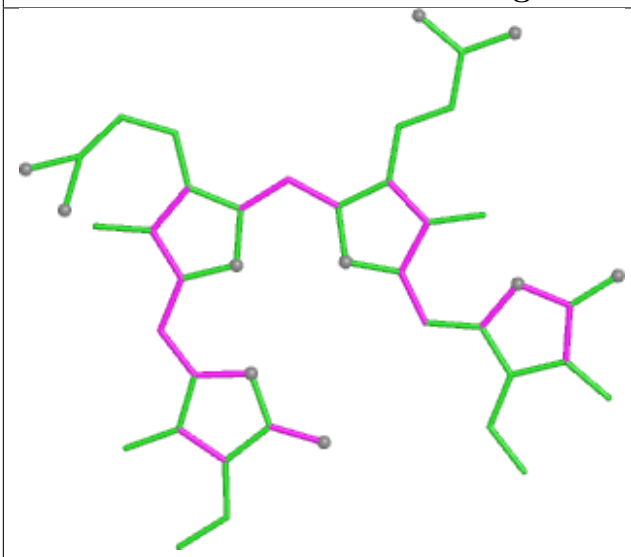


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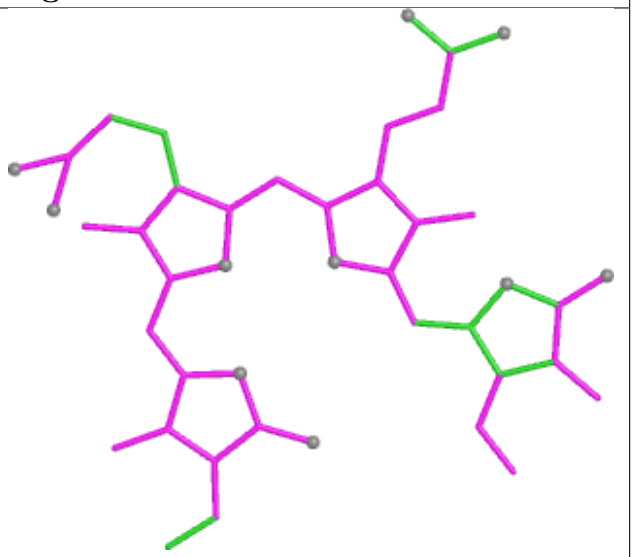


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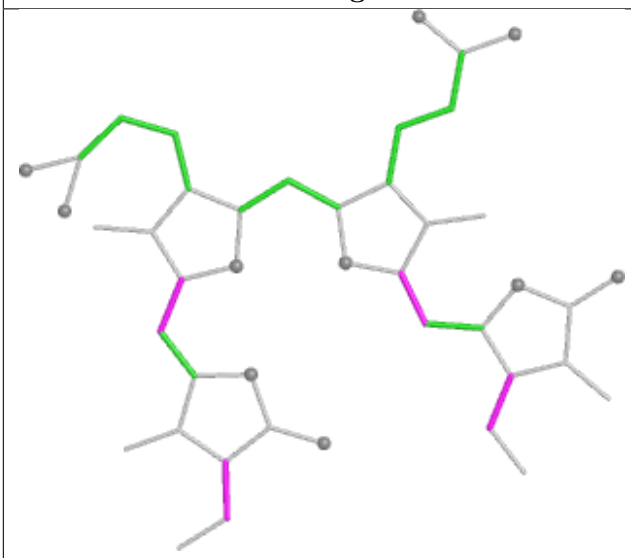
Ligand CYC gC 301



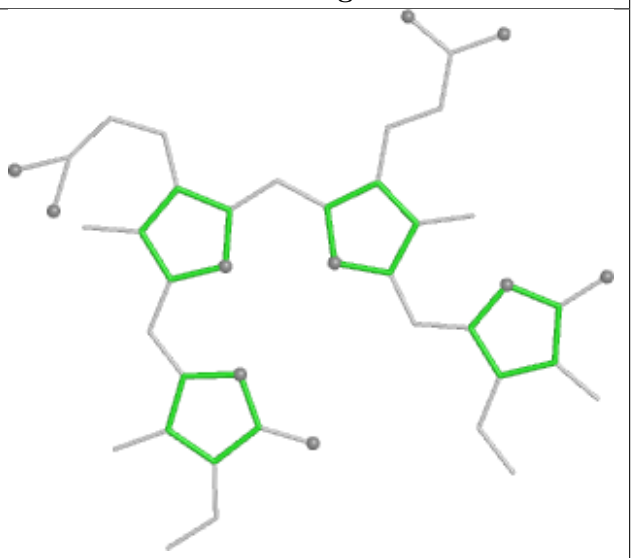
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Bond angles

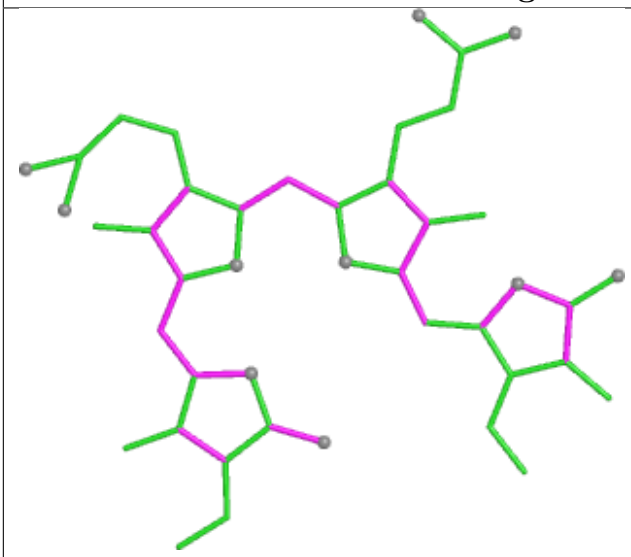


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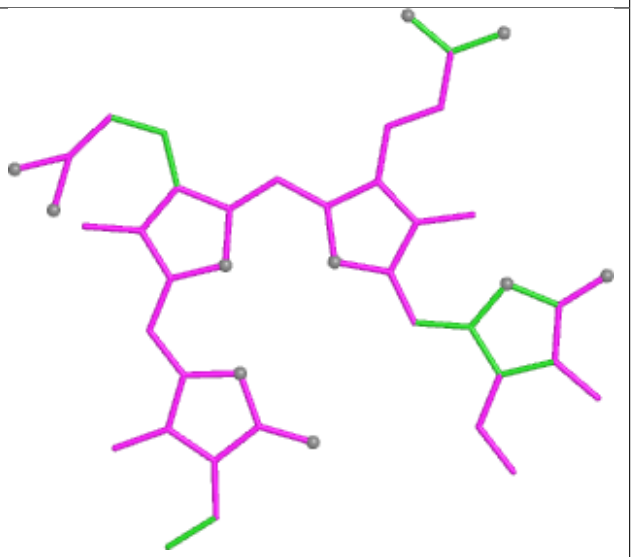


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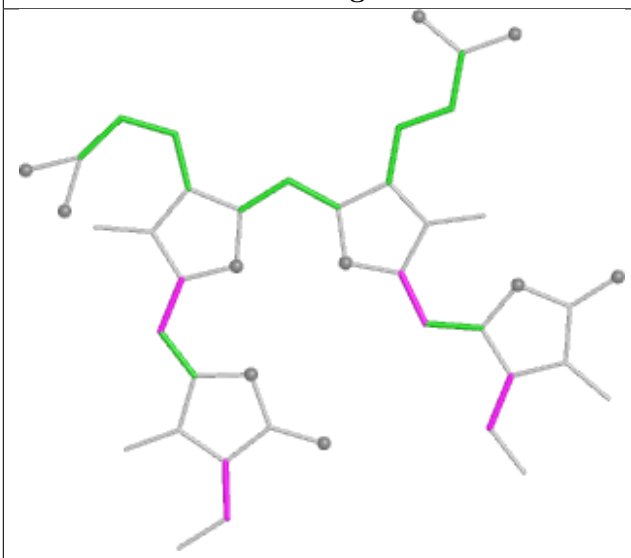
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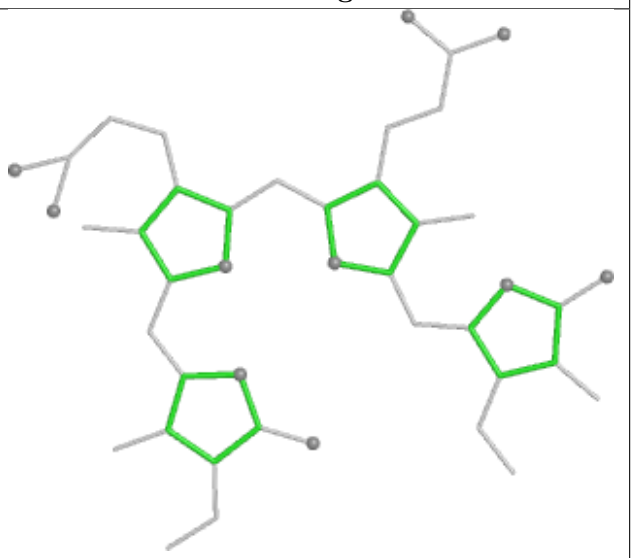
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Bond angles

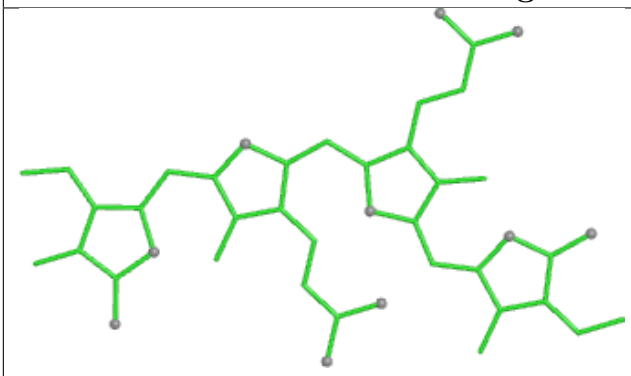


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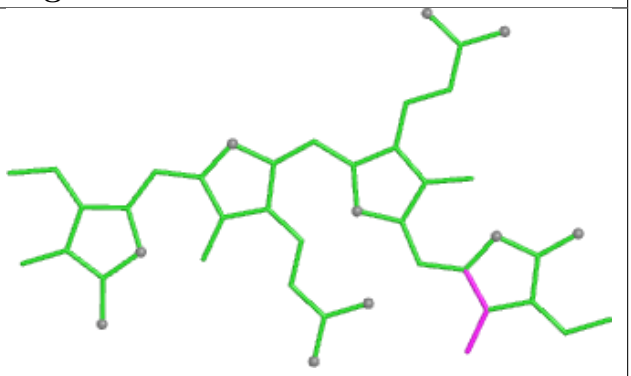


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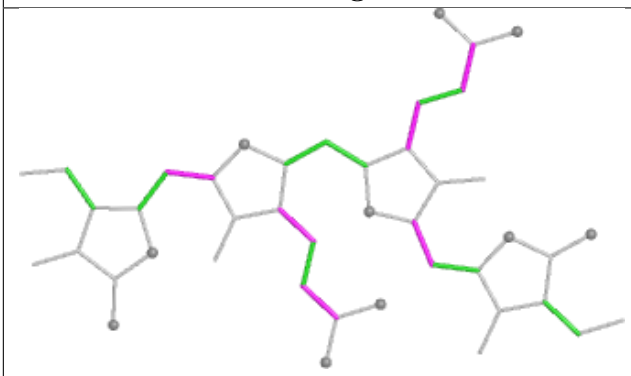
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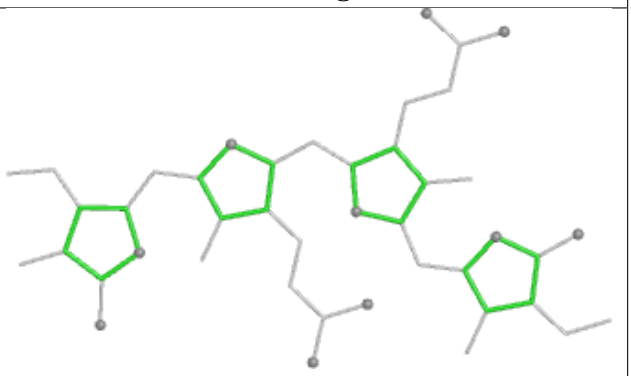
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Bond angles

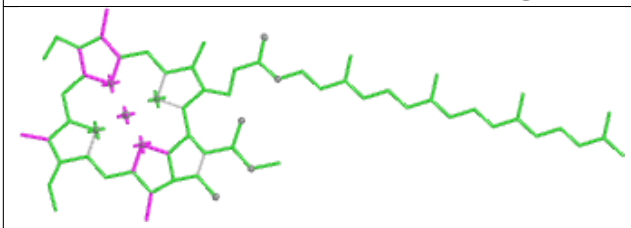


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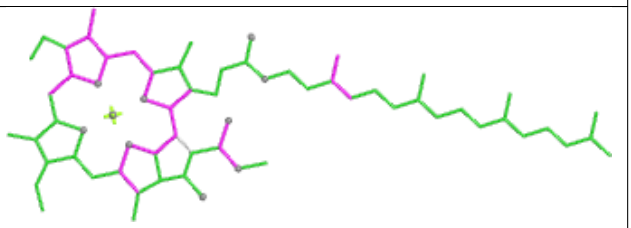


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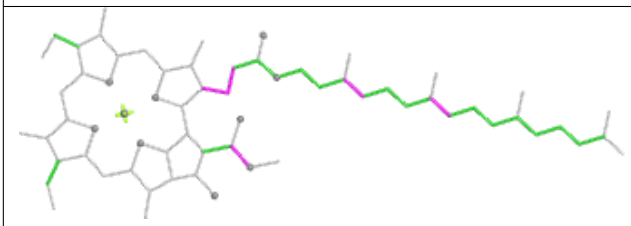
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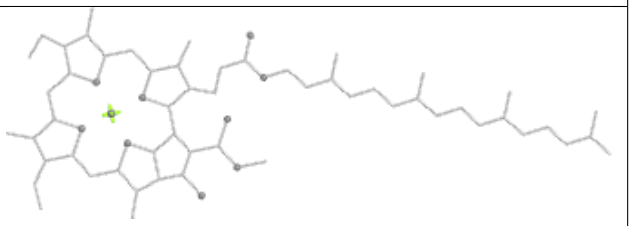
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Bond angles

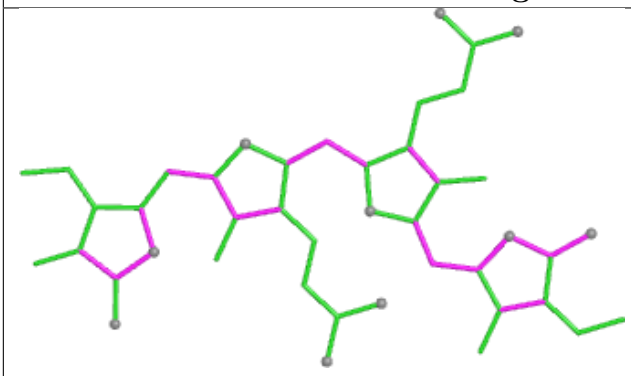


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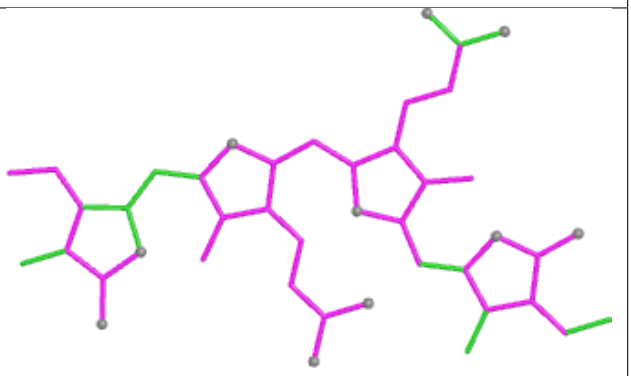


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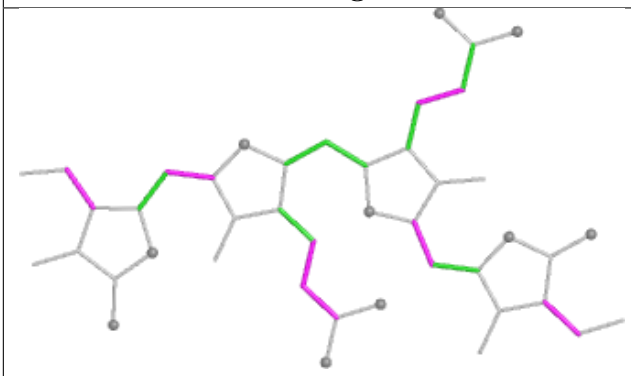
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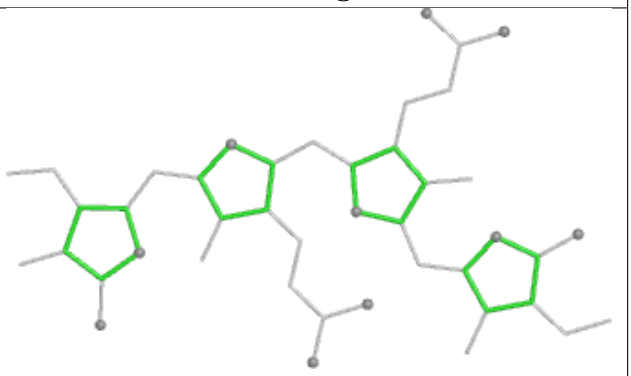
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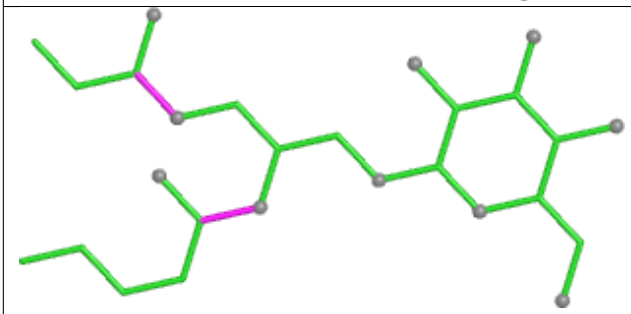


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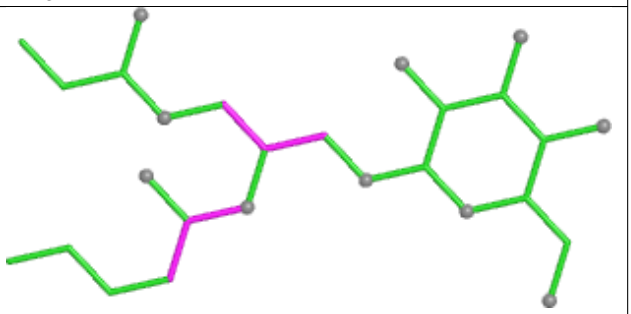


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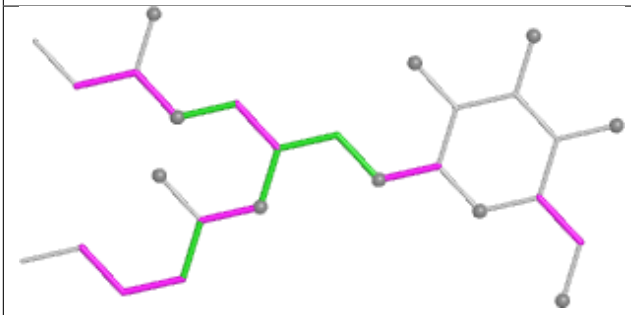
Ligand LMG jE 102



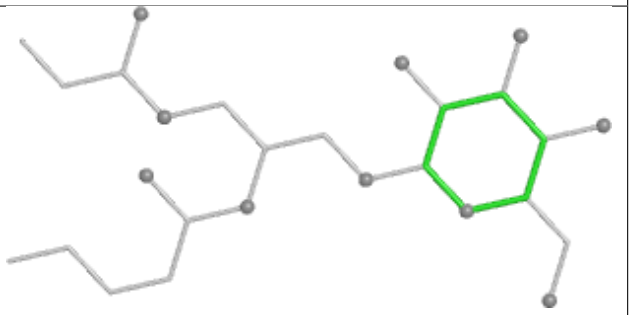
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Bond angles

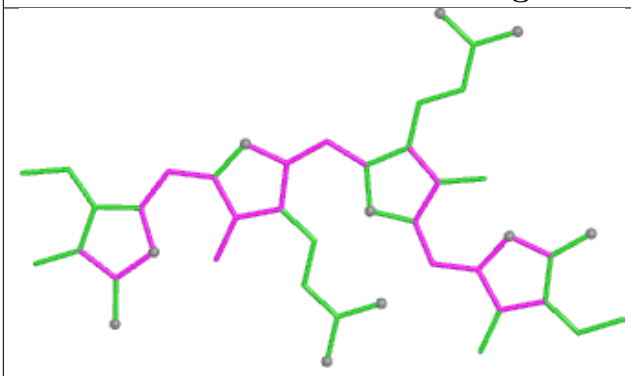


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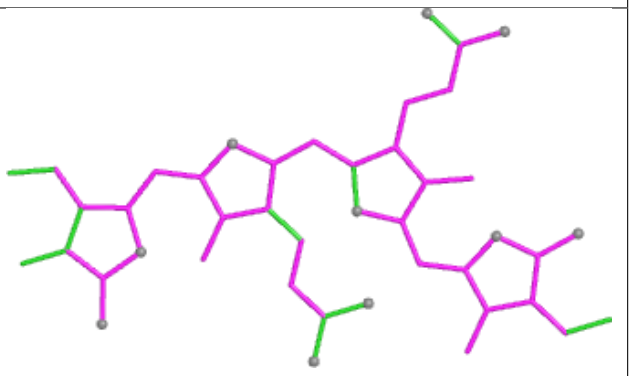


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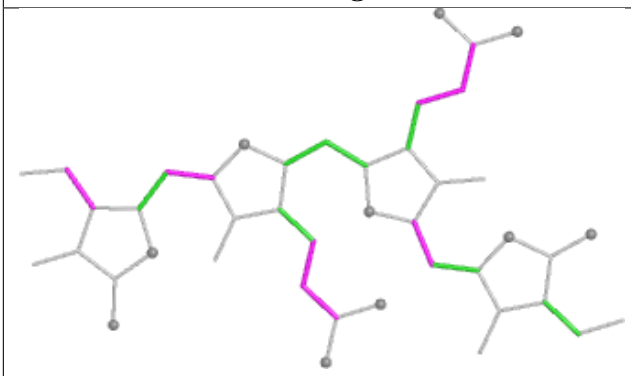
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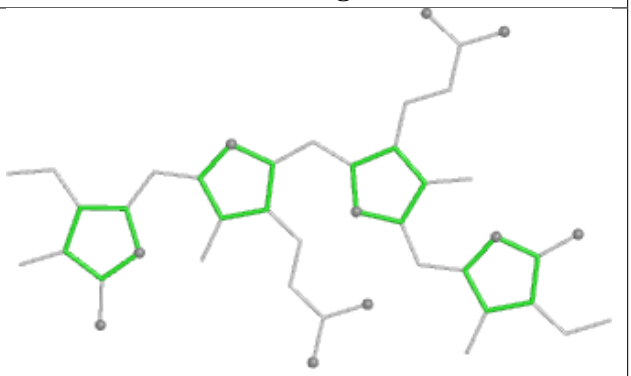
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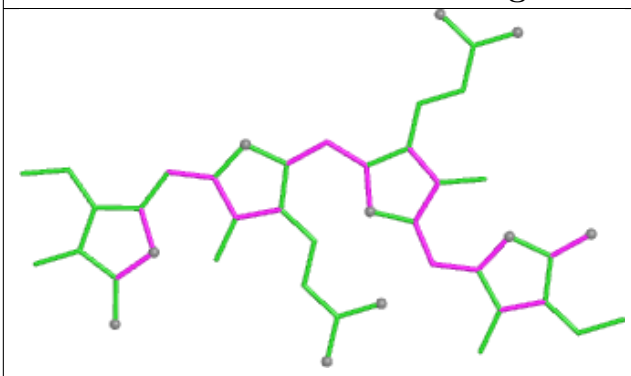


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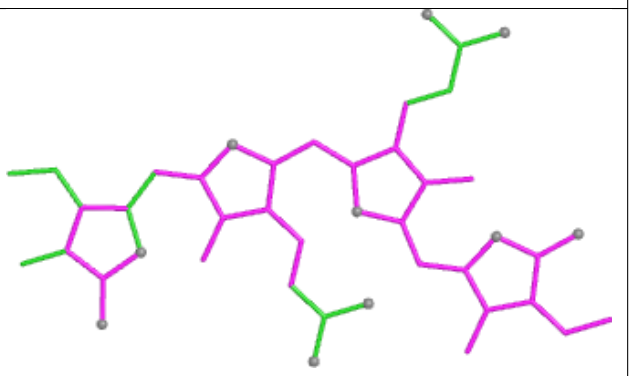


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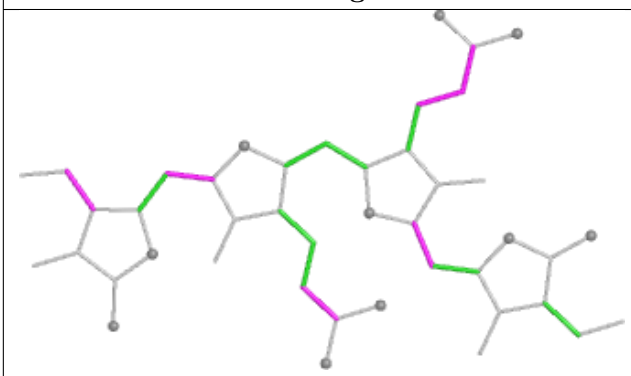
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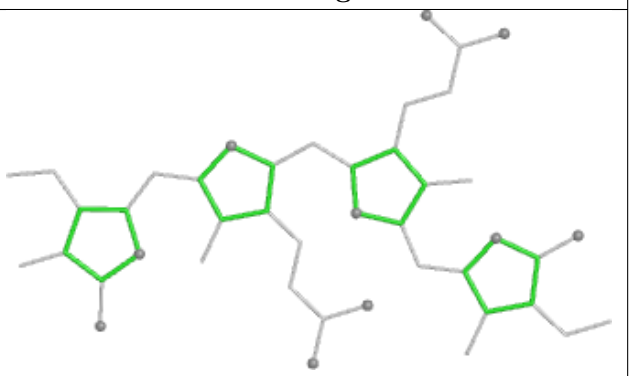
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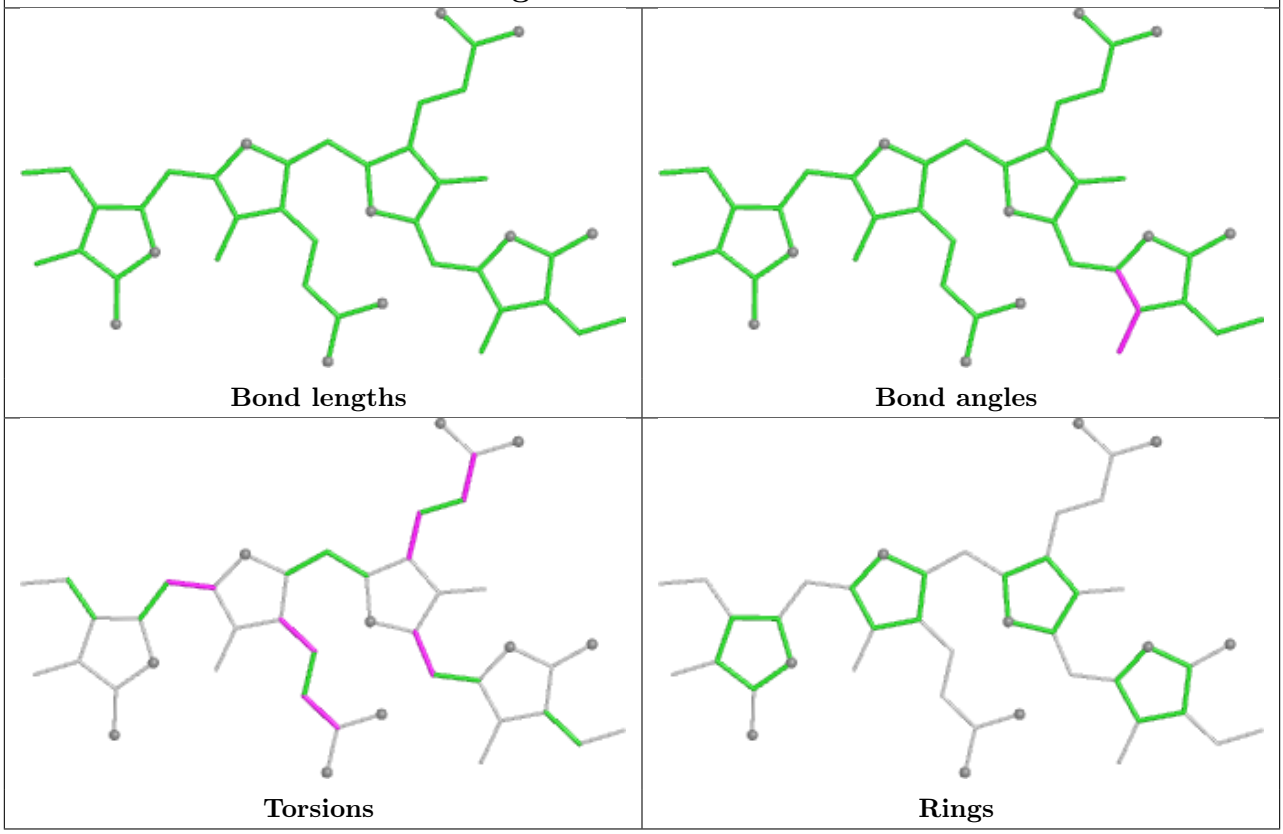


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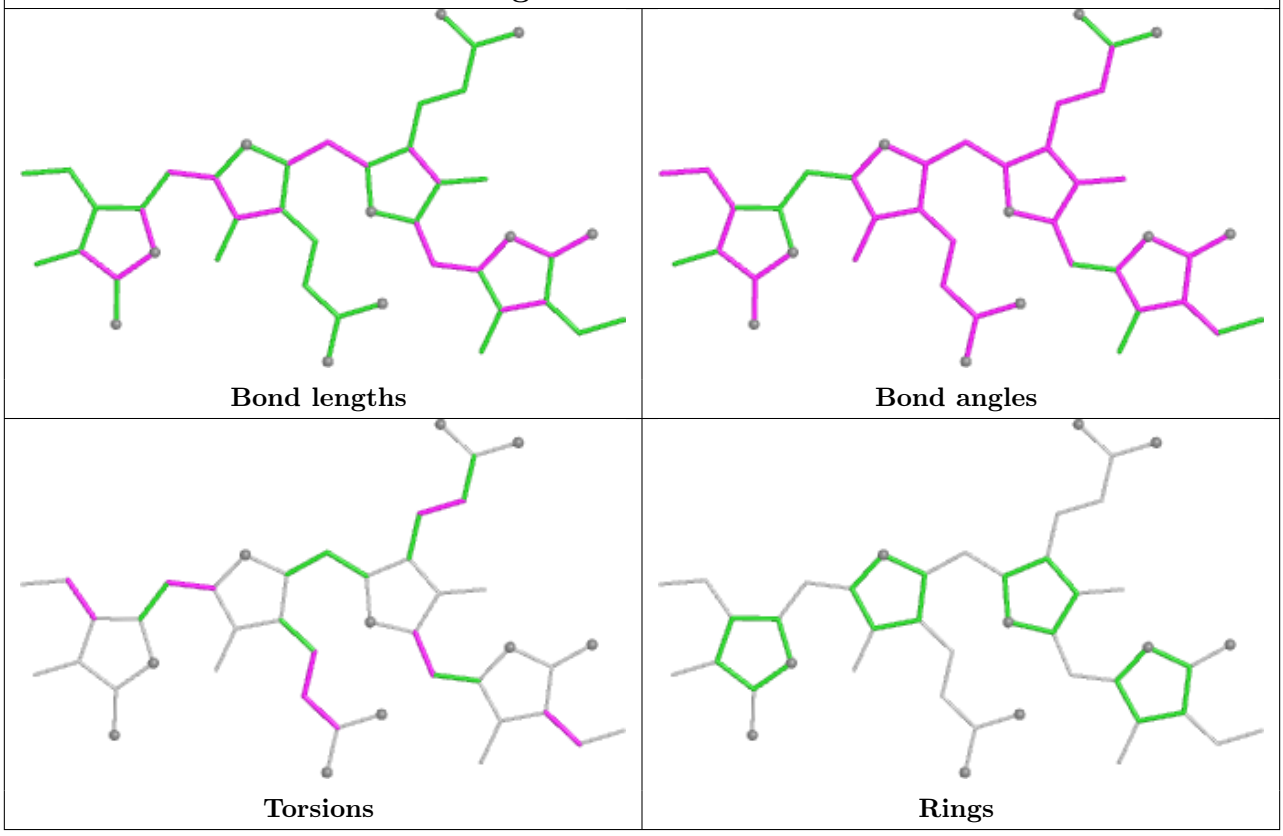


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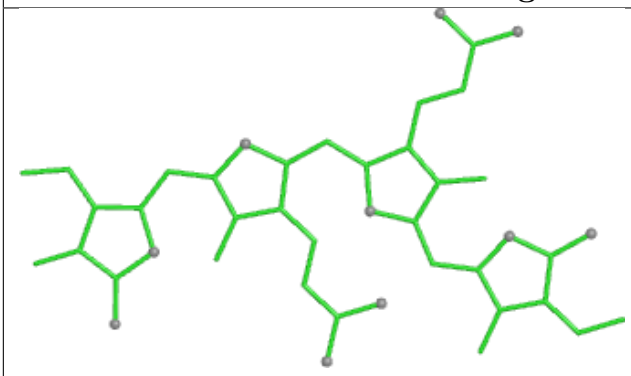
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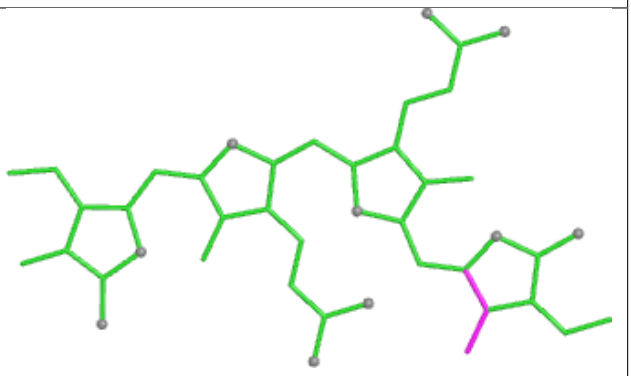
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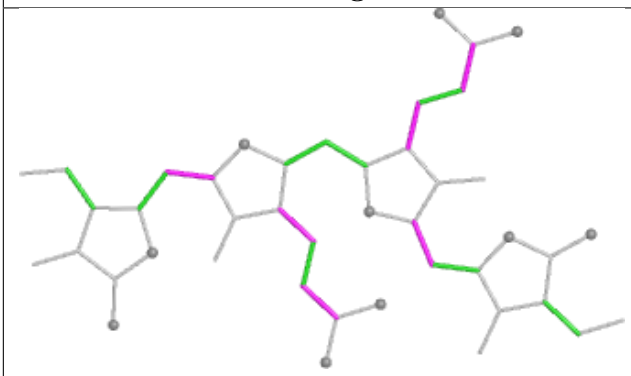
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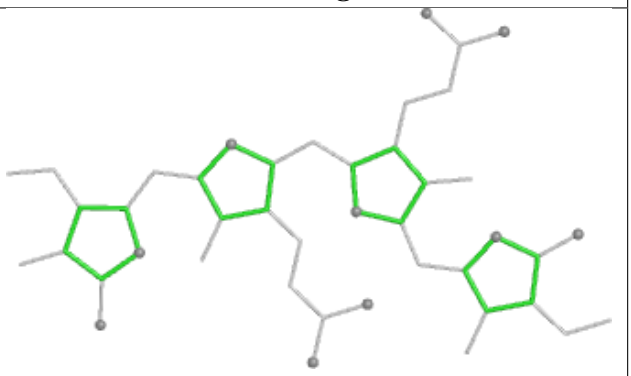
Bond lengths



Bond angles

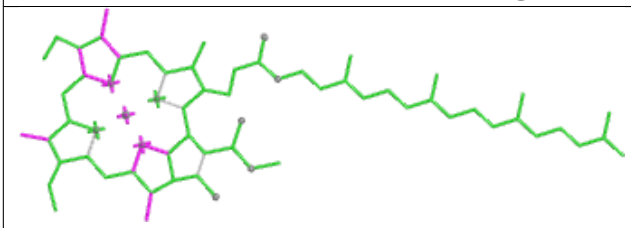


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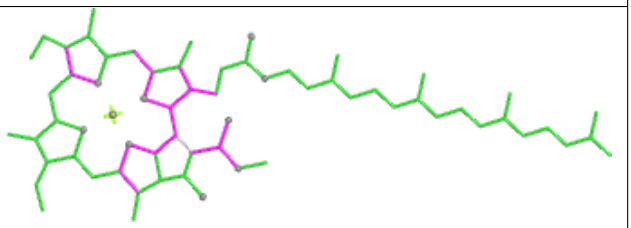


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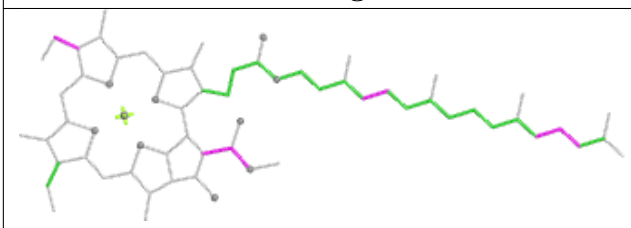
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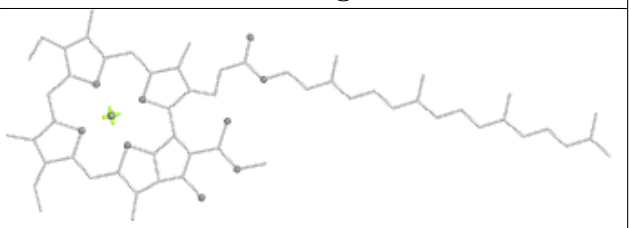
Bond lengths



Bond angles

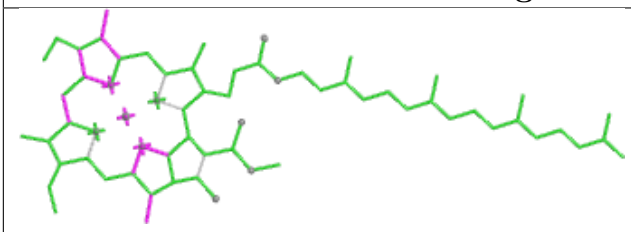


Torsions

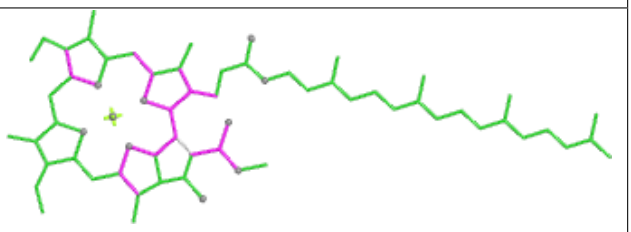


Rings

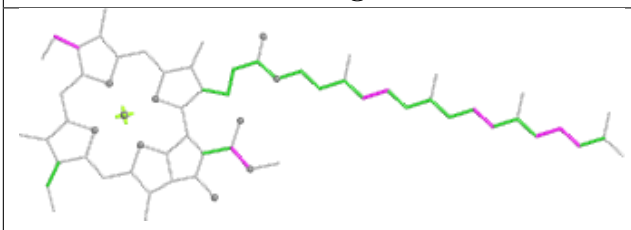
Ligand CLA cD 505



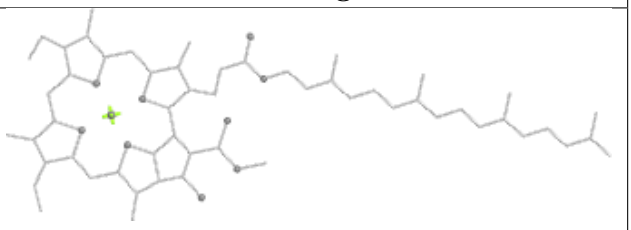
Bond lengths



Bond angles

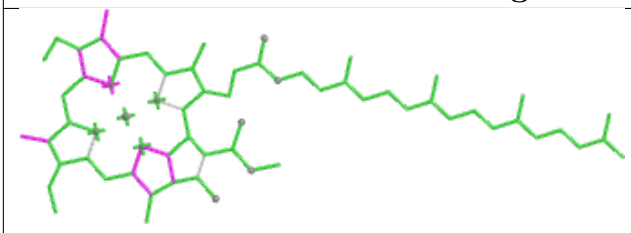


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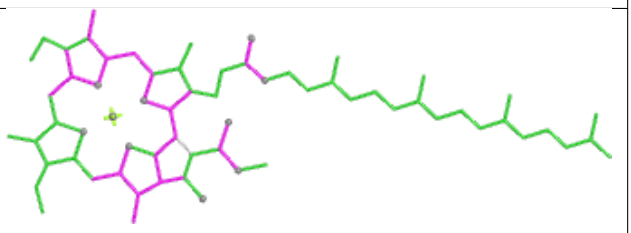


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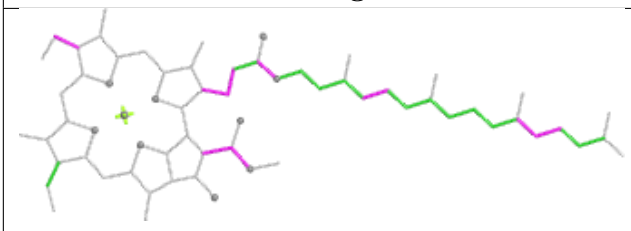
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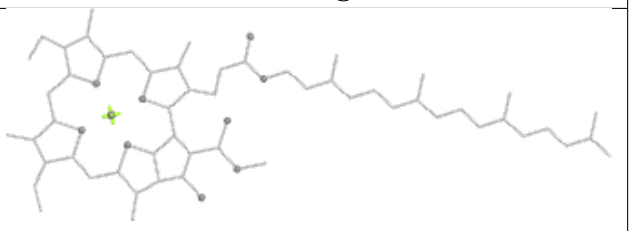
Bond lengths



Bond angles

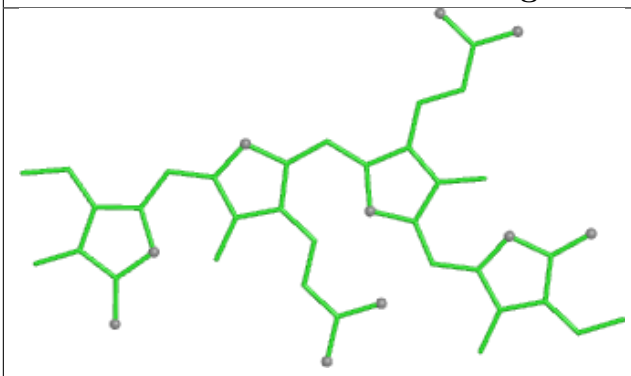


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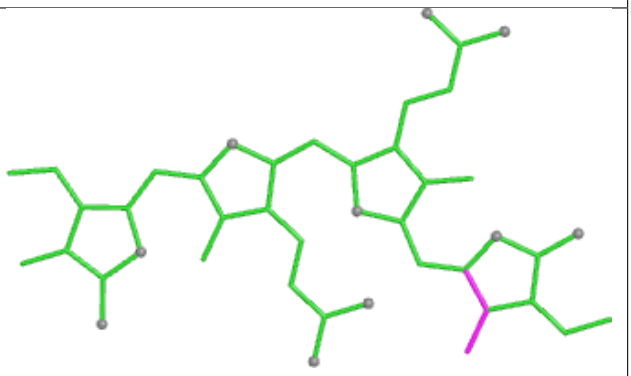


Rings

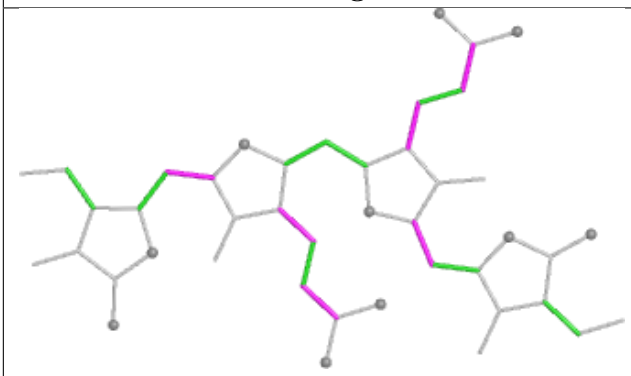
Ligand CYC eI 202



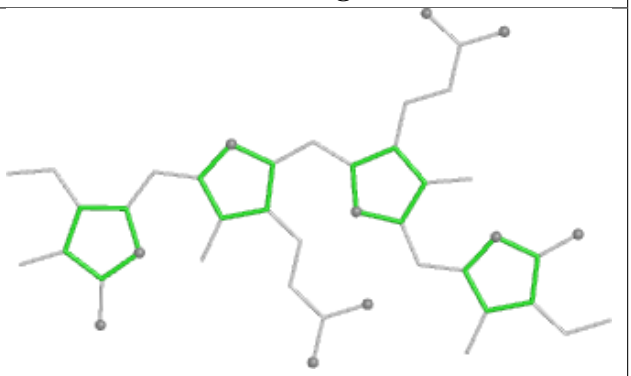
Bond lengths



Bond angles

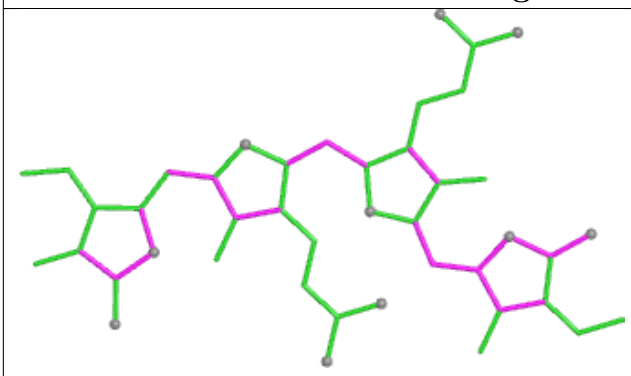


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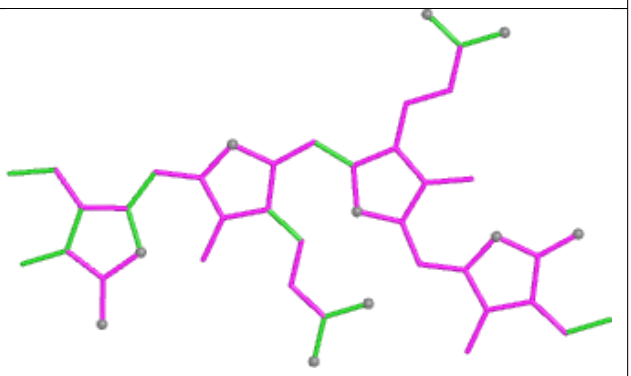


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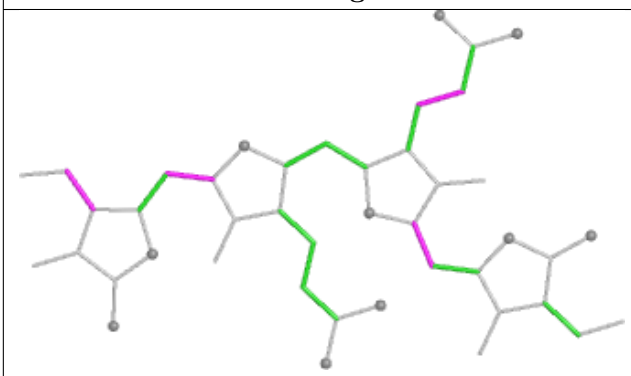
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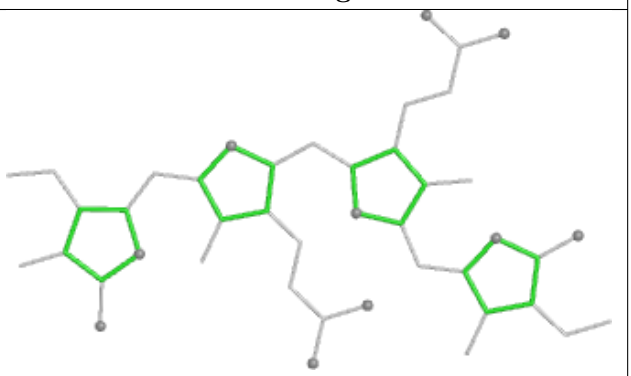
Bond lengths



Bond angles

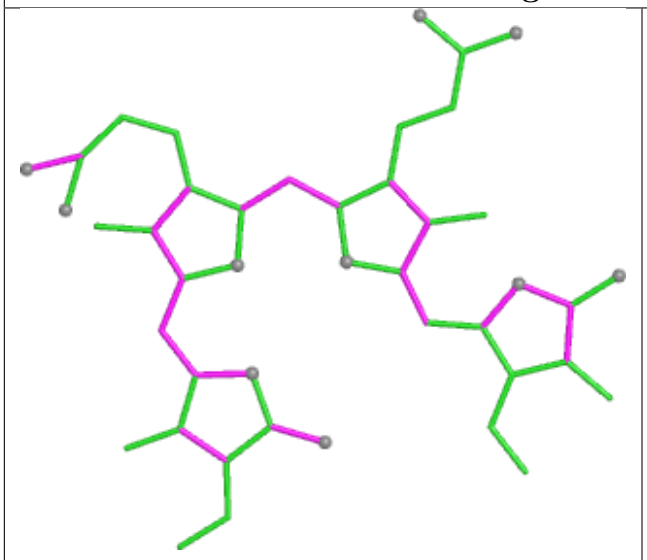


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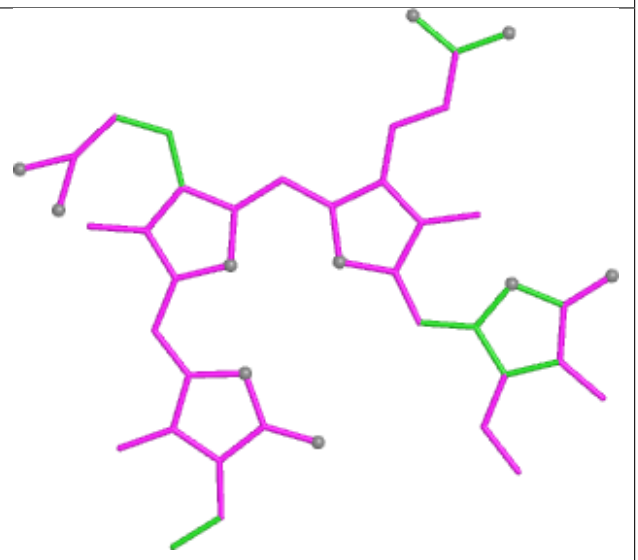


Rings

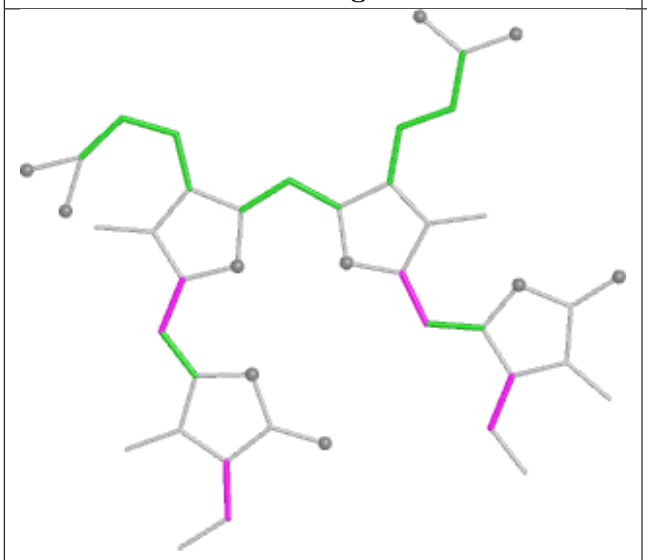
Ligand CYC i9 202



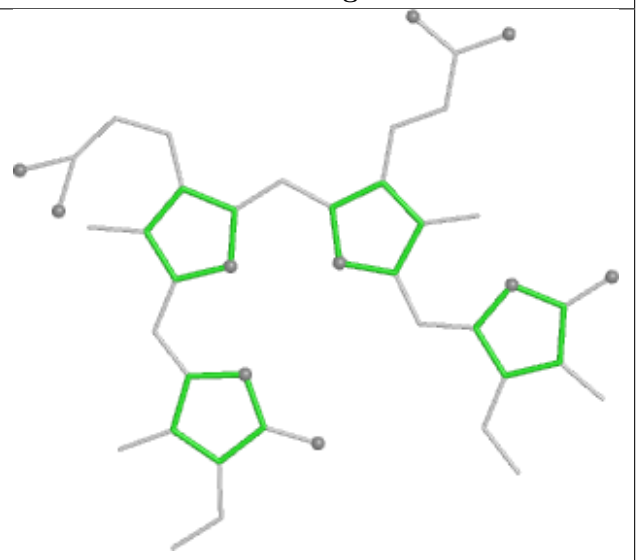
Bond lengths



Bond angles

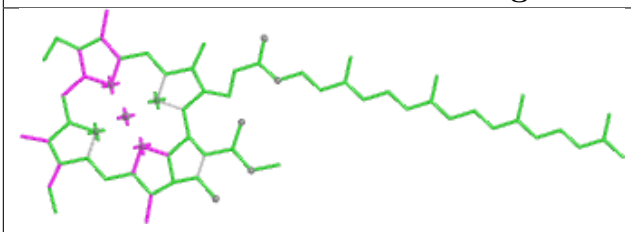


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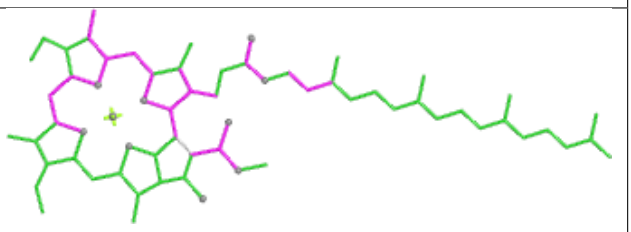


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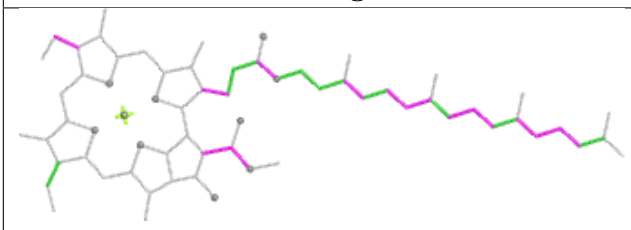
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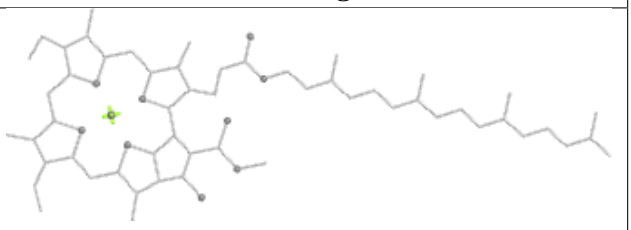
Bond lengths



Bond angles

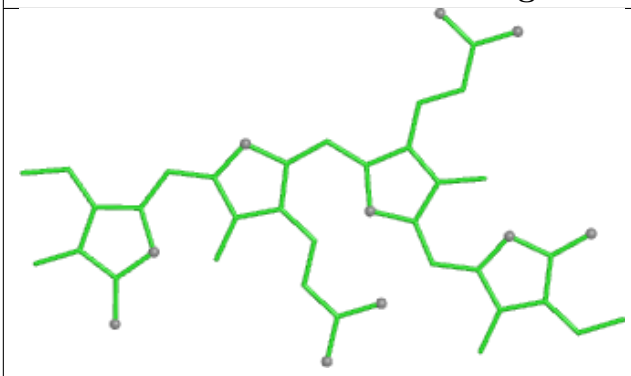


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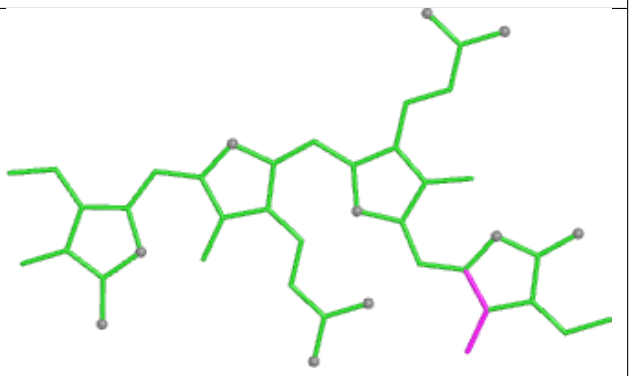


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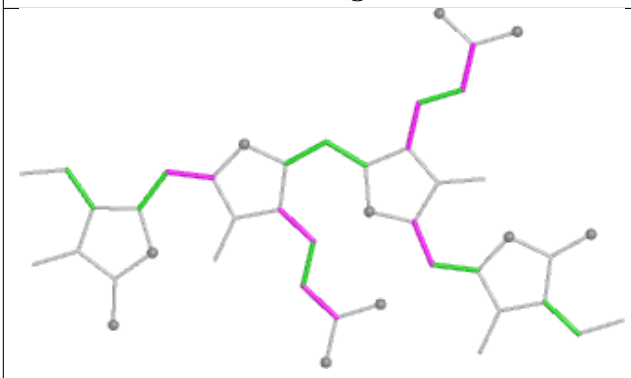
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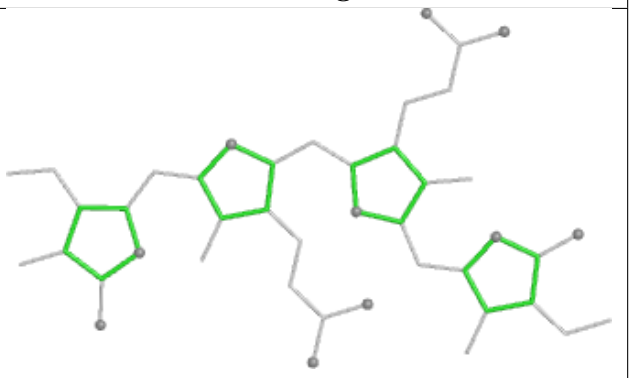
Bond lengths



Bond angles

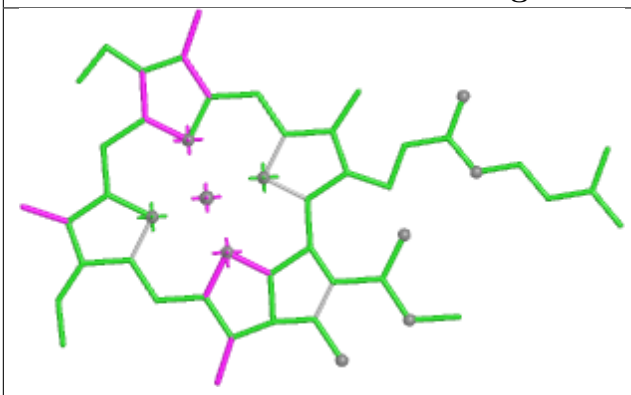


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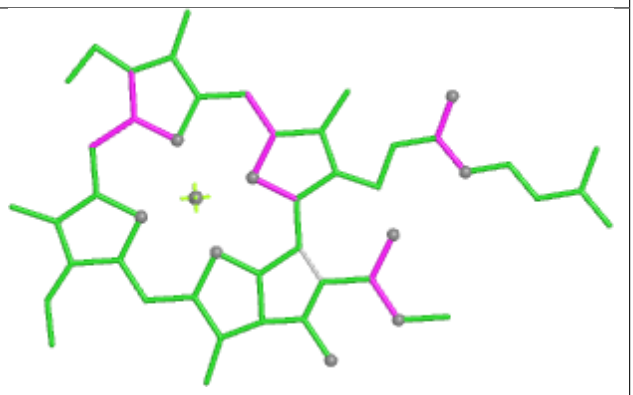


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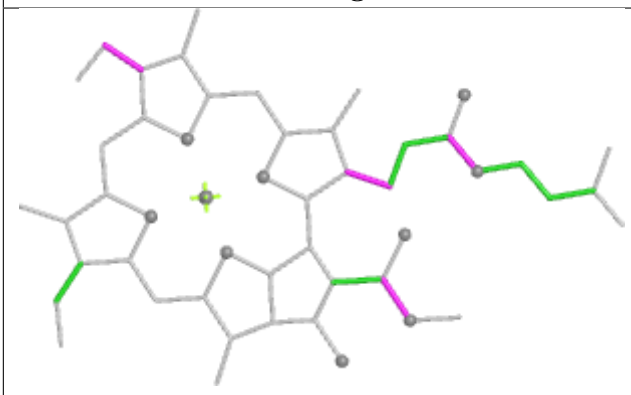
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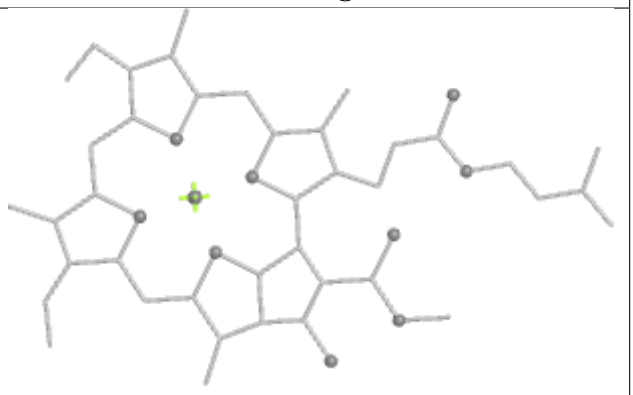
Bond lengths



Bond angles



Torsions

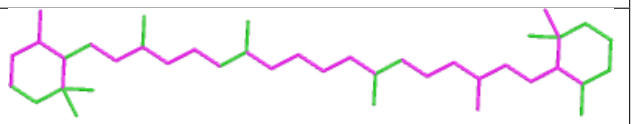


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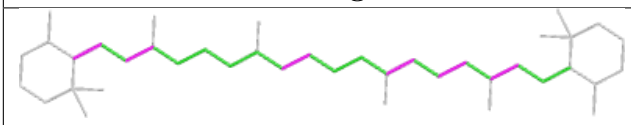
Ligand BCR I1 102



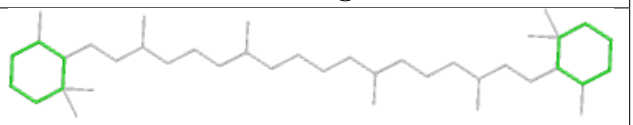
Bond lengths



Bond angles

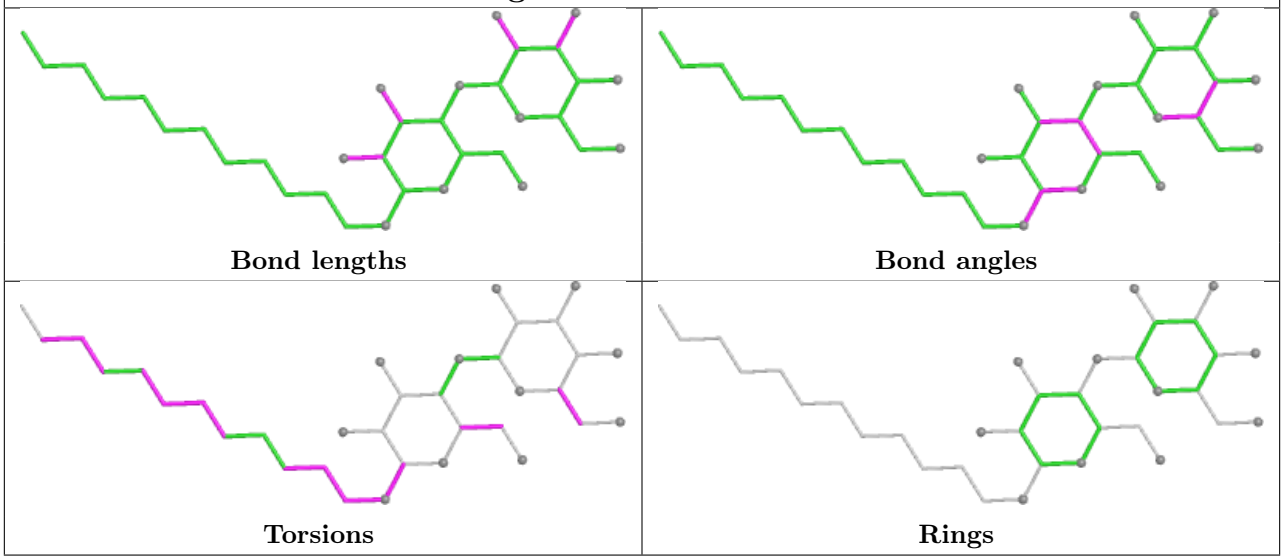


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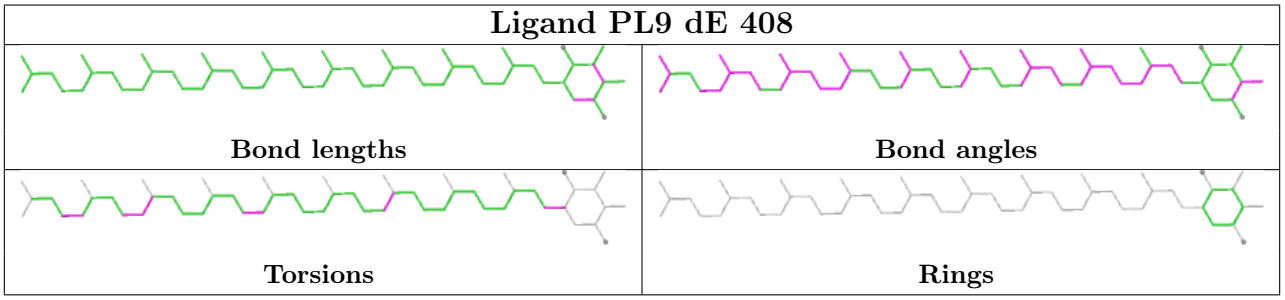


Rings

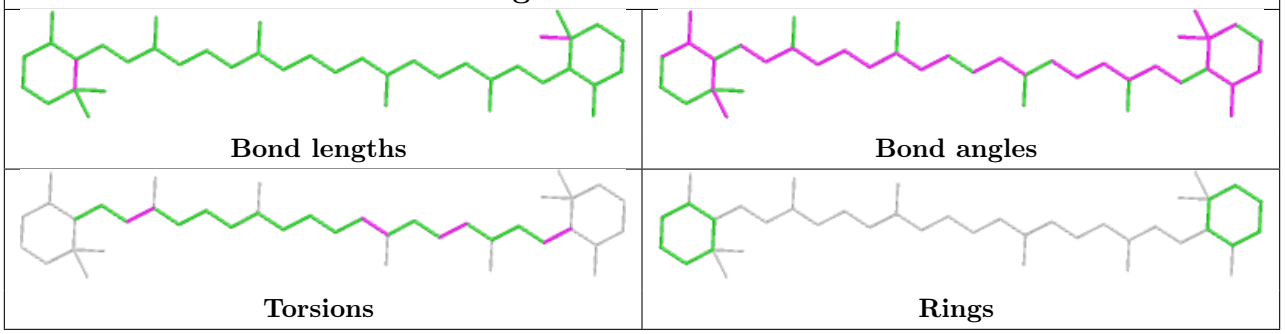
Ligand LMT AD 412



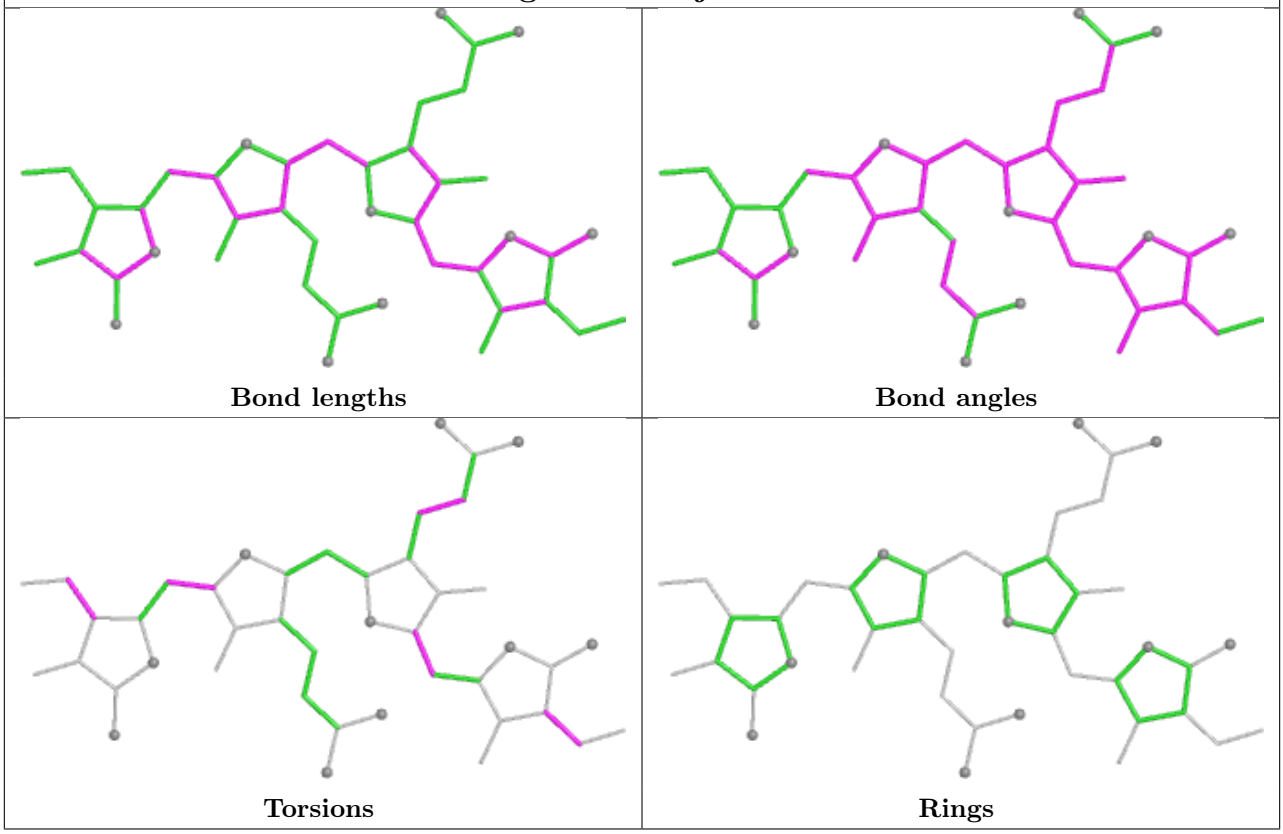
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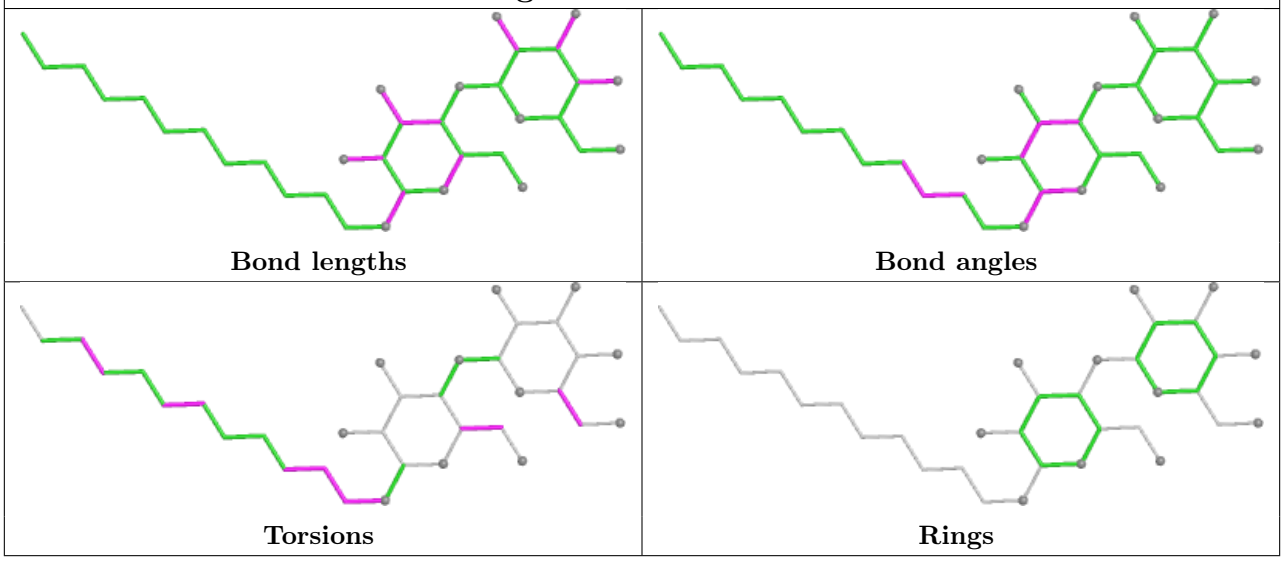
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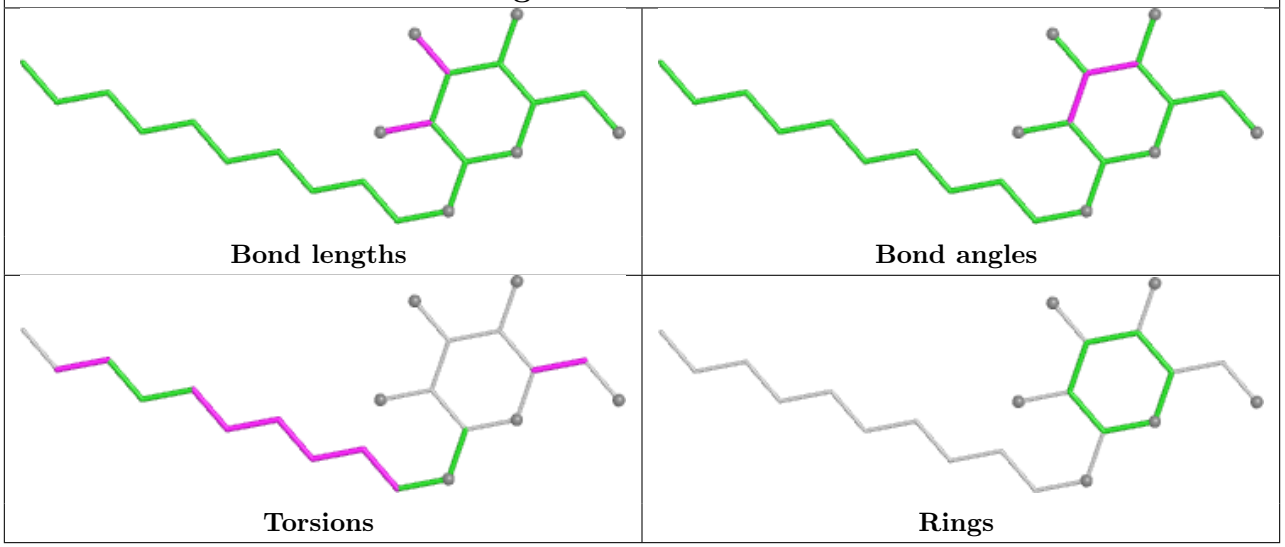
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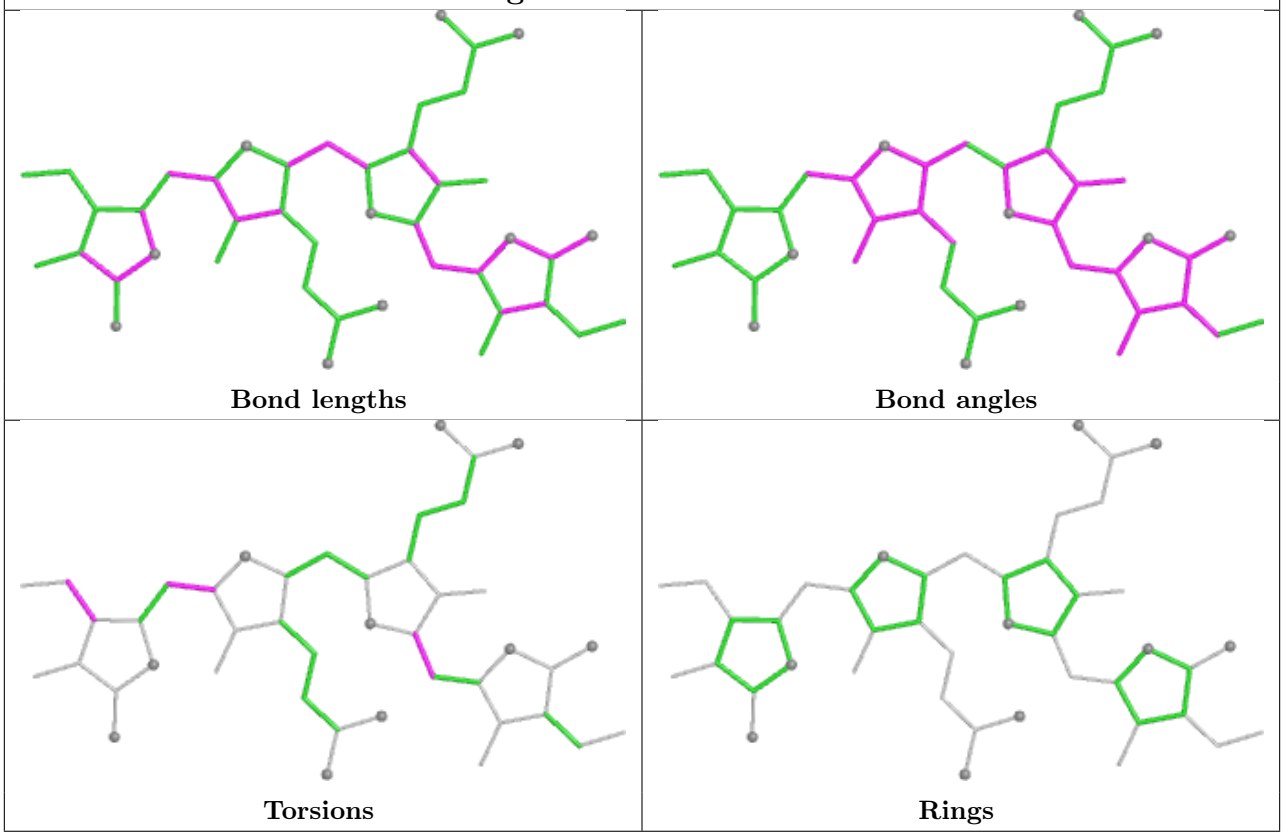
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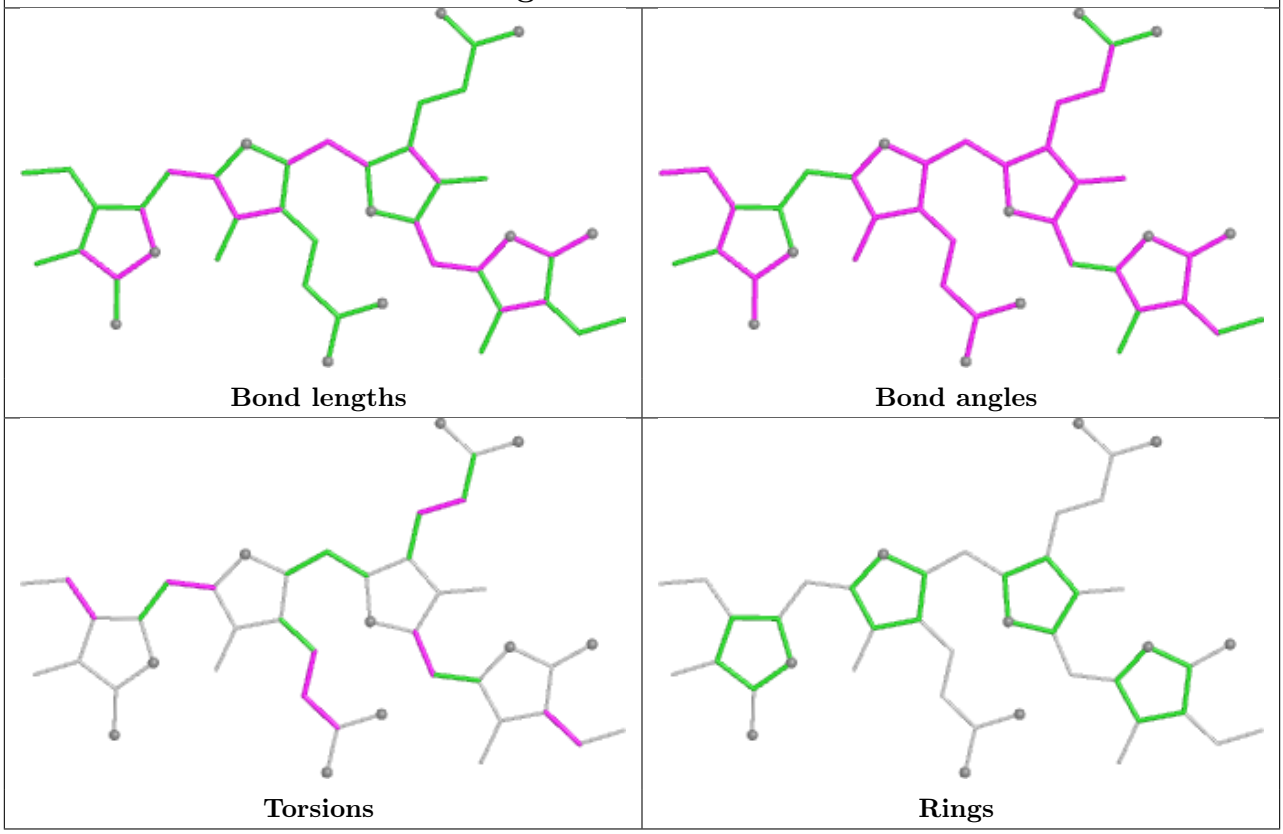
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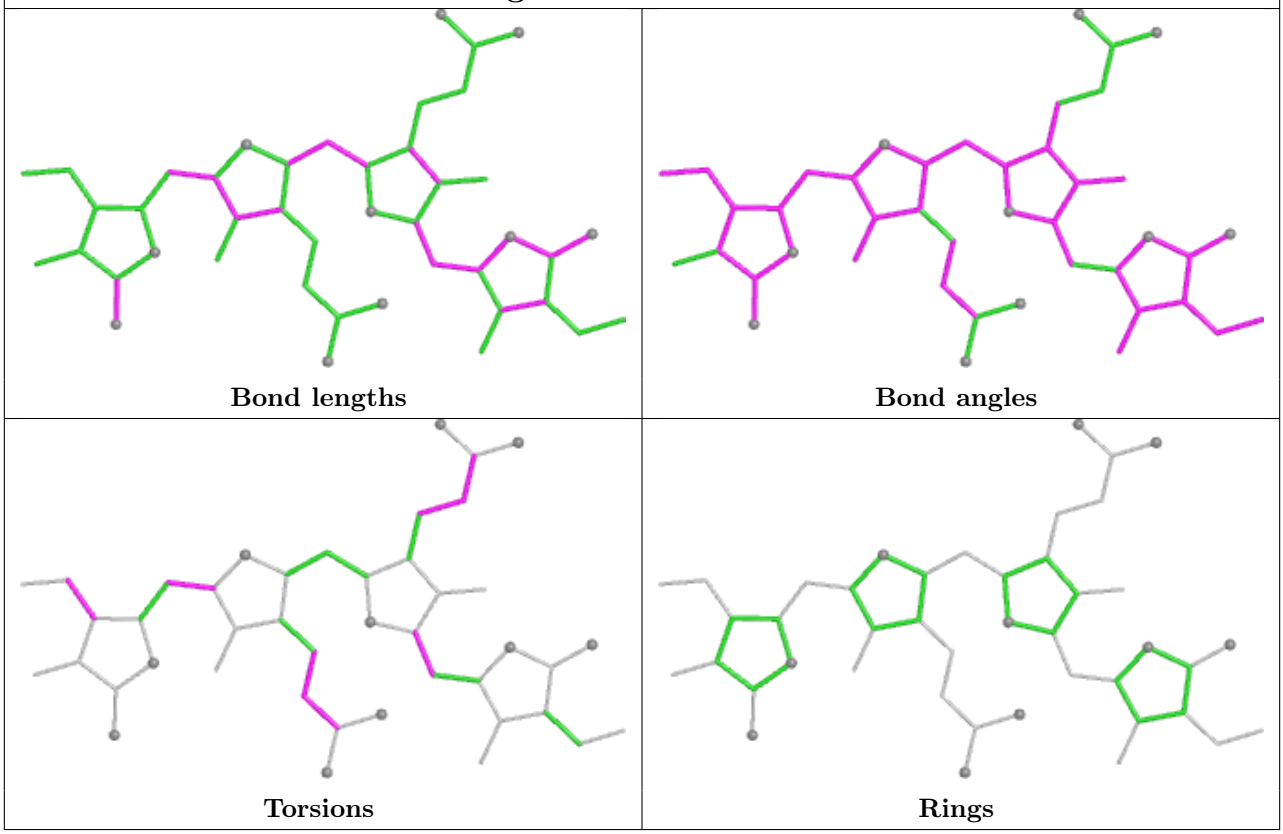
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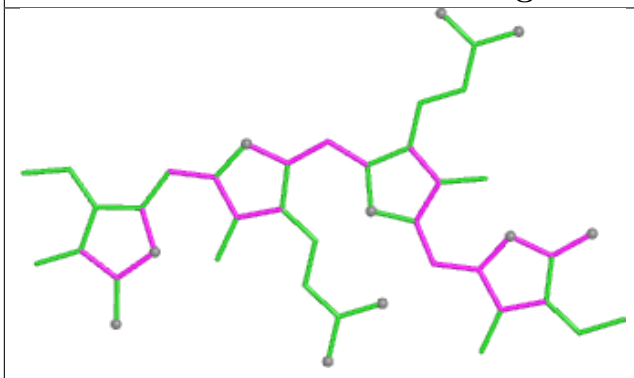
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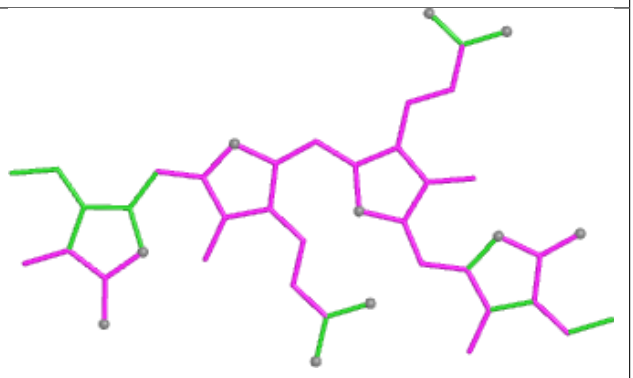
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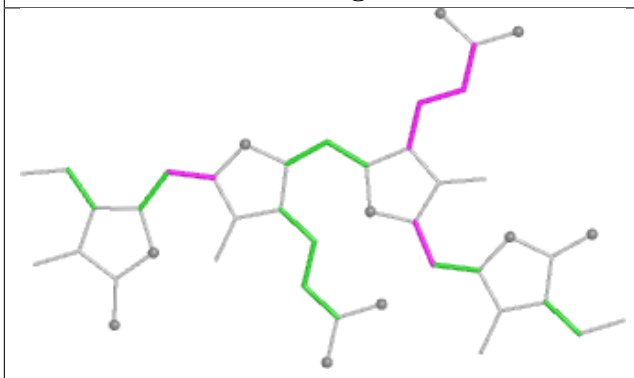
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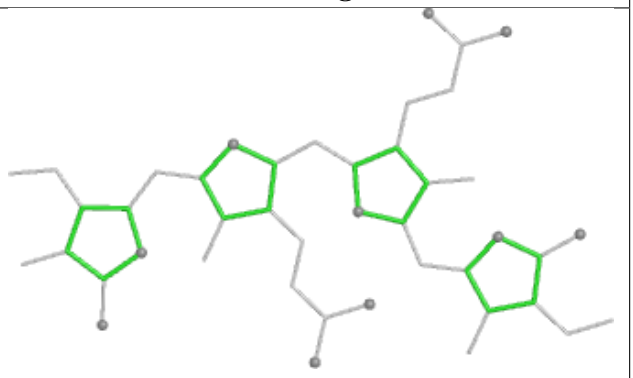
Bond lengths



Bond angles

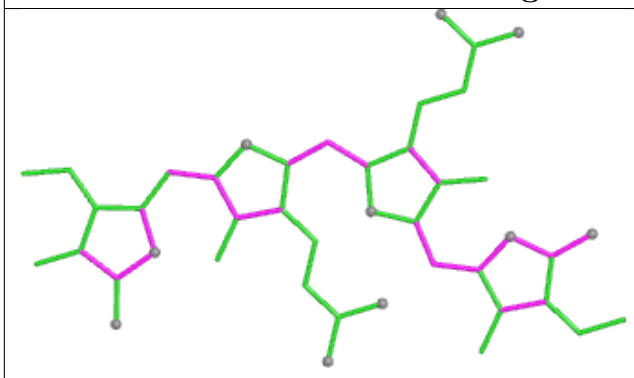


Torsions

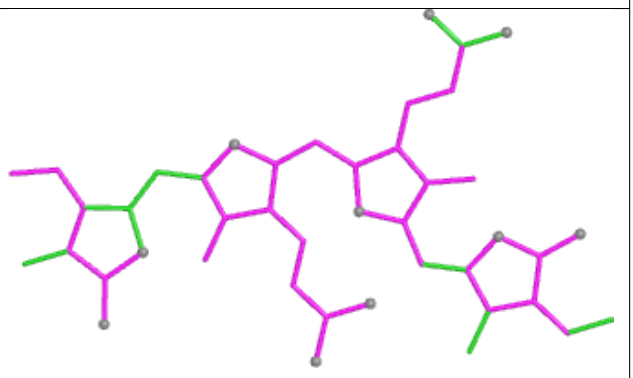


Rings

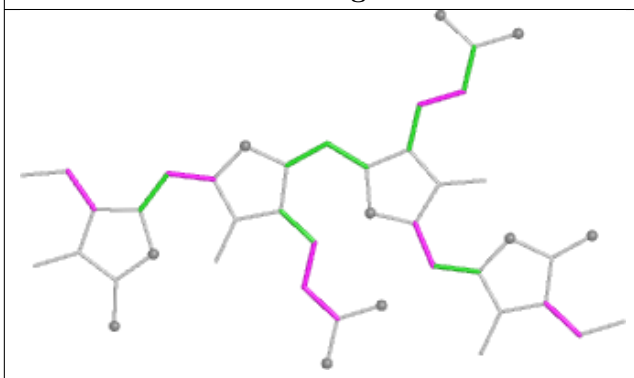
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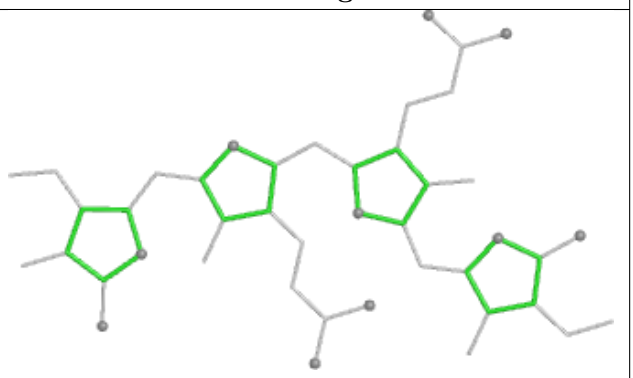
Bond lengths



Bond angles

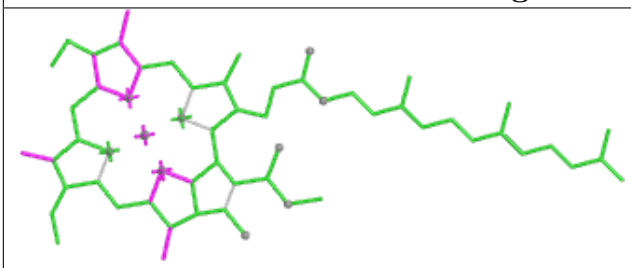


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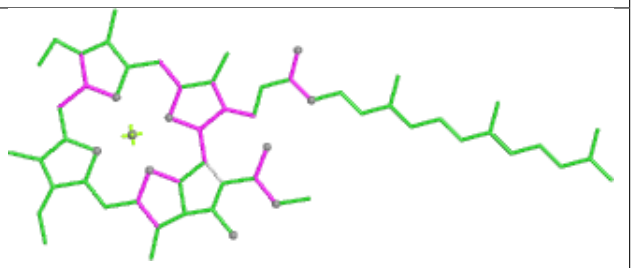


Rings

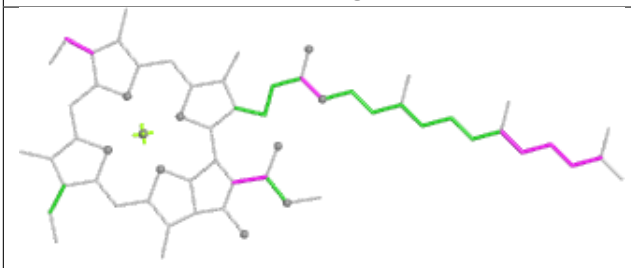
Ligand CLA HE 101



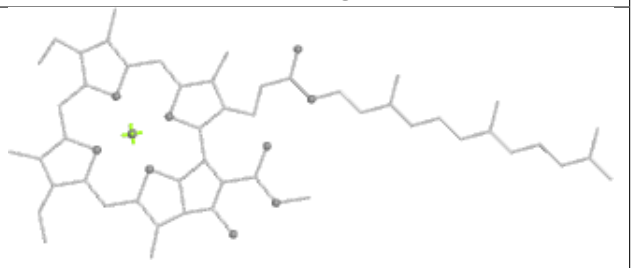
Bond lengths



Bond angles

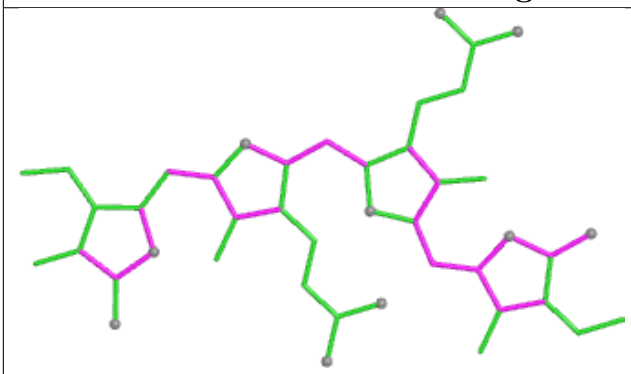


Torsions

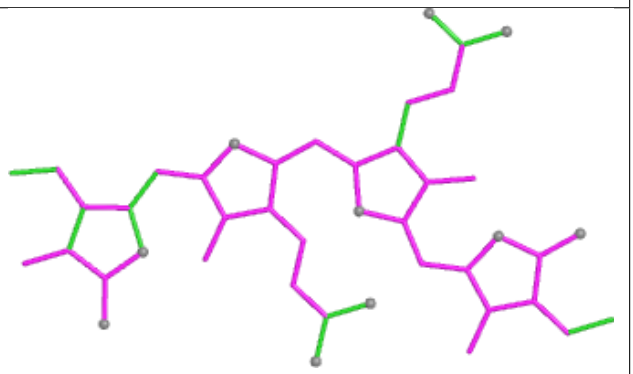


Rings

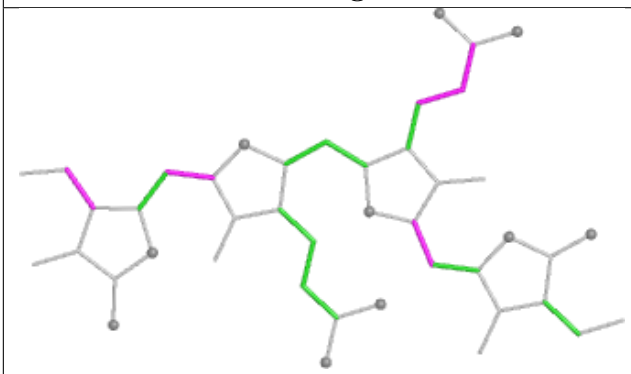
Ligand CYC 2L 201



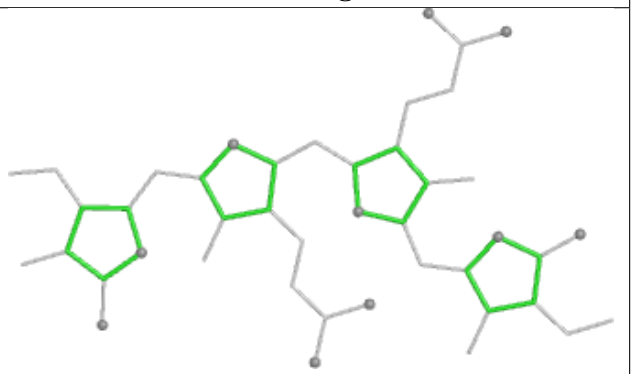
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Bond angles

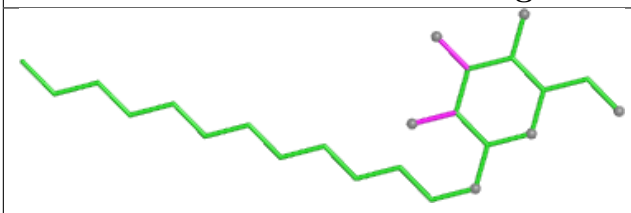


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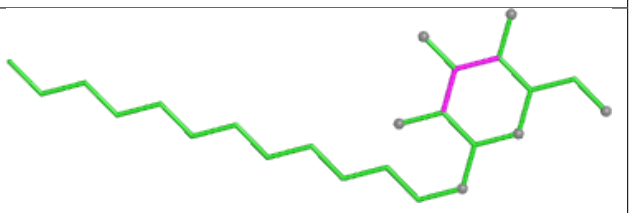


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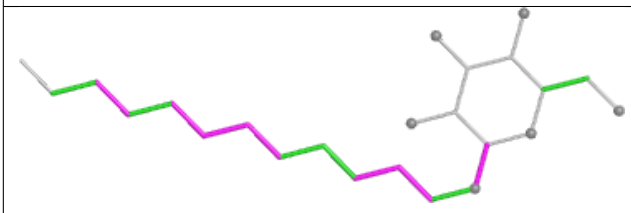
Ligand LMT d1 404



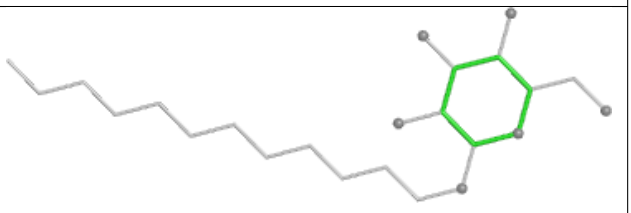
Bond lengths



Bond angles

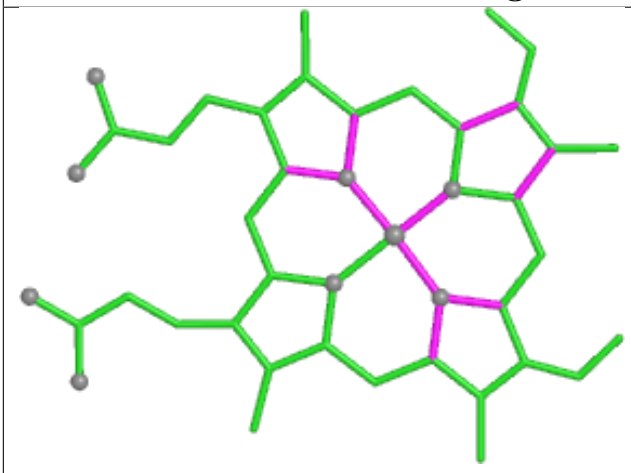


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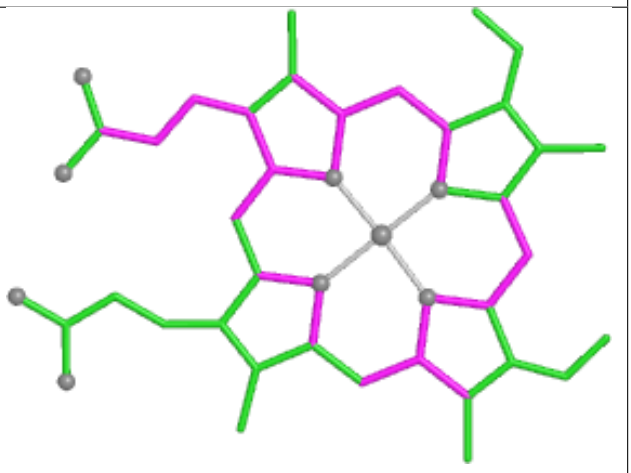


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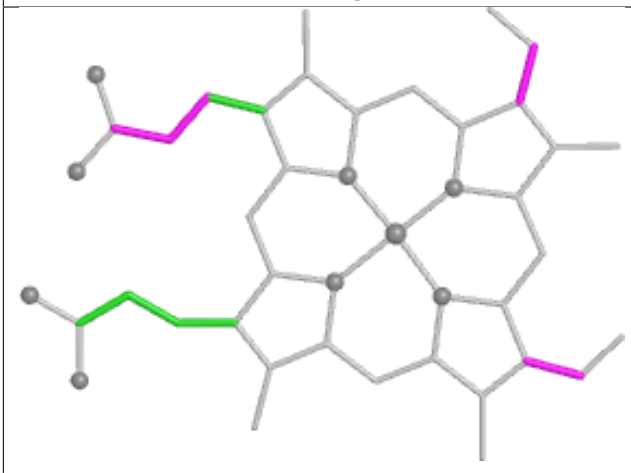
Ligand HEM VE 201



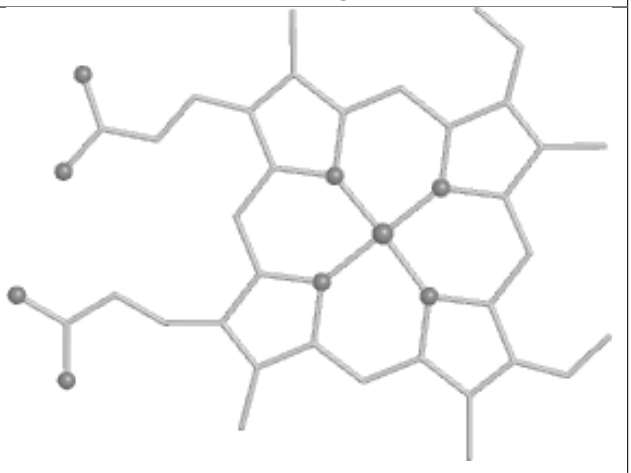
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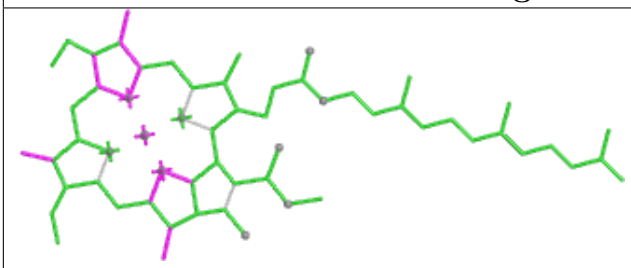
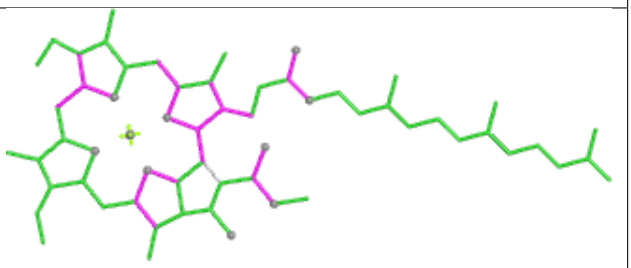
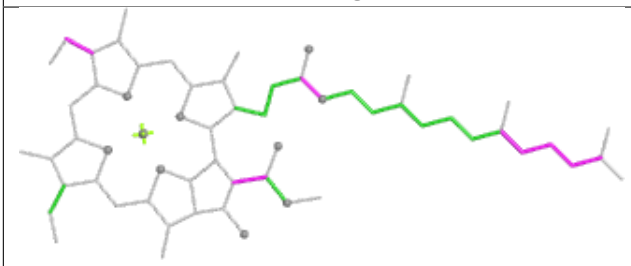
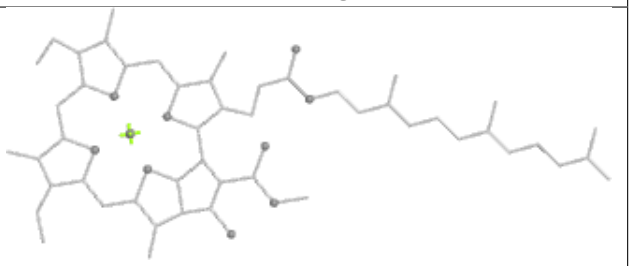
Bond angles

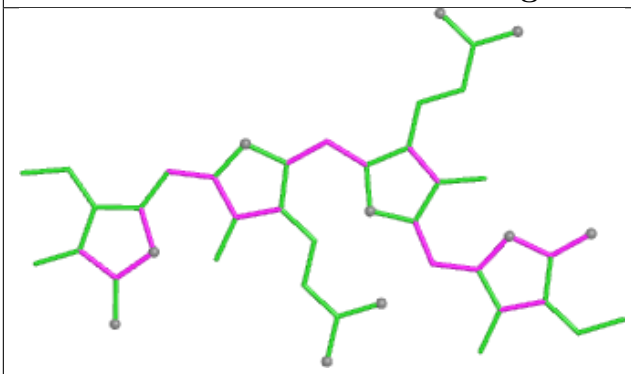
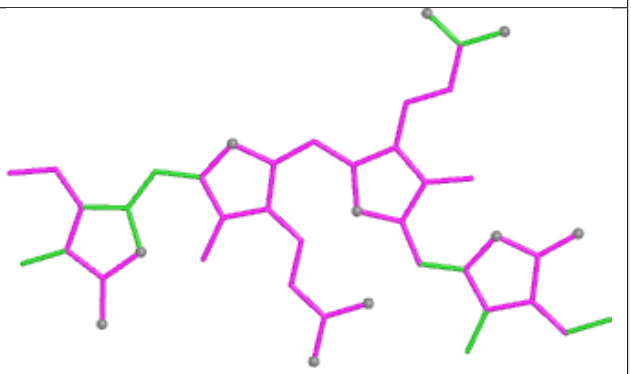
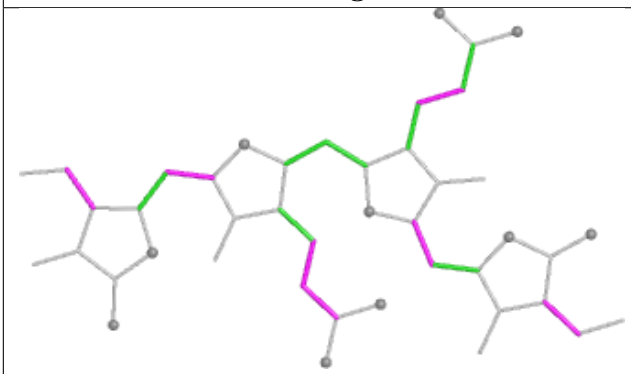
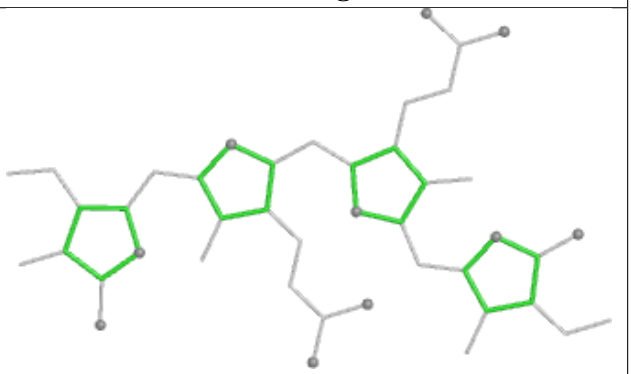


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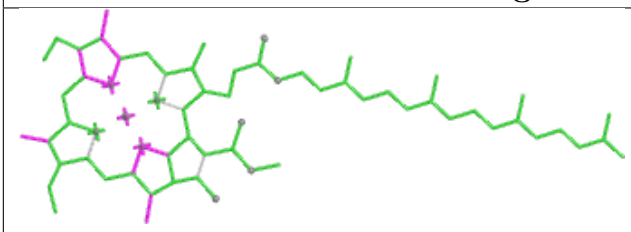


Rings

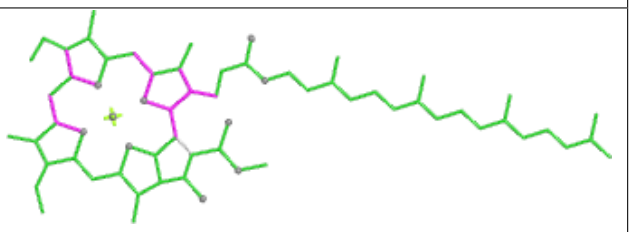
Ligand CLA hD 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CYC f8 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

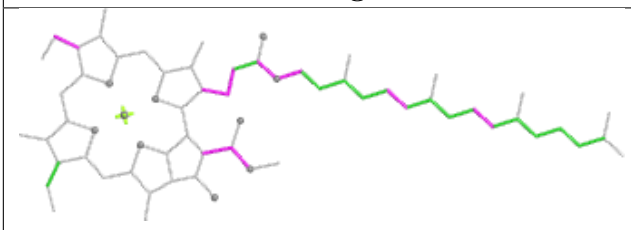
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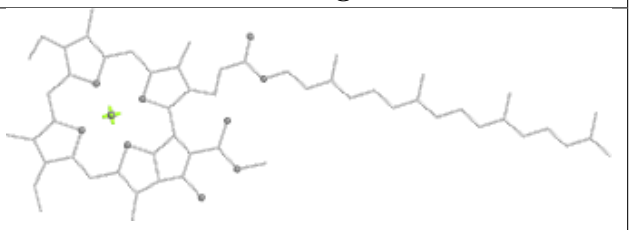
Bond lengths



Bond angles



Torsions



Rings

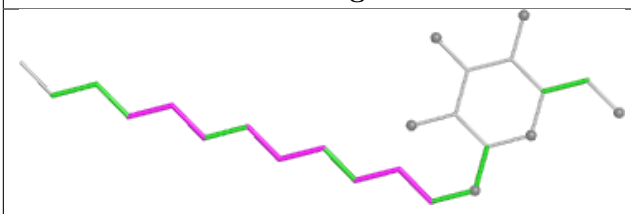
Ligand LMT B1 619



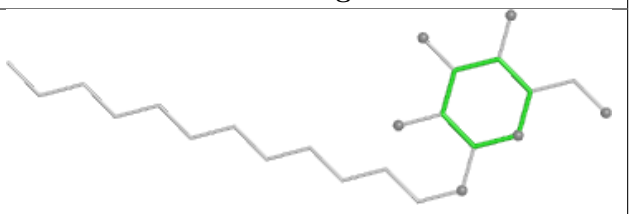
Bond lengths



Bond angles

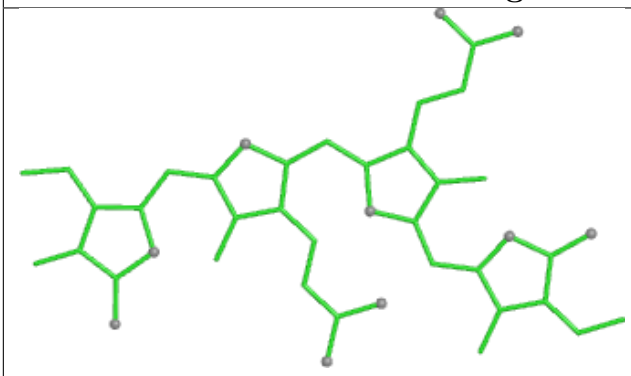


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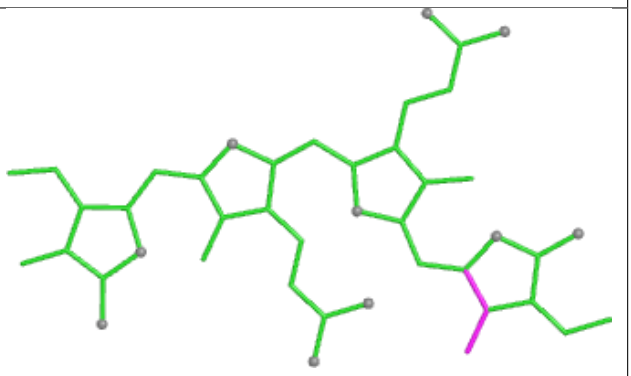


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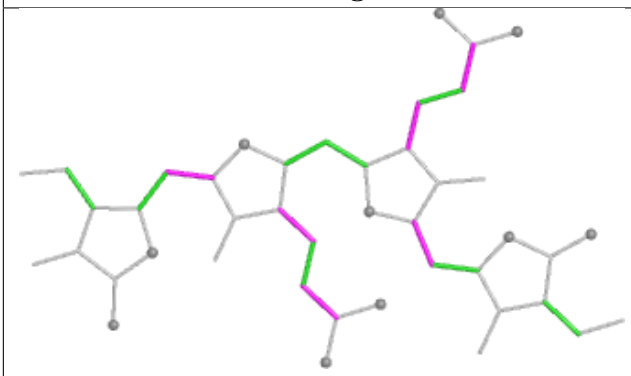
Ligand CYC mH 201



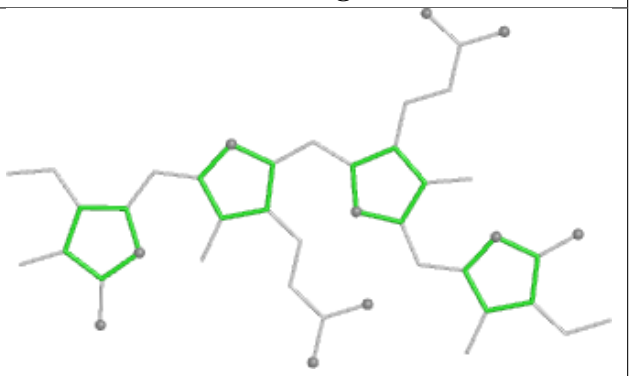
Bond lengths



Bond angles

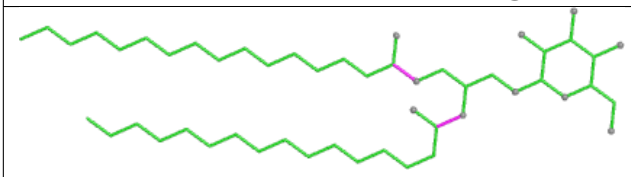


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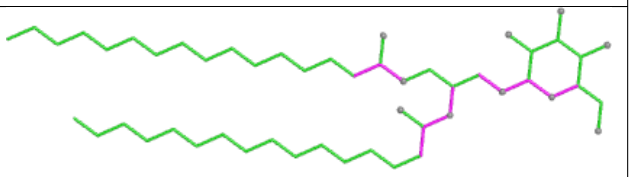


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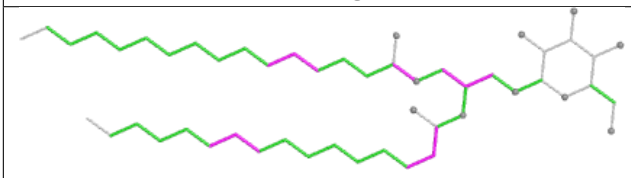
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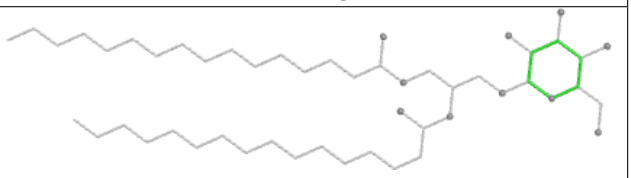
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Bond angles

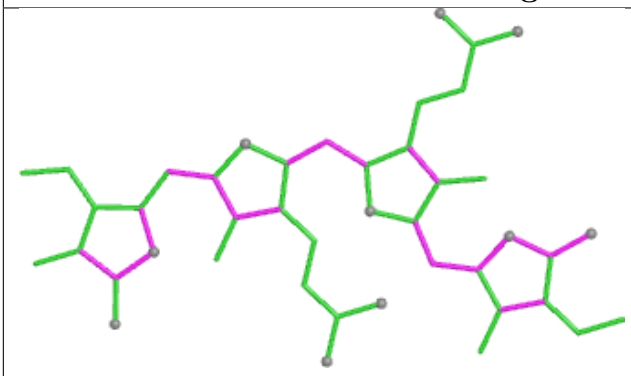


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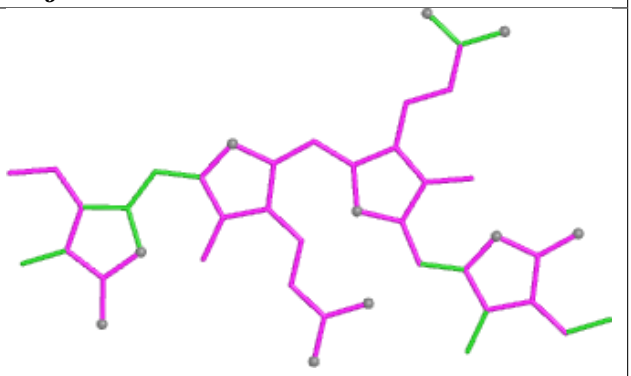


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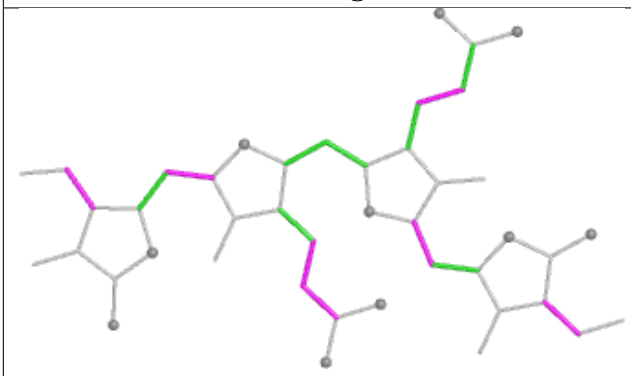
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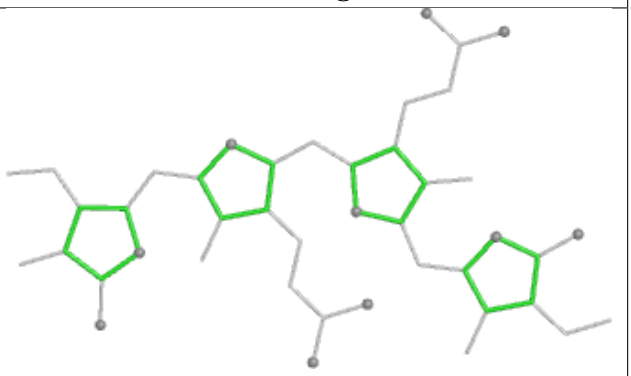
Bond lengths



Bond angles

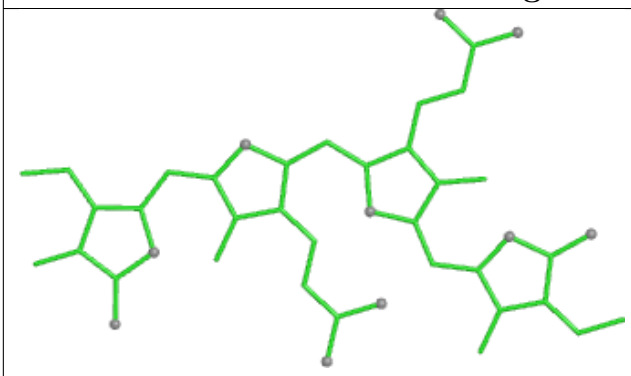


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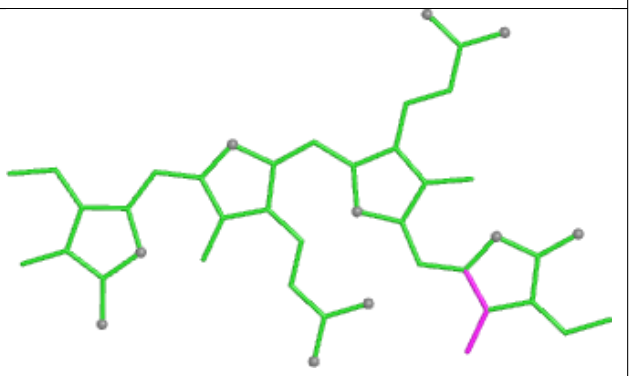


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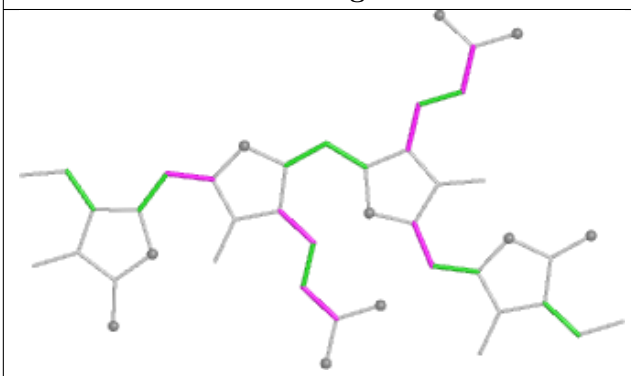
Ligand CYC iI 201



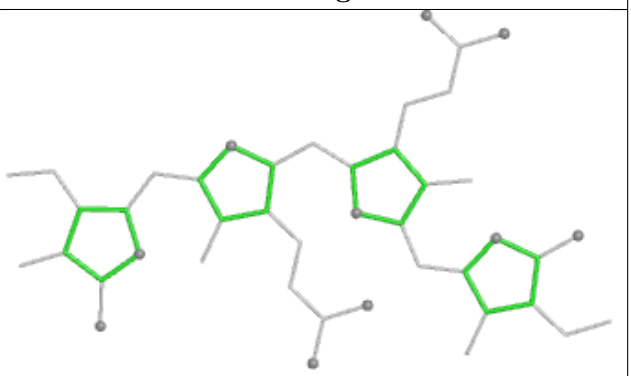
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Bond angles

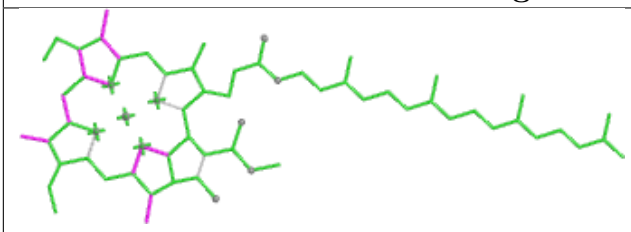


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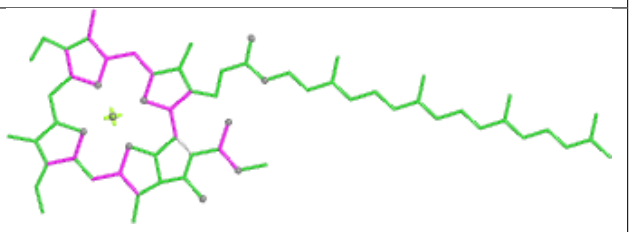


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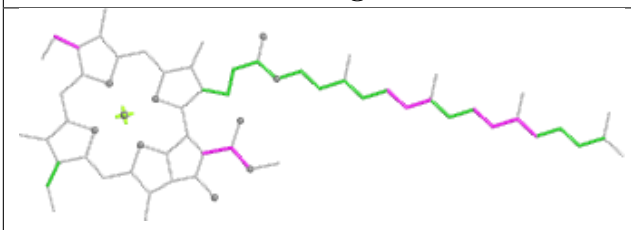
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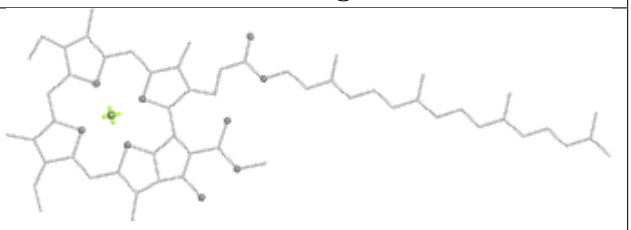
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Bond angles

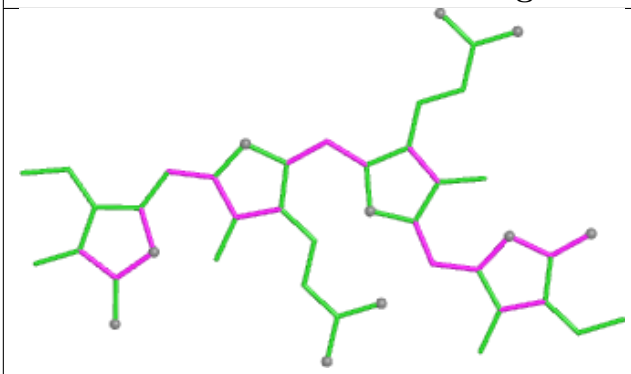


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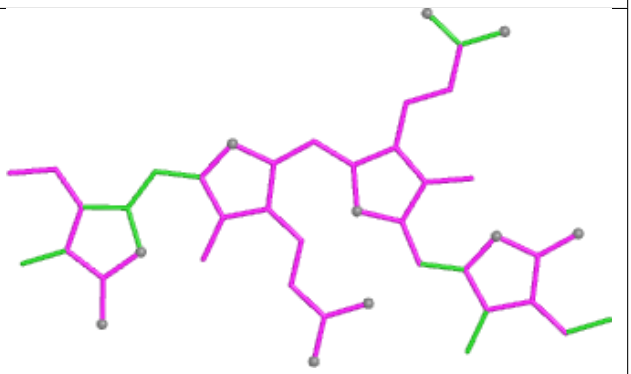


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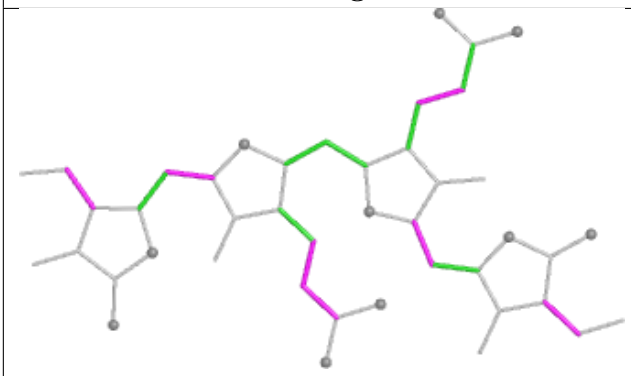
Ligand CYC b8 201



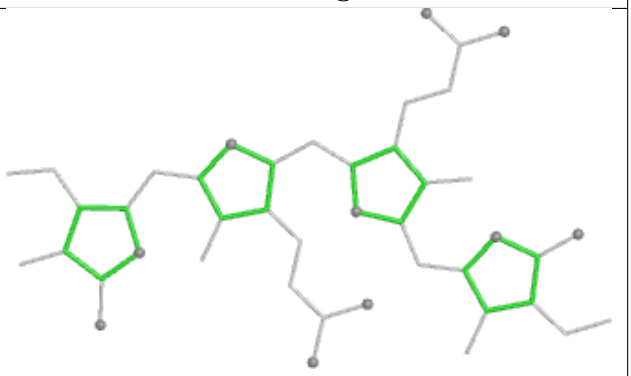
Bond lengths



Bond angles

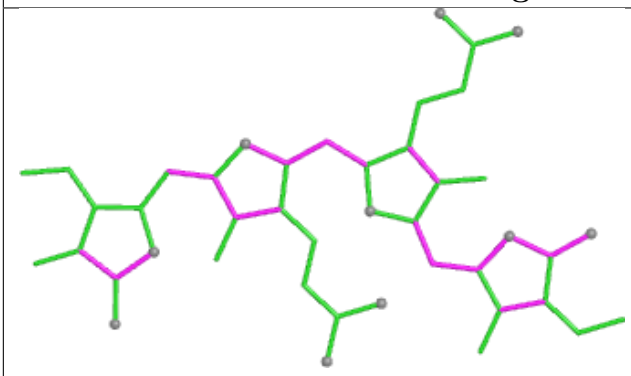


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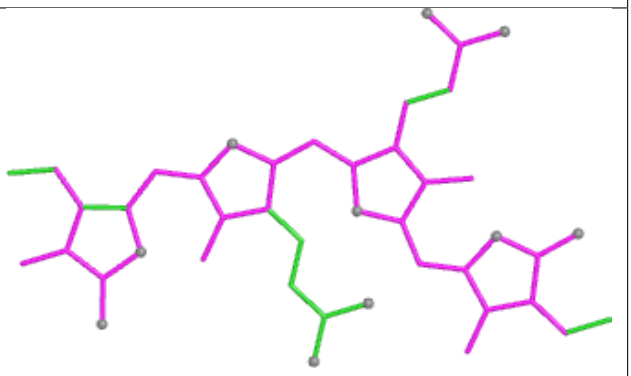


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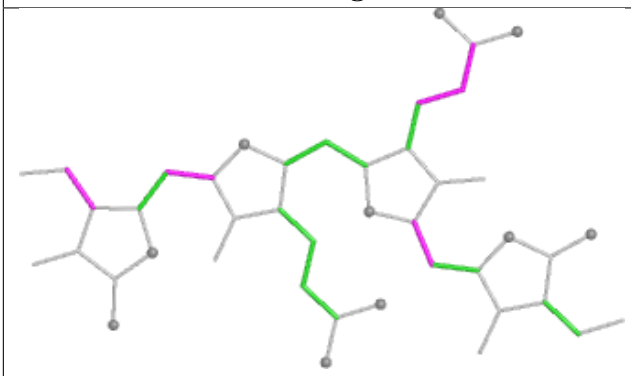
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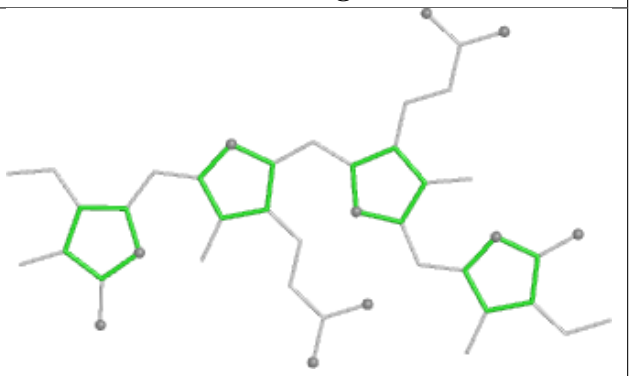
Bond lengths



Bond angles

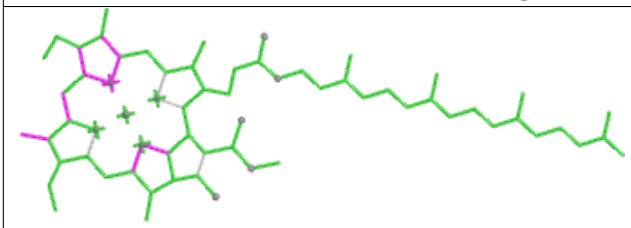


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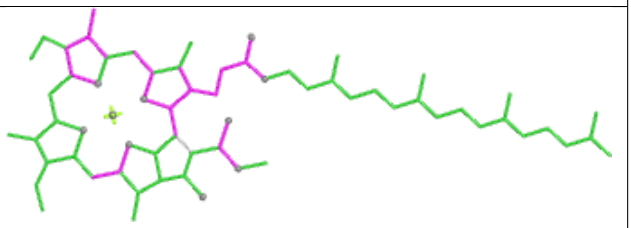


Rings

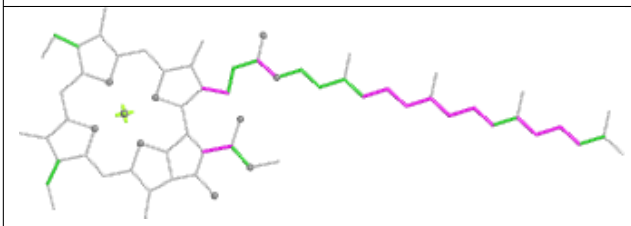
Ligand CLA B1 611



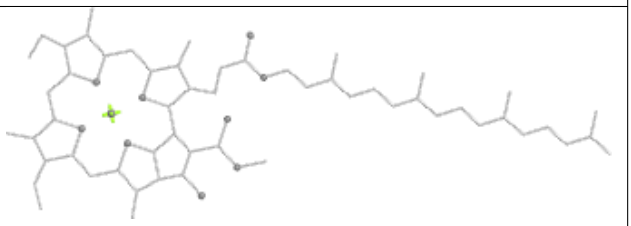
Bond lengths



Bond angles

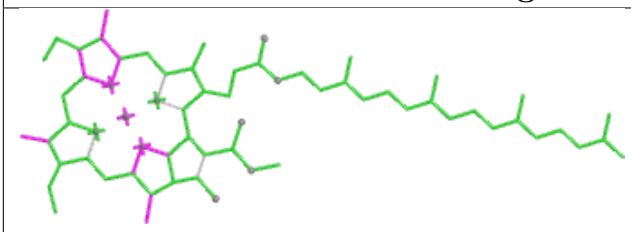


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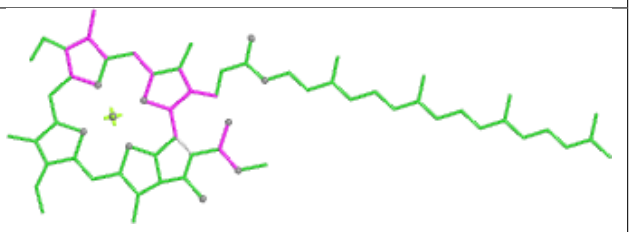


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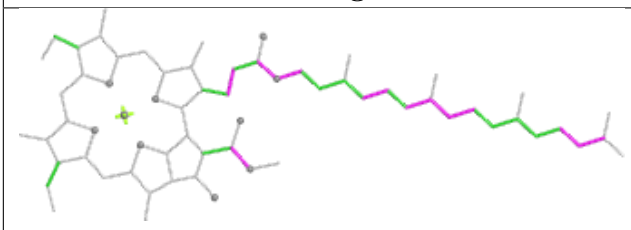
Ligand CLA cE 514



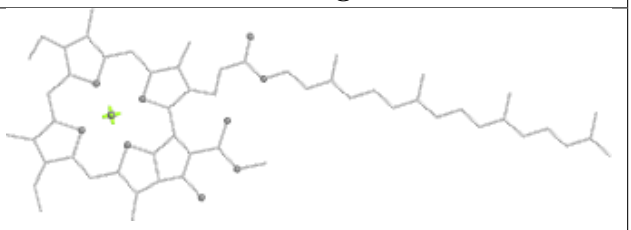
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Bond angles

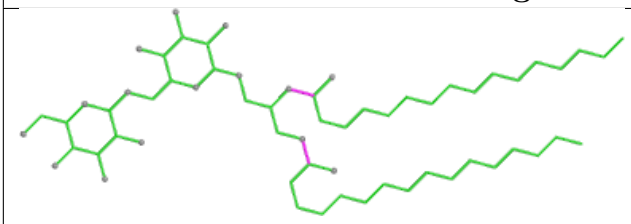


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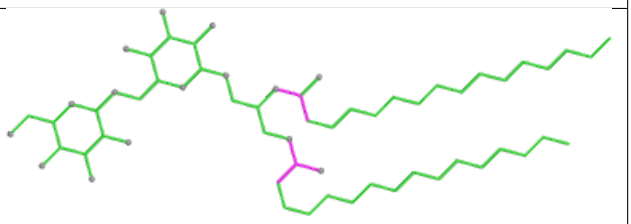


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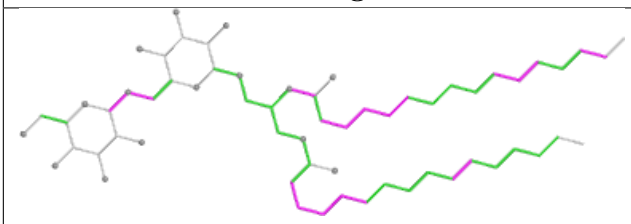
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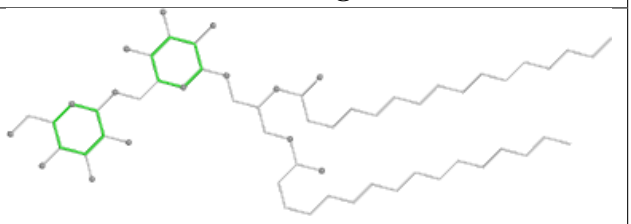
Bond lengths



Bond angles

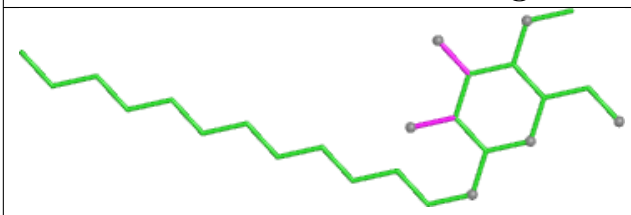


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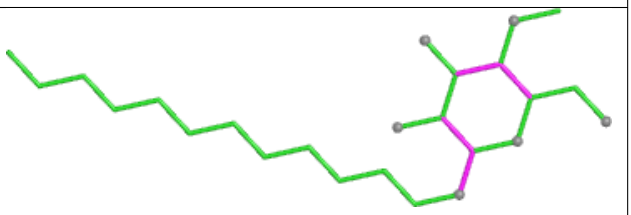


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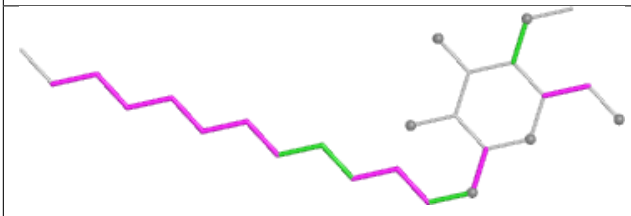
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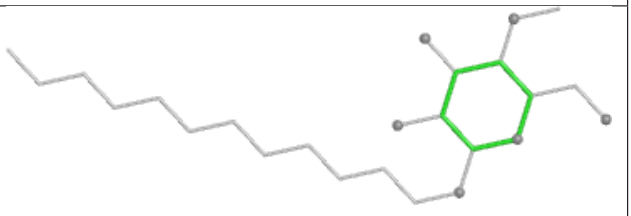
Bond lengths



Bond angles

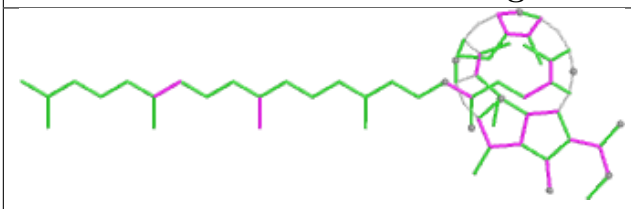


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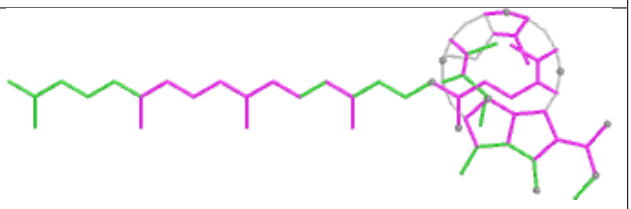


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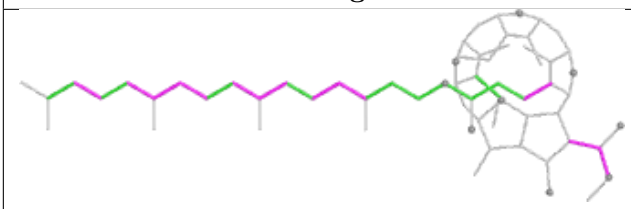
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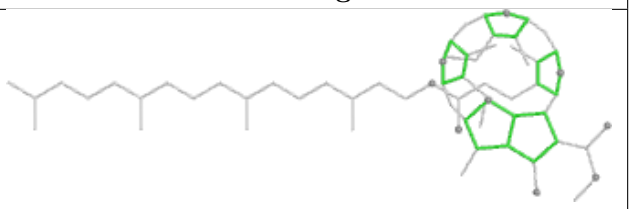
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Bond angles

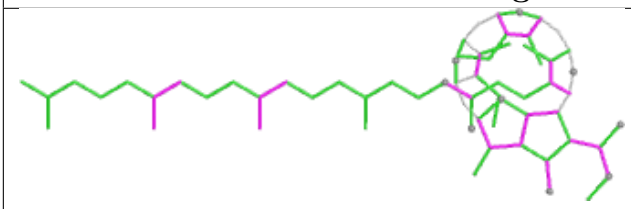


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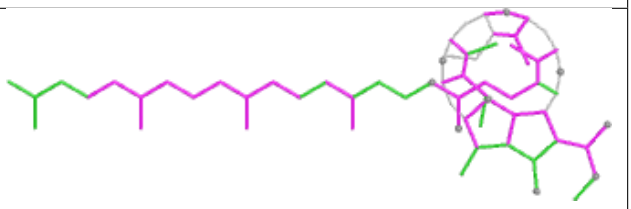


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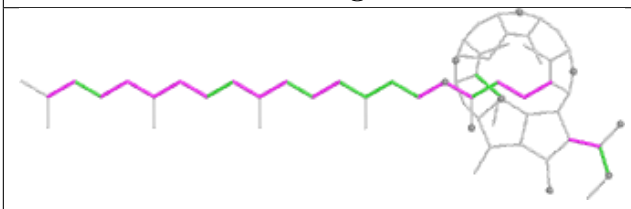
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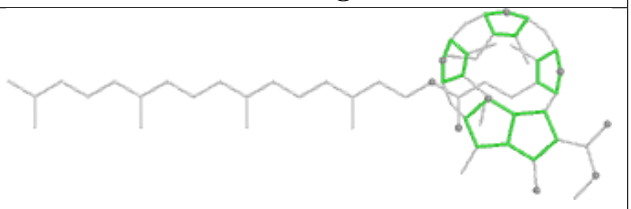
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Bond angles

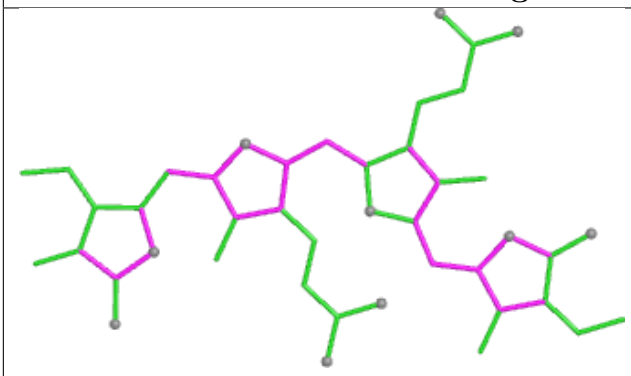


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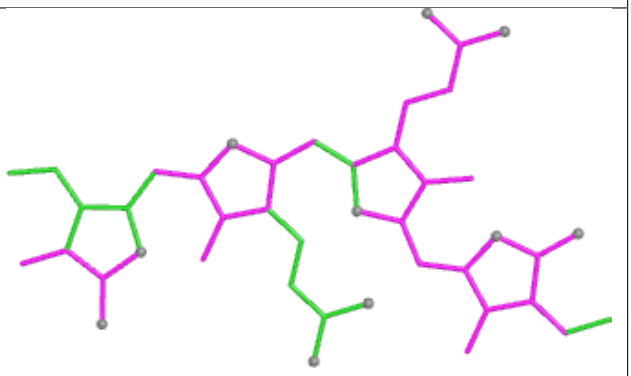


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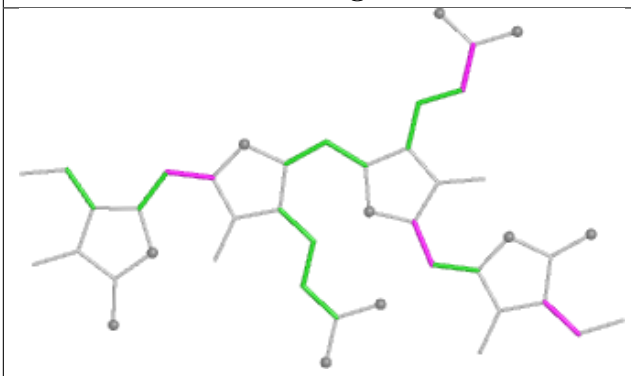
Ligand CYC hK 201



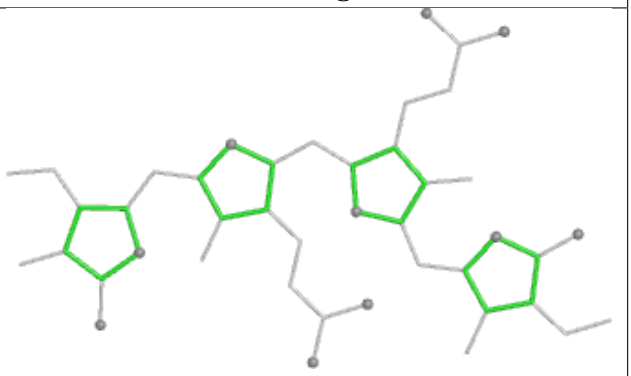
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Bond angles

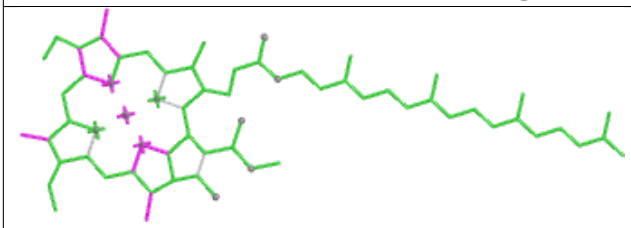


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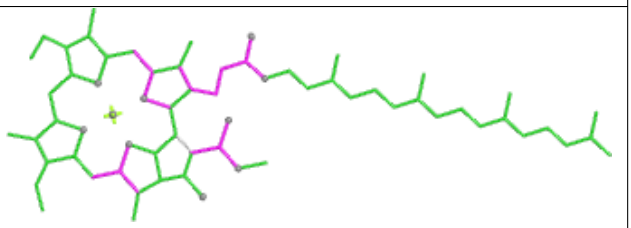


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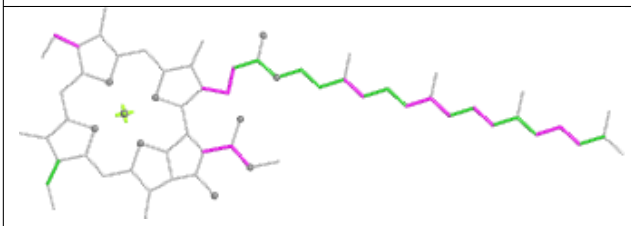
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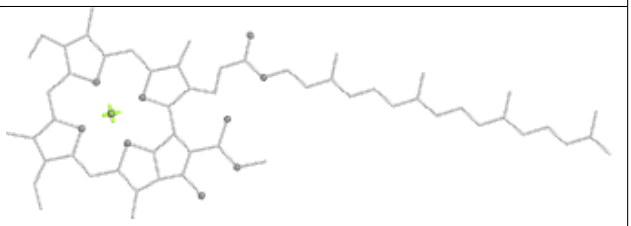
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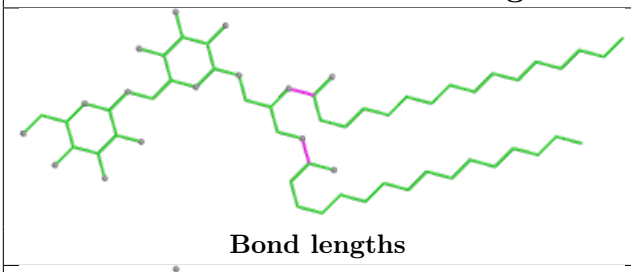


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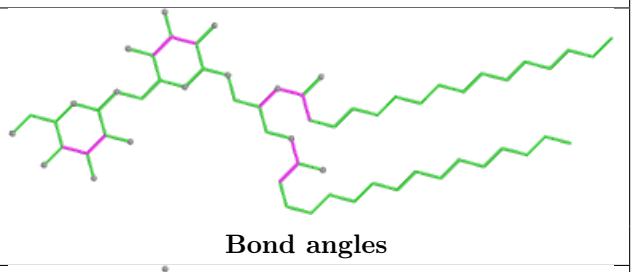


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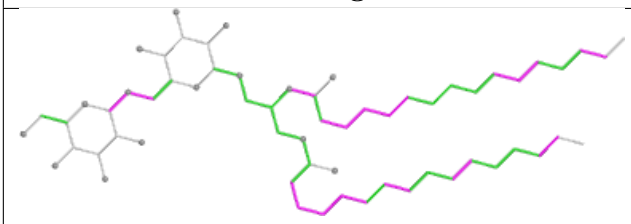
Ligand DGD CD 518



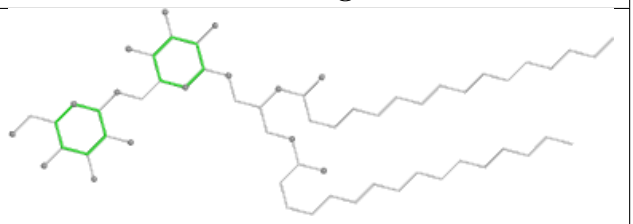
Bond lengths



Bond angles

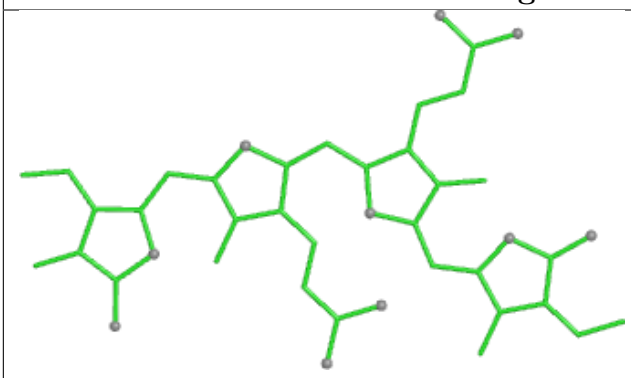


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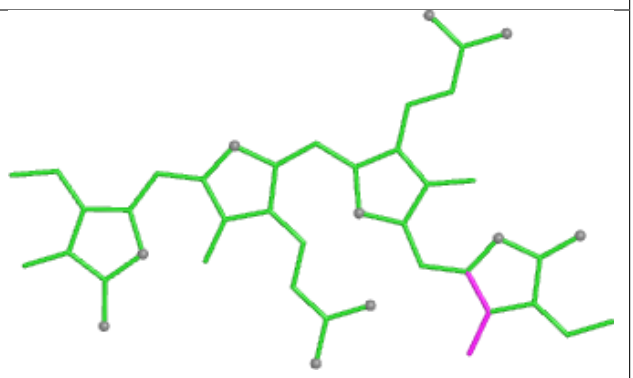


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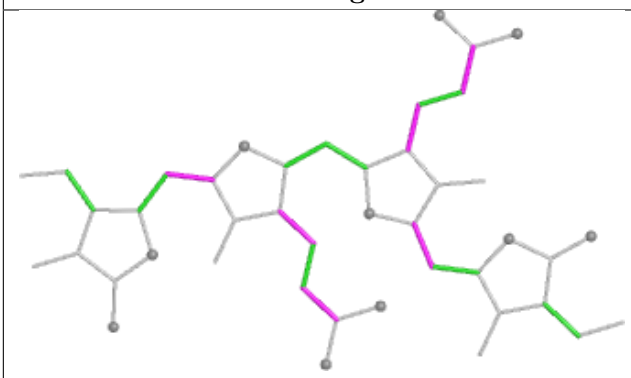
Ligand CYC e6 202



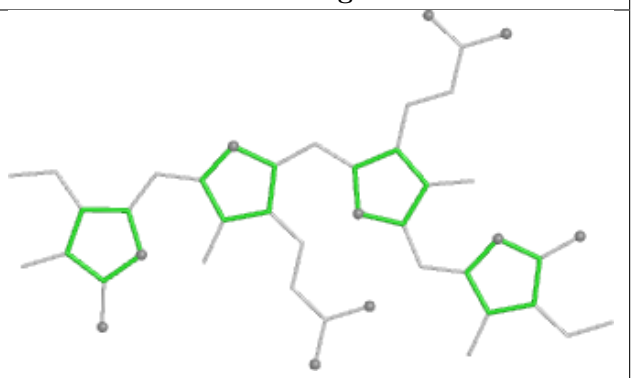
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Bond angles

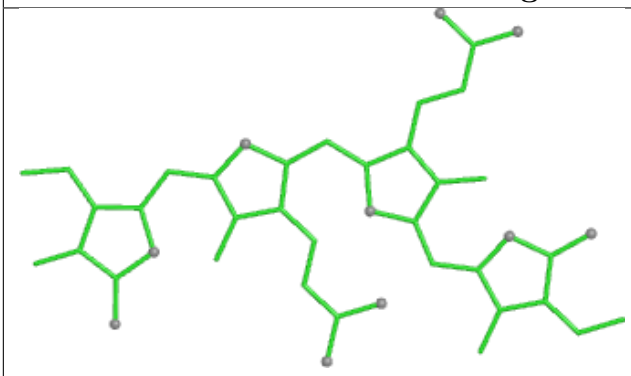


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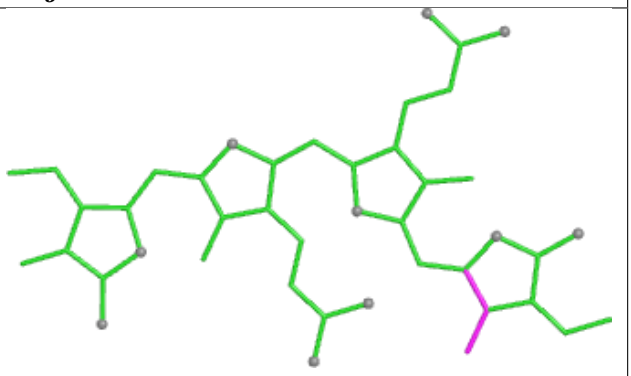


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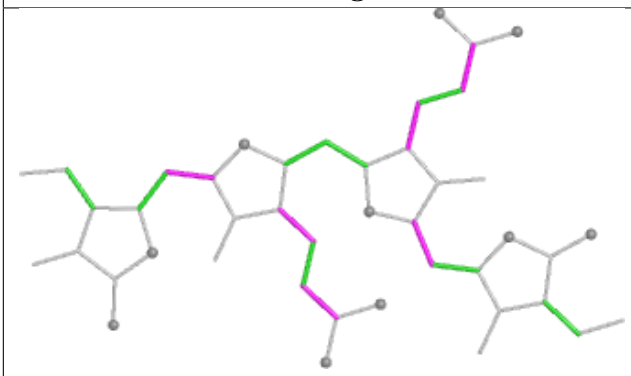
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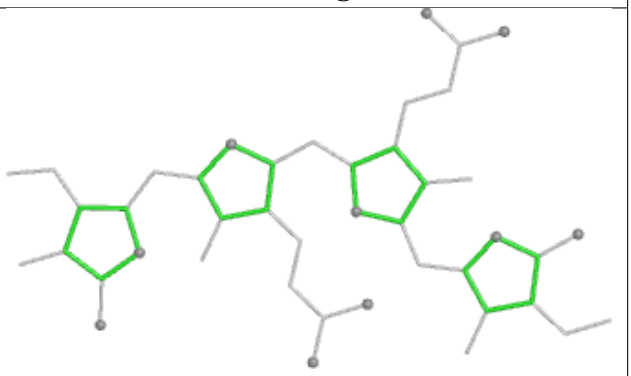
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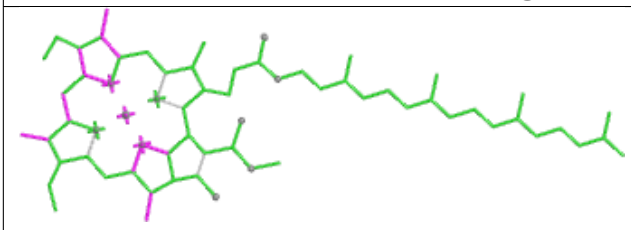


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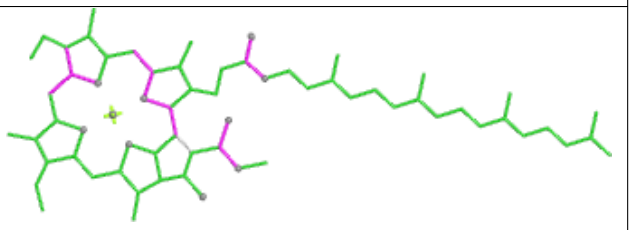


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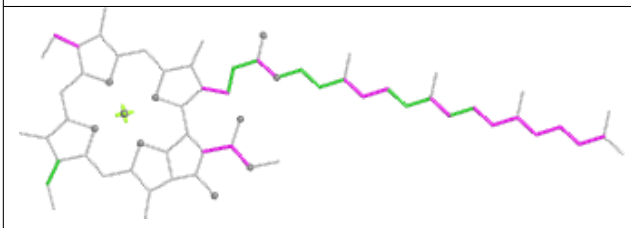
Ligand CLA x1 101



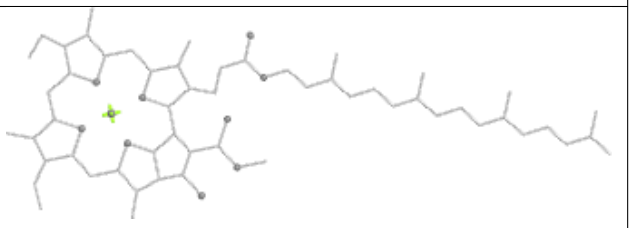
Bond lengths



Bond angles

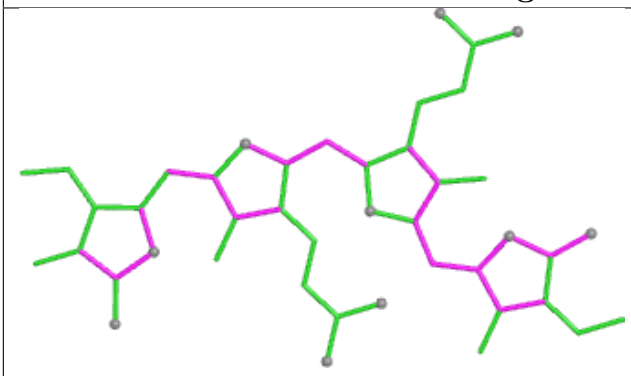


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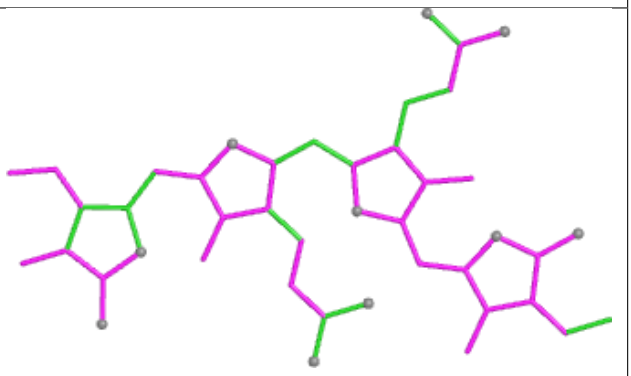


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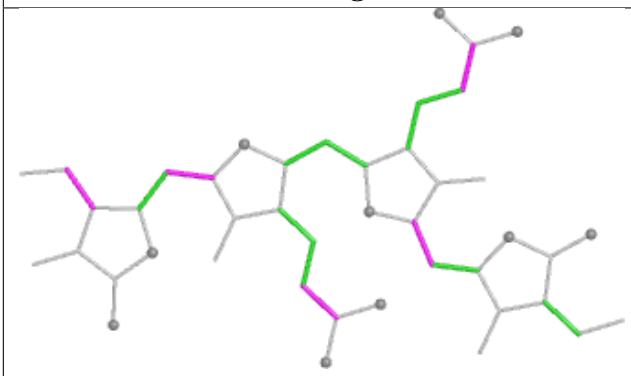
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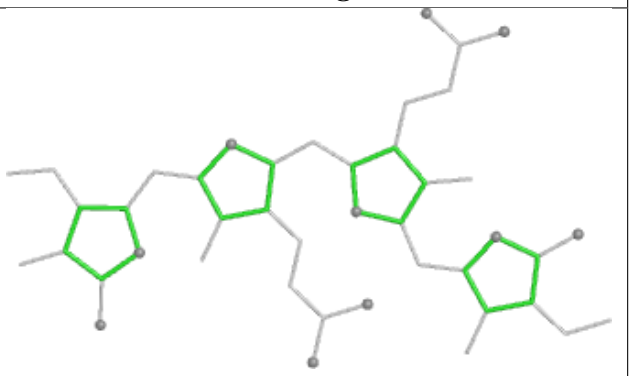
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Bond angles

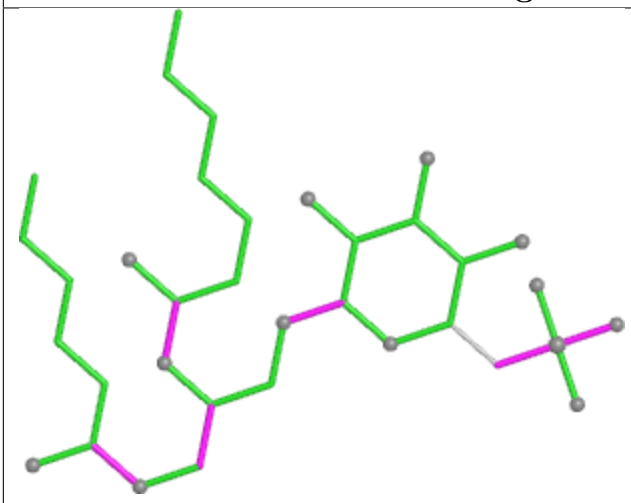


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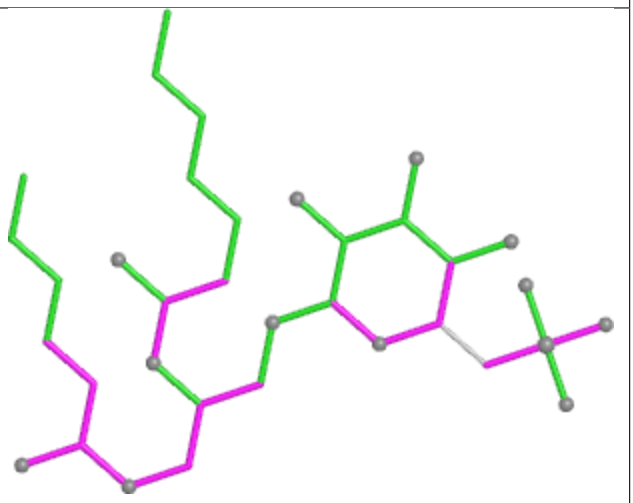


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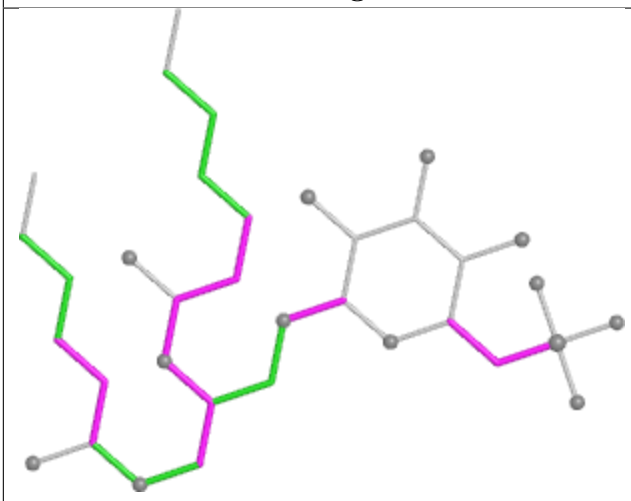
Ligand SQD hE 103



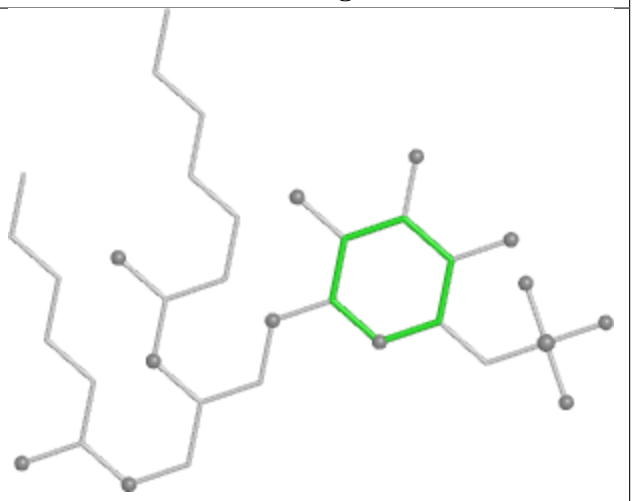
Bond lengths



Bond angles

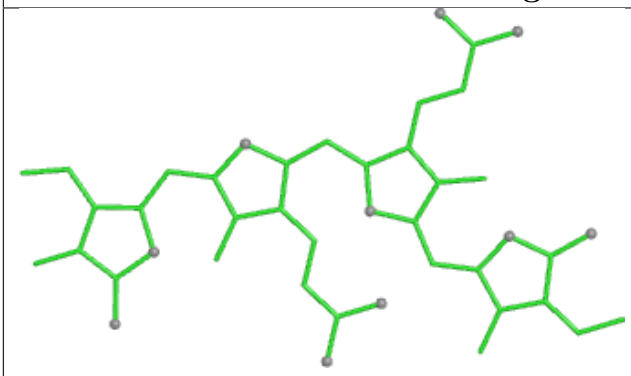


Torsions

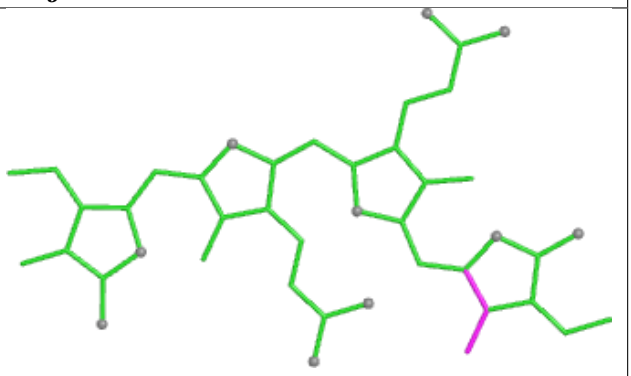


Rings

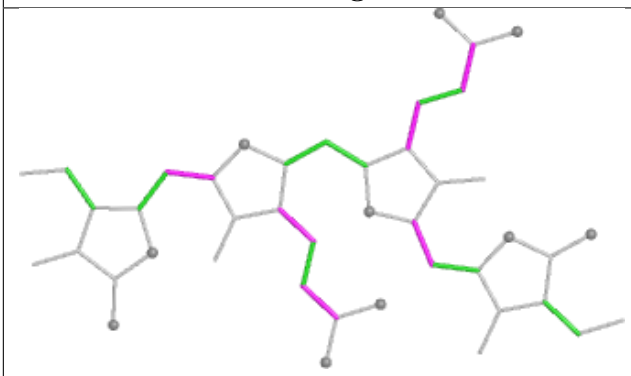
Ligand CYC jI 202



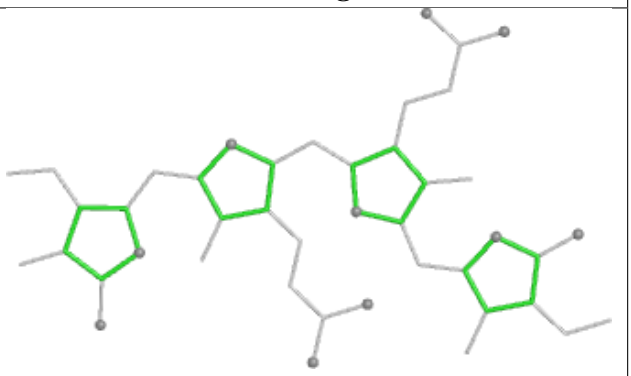
Bond lengths



Bond angles

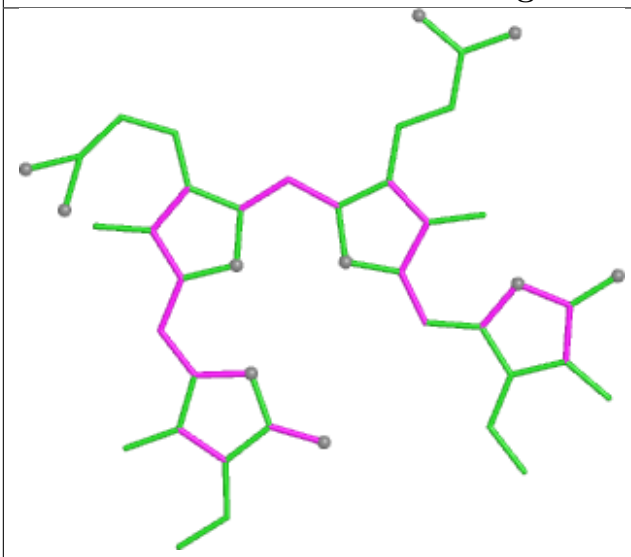


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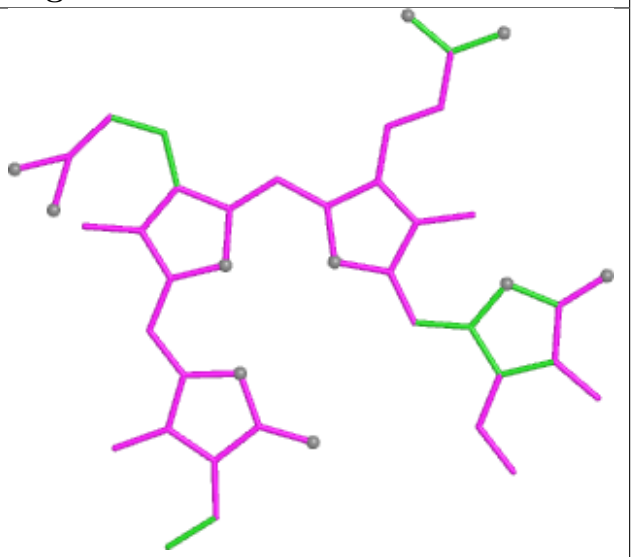


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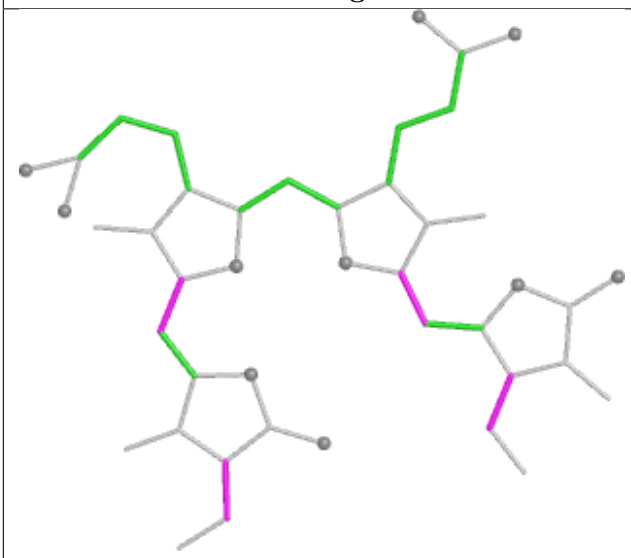
Ligand CYC g5 202



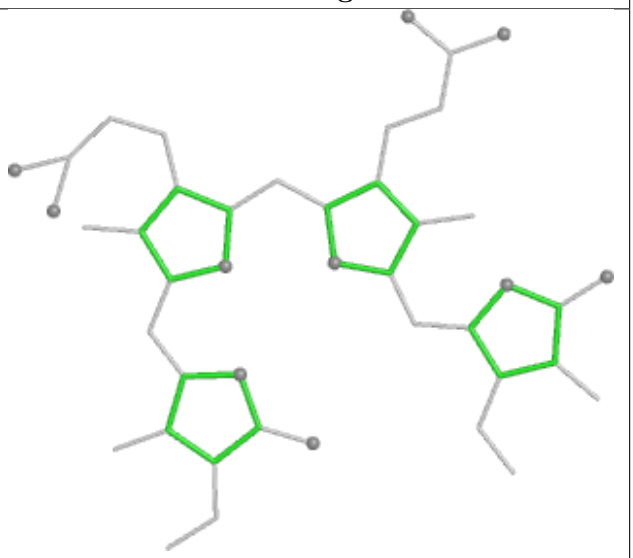
Bond lengths



Bond angles

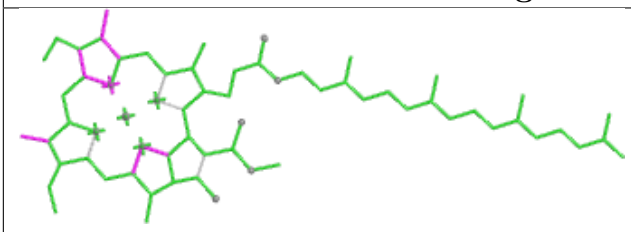


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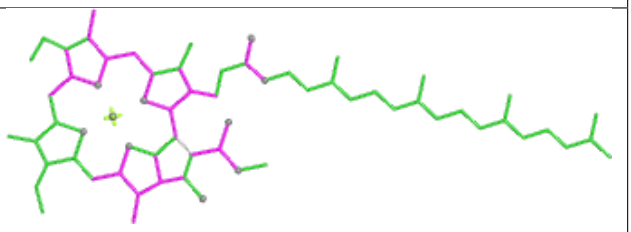


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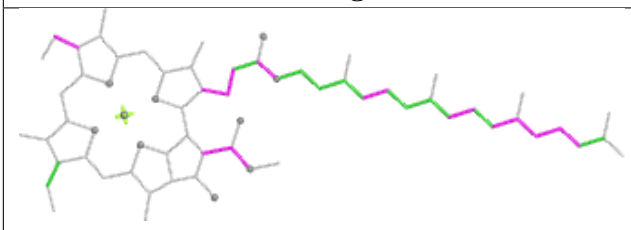
Ligand CLA cD 507



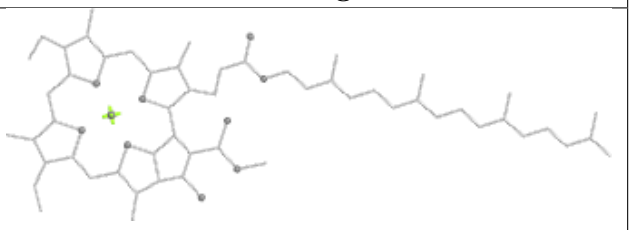
Bond lengths



Bond angles



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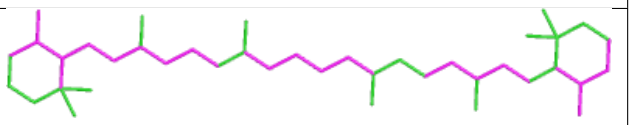


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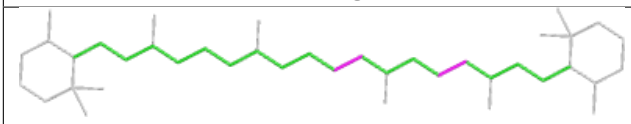
Ligand BCR bD 617



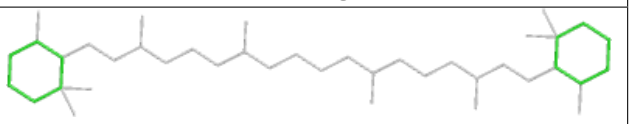
Bond lengths



Bond angles

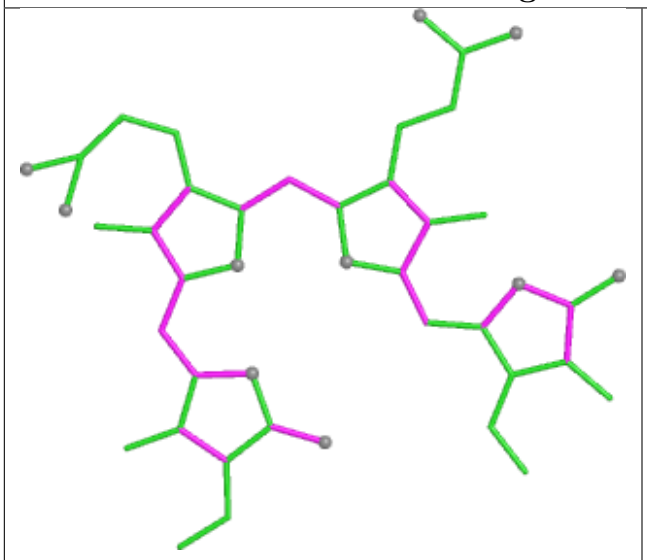


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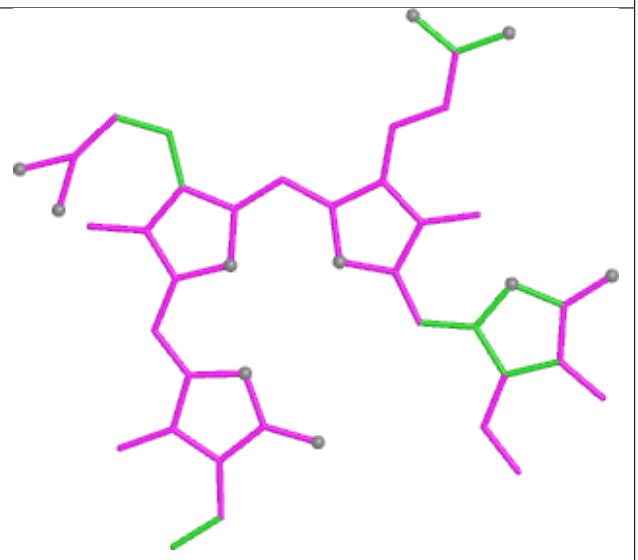


Rings

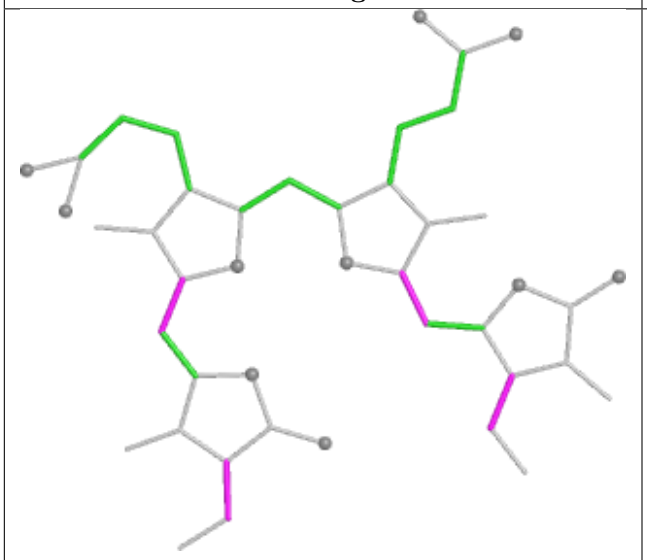
Ligand CYC e5 201



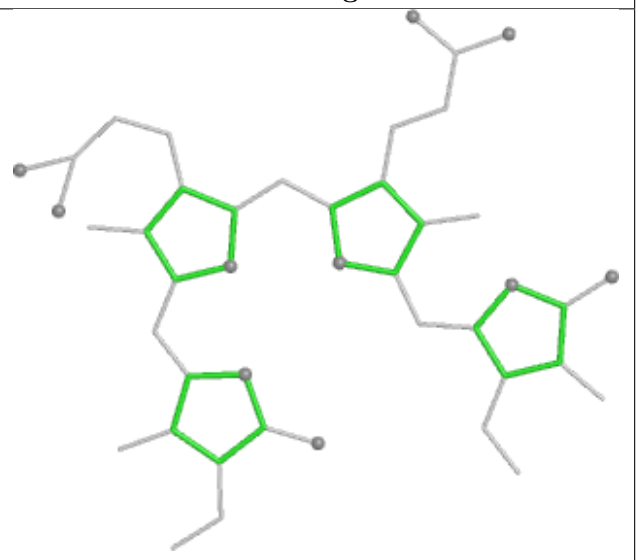
Bond lengths



Bond angles

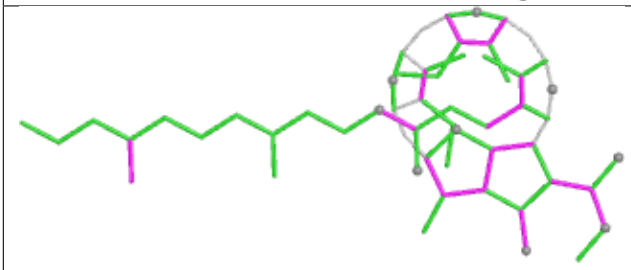


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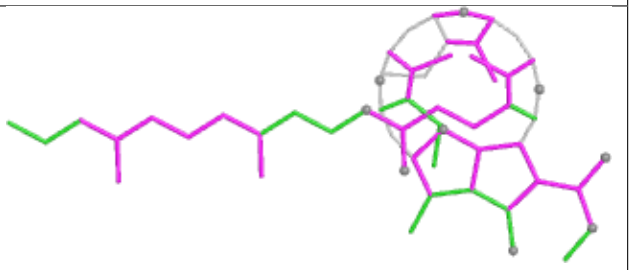


Rings

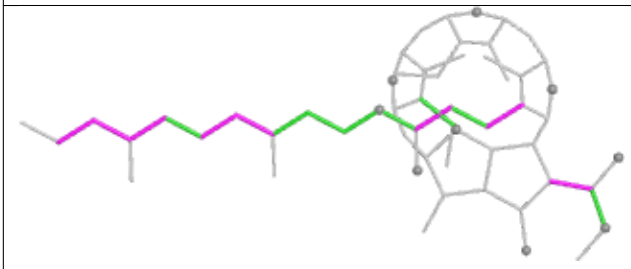
Ligand PHO aE 412



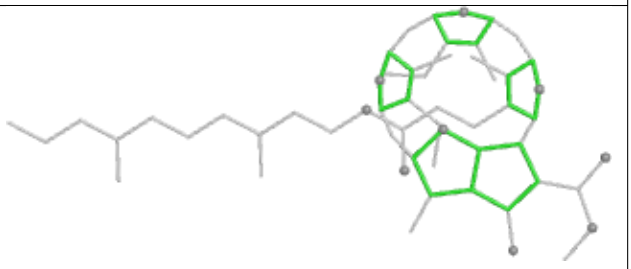
Bond lengths



Bond angles

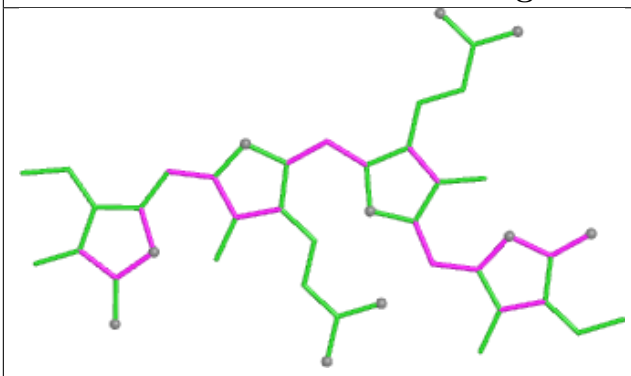


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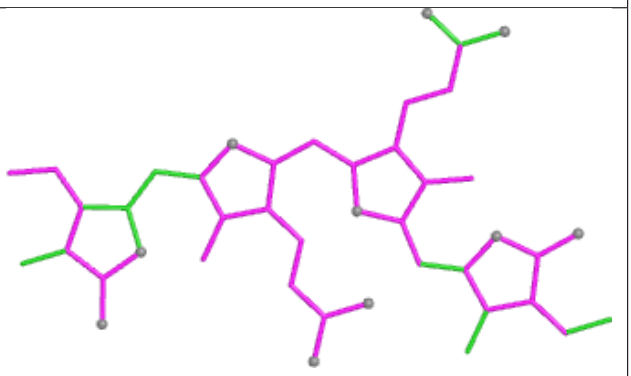


Rings

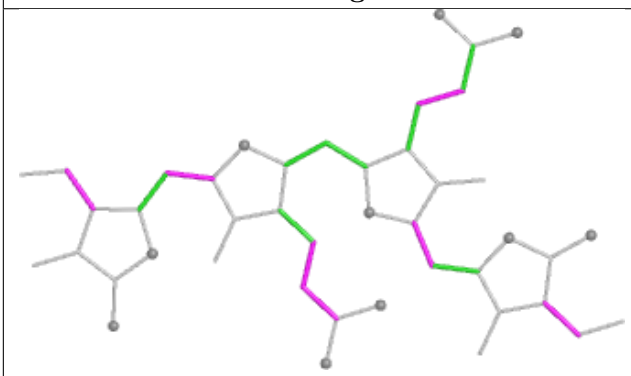
Ligand CYC b5 201



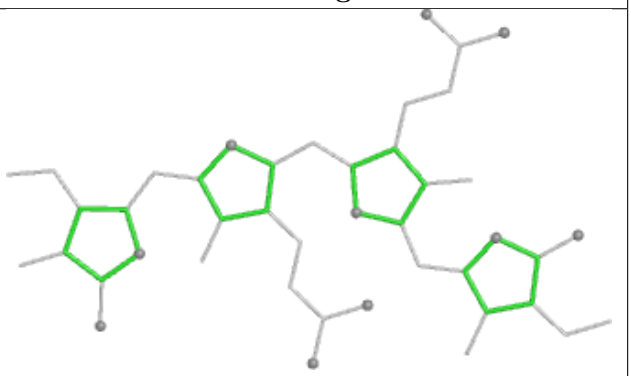
Bond lengths



Bond angles

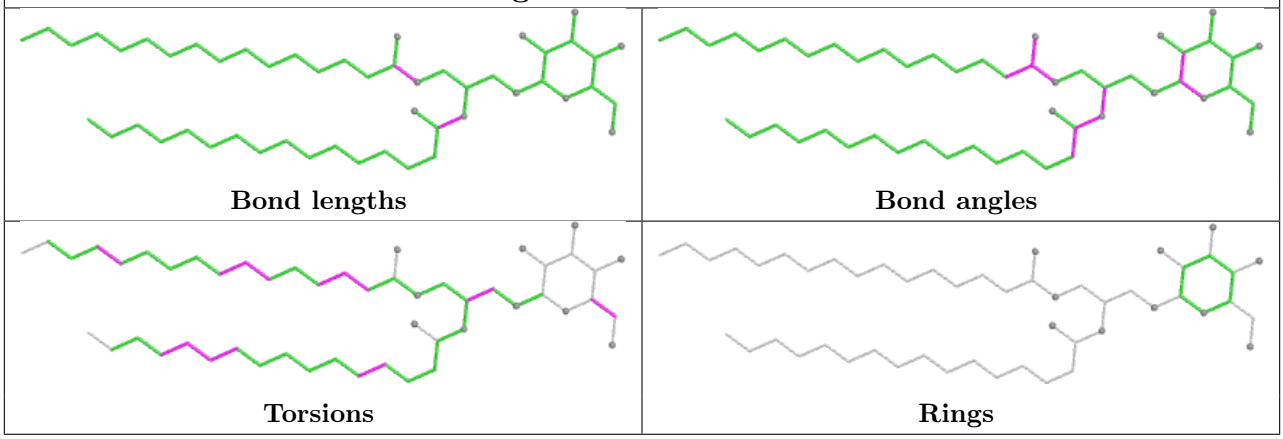


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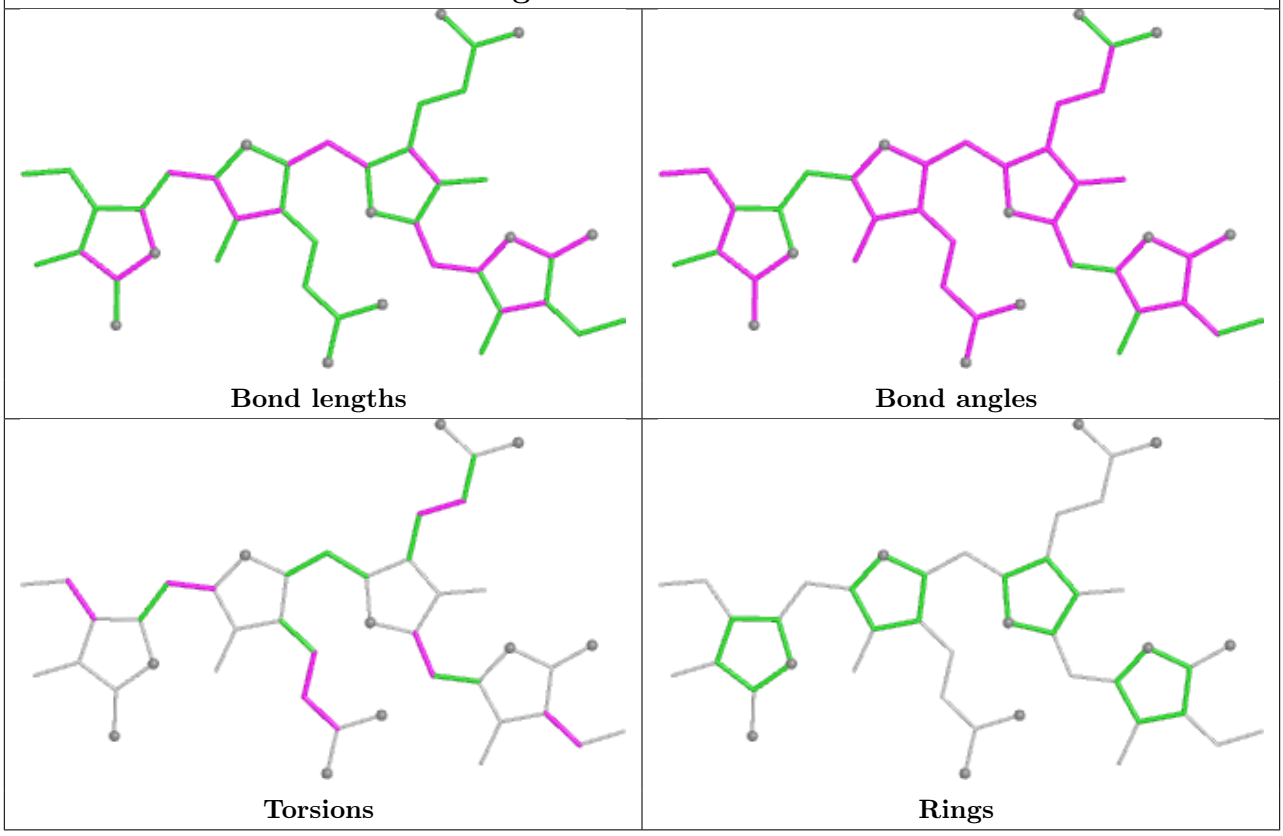


Rings

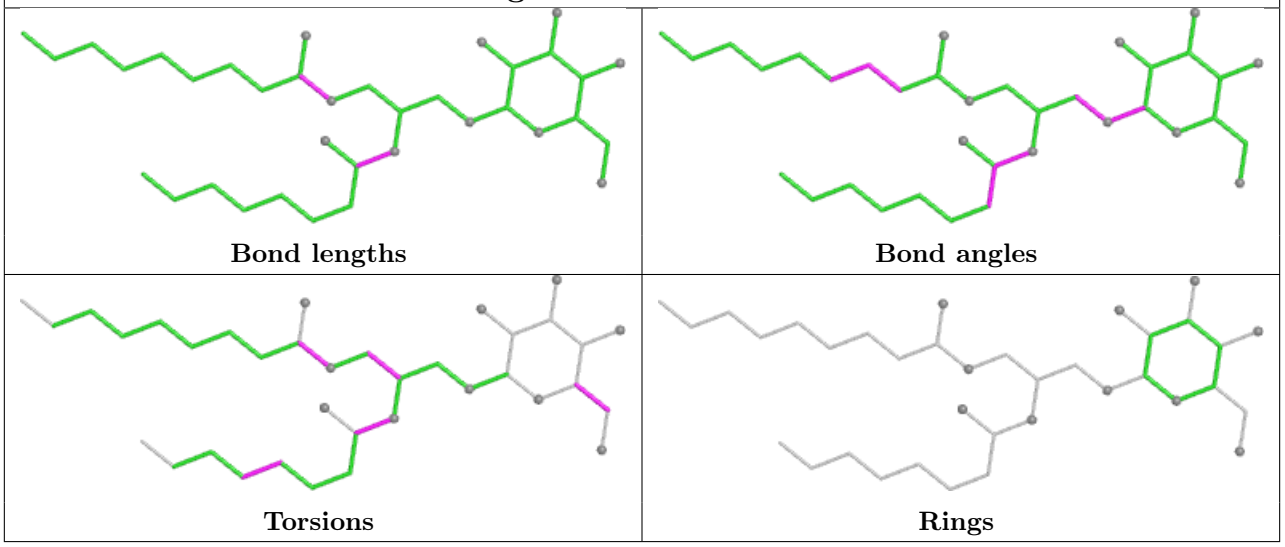
Ligand LMG dE 411



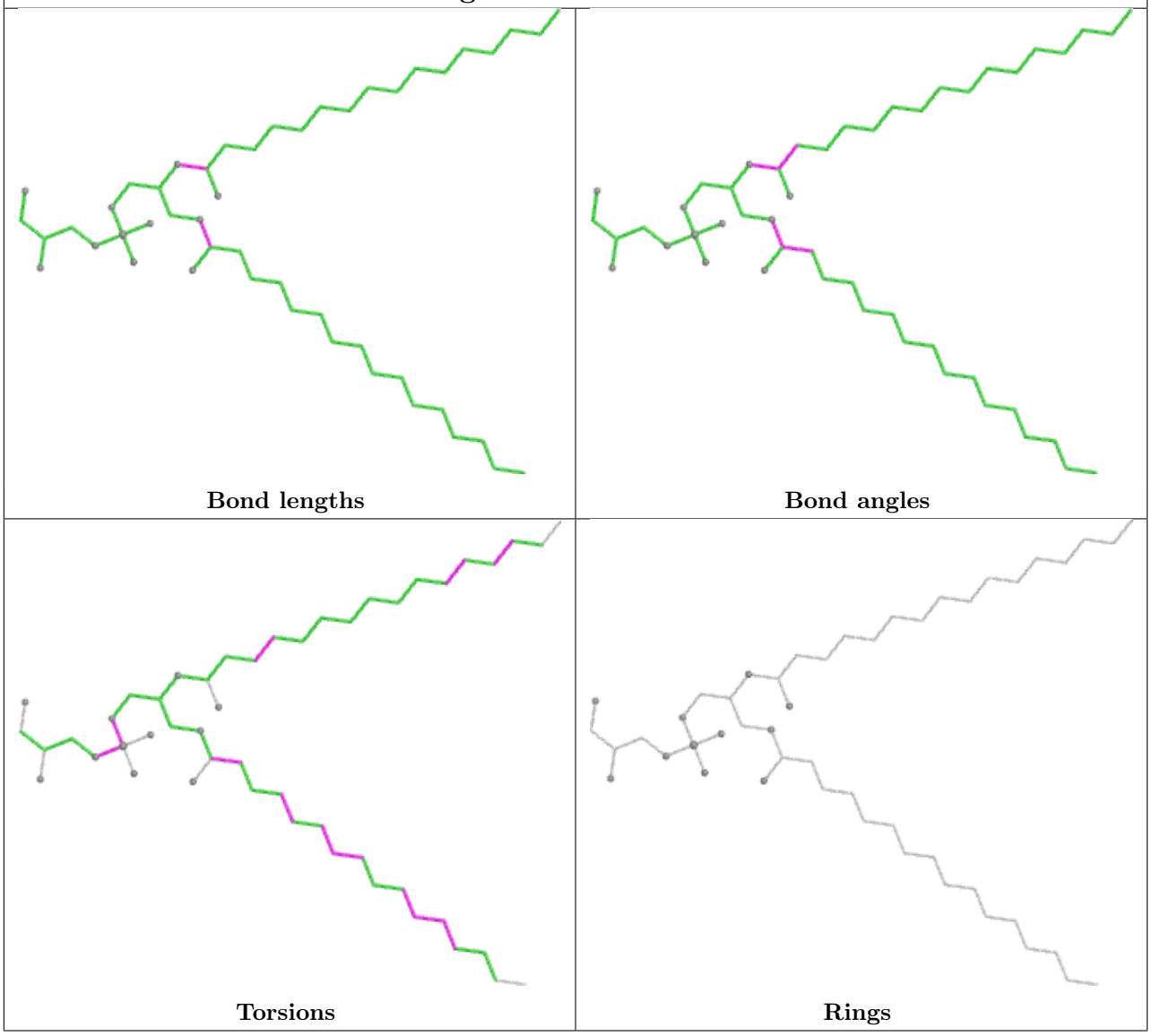
Ligand CYC hA 201



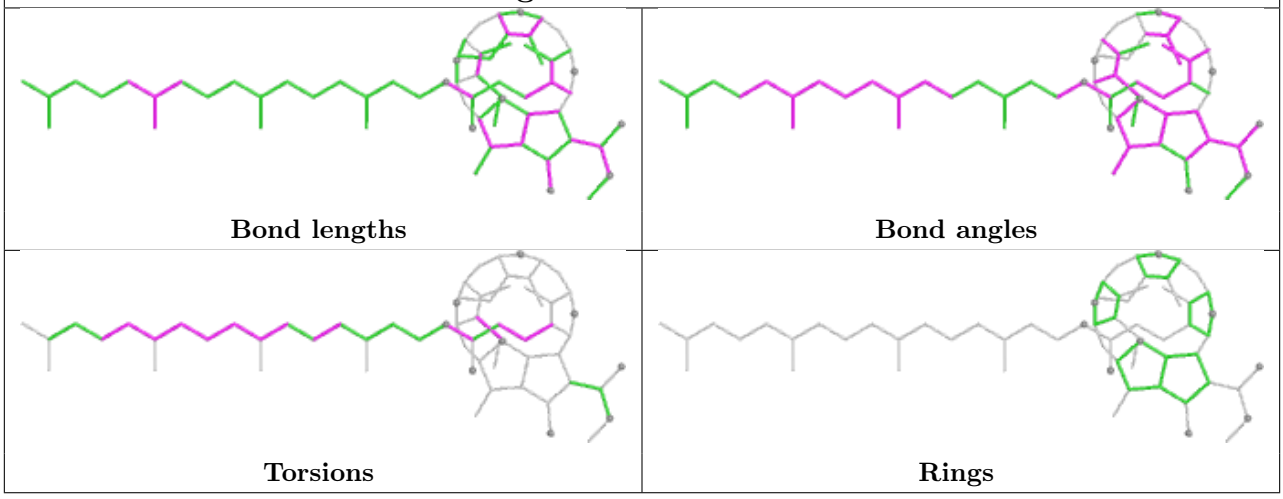
Ligand LMG TD 101



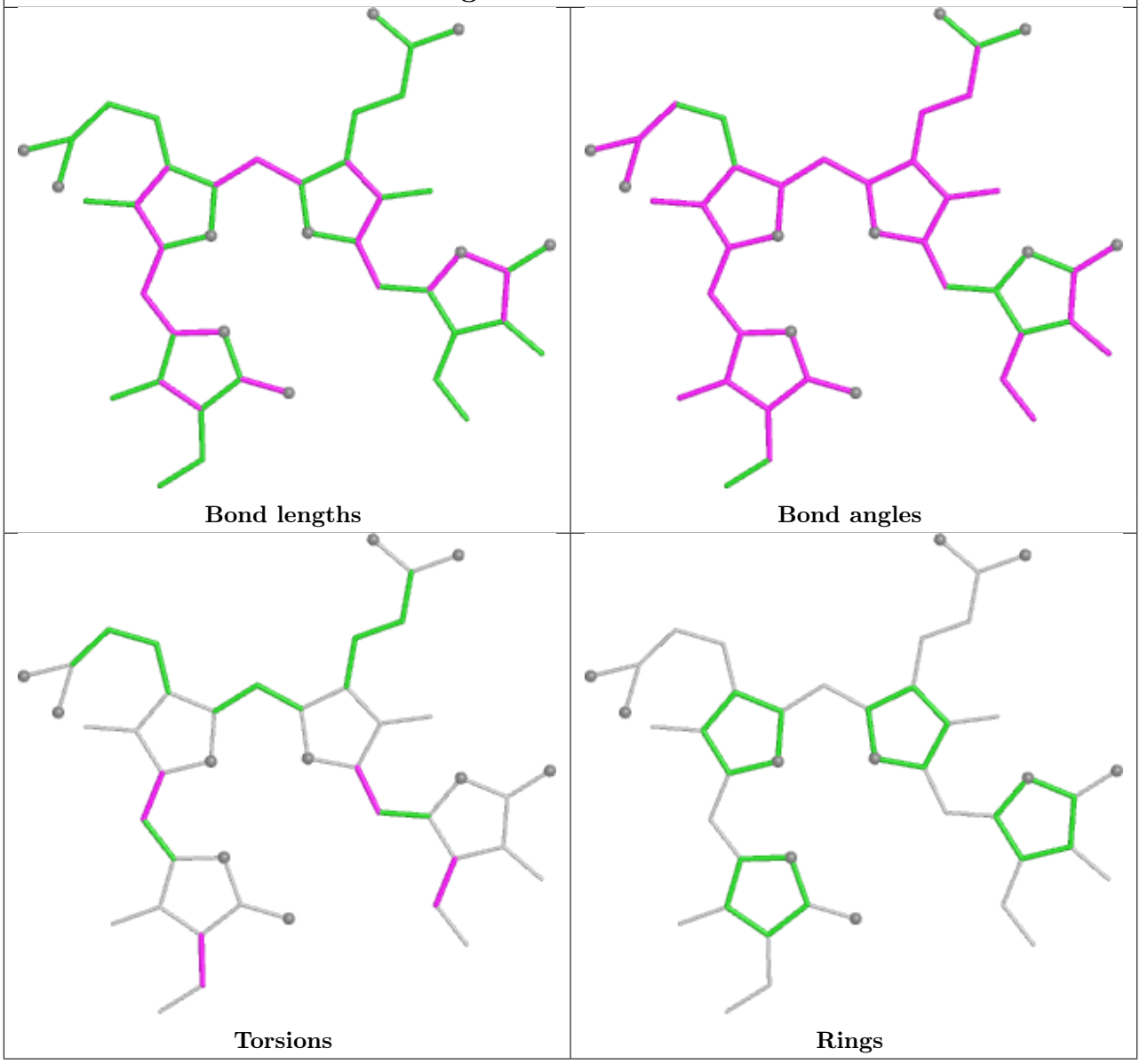
Ligand LHG dD 409



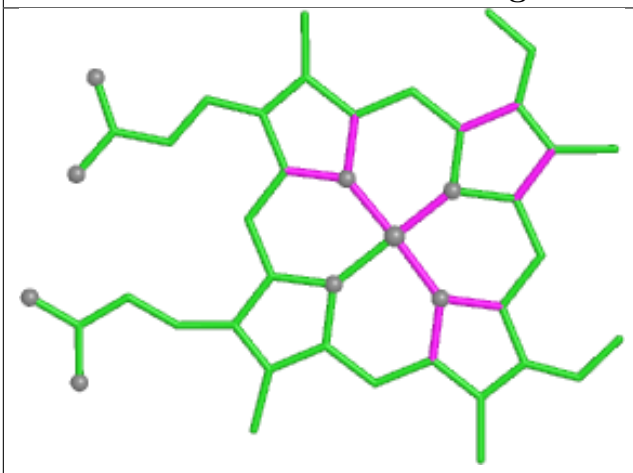
Ligand PHO d1 402



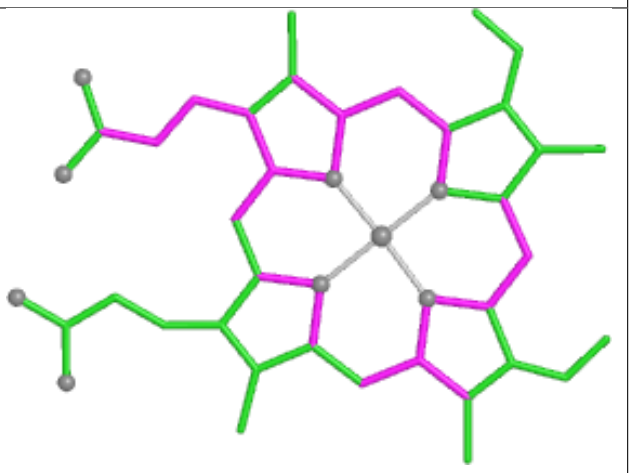
Ligand CYC e8 201



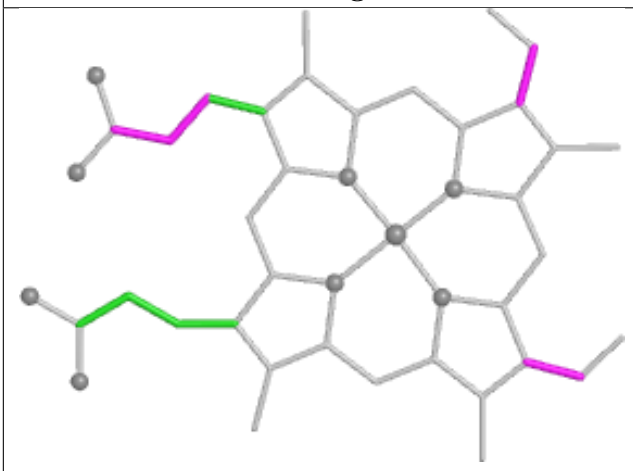
Ligand HEM V1 201



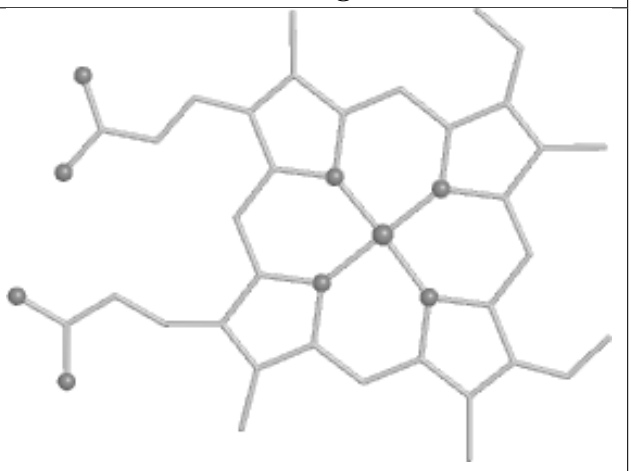
Bond lengths



Bond angles

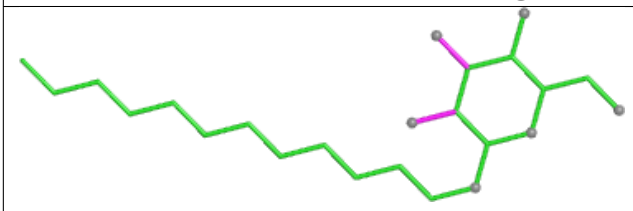


Torsions

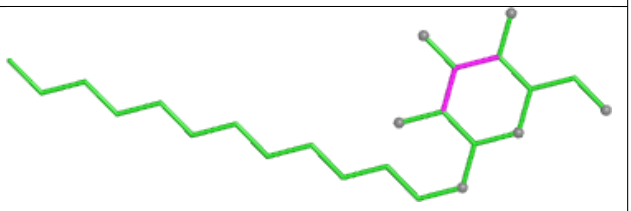


Rings

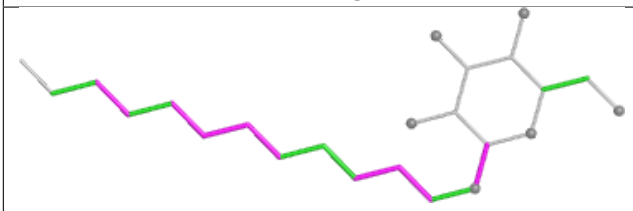
Ligand LMT dE 404



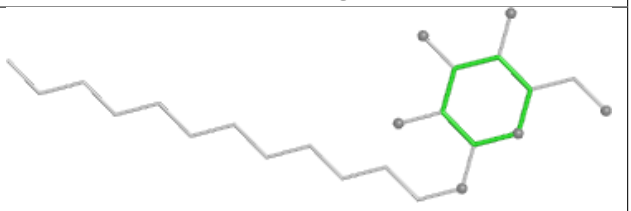
Bond lengths



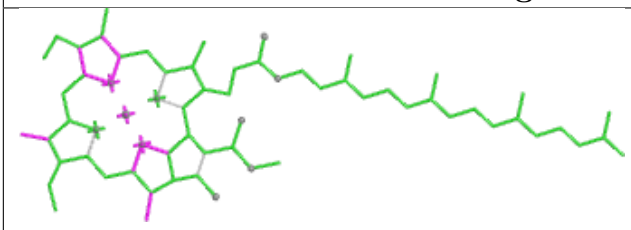
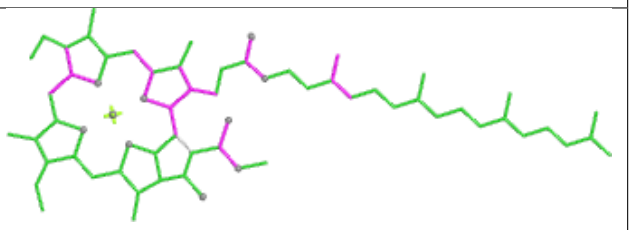
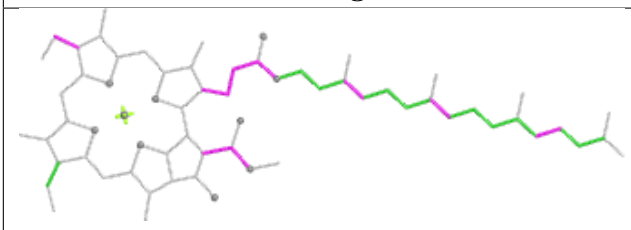
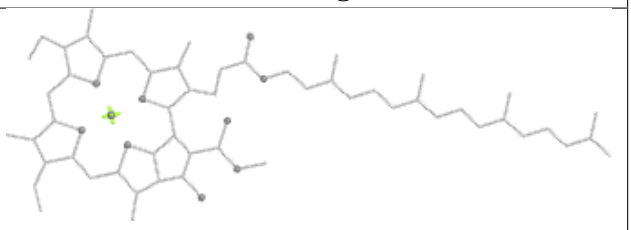
Bond angles

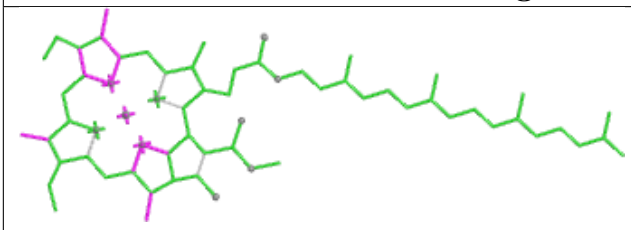
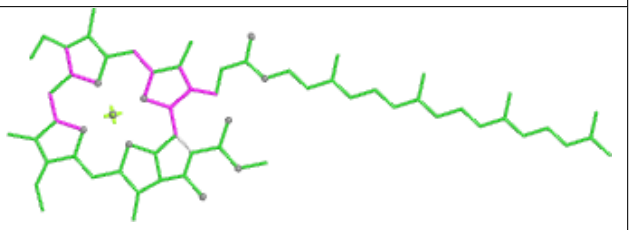
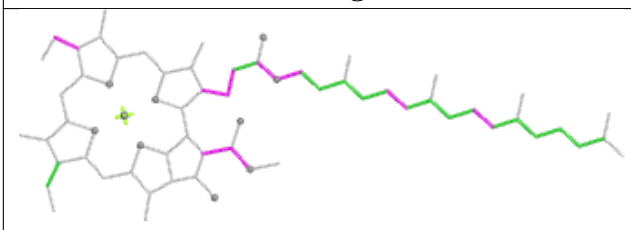
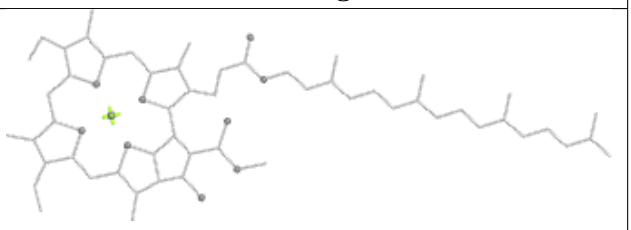


Torsions

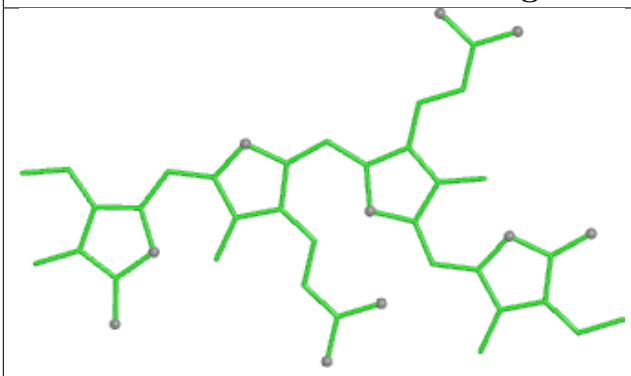


Rings

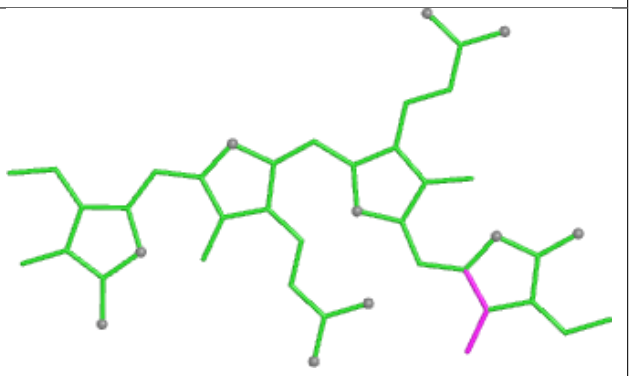
Ligand CLA C1 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA dE 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

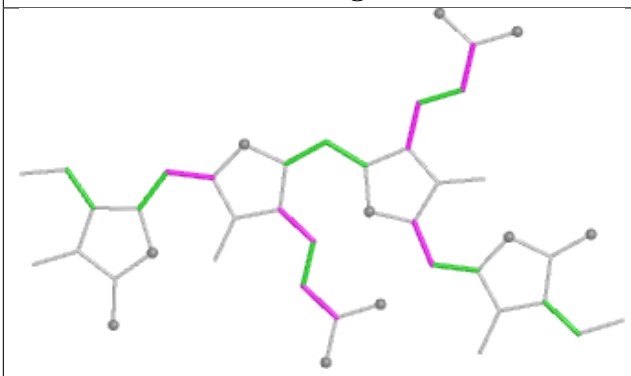
Ligand CYC i2 201



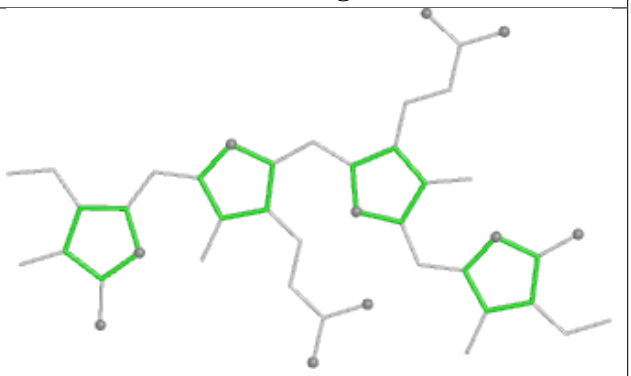
Bond lengths



Bond angles

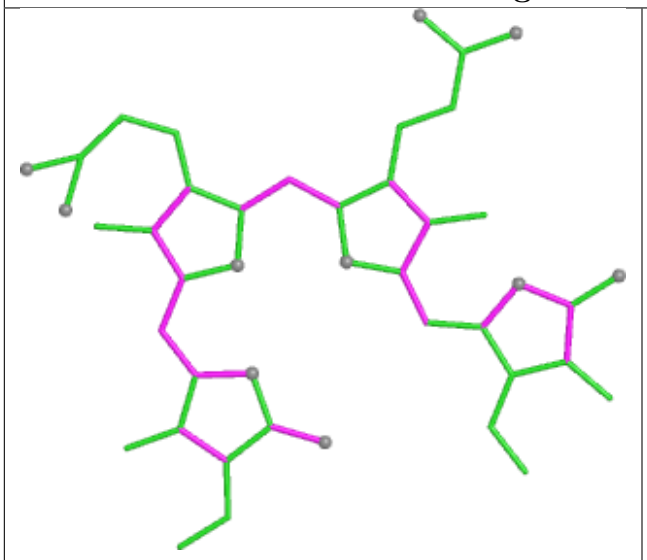


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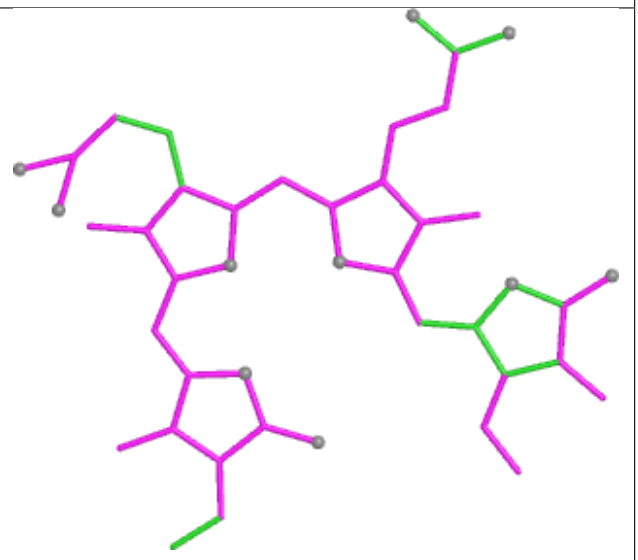


Rings

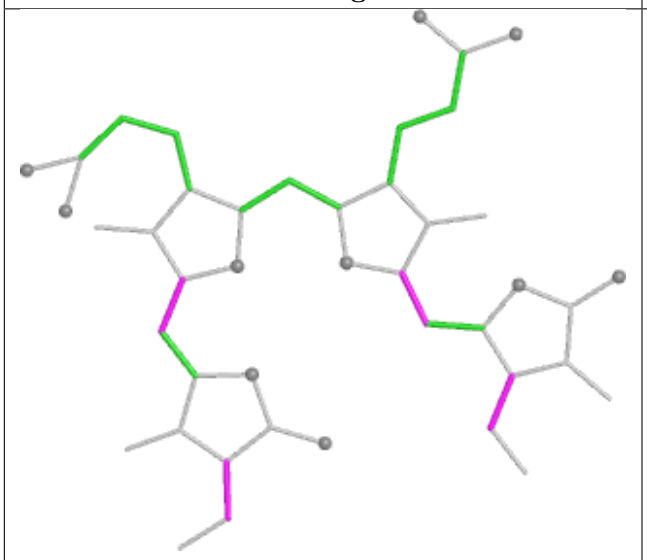
Ligand CYC kC 201



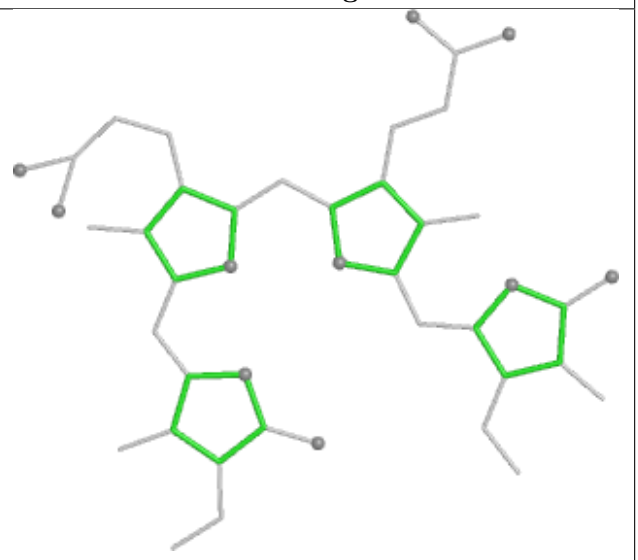
Bond lengths



Bond angles

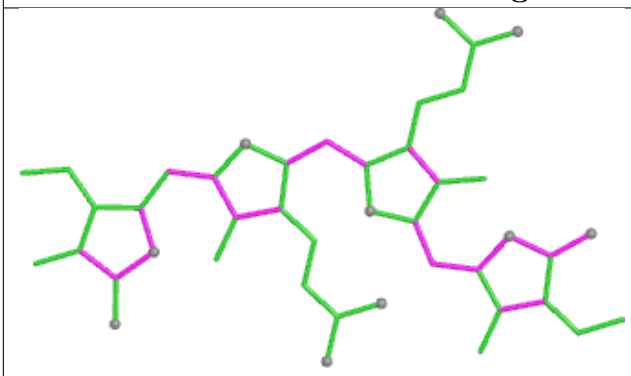


Torsions

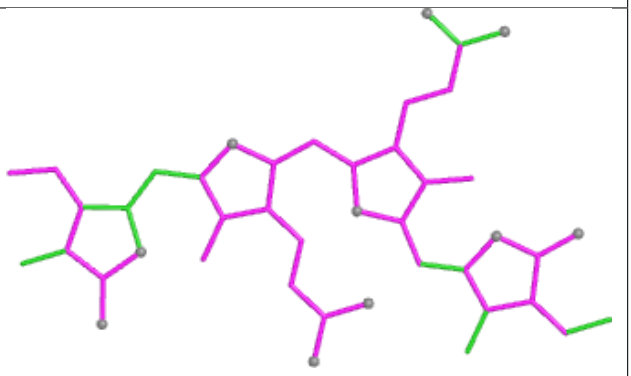


Rings

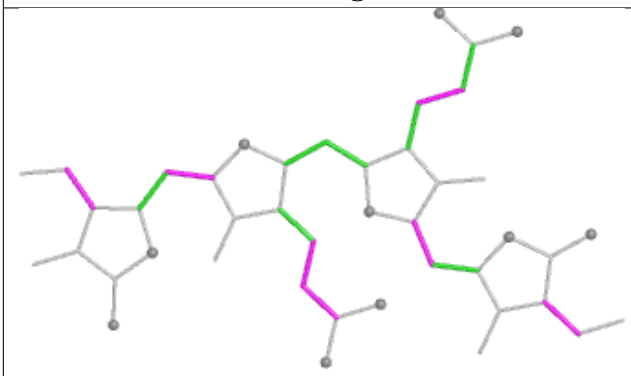
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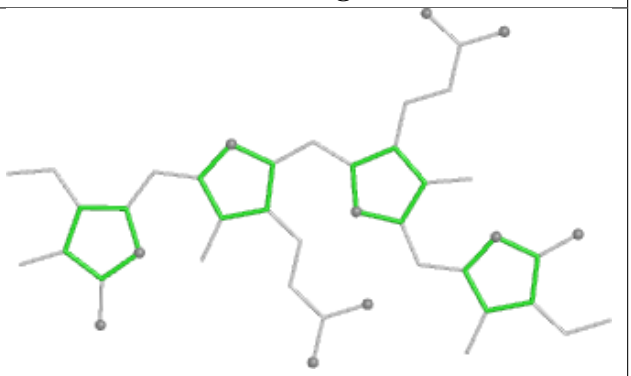
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Bond angles

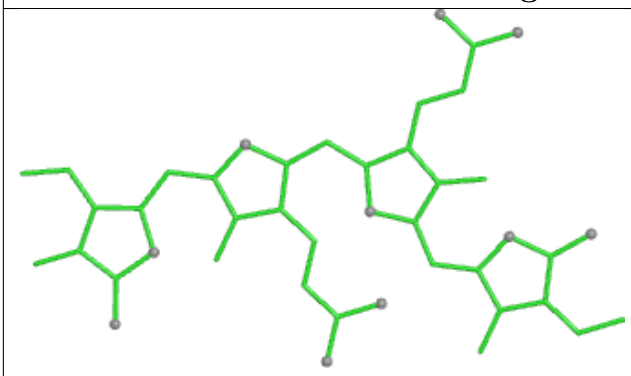


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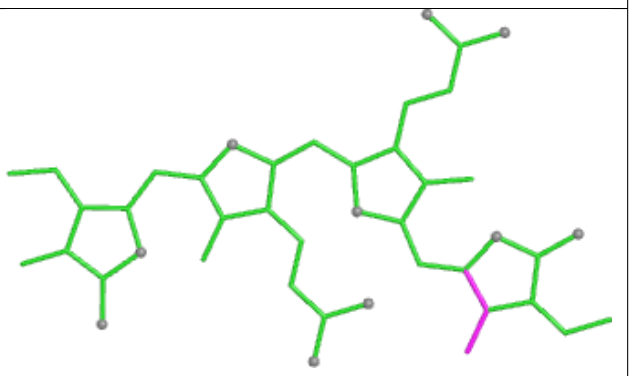


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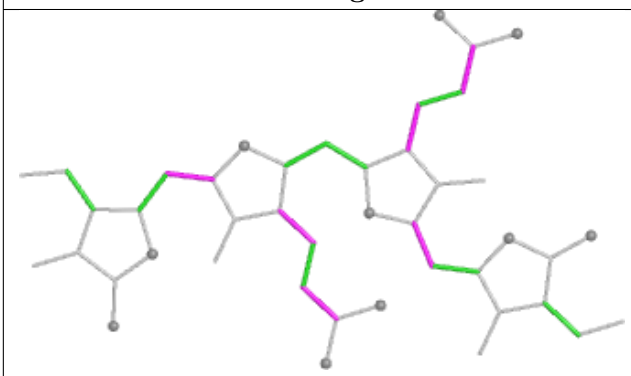
Ligand CYC cI 202



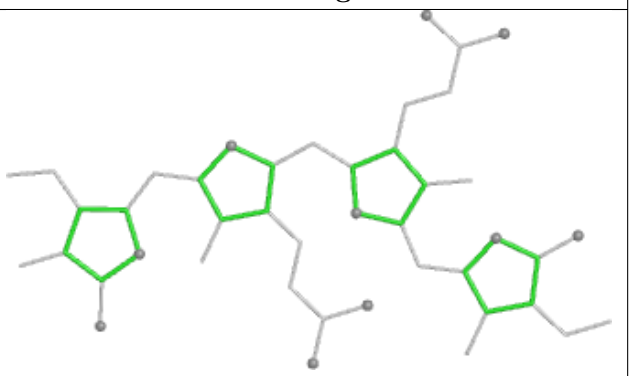
Bond lengths



Bond angles

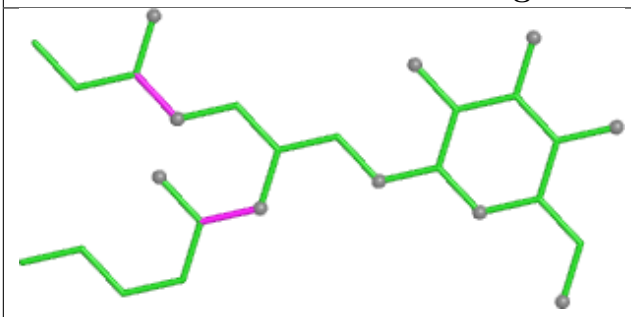


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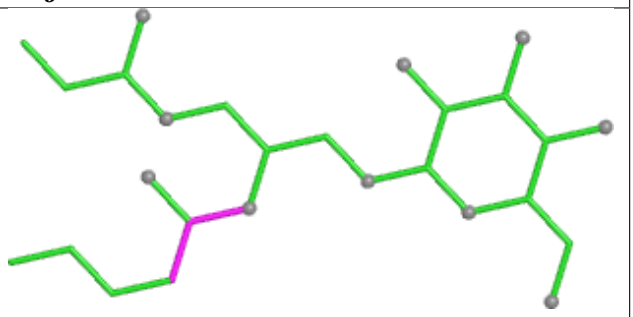


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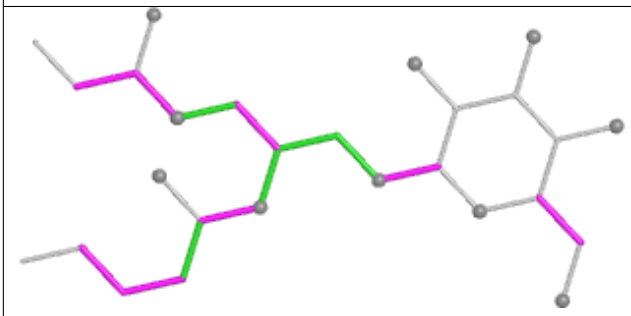
Ligand LMG jD 102



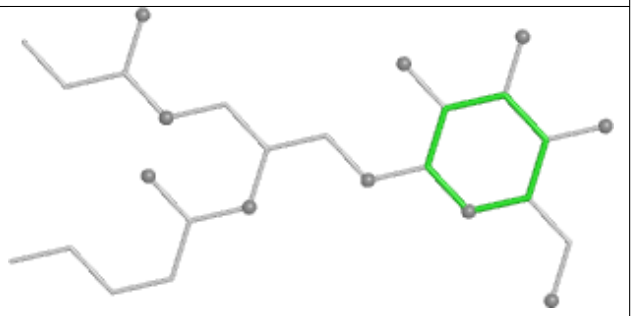
Bond lengths



Bond angles

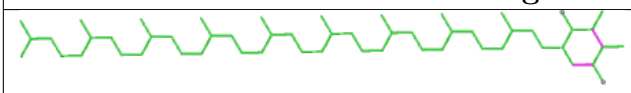


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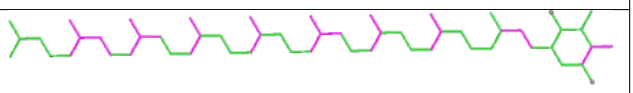


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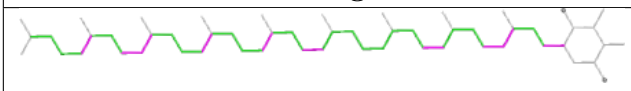
Ligand PL9 aE 408



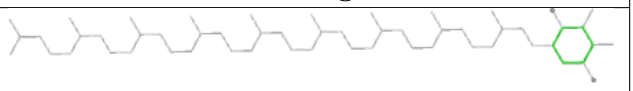
Bond lengths



Bond angles

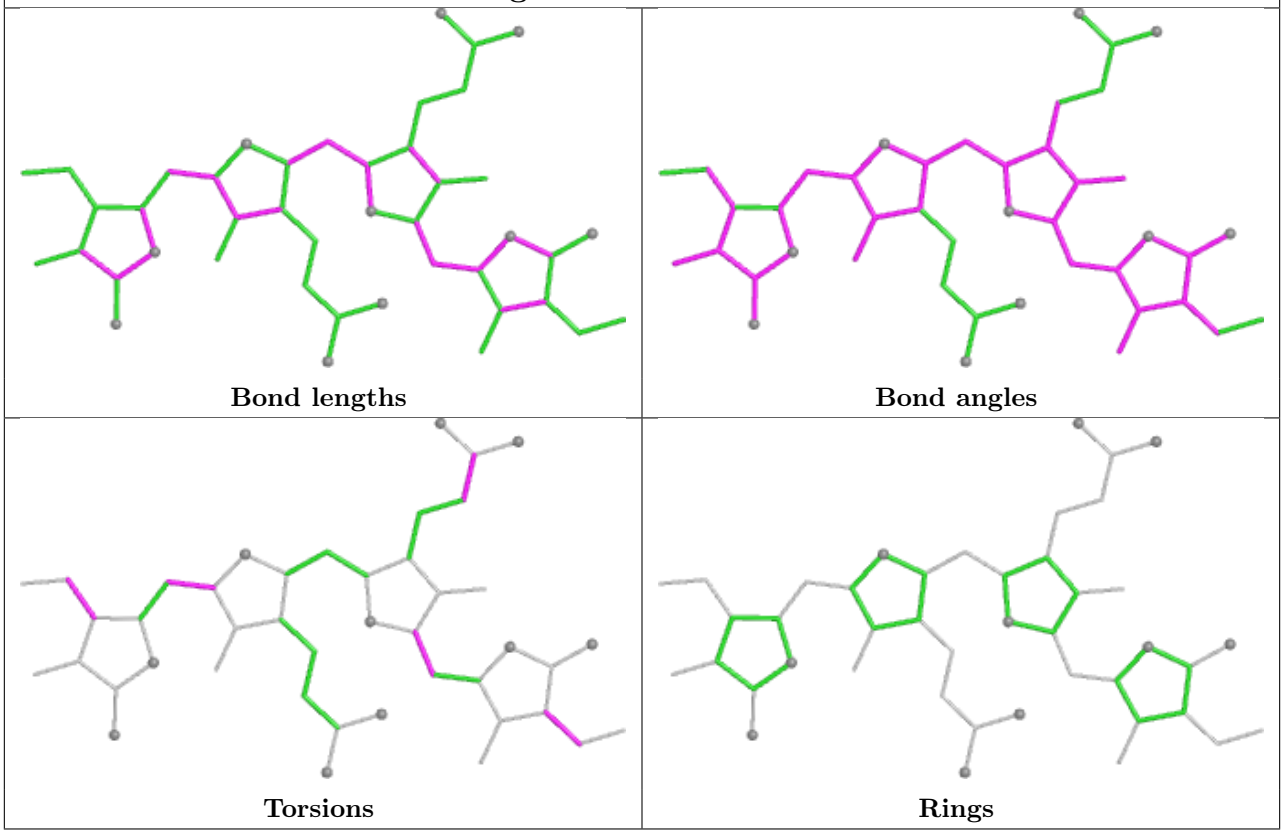


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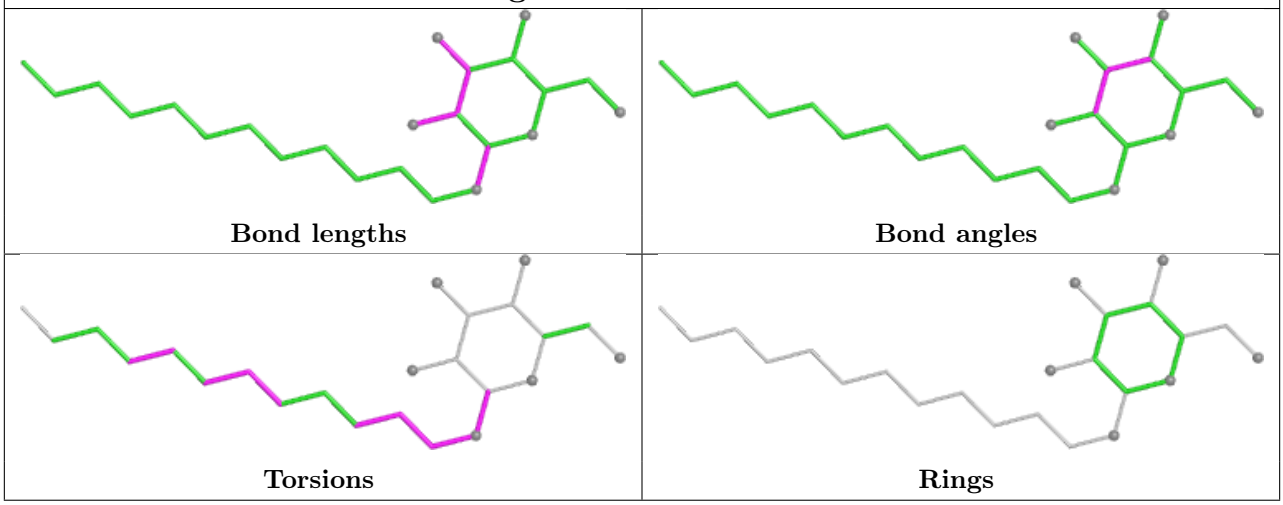


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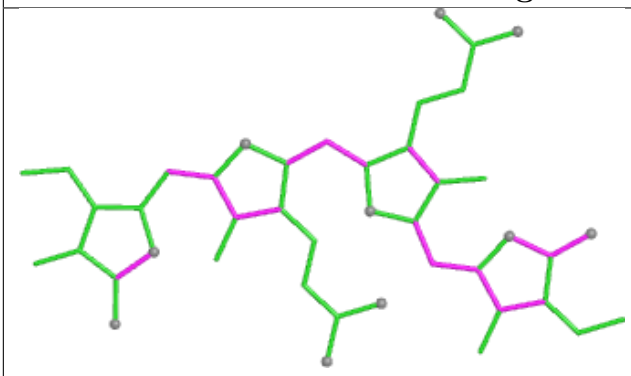
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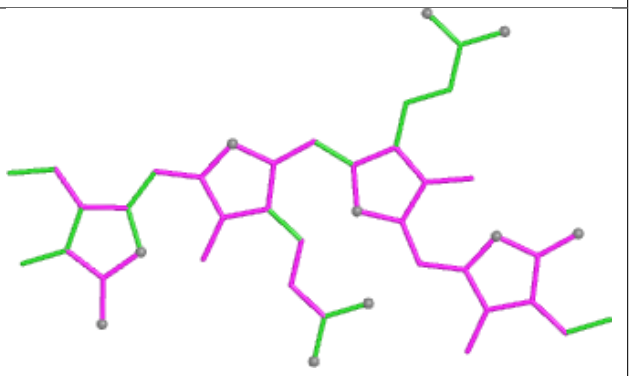
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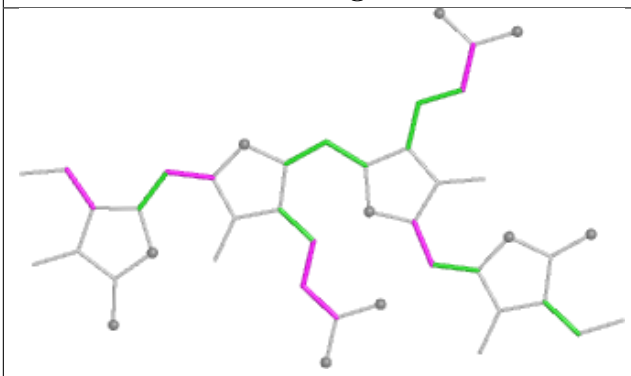
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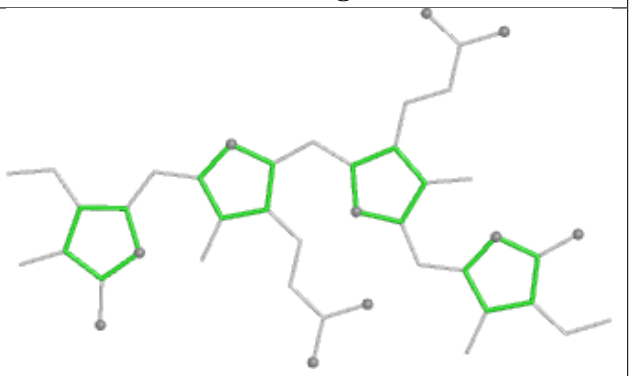
Bond lengths



Bond angles

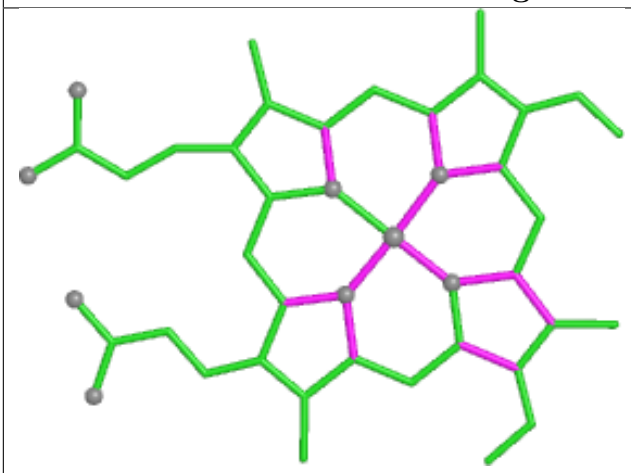


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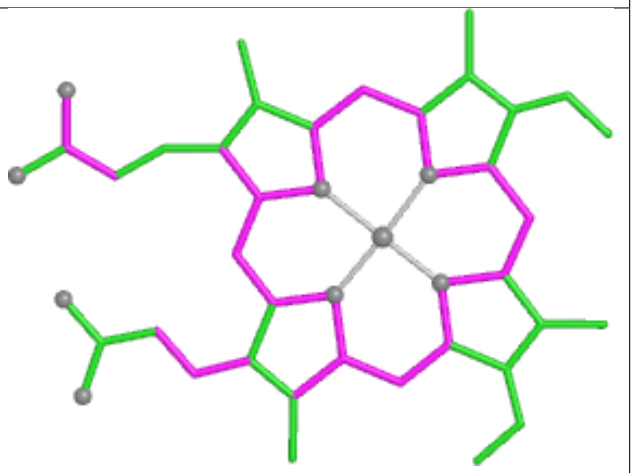


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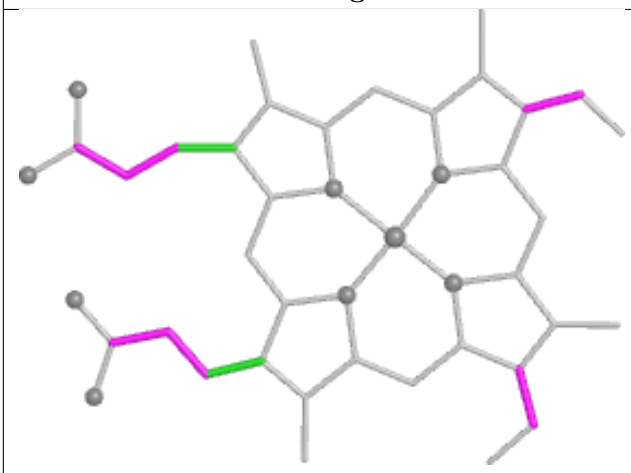
Ligand HEM fD 101



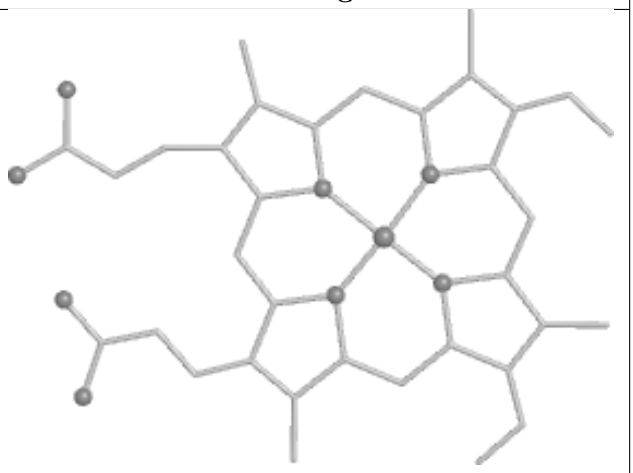
Bond lengths



Bond angles

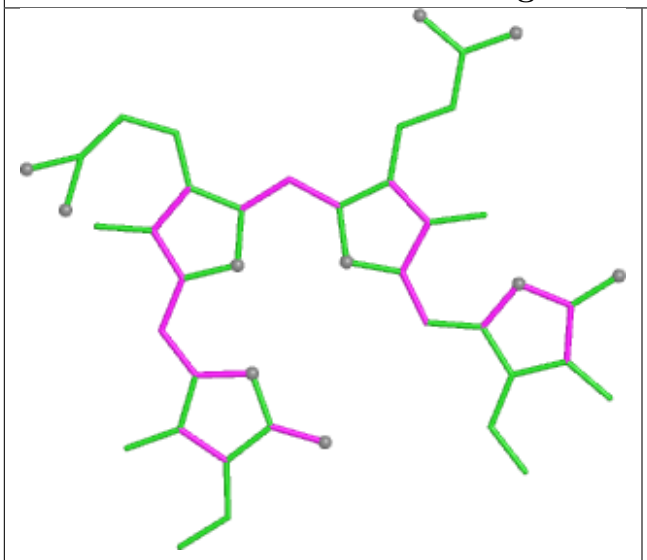


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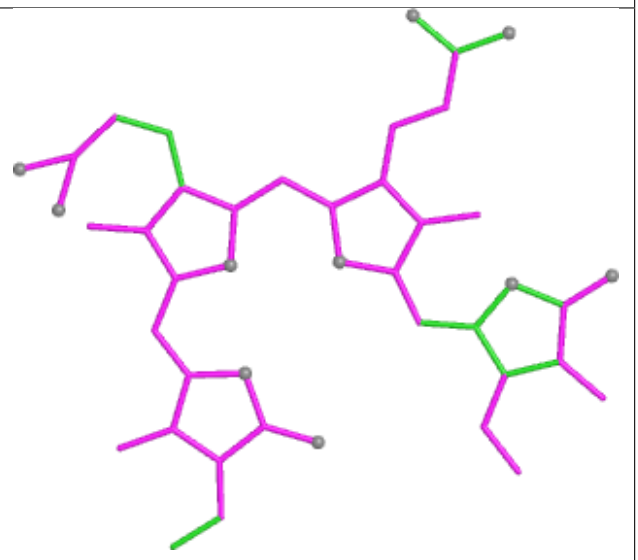


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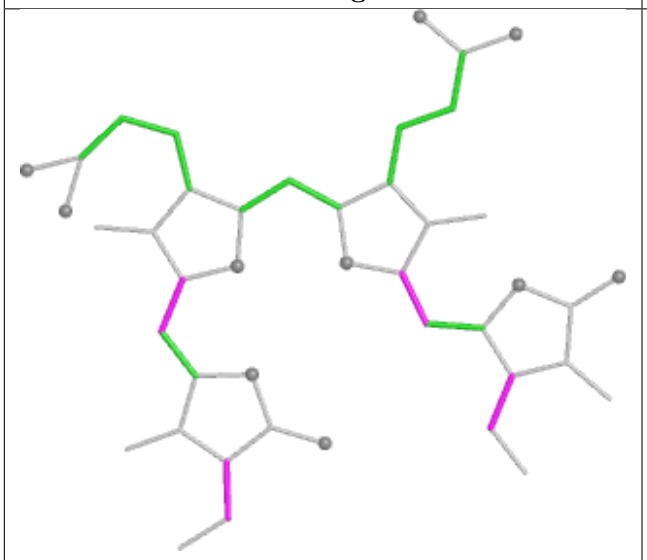
Ligand CYC kJ 201



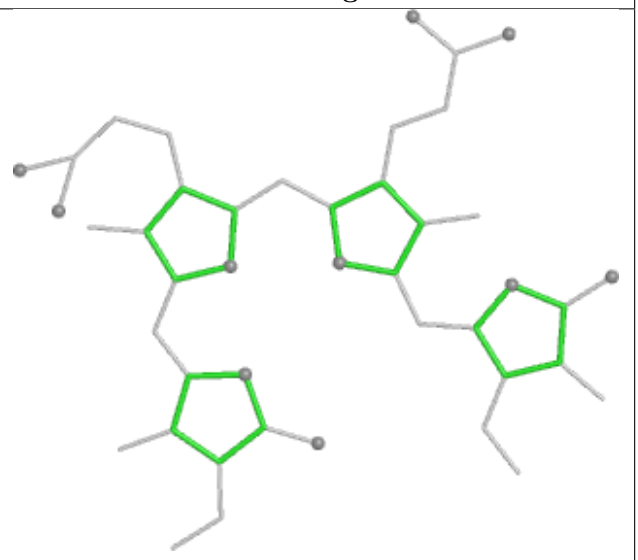
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Bond angles

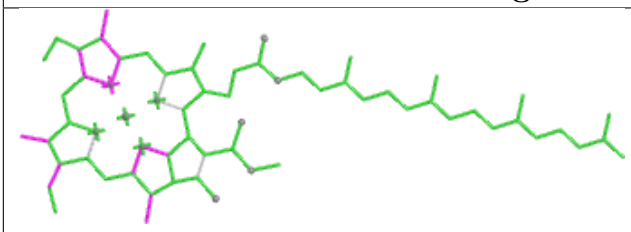


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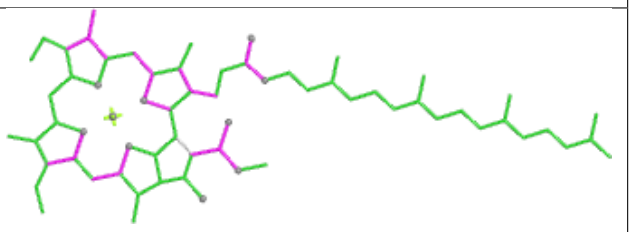


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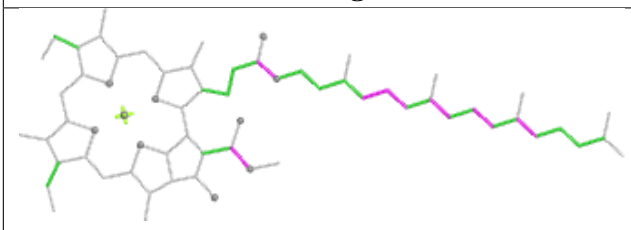
Ligand CLA BE 605



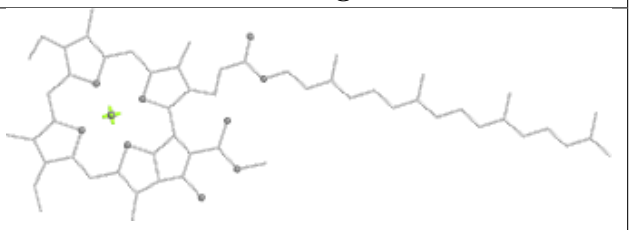
Bond lengths



Bond angles



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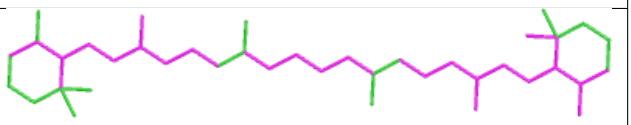


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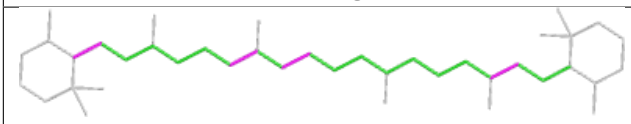
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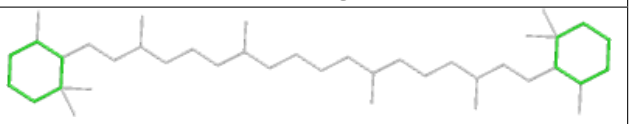
Bond lengths



Bond angles

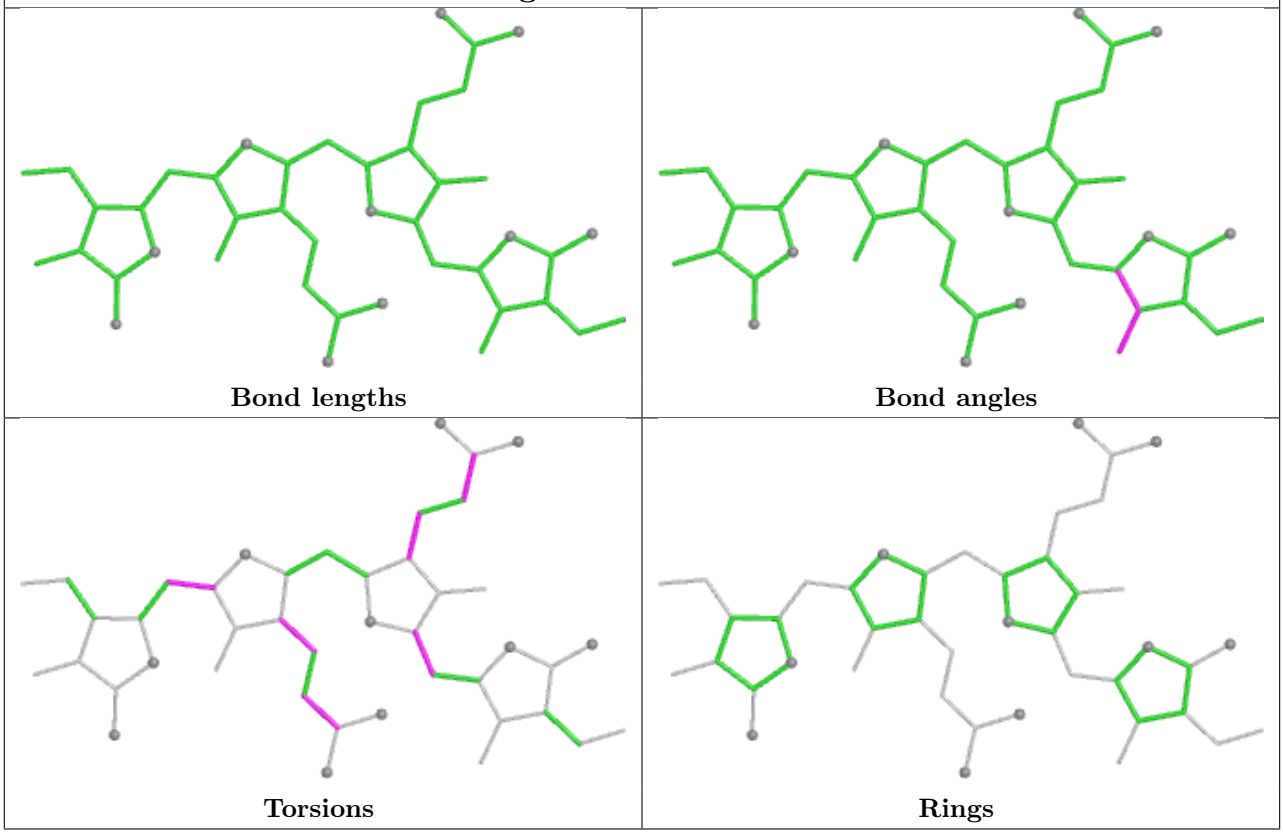


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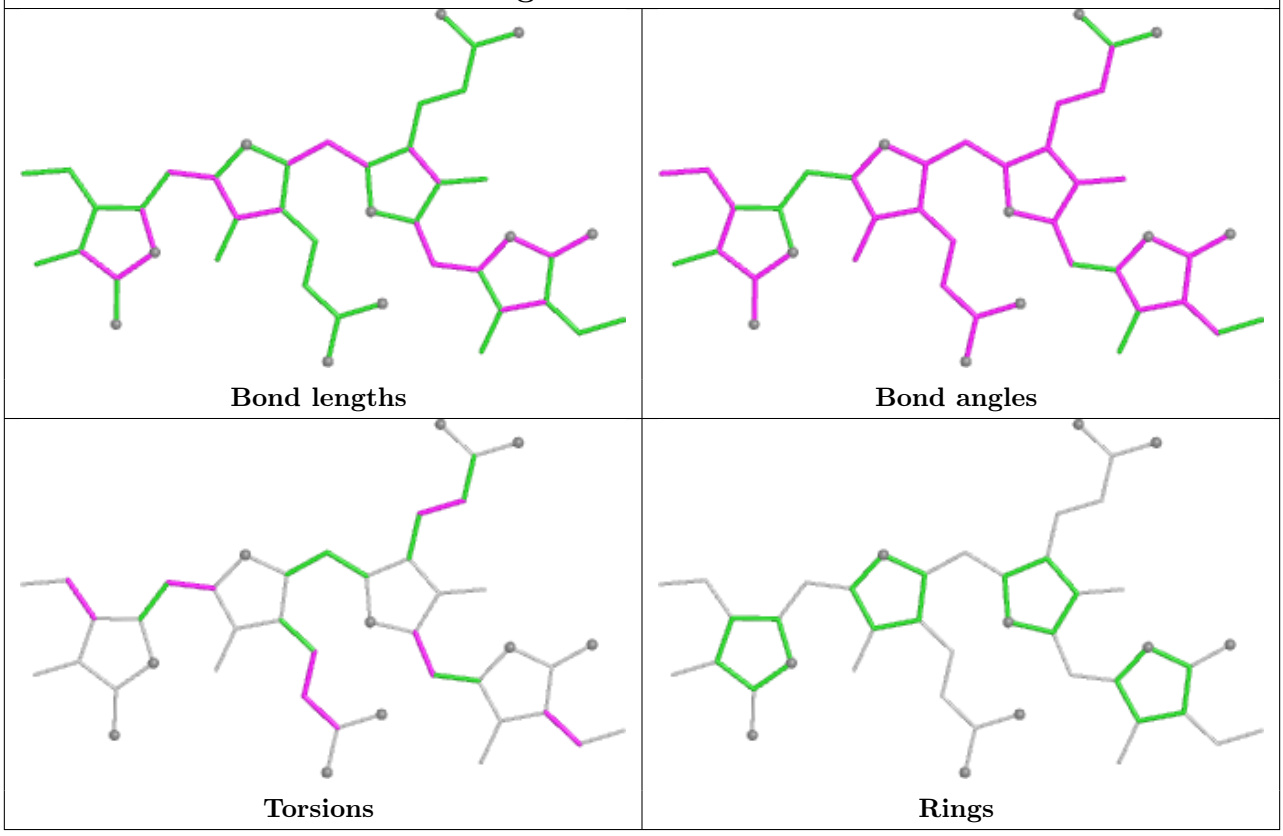


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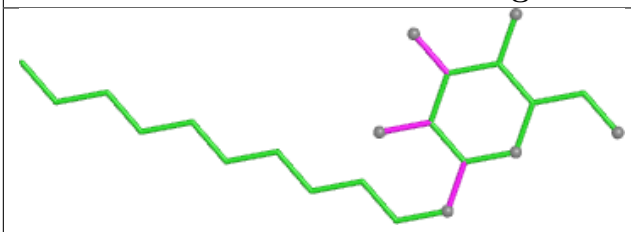
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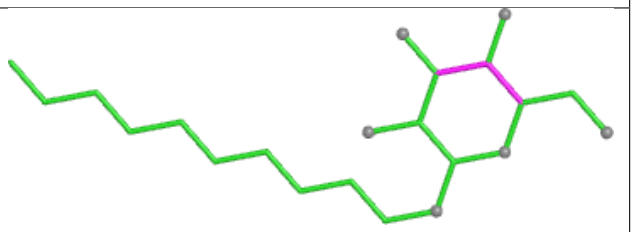
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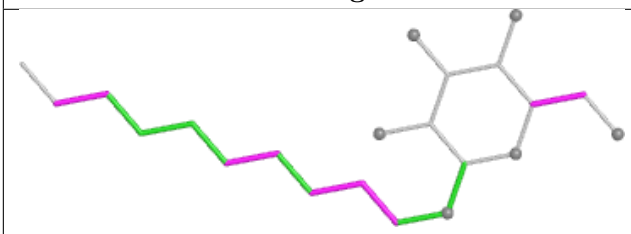
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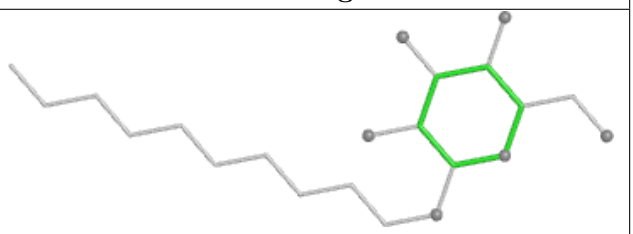
Bond lengths



Bond angles

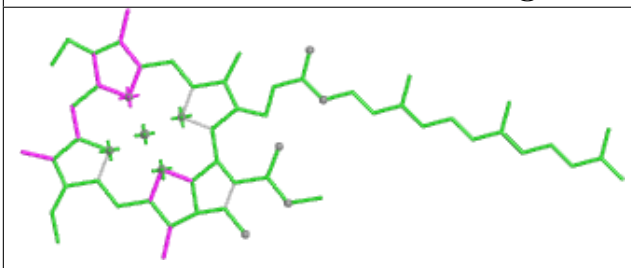


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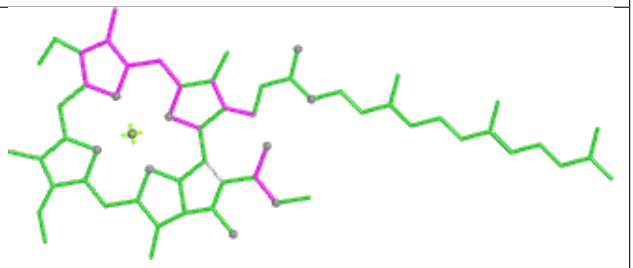


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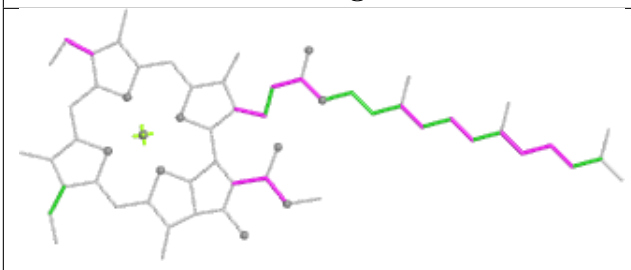
Ligand CLA IE 101



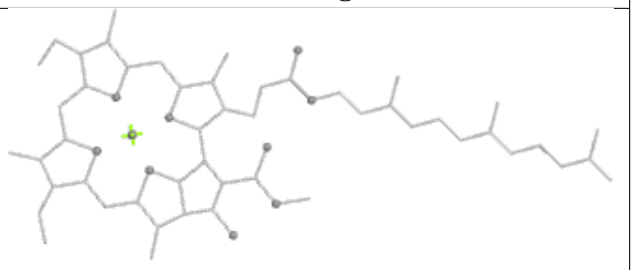
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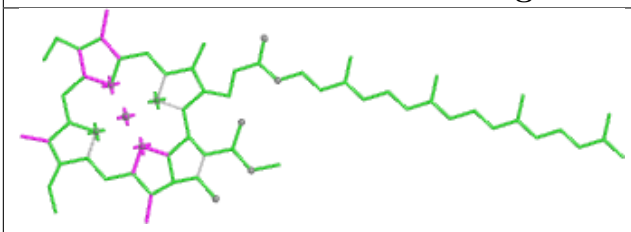
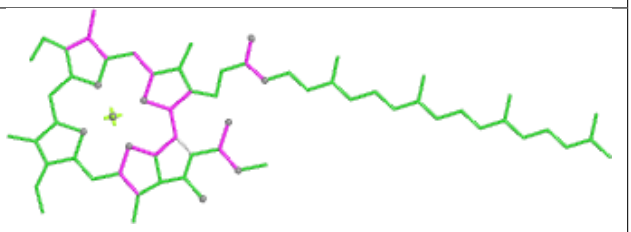
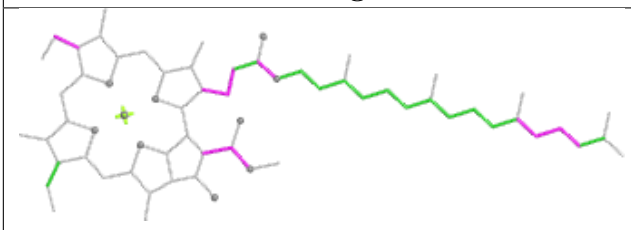
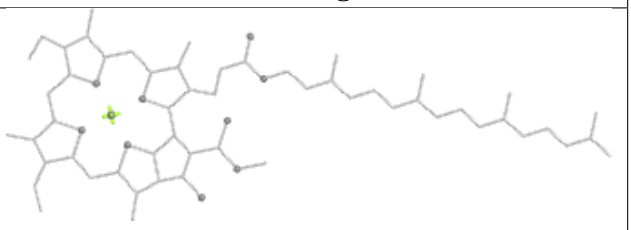
Bond angles



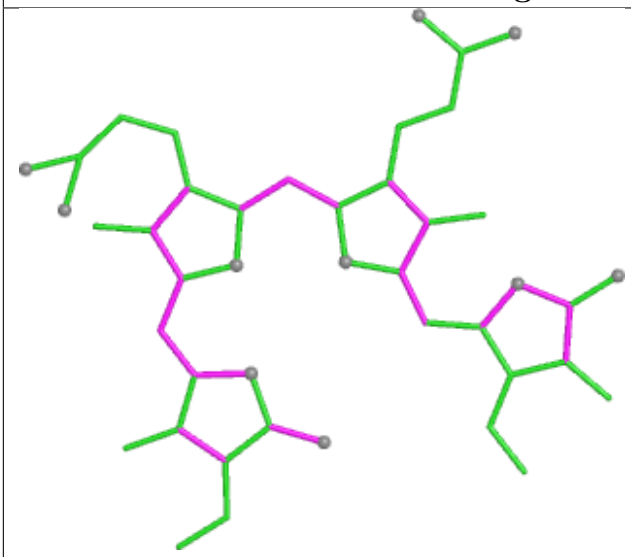
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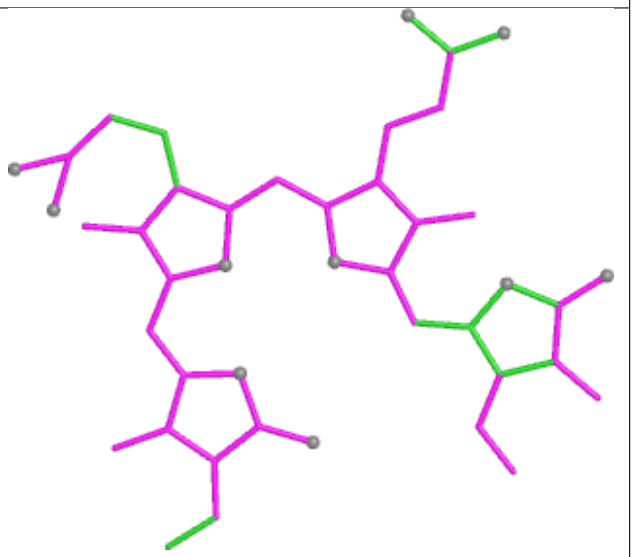
Rings

Ligand CLA bE 609	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

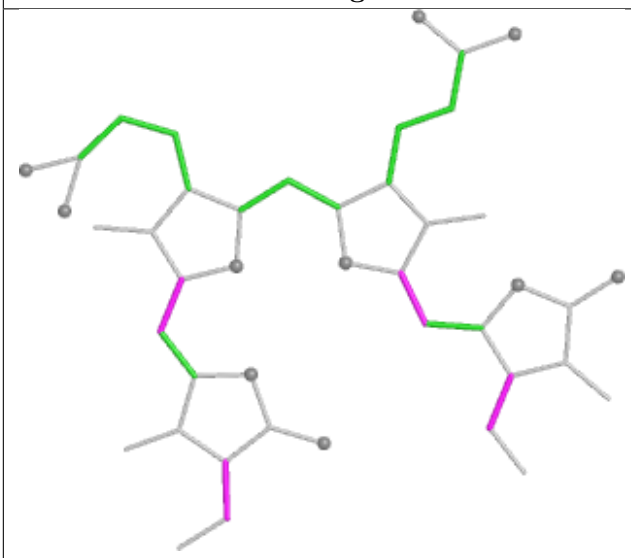
Ligand CYC eC 201



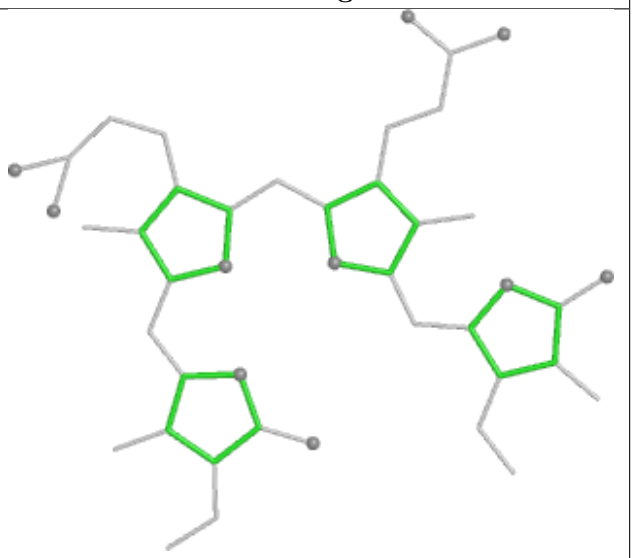
Bond lengths



Bond angles



Torsions

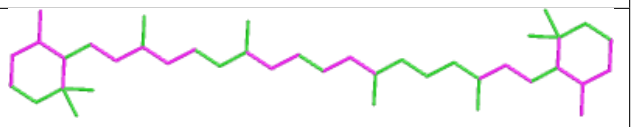


Rings

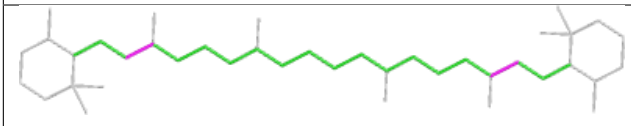
Ligand BCR b1 618



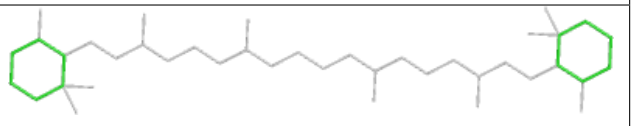
Bond lengths



Bond angles

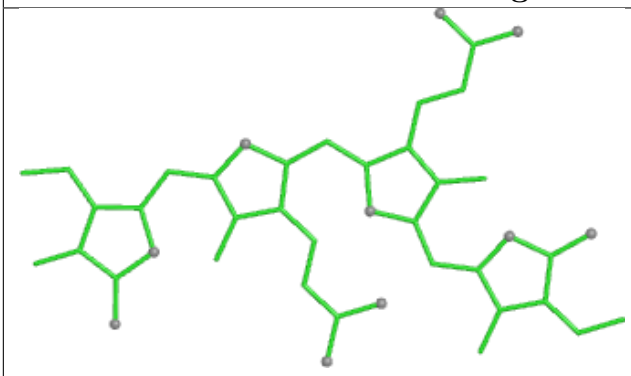


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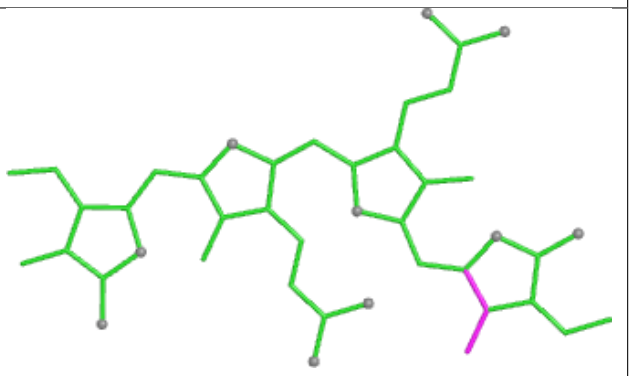


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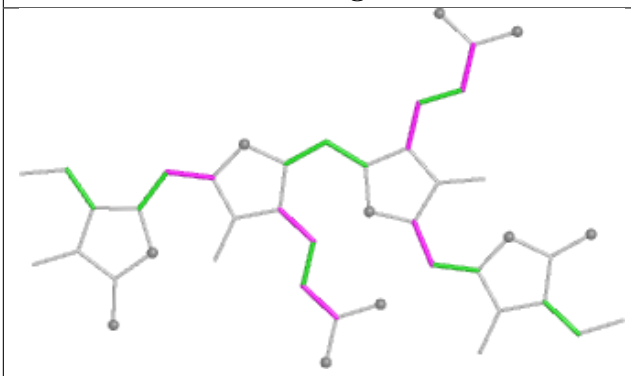
Ligand CYC m8 201



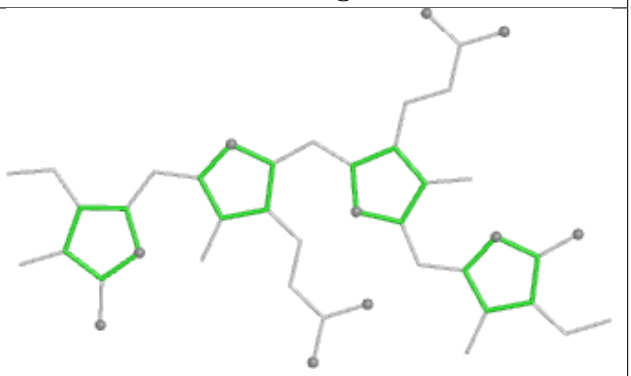
Bond lengths



Bond angles

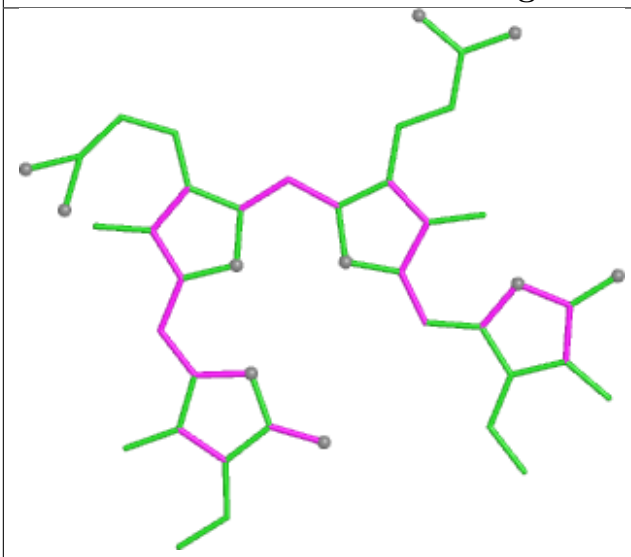


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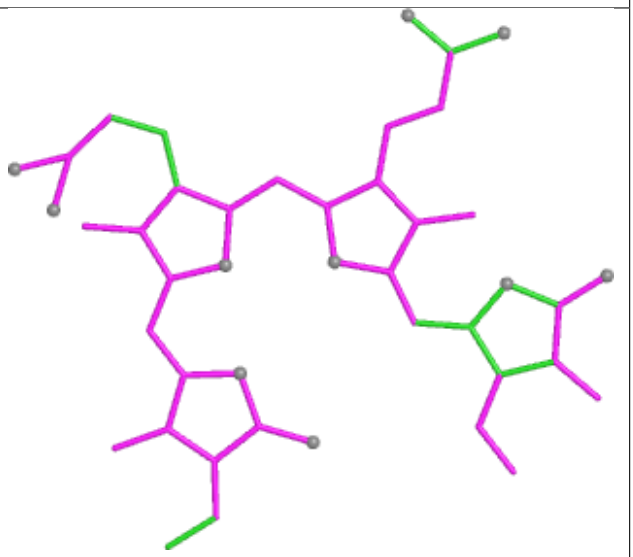


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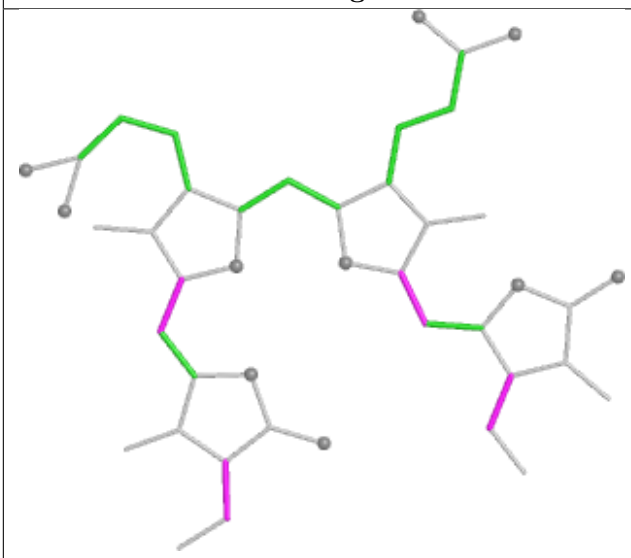
Ligand CYC e7 201



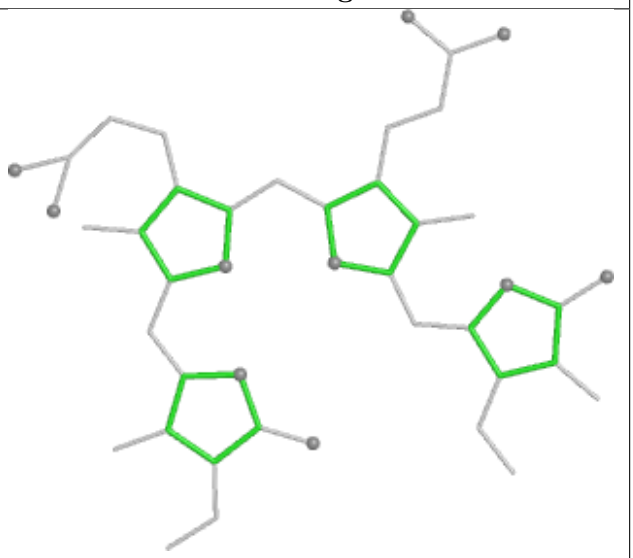
Bond lengths



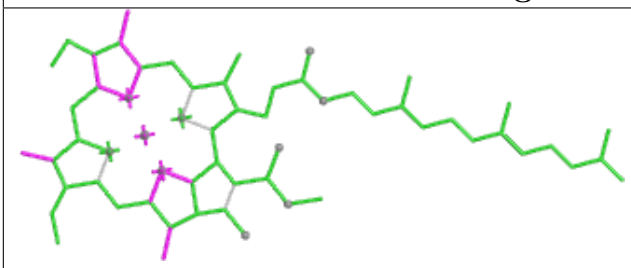
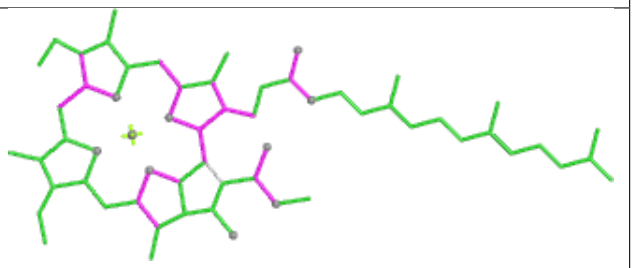
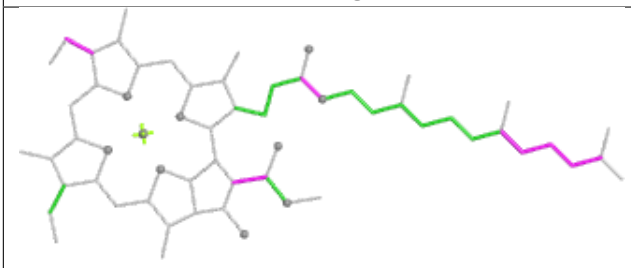
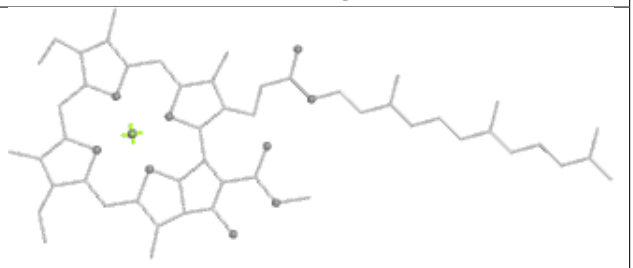
Bond angles

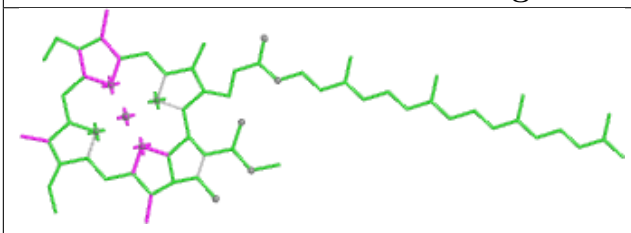
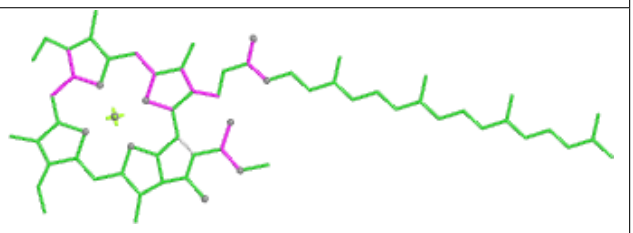
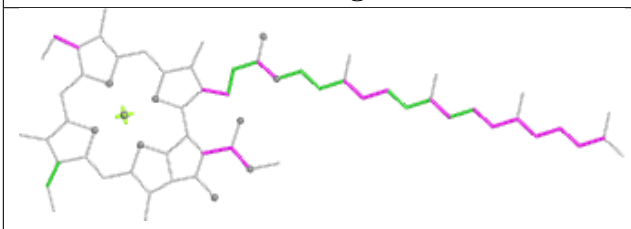
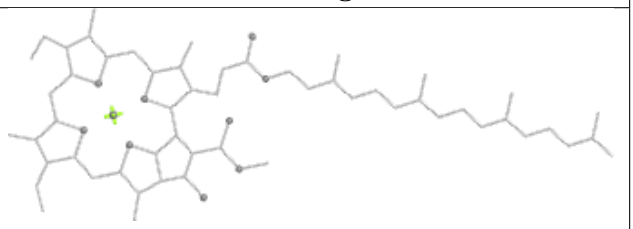


Torsions

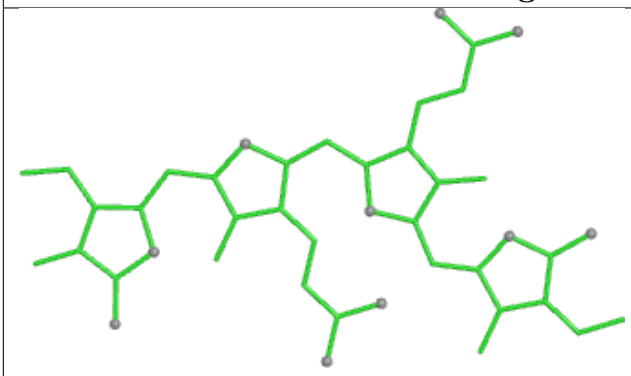


Rings

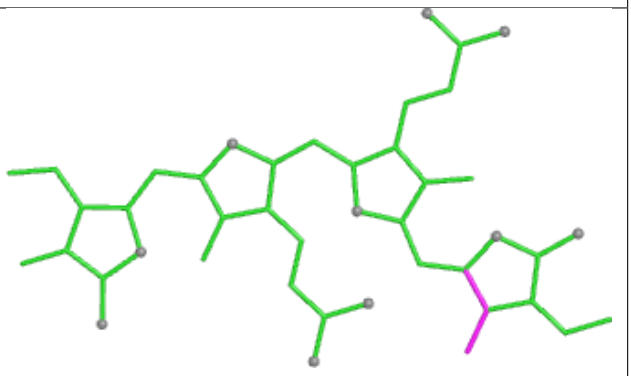
Ligand CLA H1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA XE 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

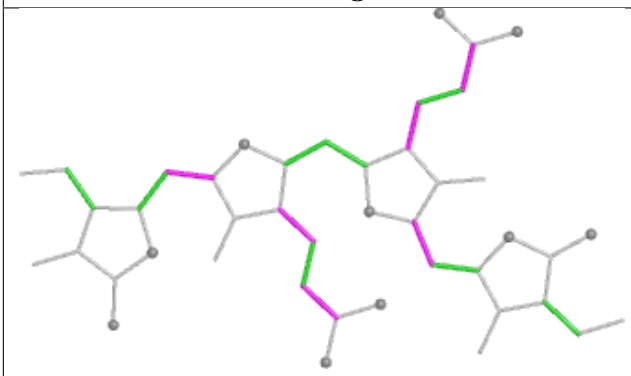
Ligand CYC e3 202



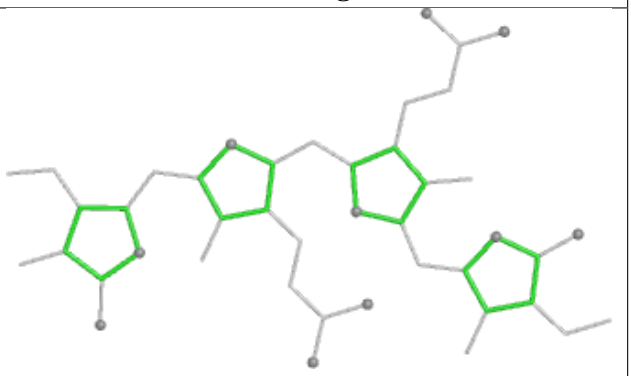
Bond lengths



Bond angles

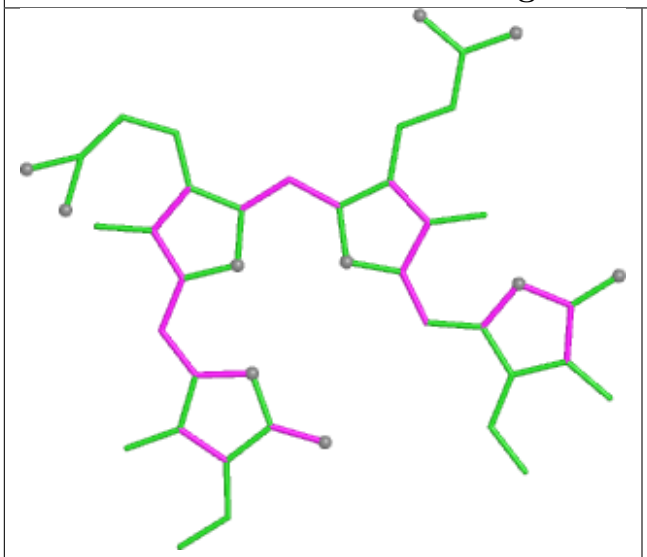


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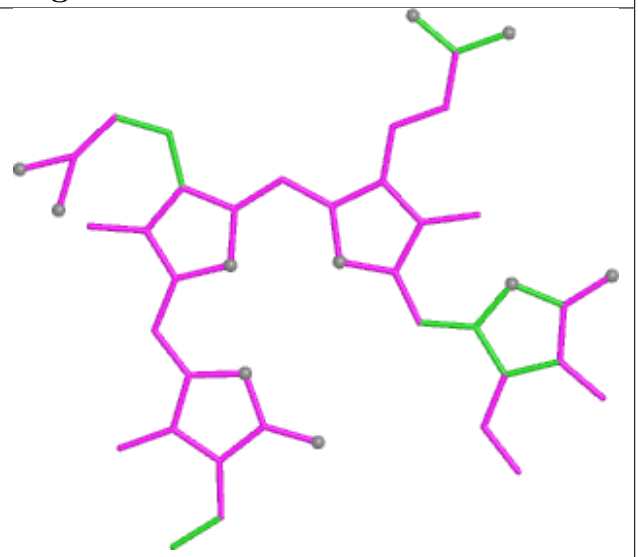


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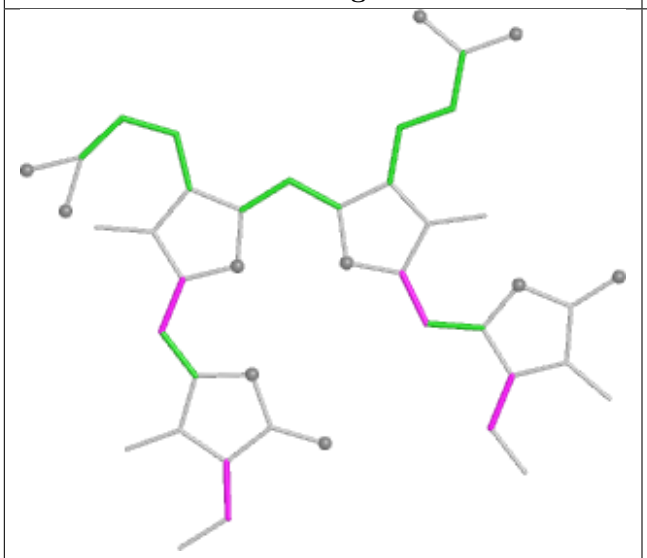
Ligand CYC g6 202



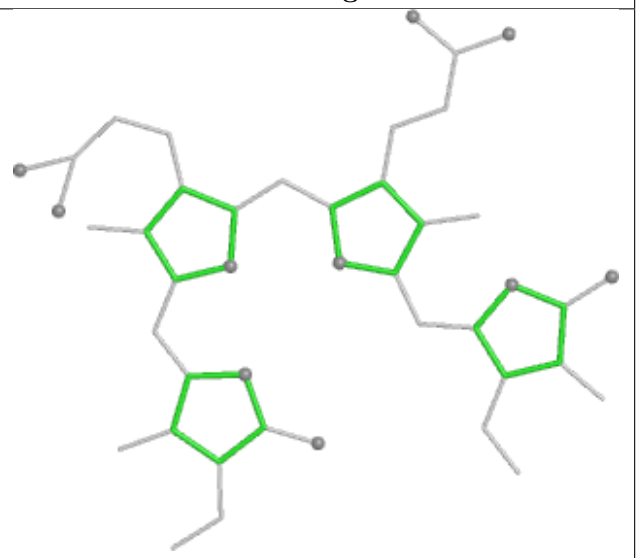
Bond lengths



Bond angles

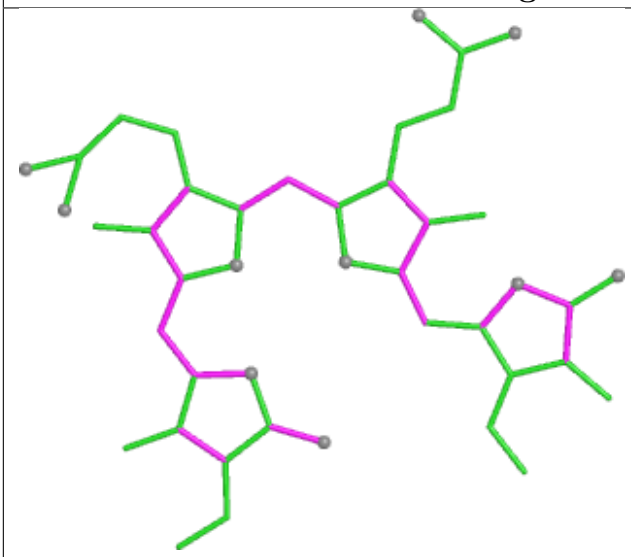


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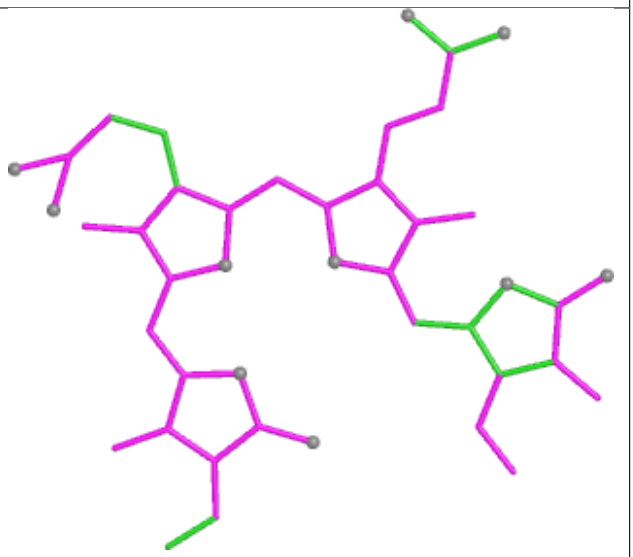


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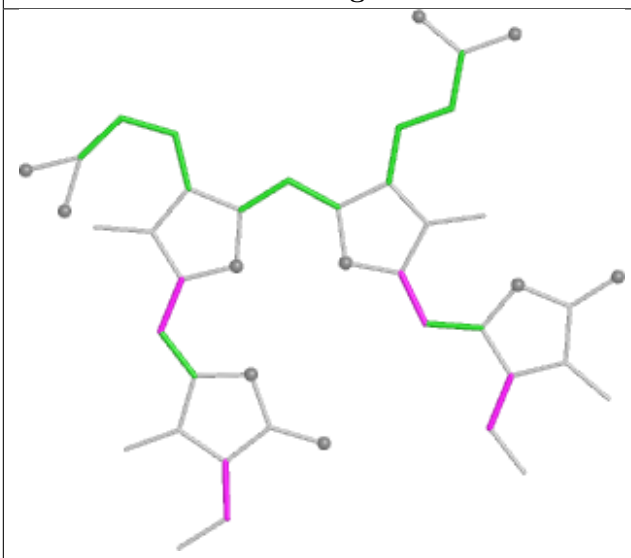
Ligand CYC kI 201



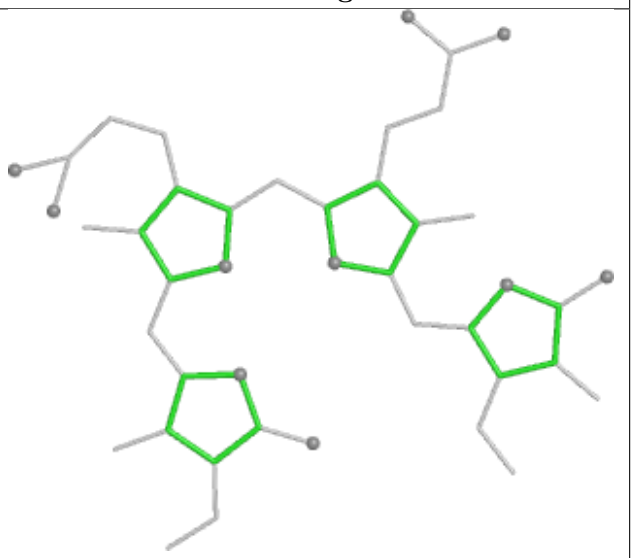
Bond lengths



Bond angles

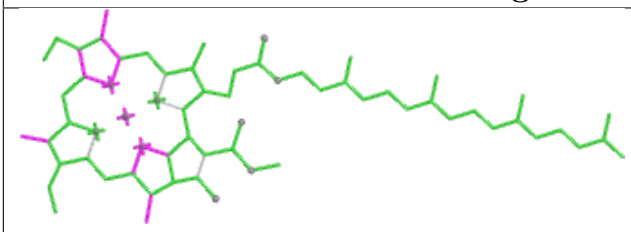


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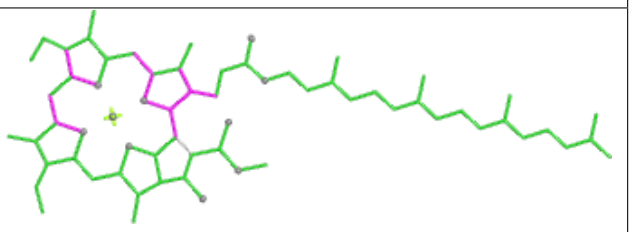


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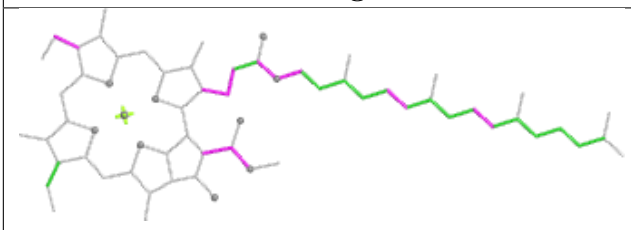
Ligand CLA DE 405



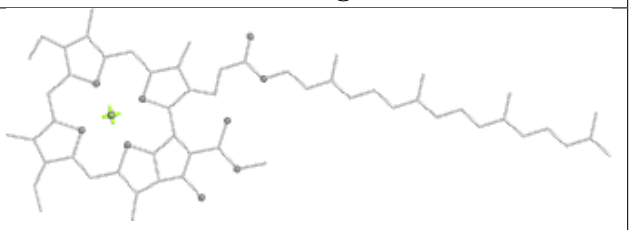
Bond lengths



Bond angles

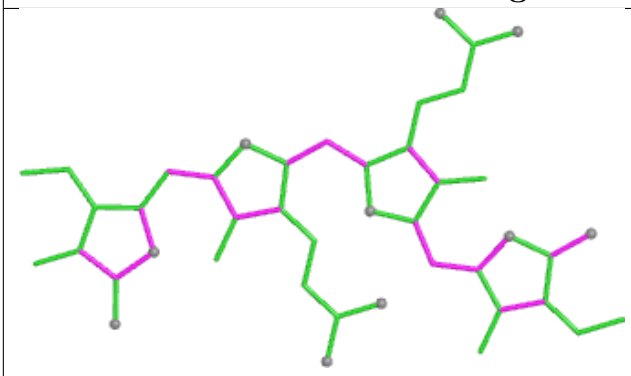


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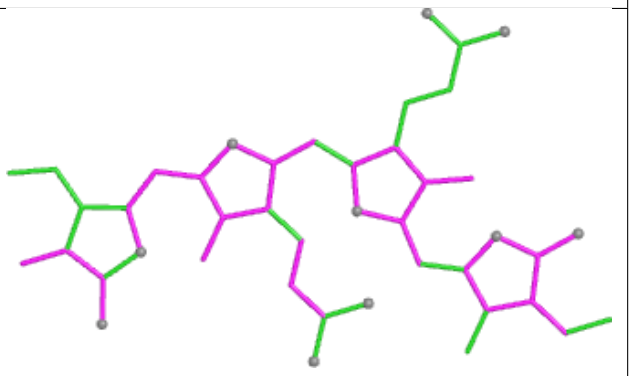


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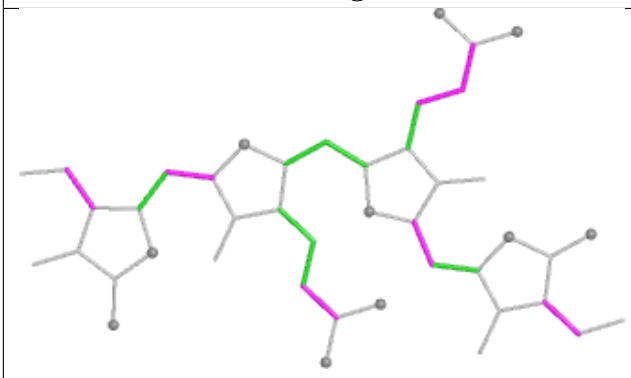
Ligand CYC wB 201



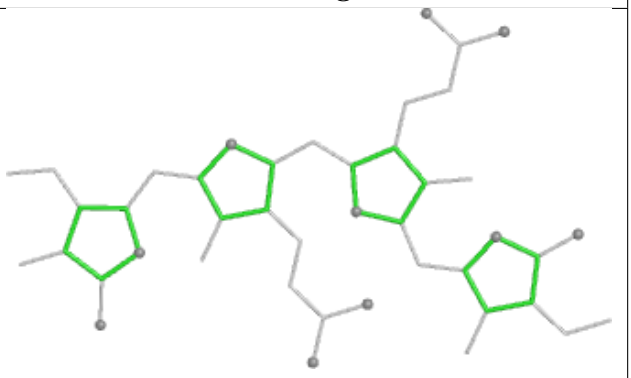
Bond lengths



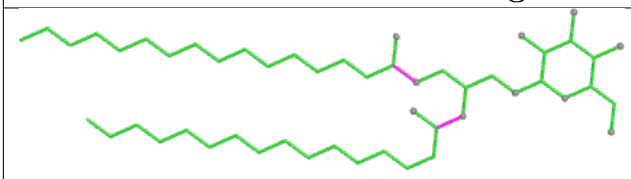
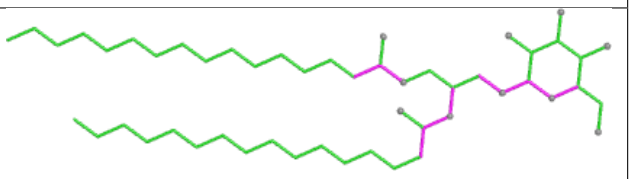
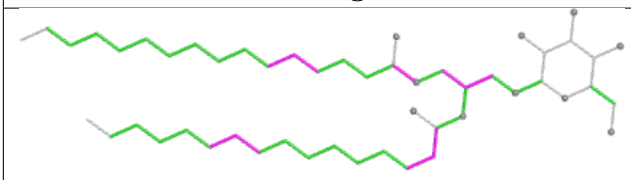
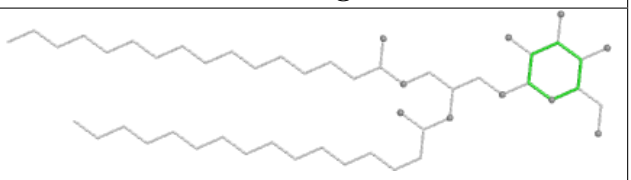
Bond angles

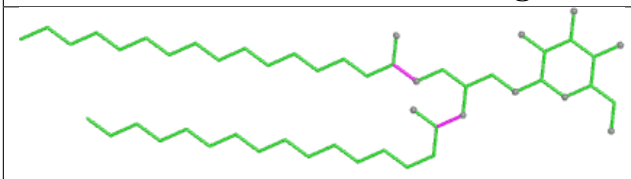
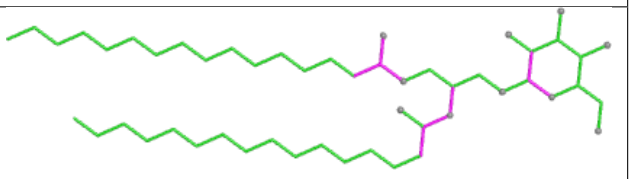
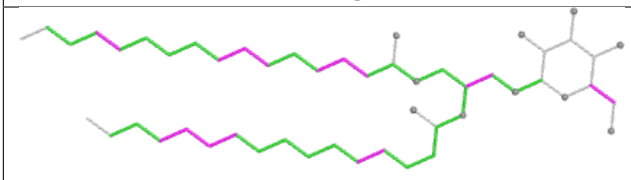
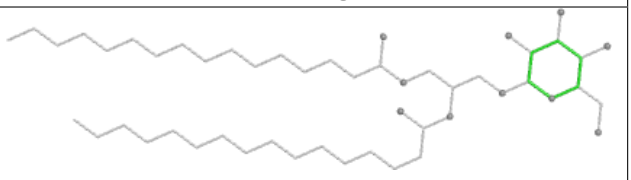


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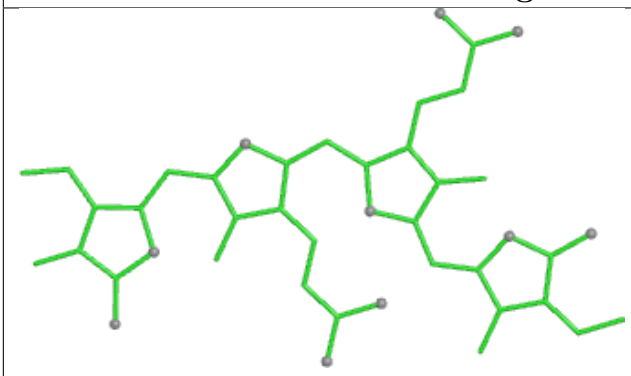


Rings

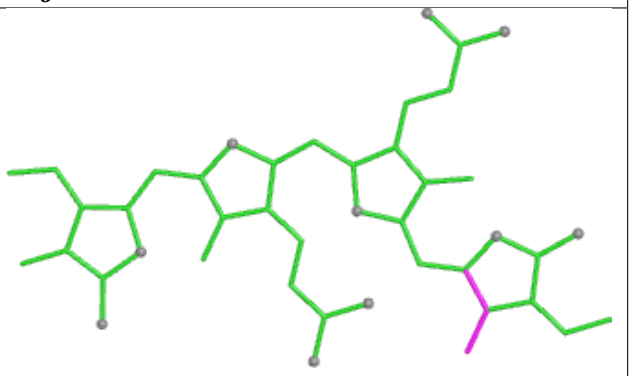
Ligand LMG CE 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG d1 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

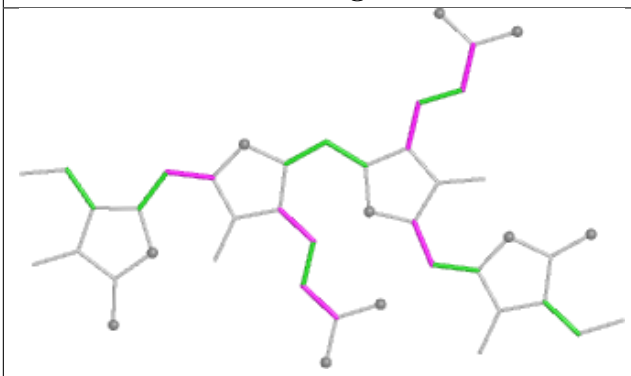
Ligand CYC jA 202



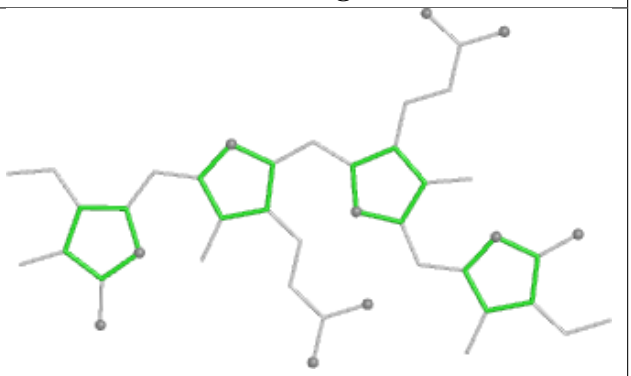
Bond lengths



Bond angles

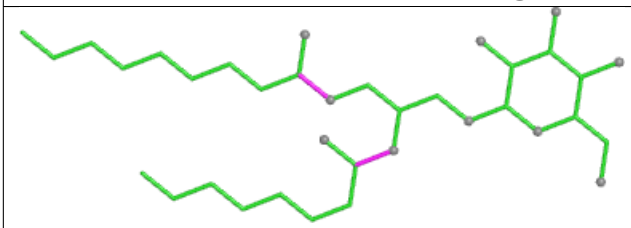


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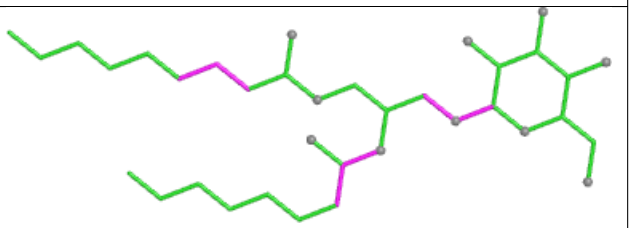


Rings

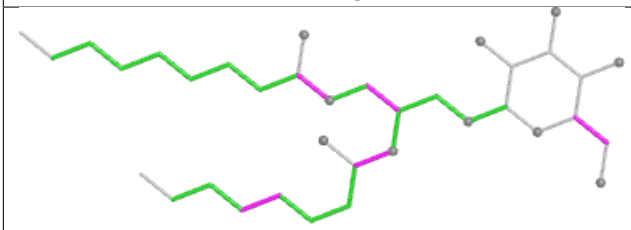
Ligand LMG T1 101



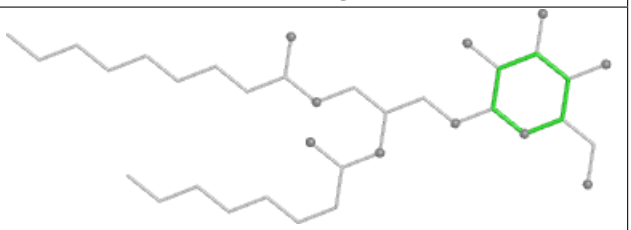
Bond lengths



Bond angles

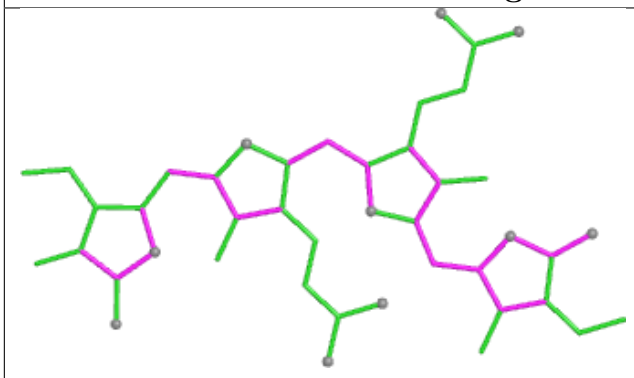


Torsions

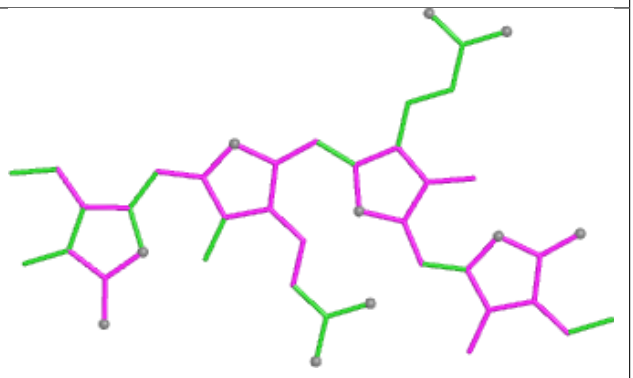


Rings

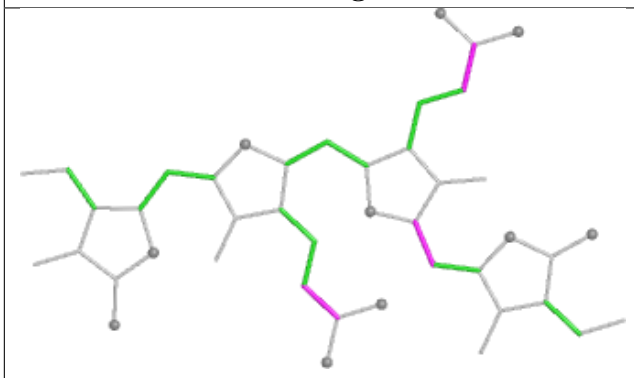
Ligand CYC C4 1001



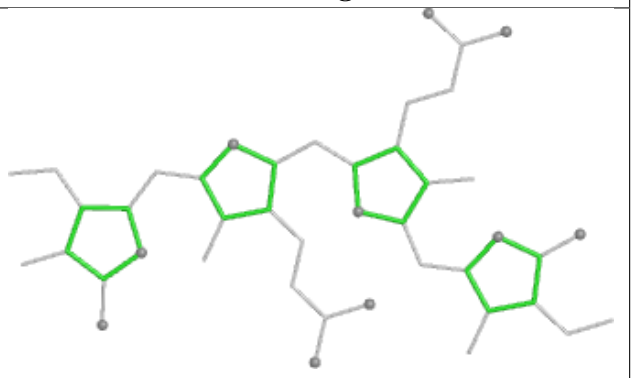
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Bond angles

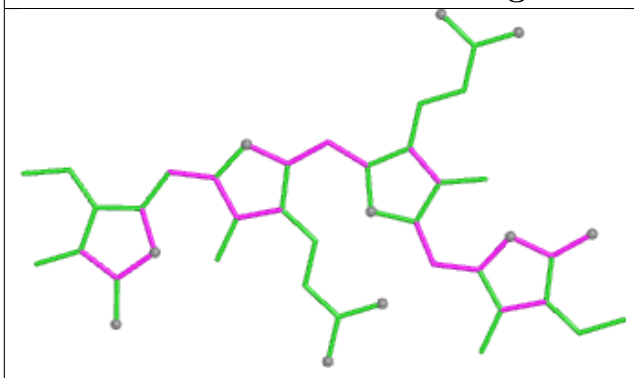


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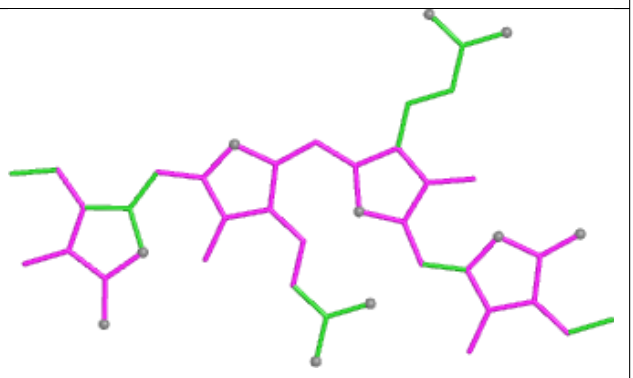


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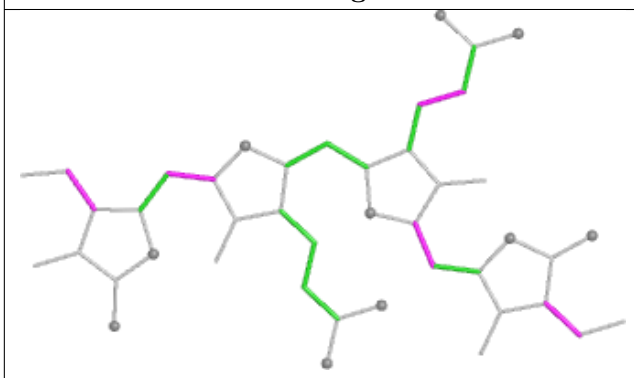
Ligand CYC GG 201



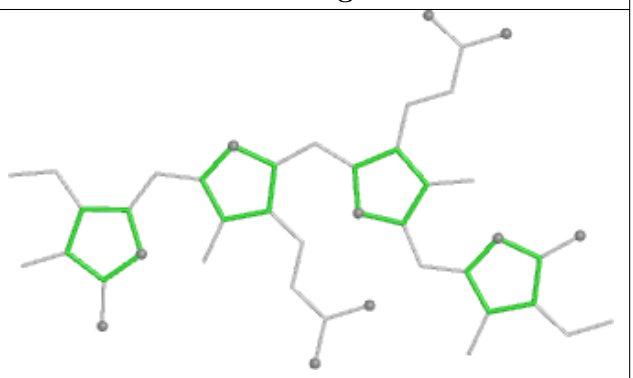
Bond lengths



Bond angles

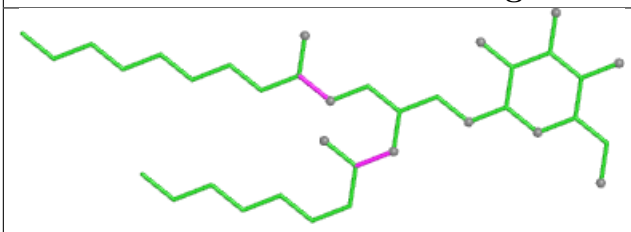


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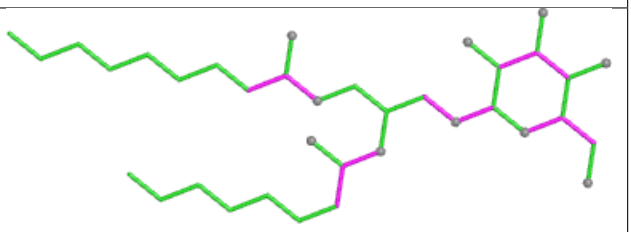


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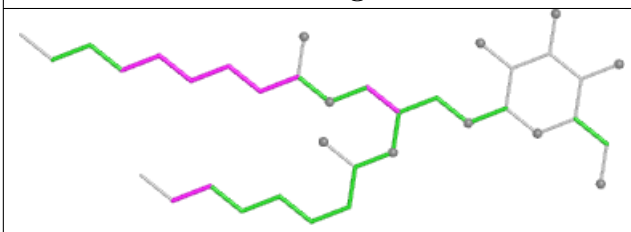
Ligand LMG AD 408



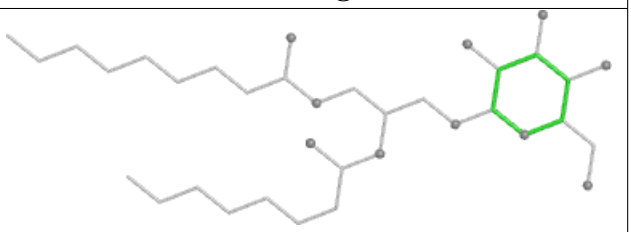
Bond lengths



Bond angles

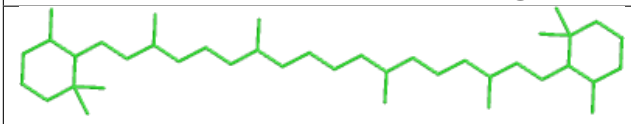


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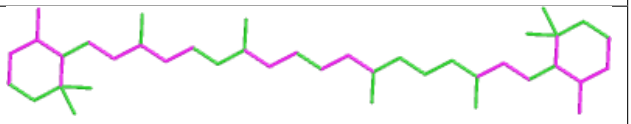


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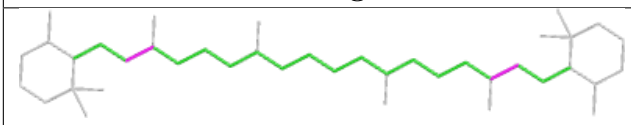
Ligand BCR bD 618



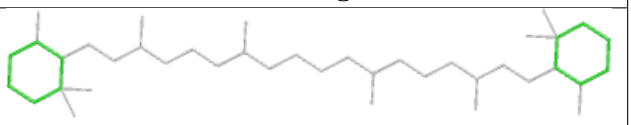
Bond lengths



Bond angles

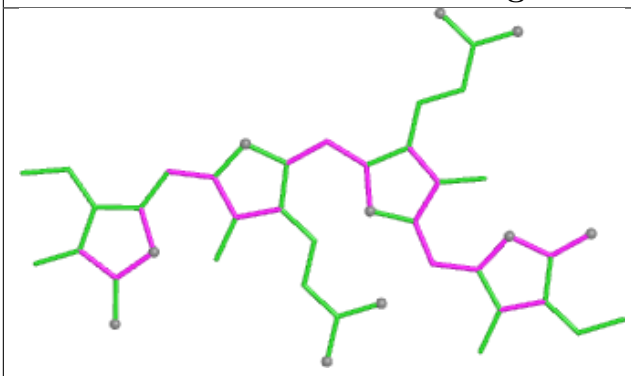


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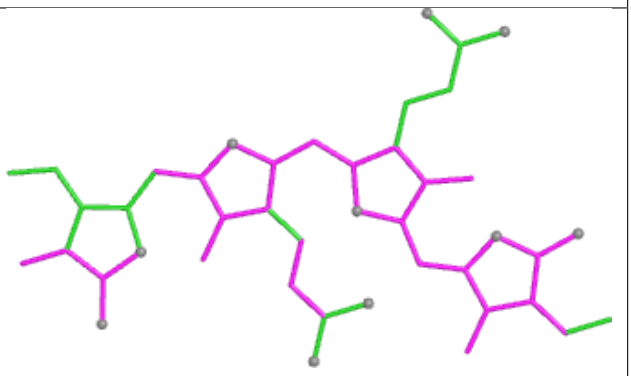


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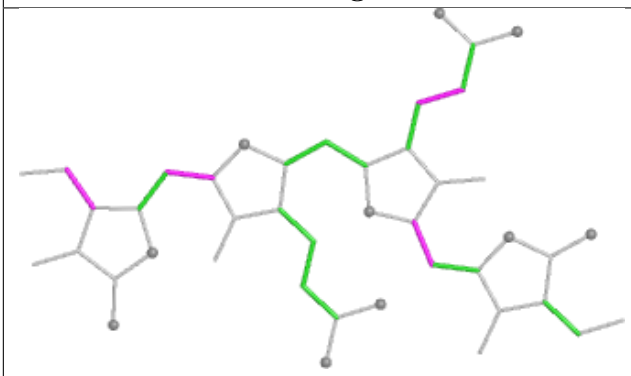
Ligand CYC OG 201



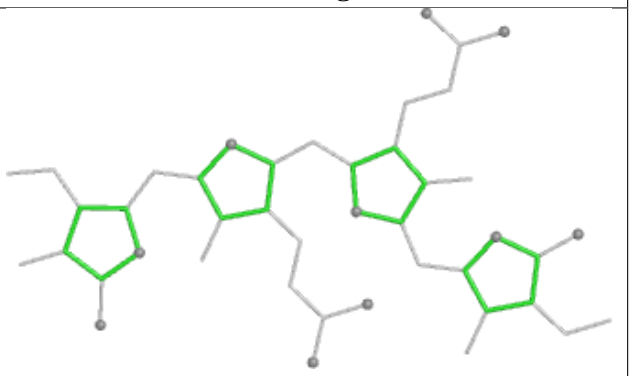
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Bond angles

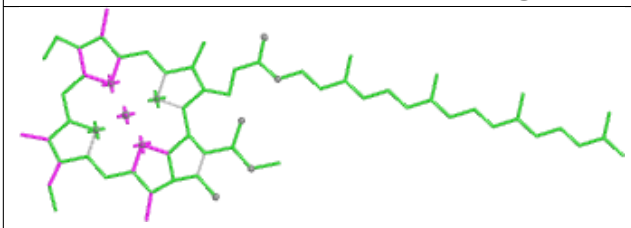


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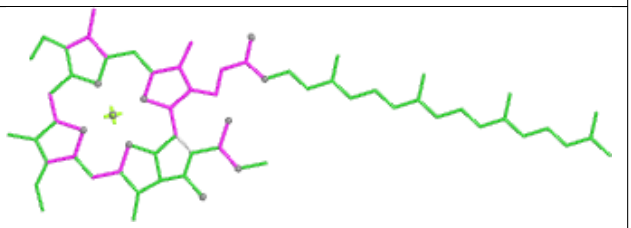


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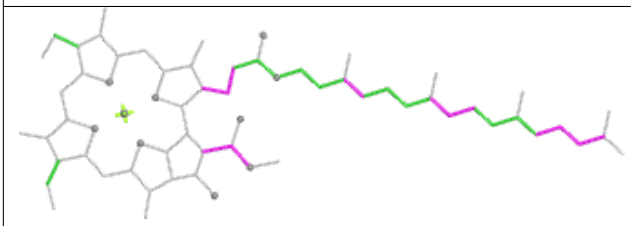
Ligand CLA cD 506



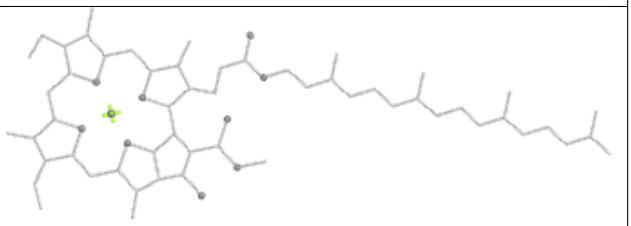
Bond lengths



Bond angles

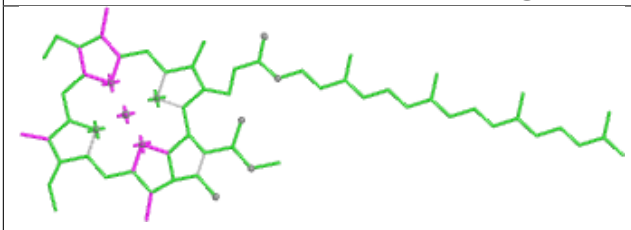


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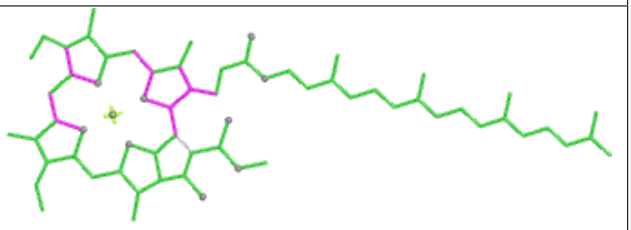


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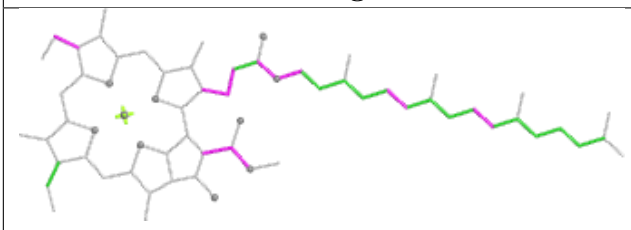
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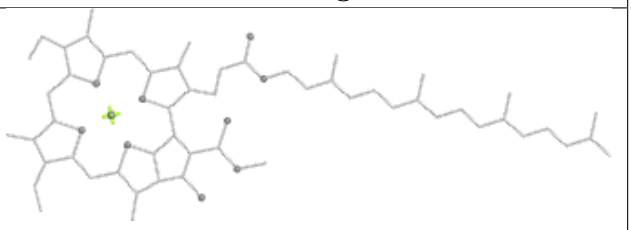
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Bond angles

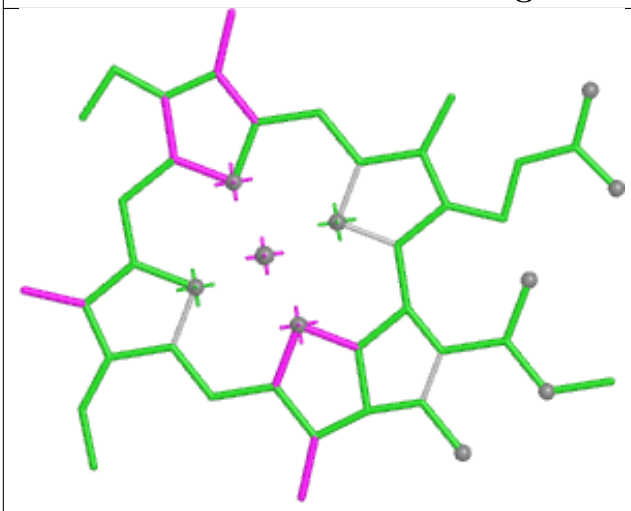


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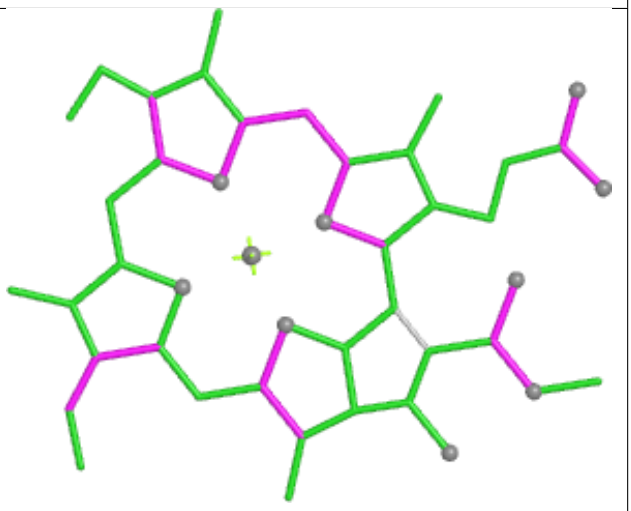


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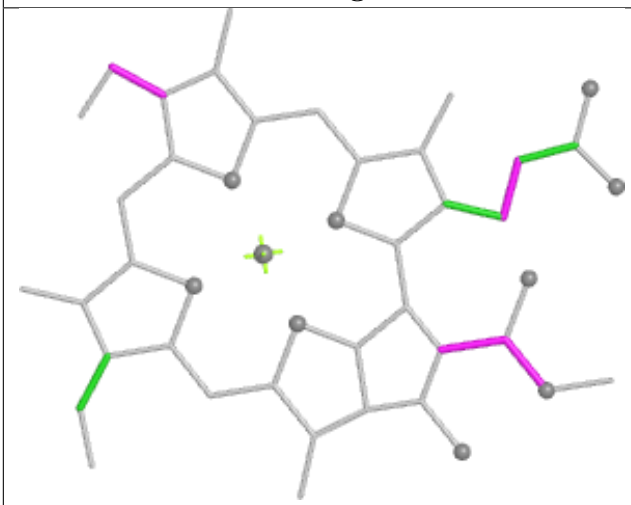
Ligand CLA bE 603



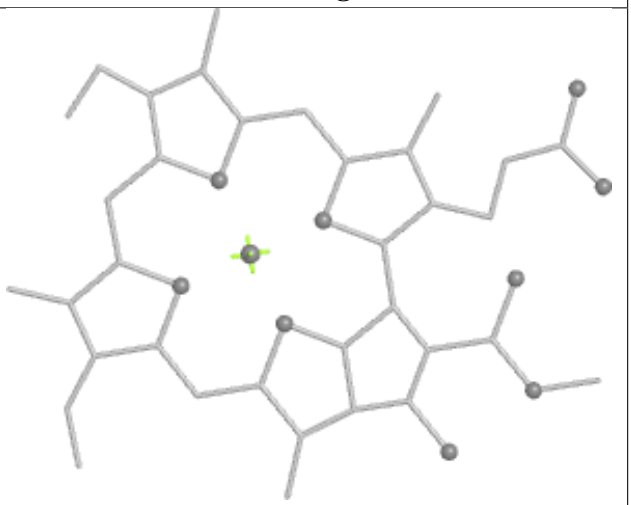
Bond lengths



Bond angles

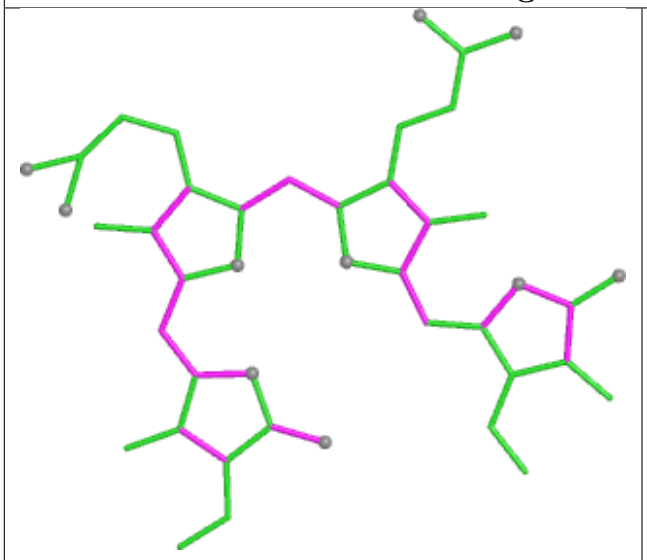


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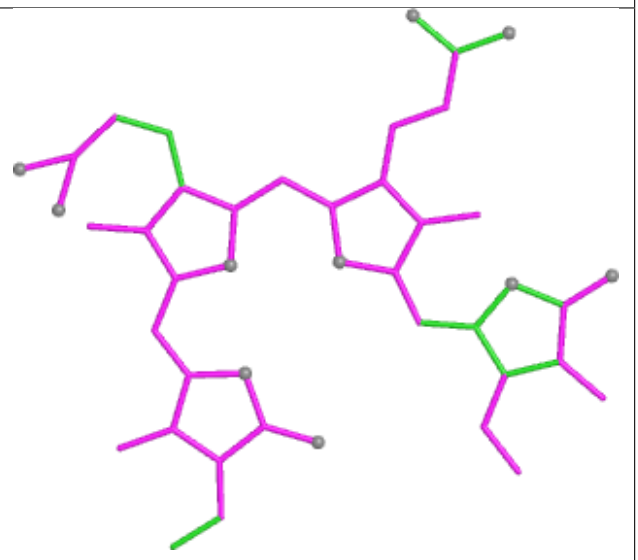


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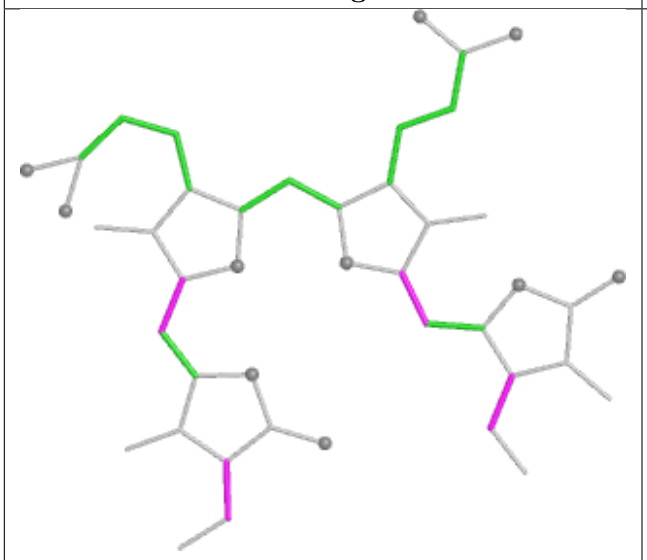
Ligand CYC k3 201



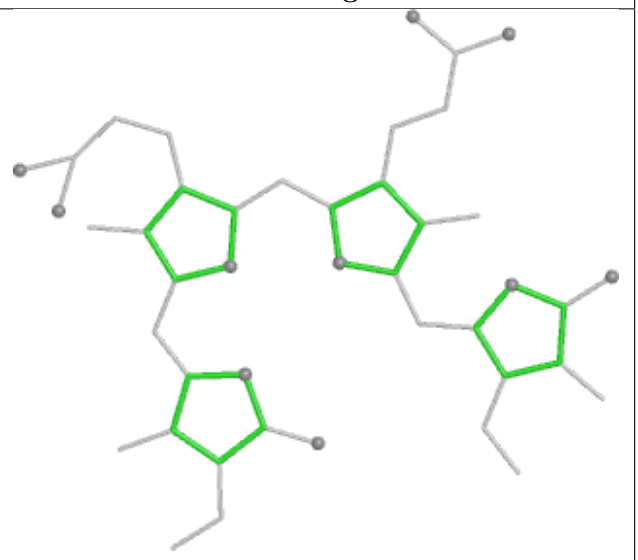
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Bond angles

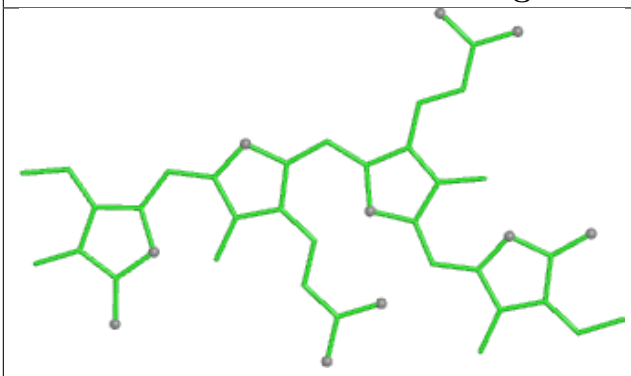


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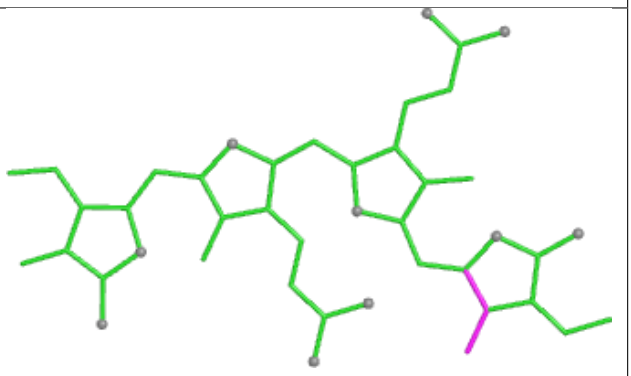


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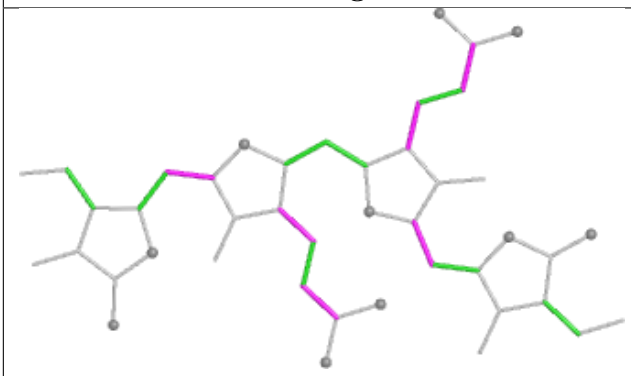
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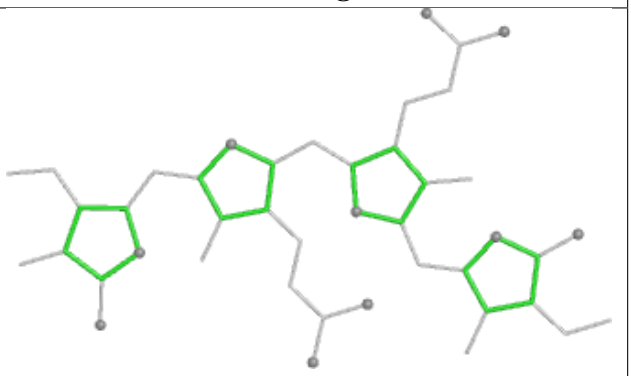
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Bond angles

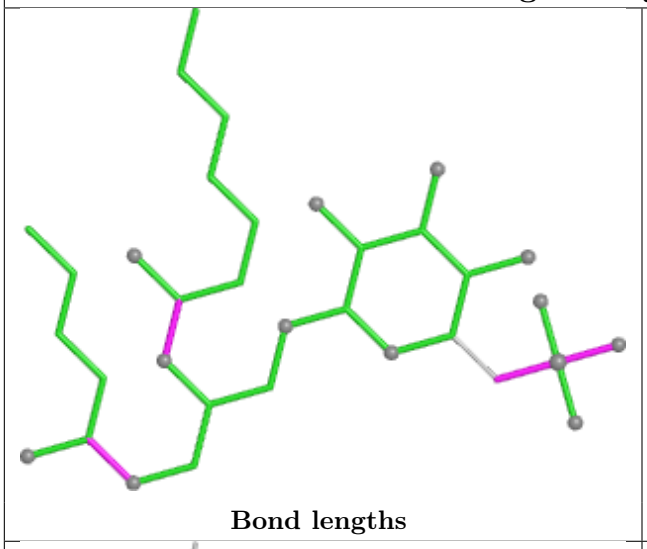


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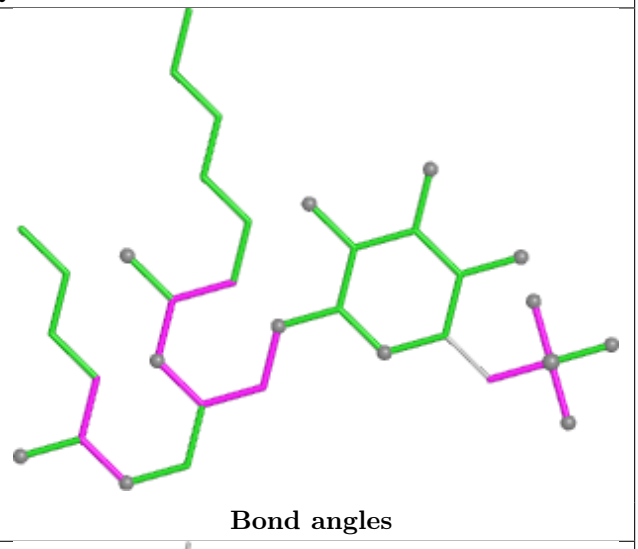


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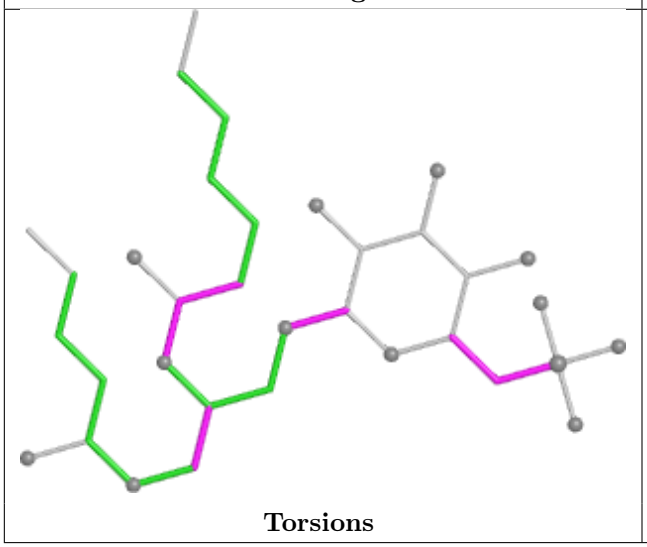
Ligand SQD d1 414



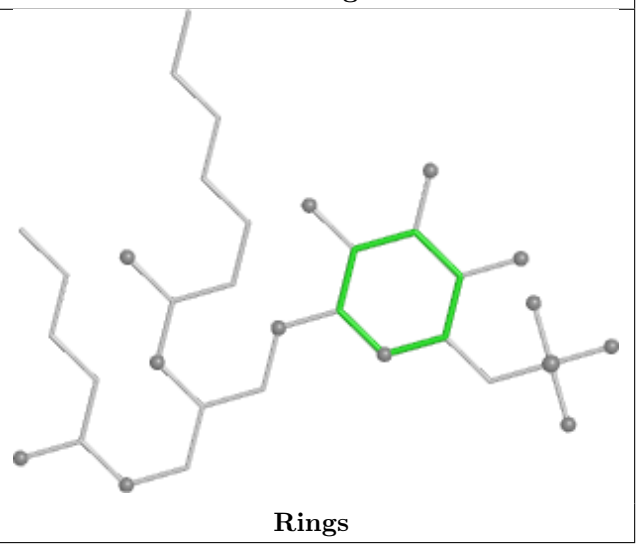
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Bond angles

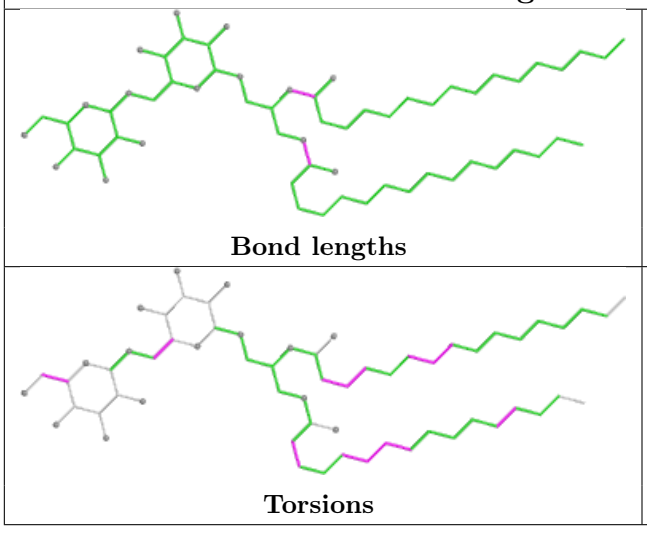


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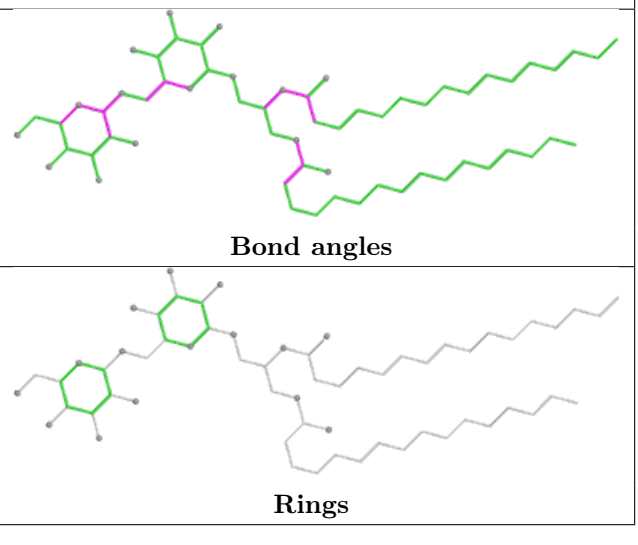


Rings

Ligand DGD c1 518



Bond lengths

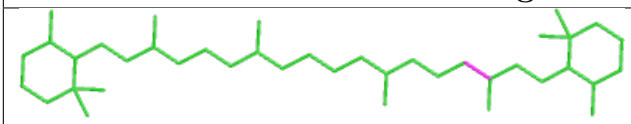


Bond angles

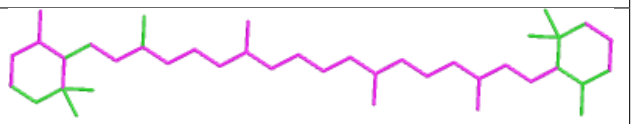
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Rings

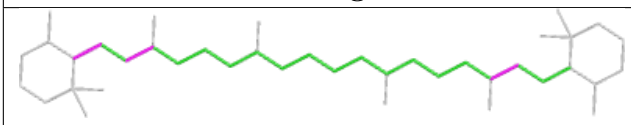
Ligand BCR iD 102



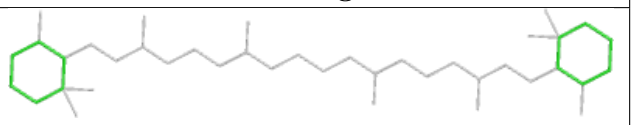
Bond lengths



Bond angles

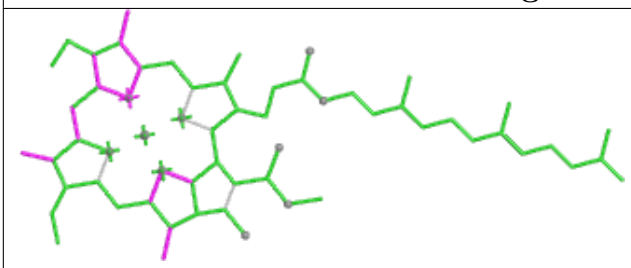


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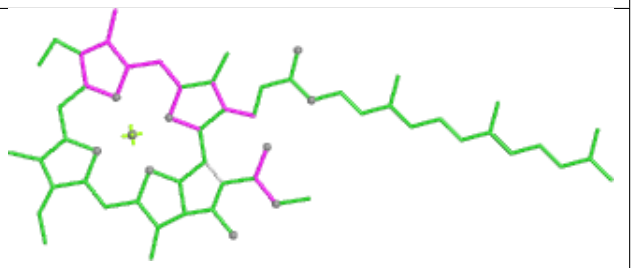


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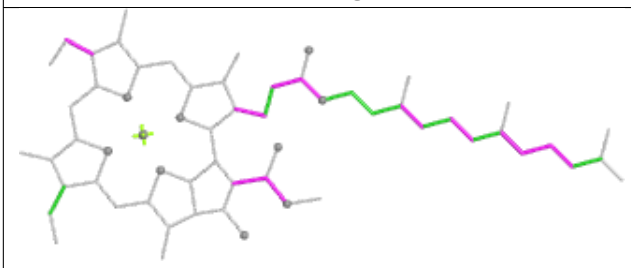
Ligand CLA I1 101



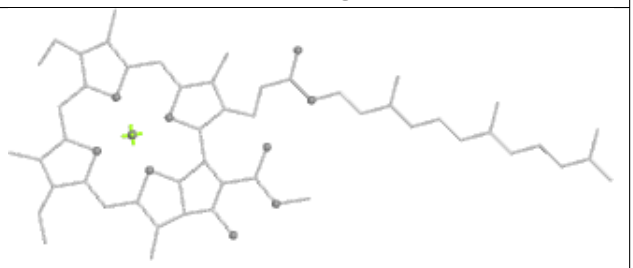
Bond lengths



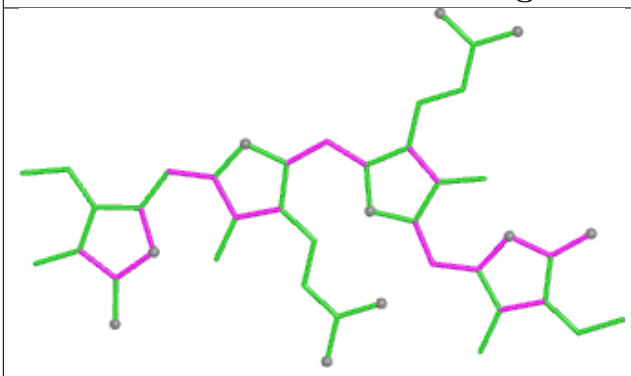
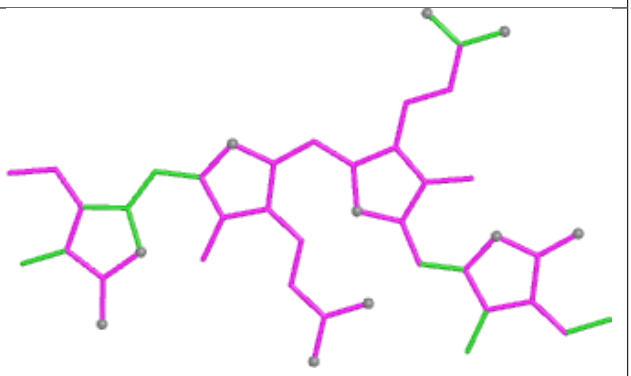
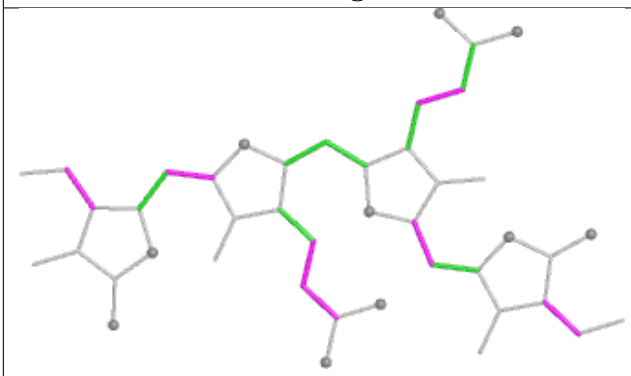
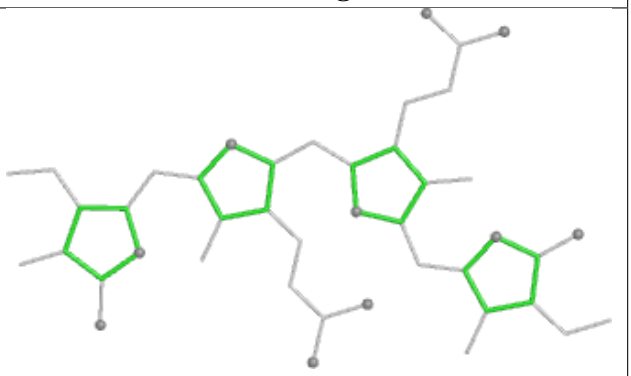
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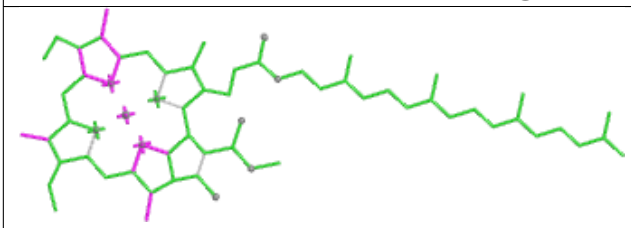
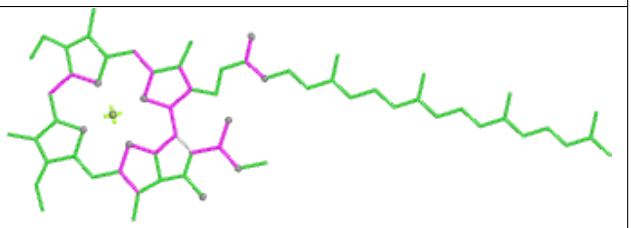
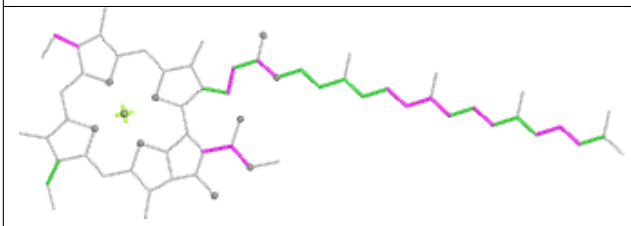
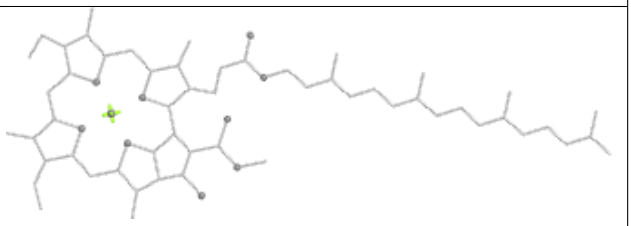


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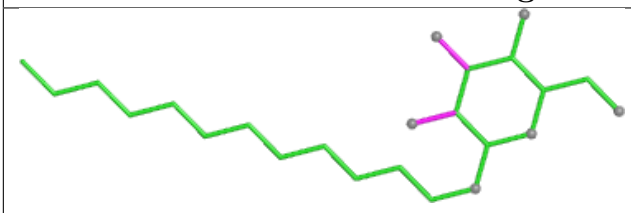


Rings

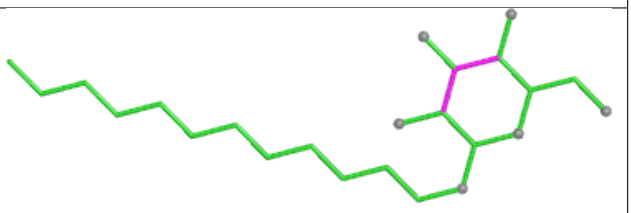
Ligand CYC b2 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA aE 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

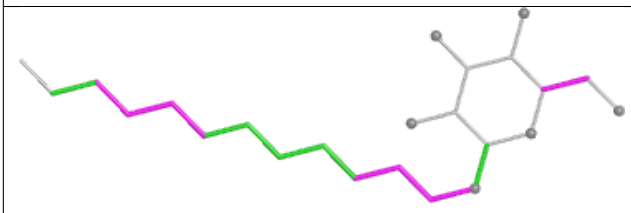
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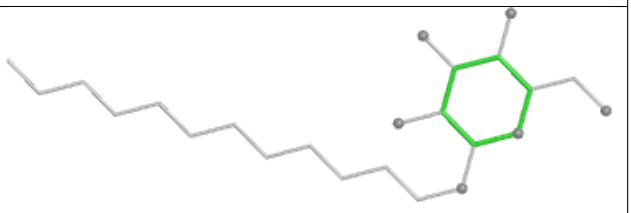
Bond lengths



Bond angles

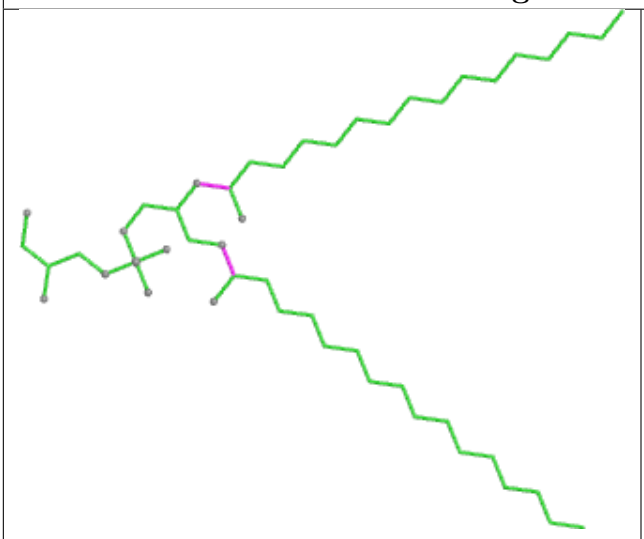


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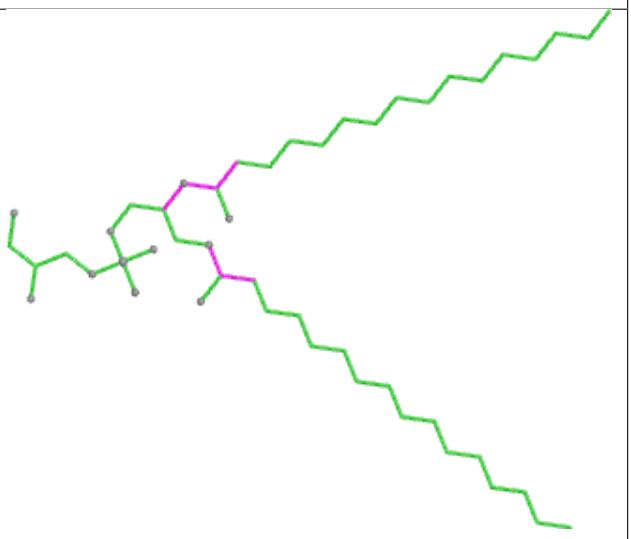


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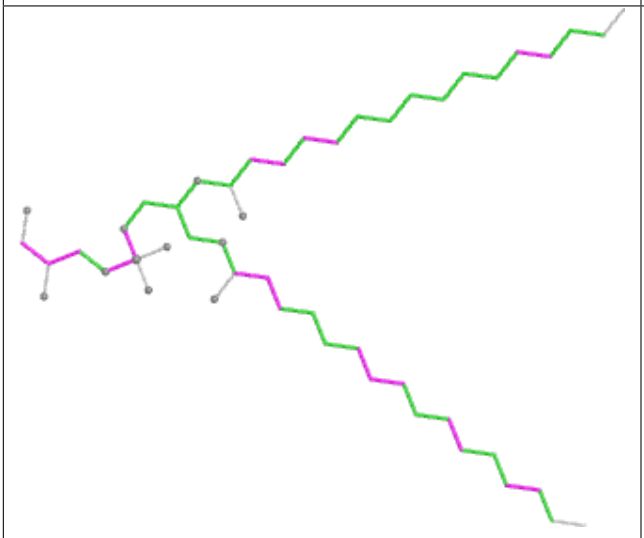
Ligand LHG dD 410



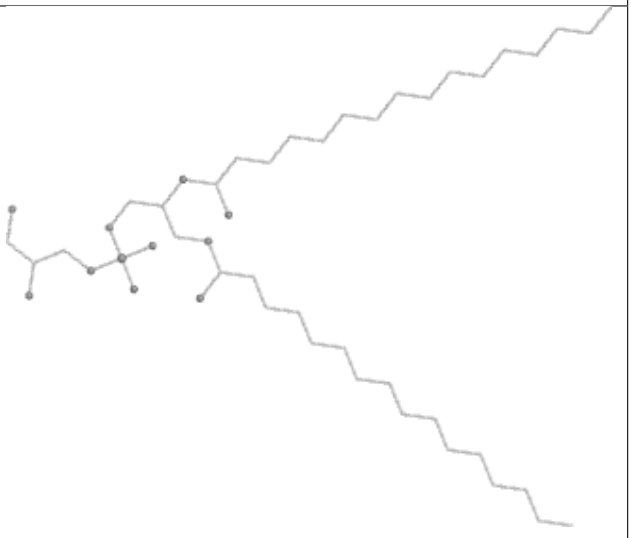
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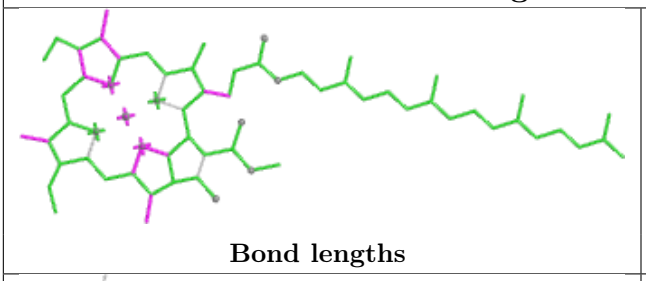


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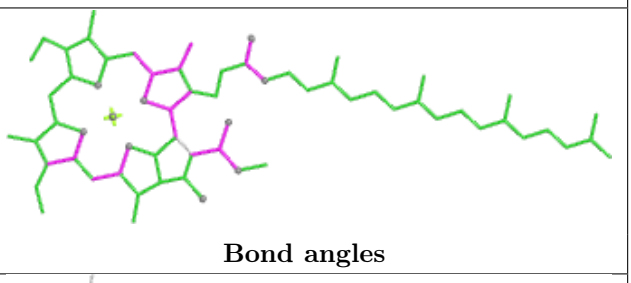


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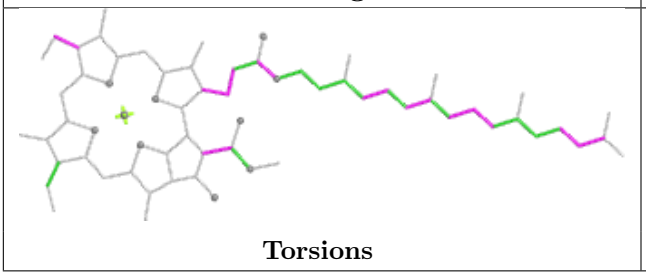
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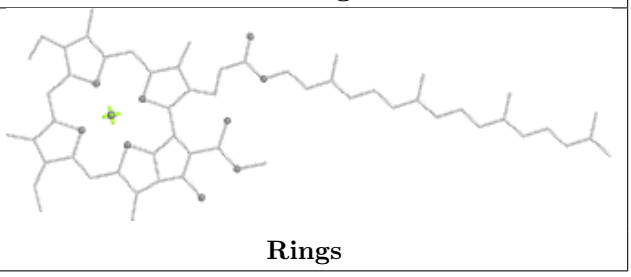
Bond lengths



Bond angles



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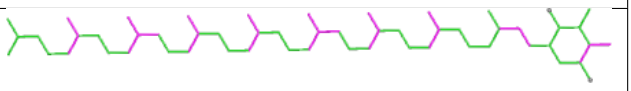


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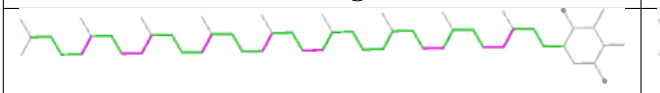
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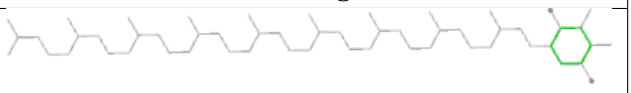
Bond lengths



Bond angles

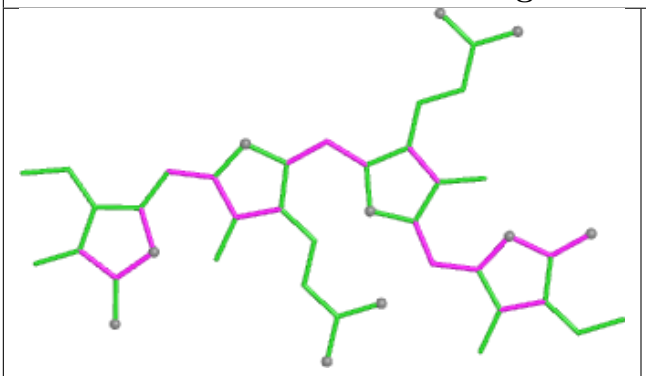


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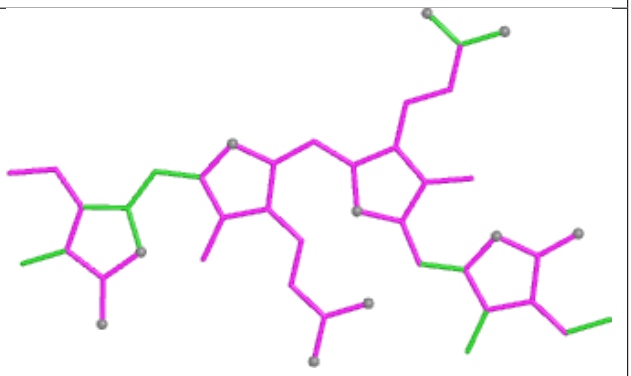


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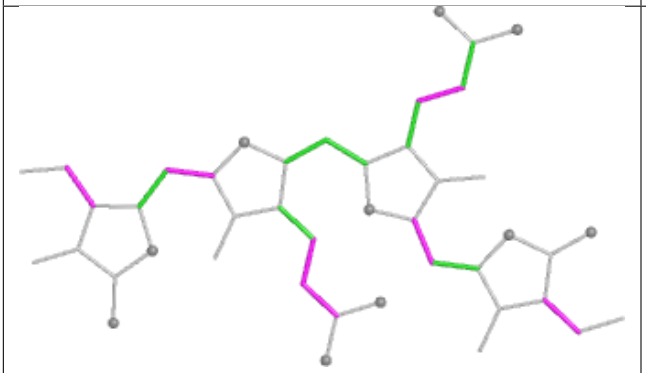
Ligand CYC d3 201



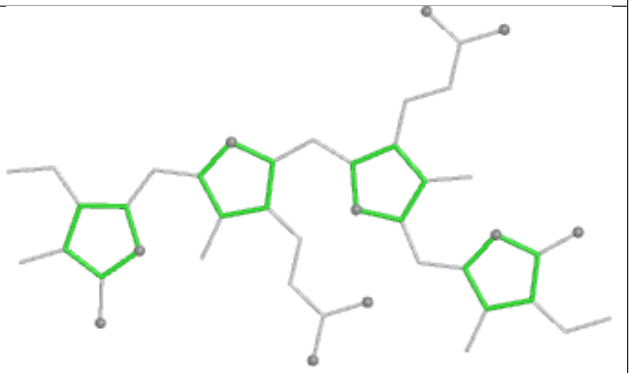
Bond lengths



Bond angles

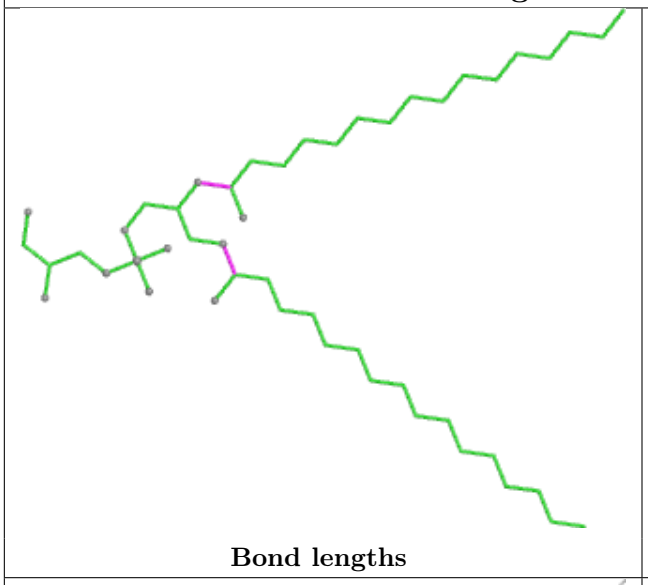


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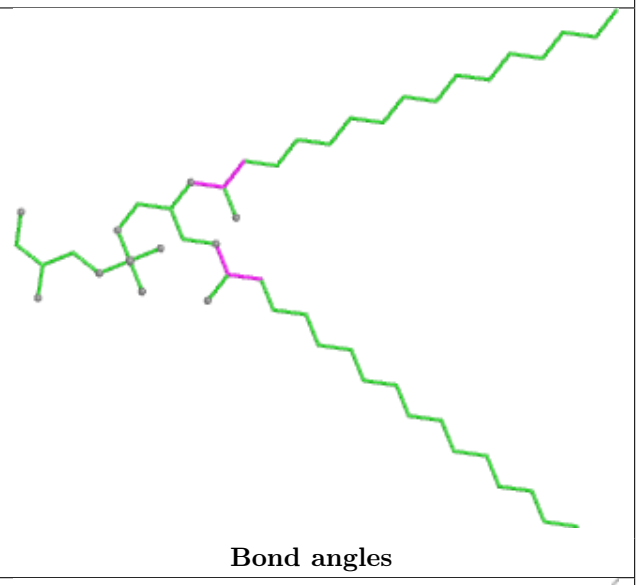


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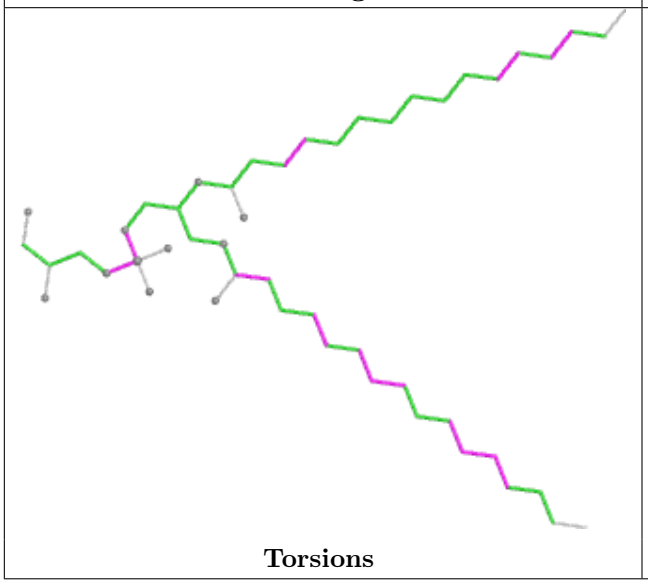
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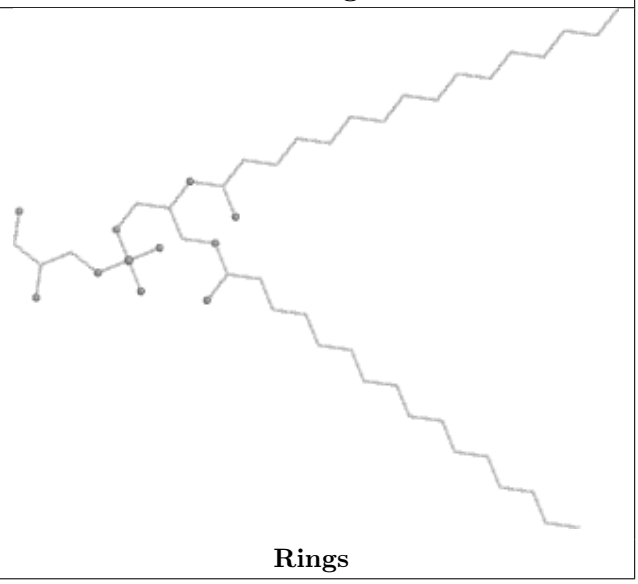
Bond lengths



Bond angles



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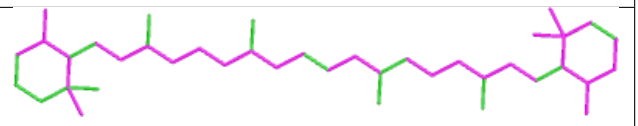


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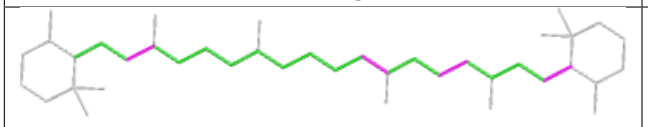
Ligand BCR h1 105



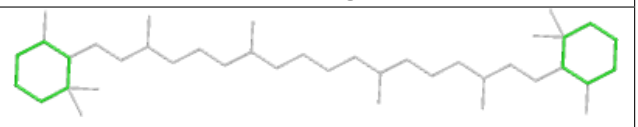
Bond lengths



Bond angles

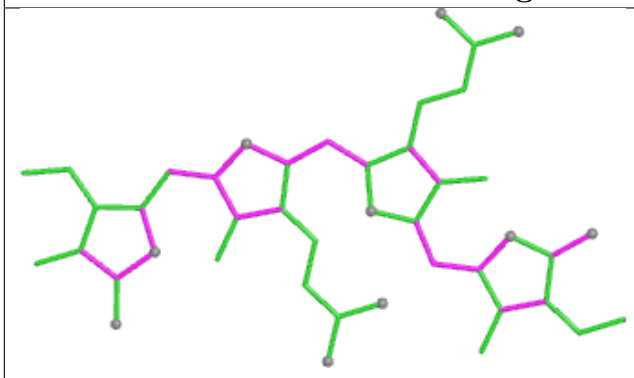


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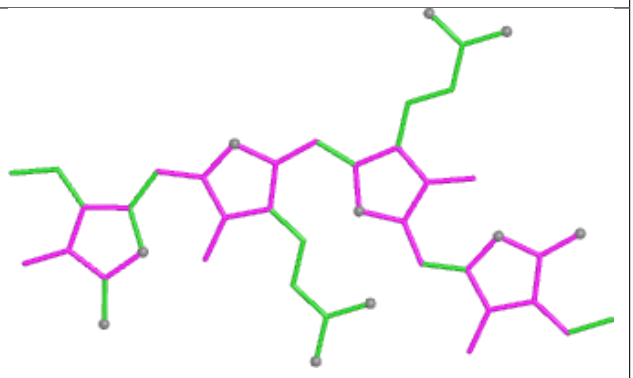


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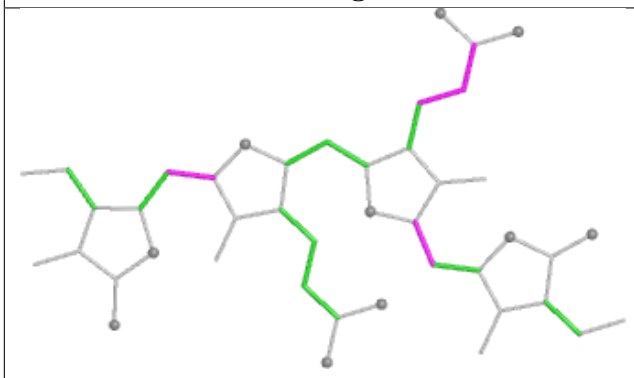
Ligand CYC 9F 201



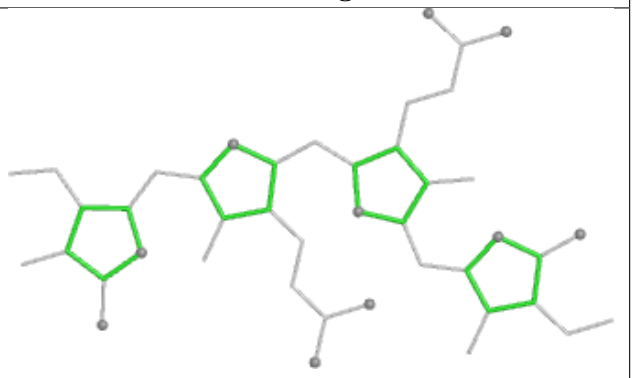
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Bond angles

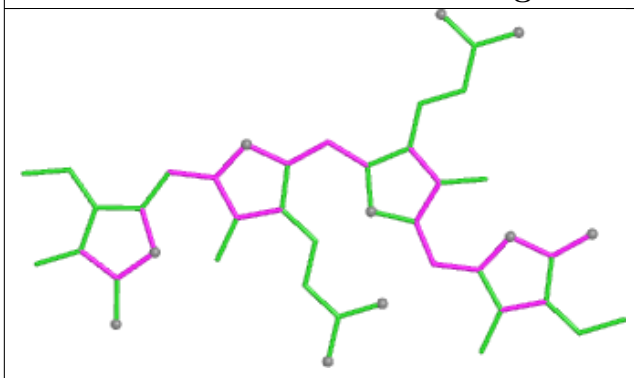


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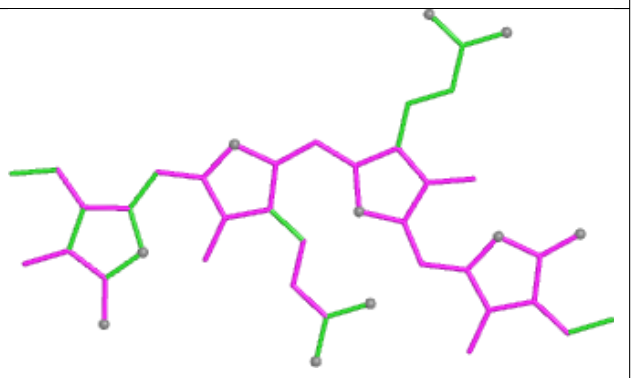


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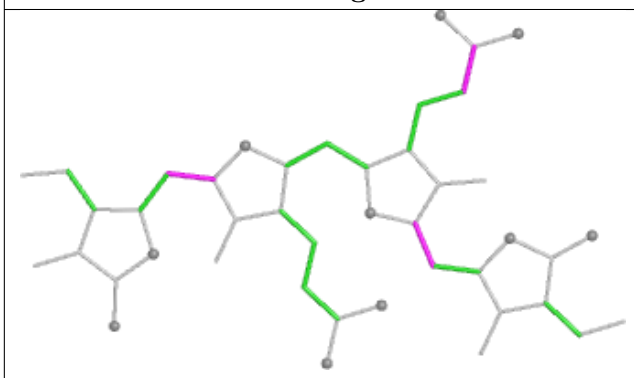
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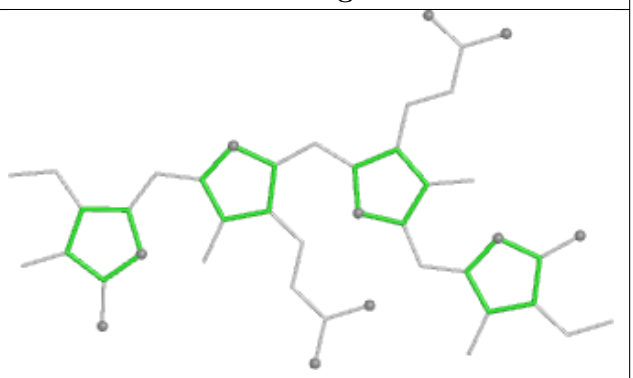
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Bond angles

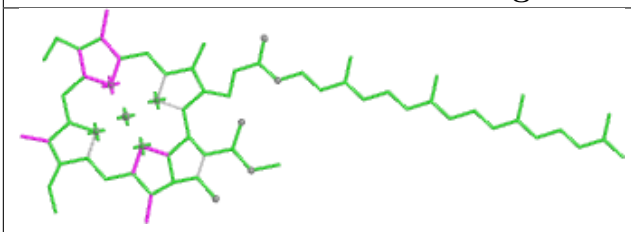


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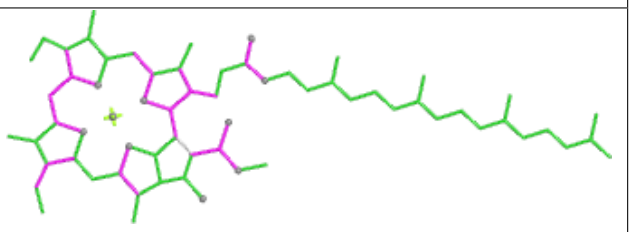


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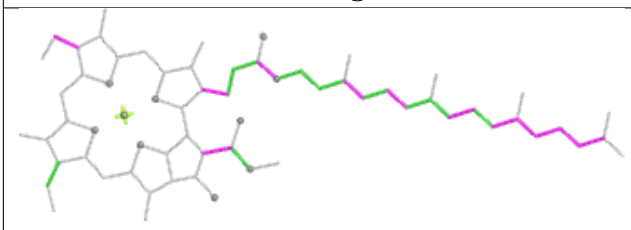
Ligand CLA BE 604



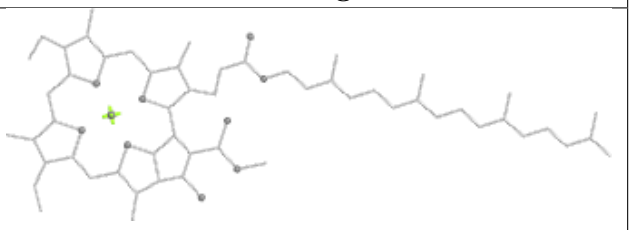
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Bond angles

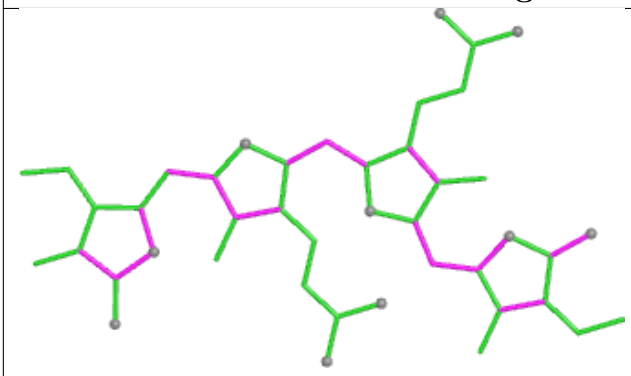


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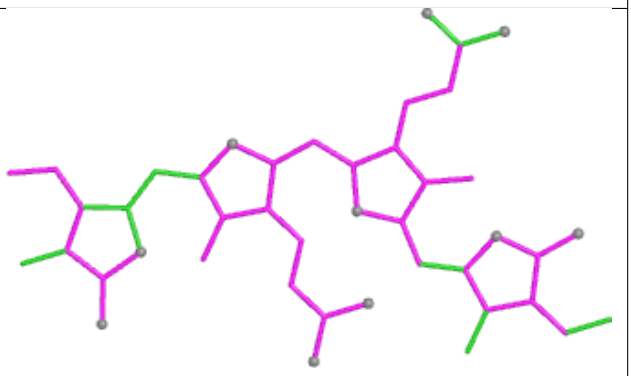


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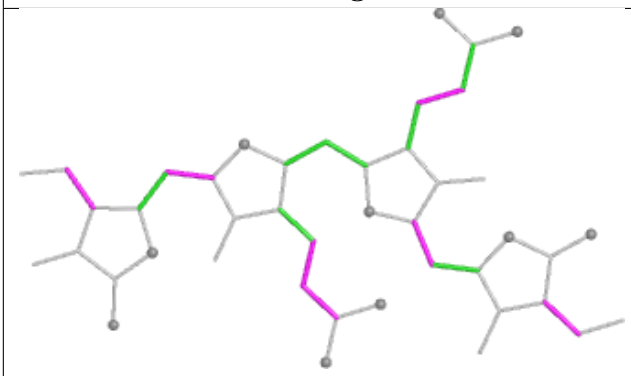
Ligand CYC bJ 201



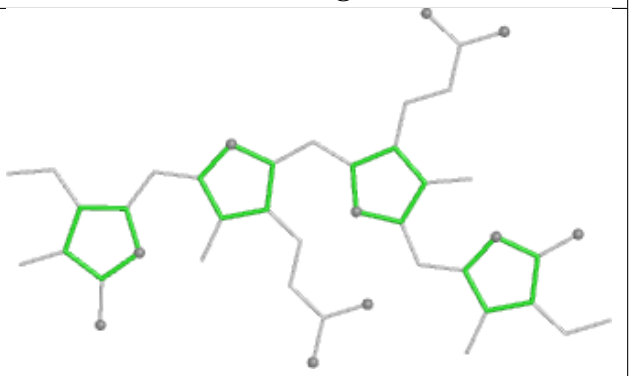
Bond lengths



Bond angles

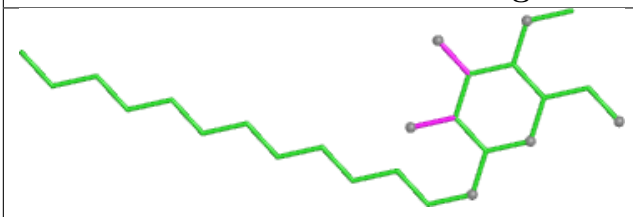


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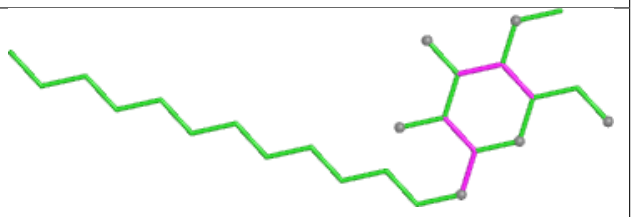


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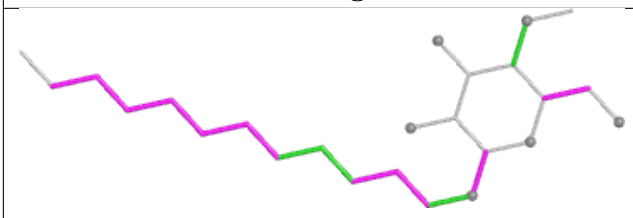
Ligand LMT dE 412



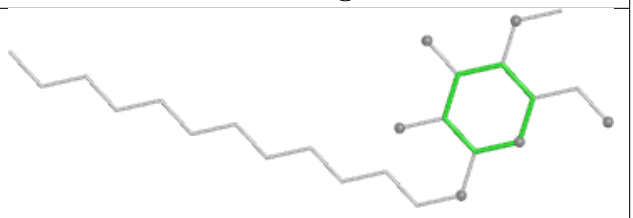
Bond lengths



Bond angles

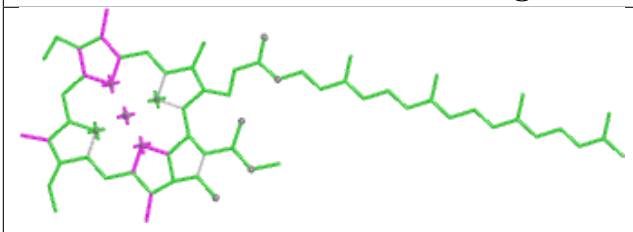


Torsions

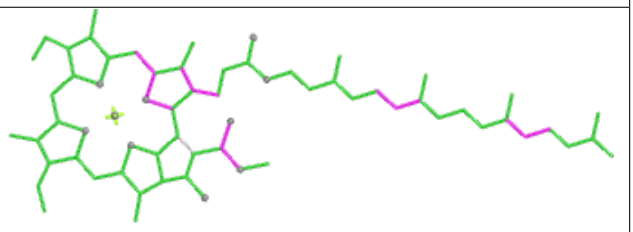


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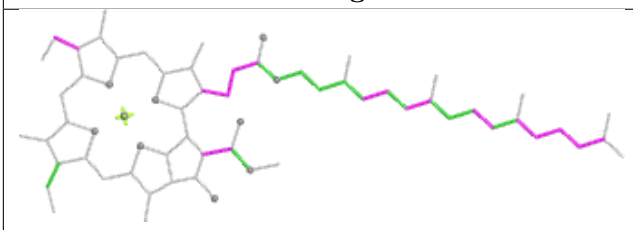
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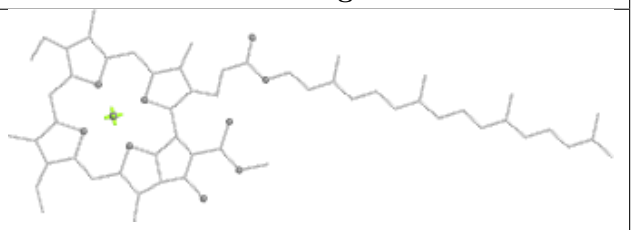
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Bond angles

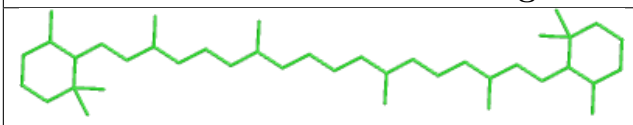


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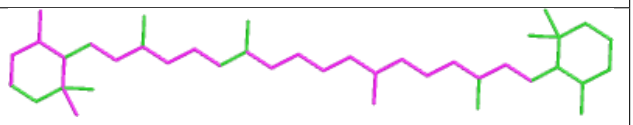


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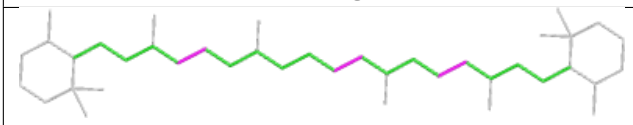
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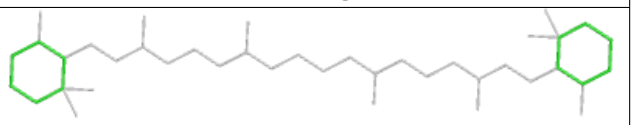
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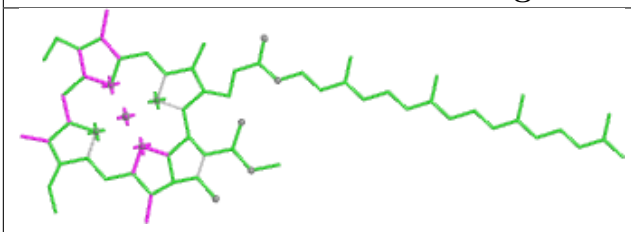


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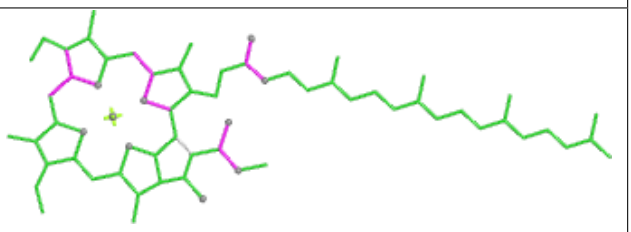


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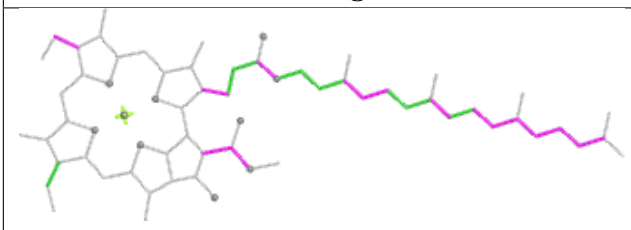
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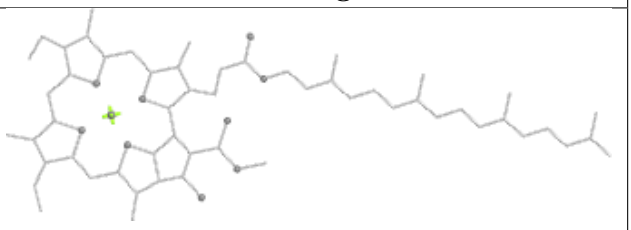
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Bond angles



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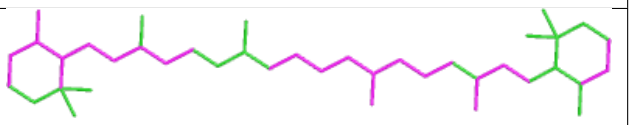


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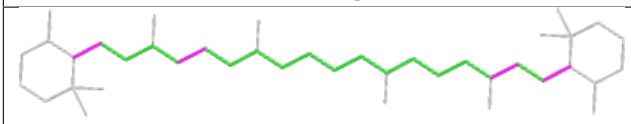
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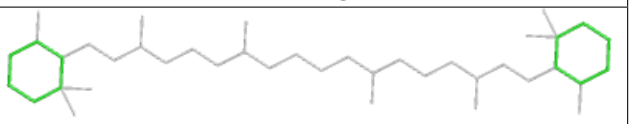
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Bond angles

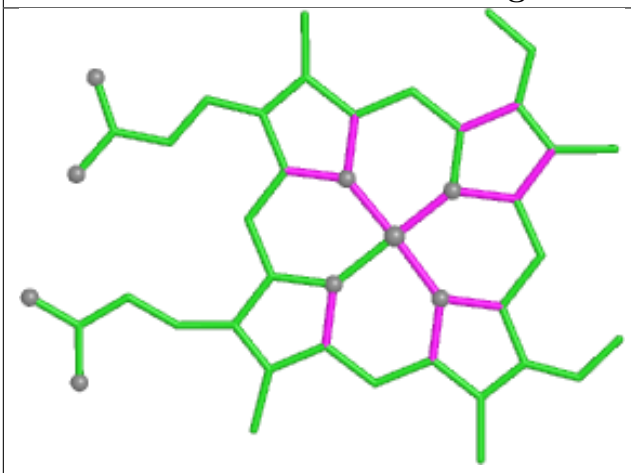


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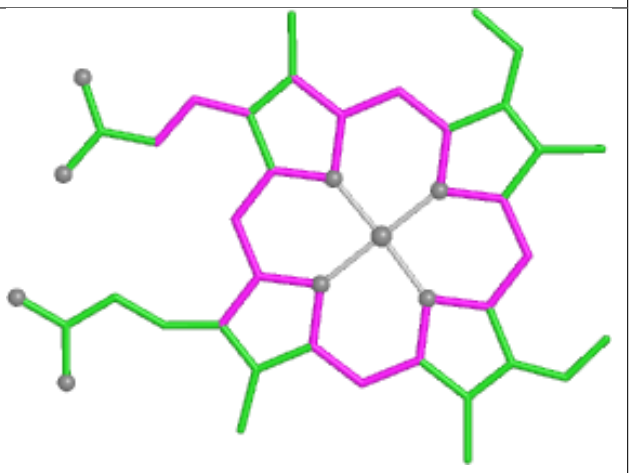


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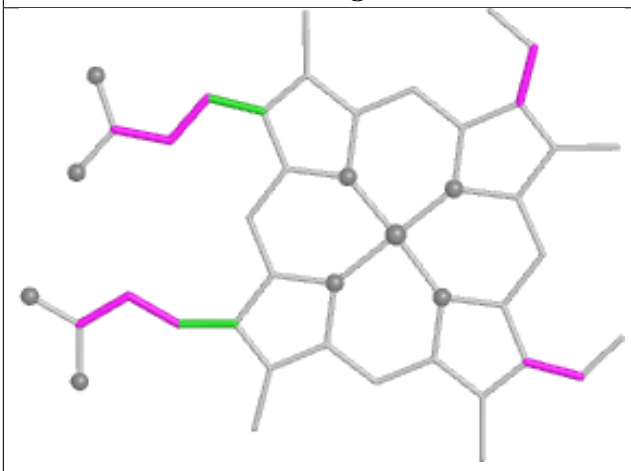
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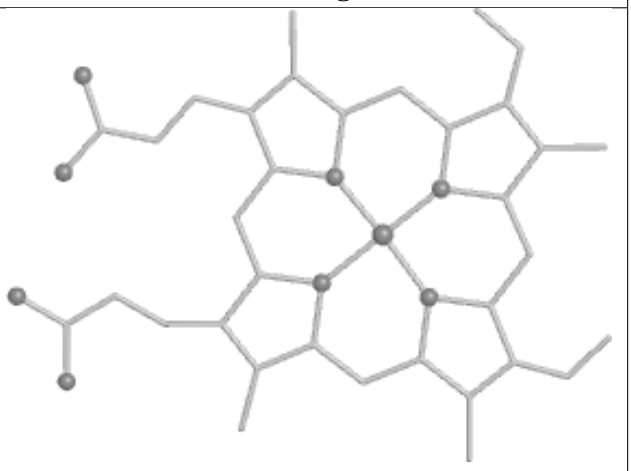
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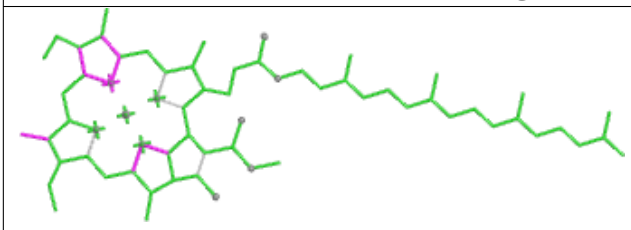


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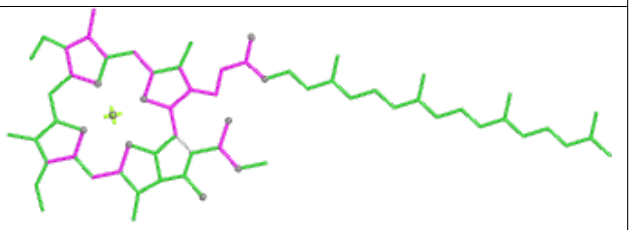


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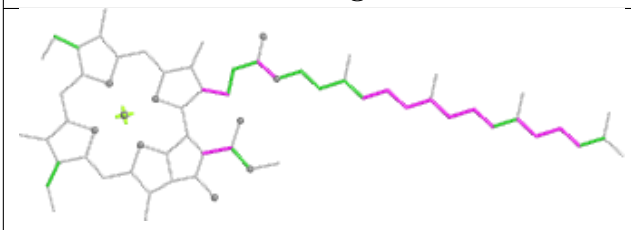
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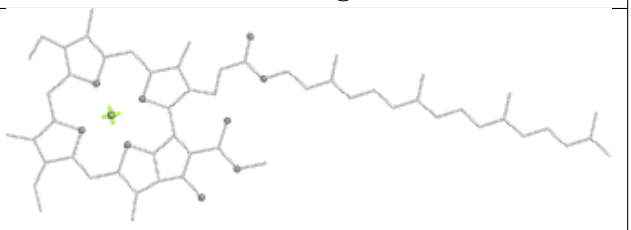
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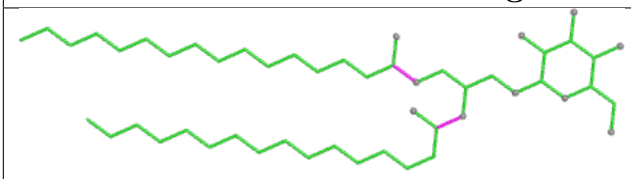


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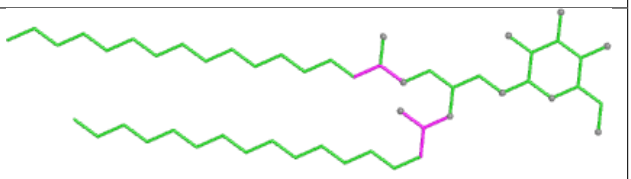


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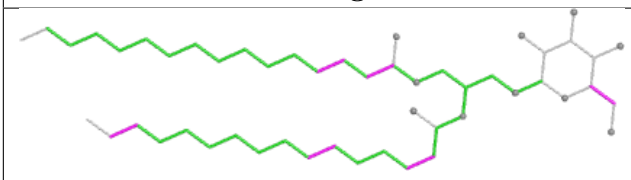
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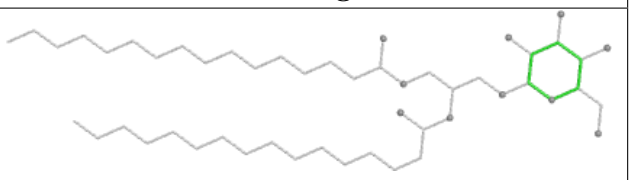
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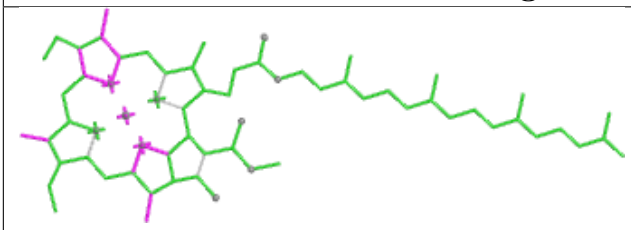


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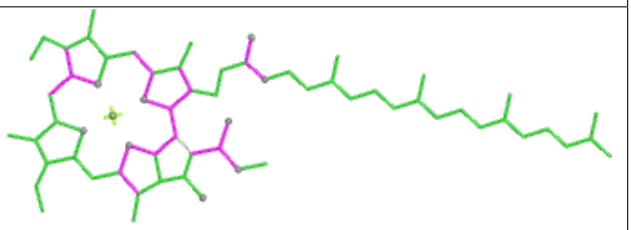


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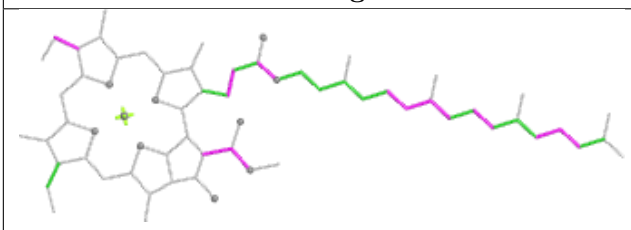
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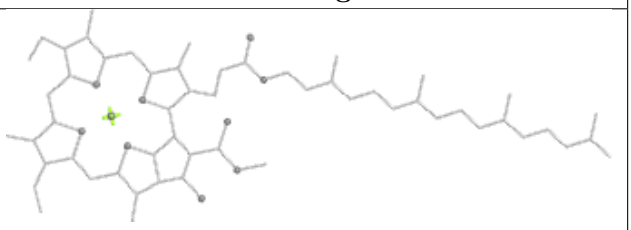
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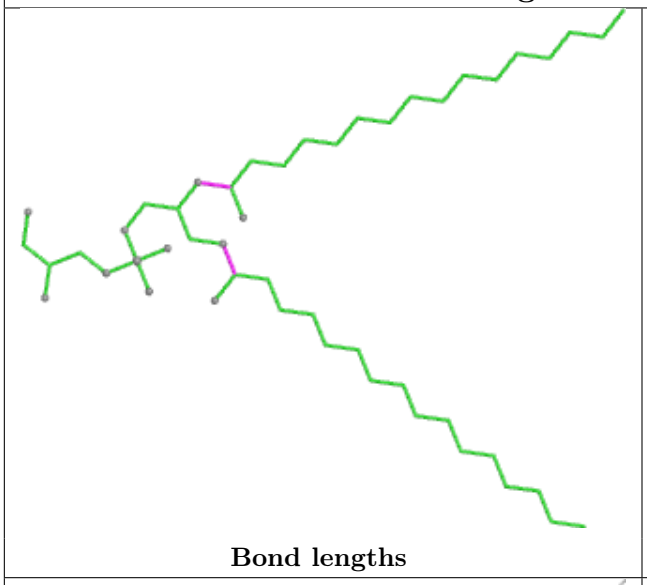


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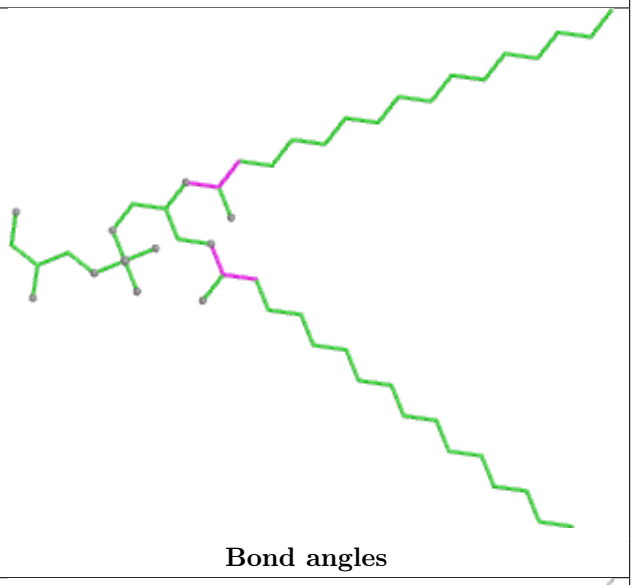


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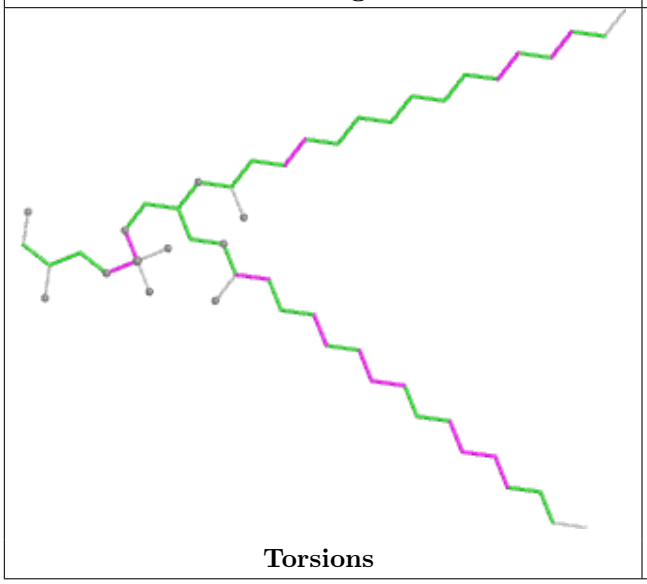
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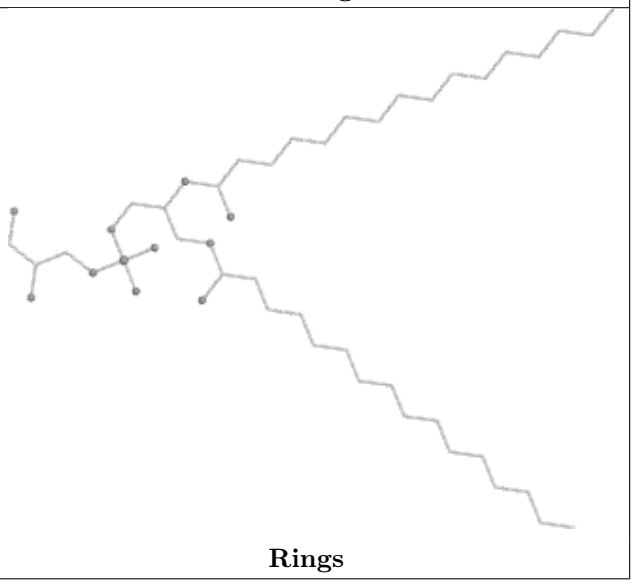
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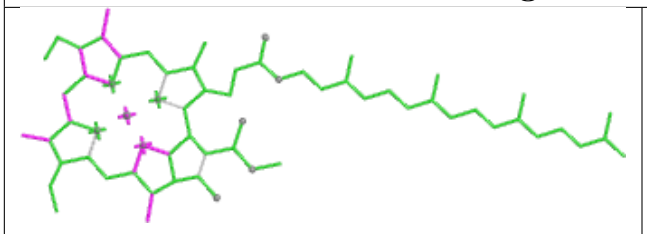


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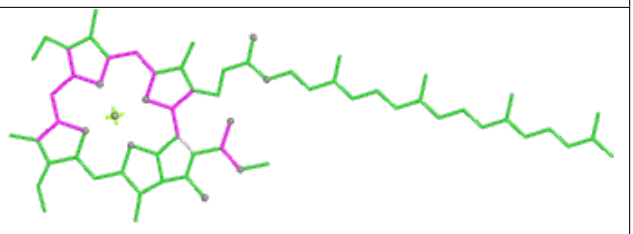


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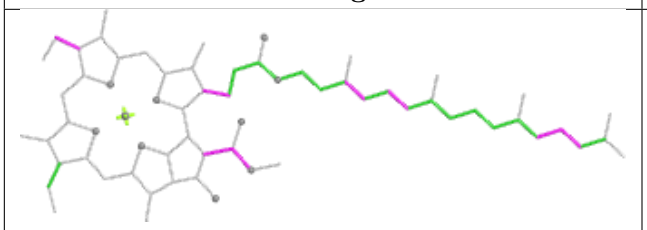
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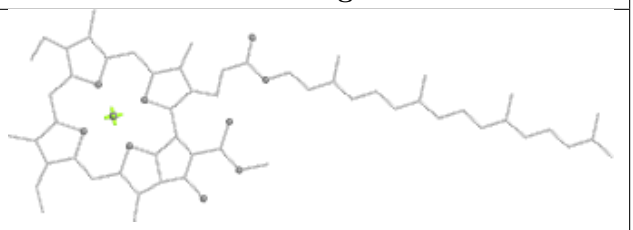
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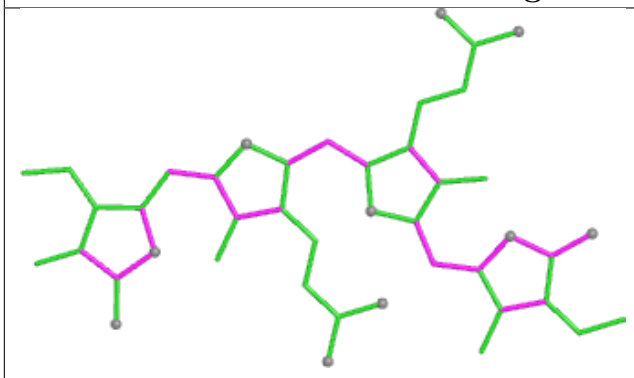


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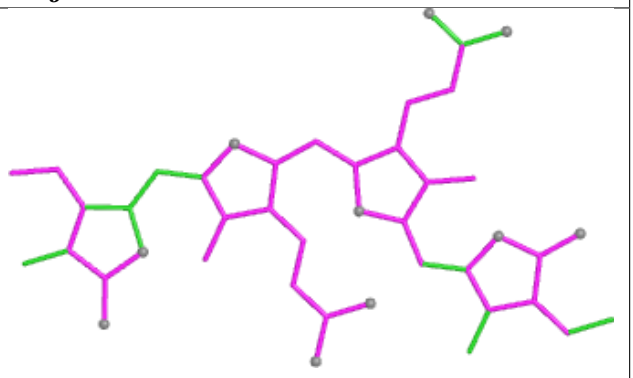


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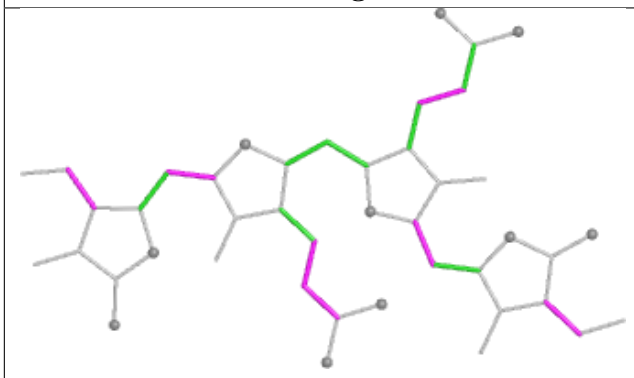
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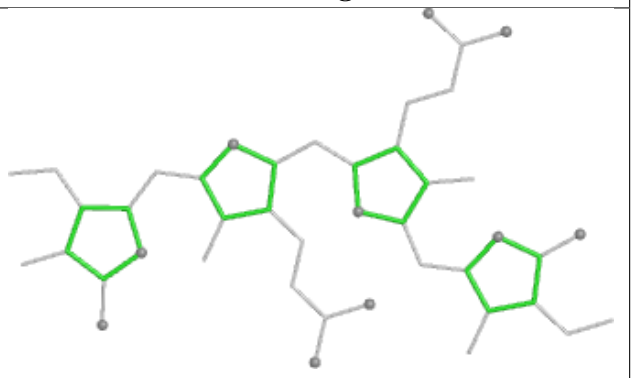
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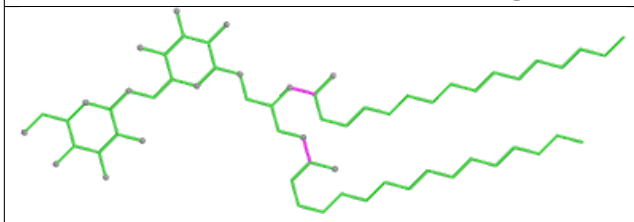


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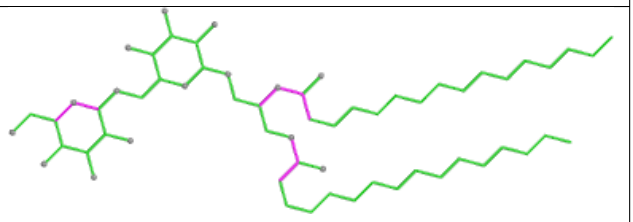


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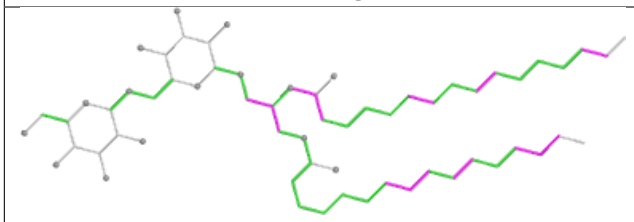
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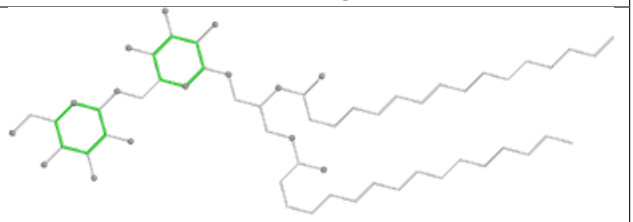
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Bond angles

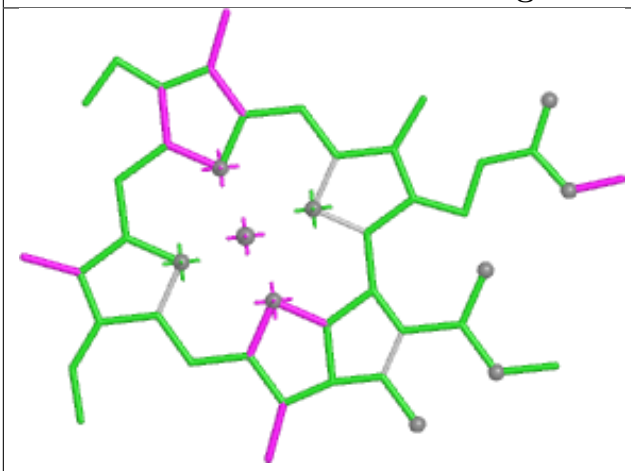


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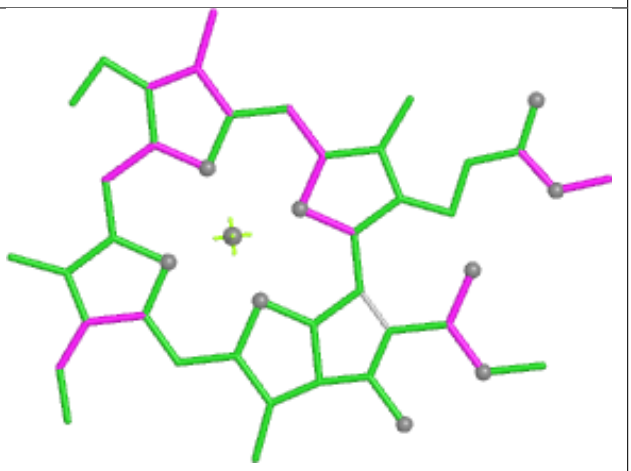


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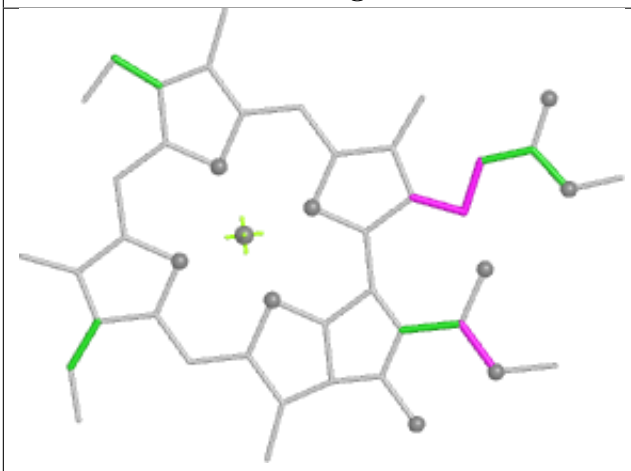
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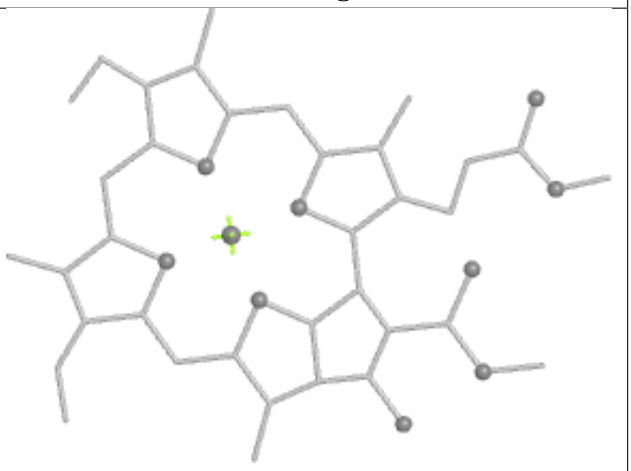
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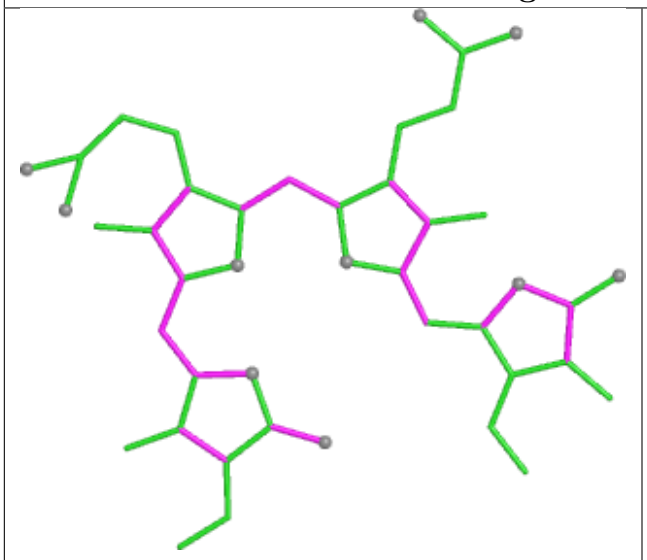


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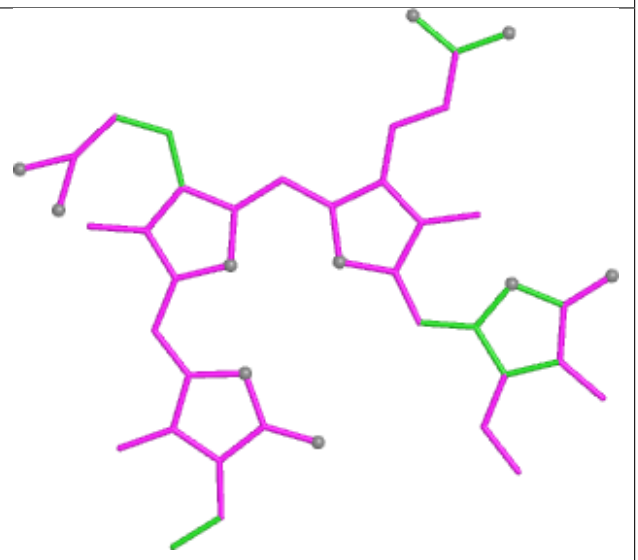


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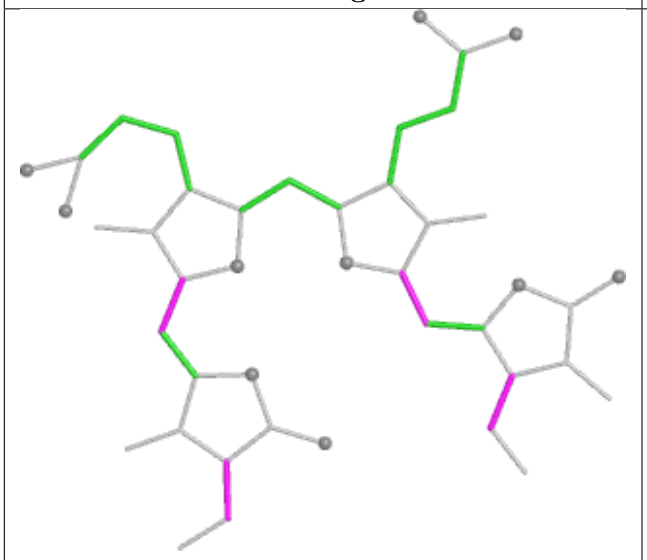
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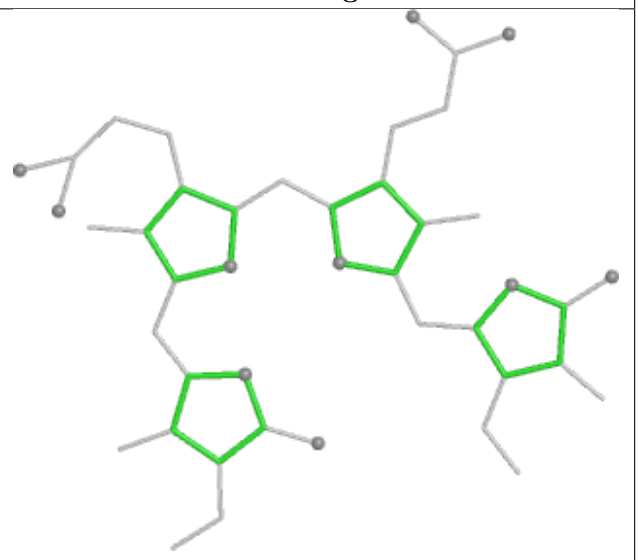
Bond lengths



Bond angles

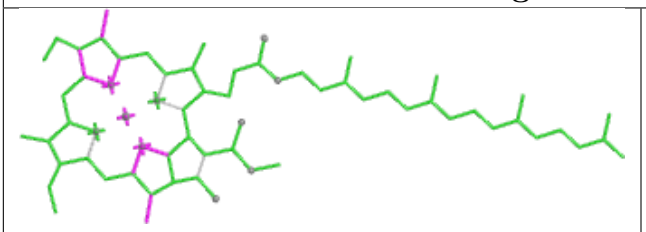


Torsions

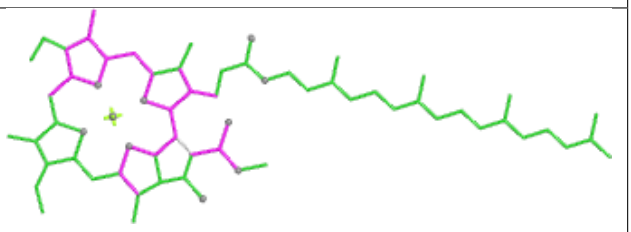


Rings

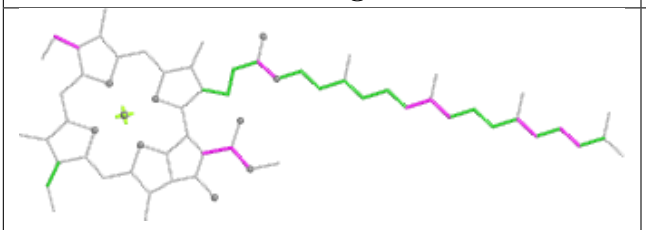
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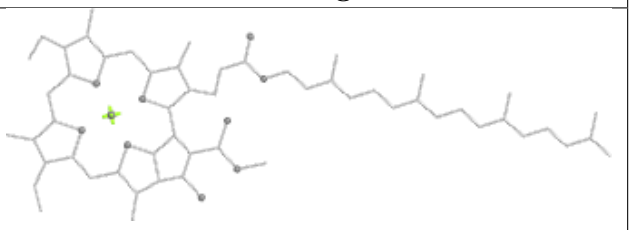
Bond lengths



Bond angles

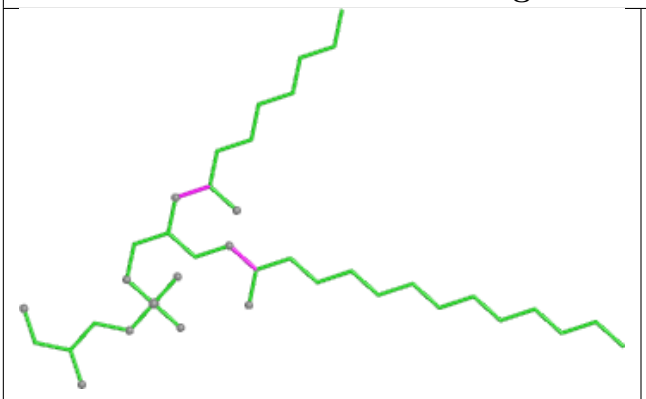


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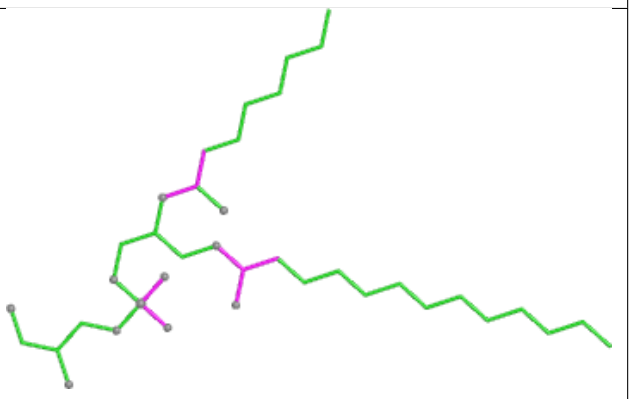


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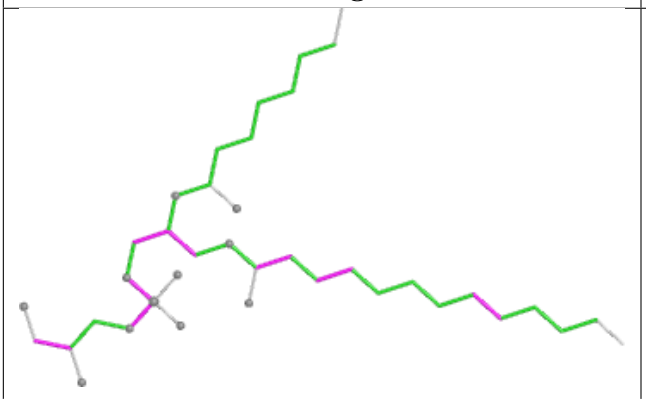
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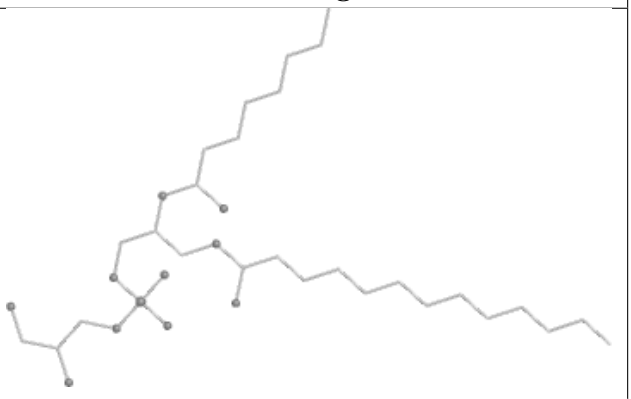
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Bond angles

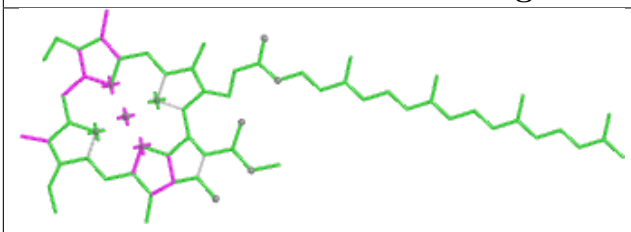


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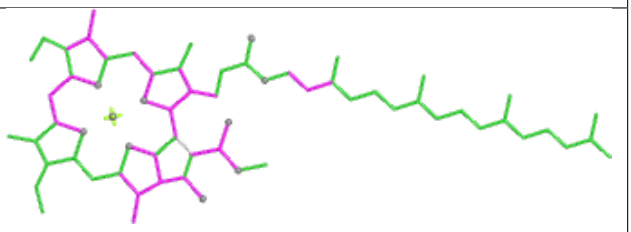


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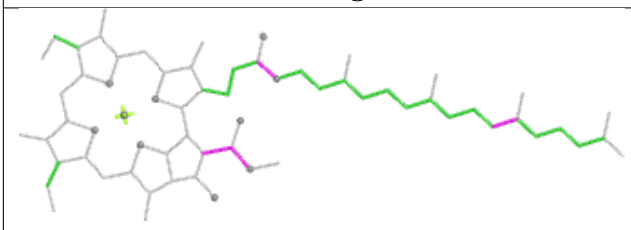
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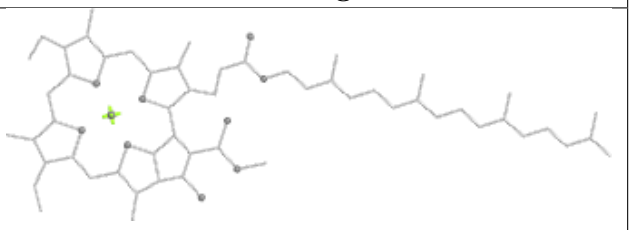
Bond lengths



Bond angles

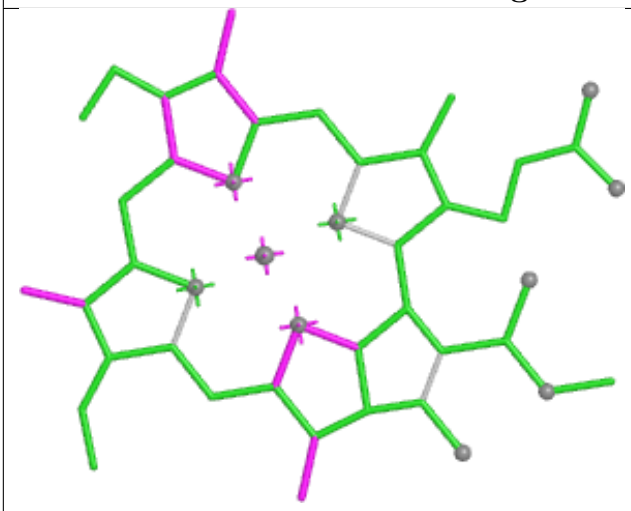


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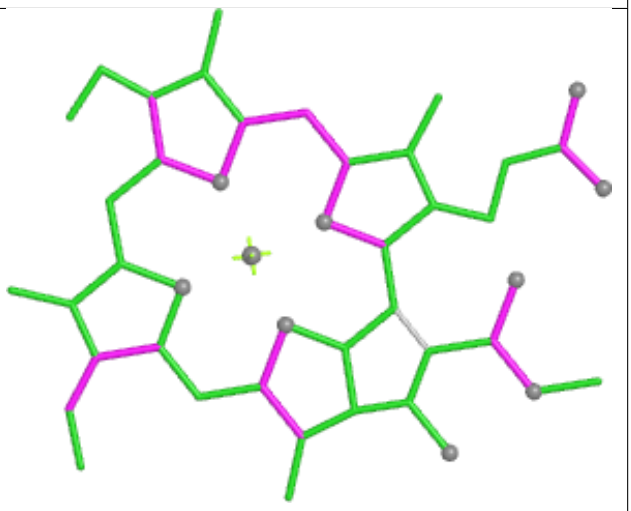


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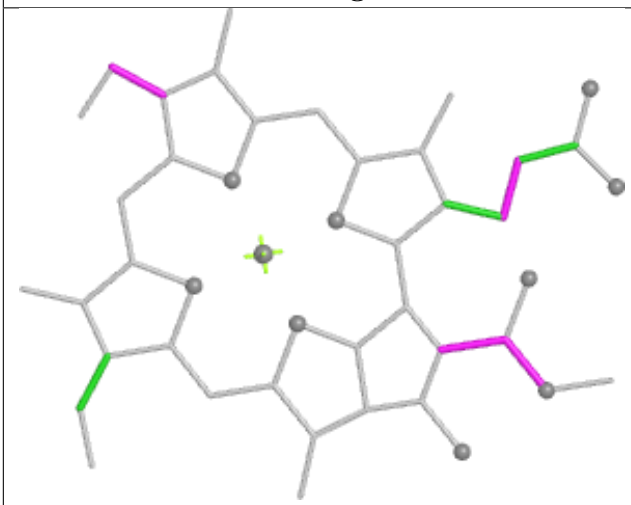
Ligand CLA BD 601



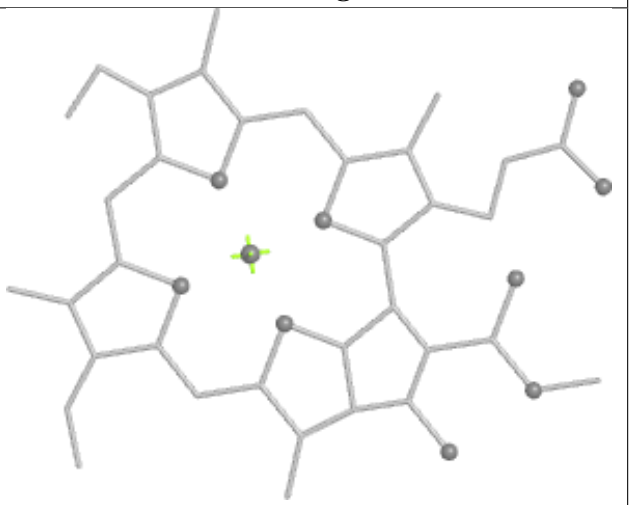
Bond lengths



Bond angles

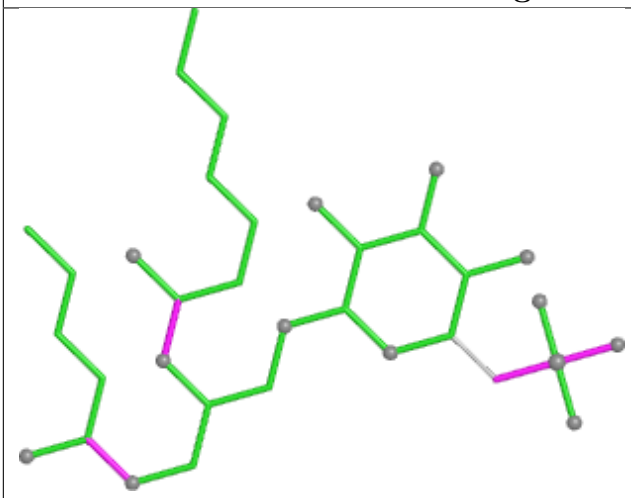


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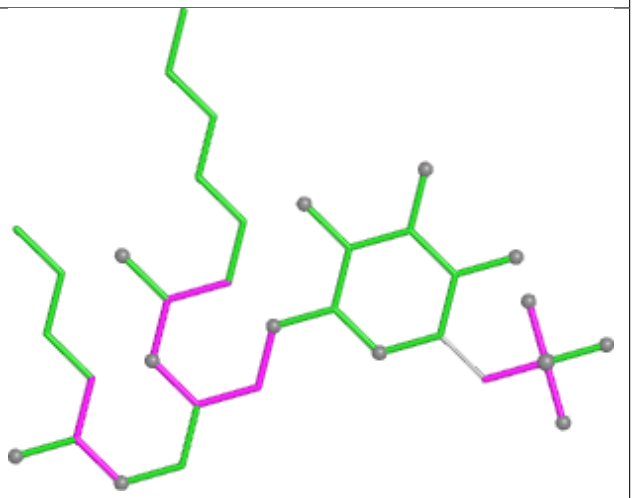


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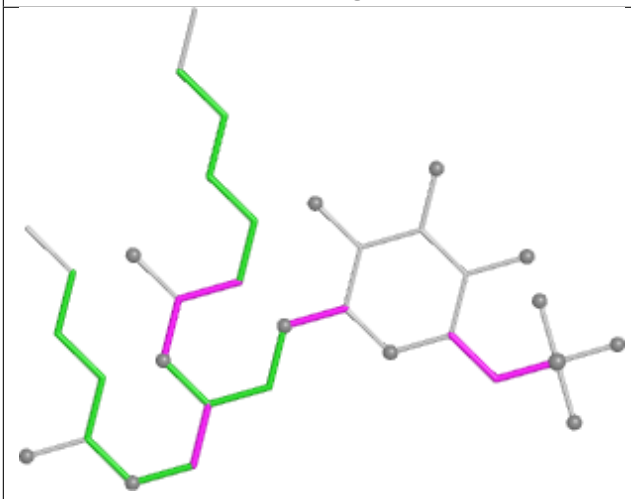
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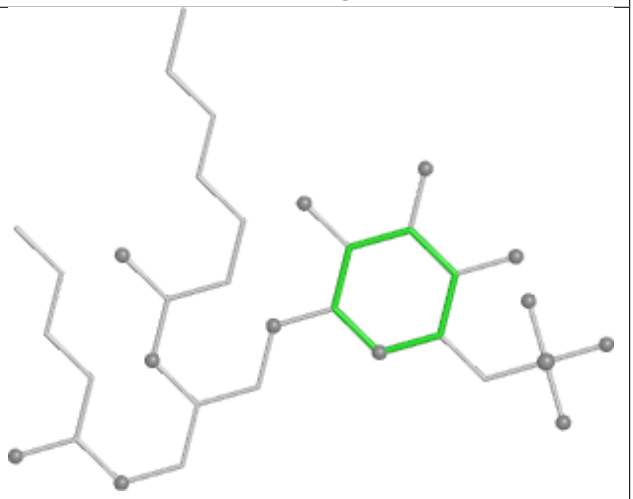
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Bond angles

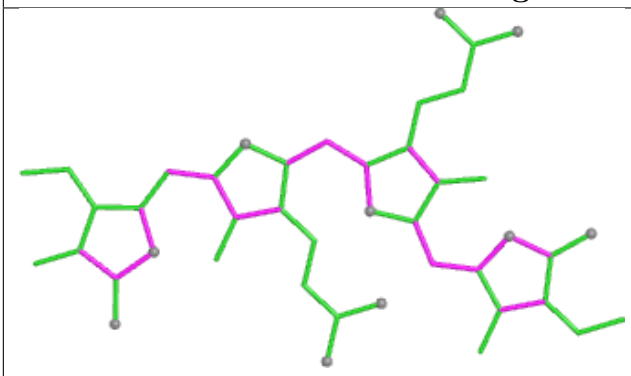


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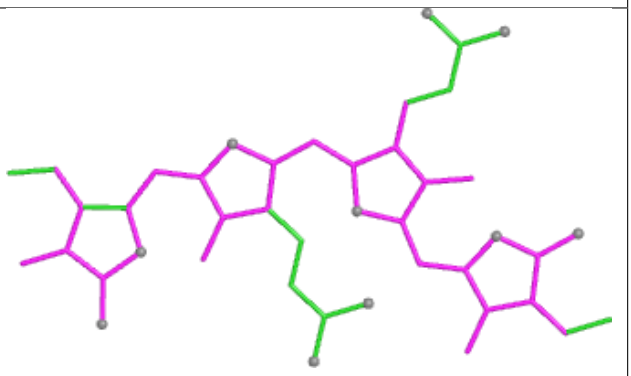


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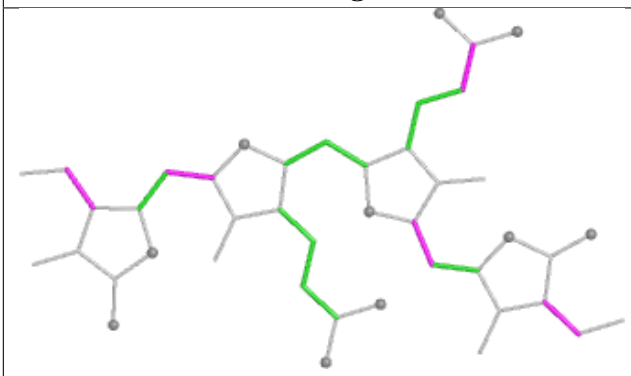
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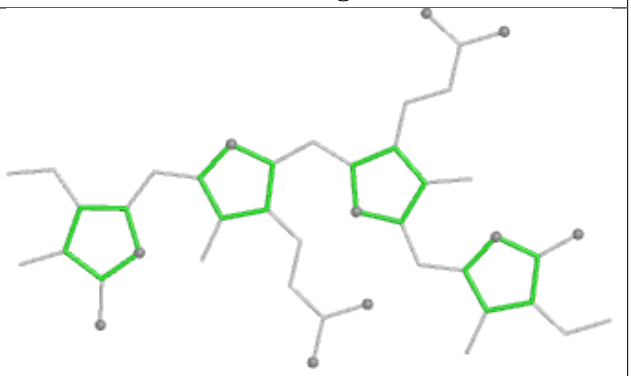
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Bond angles

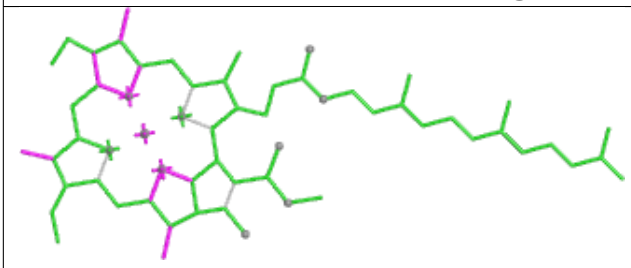


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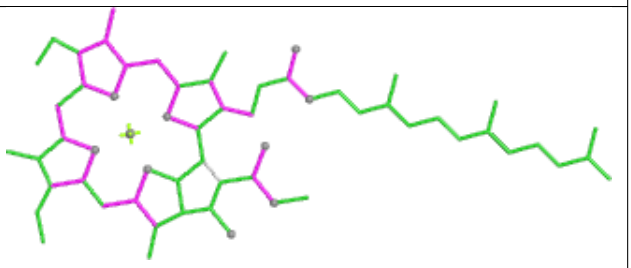


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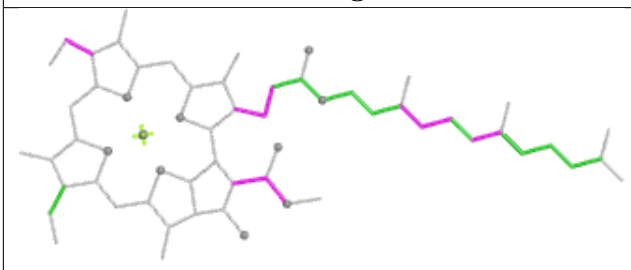
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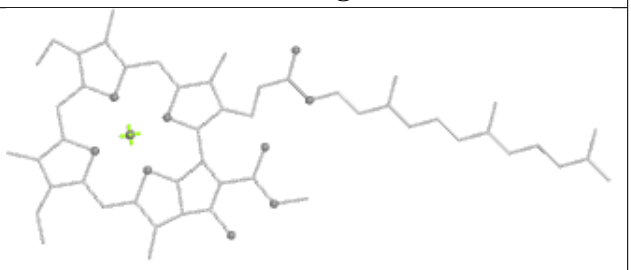
Bond lengths



Bond angles

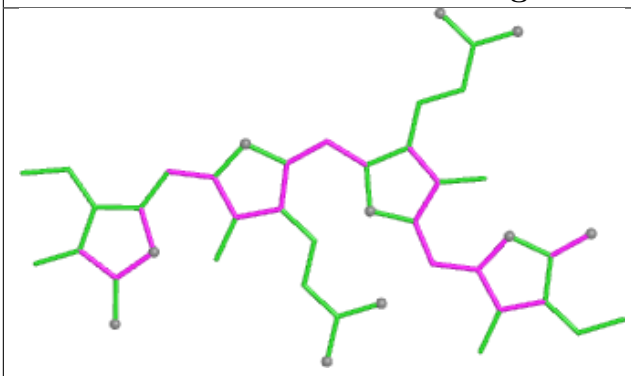


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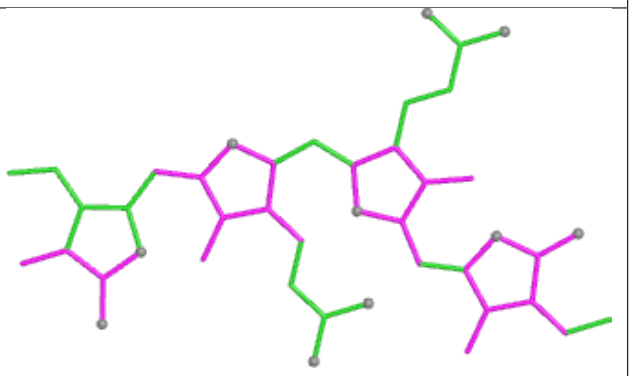


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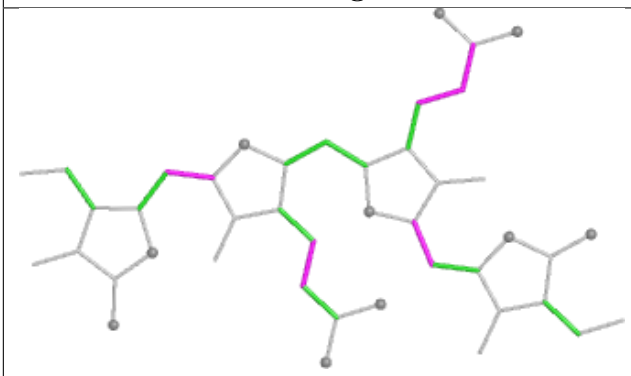
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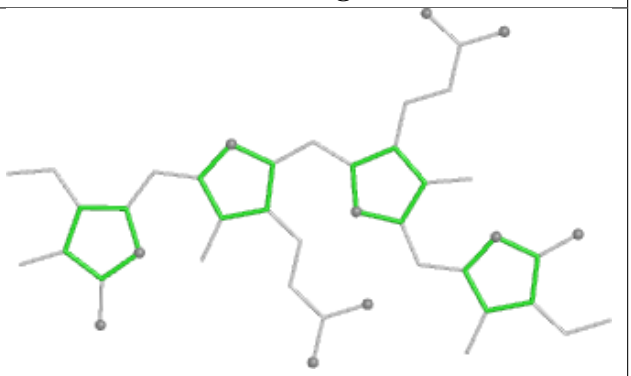
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Bond angles

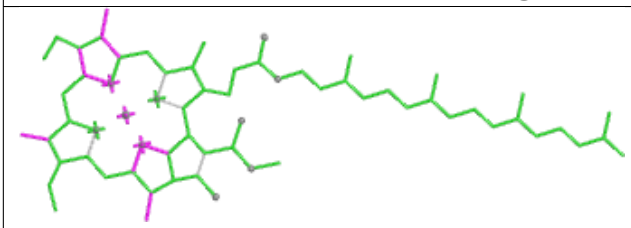


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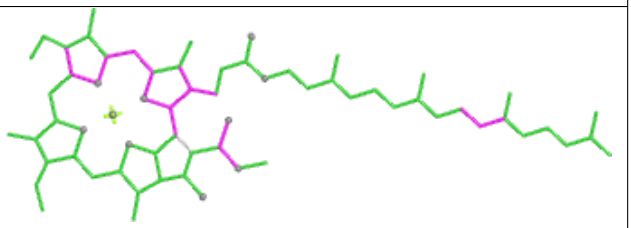


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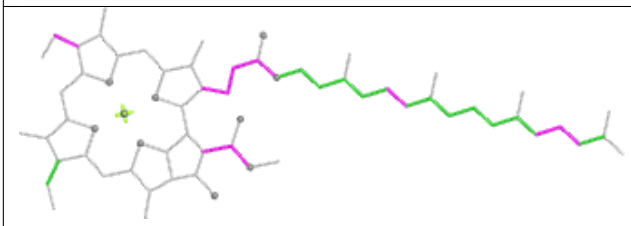
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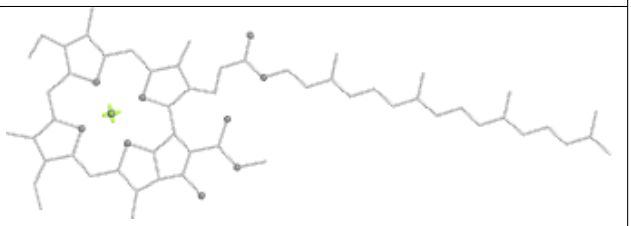
Bond lengths



Bond angles

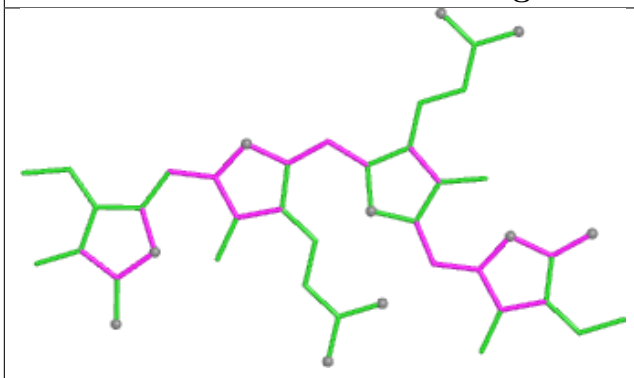


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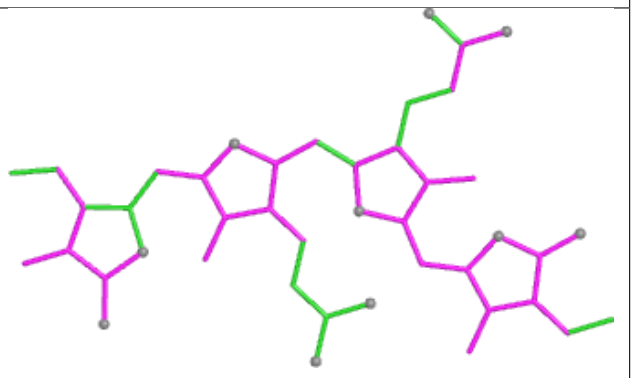


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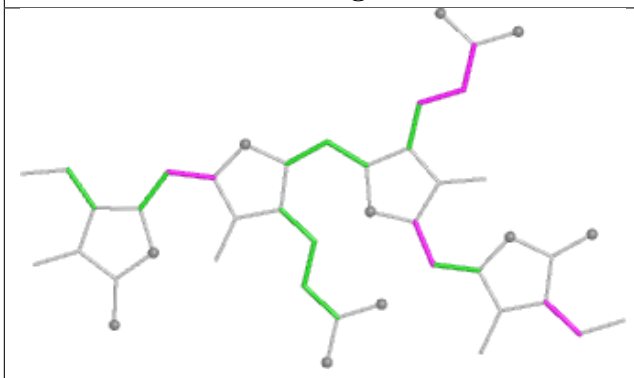
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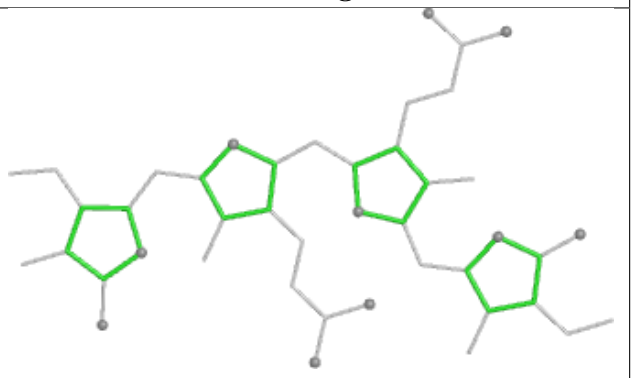
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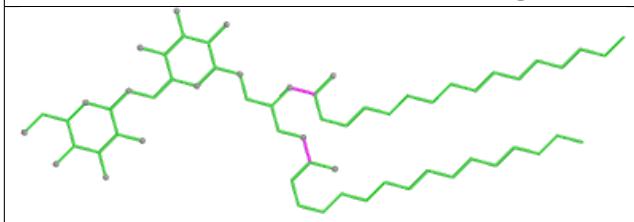


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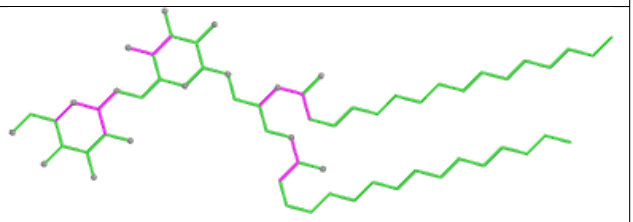


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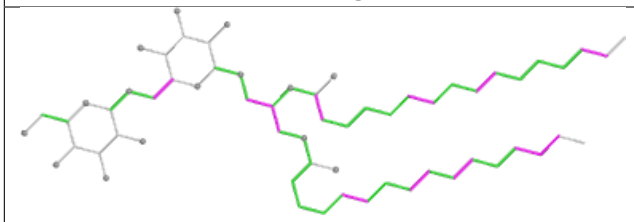
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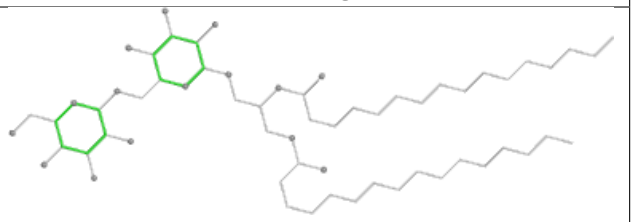
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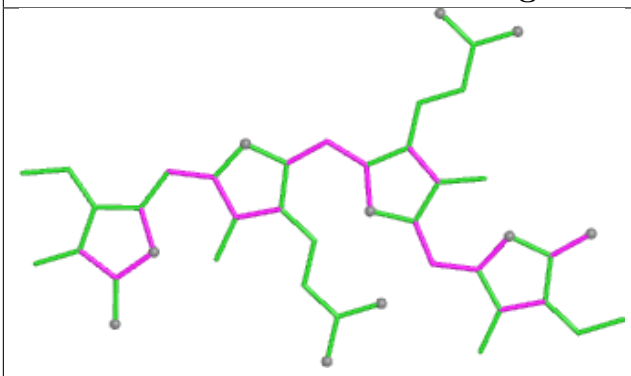


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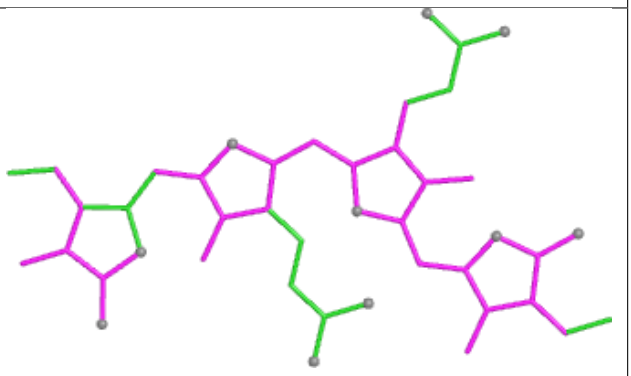


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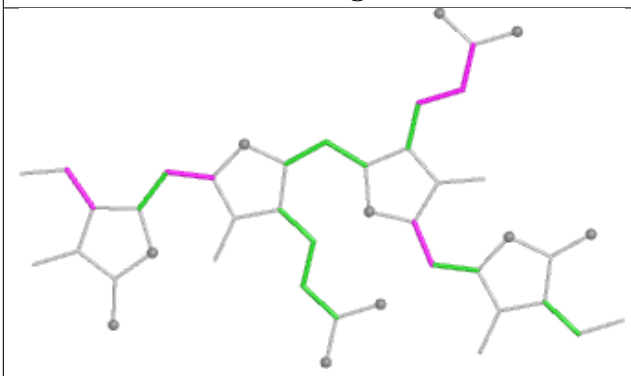
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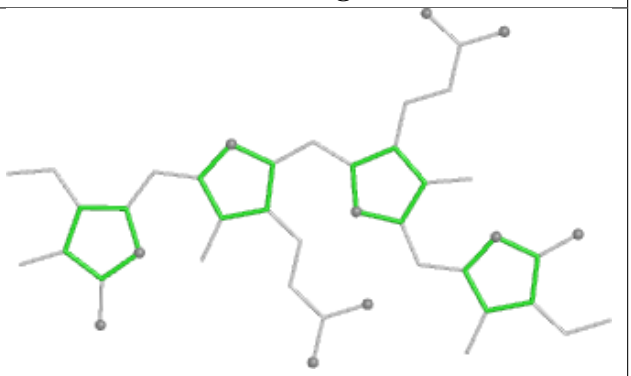
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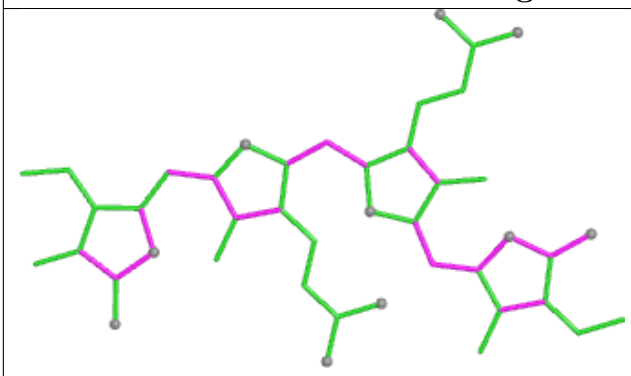


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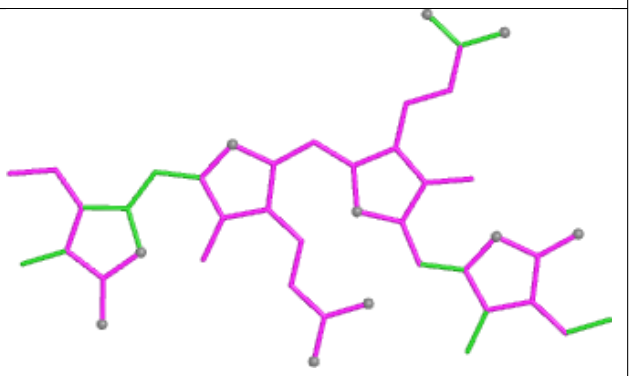


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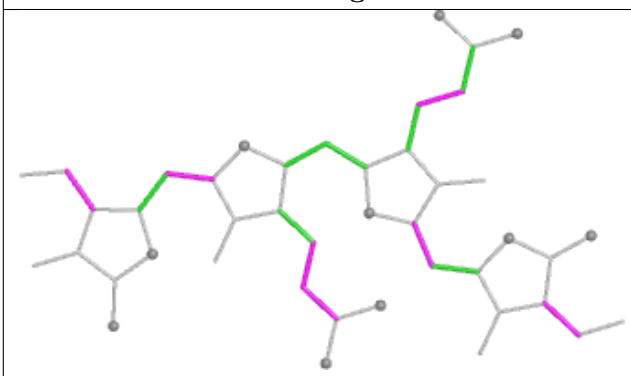
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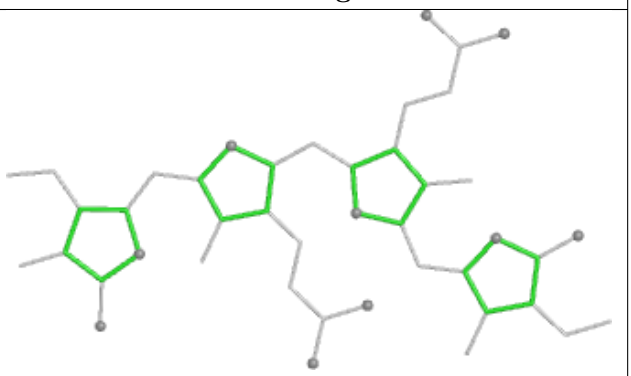
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Bond angles

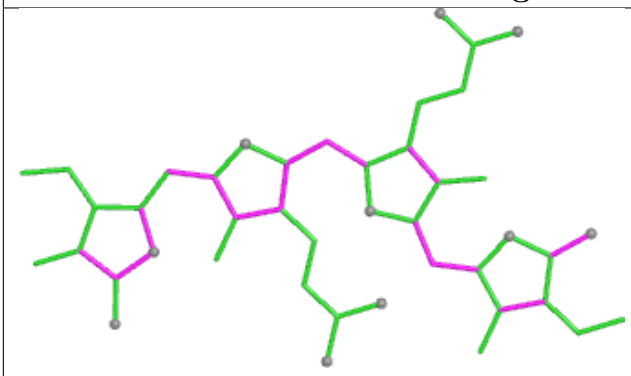


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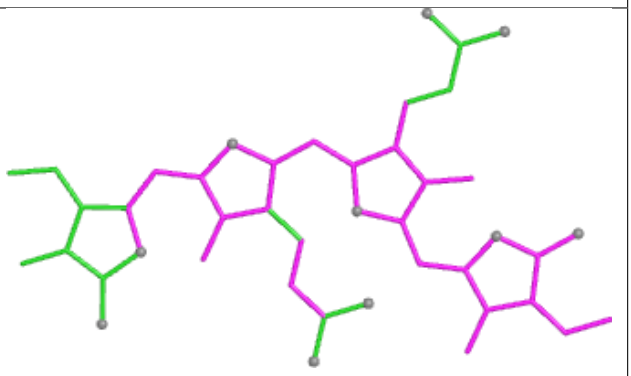


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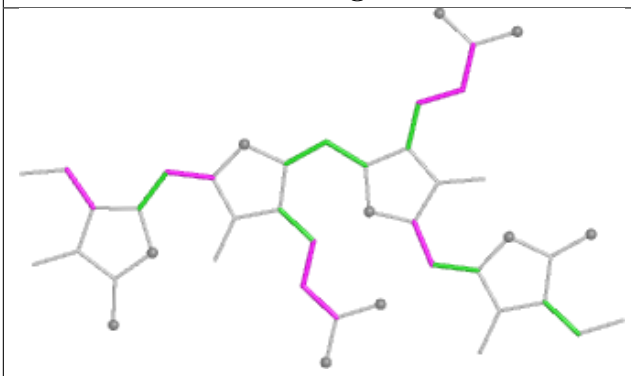
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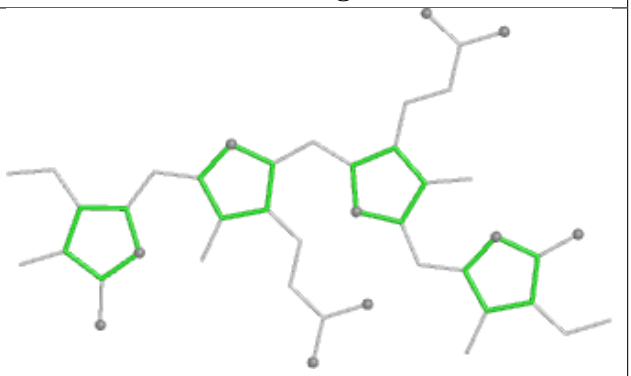
Bond lengths



Bond angles

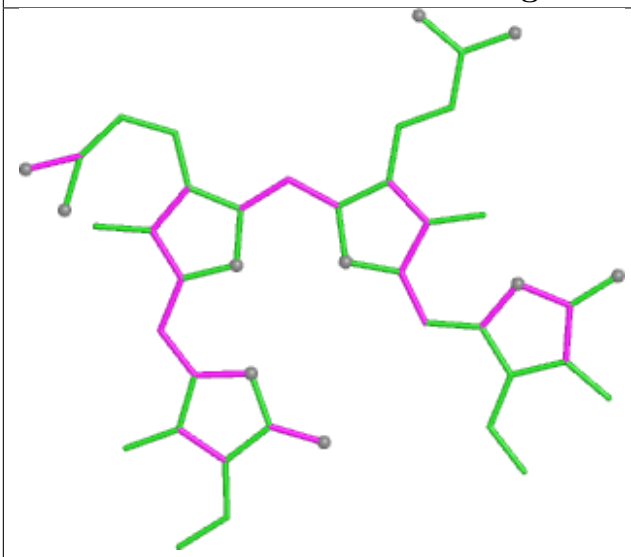


Torsions

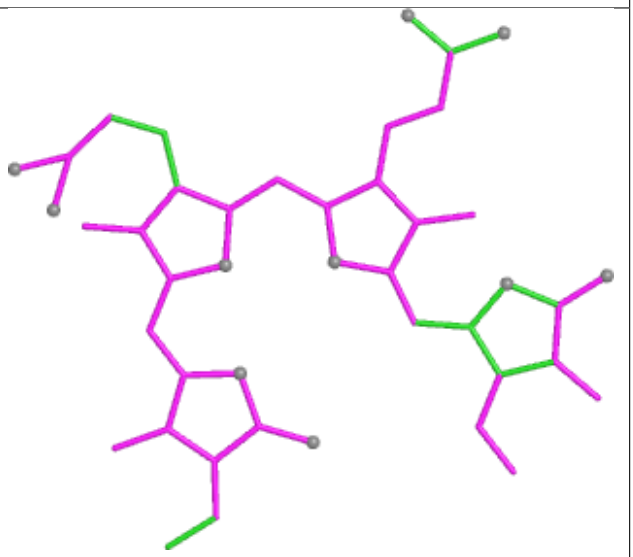


Rings

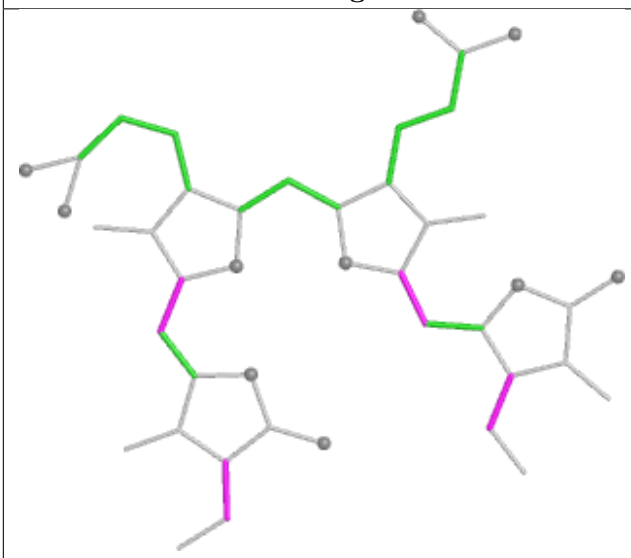
Ligand CYC i8 202



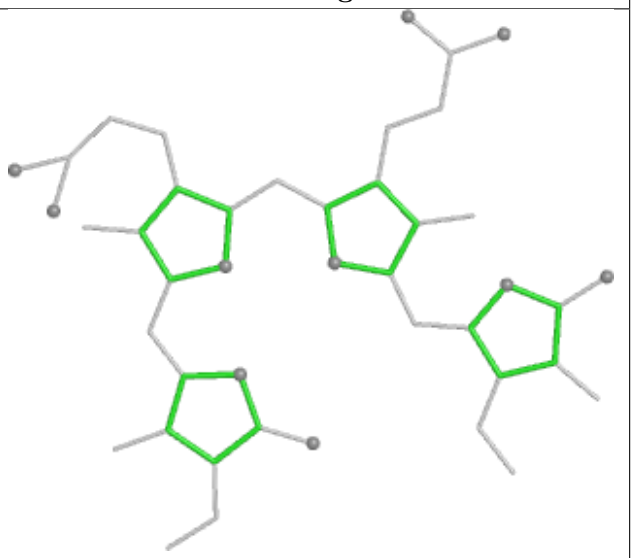
Bond lengths



Bond angles

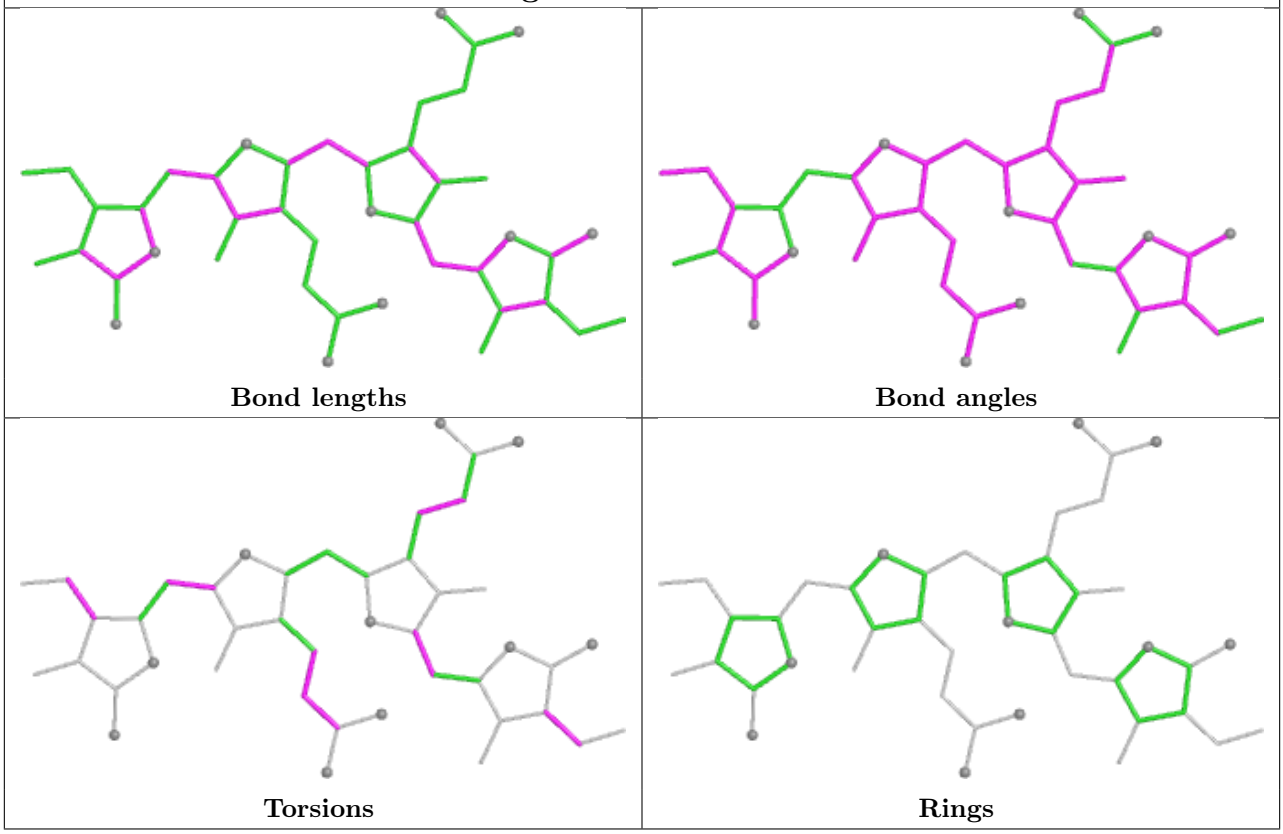


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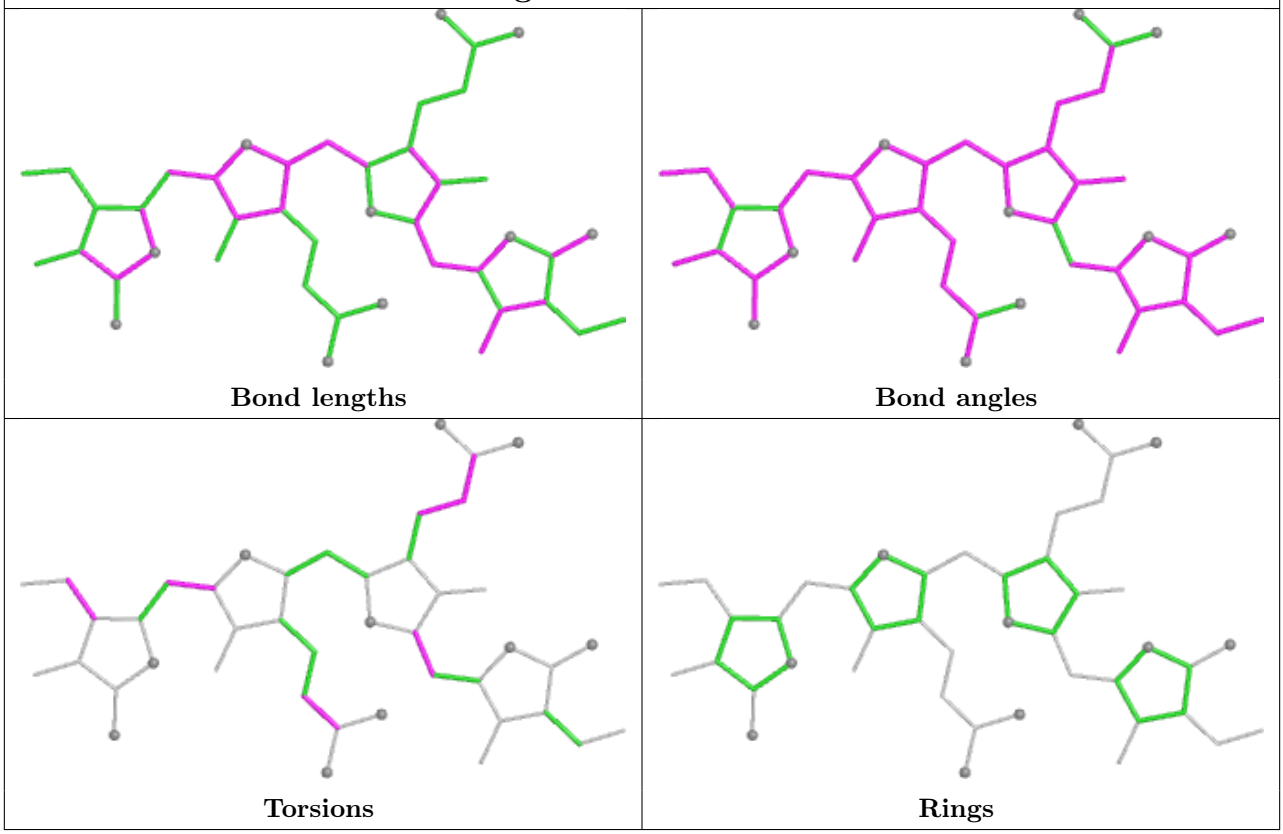


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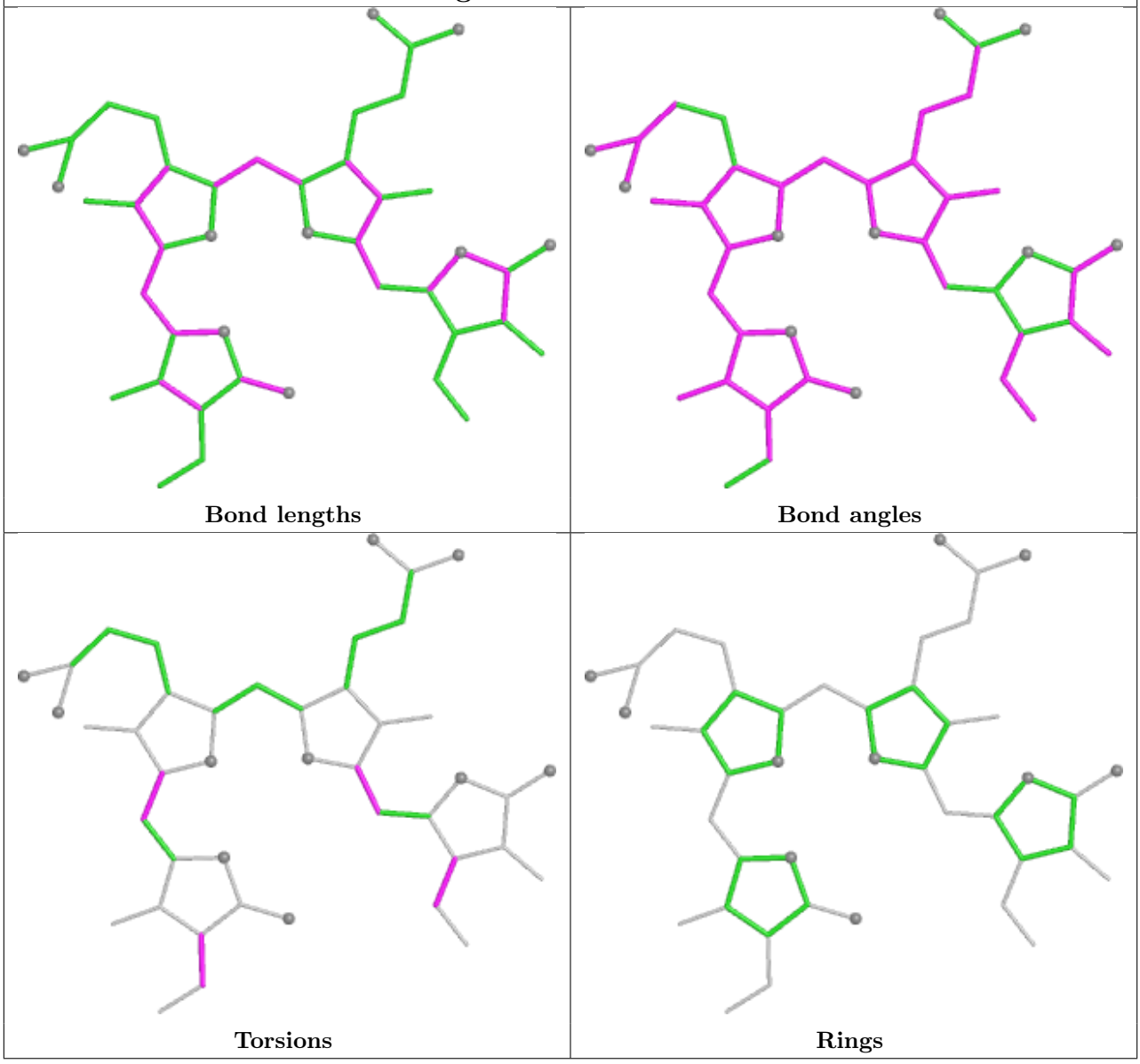
Ligand CYC lJ 201



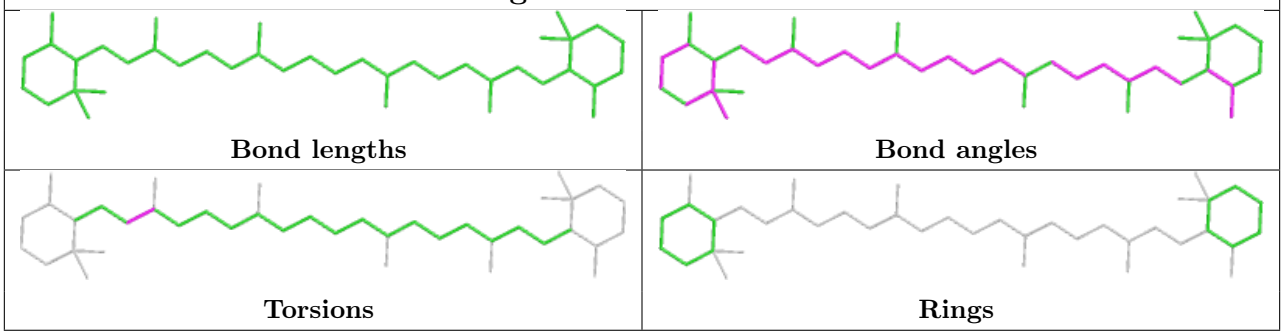
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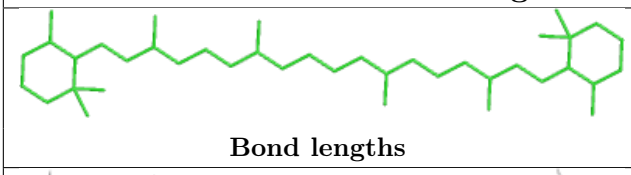
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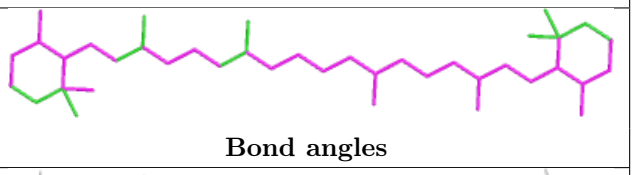
Ligand BCR CD 520



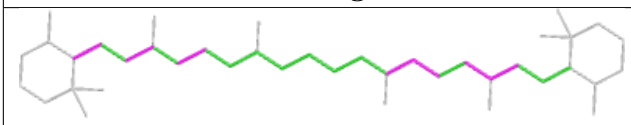
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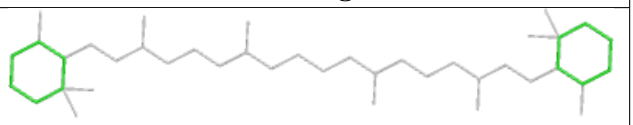
Bond lengths



Bond angles

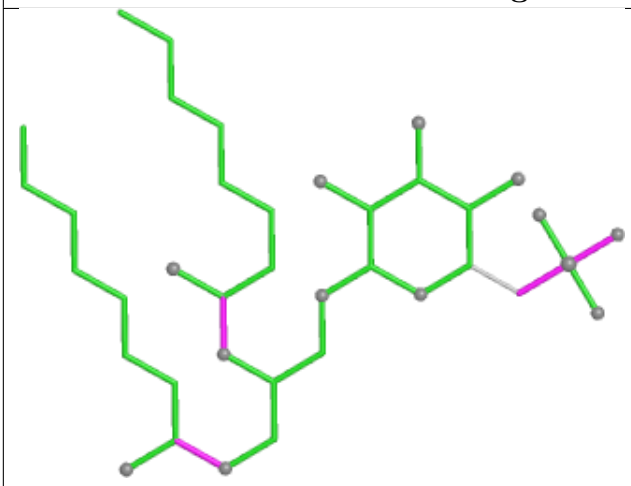


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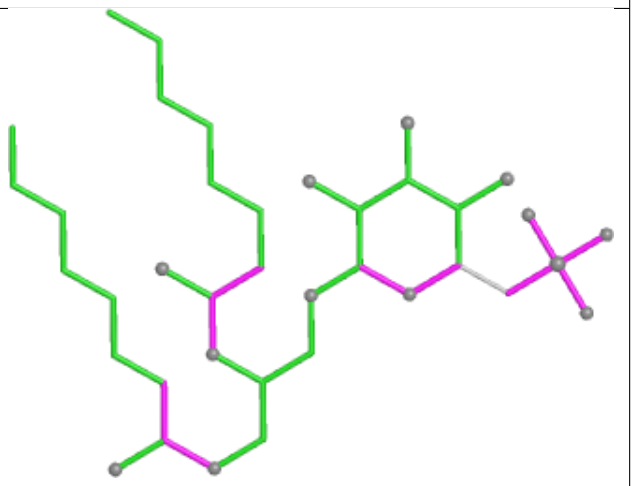


Rings

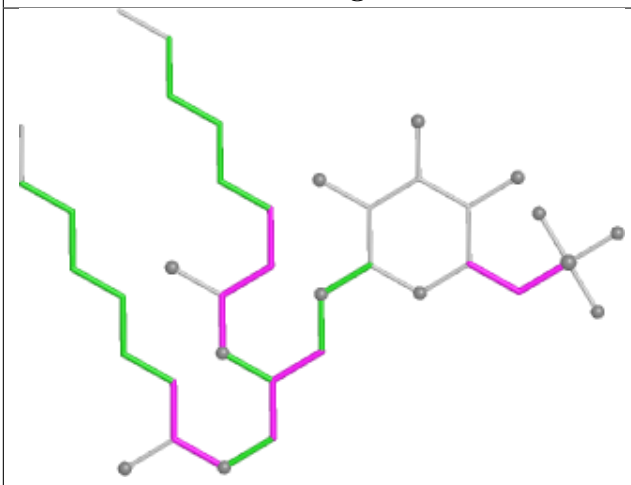
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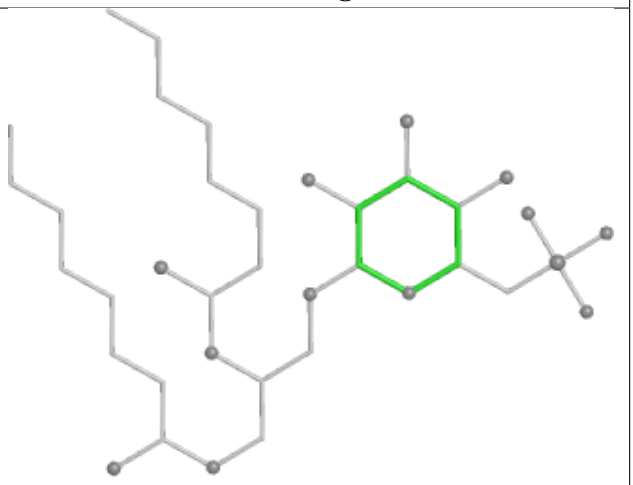
Bond lengths



Bond angles

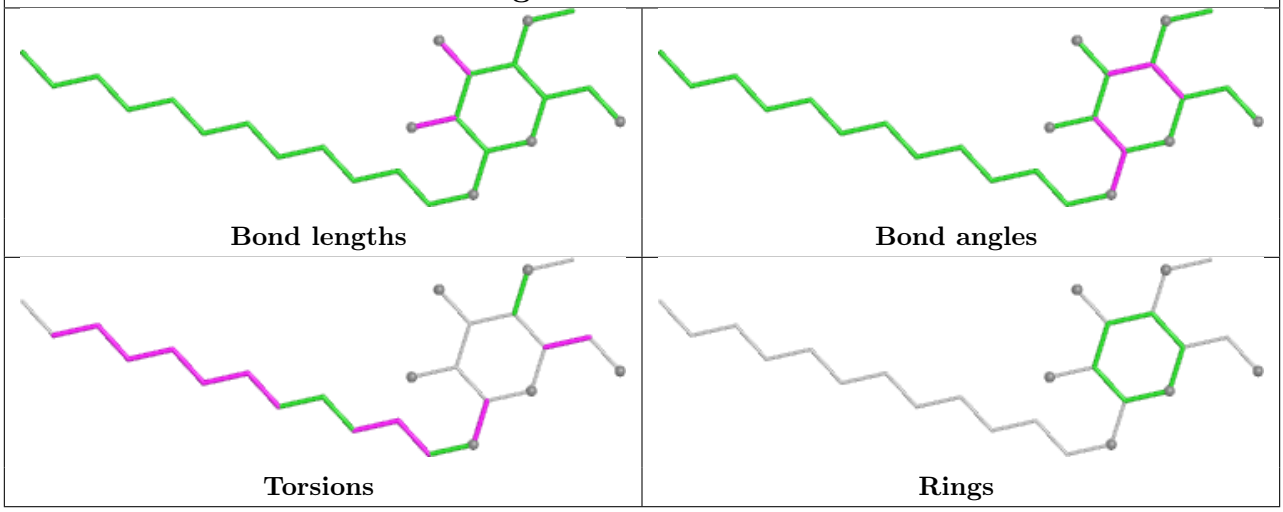


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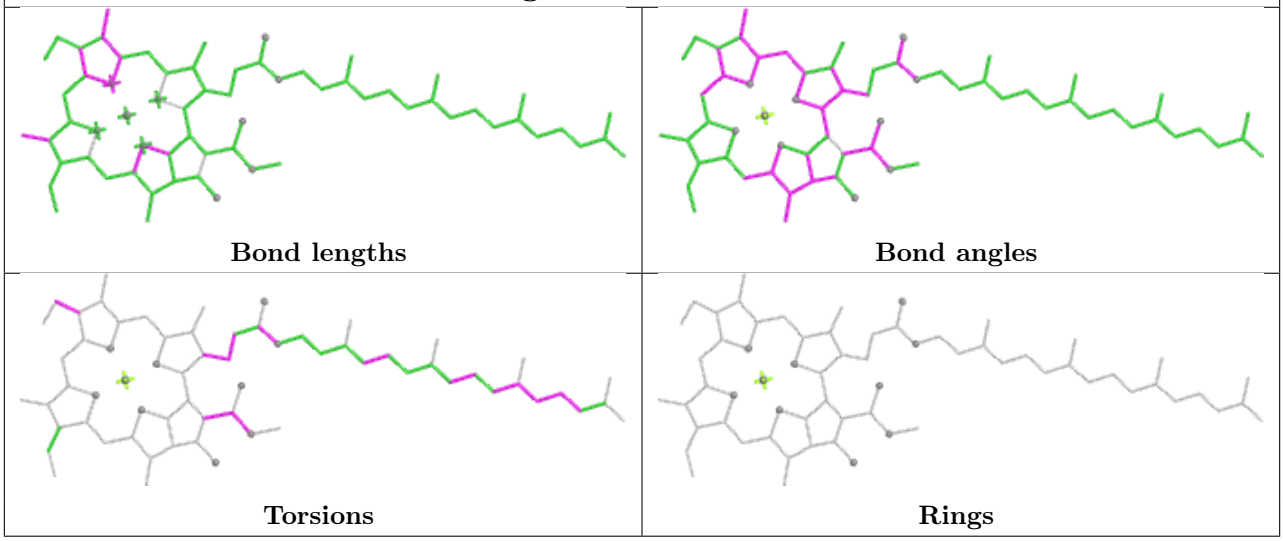


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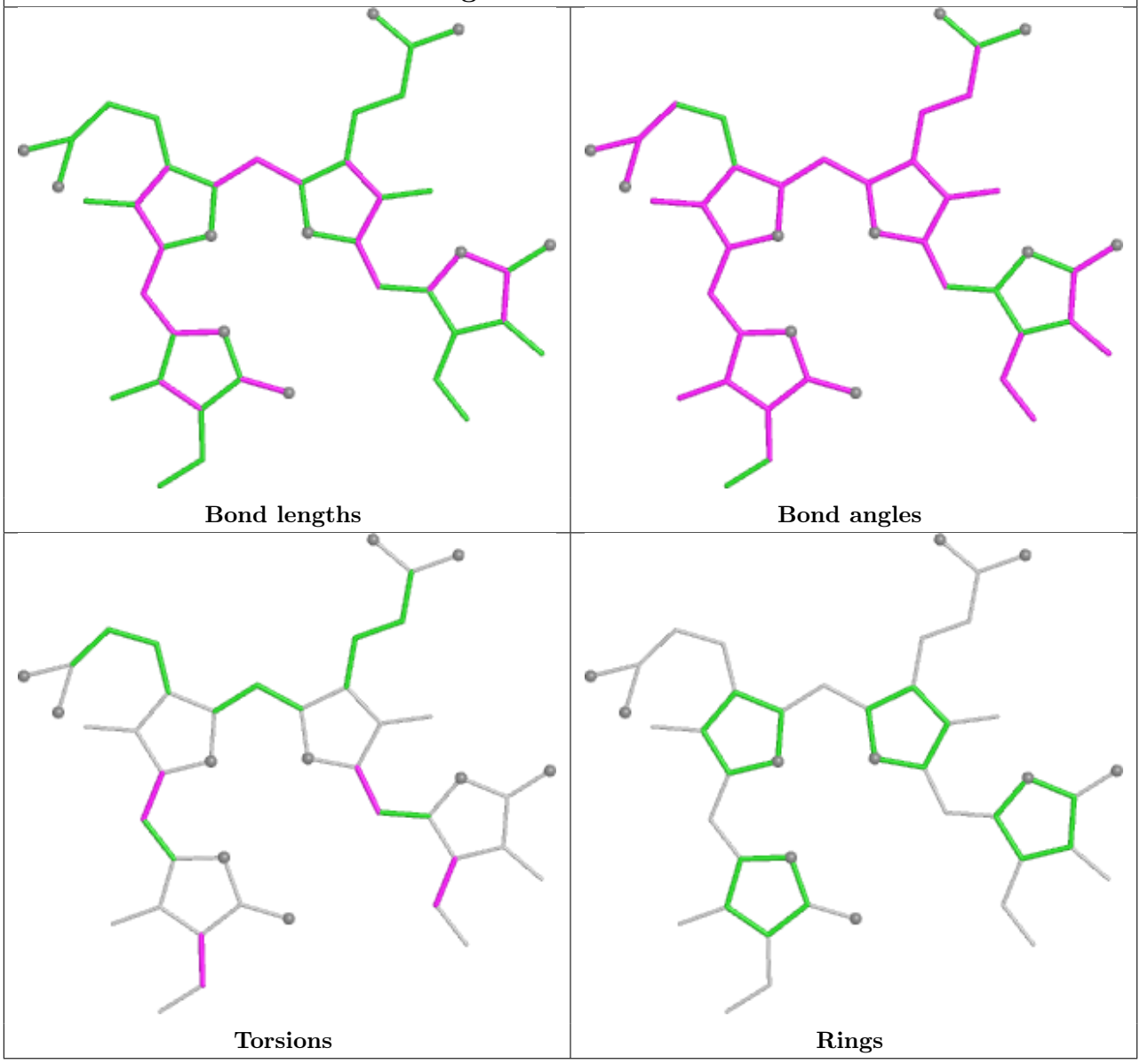
Ligand LMT D1 411



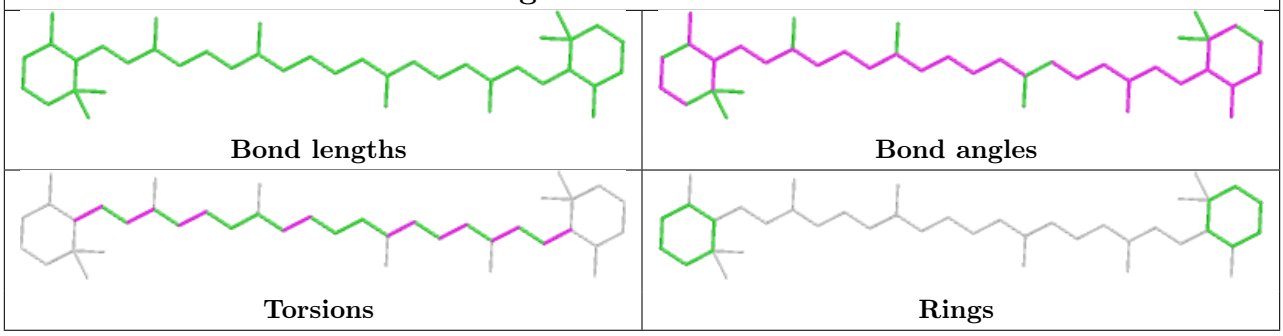
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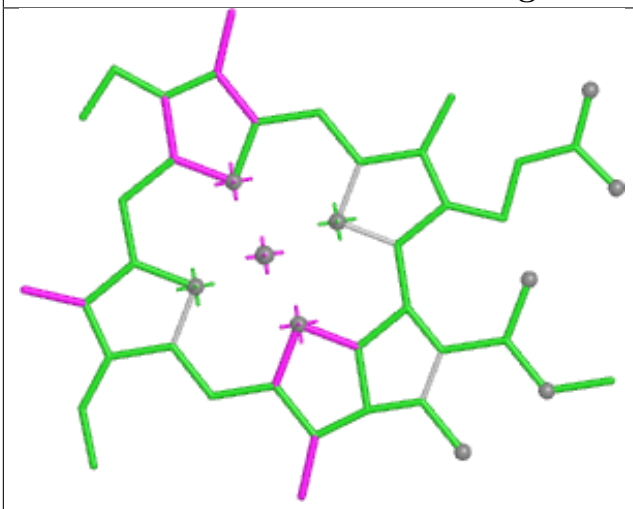
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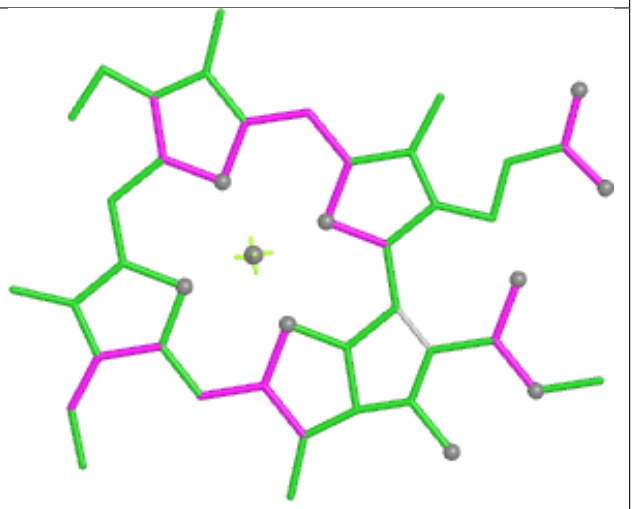
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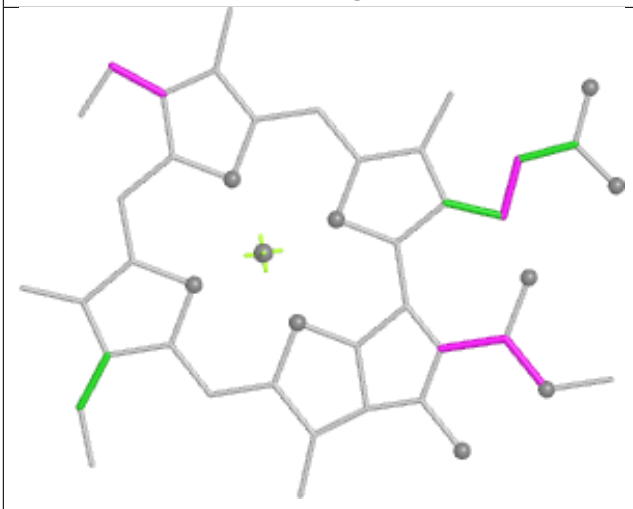
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Bond lengths



Bond angles

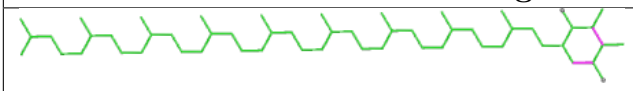


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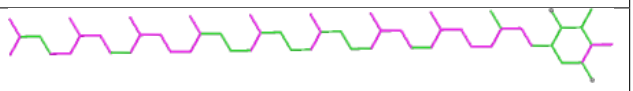


Rings

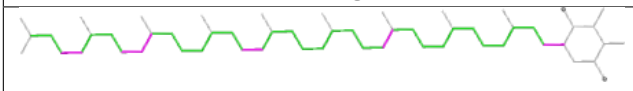
Ligand PL9 DD 408



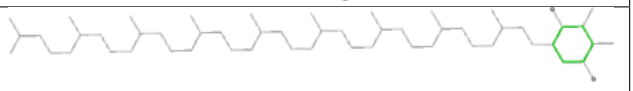
Bond lengths



Bond angles

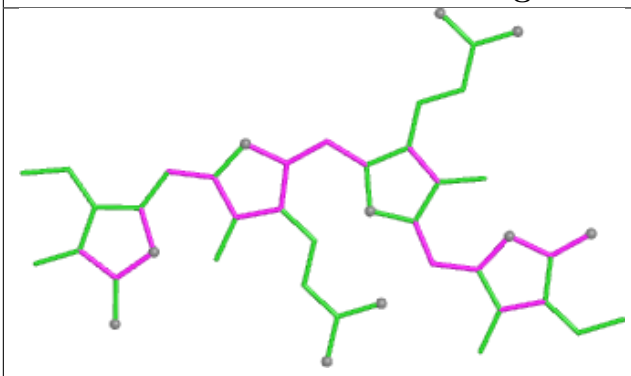


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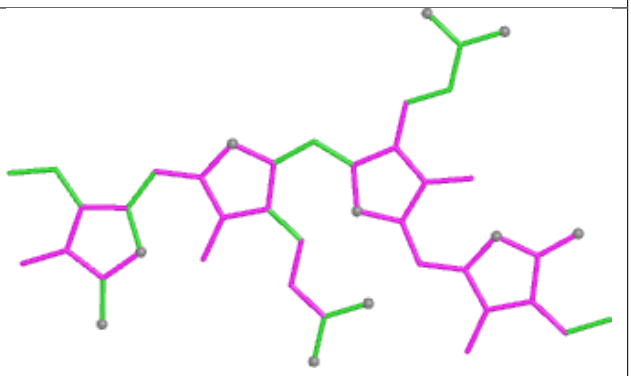


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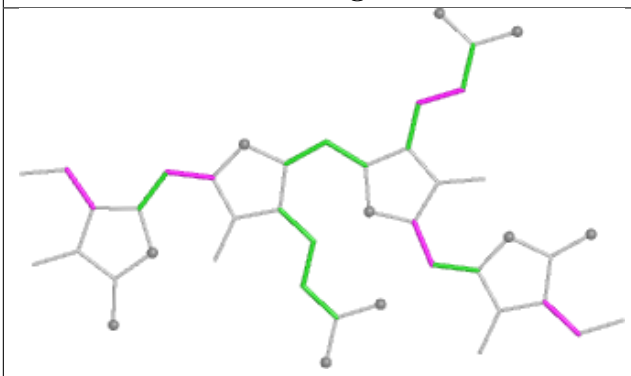
Ligand CYC nF 202



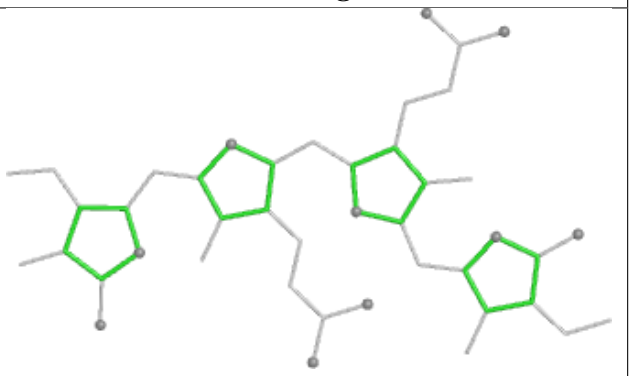
Bond lengths



Bond angles

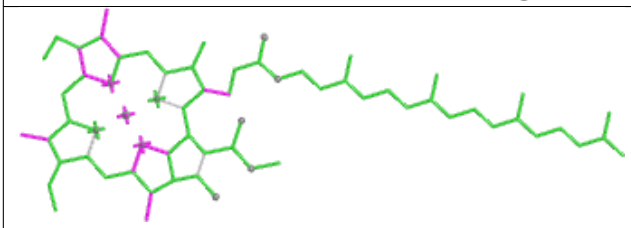


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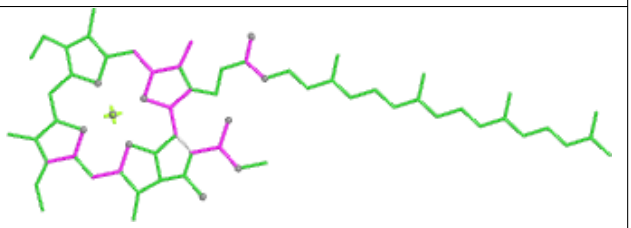


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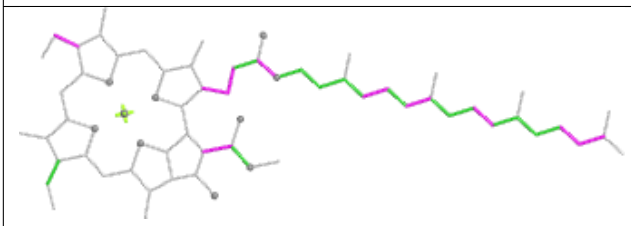
Ligand CLA bE 604



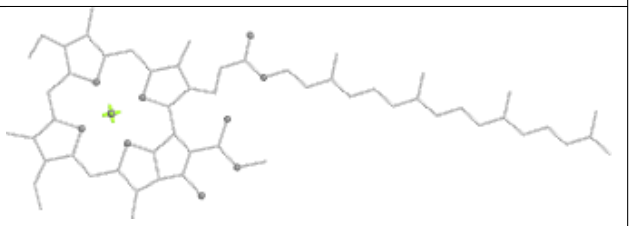
Bond lengths



Bond angles

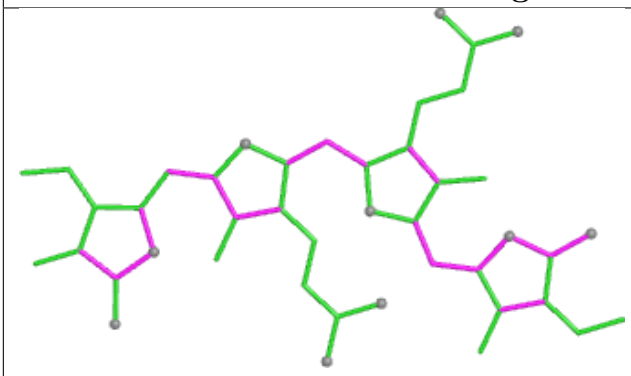


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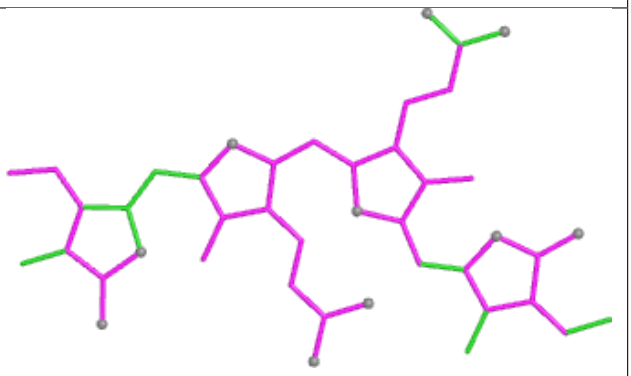


Rings

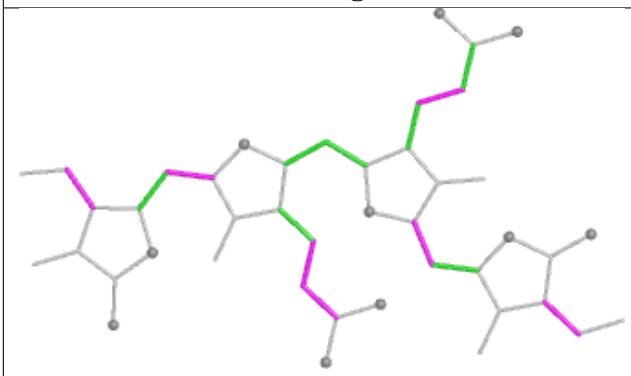
Ligand CYC bA 201



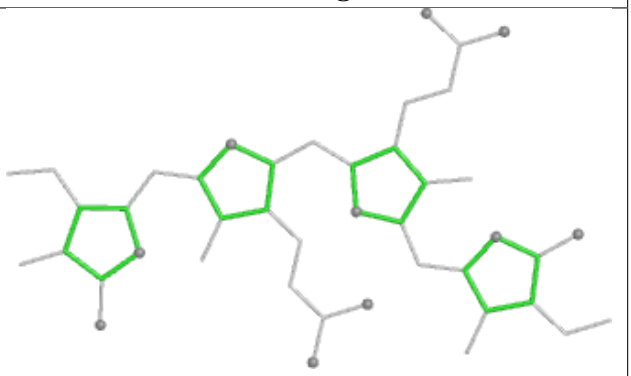
Bond lengths



Bond angles

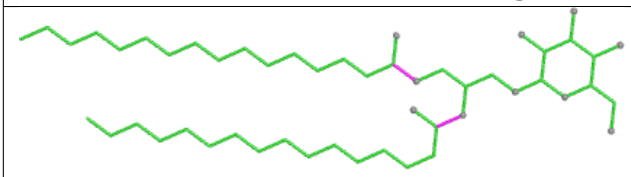


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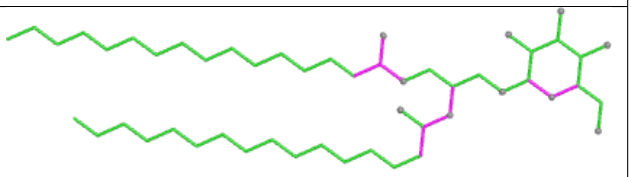


Rings

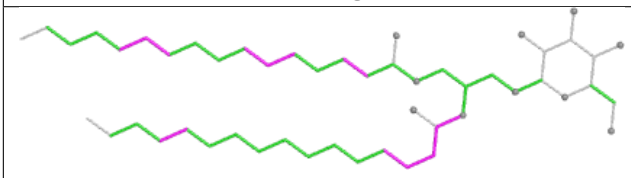
Ligand LMG C1 521



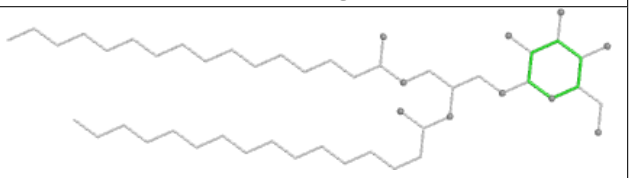
Bond lengths



Bond angles

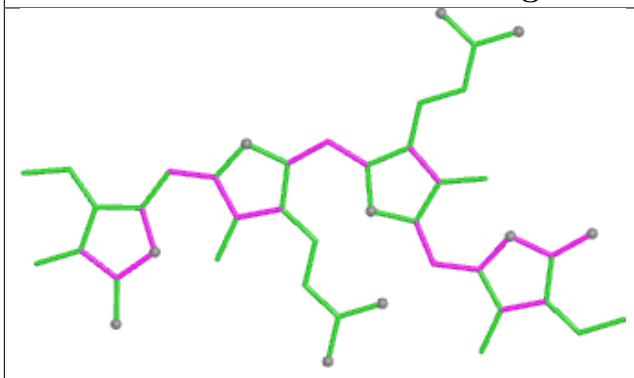


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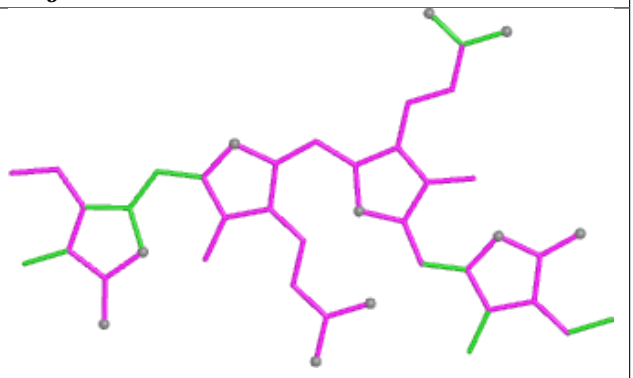


Rings

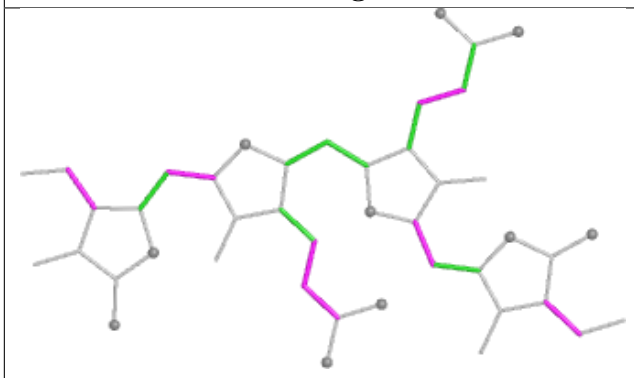
Ligand CYC j6 201



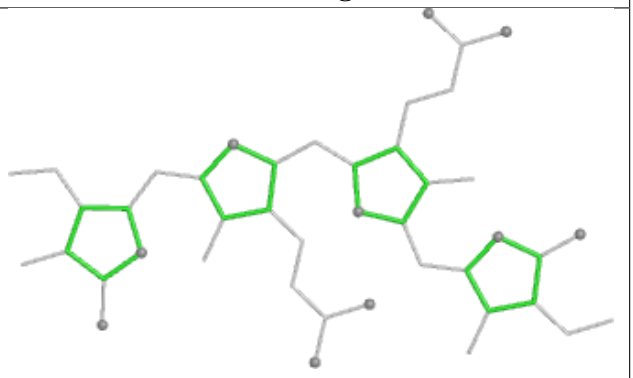
Bond lengths



Bond angles

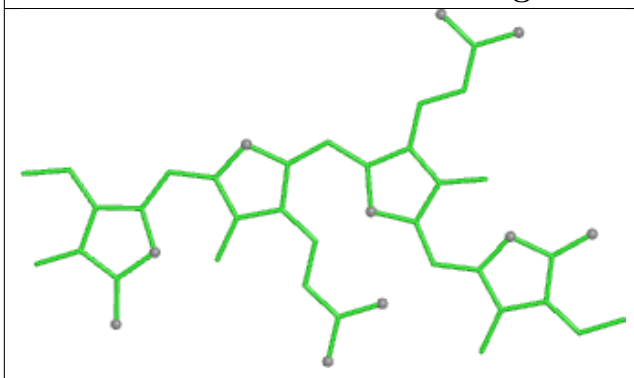


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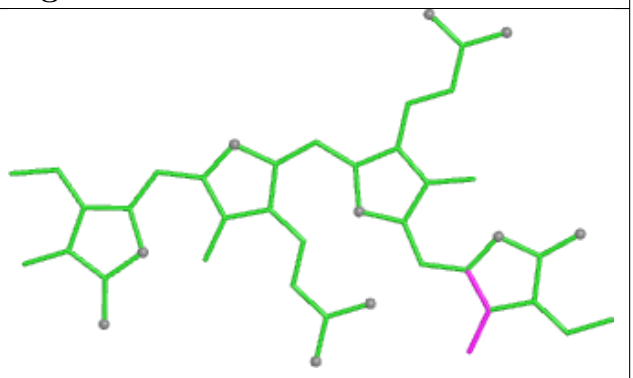


Rings

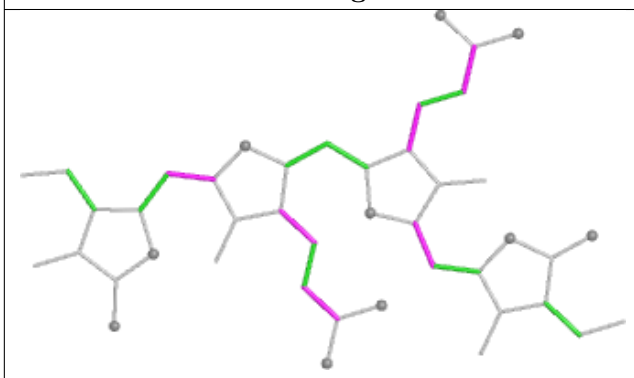
Ligand CYC gH 201



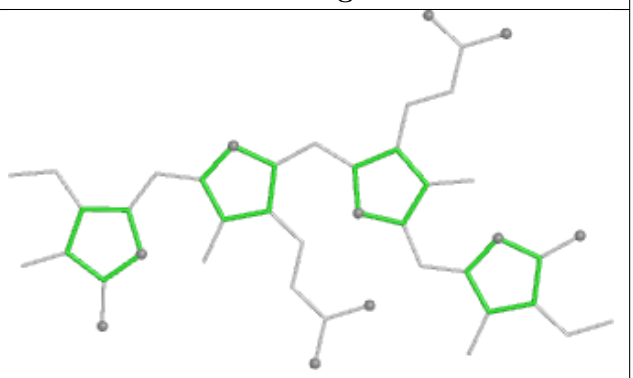
Bond lengths



Bond angles

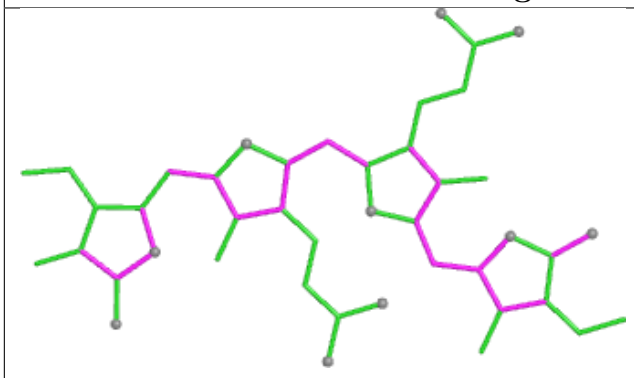


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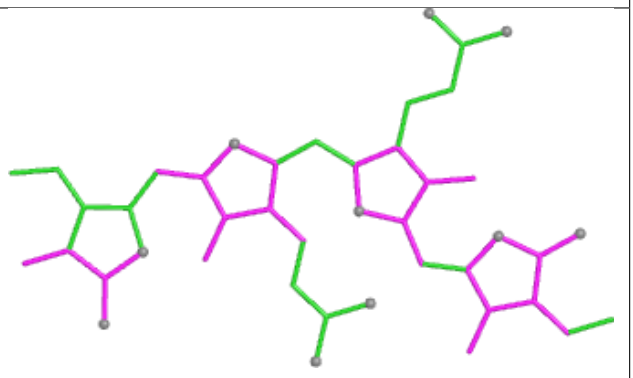


Rings

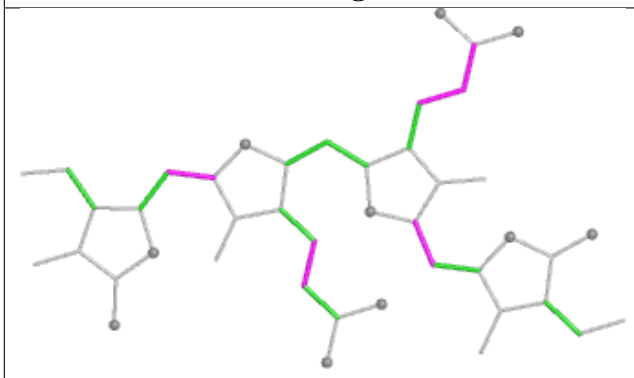
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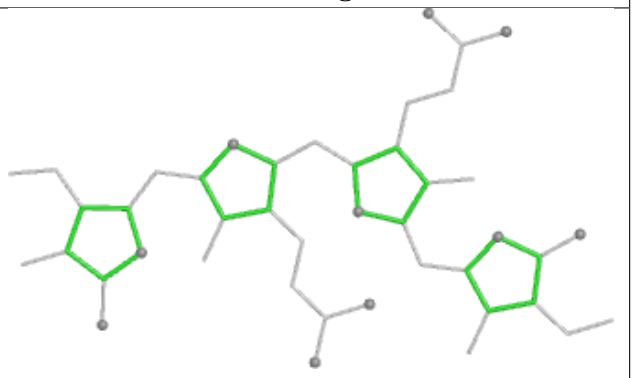
Bond lengths



Bond angles

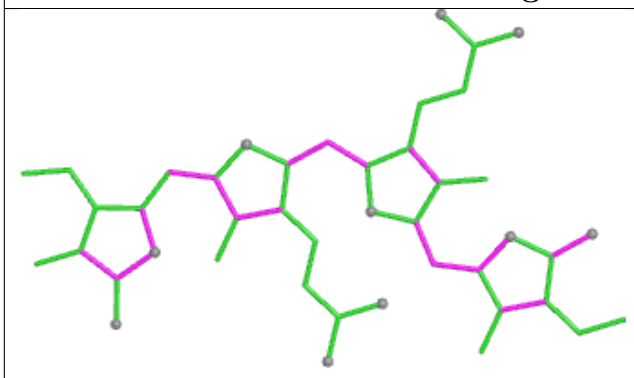


Torsions

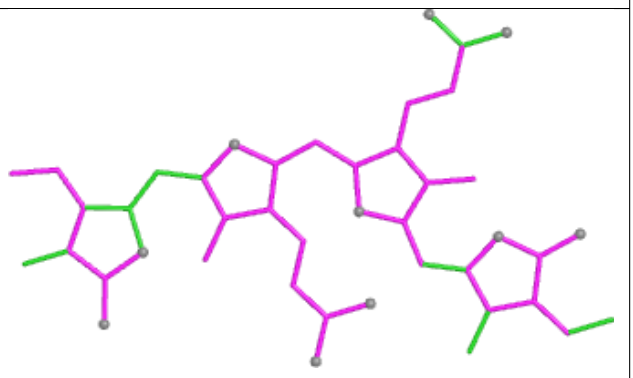


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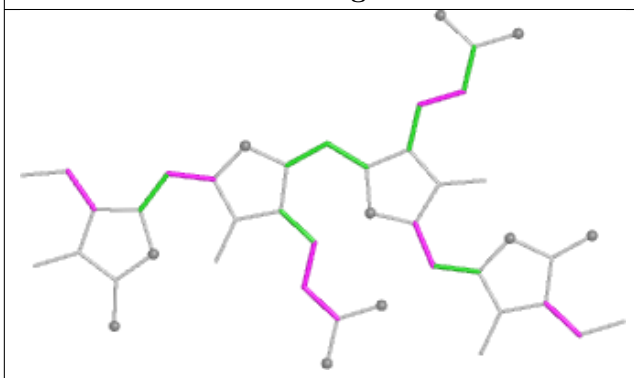
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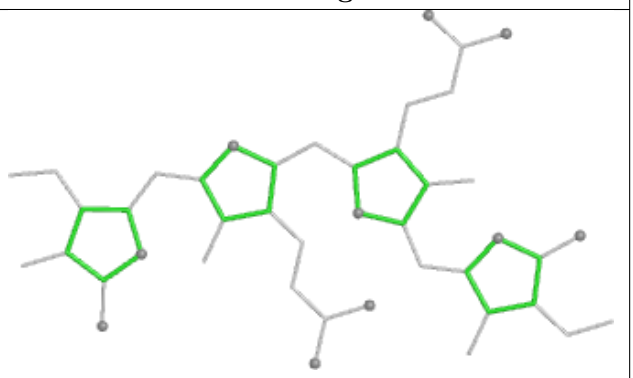
Bond lengths



Bond angles

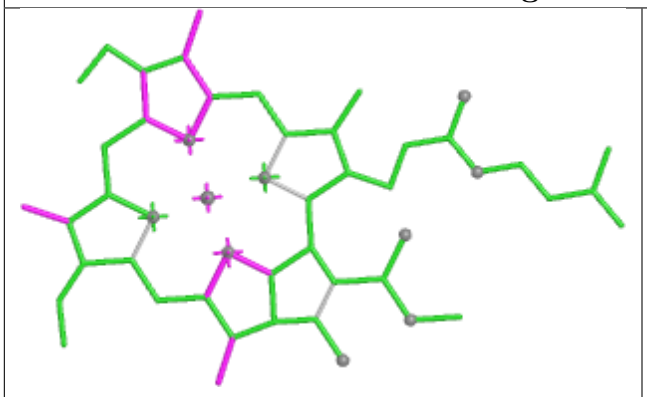


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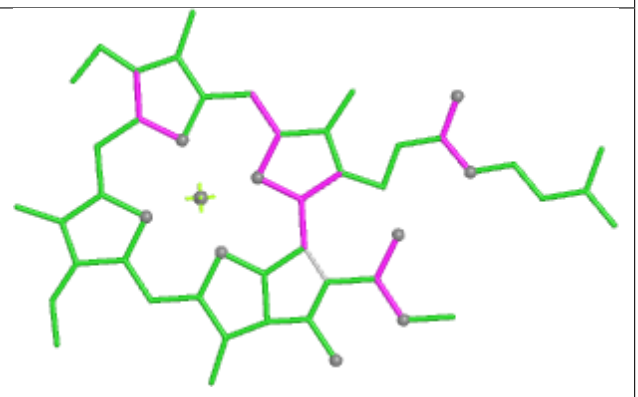


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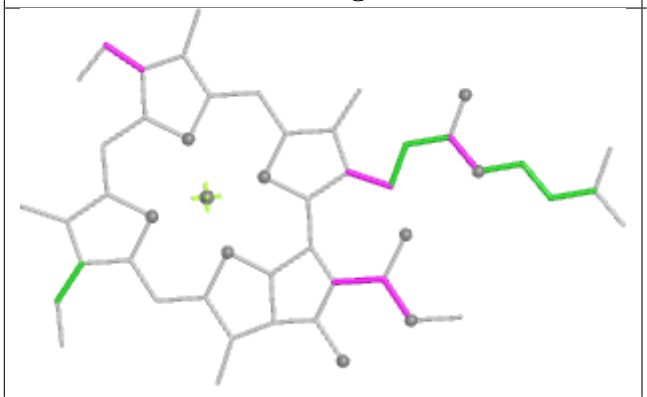
Ligand CLA c1 513



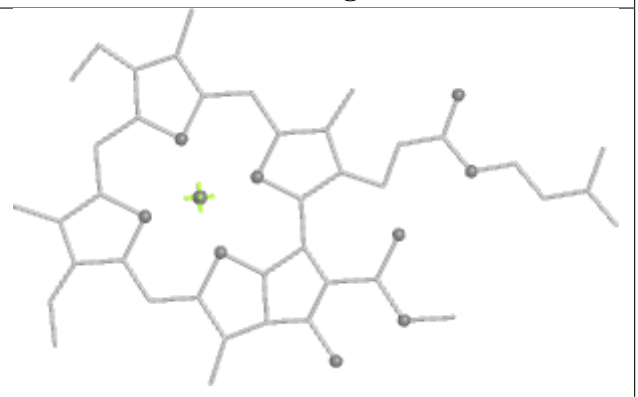
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Bond angles

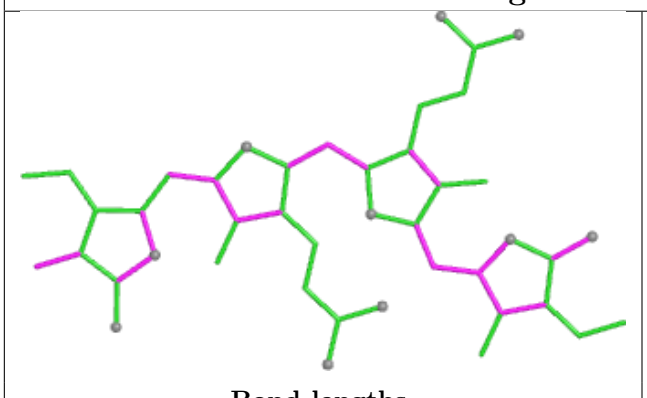


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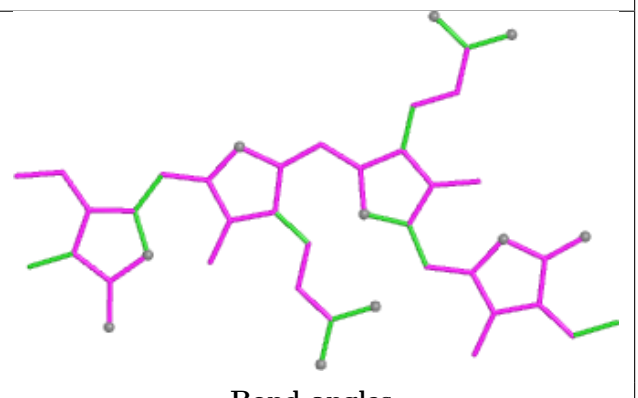


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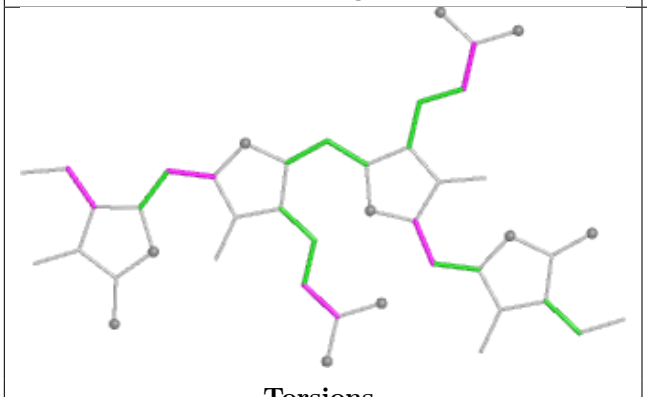
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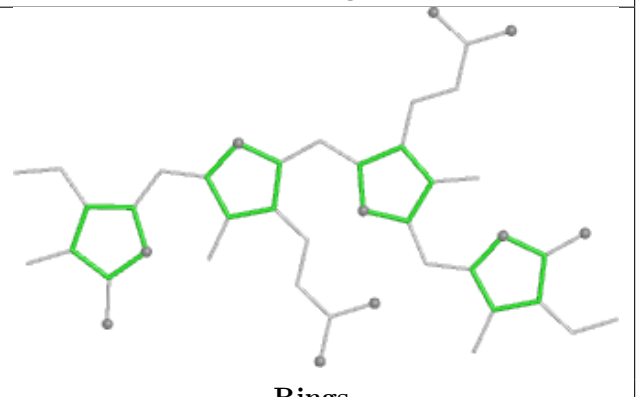
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Bond angles

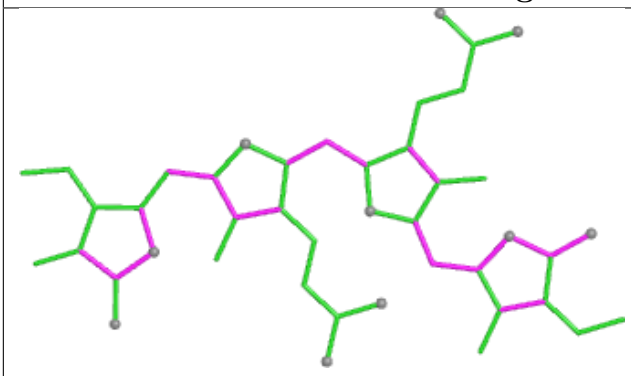


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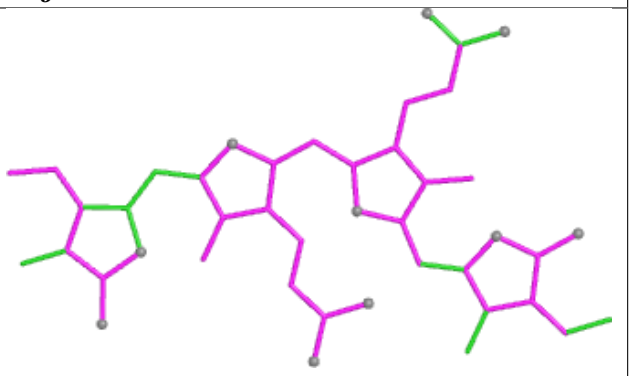


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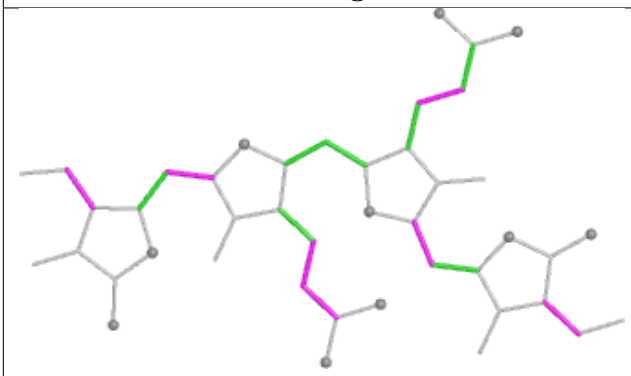
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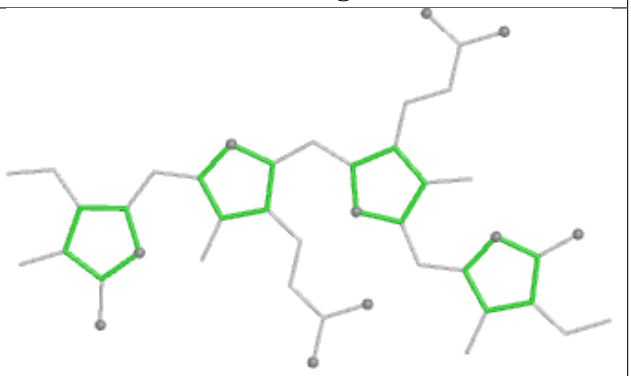
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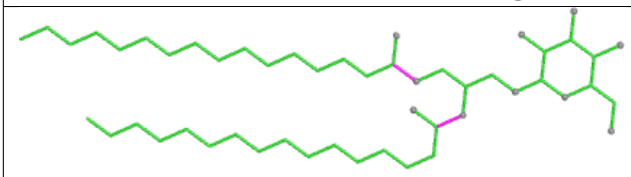


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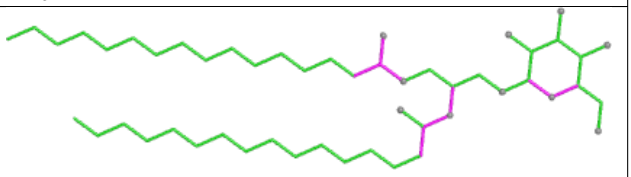


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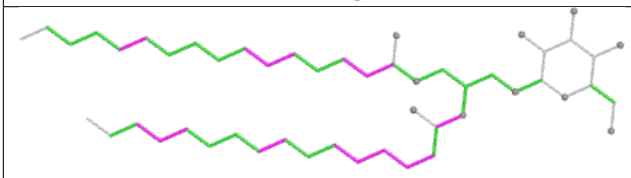
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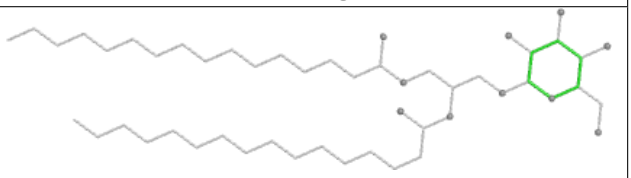
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Bond angles

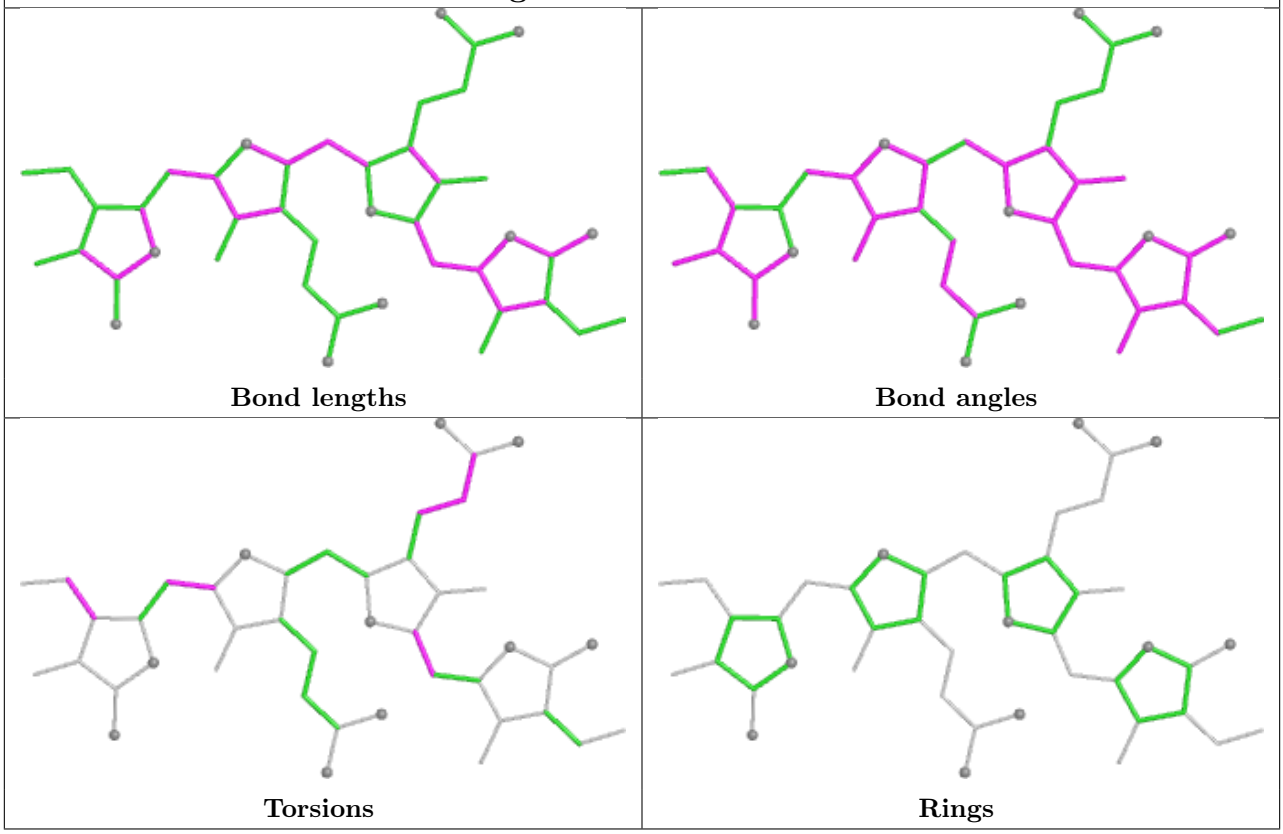


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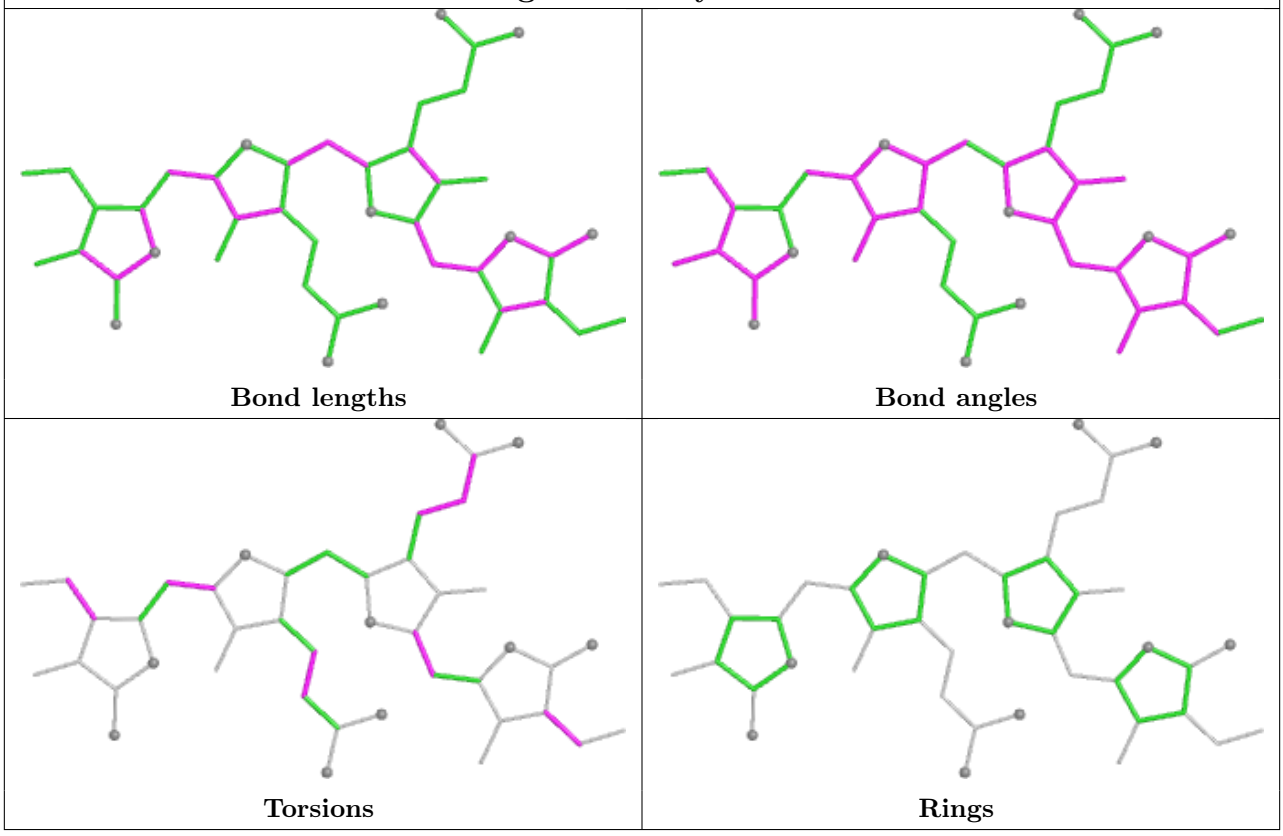


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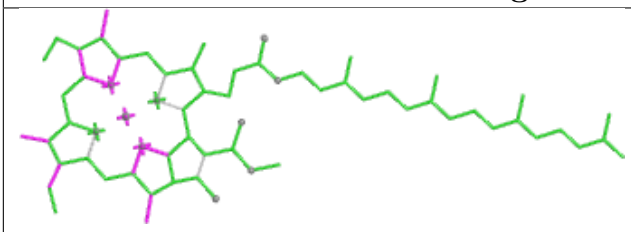
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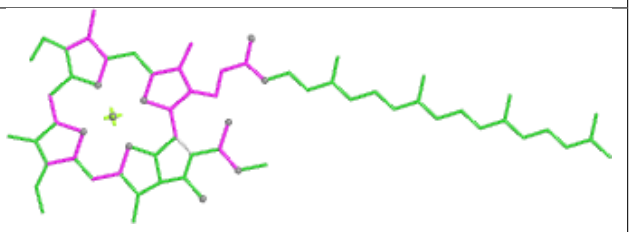
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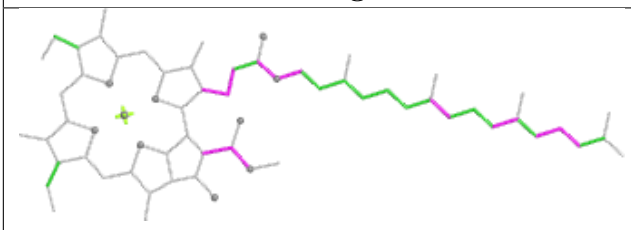
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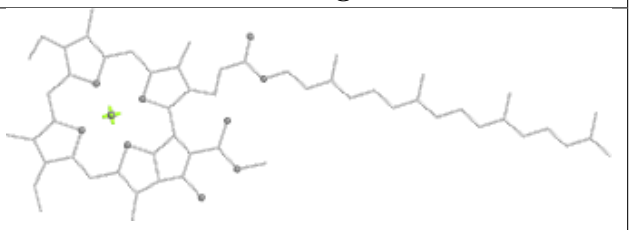
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Bond angles

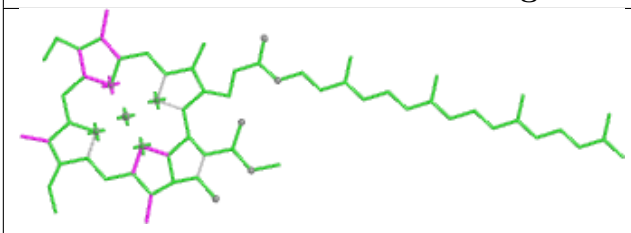


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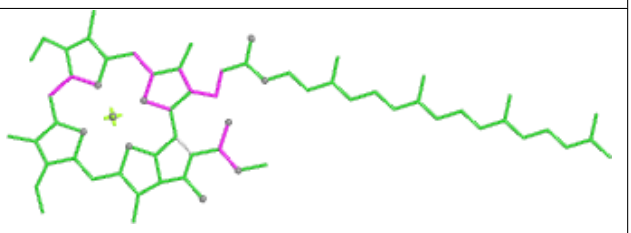


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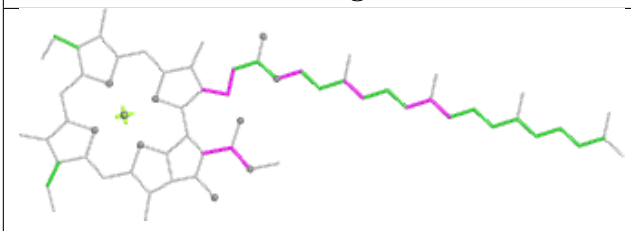
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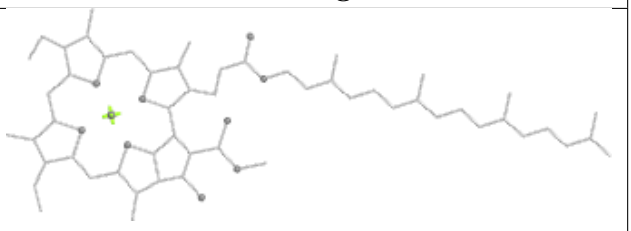
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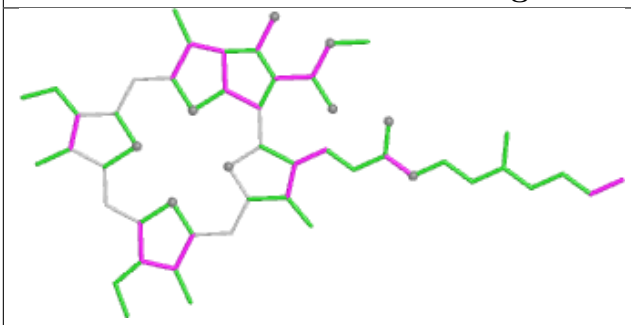


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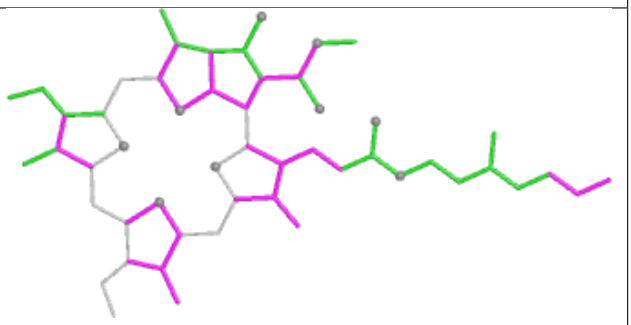


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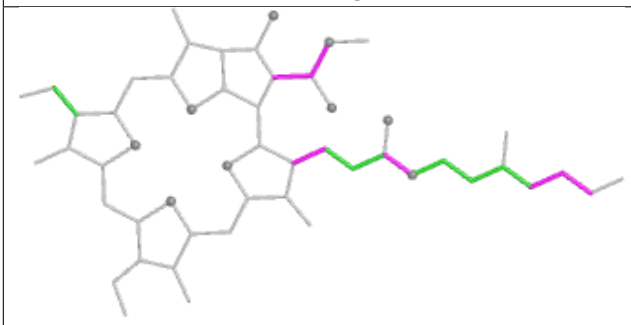
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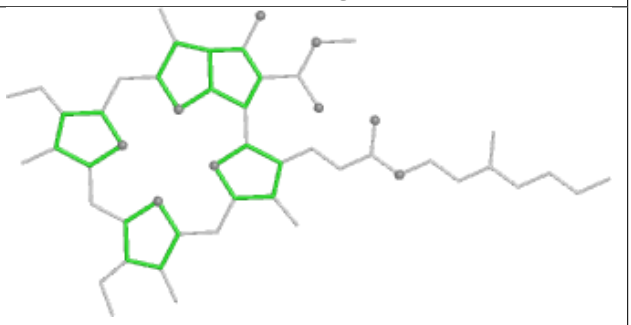
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Bond angles

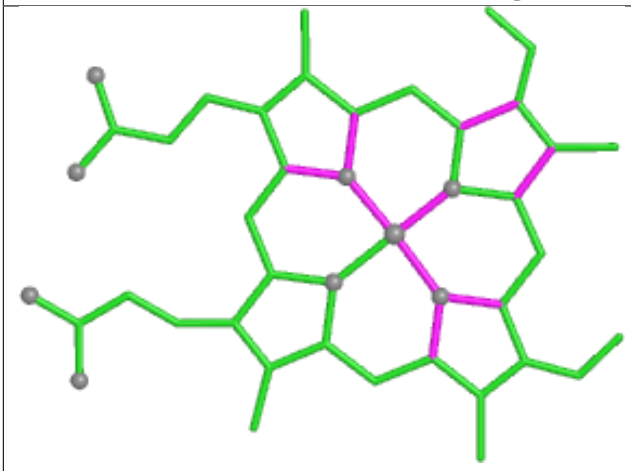


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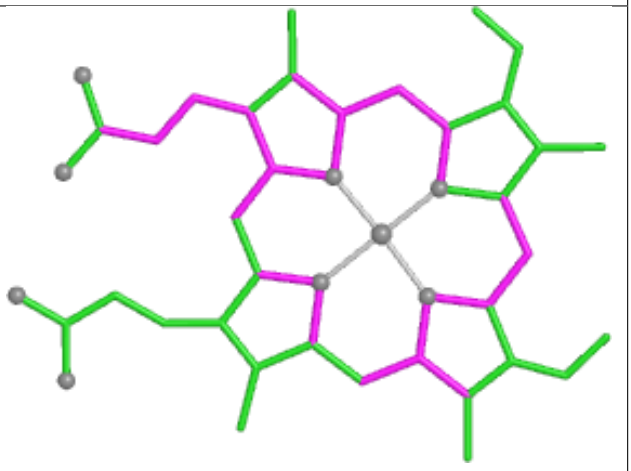


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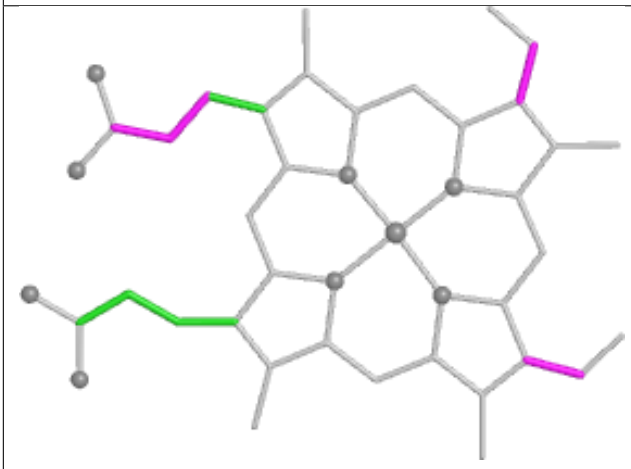
Ligand HEM vD 201



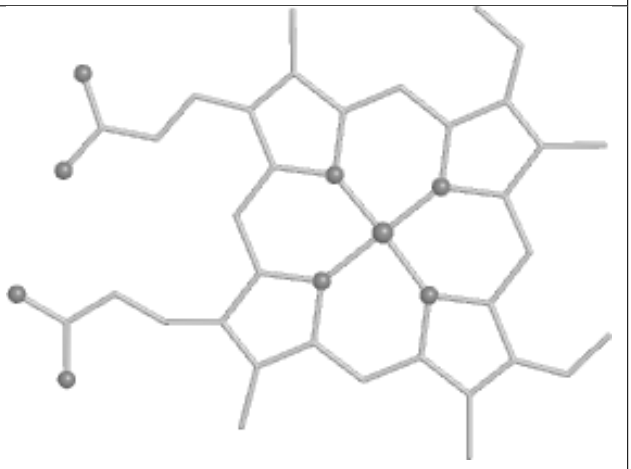
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Bond angles

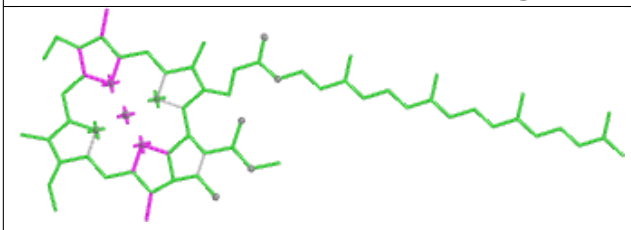


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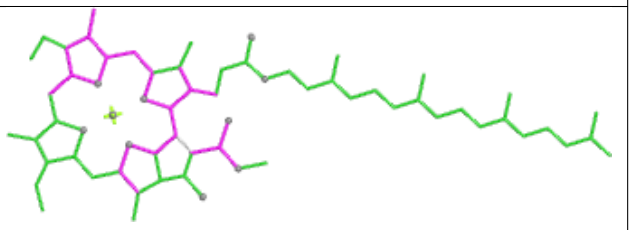


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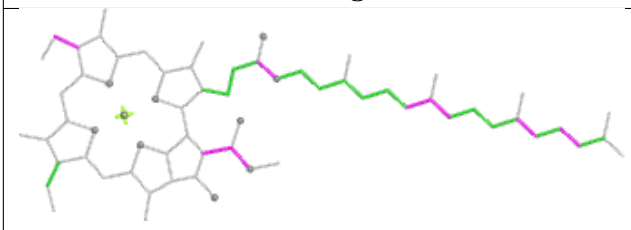
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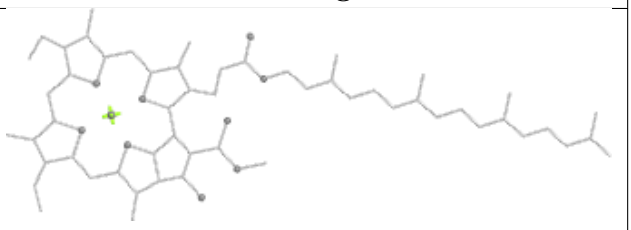
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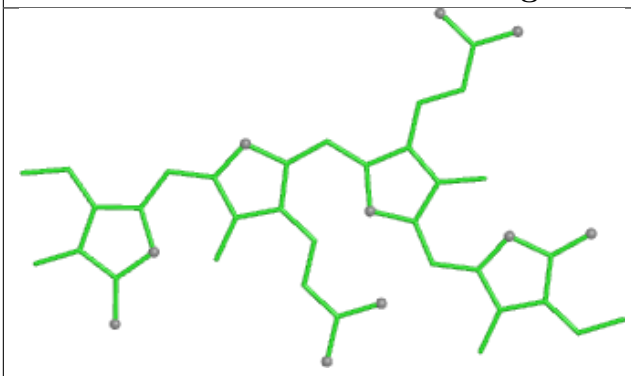


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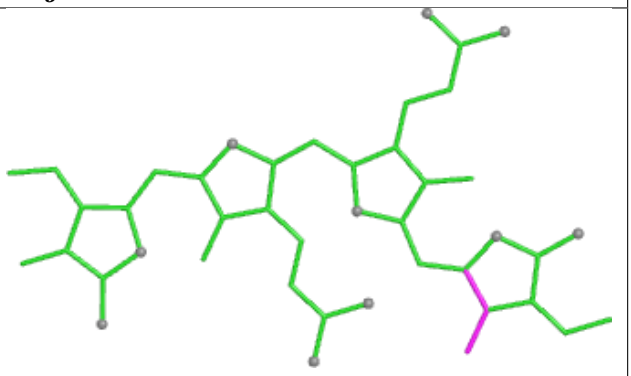


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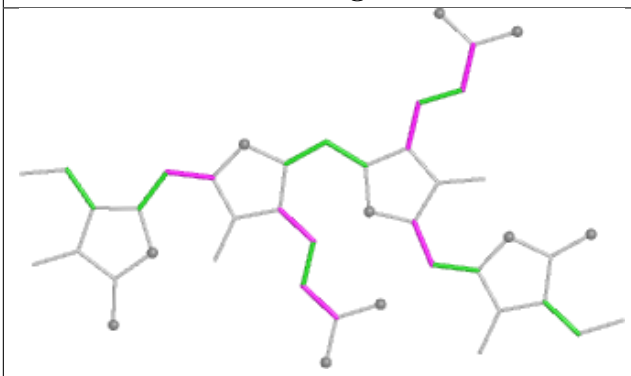
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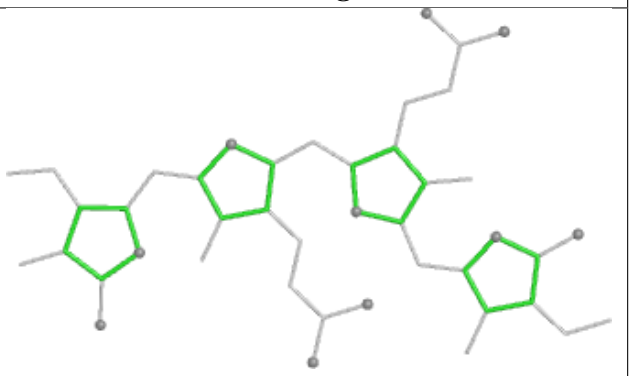
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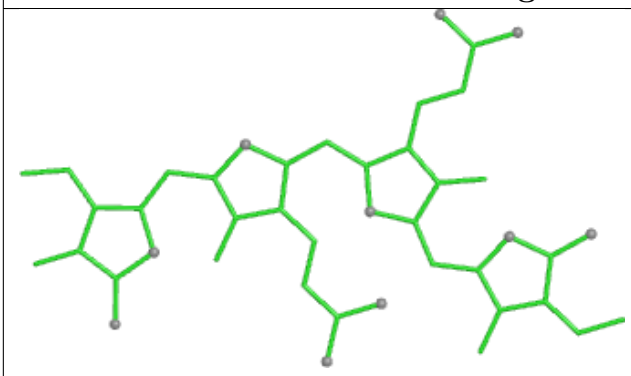


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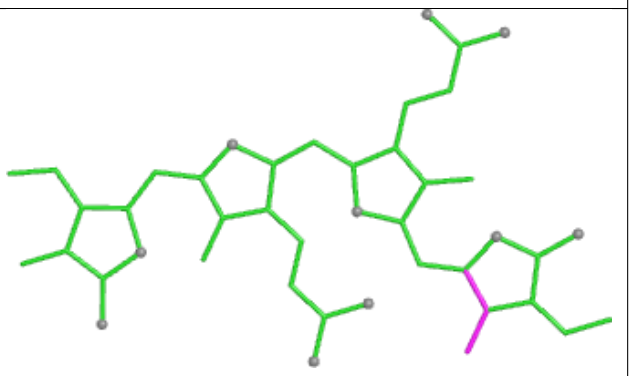


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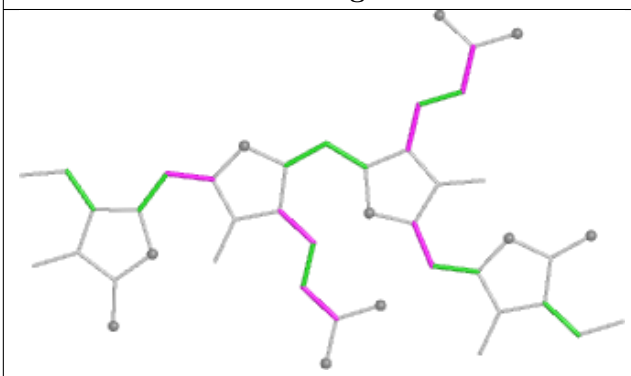
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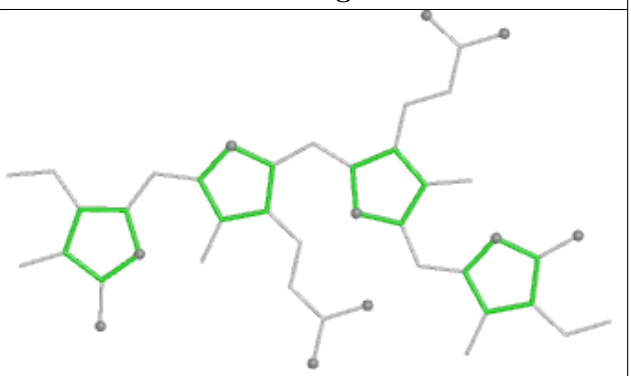
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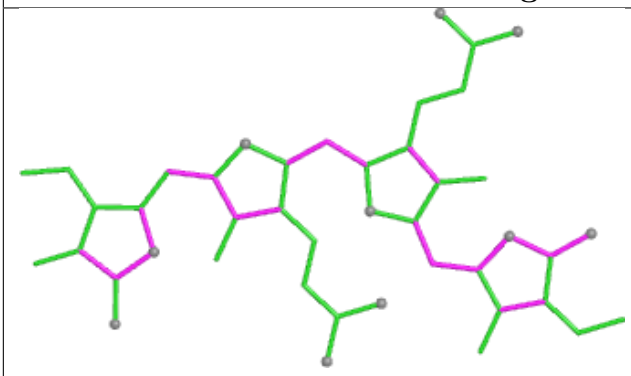


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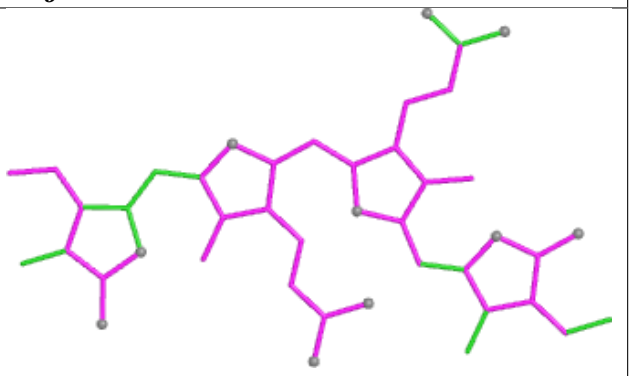


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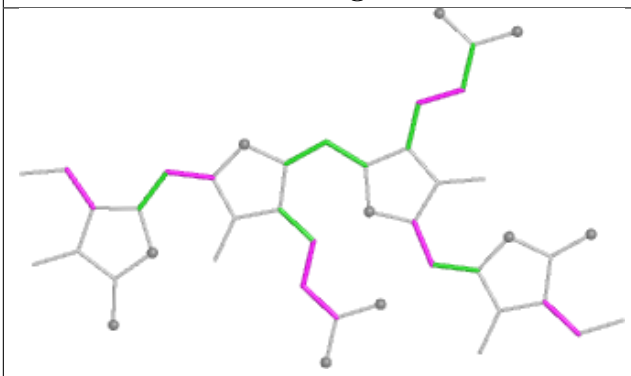
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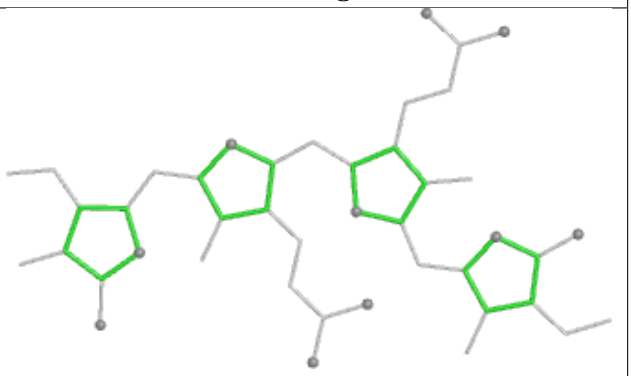
Bond lengths



Bond angles

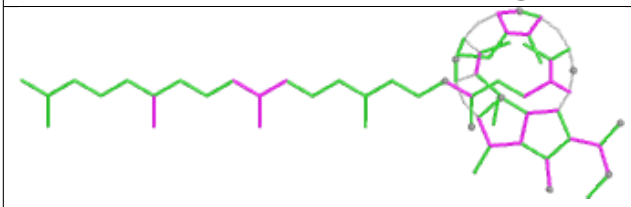


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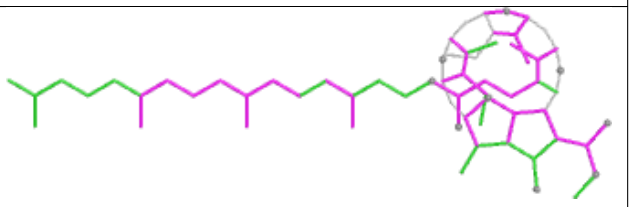


Rings

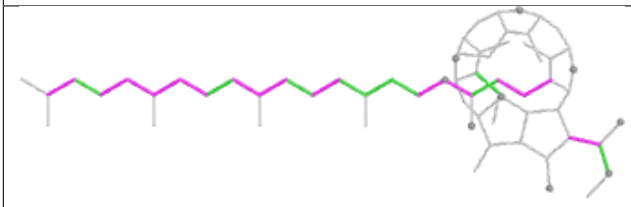
Ligand PHO aD 412



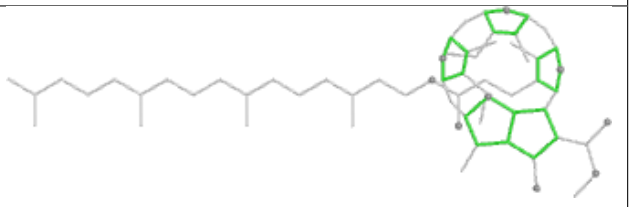
Bond lengths



Bond angles

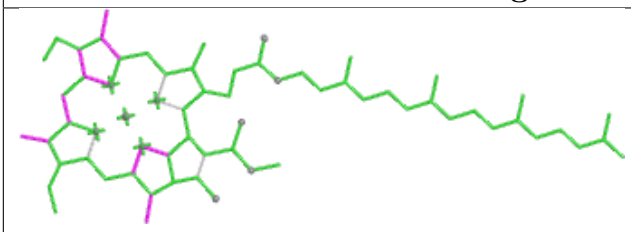


Torsions

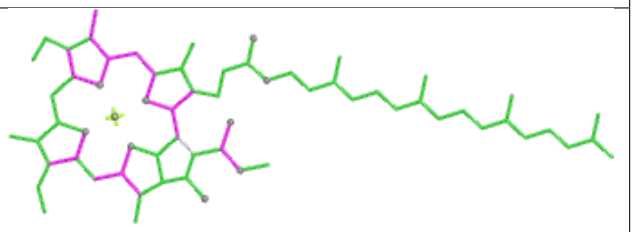


Rings

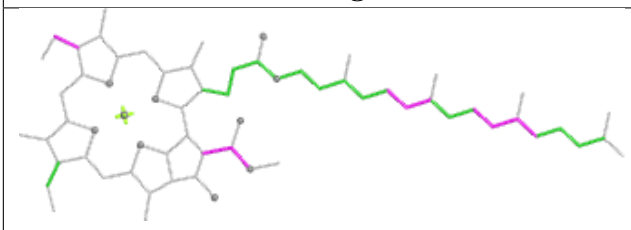
Ligand CLA BD 614



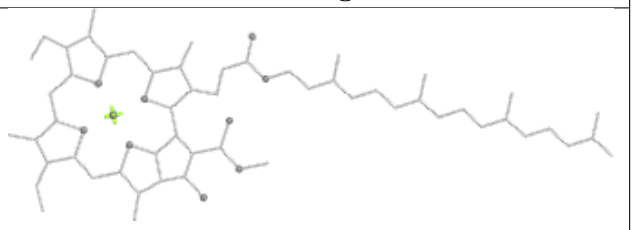
Bond lengths



Bond angles

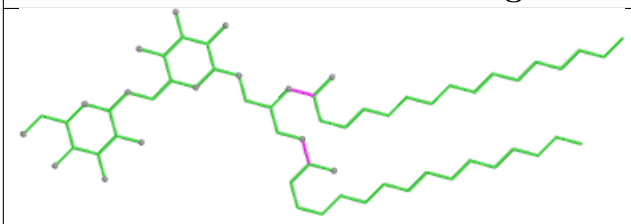


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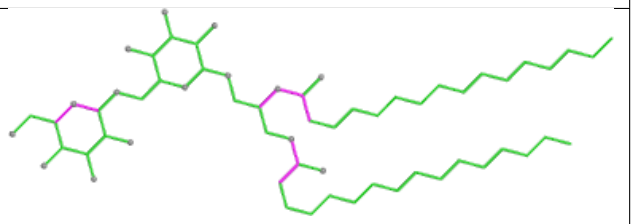


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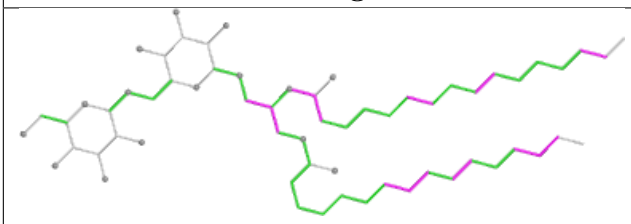
Ligand DGD HD 102



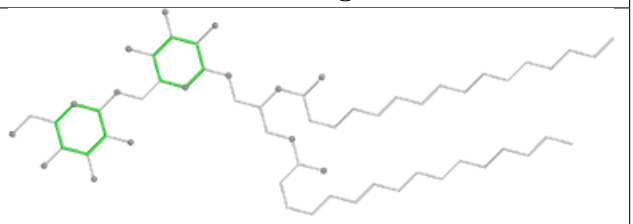
Bond lengths



Bond angles

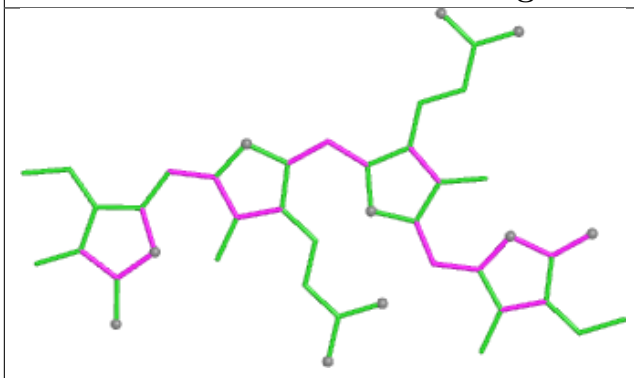


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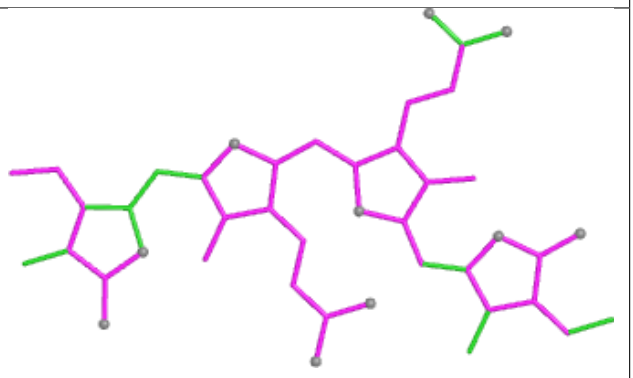


Rings

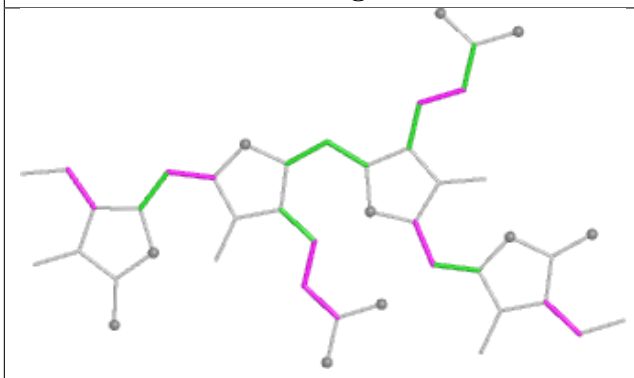
Ligand CYC d9 201



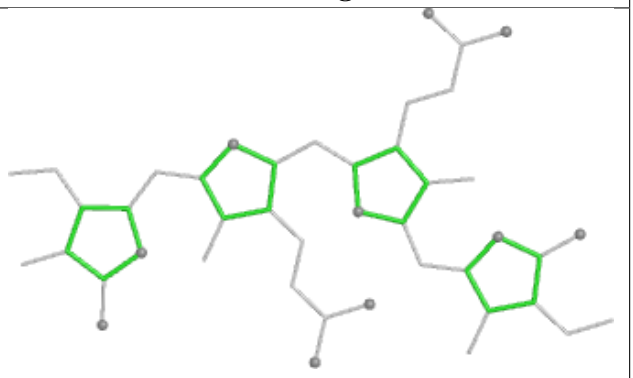
Bond lengths



Bond angles

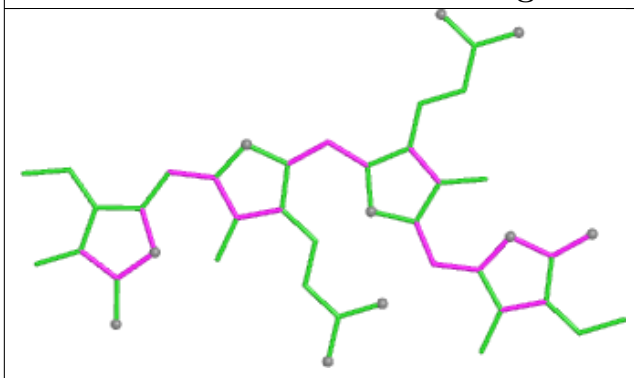


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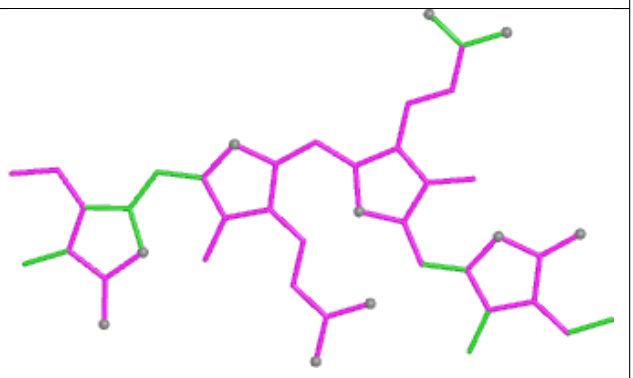


Rings

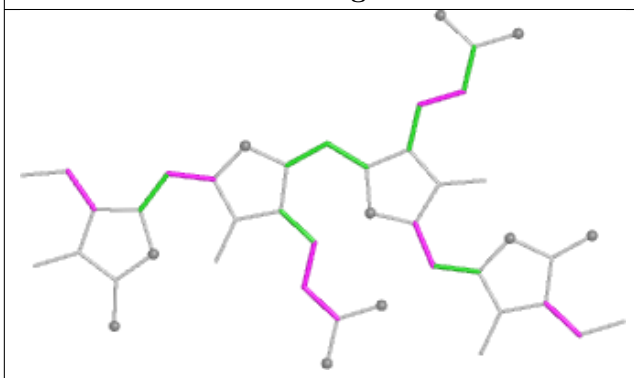
Ligand CYC h7 201



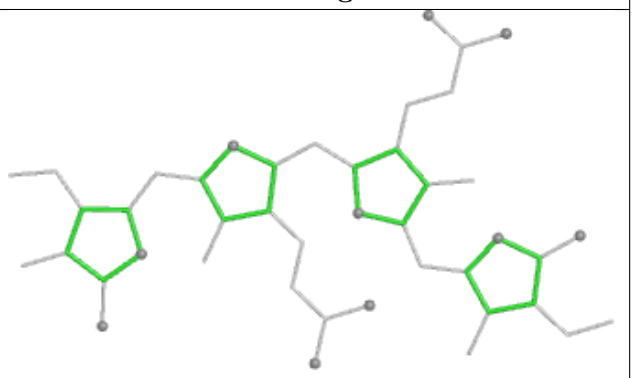
Bond lengths



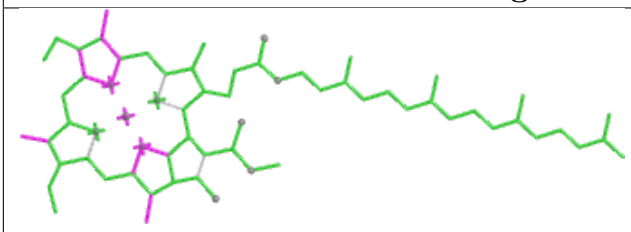
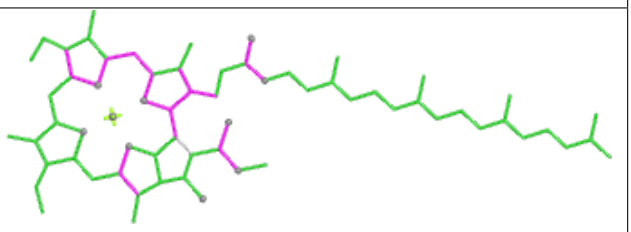
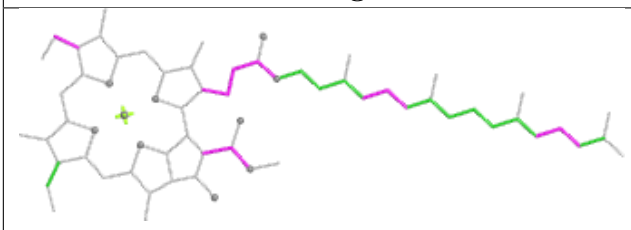
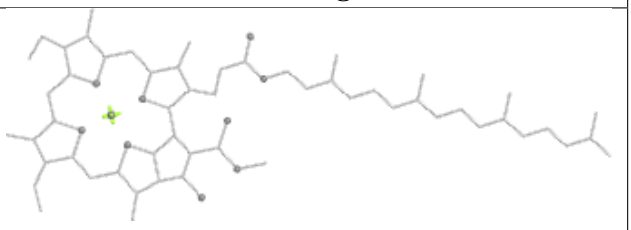
Bond angles



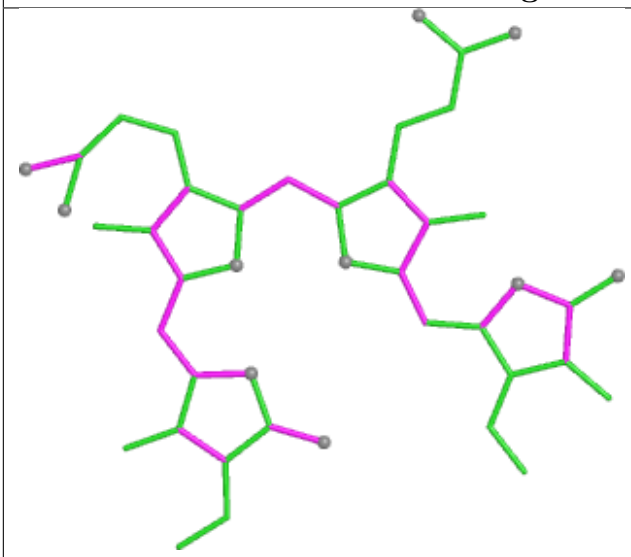
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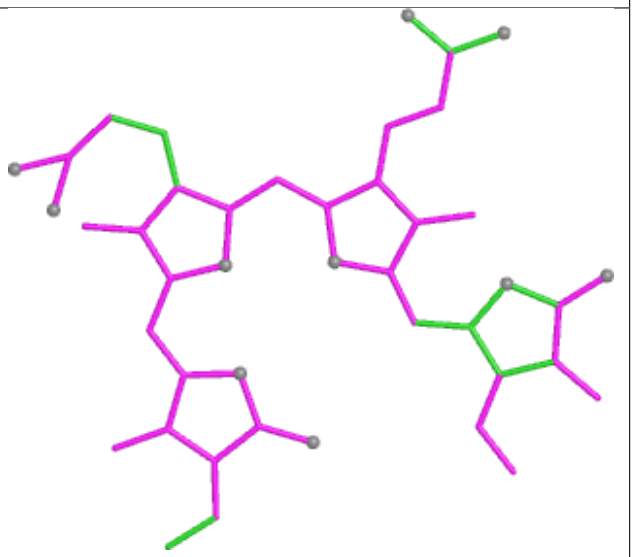
Rings

Ligand CLA CD 503	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

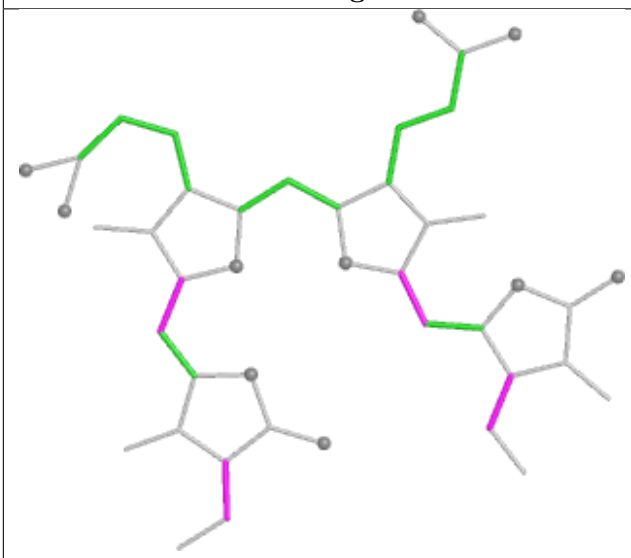
Ligand CYC i6 202



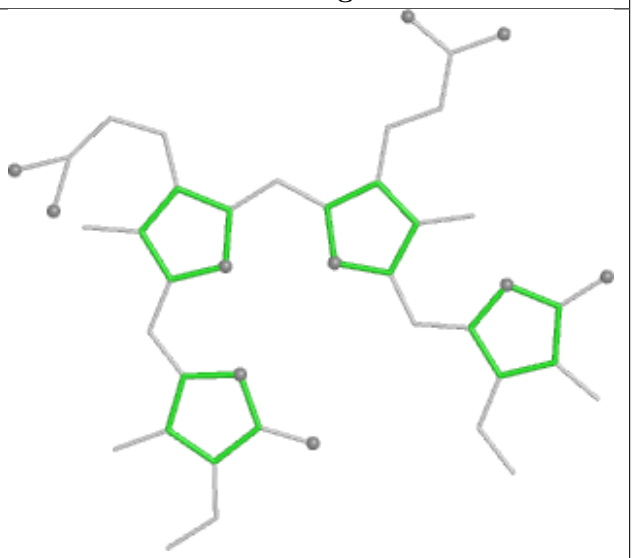
Bond lengths



Bond angles

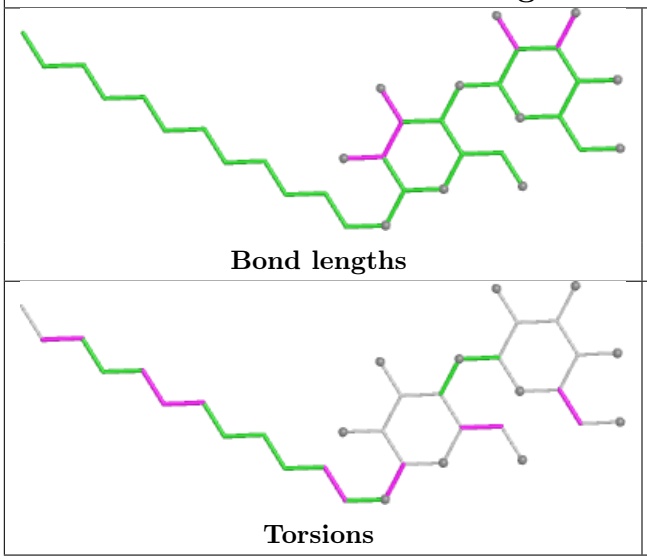


Torsions

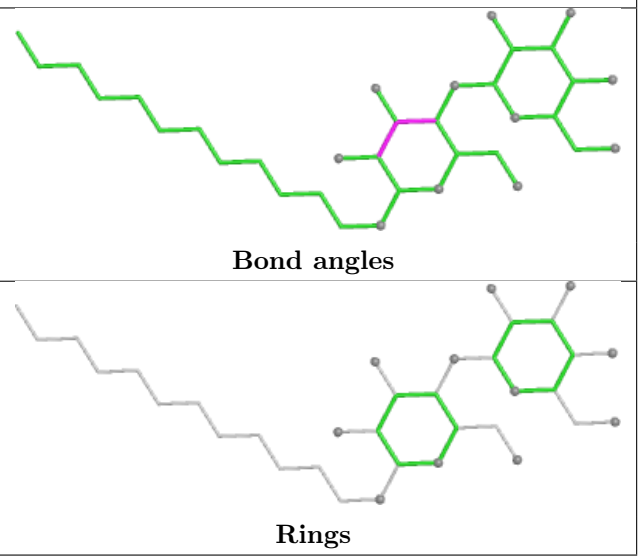


Rings

Ligand LMT a1 401



Bond lengths

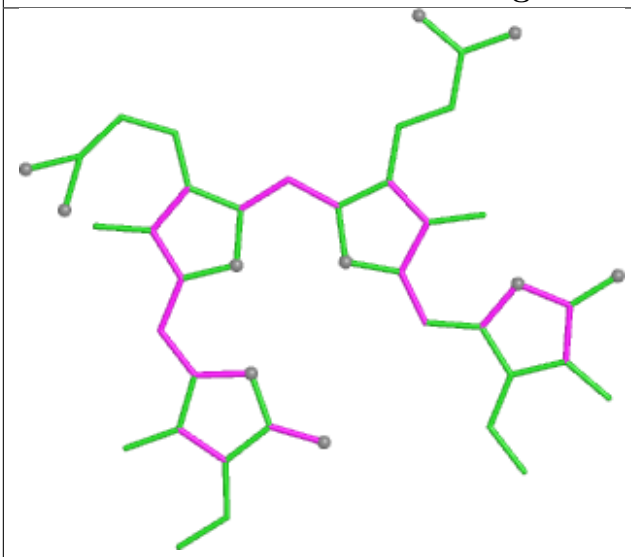


Bond angles

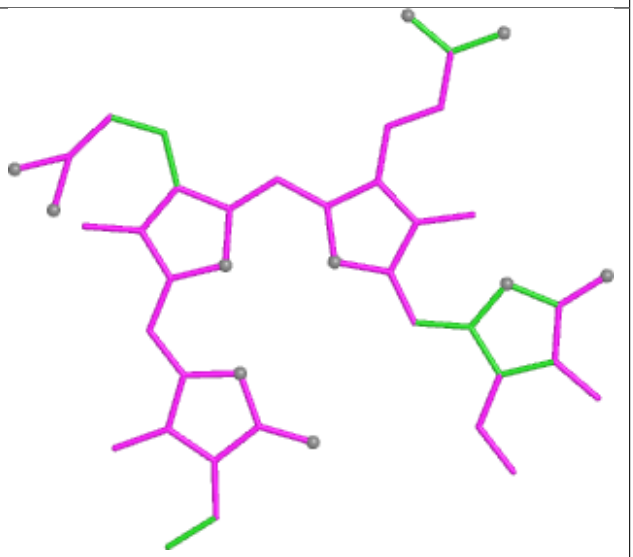
Torsions

Rings

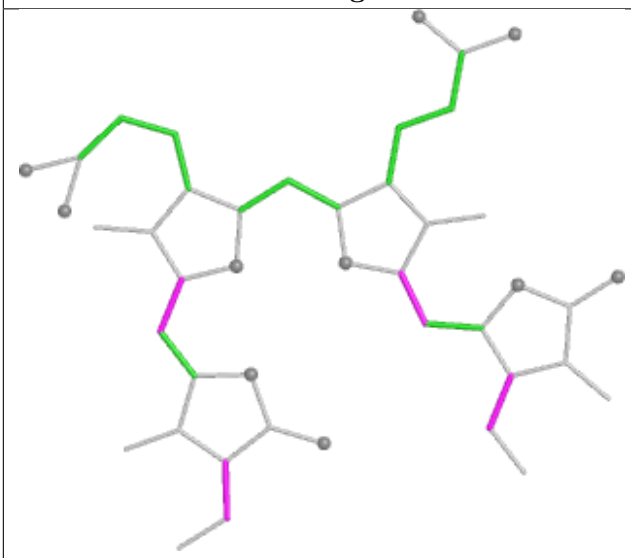
Ligand CYC eH 201



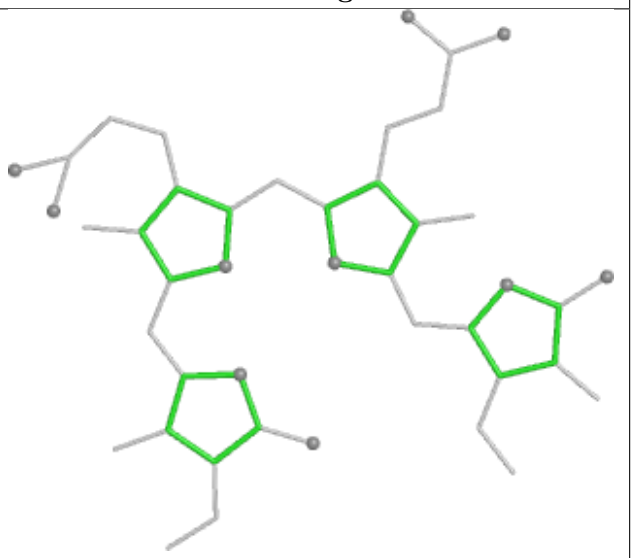
Bond lengths



Bond angles

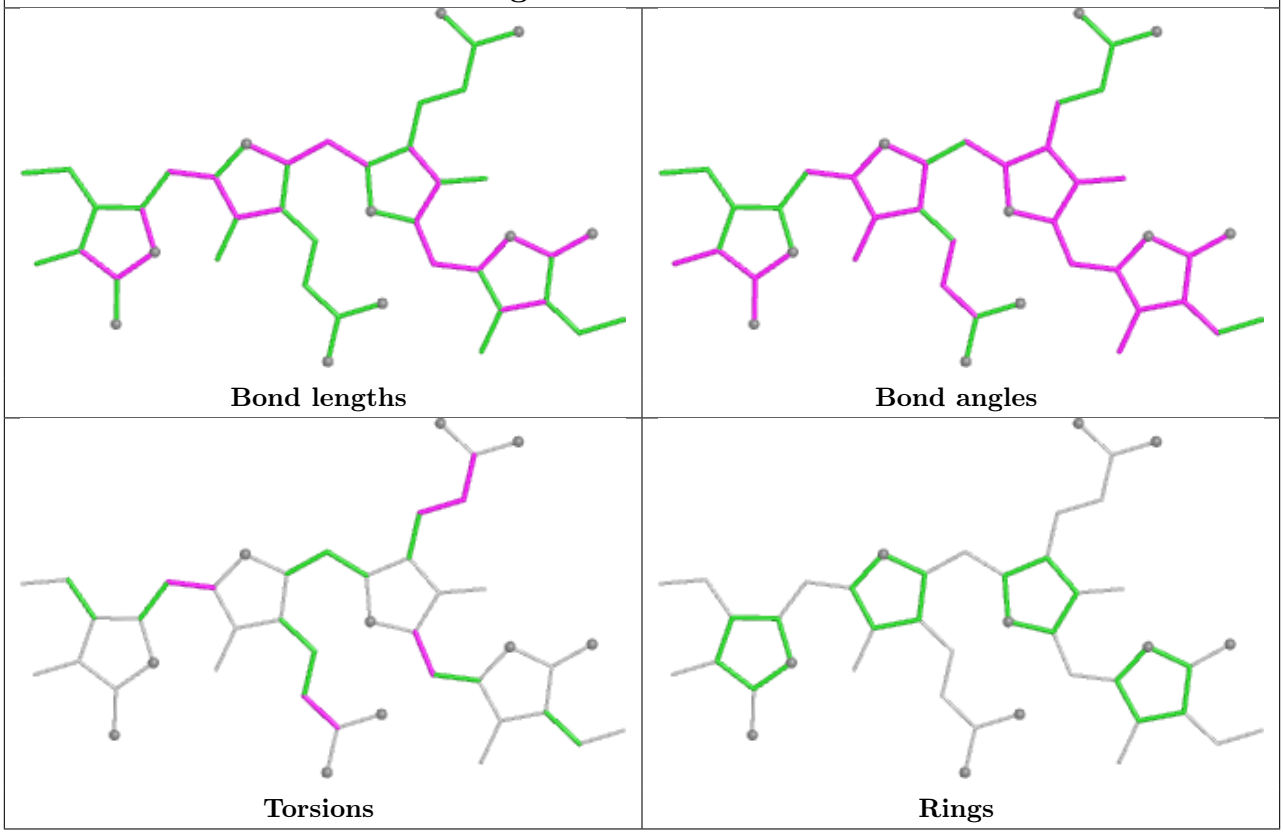


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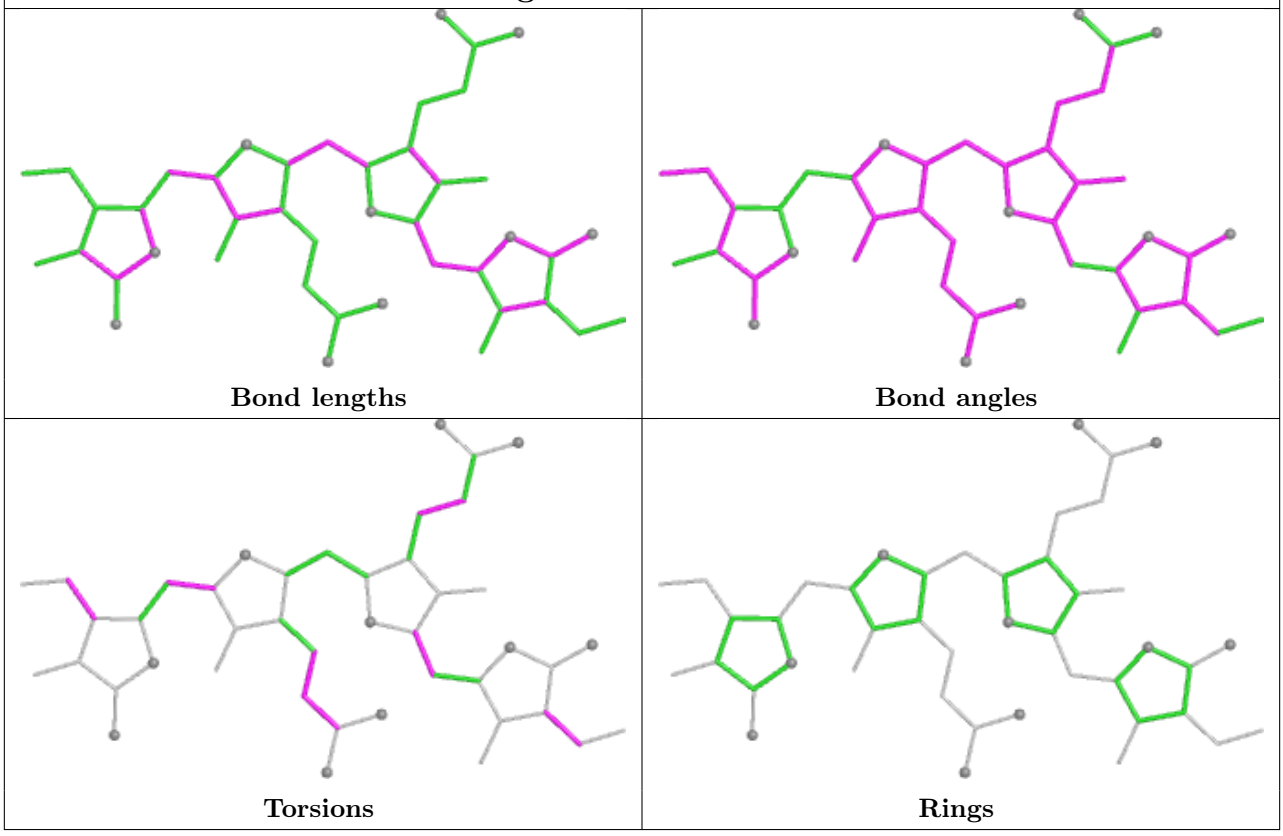


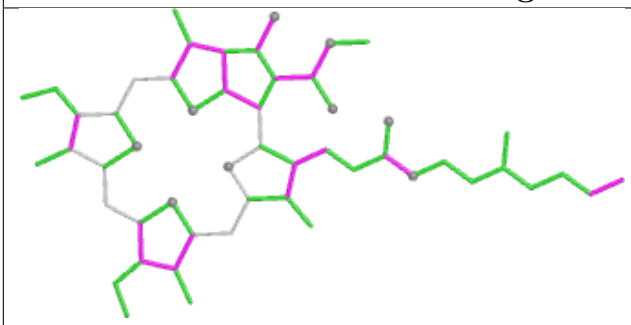
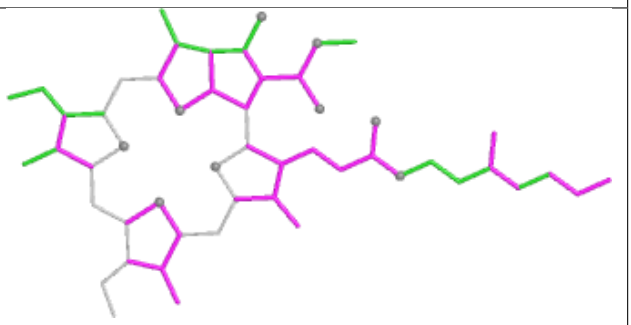
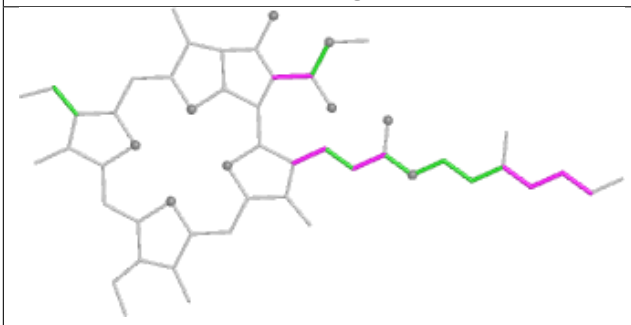
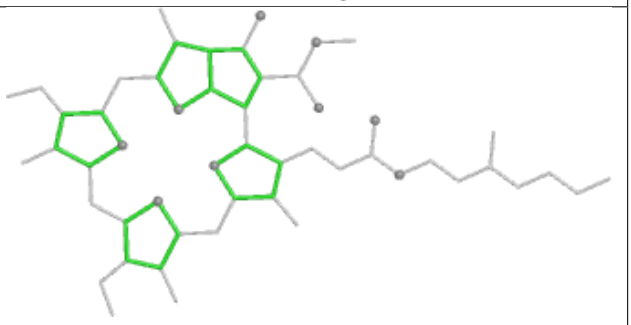
Rings

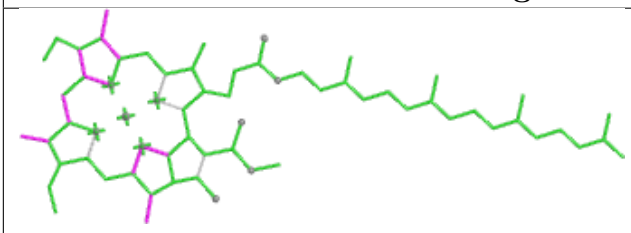
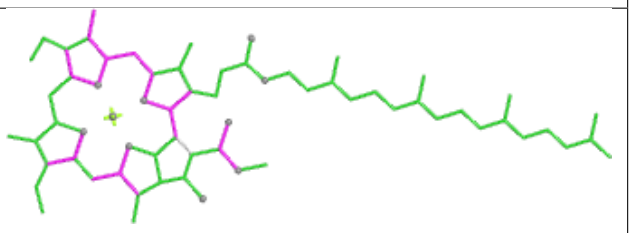
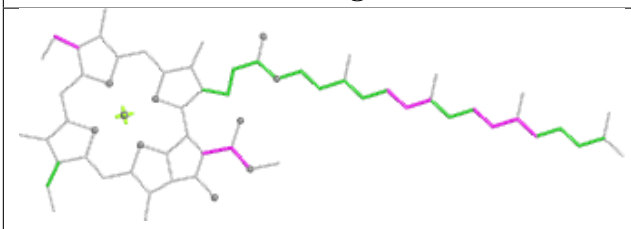
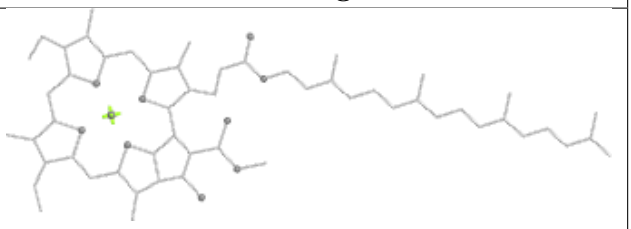
Ligand CYC RB 201



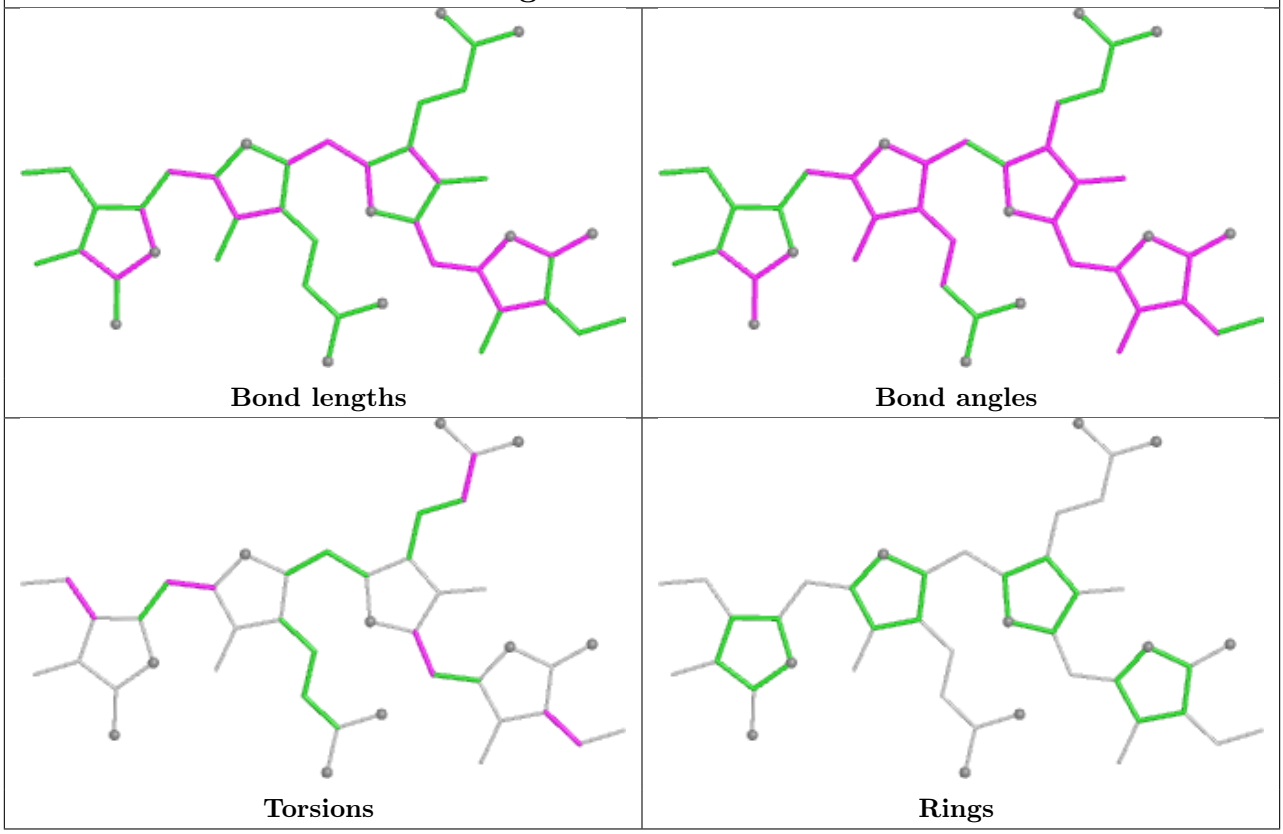
Ligand CYC b7 201



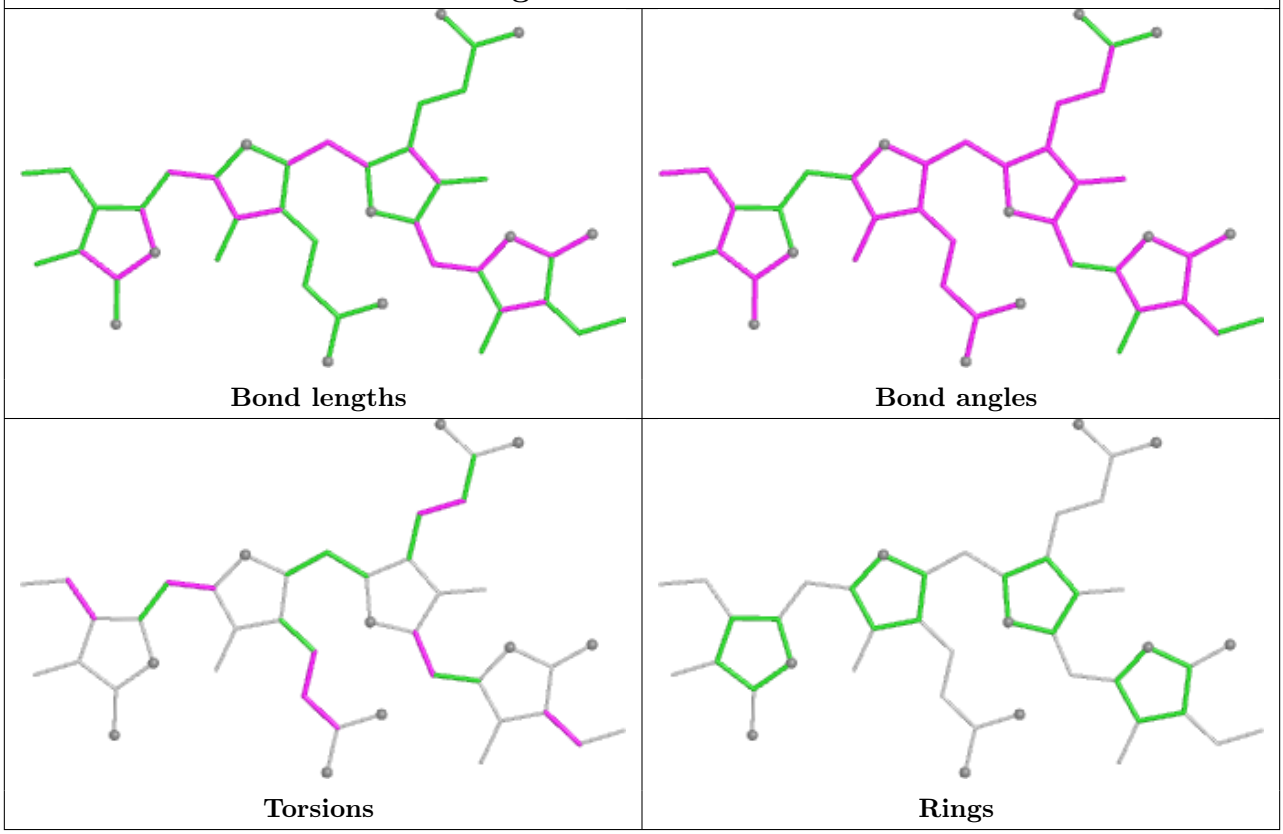
Ligand PHO a1 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bD 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

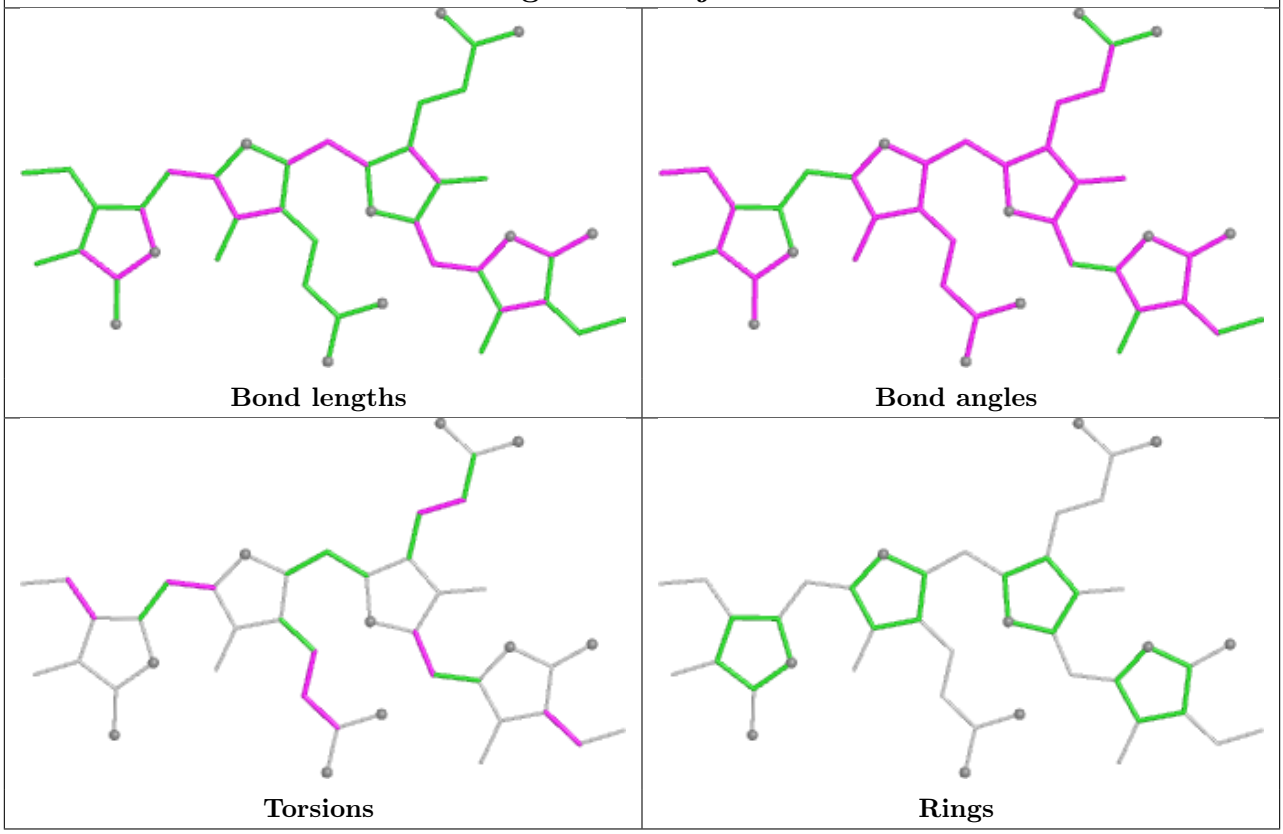
Ligand CYC fF 201



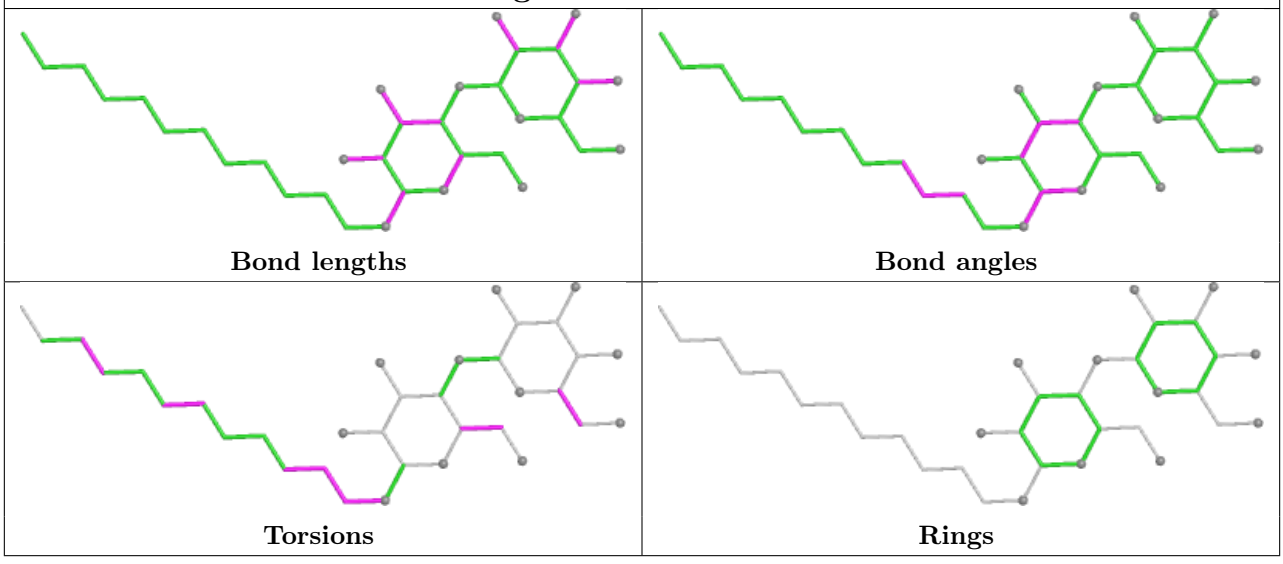
Ligand CYC bH 201



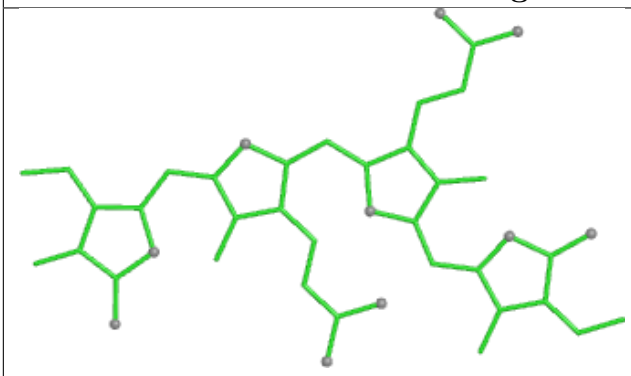
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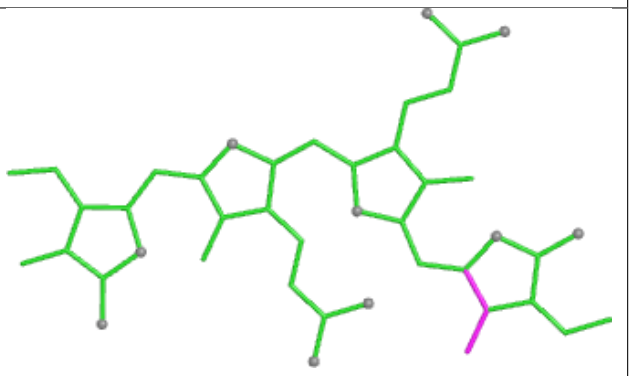
Ligand LMT bE 601



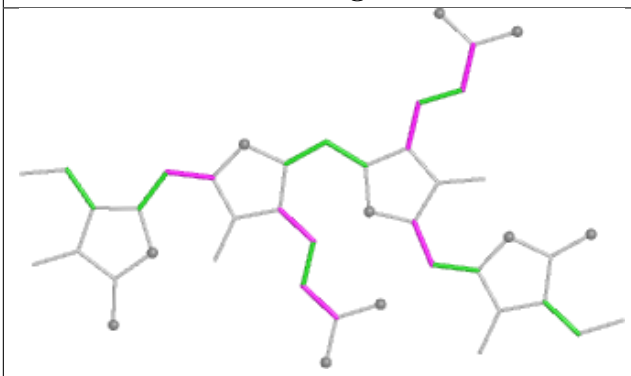
Ligand CYC mJ 201



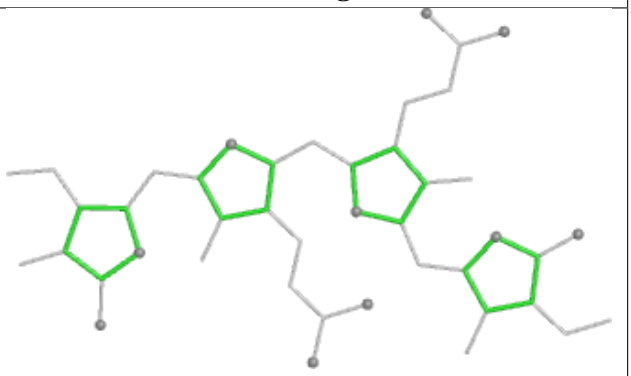
Bond lengths



Bond angles

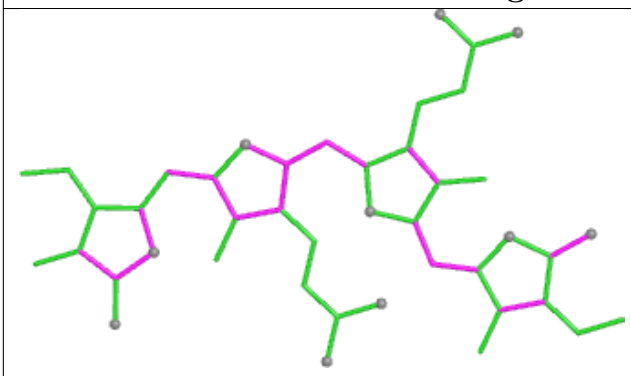


Torsions

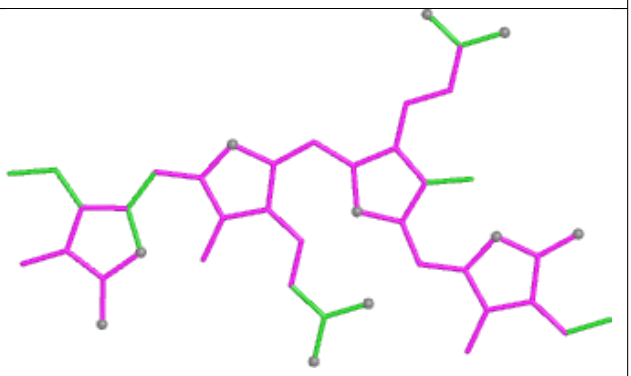


Rings

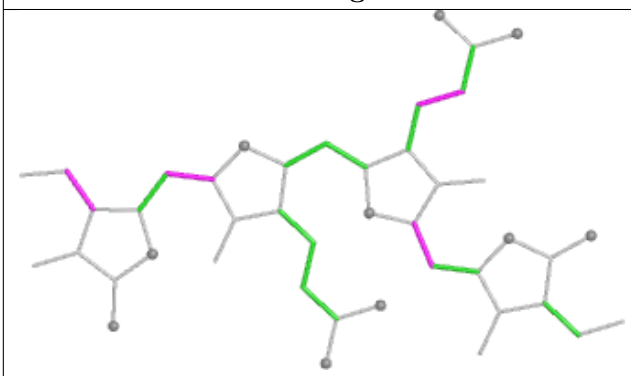
Ligand CYC HG 201



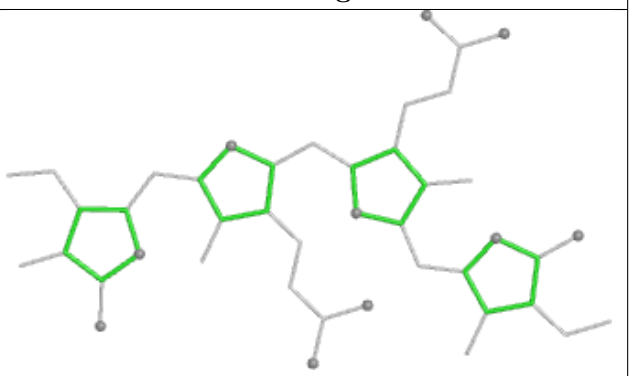
Bond lengths



Bond angles

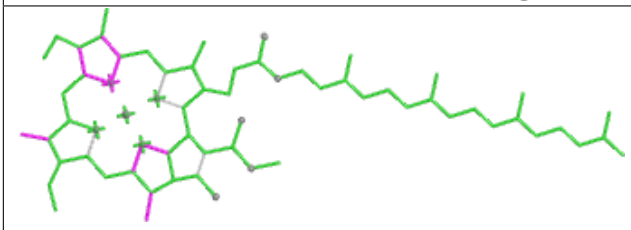


Torsions

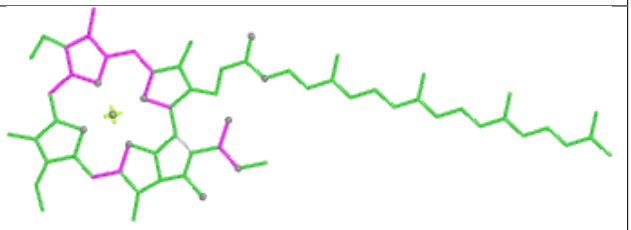


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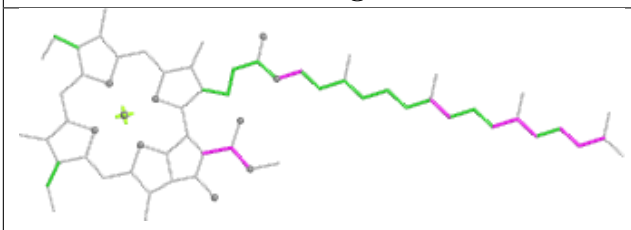
Ligand CLA dE 403



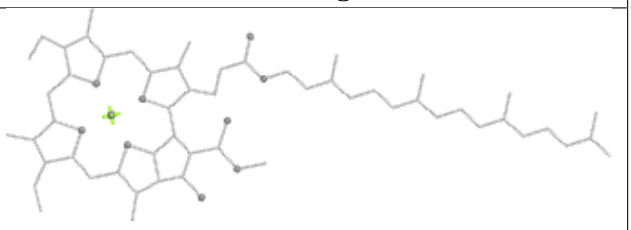
Bond lengths



Bond angles

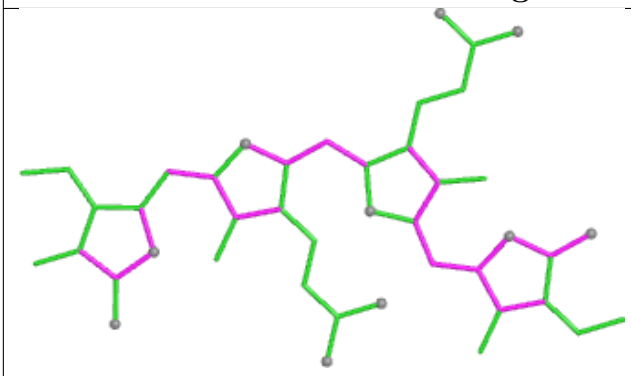


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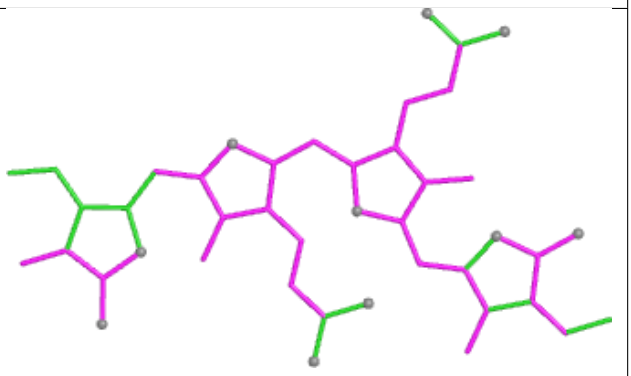


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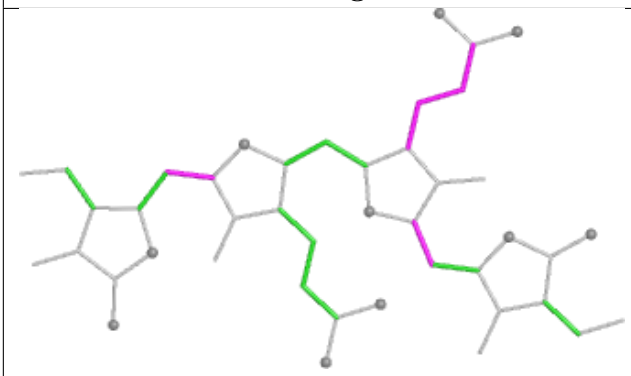
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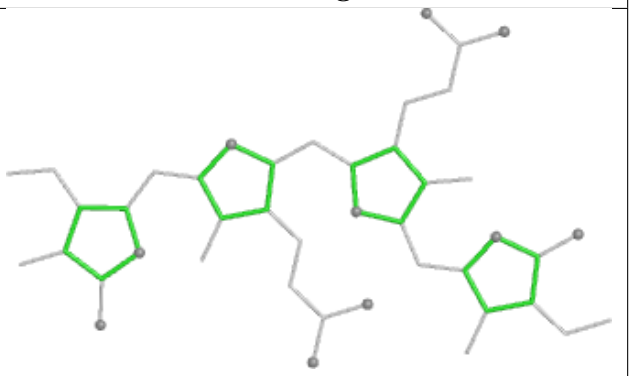
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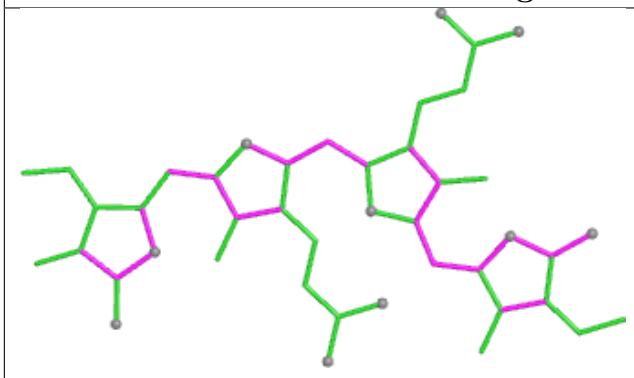


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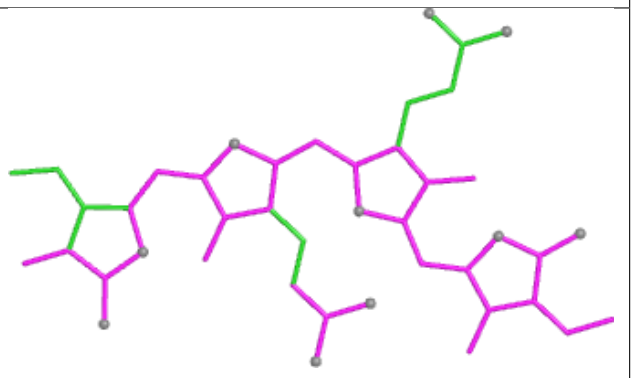


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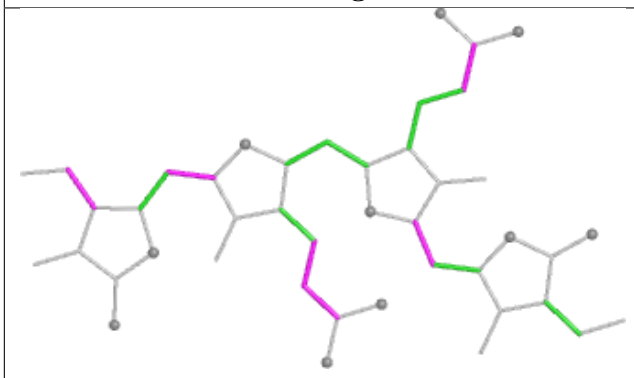
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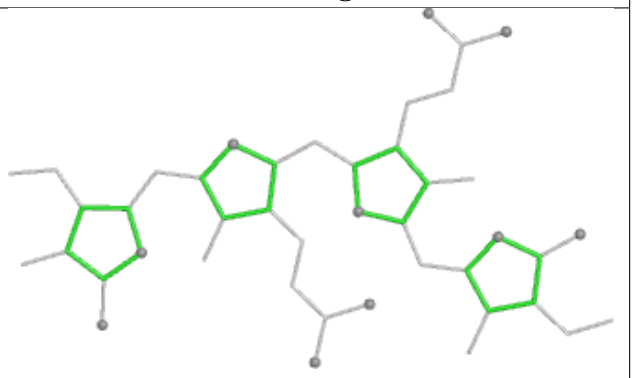
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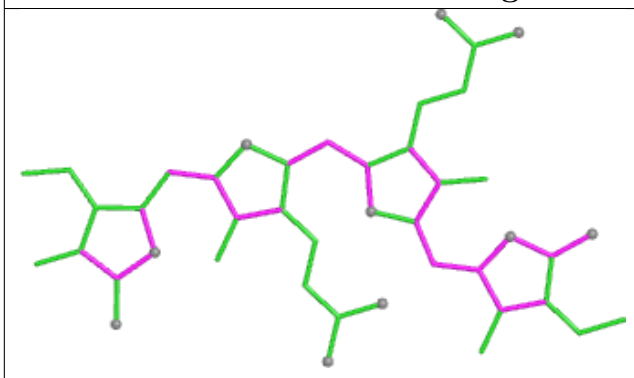


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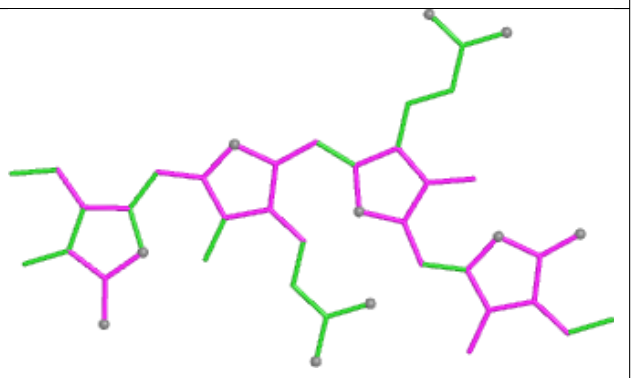


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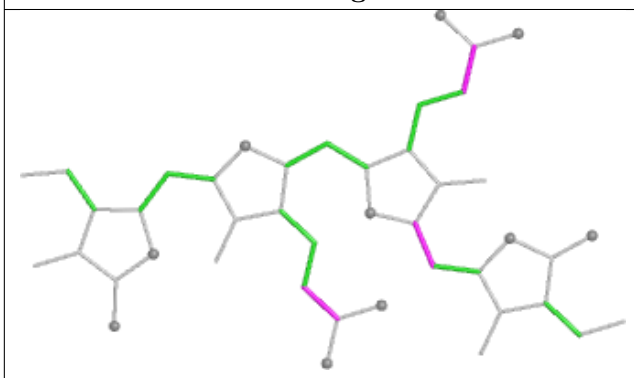
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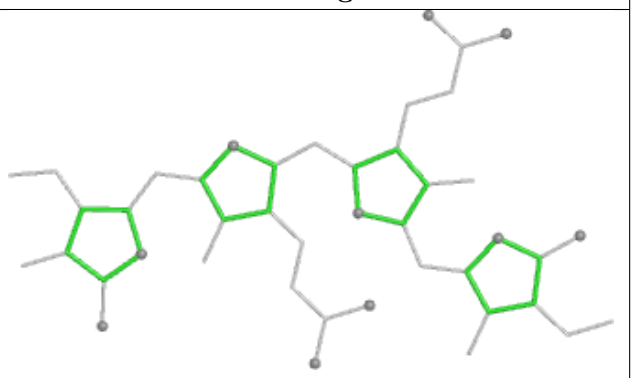
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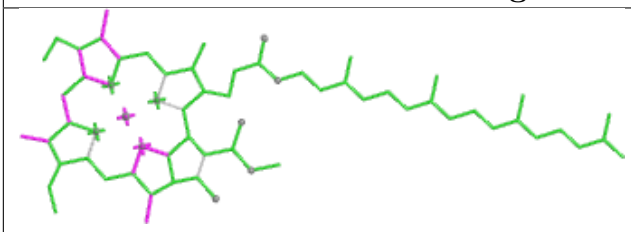


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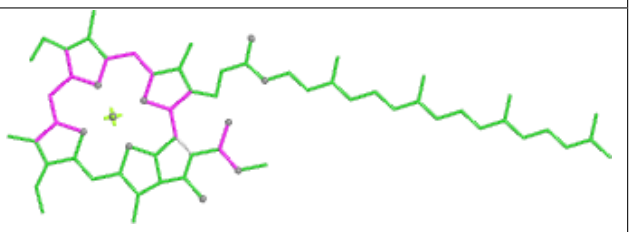


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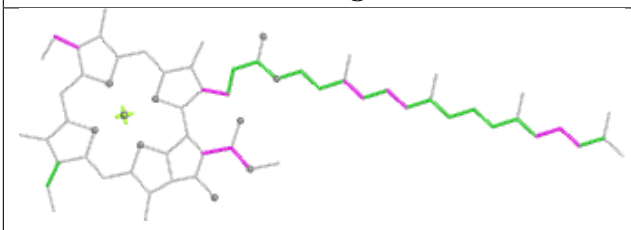
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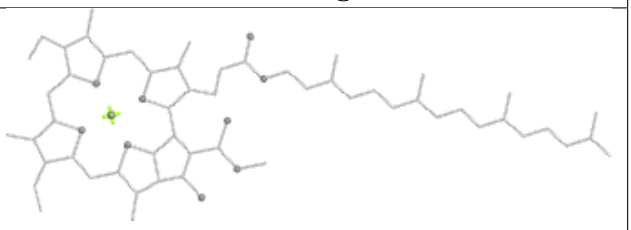
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Bond angles

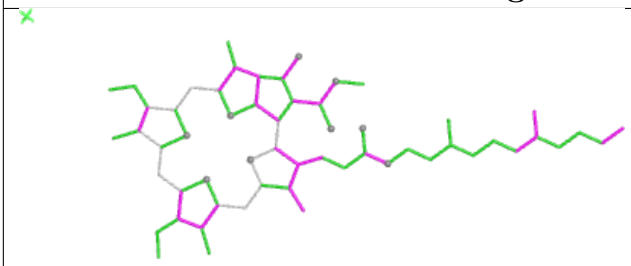


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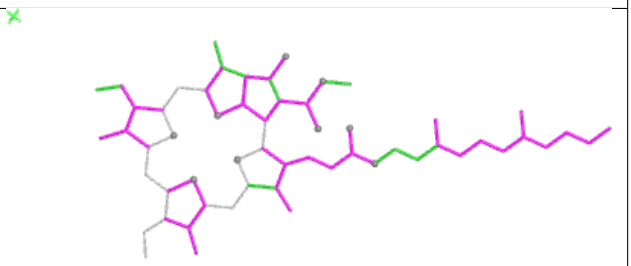


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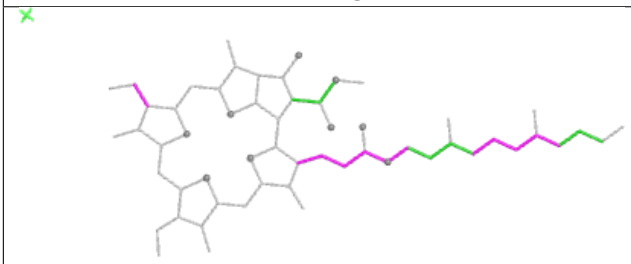
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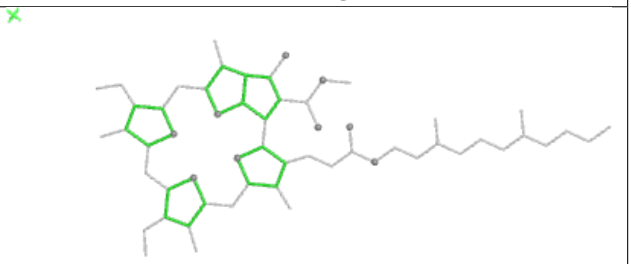
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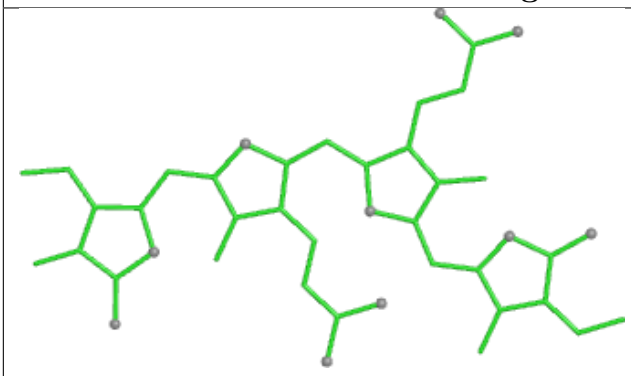


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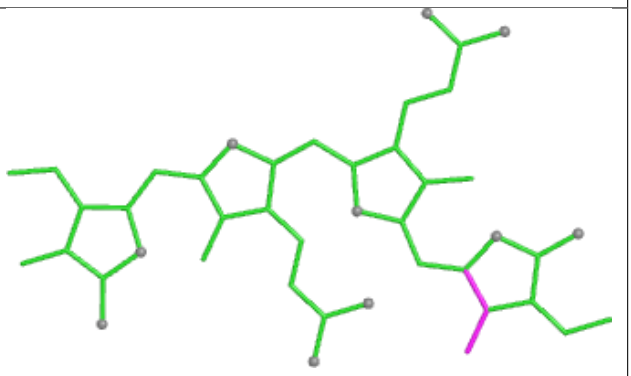


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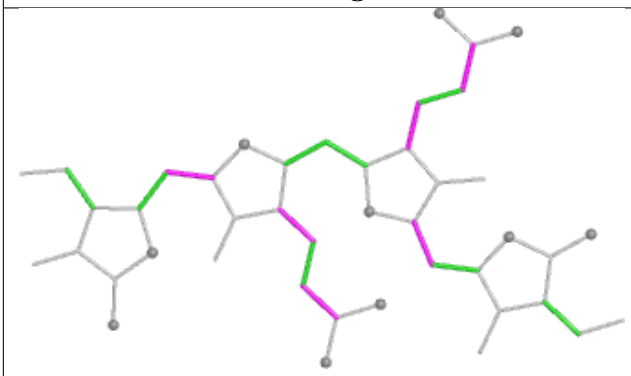
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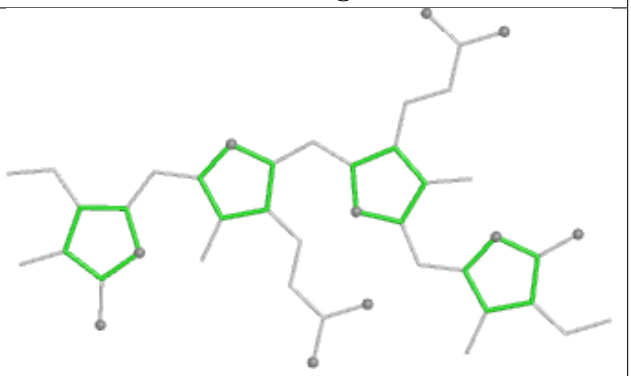
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Bond angles

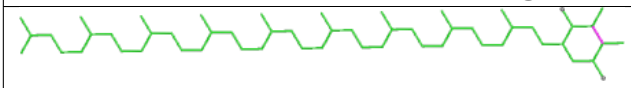


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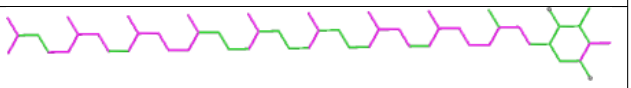


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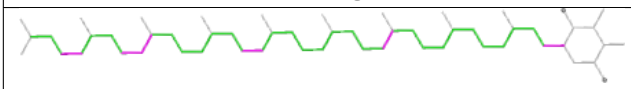
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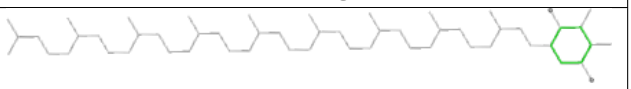
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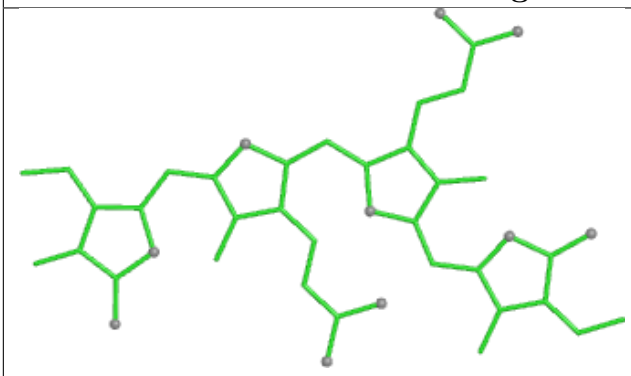


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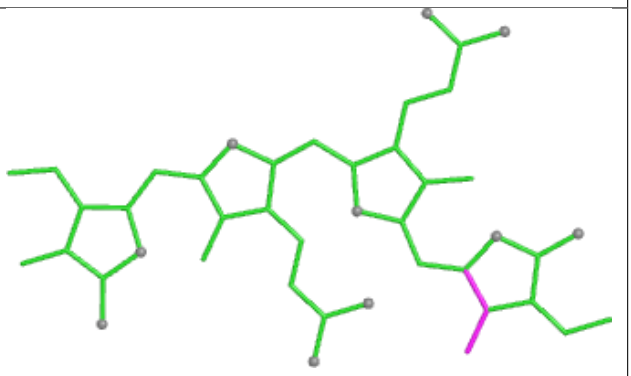


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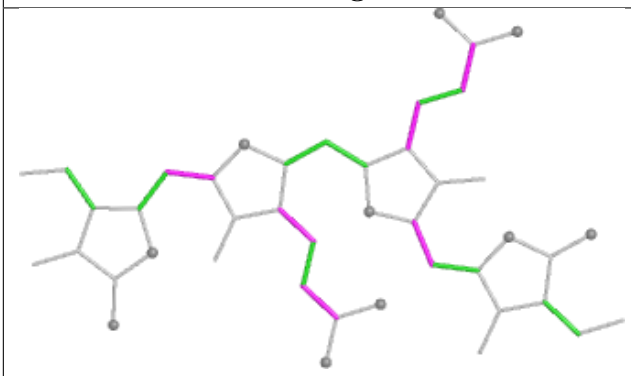
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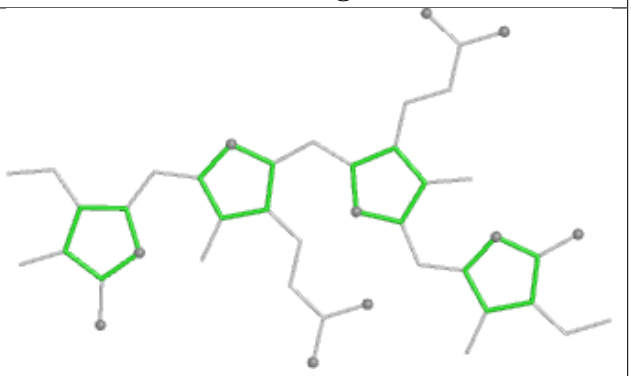
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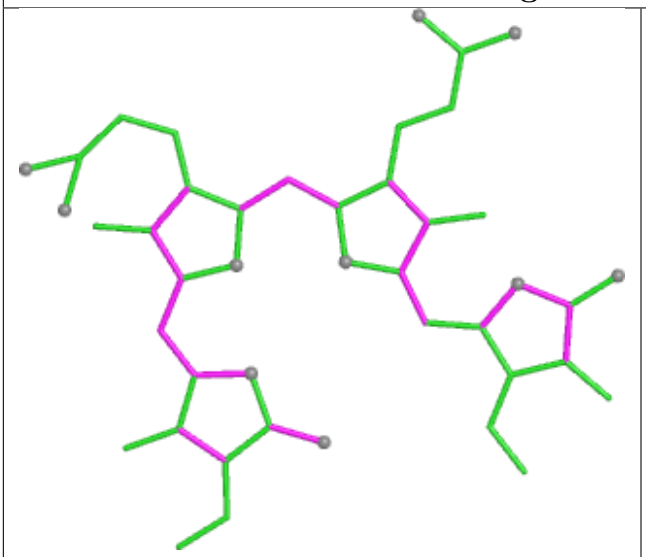


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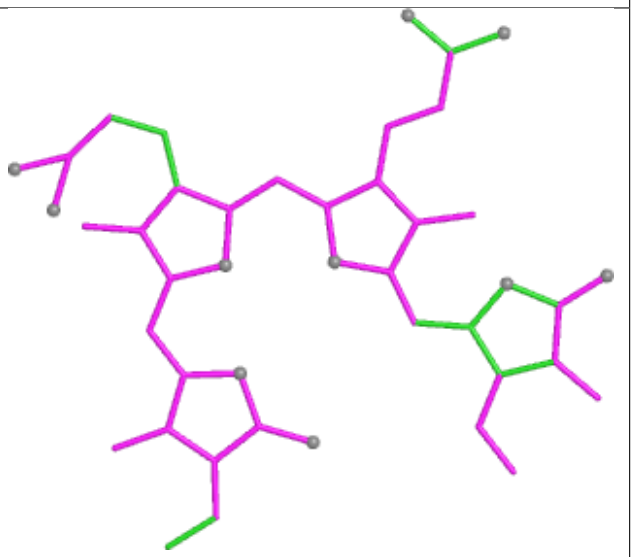


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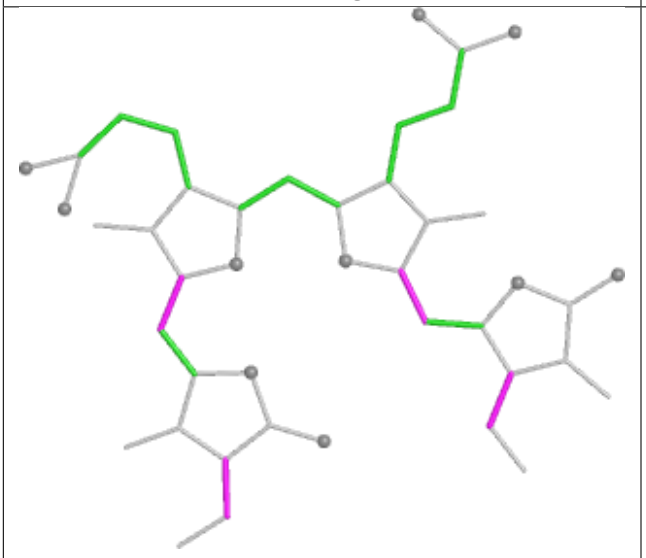
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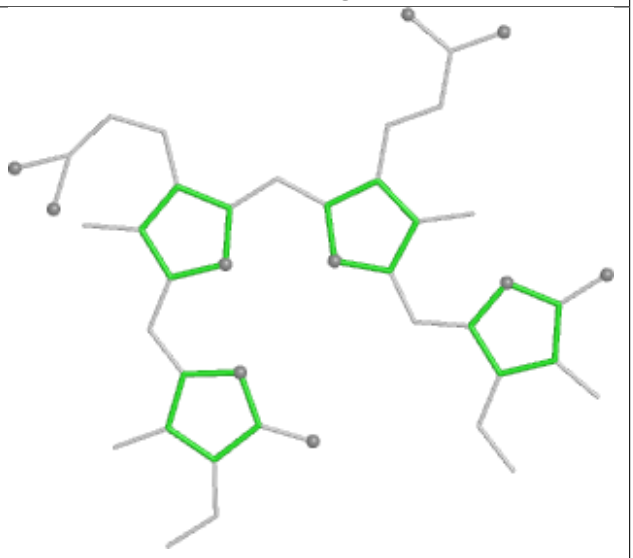
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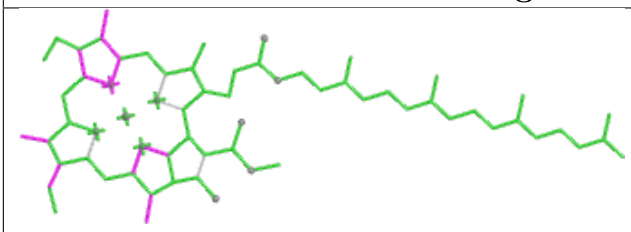


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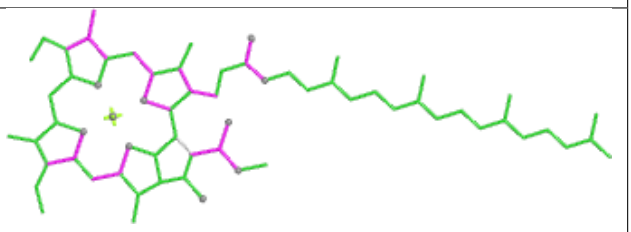


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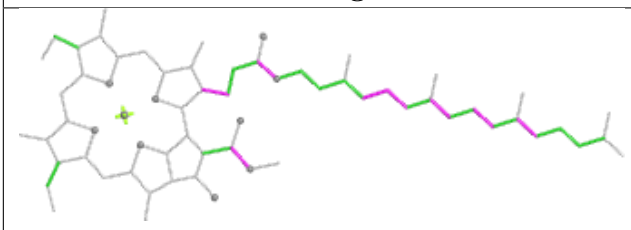
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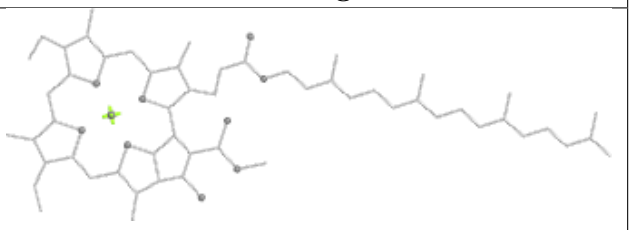
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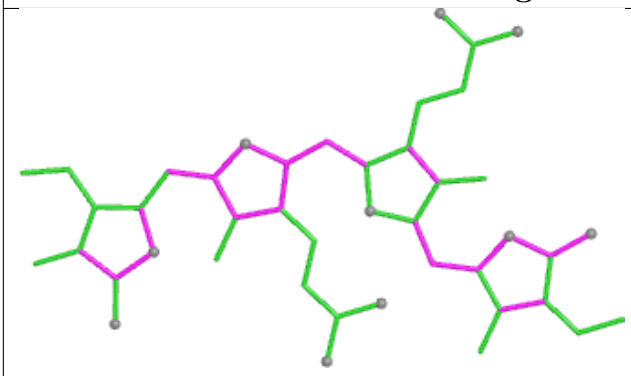


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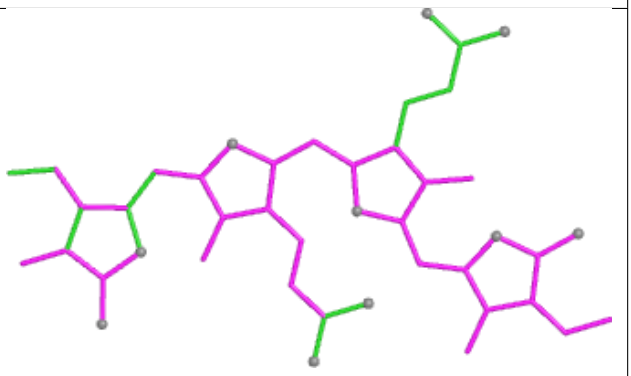


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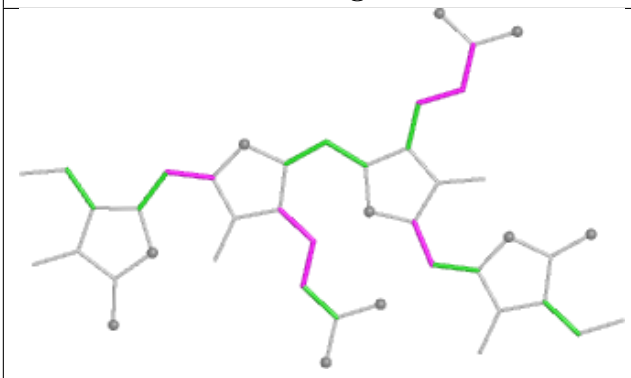
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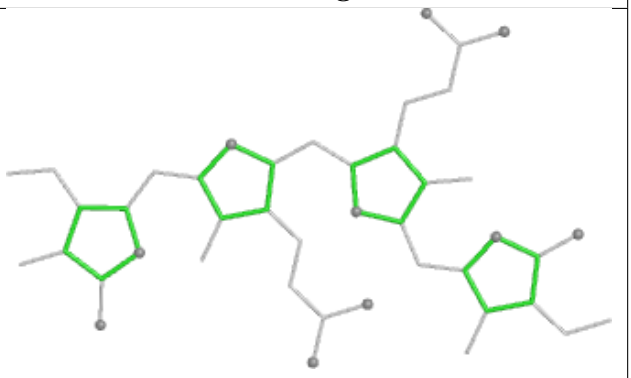
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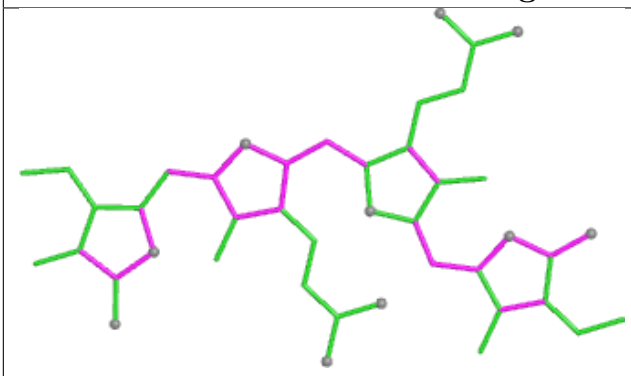


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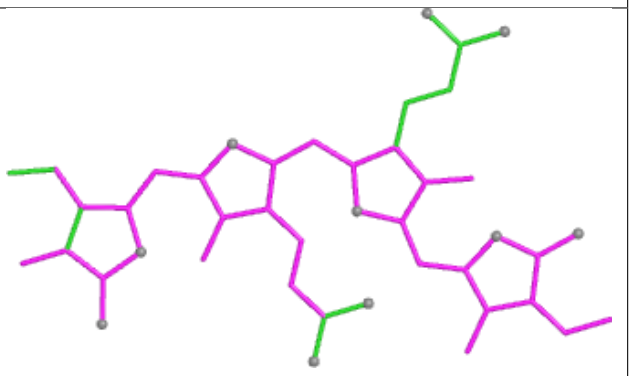


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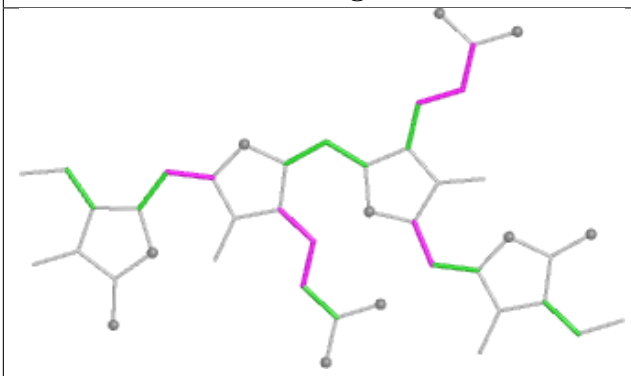
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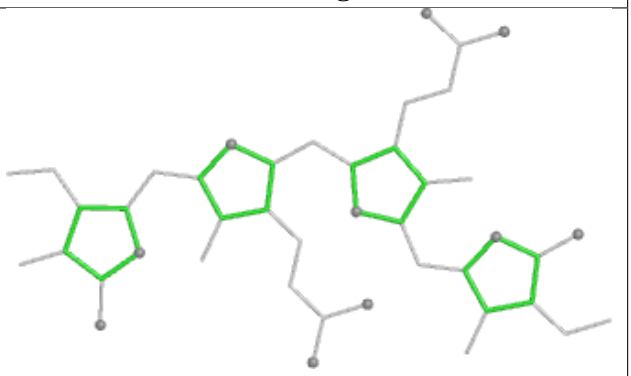
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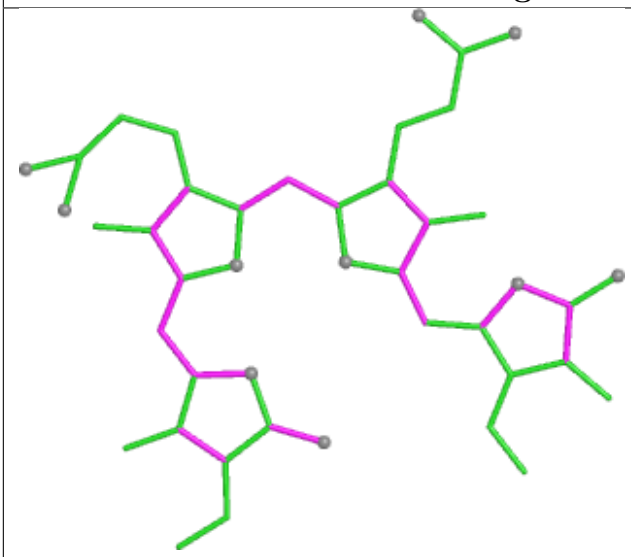


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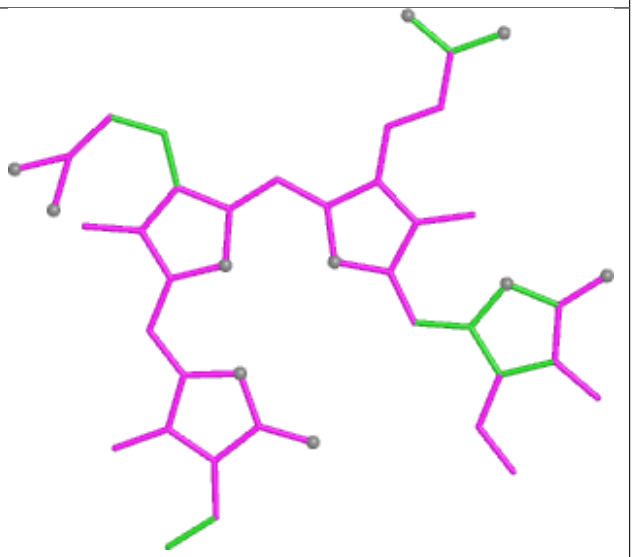


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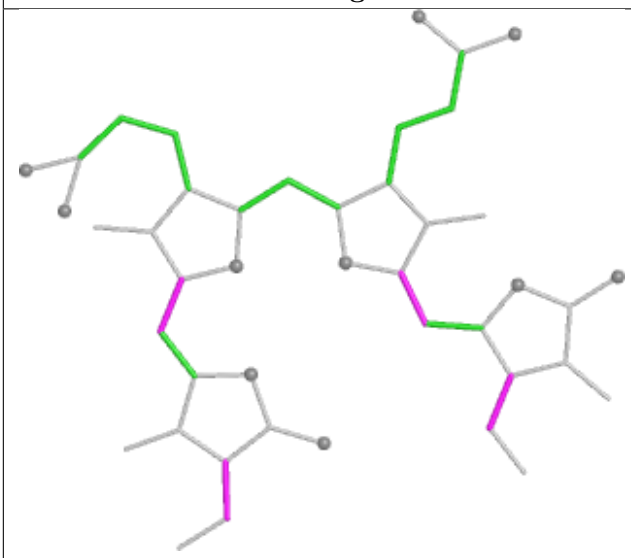
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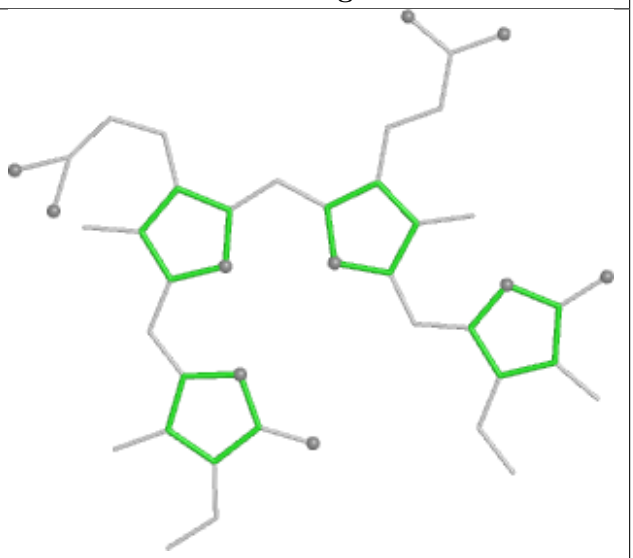
Bond lengths



Bond angles

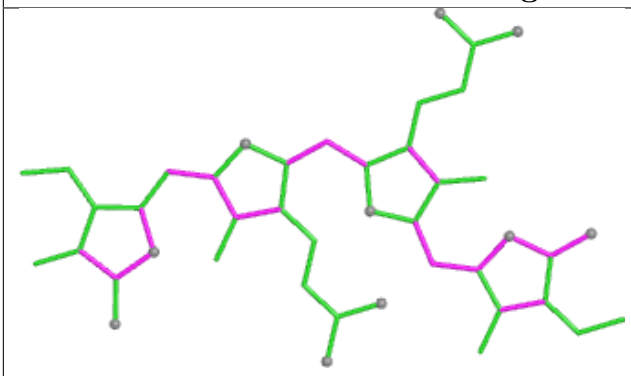


Torsions

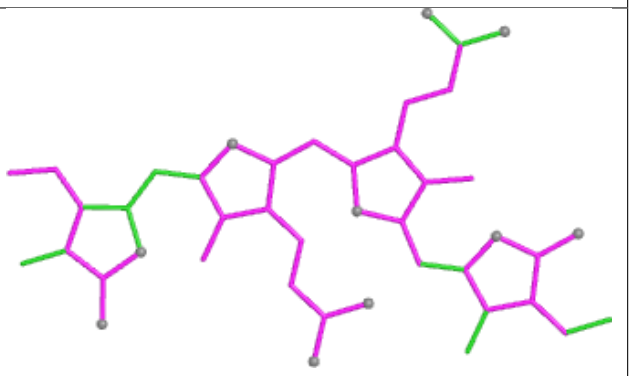


Rings

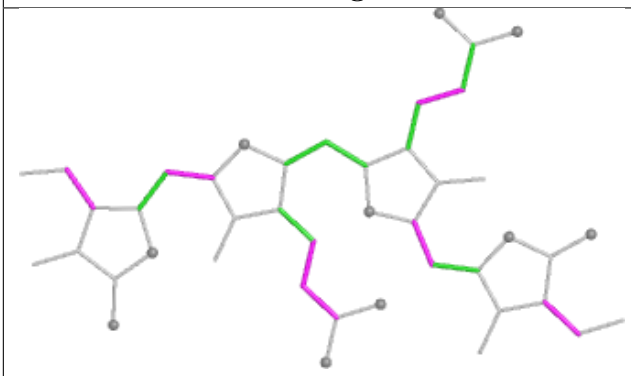
Ligand CYC f6 201



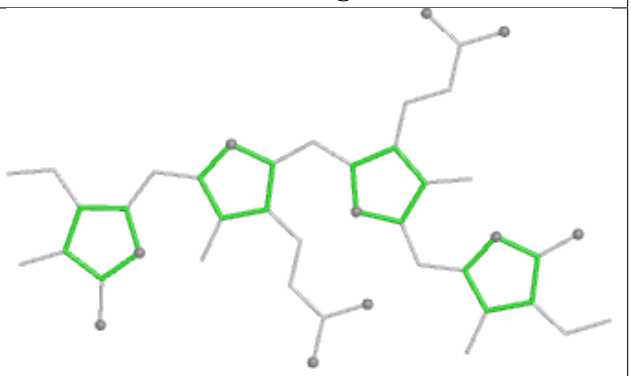
Bond lengths



Bond angles

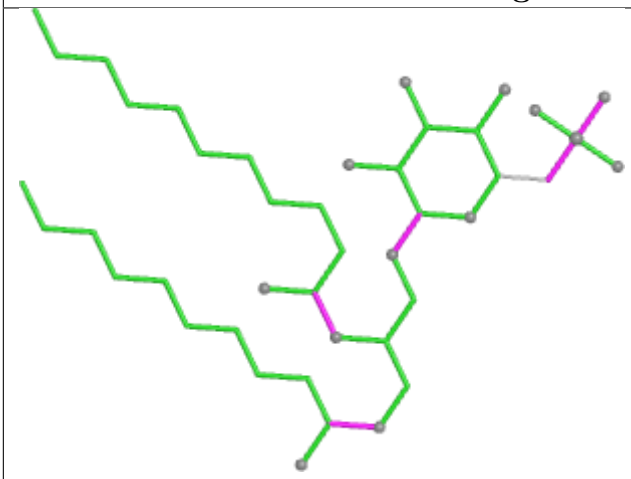


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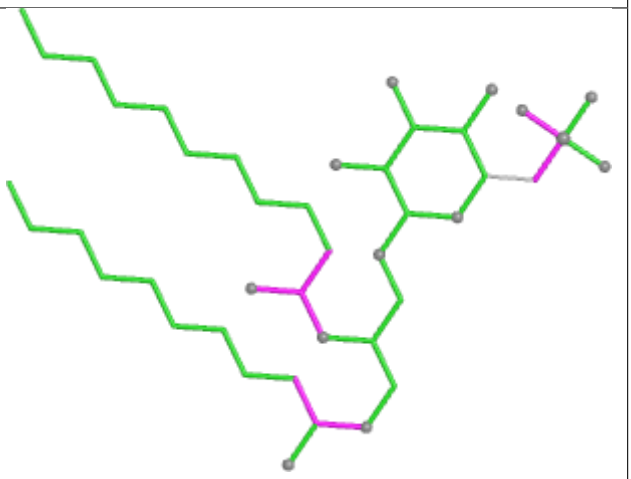


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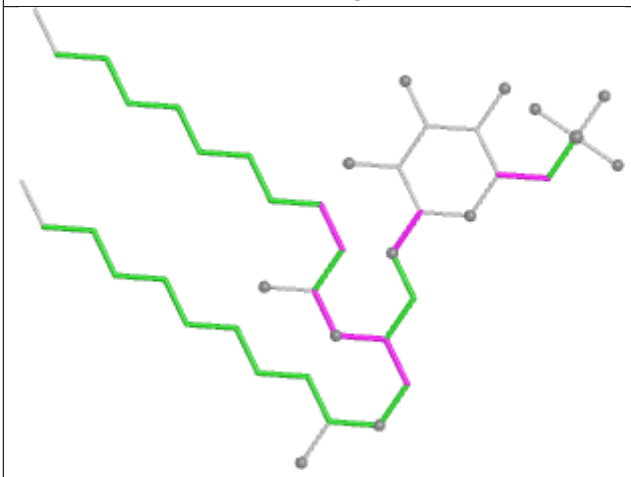
Ligand SQD LD 102



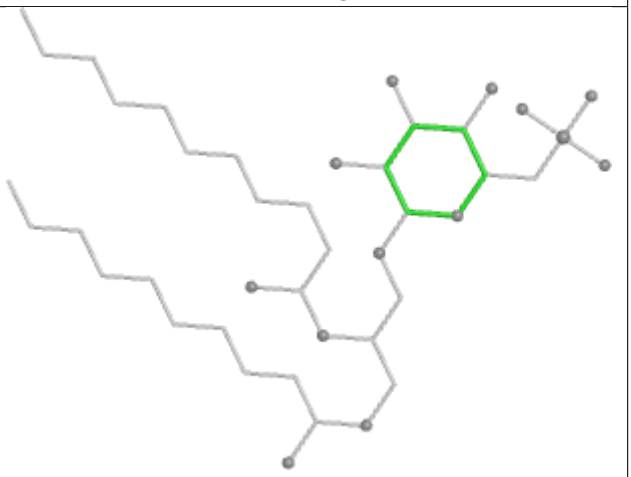
Bond lengths



Bond angles

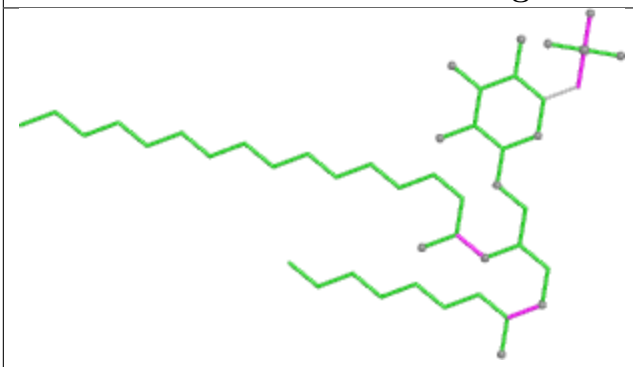


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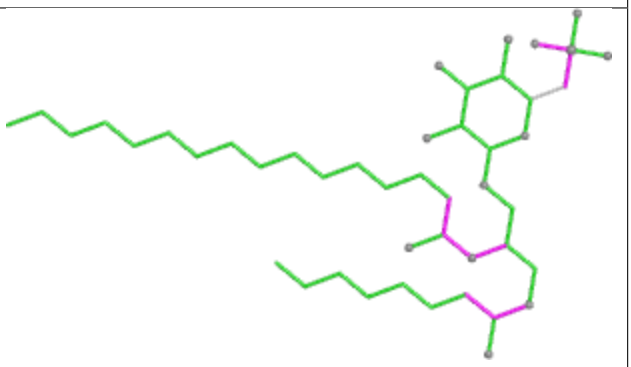


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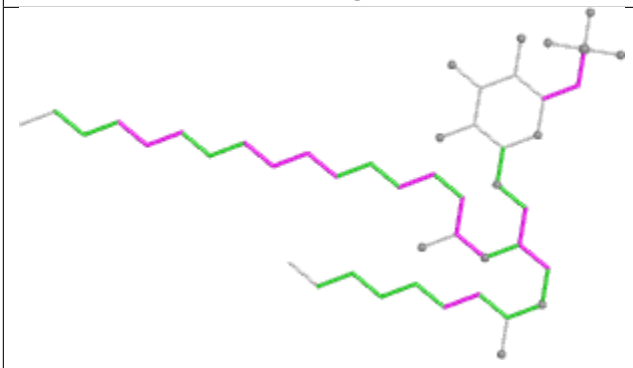
Ligand SQD AE 407



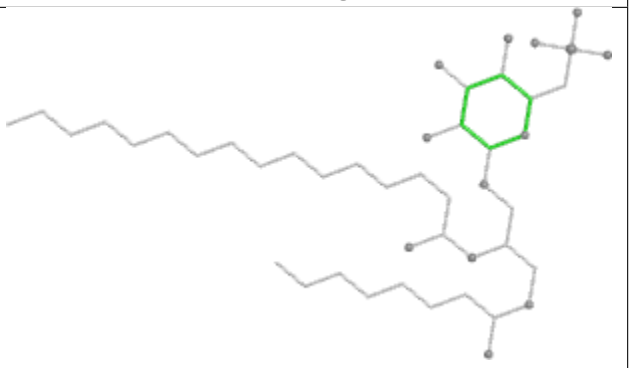
Bond lengths



Bond angles

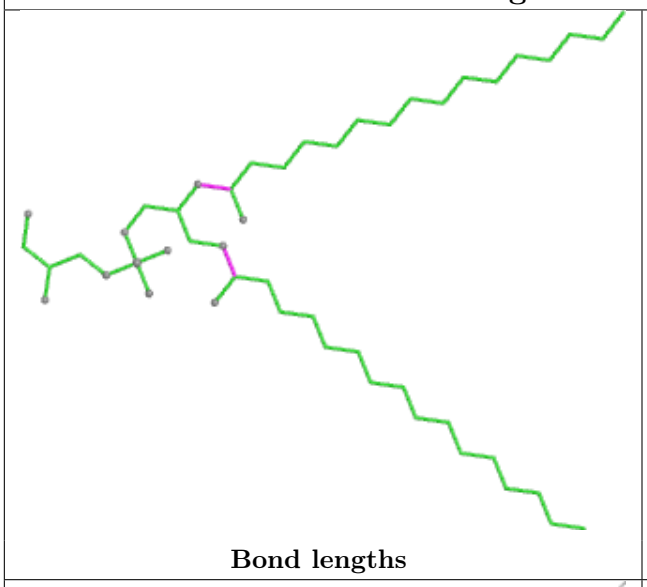


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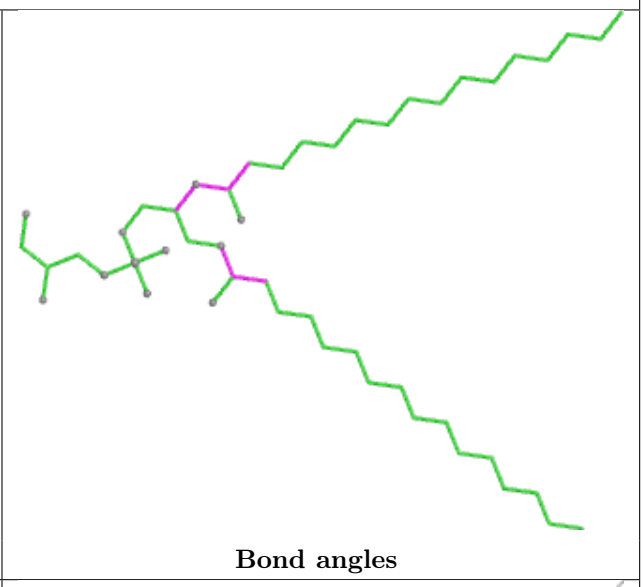


Rings

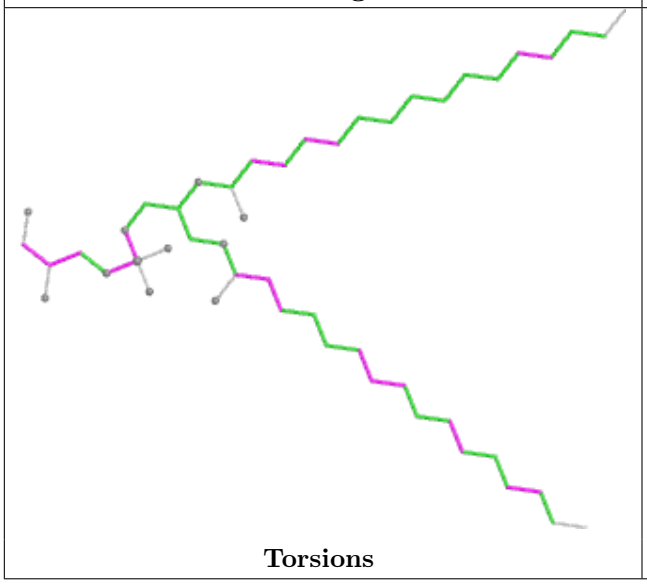
Ligand LHG DD 410



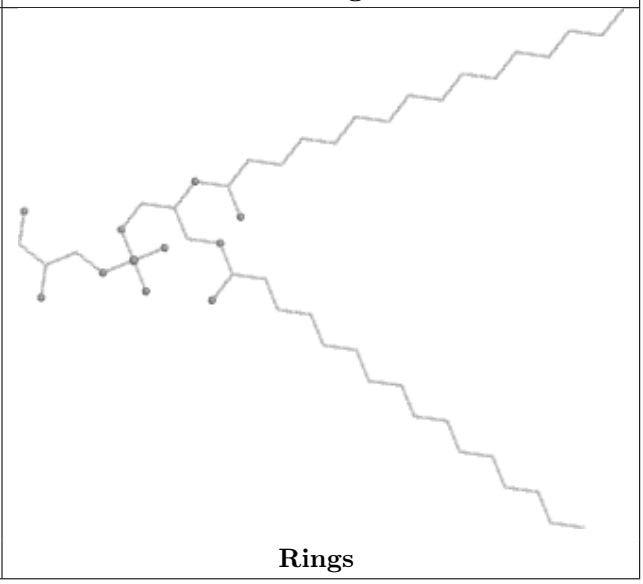
Bond lengths



Bond angles

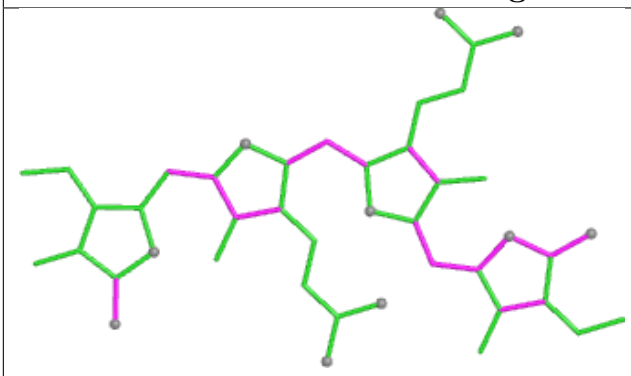


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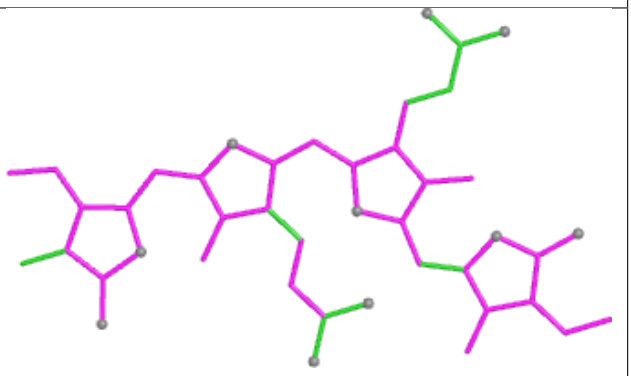


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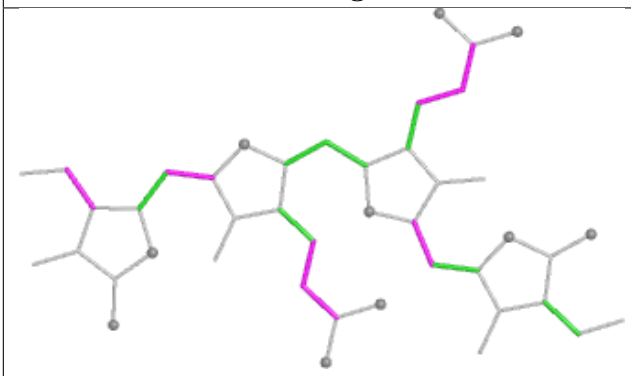
Ligand CYC mF 201



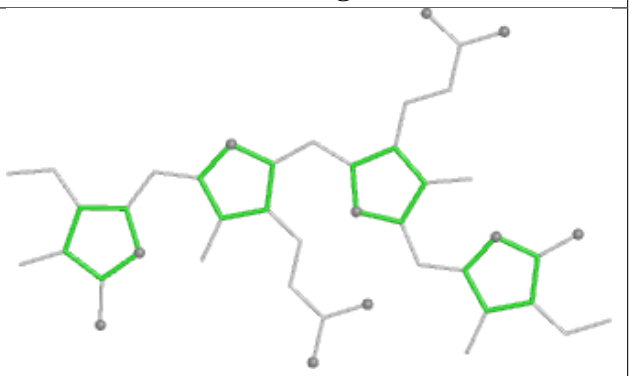
Bond lengths



Bond angles

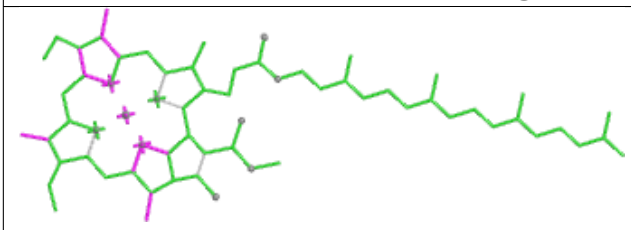


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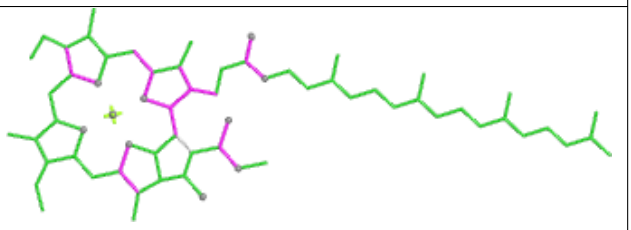


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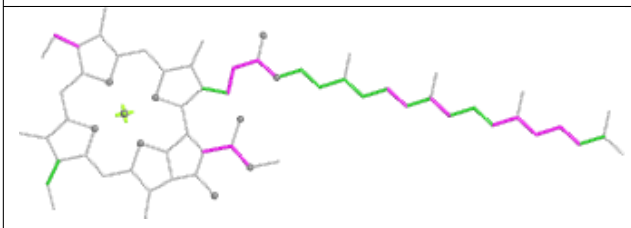
Ligand CLA bE 610



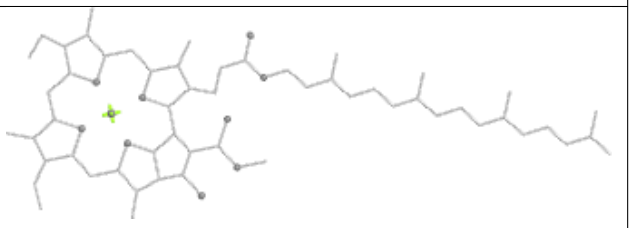
Bond lengths



Bond angles

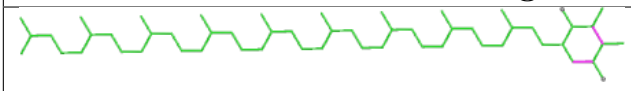


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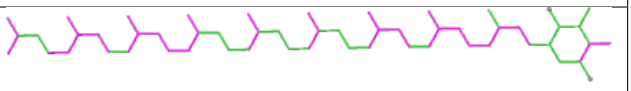


Rings

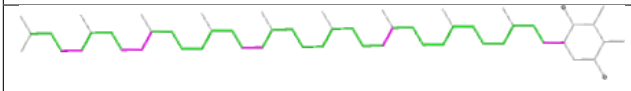
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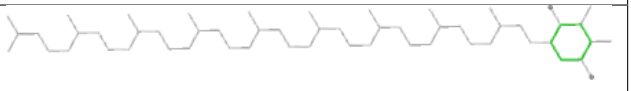
Bond lengths



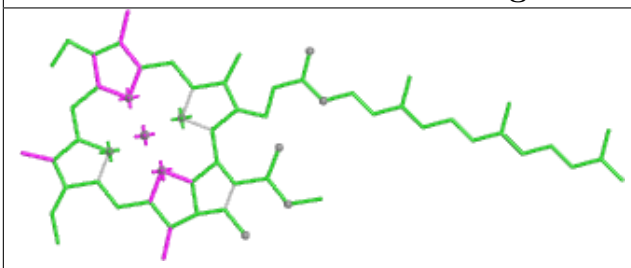
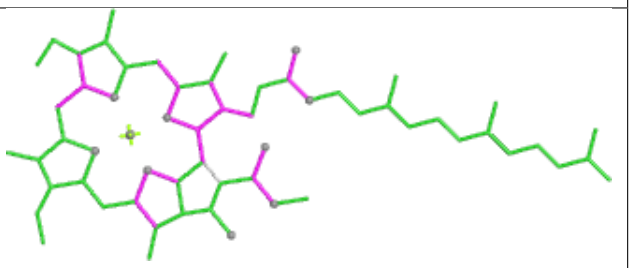
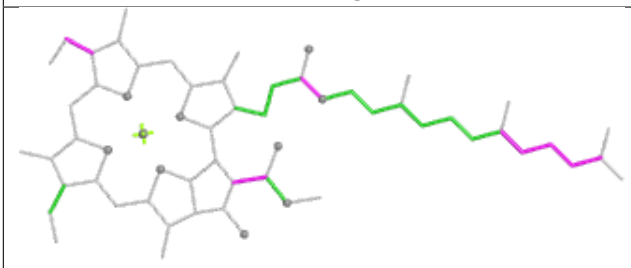
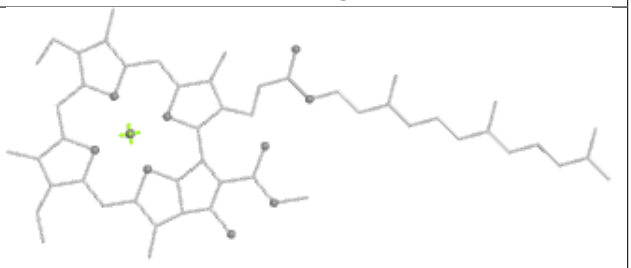
Bond angles

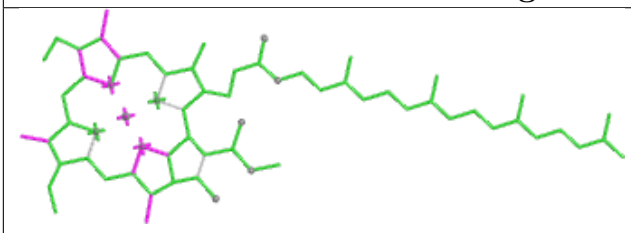
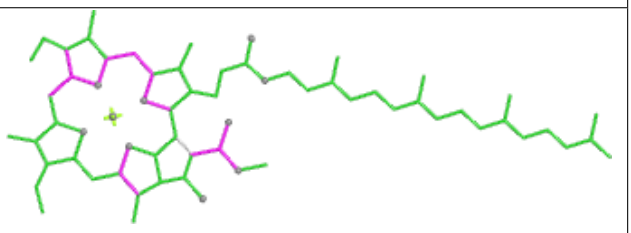
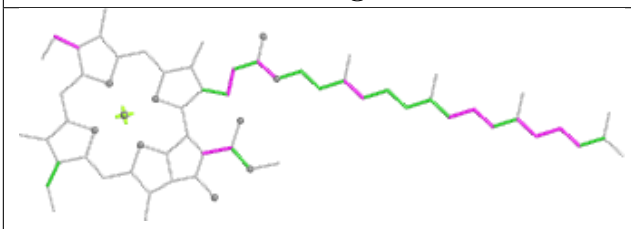
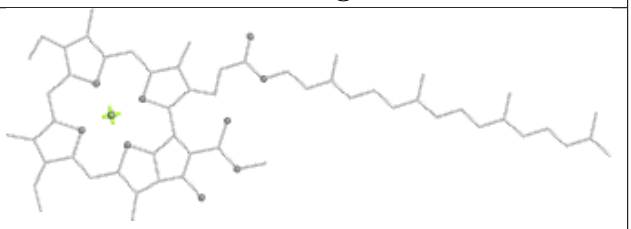


Torsions

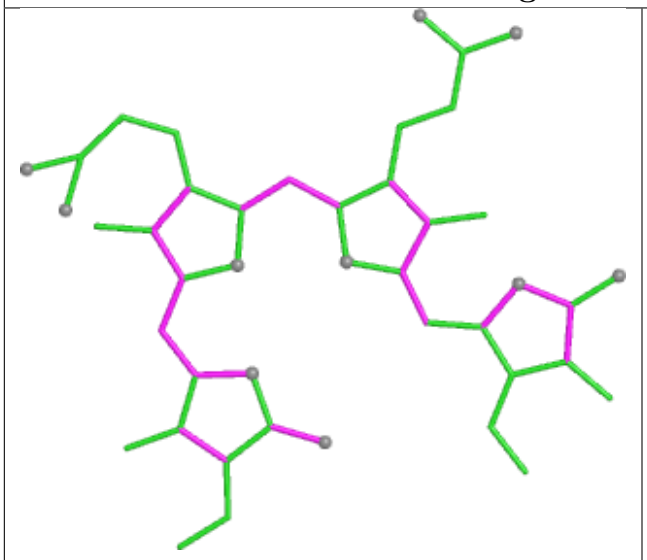


Rings

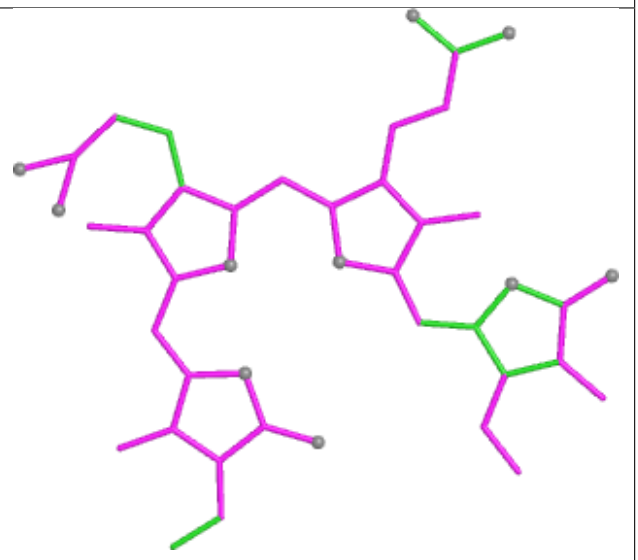
Ligand CLA HD 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b1 614	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

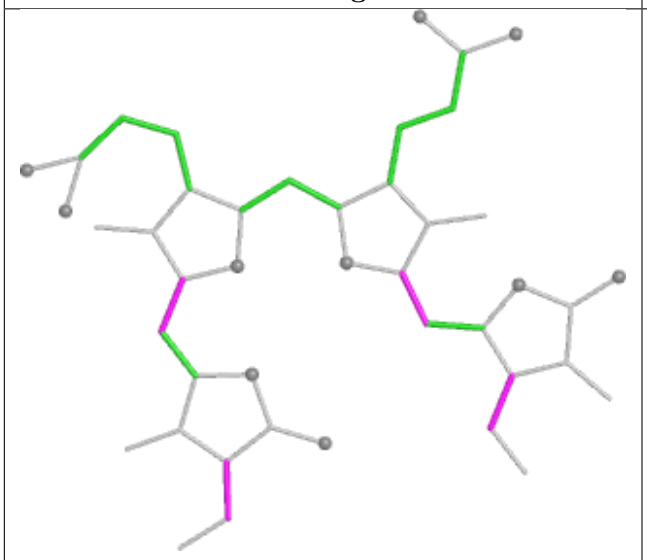
Ligand CYC e2 201



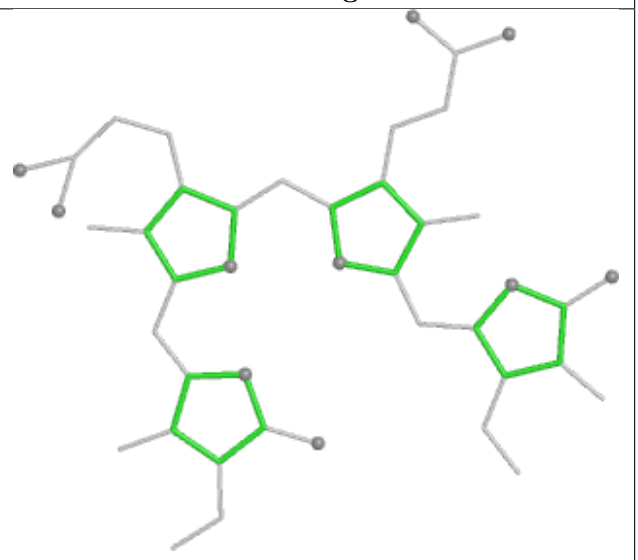
Bond lengths



Bond angles

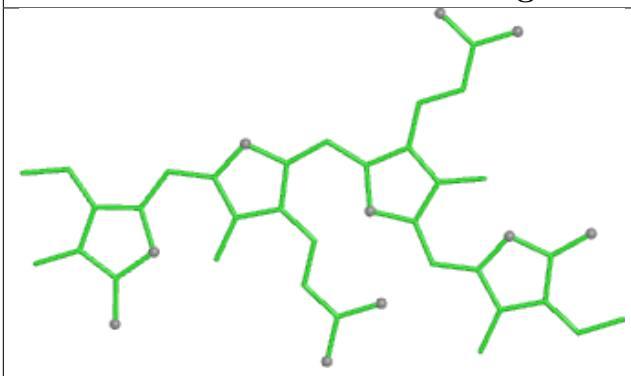


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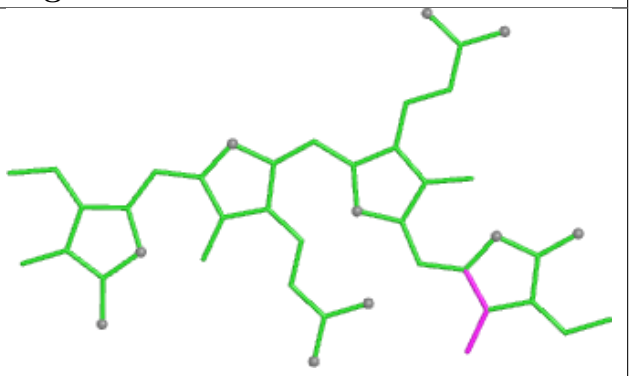


Rings

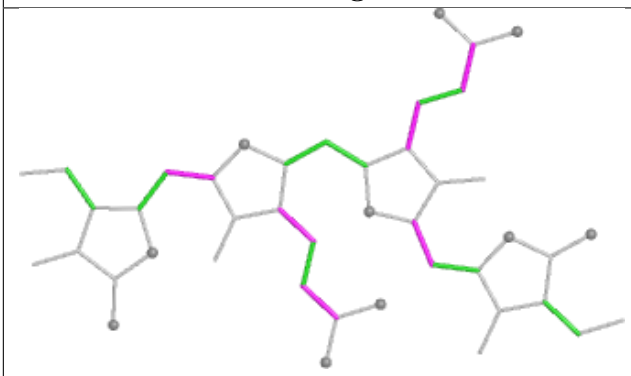
Ligand CYC g2 201



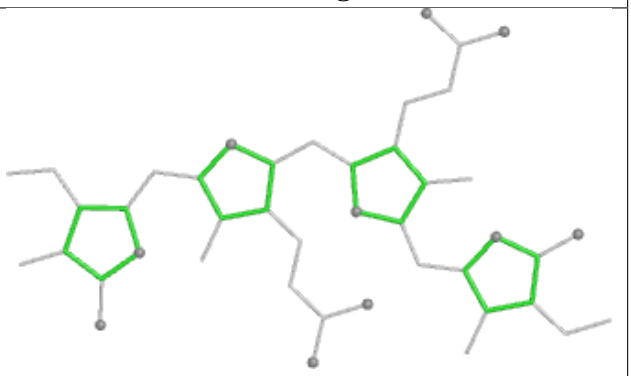
Bond lengths



Bond angles

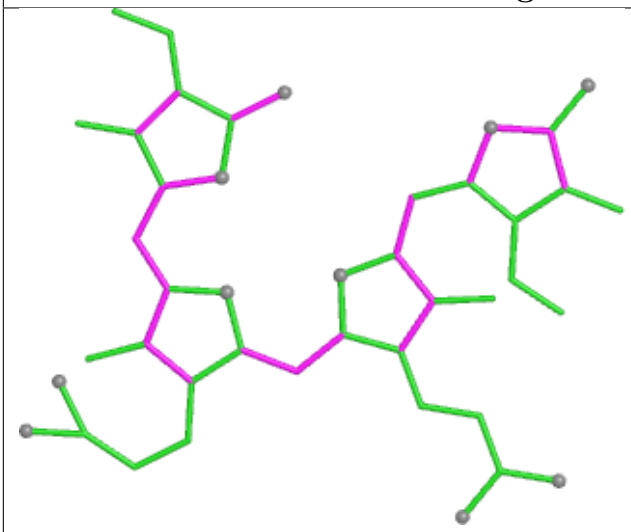


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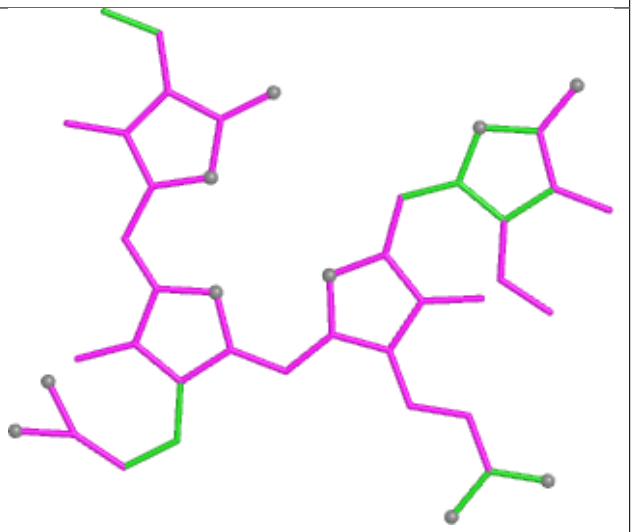


Rings

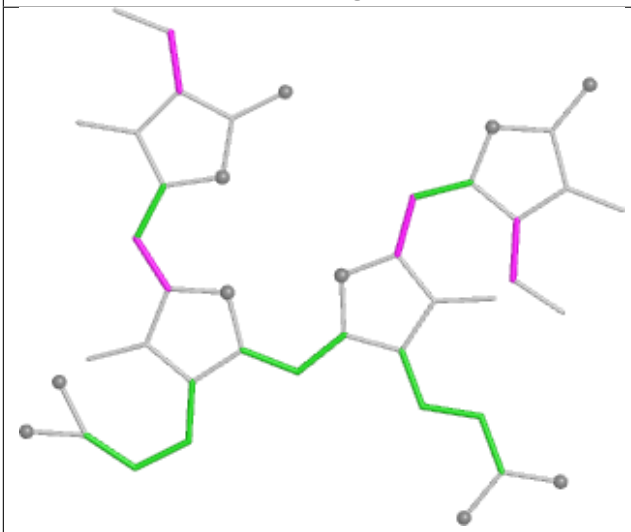
Ligand CYC k7 201



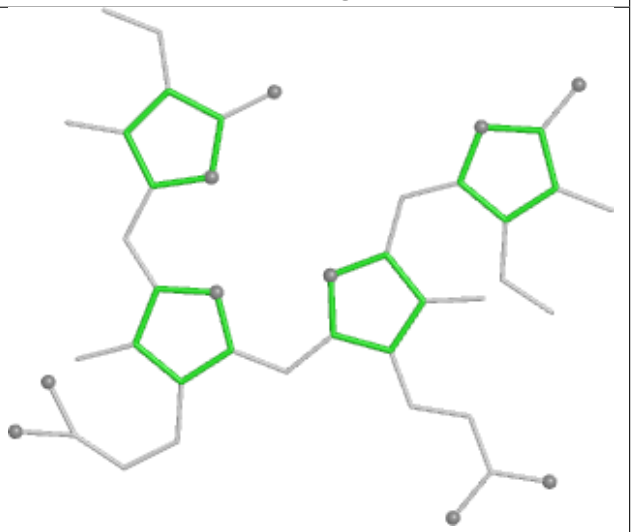
Bond lengths



Bond angles

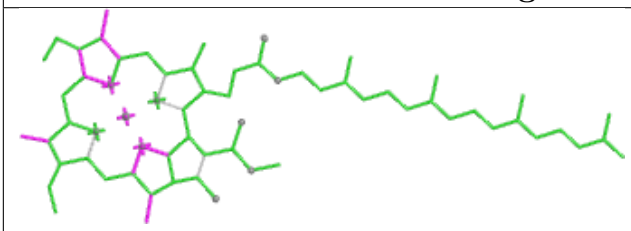


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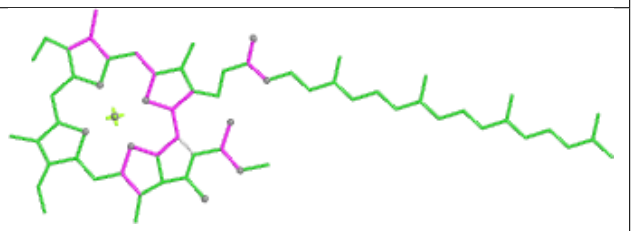


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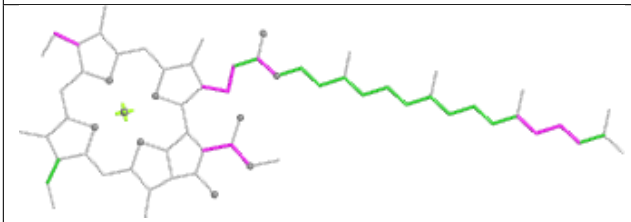
Ligand CLA b1 609



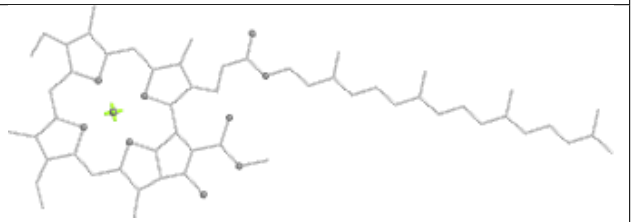
Bond lengths



Bond angles

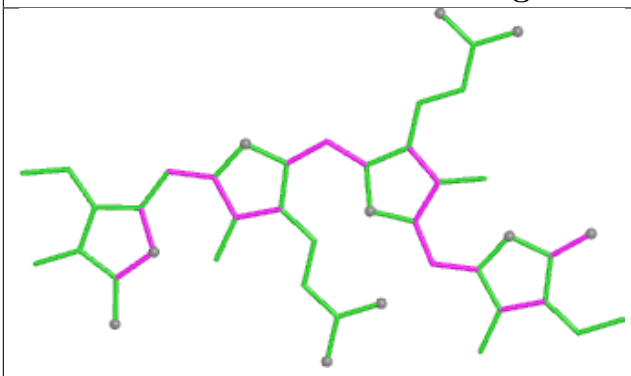


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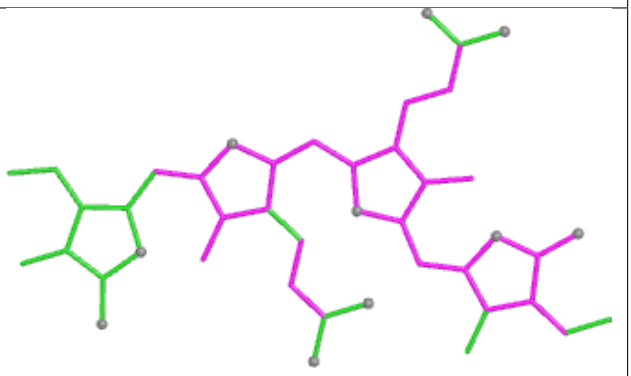


Rings

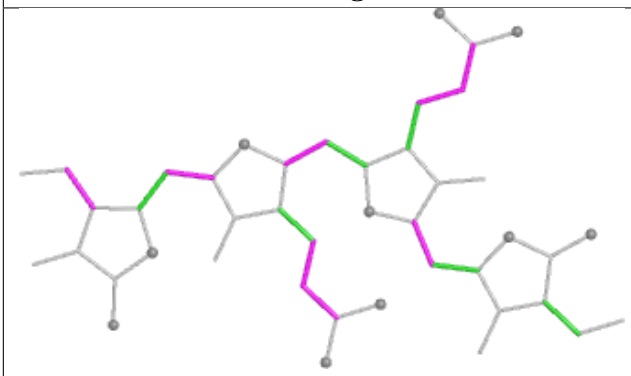
Ligand CYC V4 201



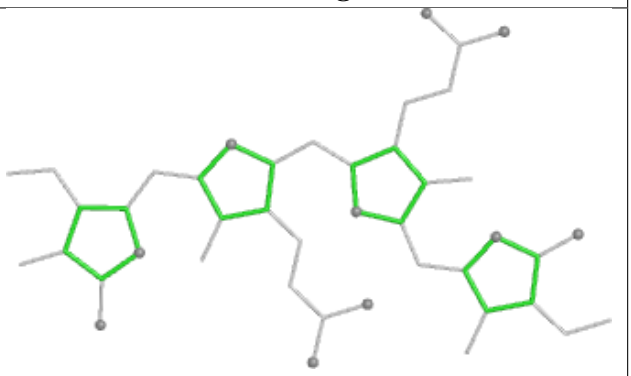
Bond lengths



Bond angles

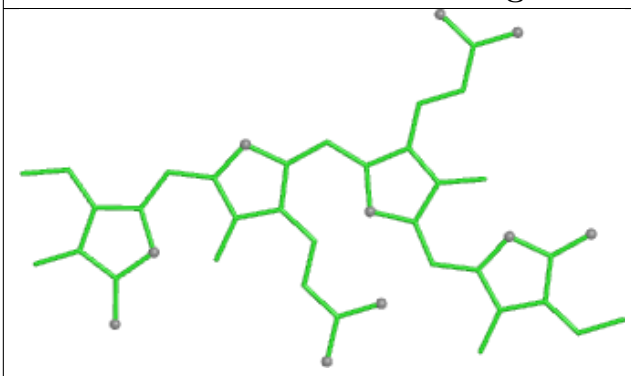


Torsions

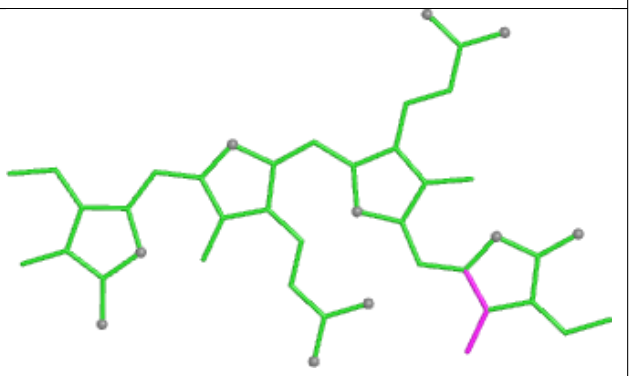


Rings

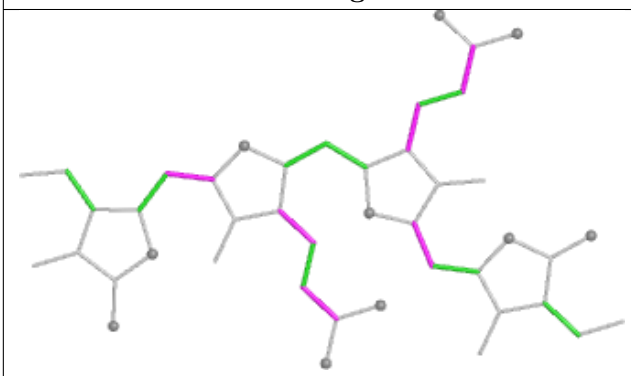
Ligand CYC mA 201



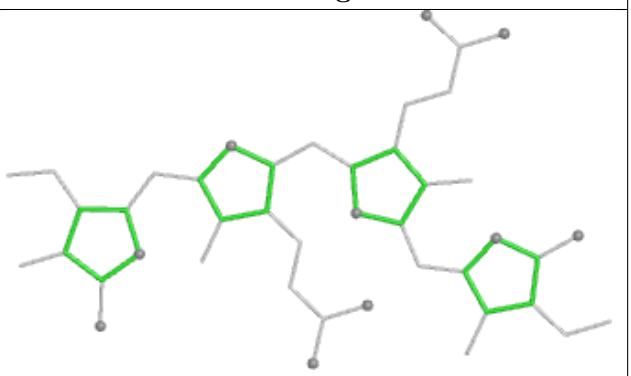
Bond lengths



Bond angles

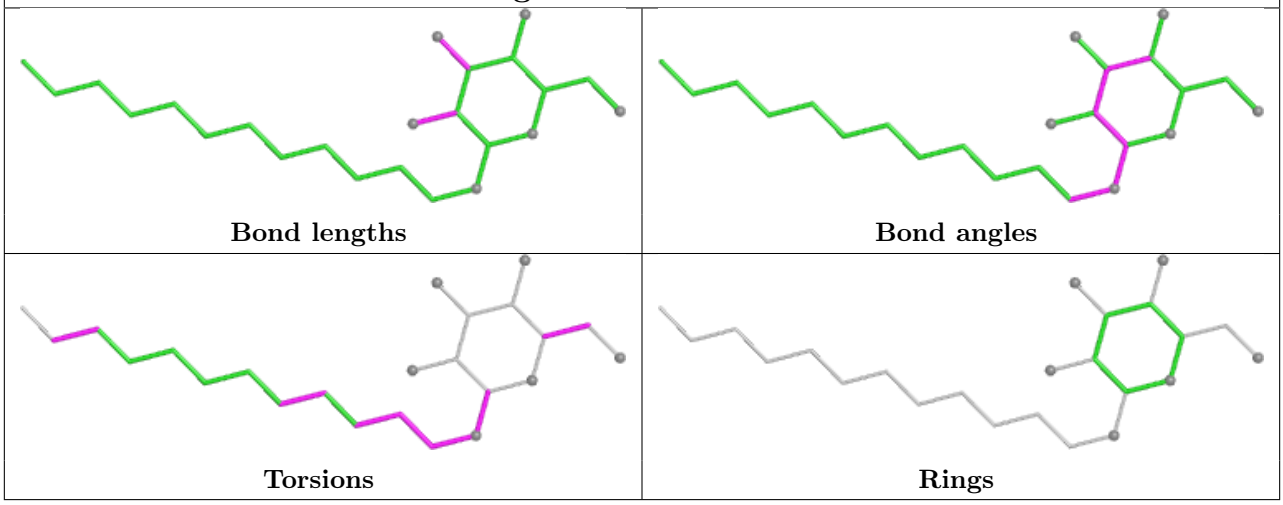


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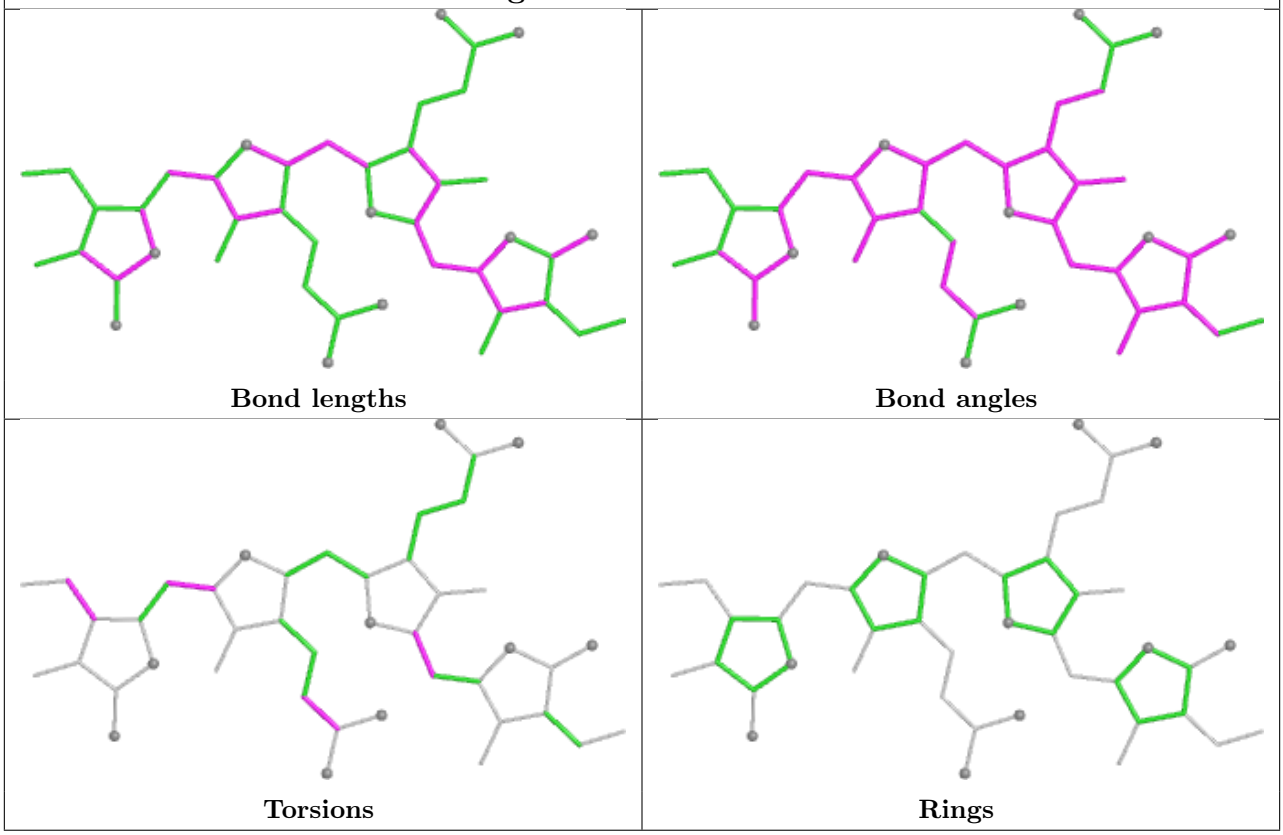


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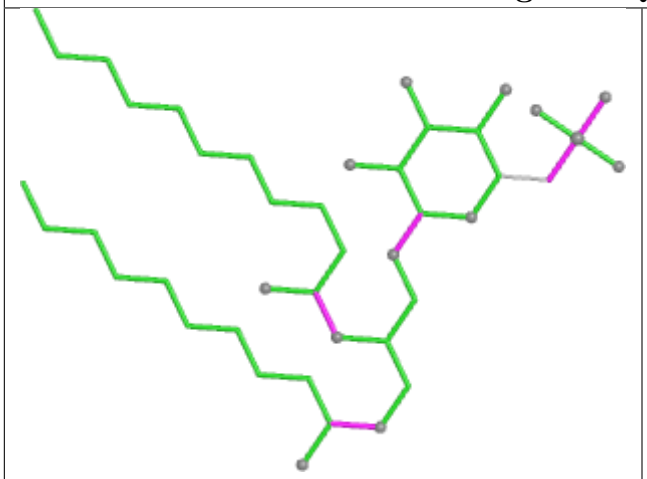
Ligand LMT bE 621



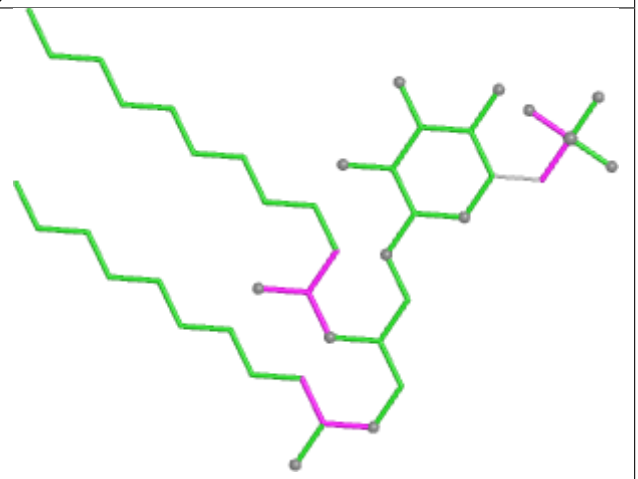
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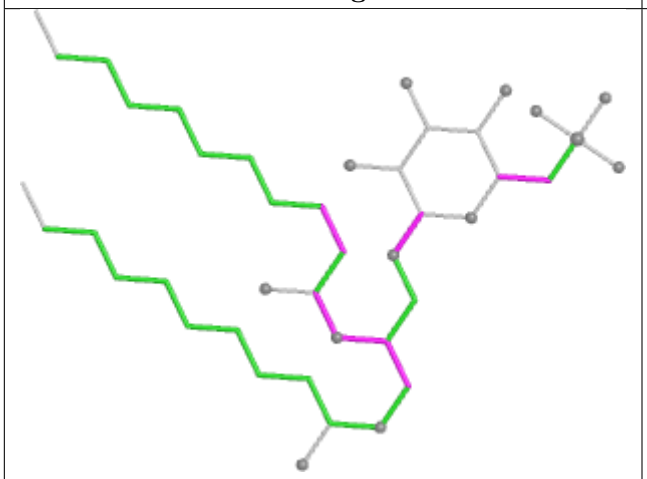
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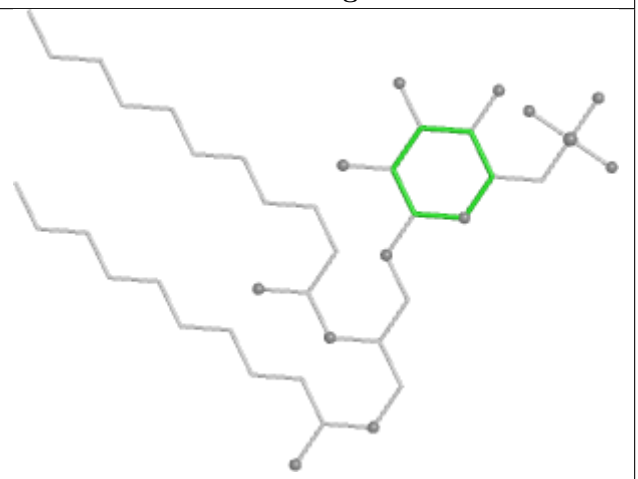
Bond lengths



Bond angles

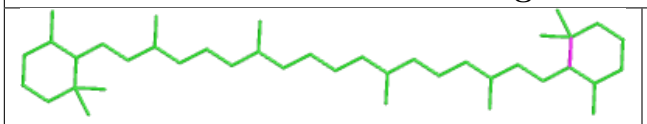


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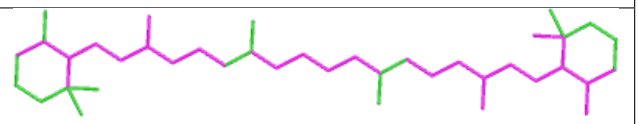


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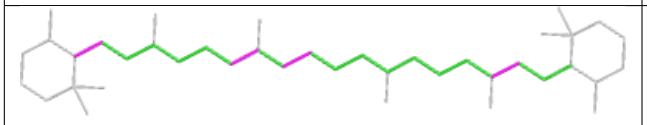
Ligand BCR B1 615



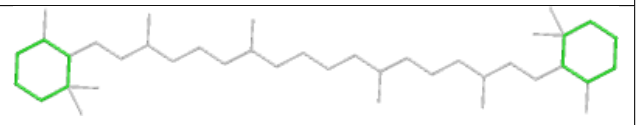
Bond lengths



Bond angles

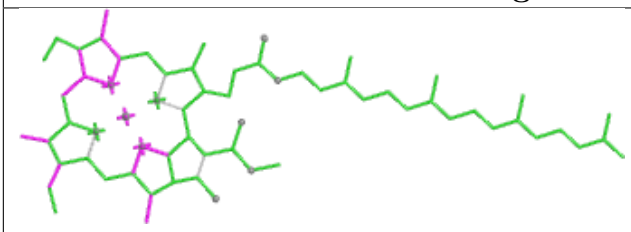


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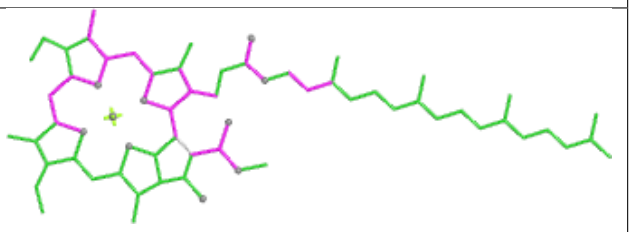


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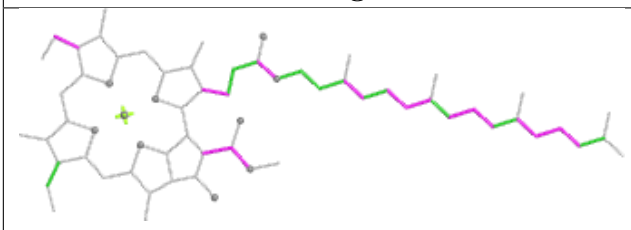
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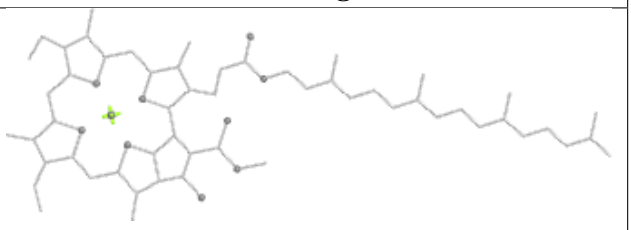
Bond lengths



Bond angles



Torsions



Rings

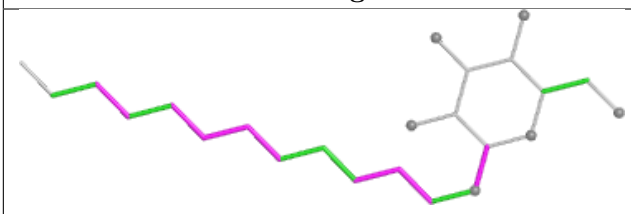
Ligand LMT dD 404



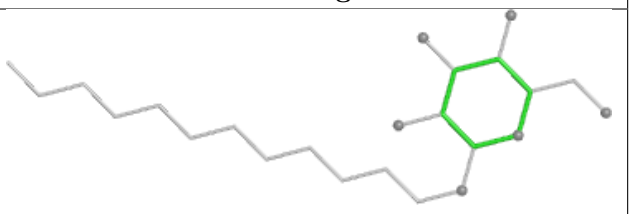
Bond lengths



Bond angles

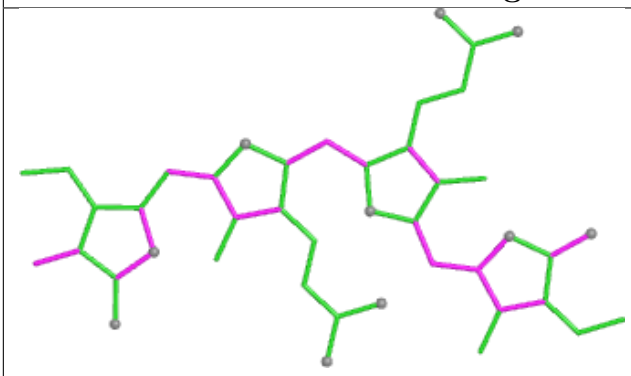


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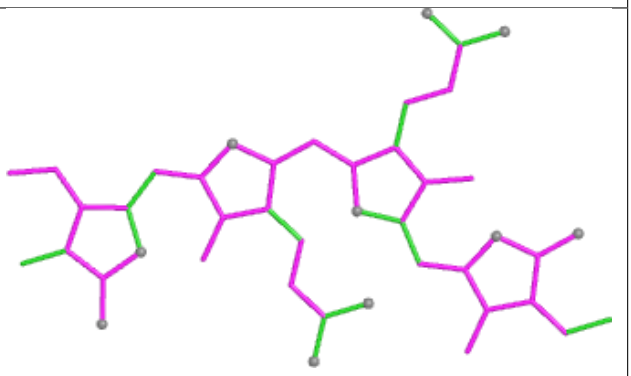


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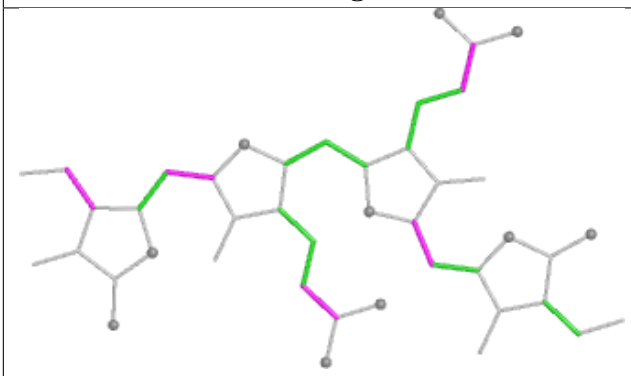
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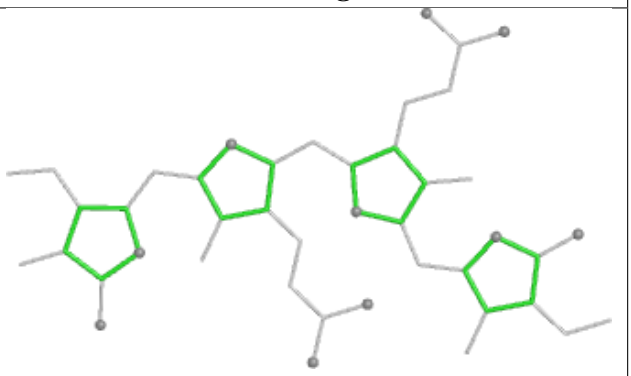
Bond lengths



Bond angles

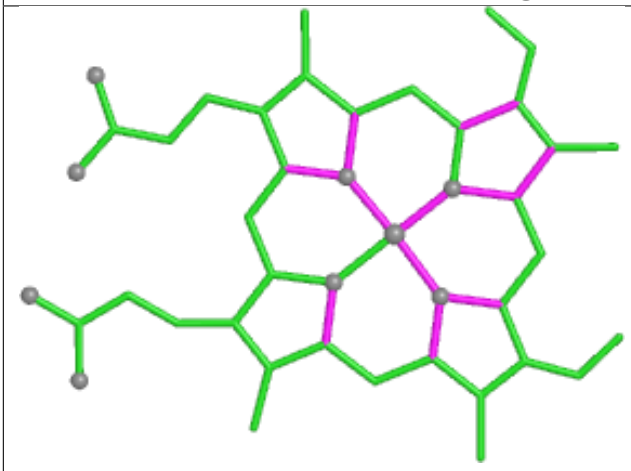


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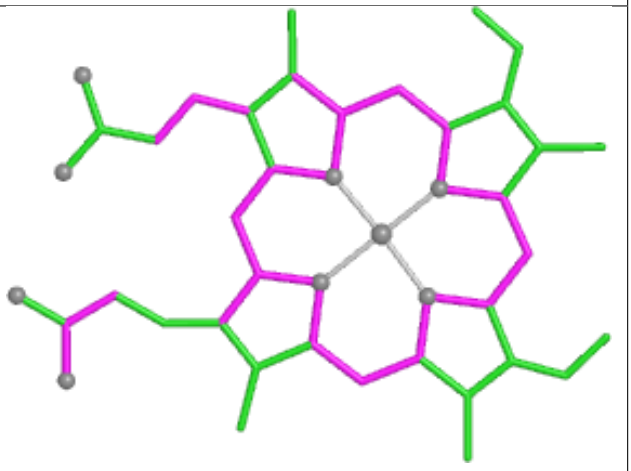


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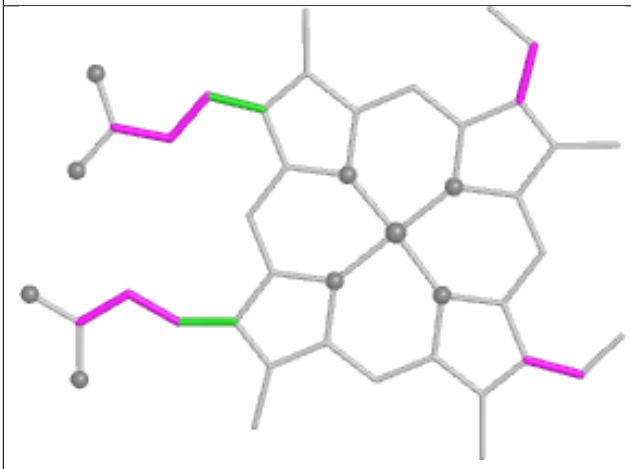
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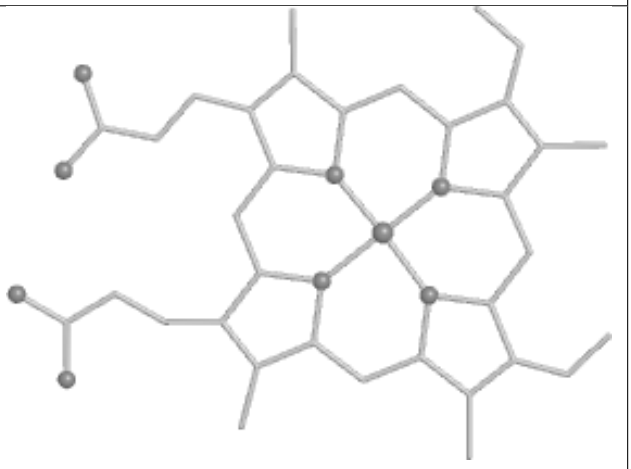
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Bond angles

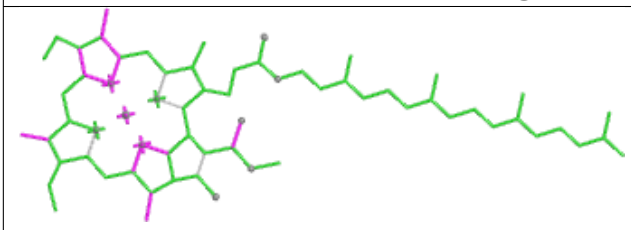


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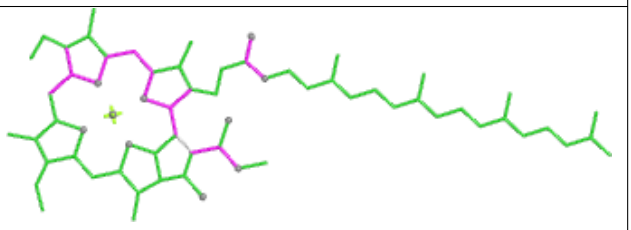


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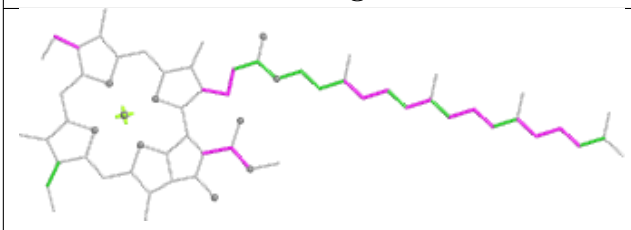
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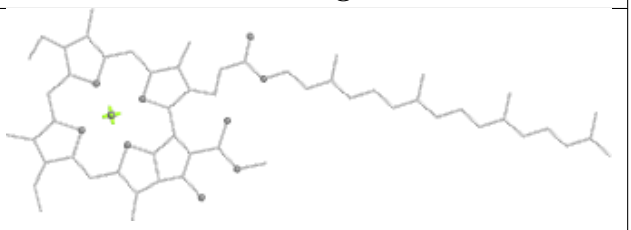
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Bond angles

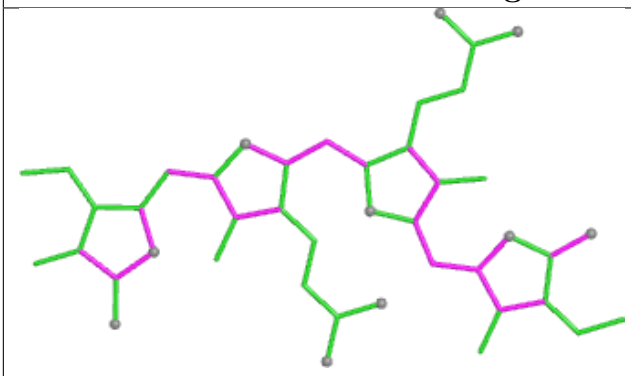


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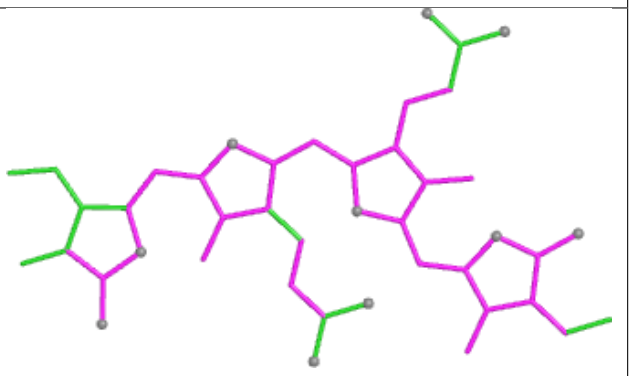


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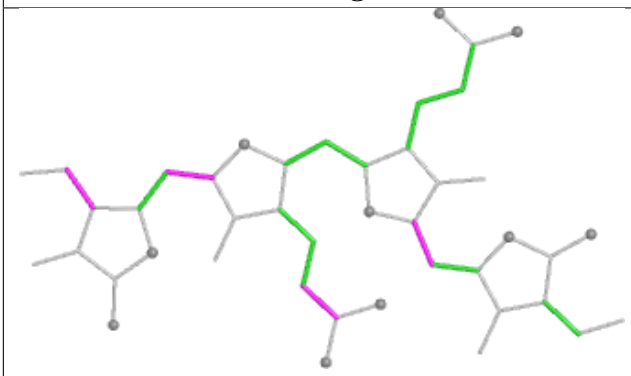
Ligand CYC MK 201



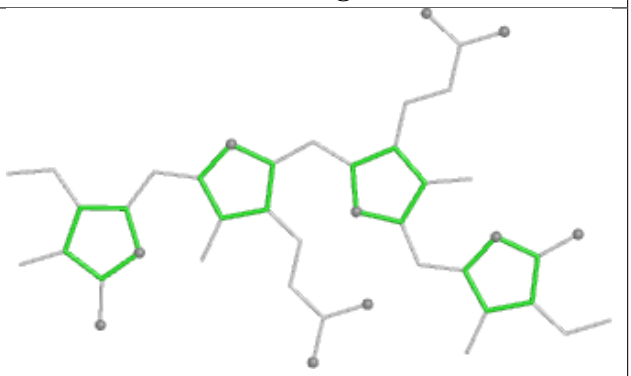
Bond lengths



Bond angles

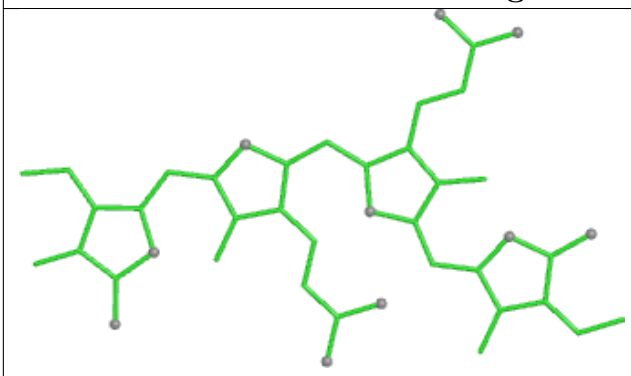


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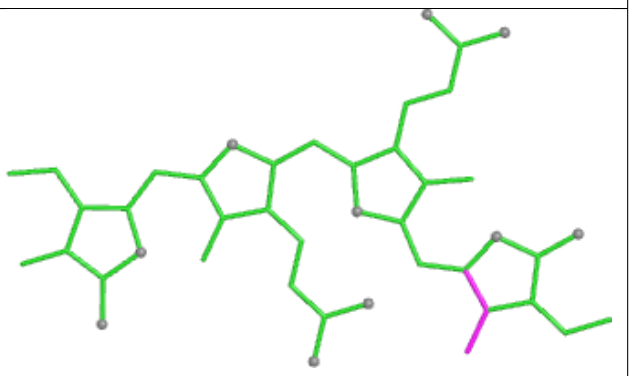


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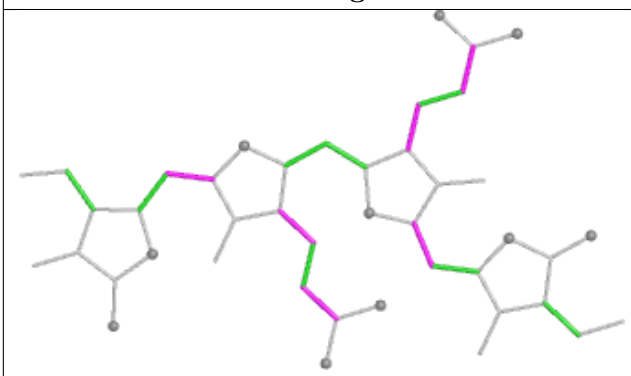
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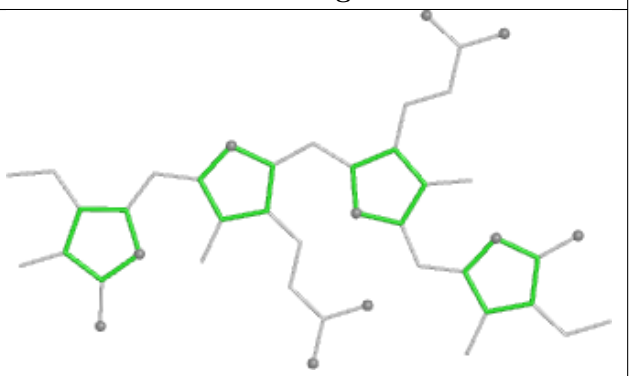
Bond lengths



Bond angles

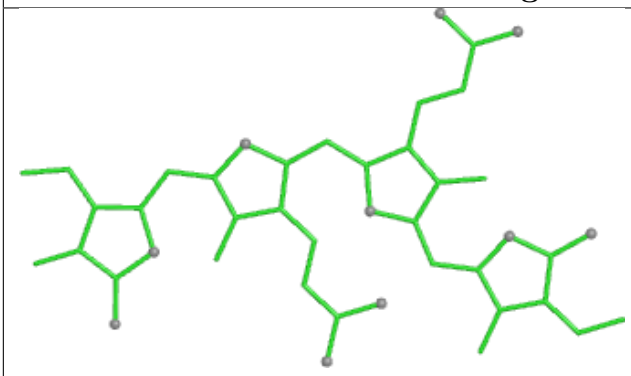


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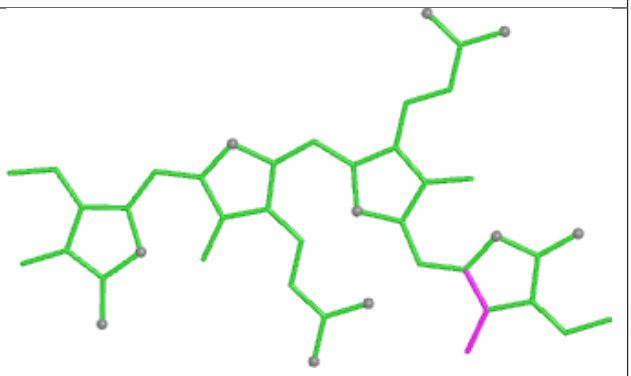


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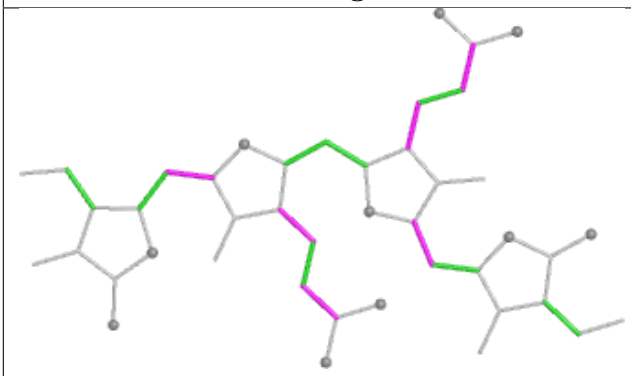
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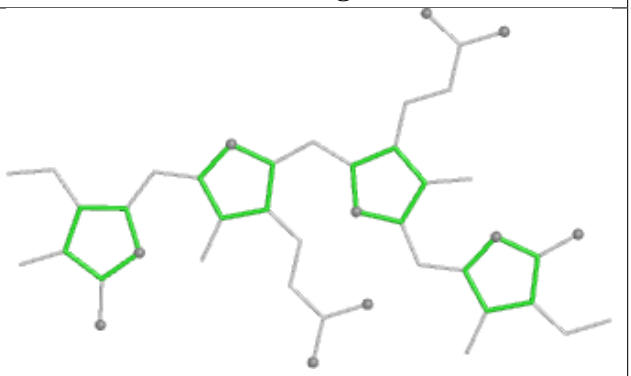
Bond lengths



Bond angles

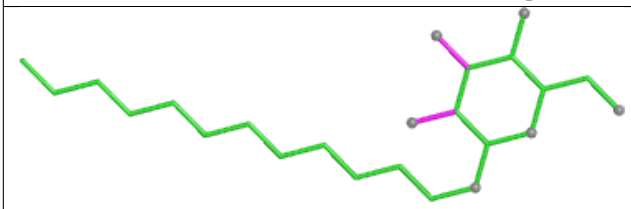


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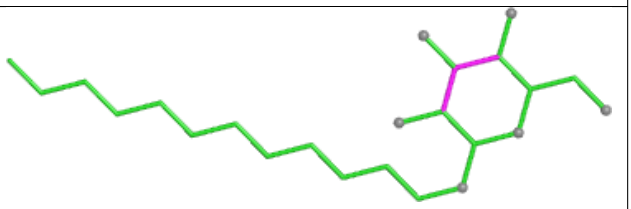


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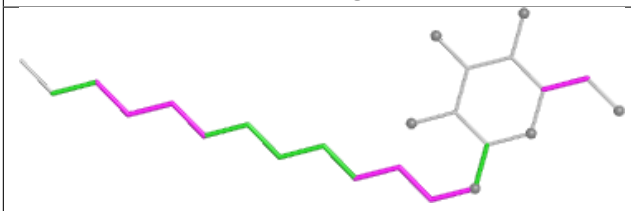
Ligand LMT i1 102



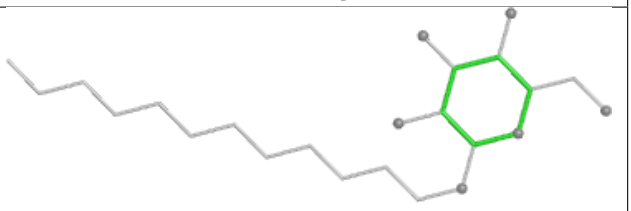
Bond lengths



Bond angles

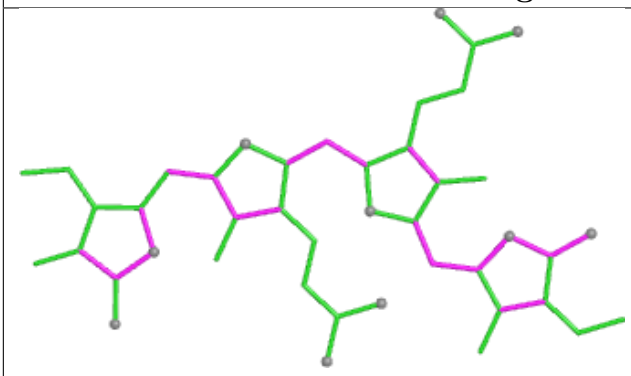


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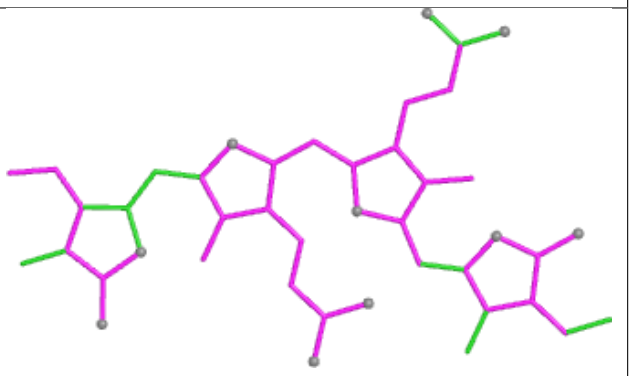


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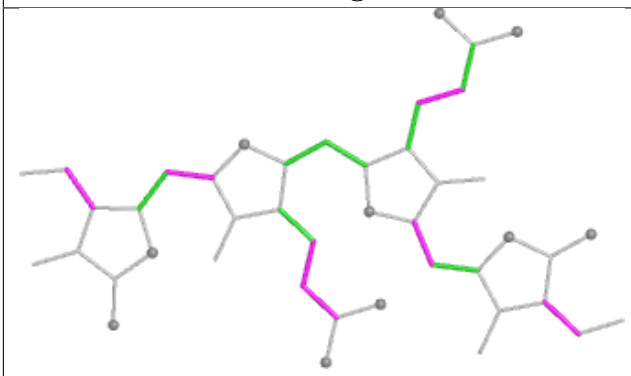
Ligand CYC d8 201



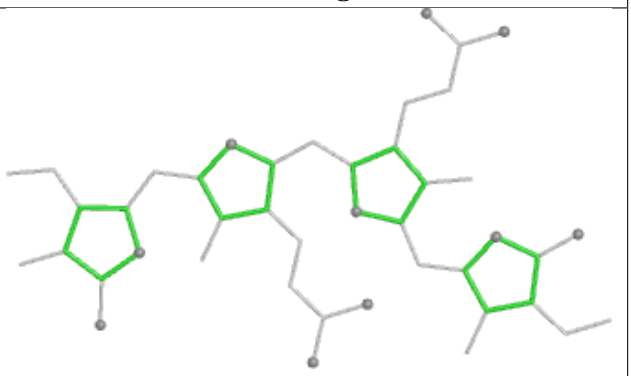
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Bond angles

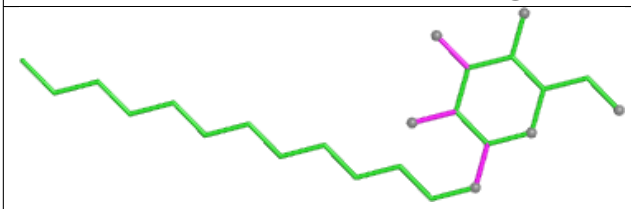


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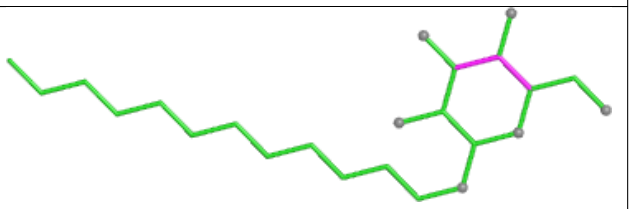


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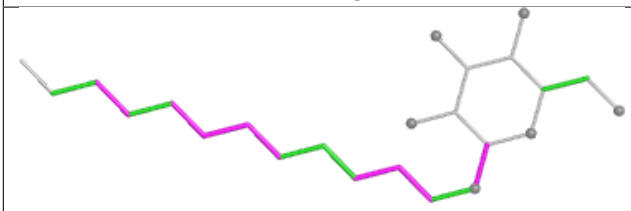
Ligand LMT DD 404



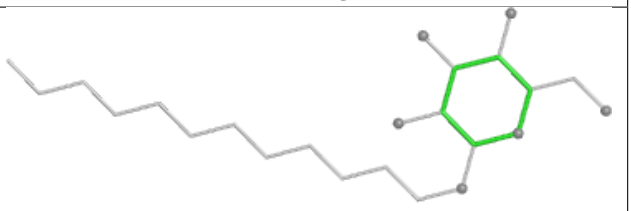
Bond lengths



Bond angles

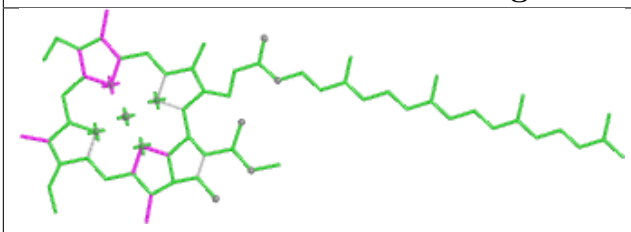


Torsions

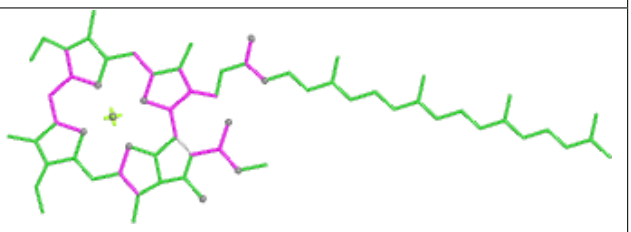


Rings

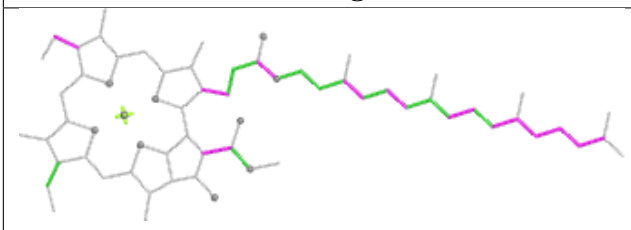
Ligand CLA BD 604



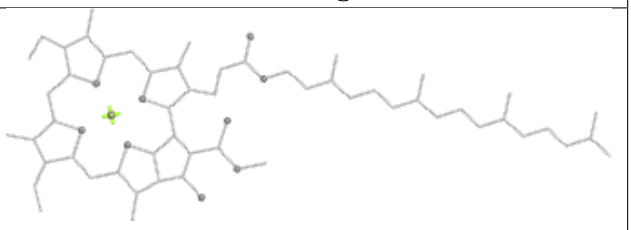
Bond lengths



Bond angles

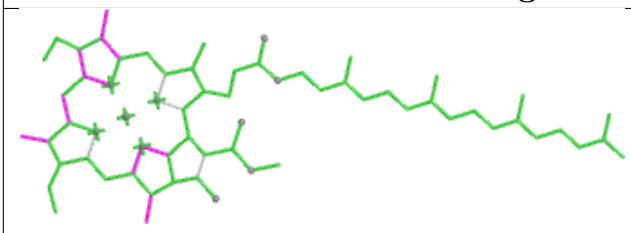


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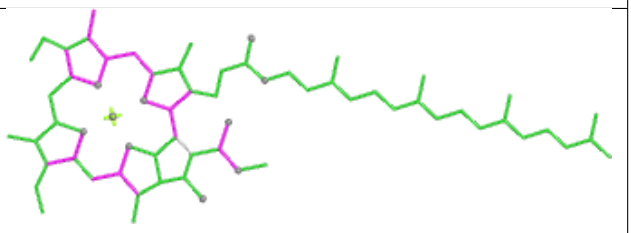


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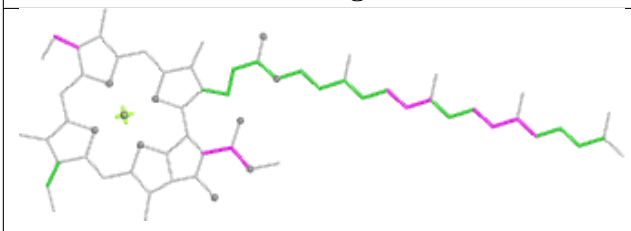
Ligand CLA b1 615



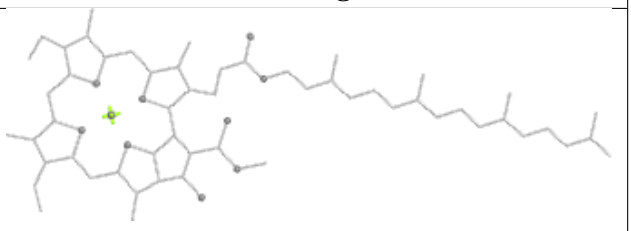
Bond lengths



Bond angles

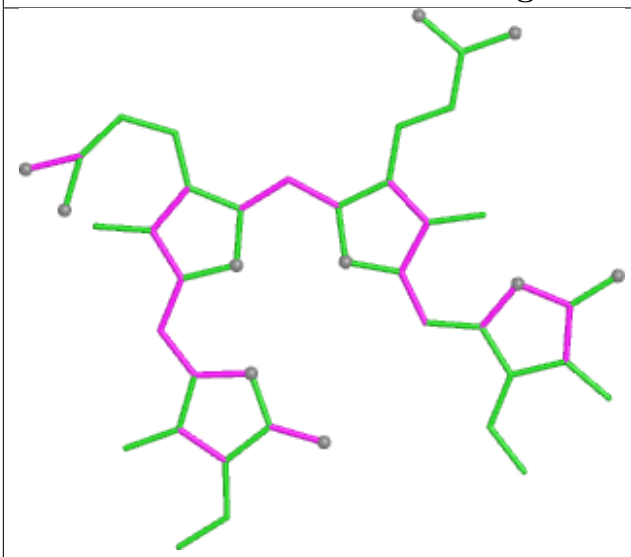


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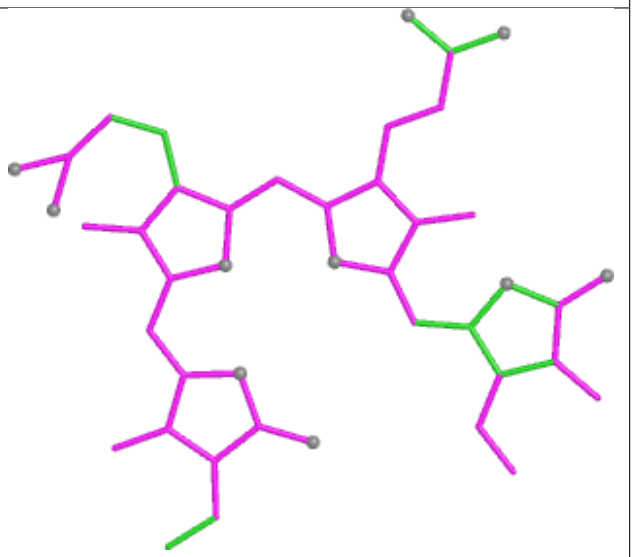


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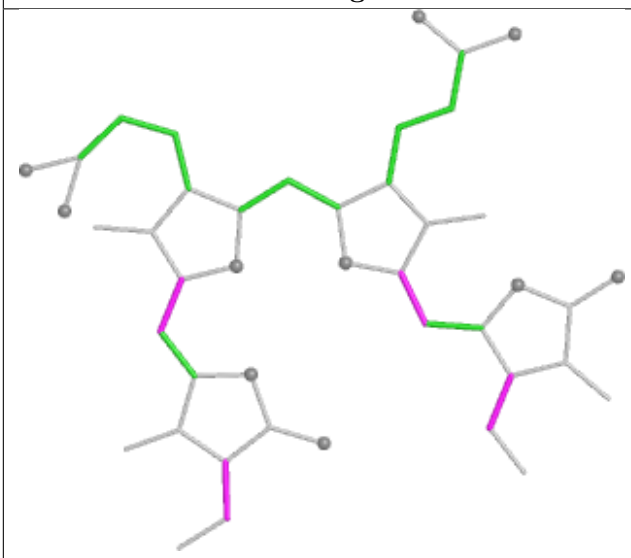
Ligand CYC iA 202



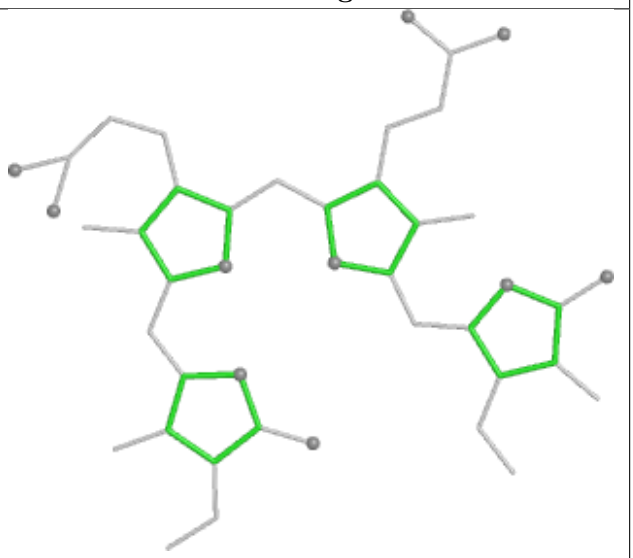
Bond lengths



Bond angles

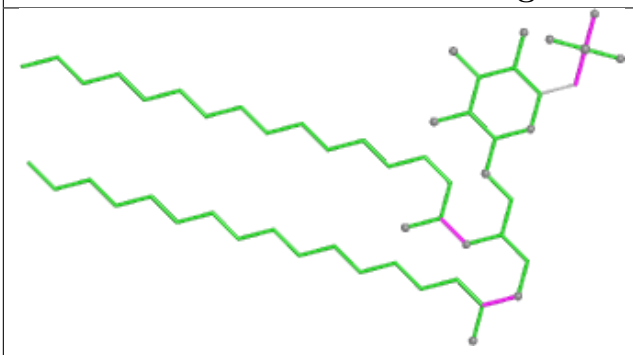


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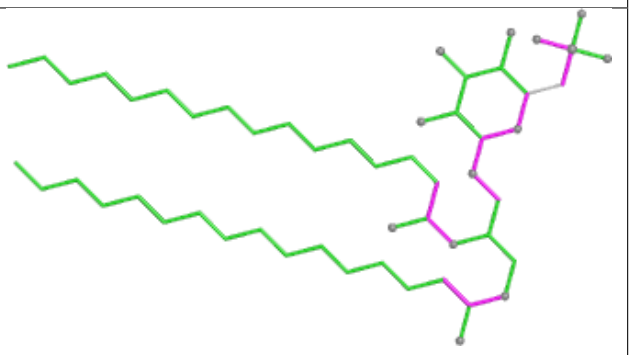


Rings

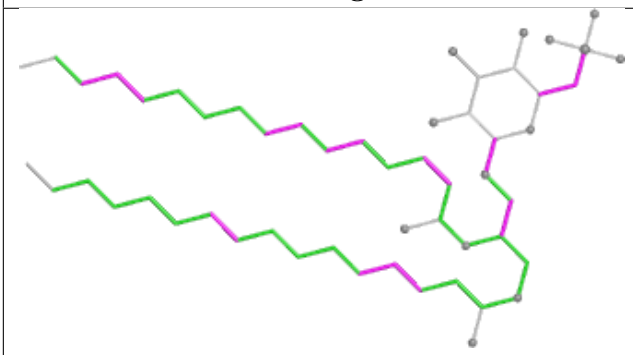
Ligand SQD cE 502



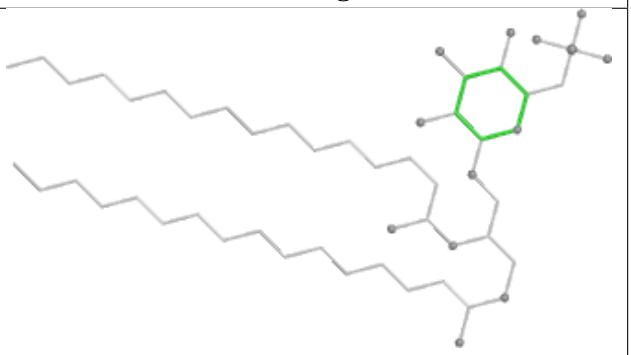
Bond lengths



Bond angles

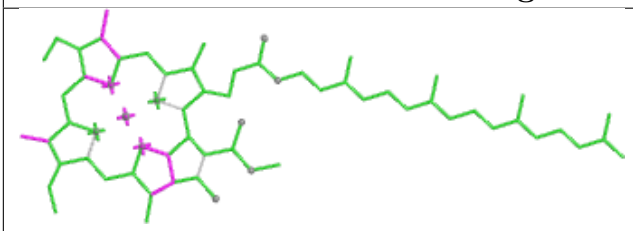


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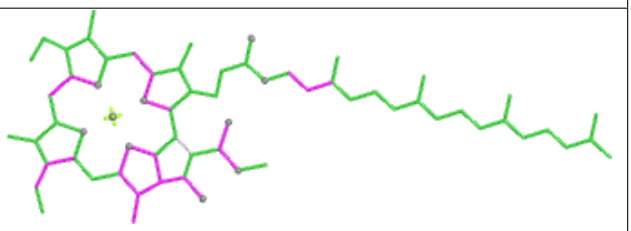


Rings

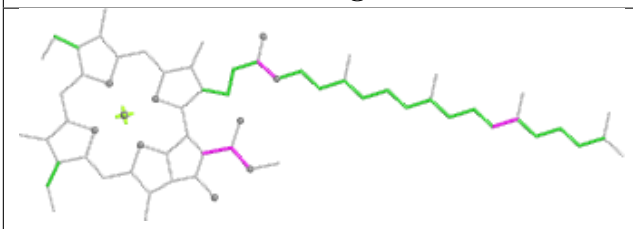
Ligand CLA cE 509



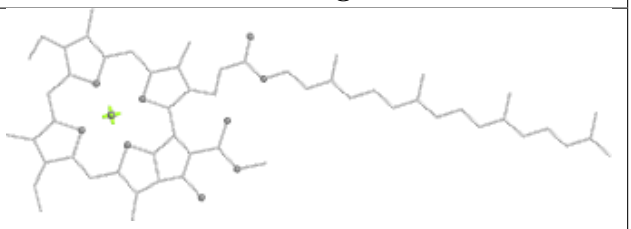
Bond lengths



Bond angles

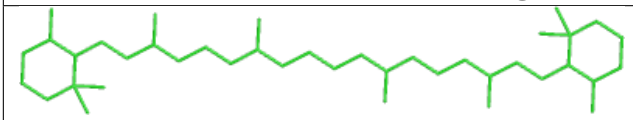


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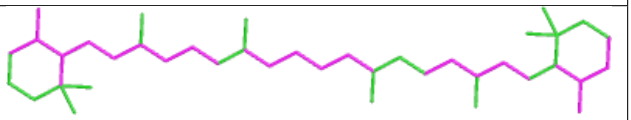


Rings

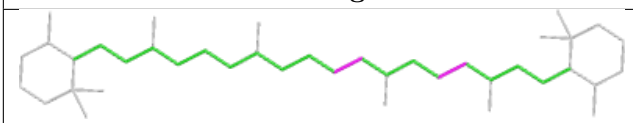
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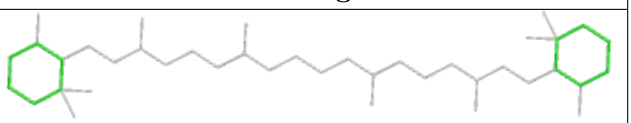
Bond lengths



Bond angles

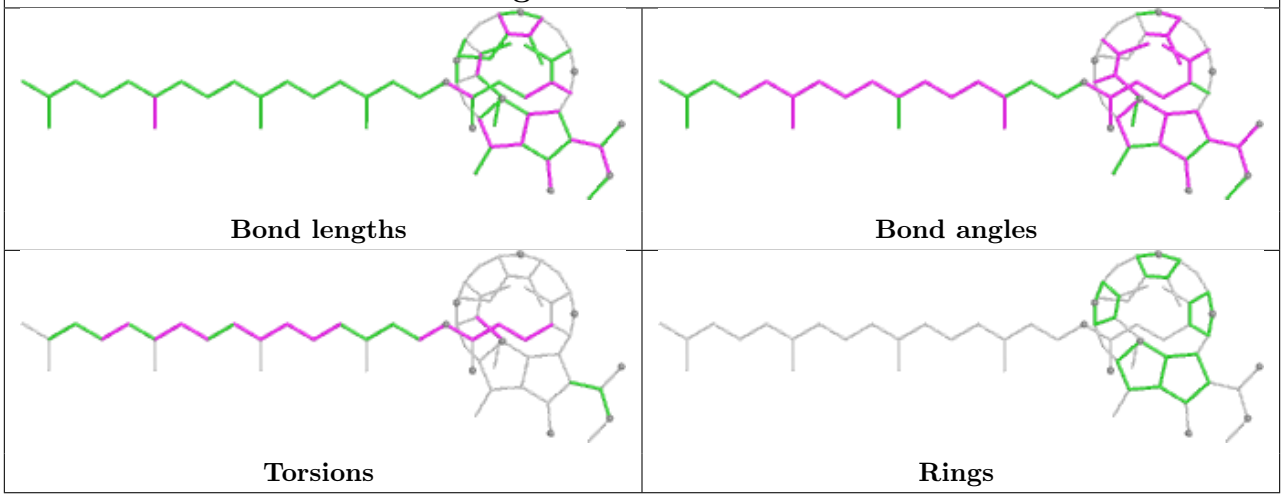


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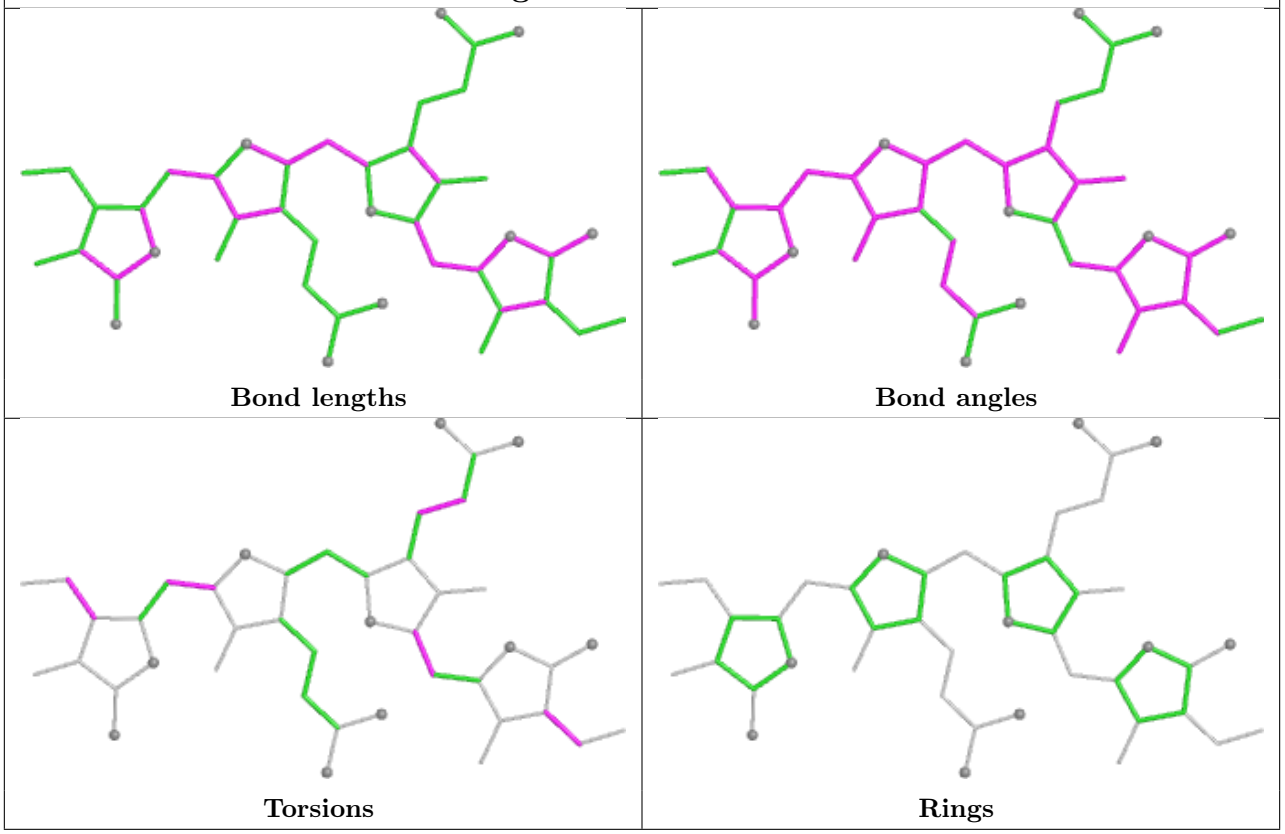


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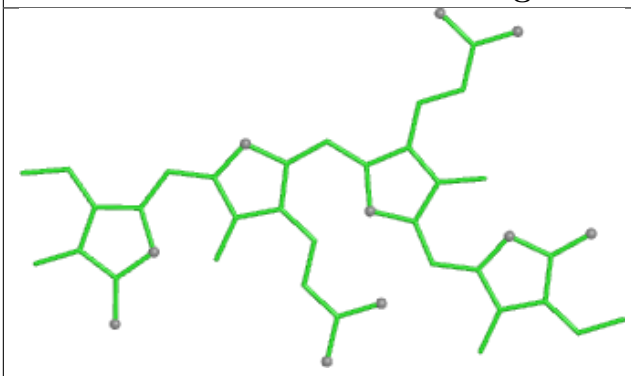
Ligand PHO D1 402



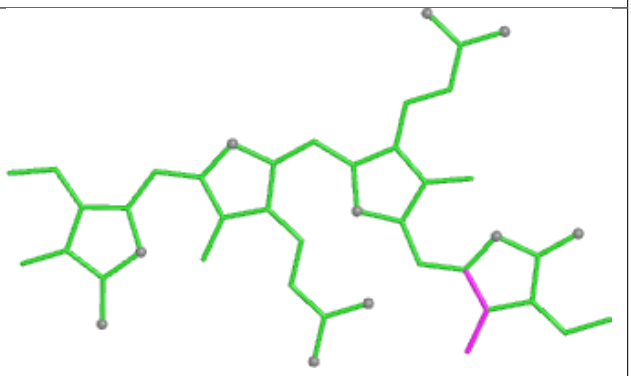
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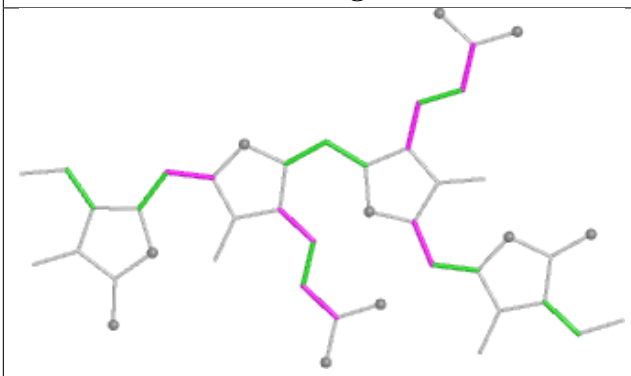
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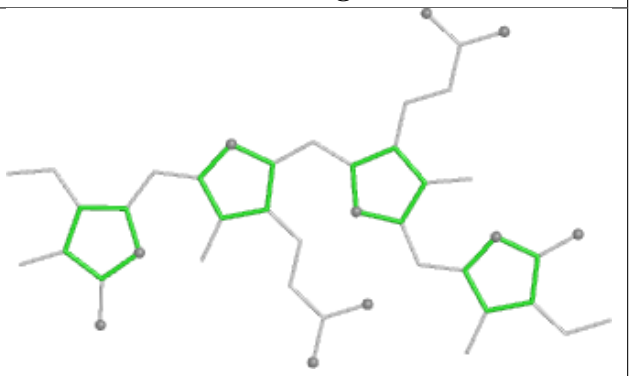
Bond lengths



Bond angles

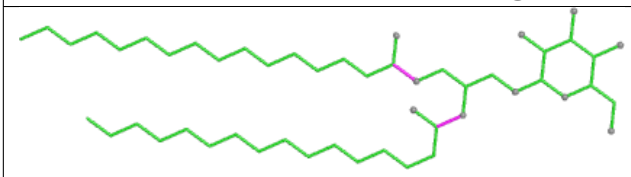


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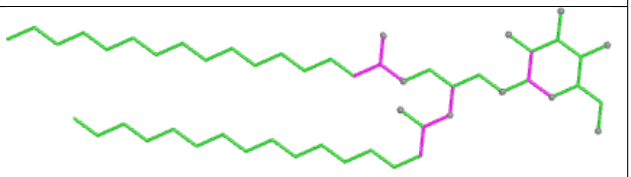


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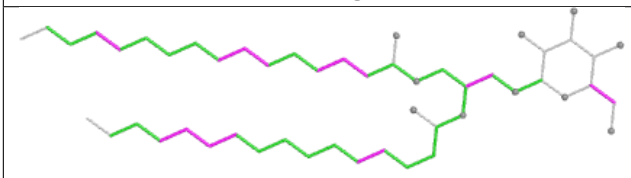
Ligand LMG dD 411



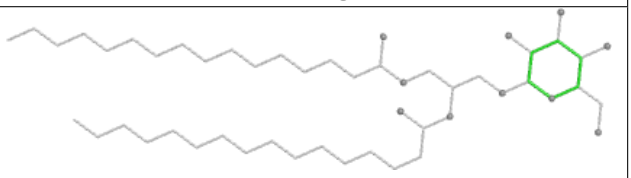
Bond lengths



Bond angles

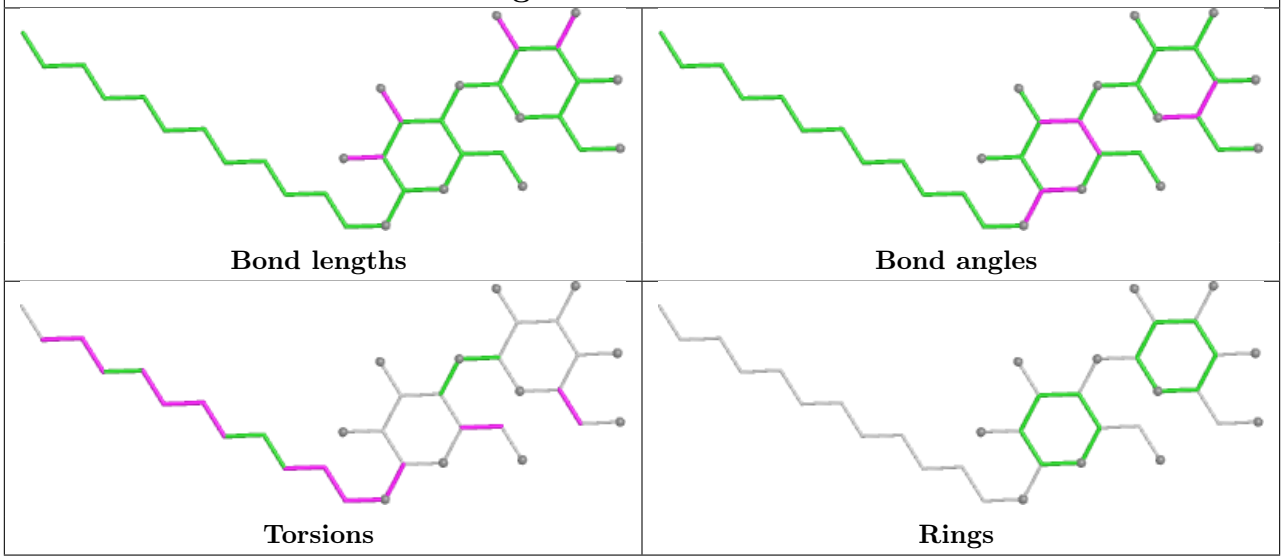


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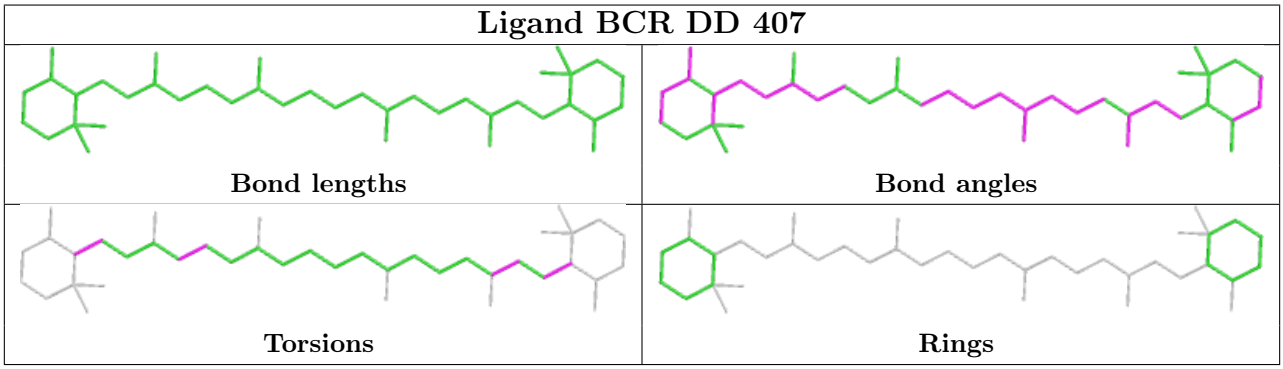


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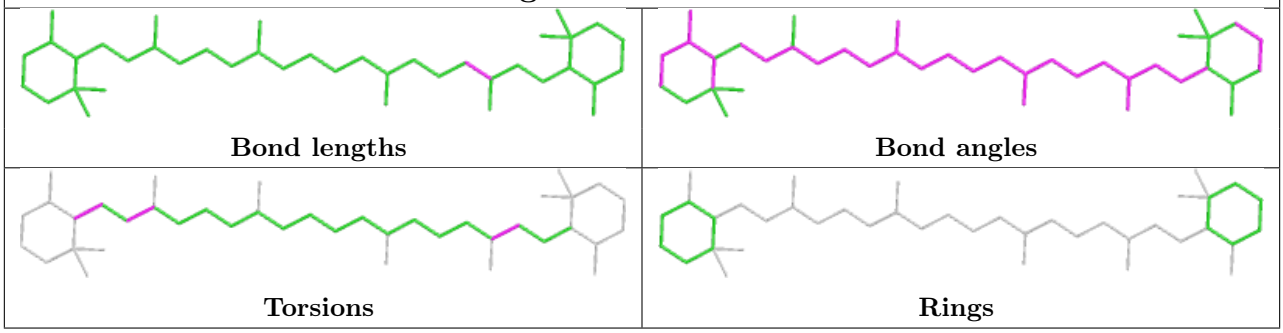
Ligand LMT A1 413



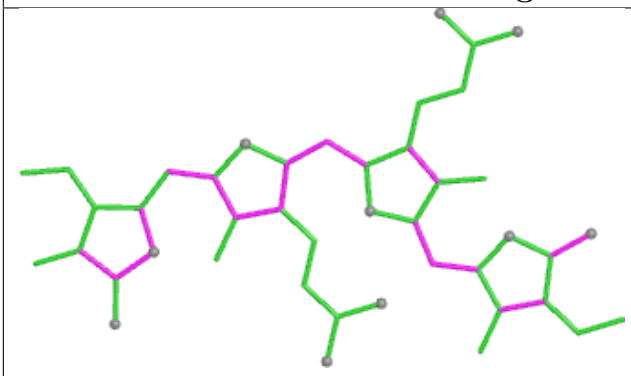
Ligand BCR DD 407



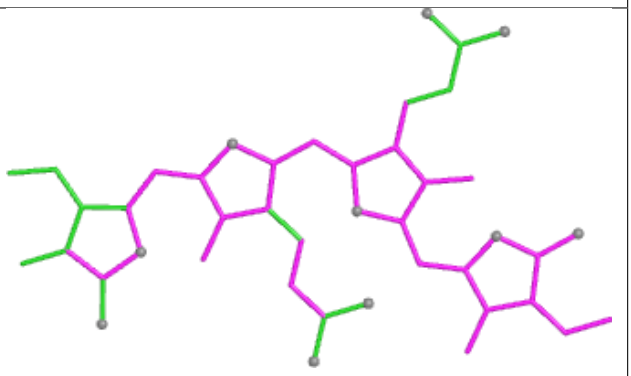
Ligand BCR iE 102



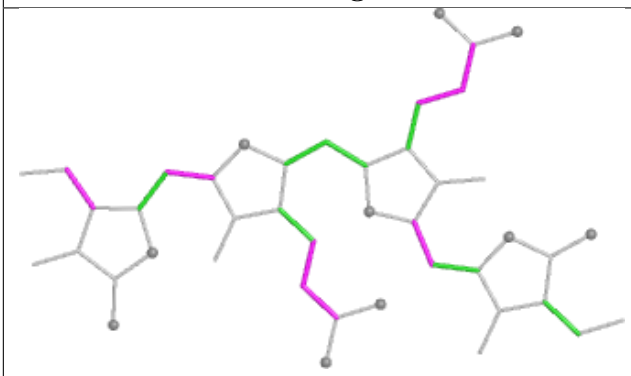
Ligand CYC S4 201



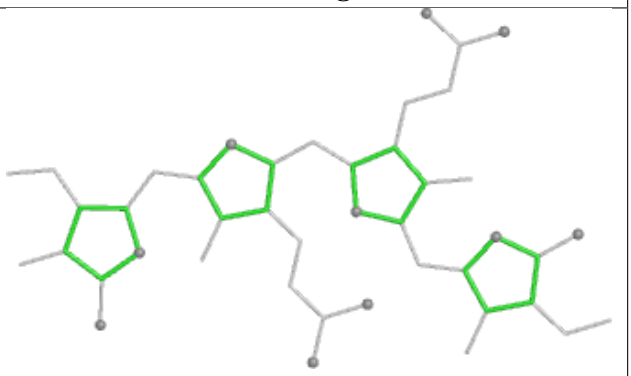
Bond lengths



Bond angles

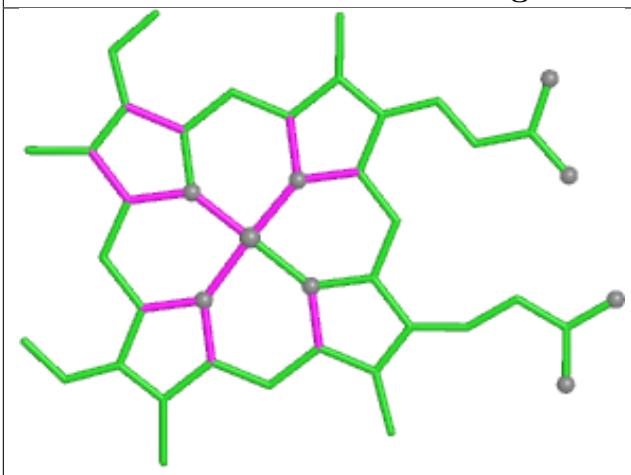


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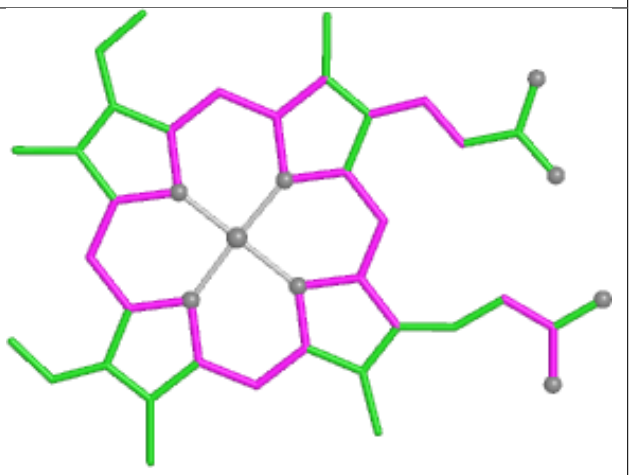


Rings

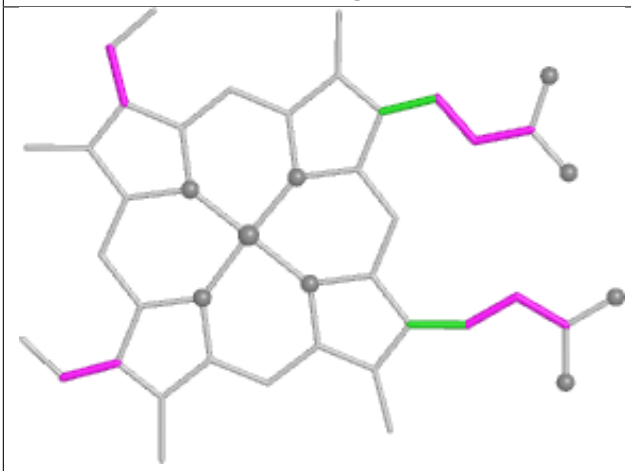
Ligand HEM E1 101



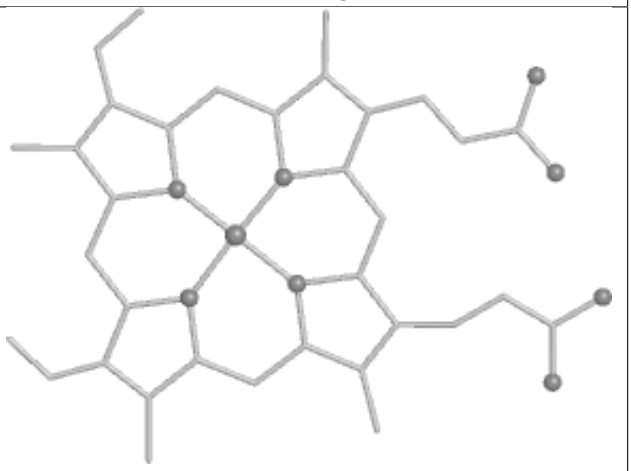
Bond lengths



Bond angles

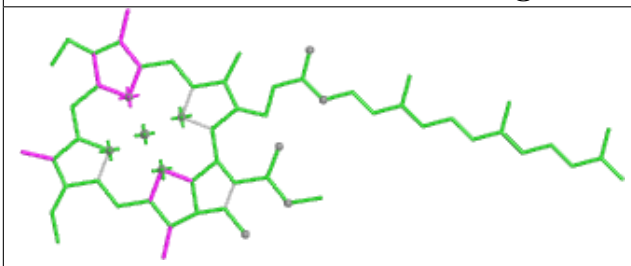


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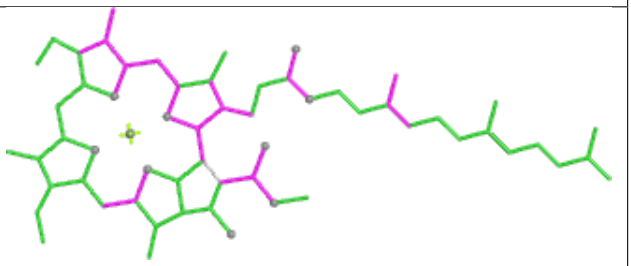


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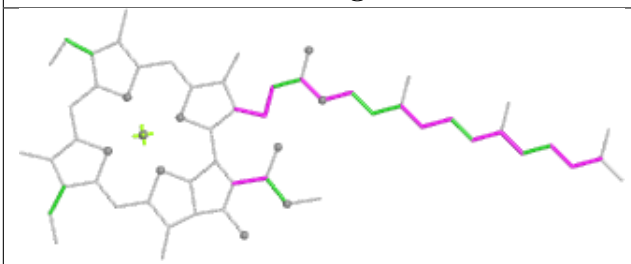
Ligand CLA aD 406



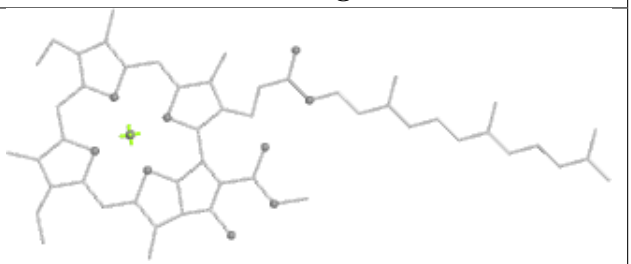
Bond lengths



Bond angles

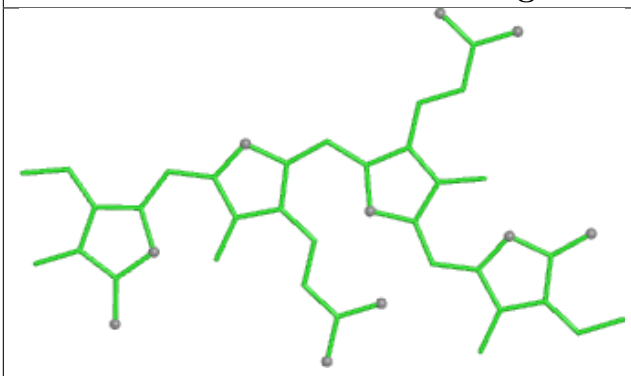


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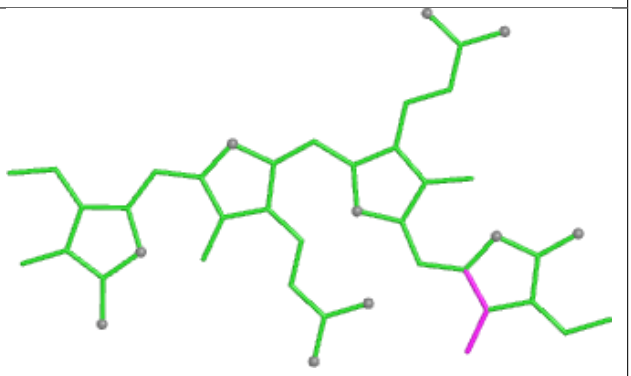


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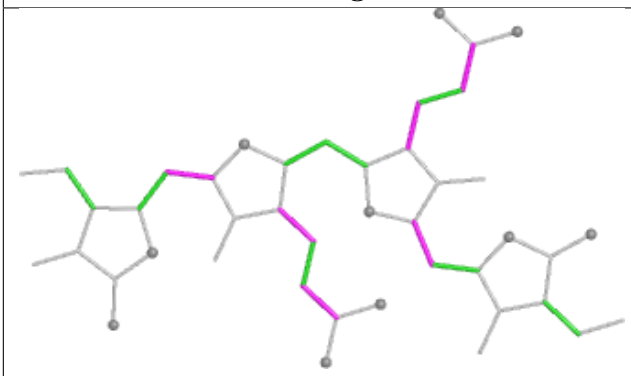
Ligand CYC cJ 202



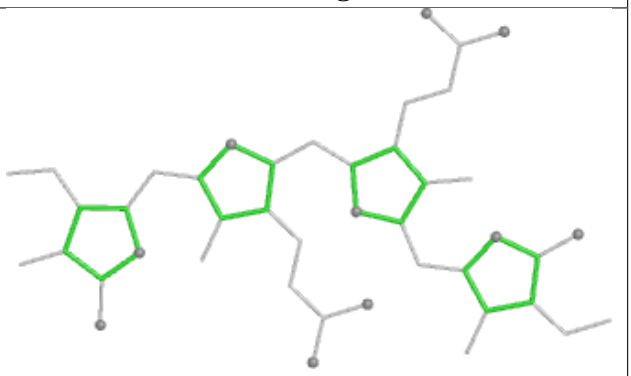
Bond lengths



Bond angles

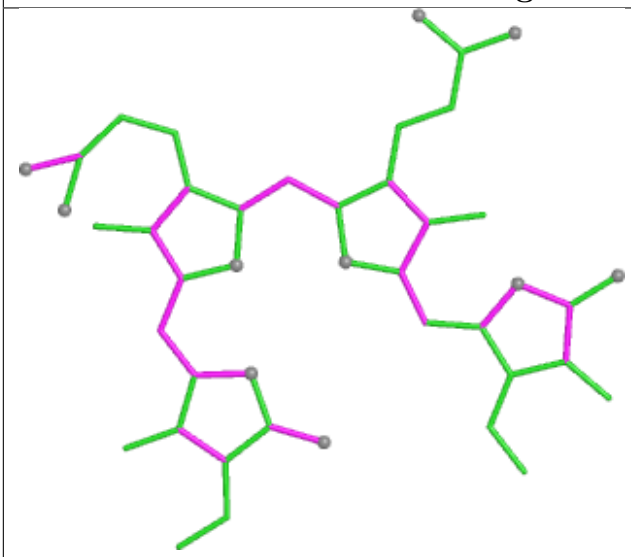


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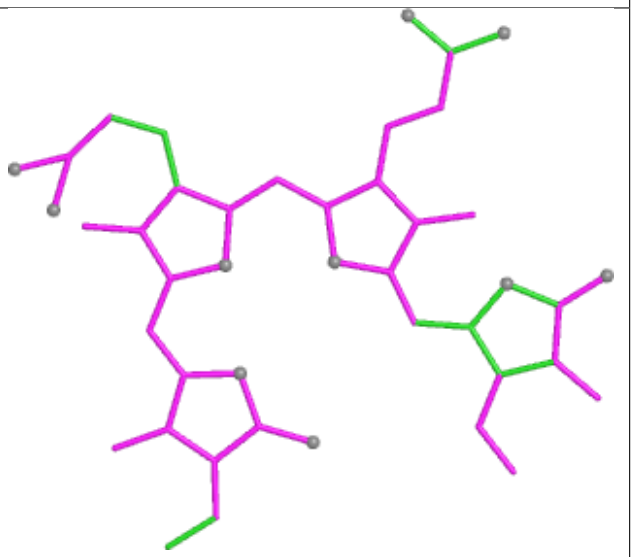


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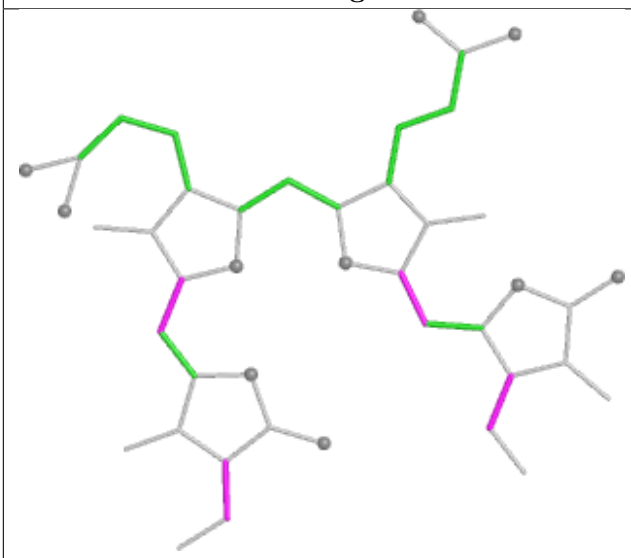
Ligand CYC iH 202



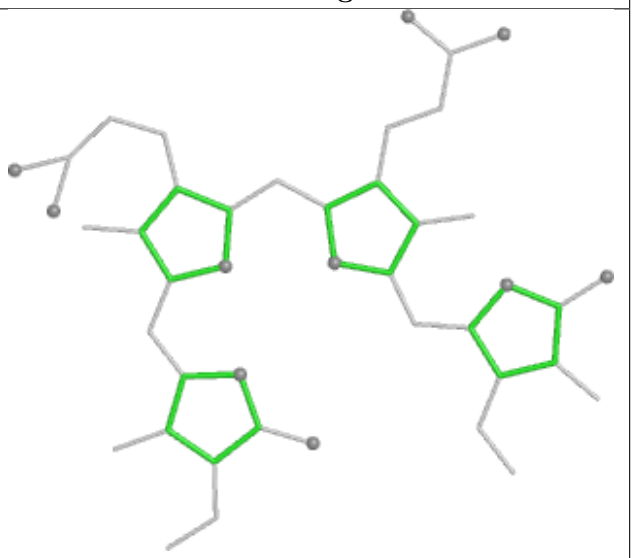
Bond lengths



Bond angles

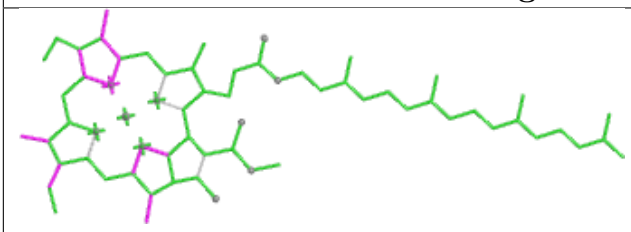


Torsions

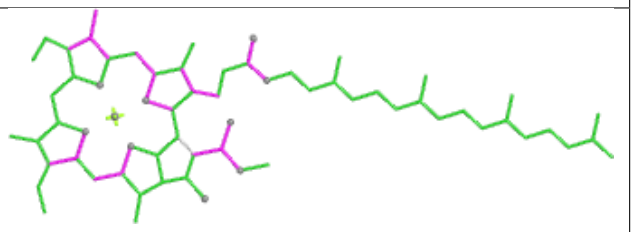


Rings

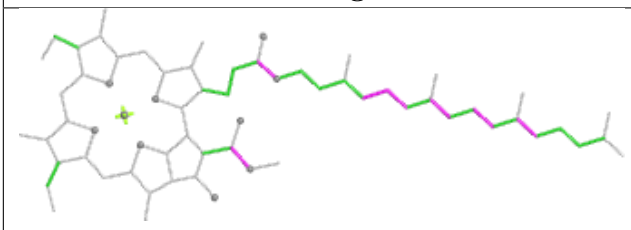
Ligand CLA b1 607



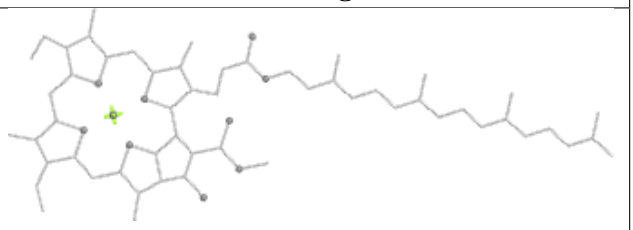
Bond lengths



Bond angles

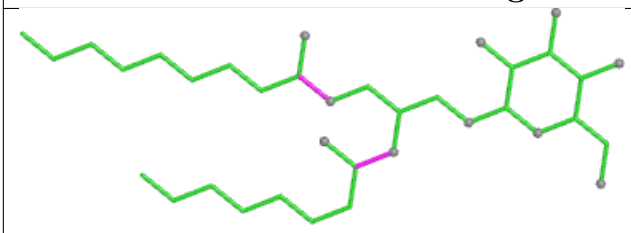


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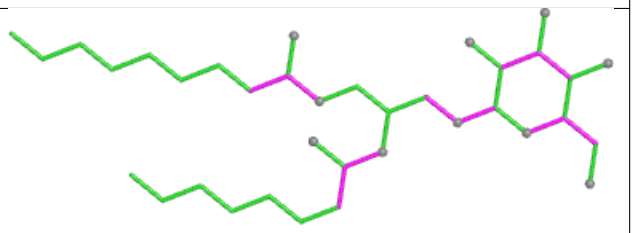


Rings

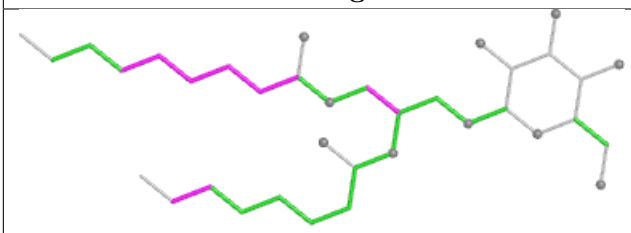
Ligand LMG AE 408



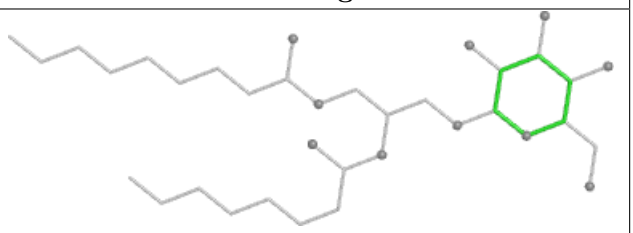
Bond lengths



Bond angles

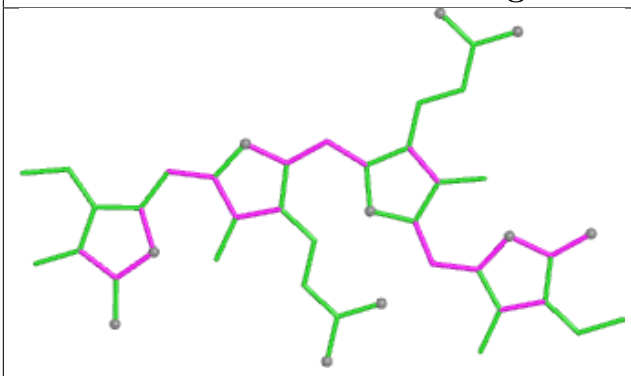


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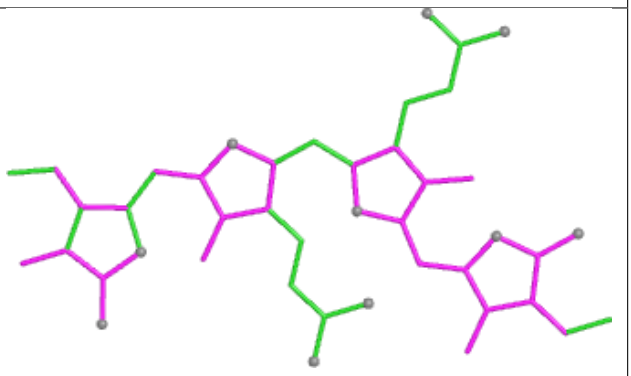


Rings

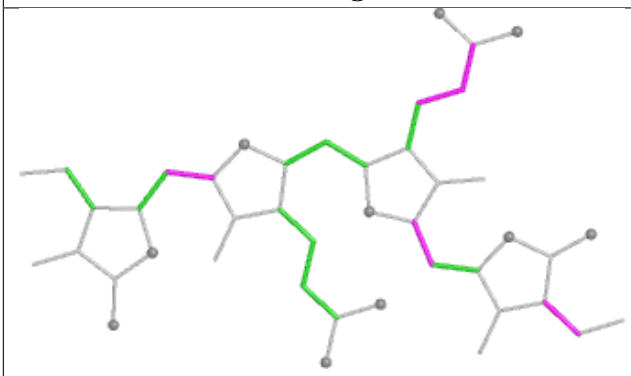
Ligand CYC KG 201



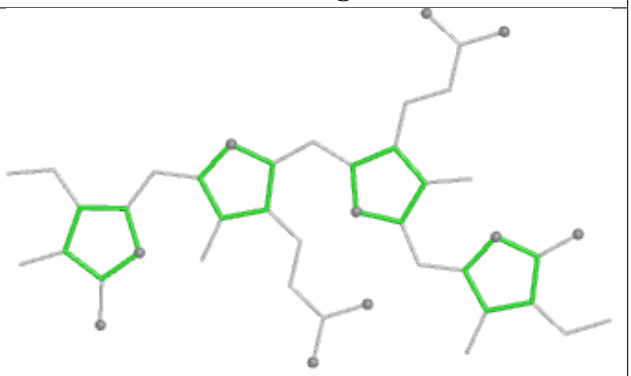
Bond lengths



Bond angles

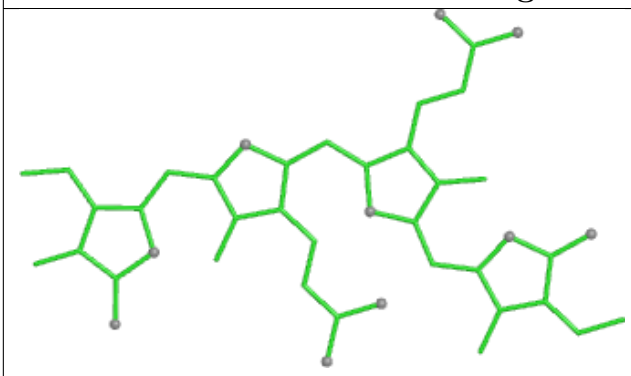


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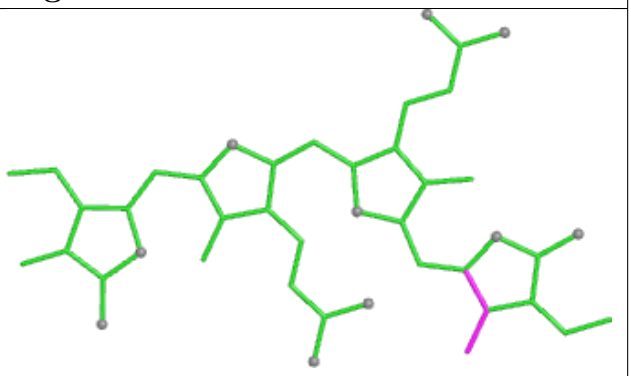


Rings

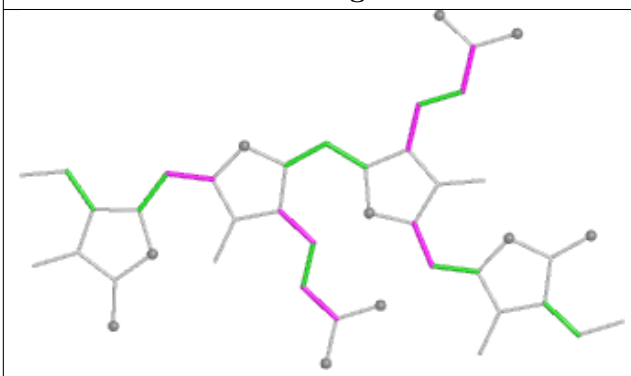
Ligand CYC g8 201



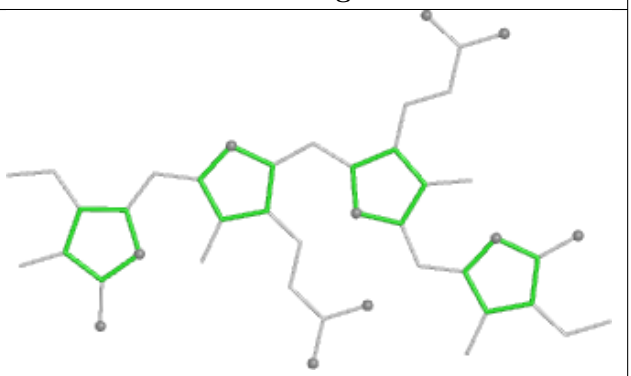
Bond lengths



Bond angles

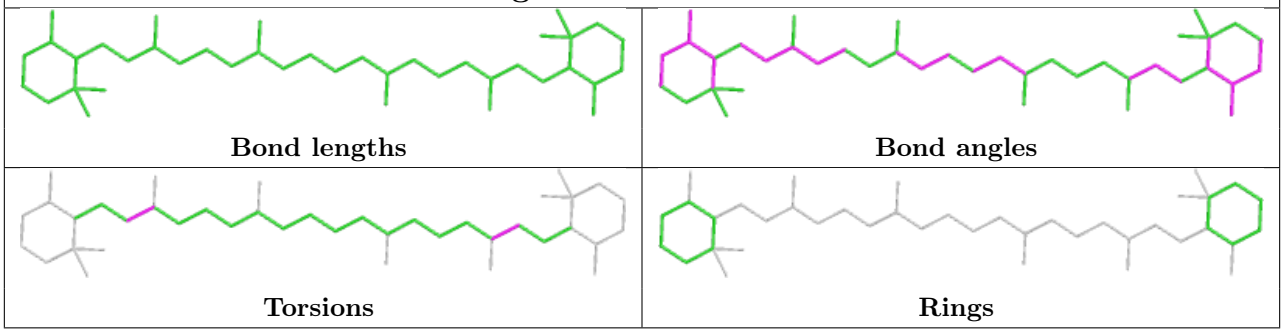


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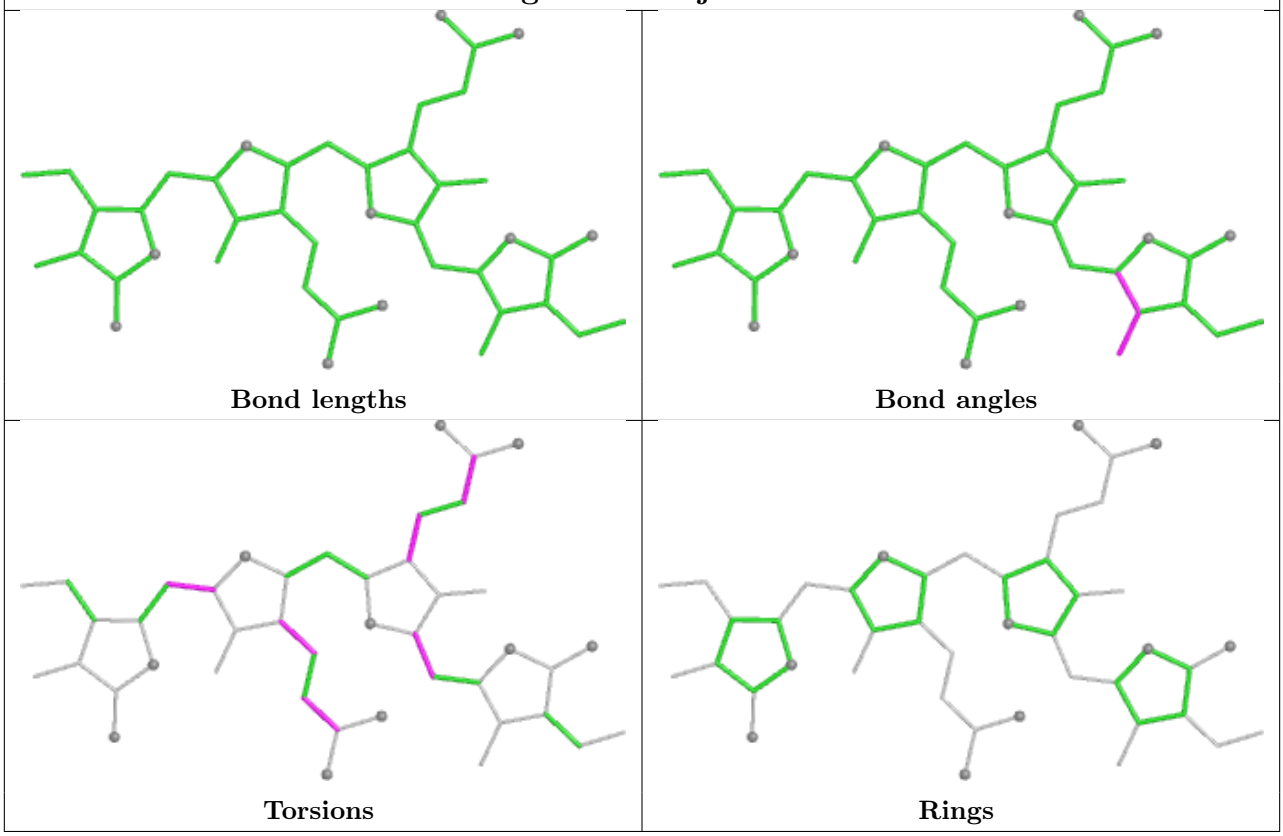


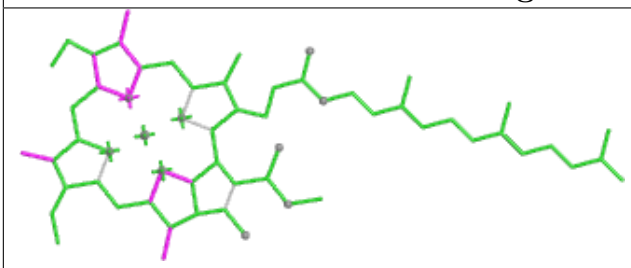
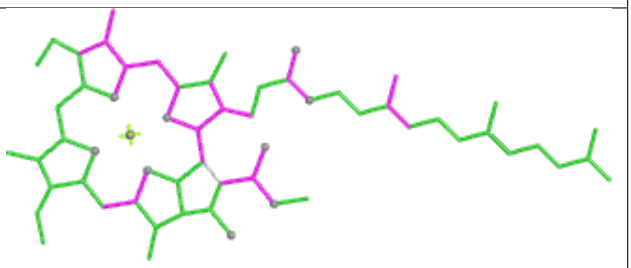
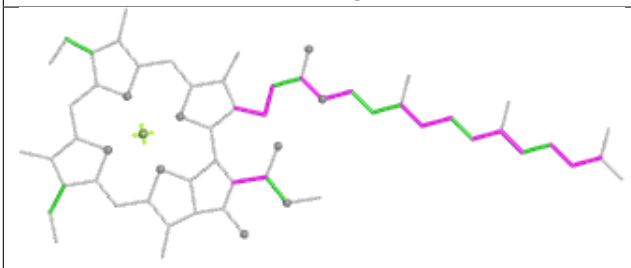
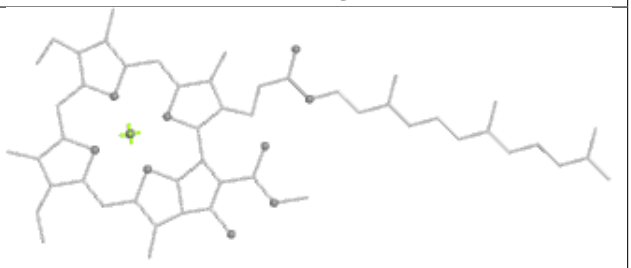
Rings

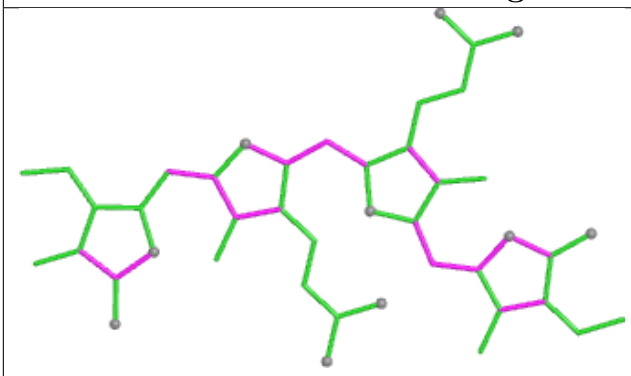
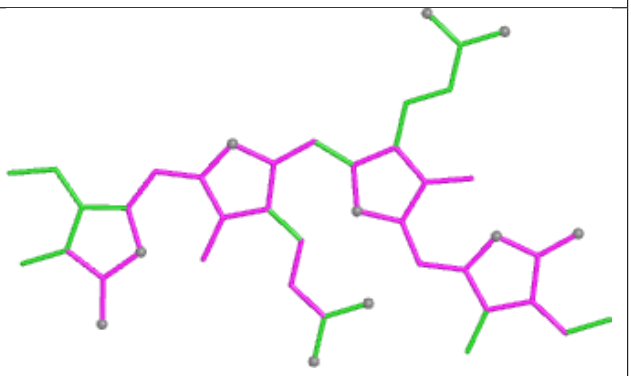
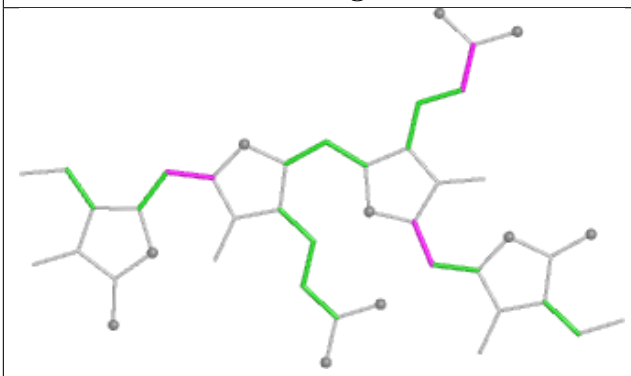
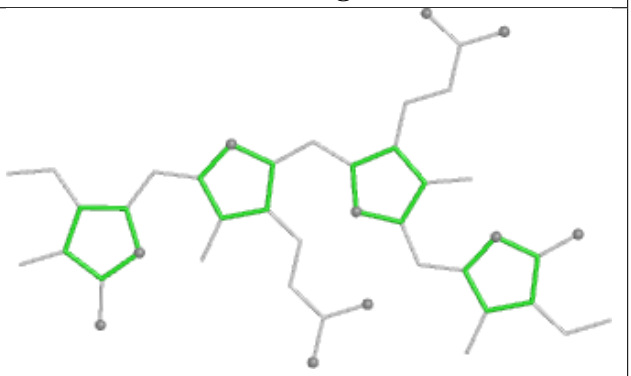
Ligand BCR BE 617



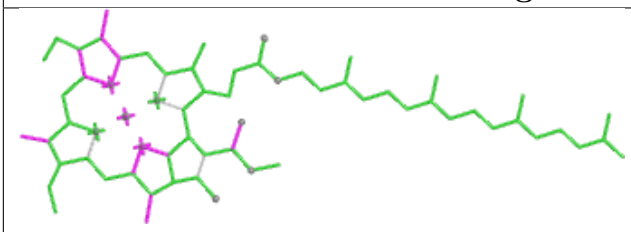
Ligand CYC jJ 202



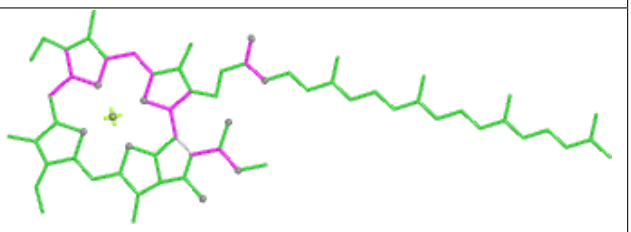
Ligand CLA aE 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CYC NG 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

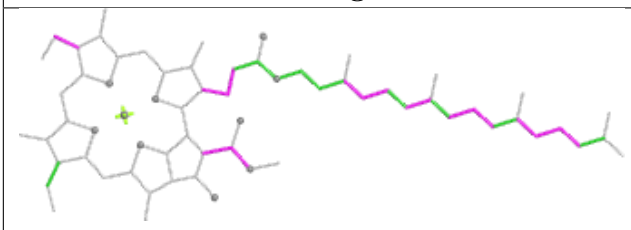
Ligand CLA bE 605



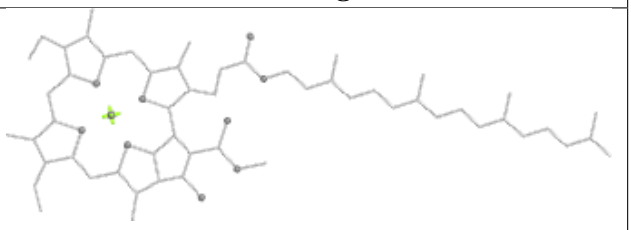
Bond lengths



Bond angles

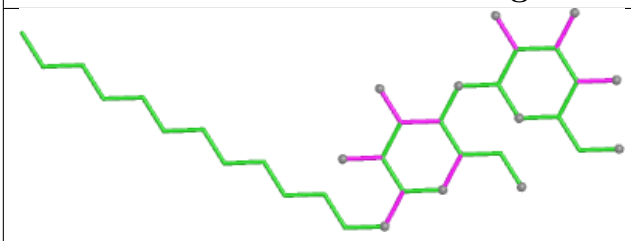


Torsions

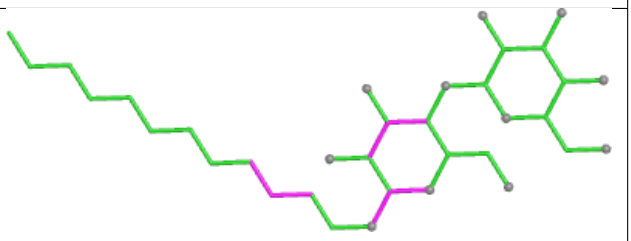


Rings

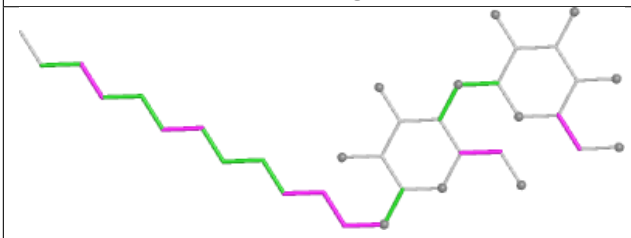
Ligand LMT bD 601



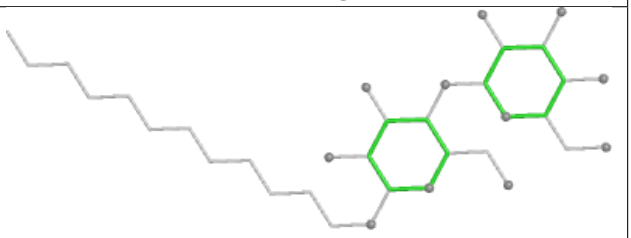
Bond lengths



Bond angles

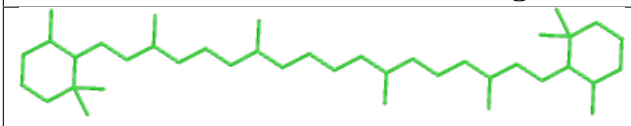


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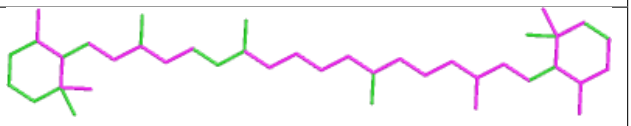


Rings

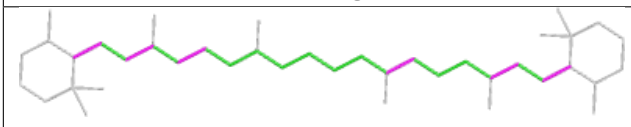
Ligand BCR CE 516



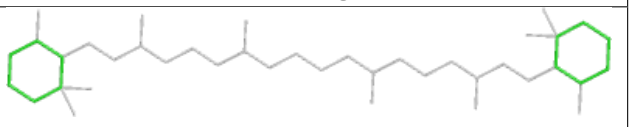
Bond lengths



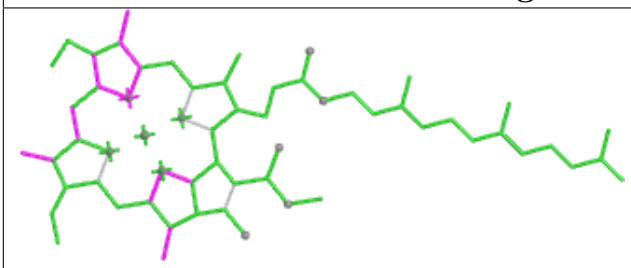
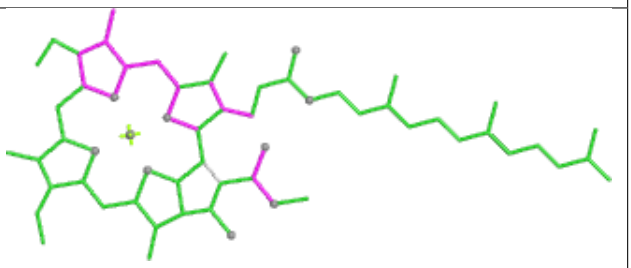
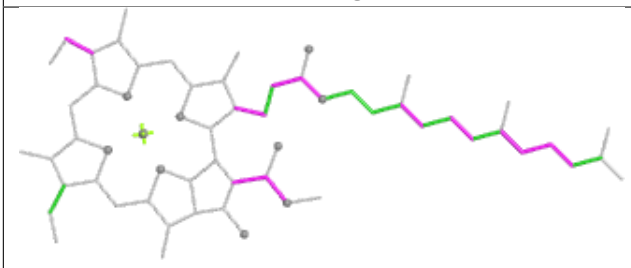
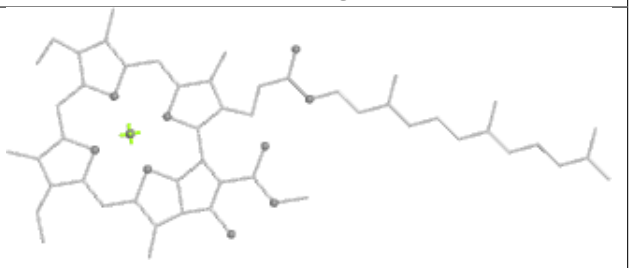
Bond angles

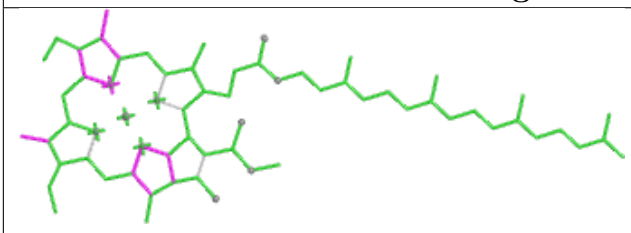
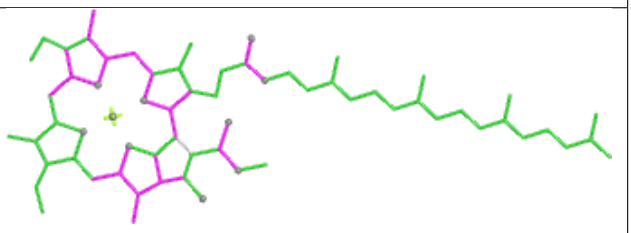
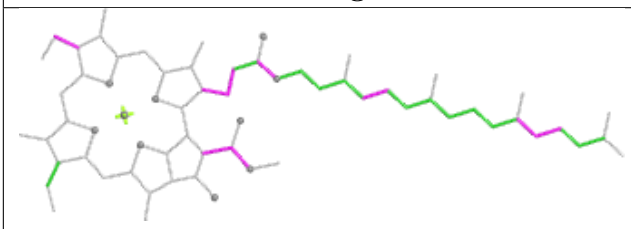
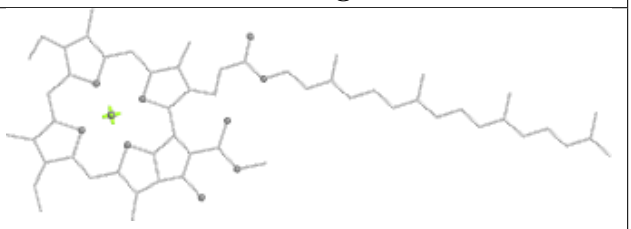


Torsions

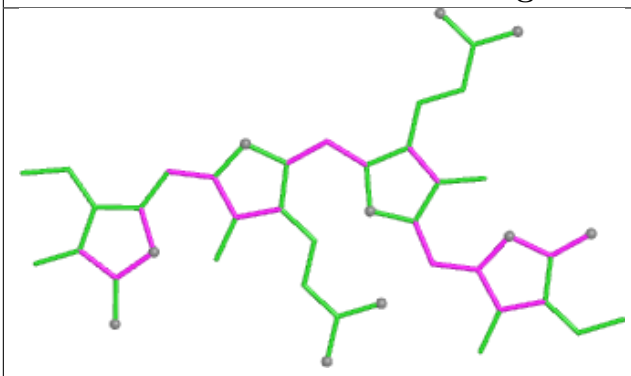


Rings

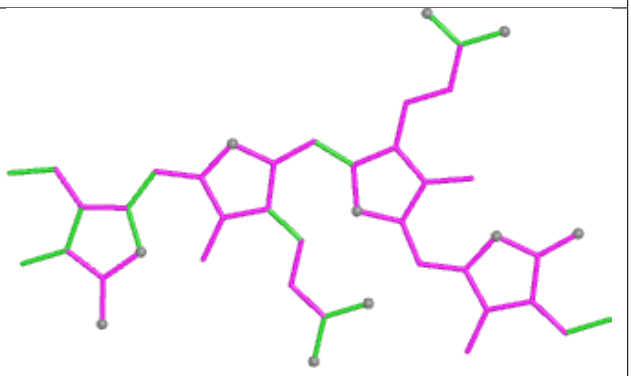
Ligand CLA ID 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA CE 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

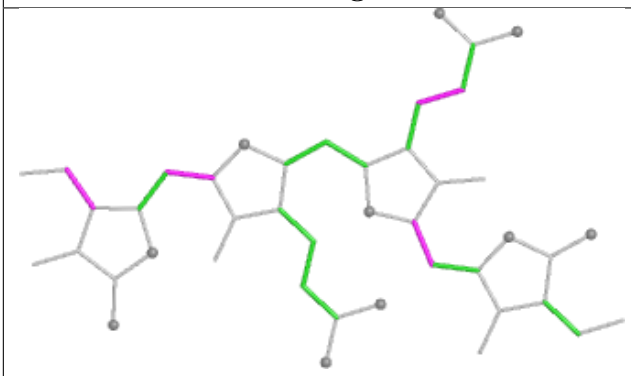
Ligand CYC v4 201



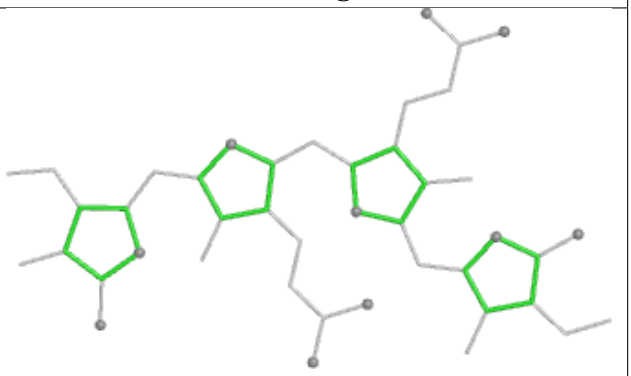
Bond lengths



Bond angles

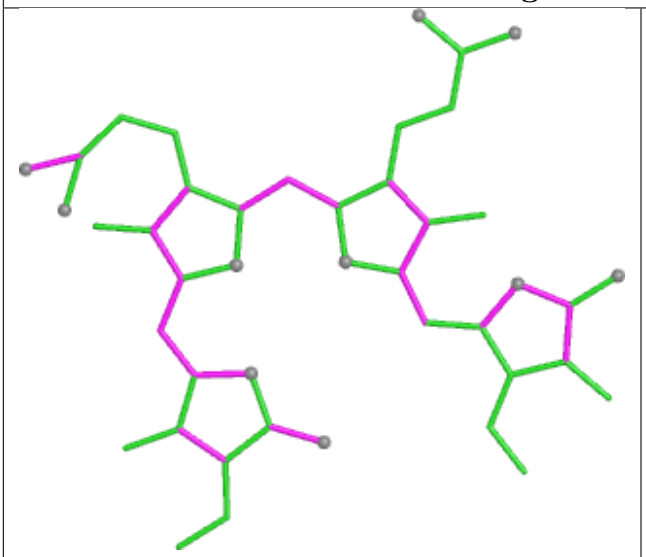


Torsions

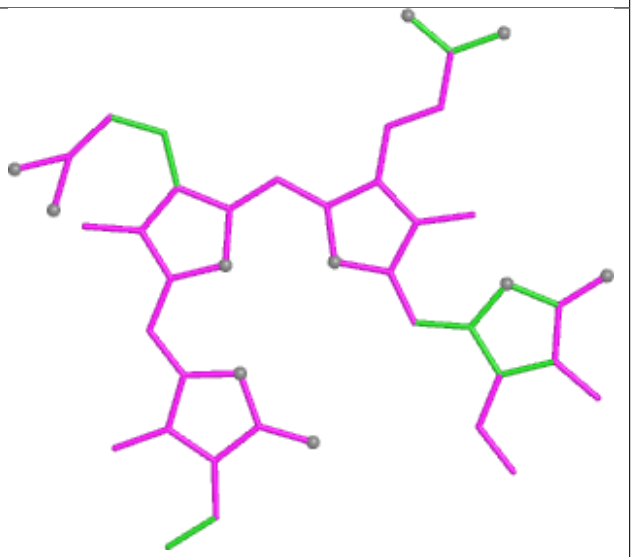


Rings

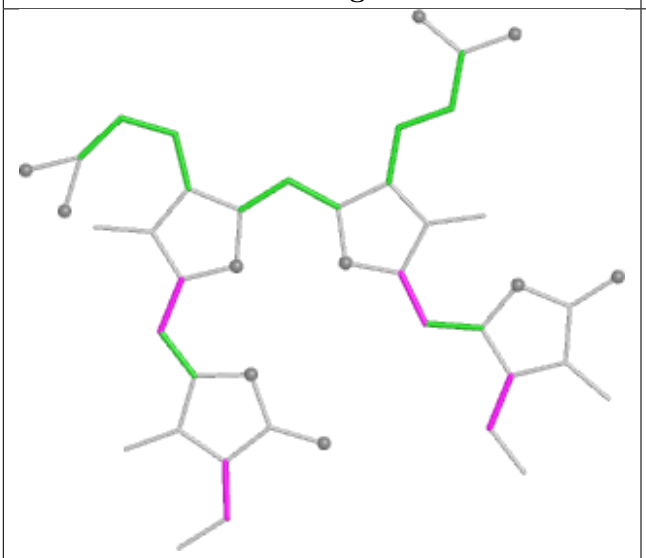
Ligand CYC i3 202



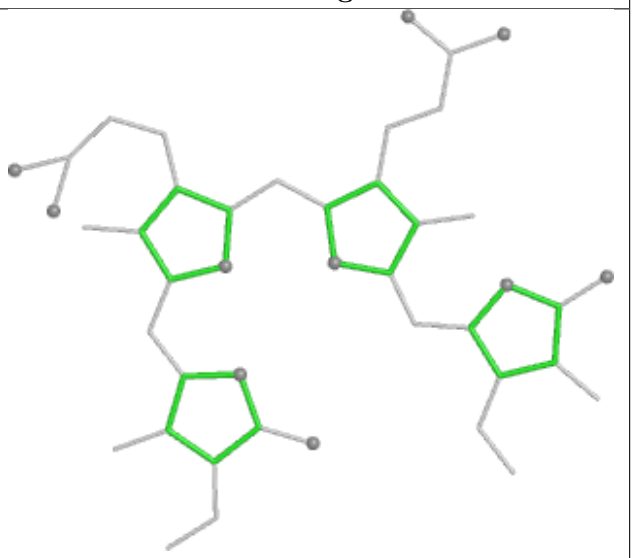
Bond lengths



Bond angles



Torsions

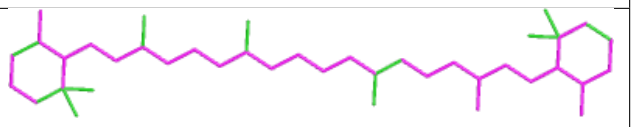


Rings

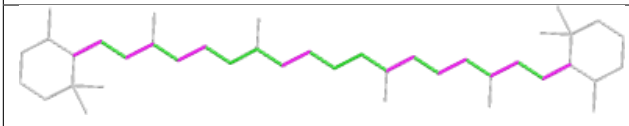
Ligand BCR cE 515



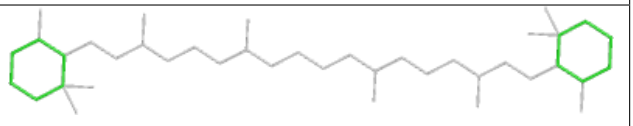
Bond lengths



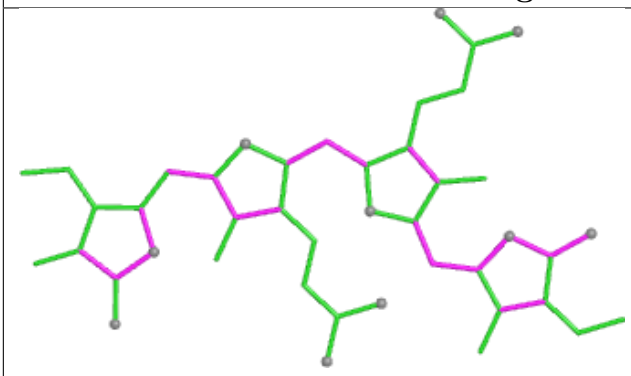
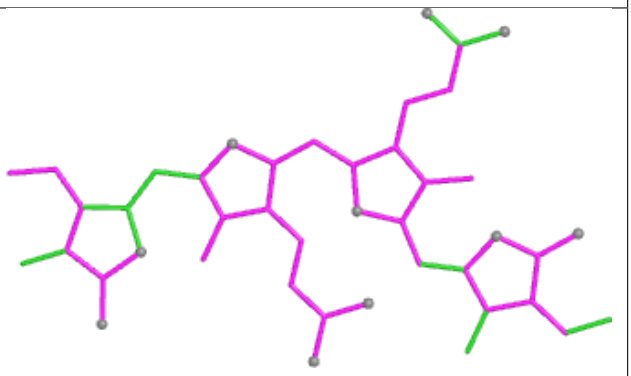
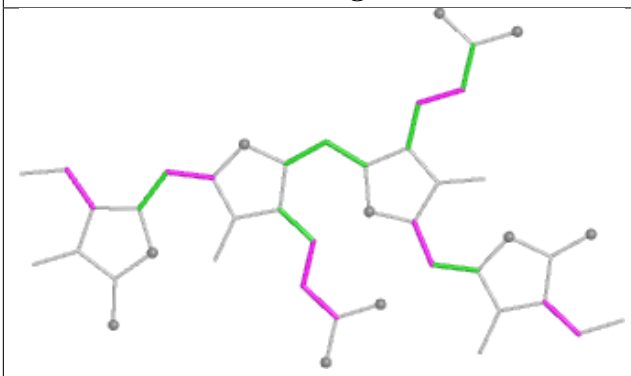
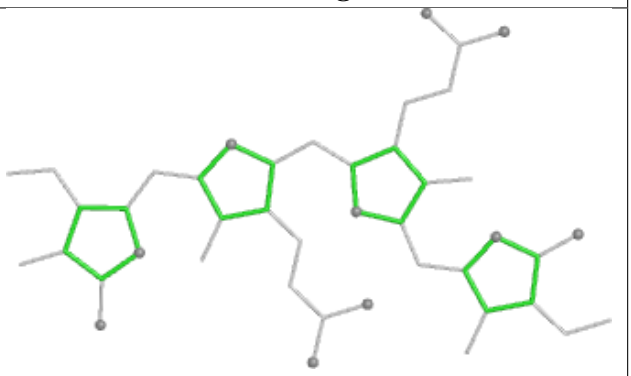
Bond angles

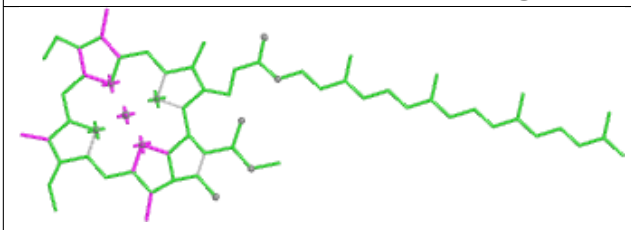
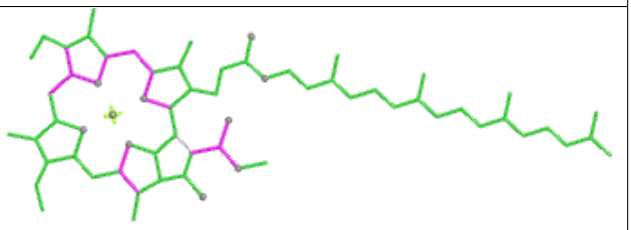
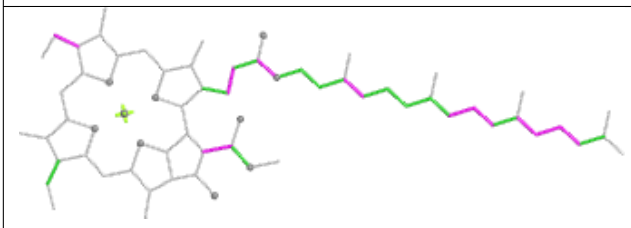
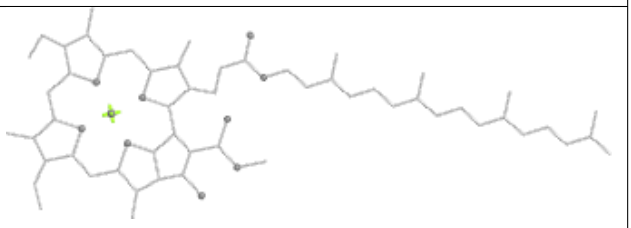


Torsions

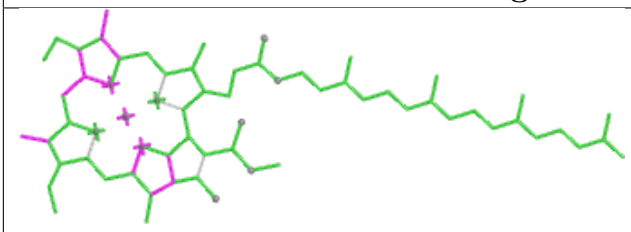


Rings

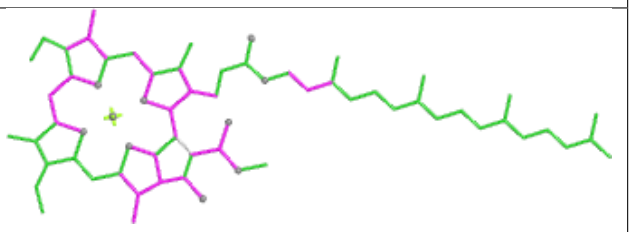
Ligand CYC d5 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA bE 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

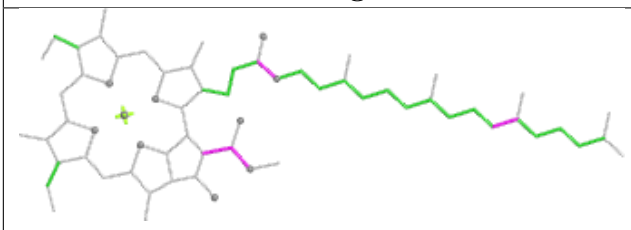
Ligand CLA CD 510



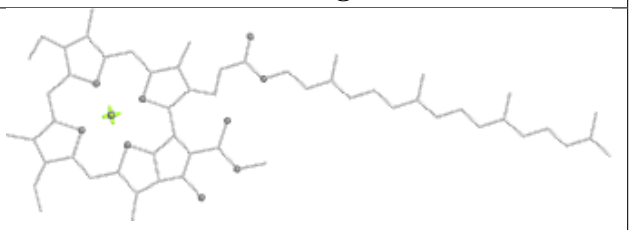
Bond lengths



Bond angles

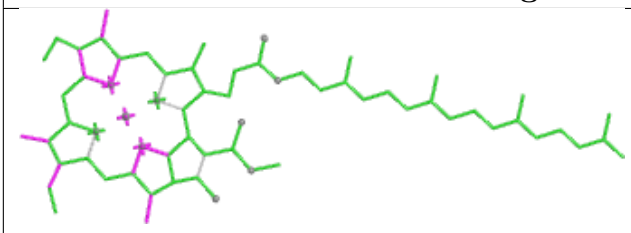


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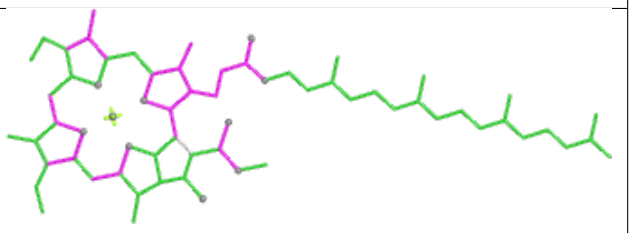


Rings

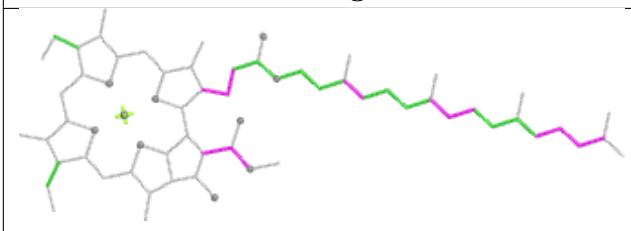
Ligand CLA c1 505



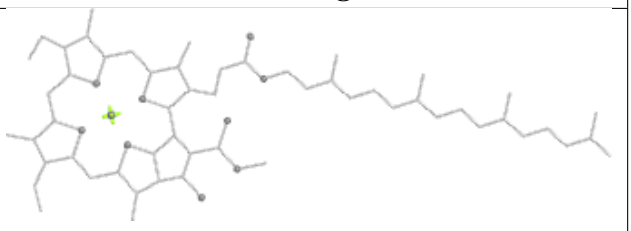
Bond lengths



Bond angles

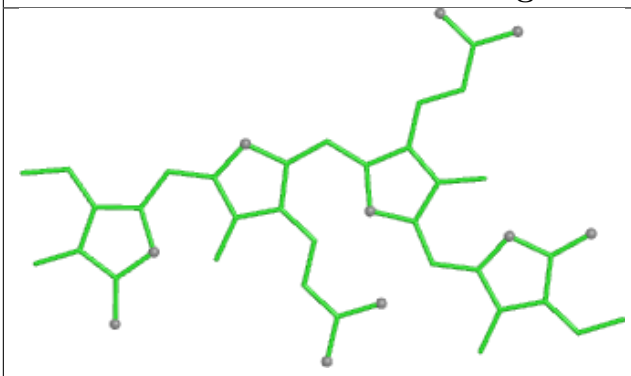


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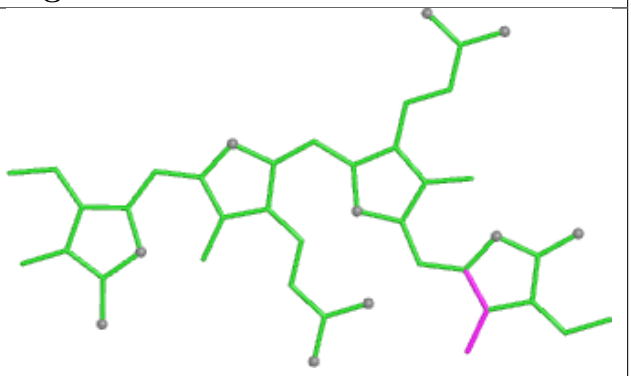


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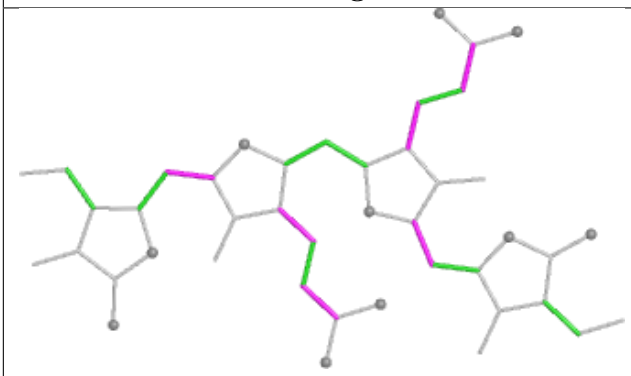
Ligand CYC gJ 201



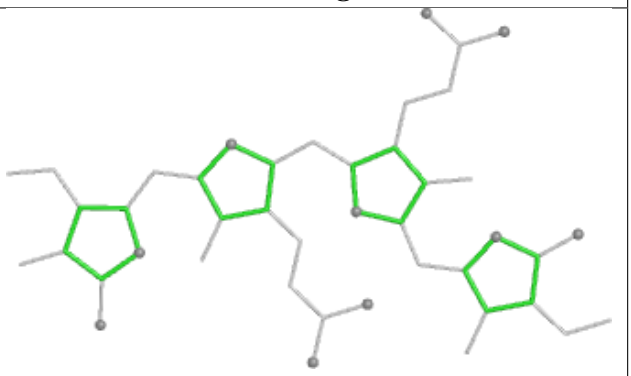
Bond lengths



Bond angles

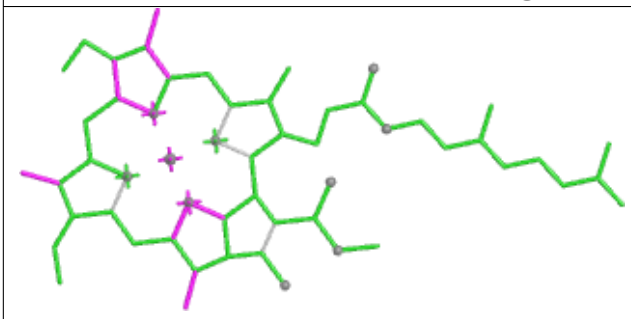


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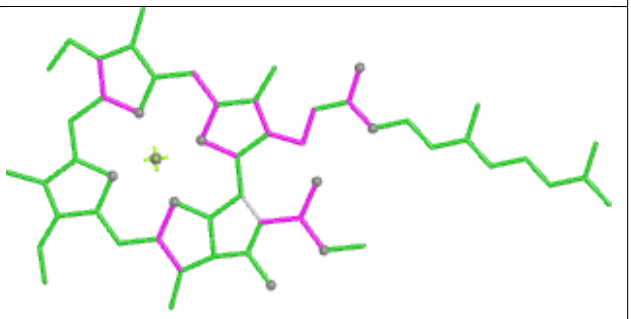


Rings

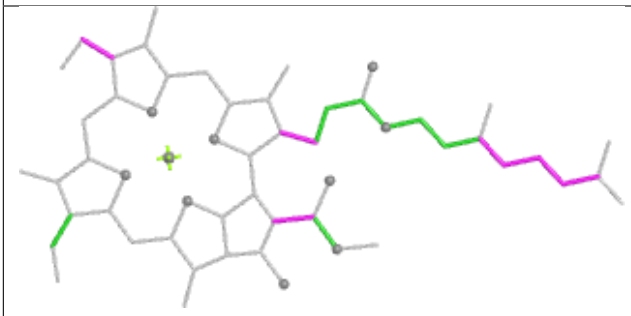
Ligand CLA iD 101



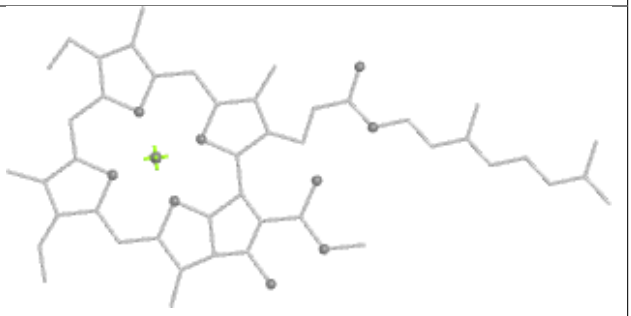
Bond lengths



Bond angles

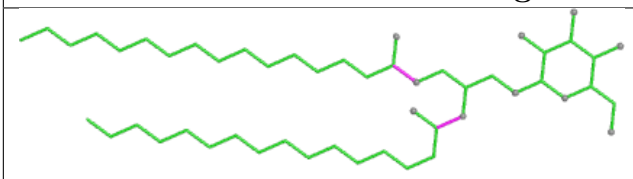


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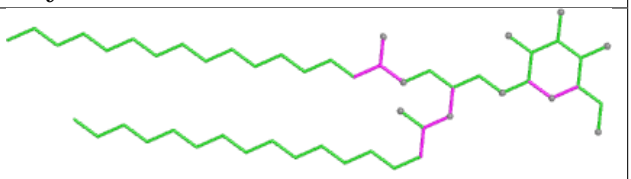


Rings

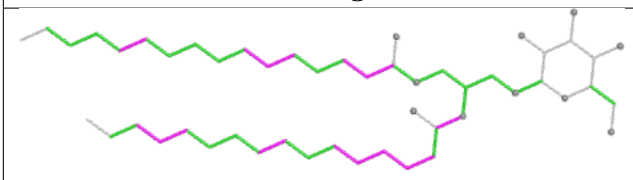
Ligand LMG y1 101



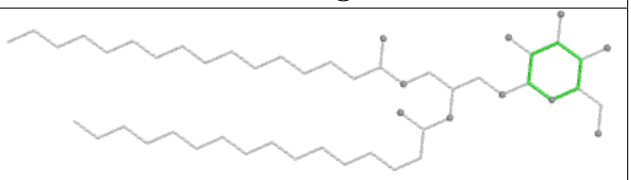
Bond lengths



Bond angles

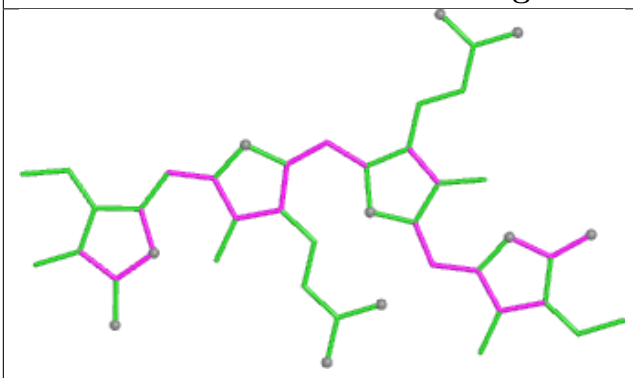


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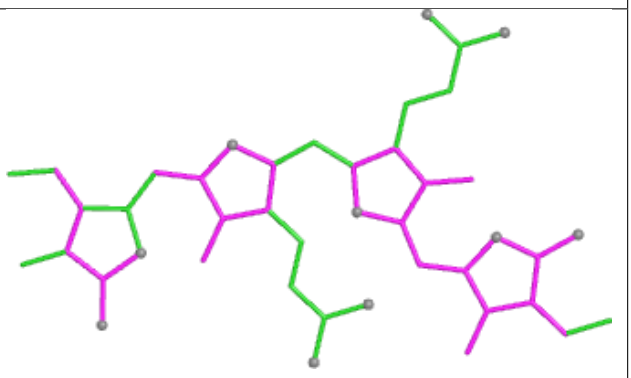


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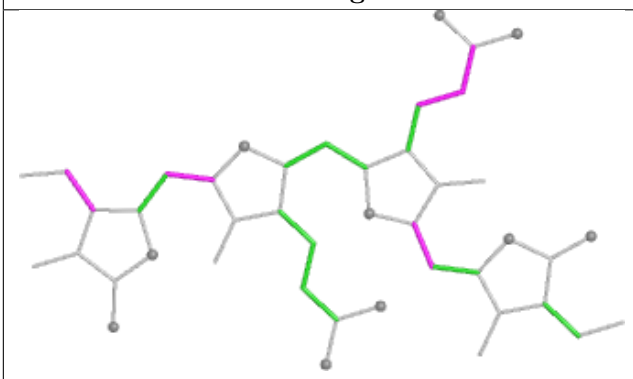
Ligand CYC O4 201



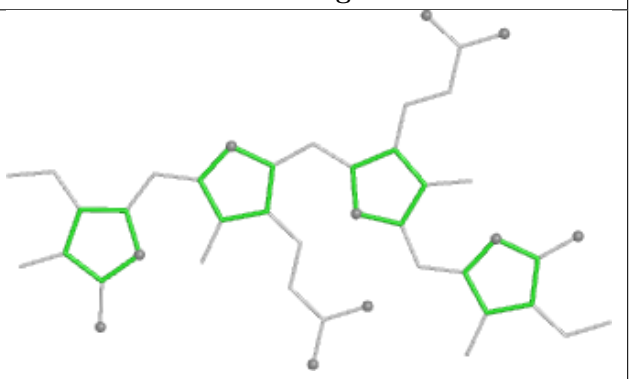
Bond lengths



Bond angles

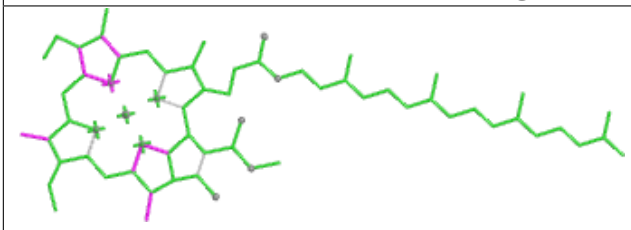


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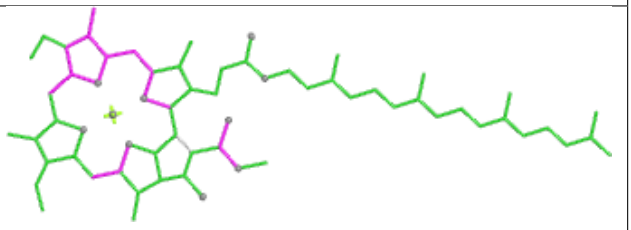


Rings

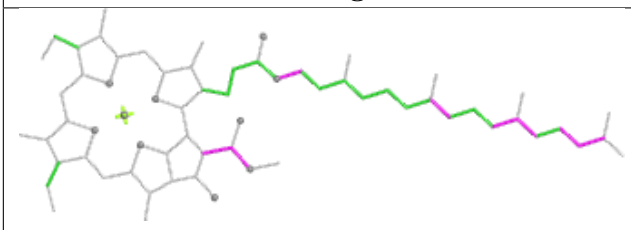
Ligand CLA dD 403



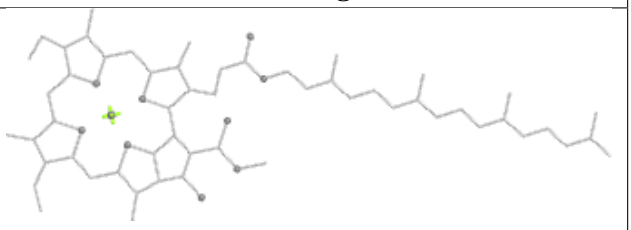
Bond lengths



Bond angles



Torsions



Rings

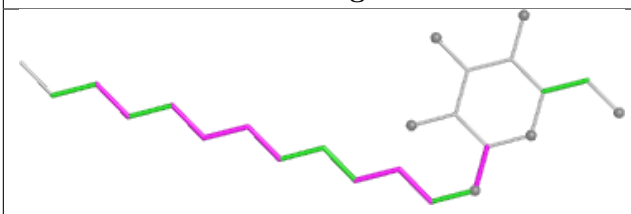
Ligand LMT DE 404



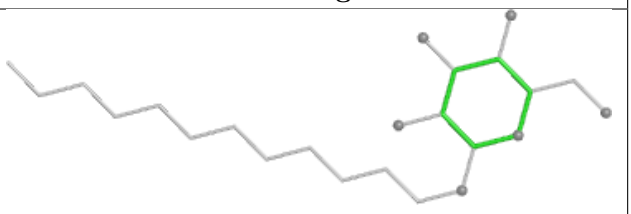
Bond lengths



Bond angles

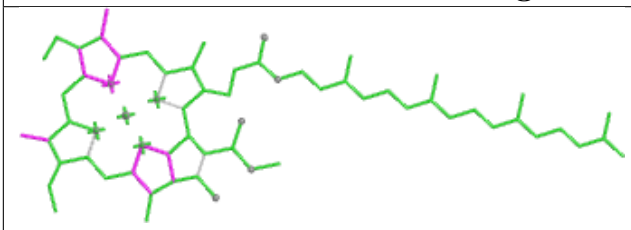


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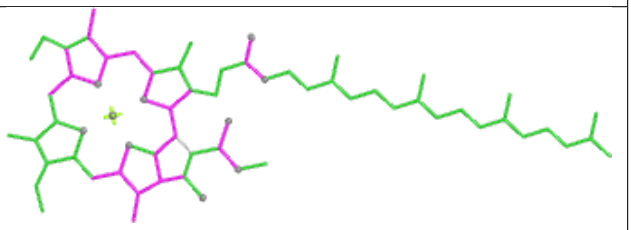


Rings

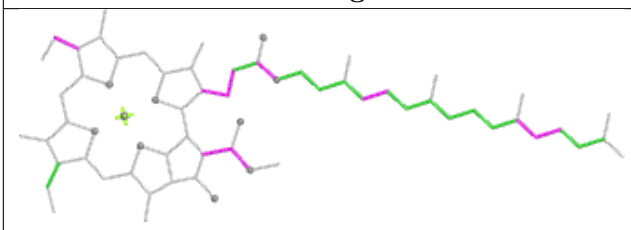
Ligand CLA C1 508



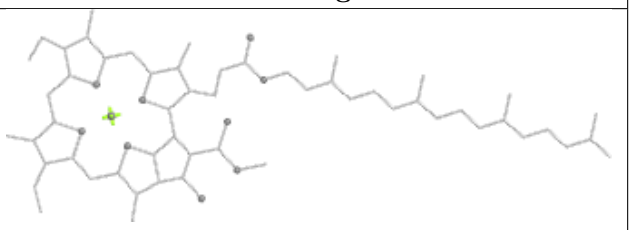
Bond lengths



Bond angles

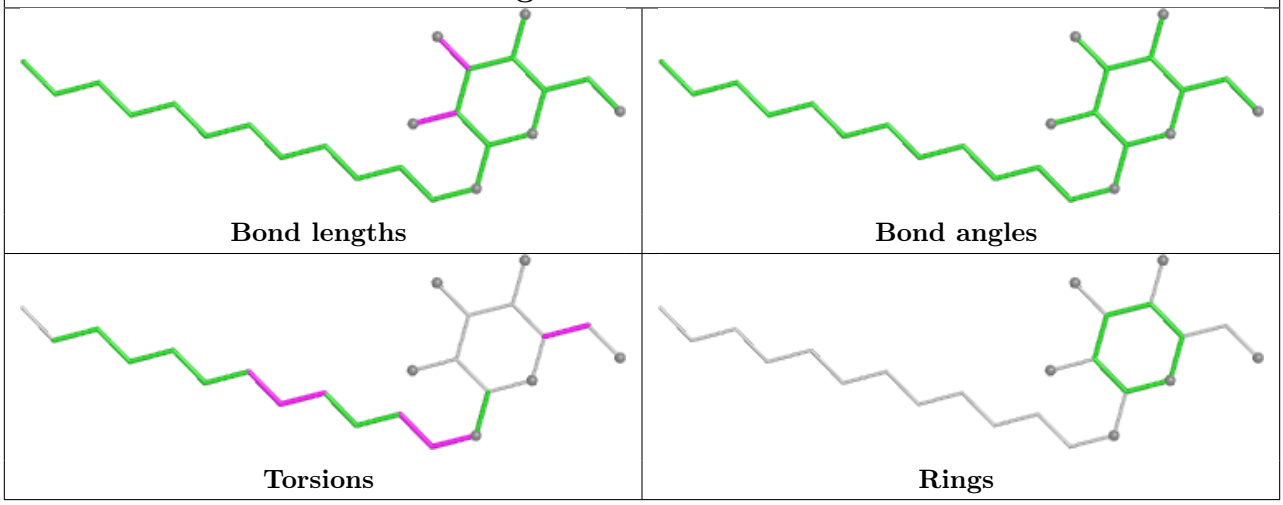


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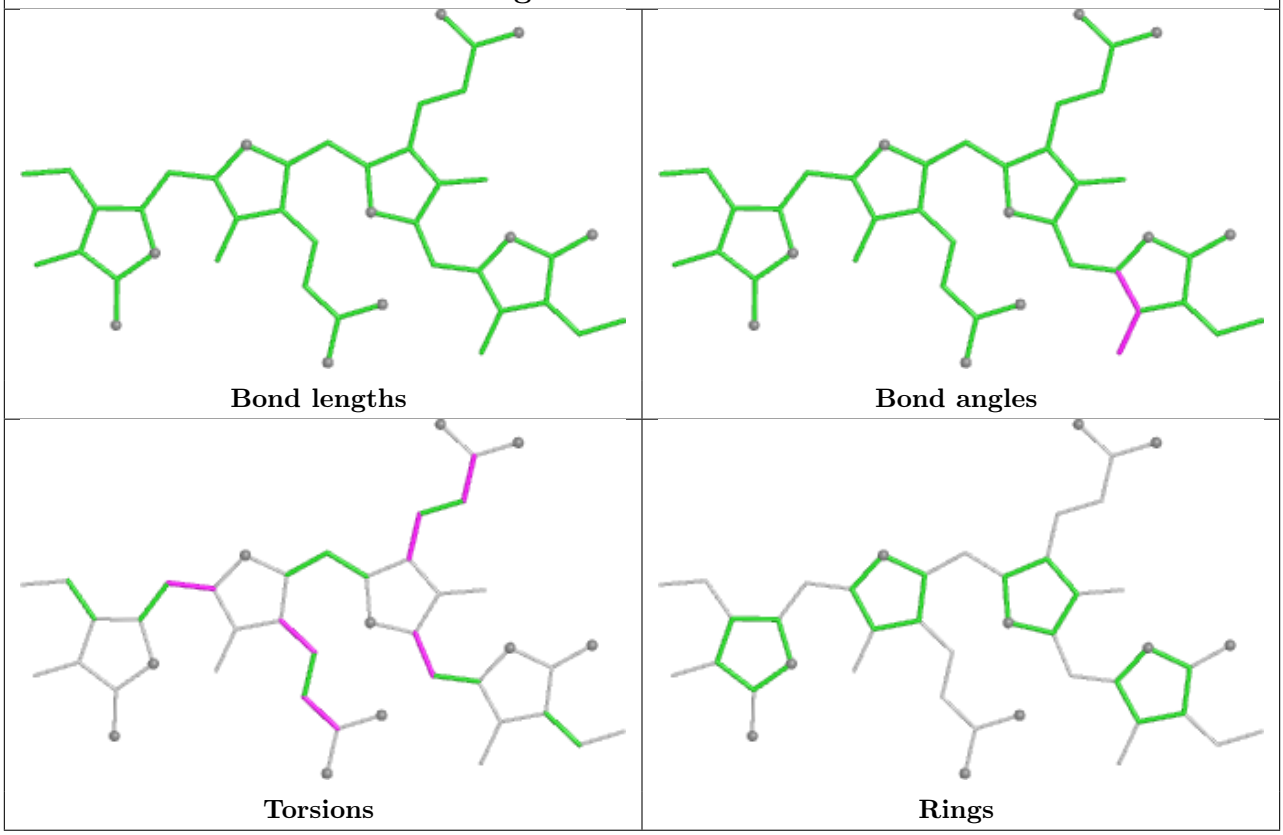


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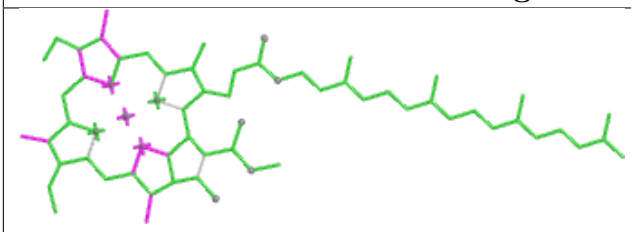
Ligand LMT b1 602



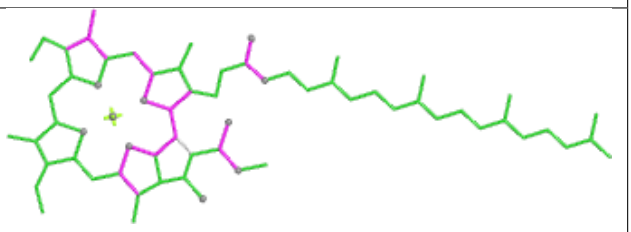
Ligand CYC cH 202



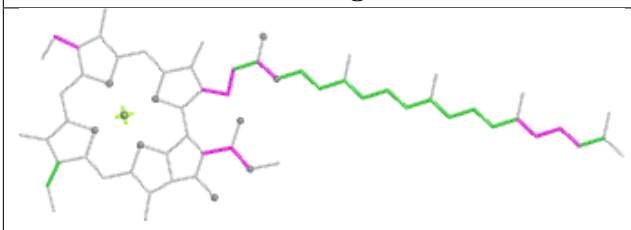
Ligand CLA bD 609



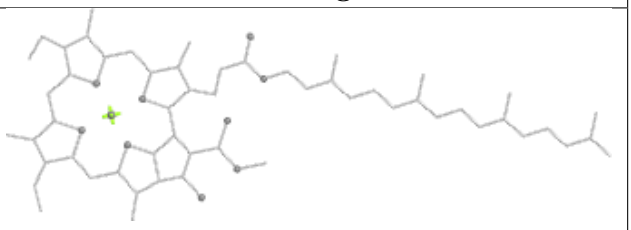
Bond lengths



Bond angles

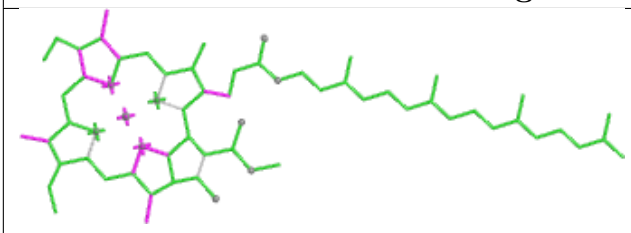


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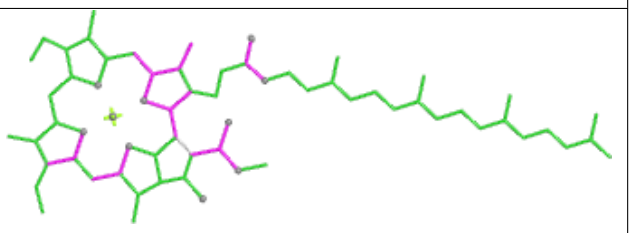


Rings

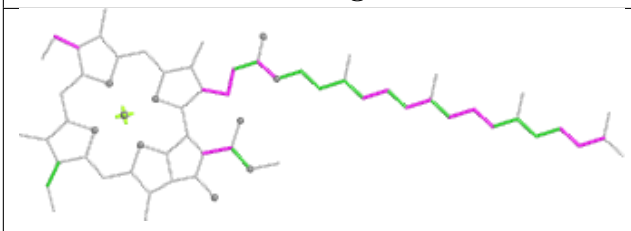
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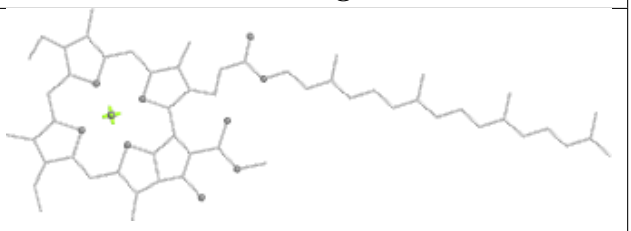
Bond lengths



Bond angles

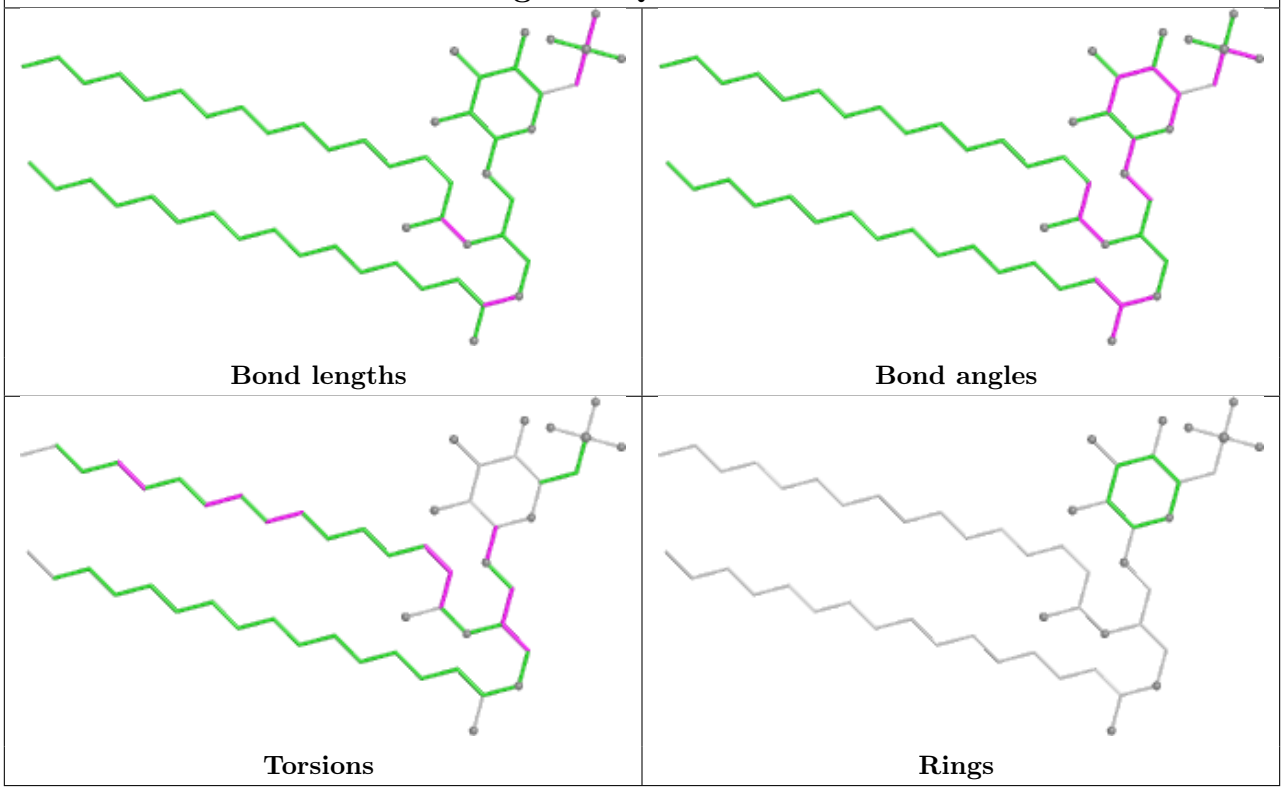


Torsions

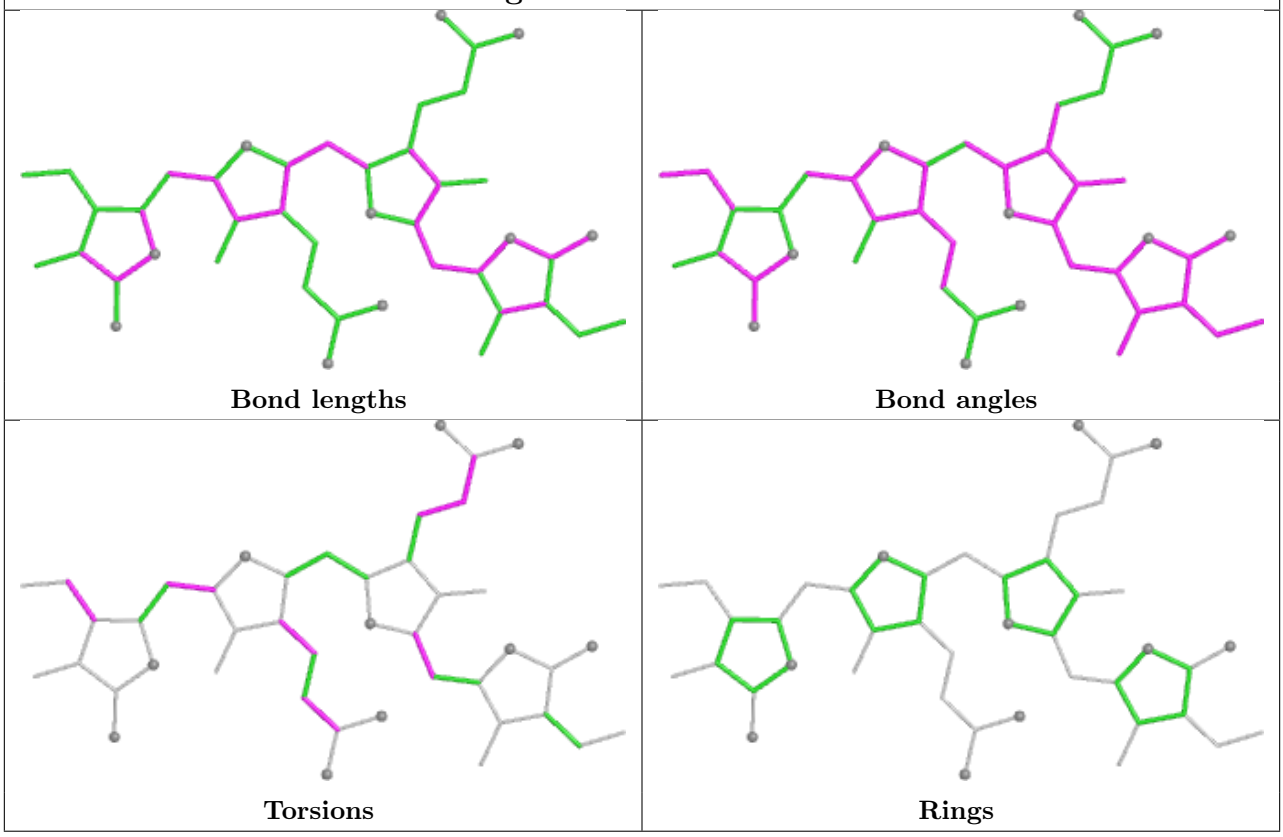


Rings

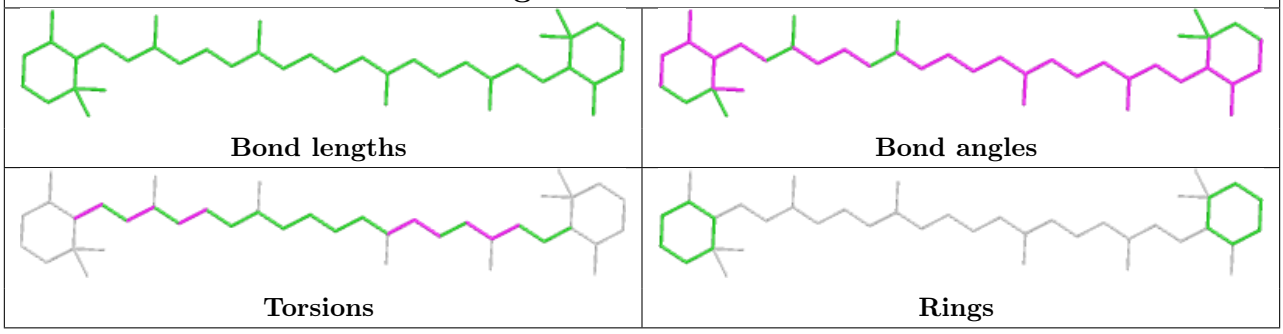
Ligand SQD CE 501



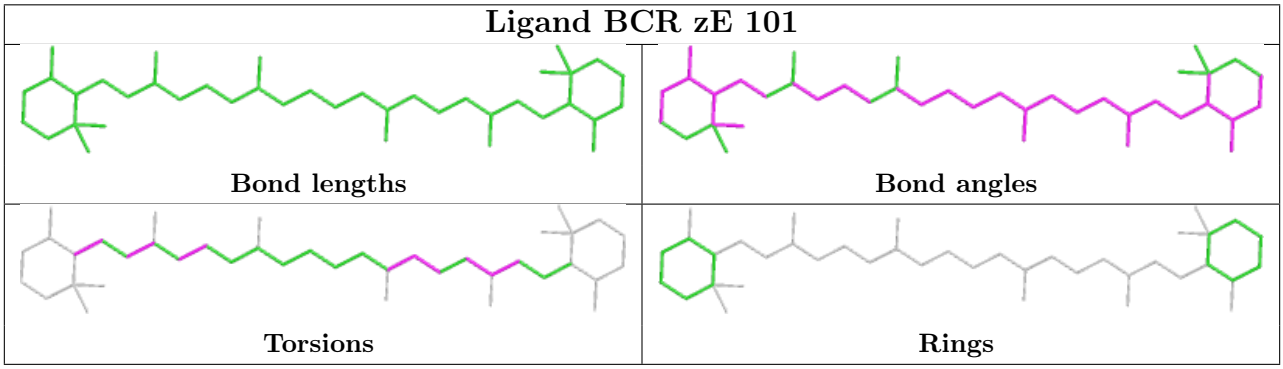
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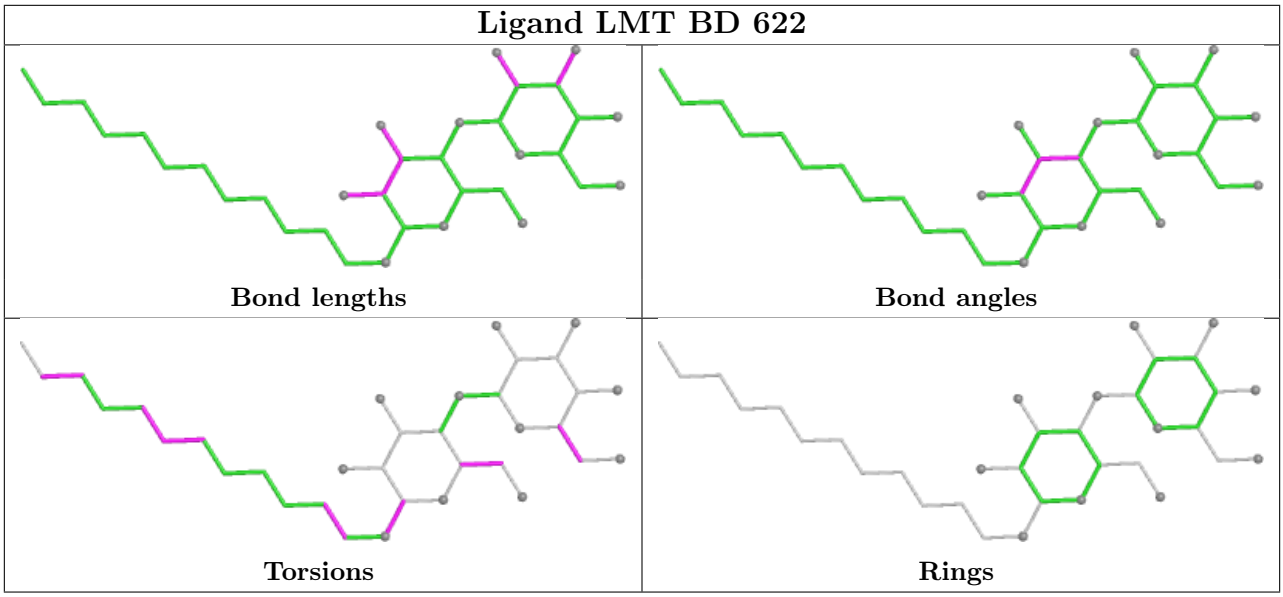
Ligand BCR ZE 101



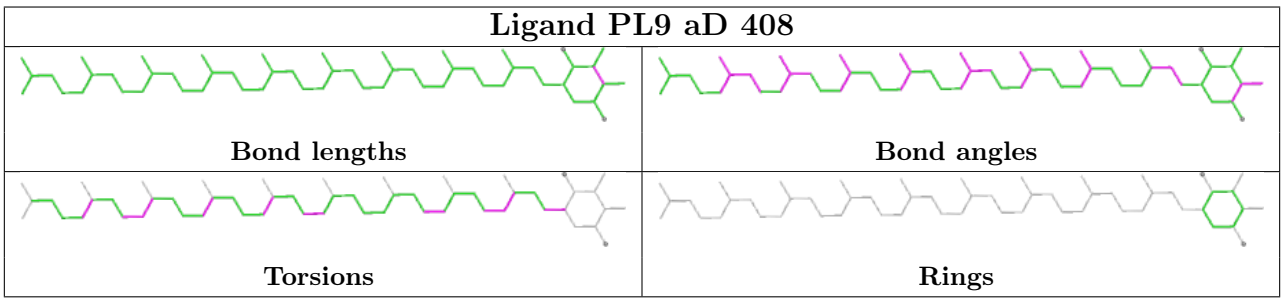
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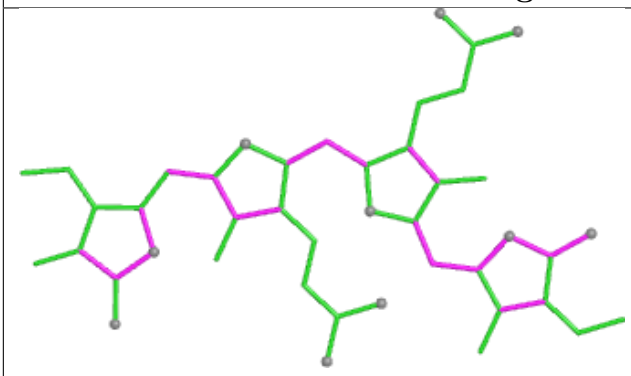
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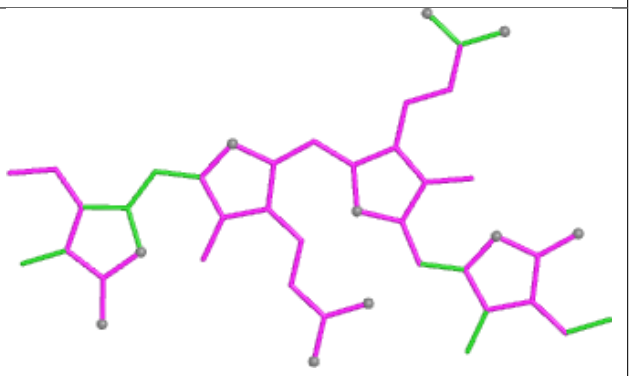
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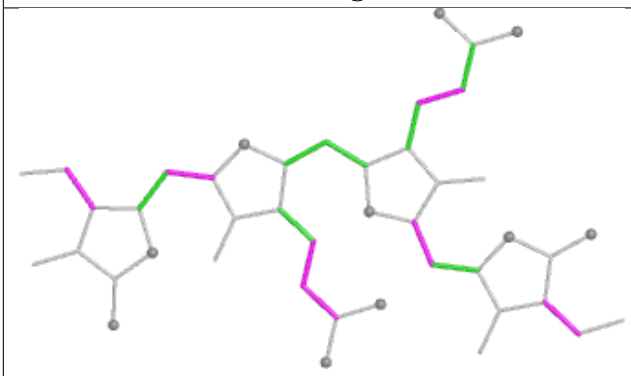
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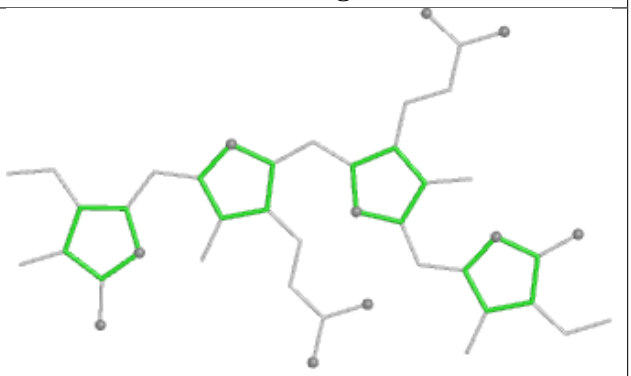
Bond lengths



Bond angles

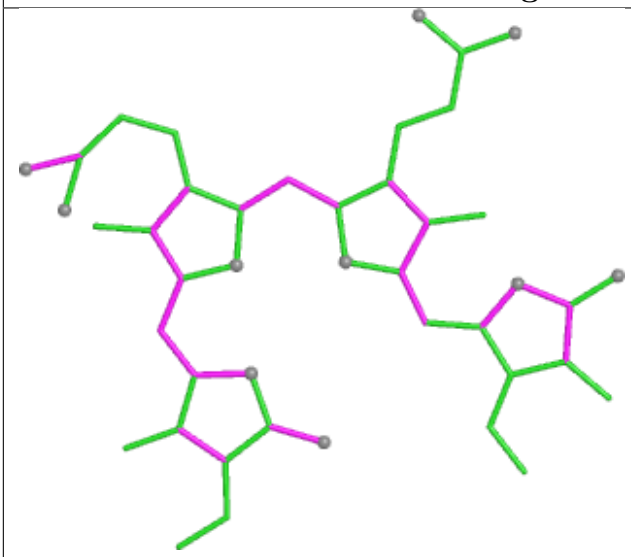


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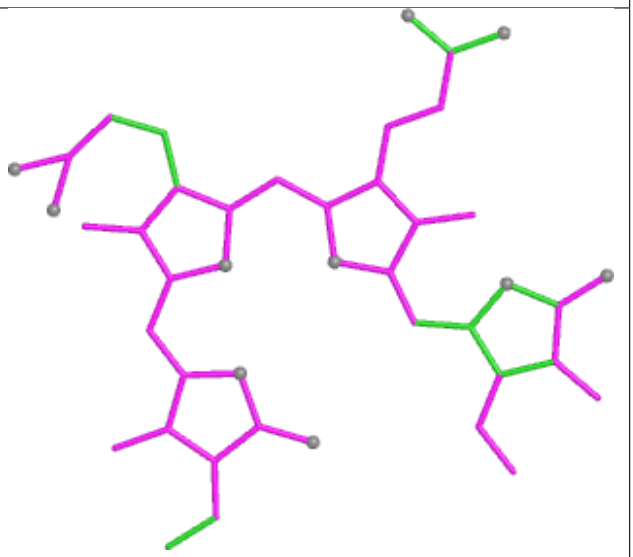


Rings

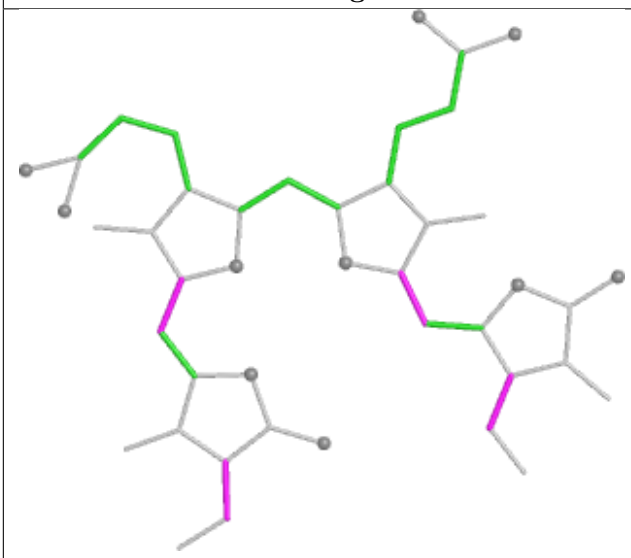
Ligand CYC i7 202



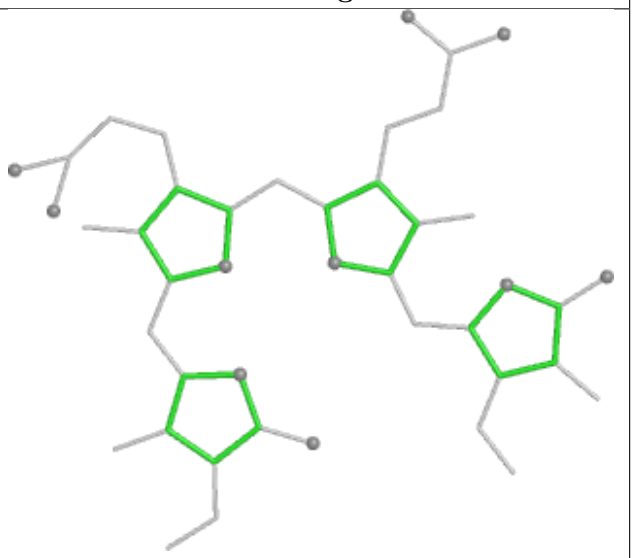
Bond lengths



Bond angles

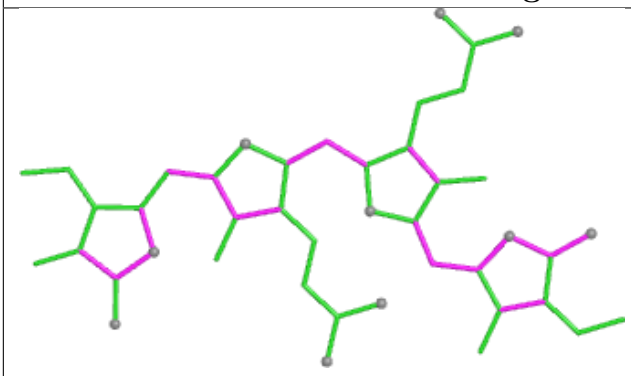


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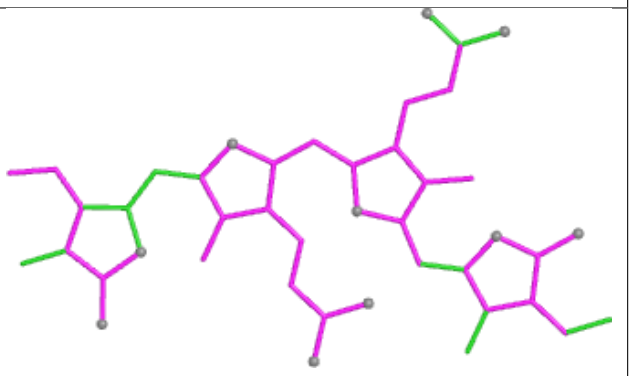


Rings

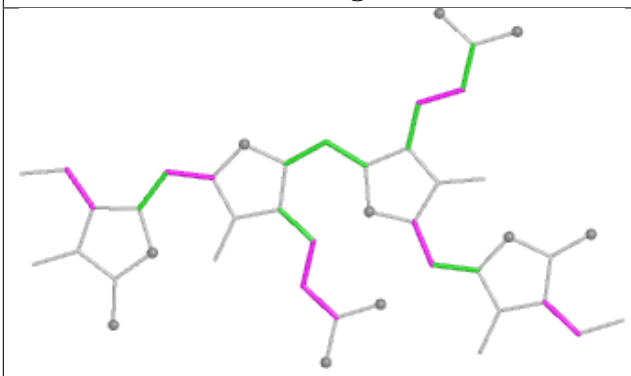
Ligand CYC fI 201



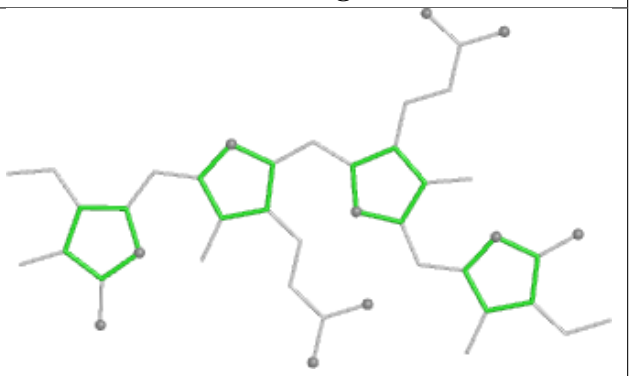
Bond lengths



Bond angles

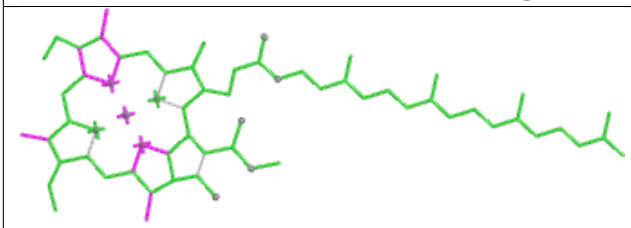


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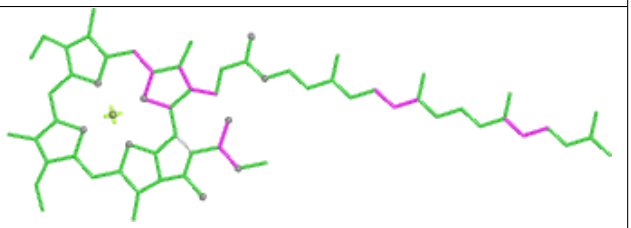


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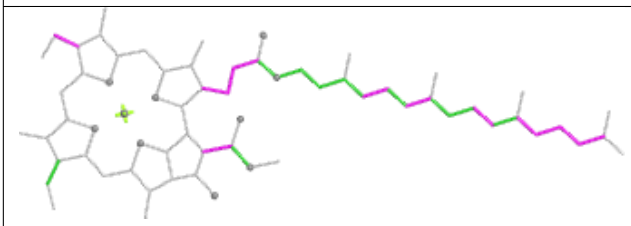
Ligand CLA b1 613



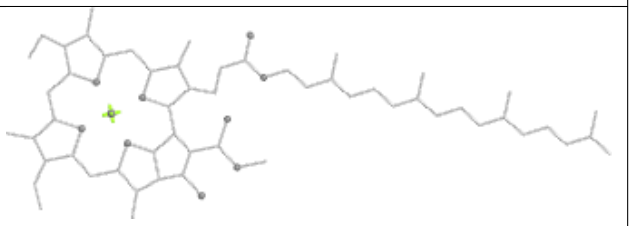
Bond lengths



Bond angles

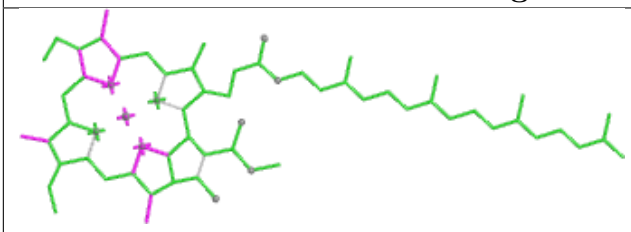


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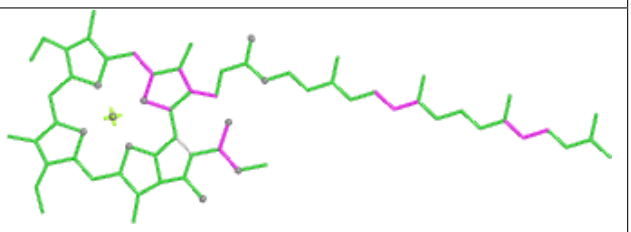


Rings

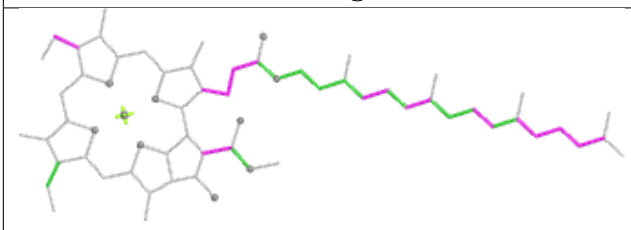
Ligand CLA BD 612



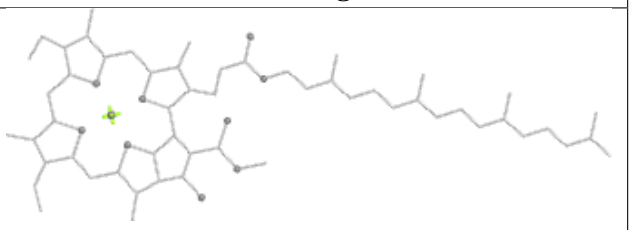
Bond lengths



Bond angles

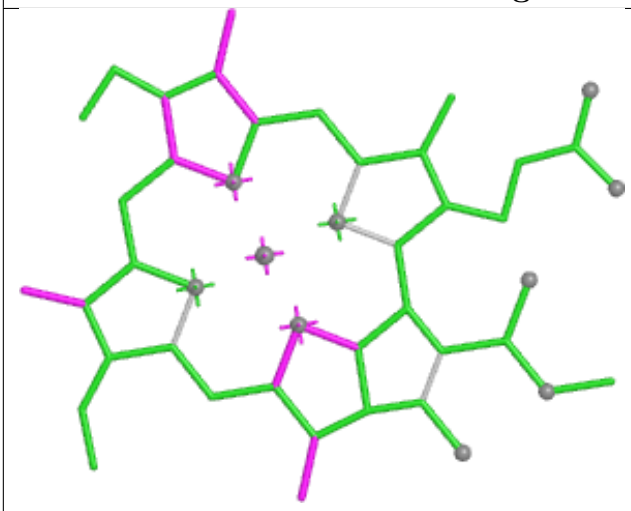


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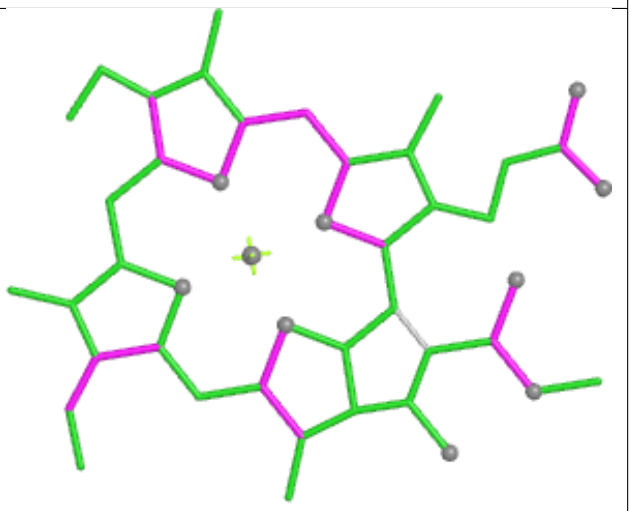


Rings

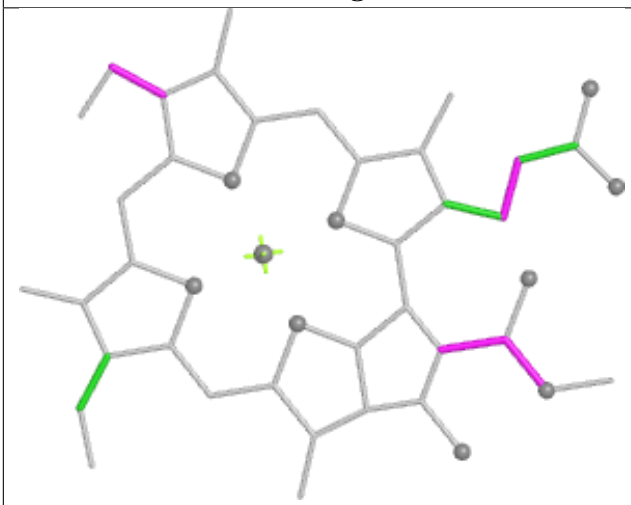
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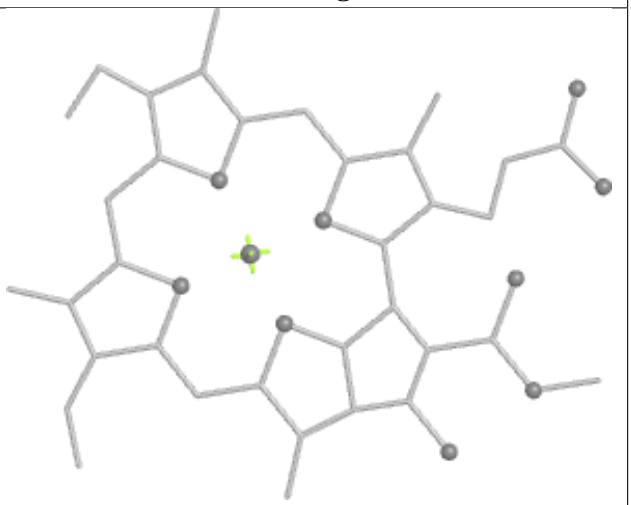
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Bond angles

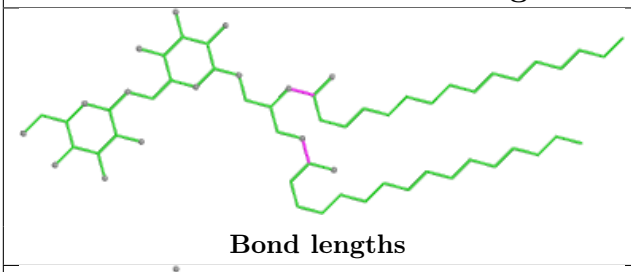


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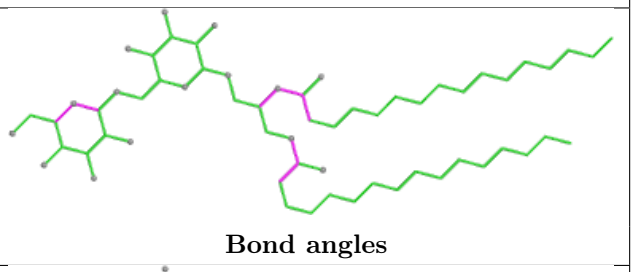


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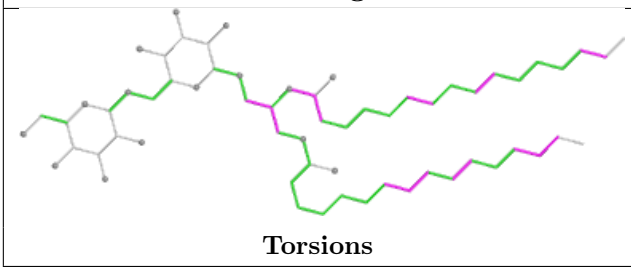
Ligand DGD H1 102



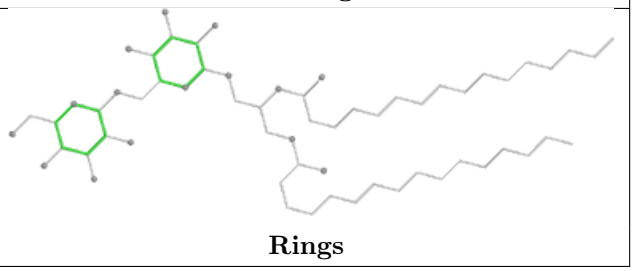
Bond lengths



Bond angles

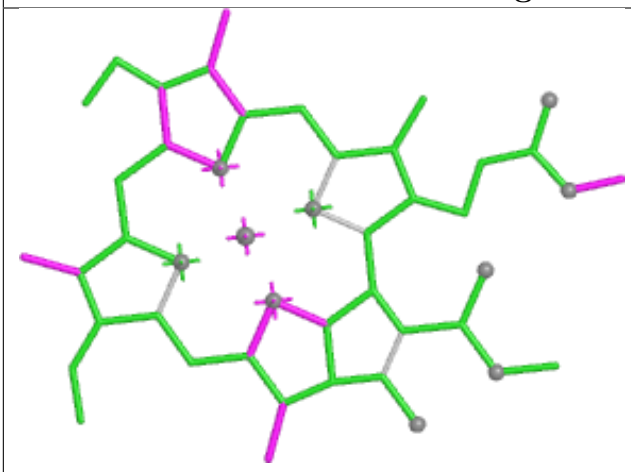


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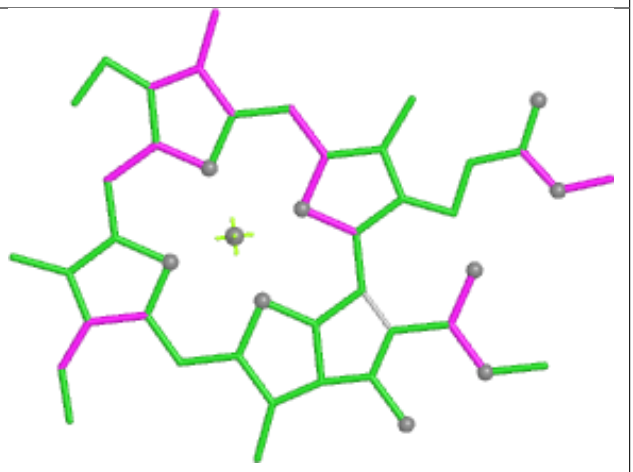


Rings

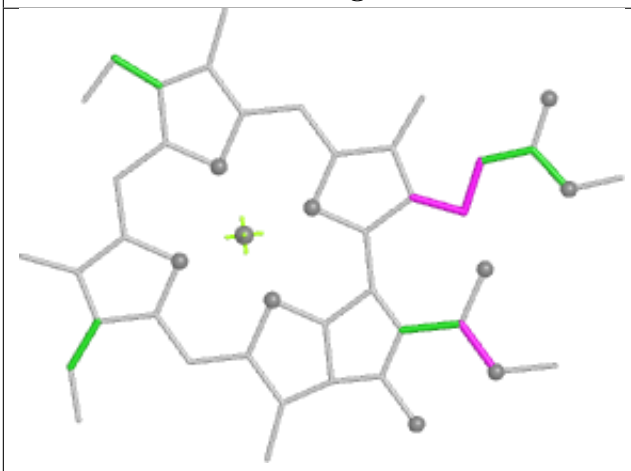
Ligand CLA aD 404



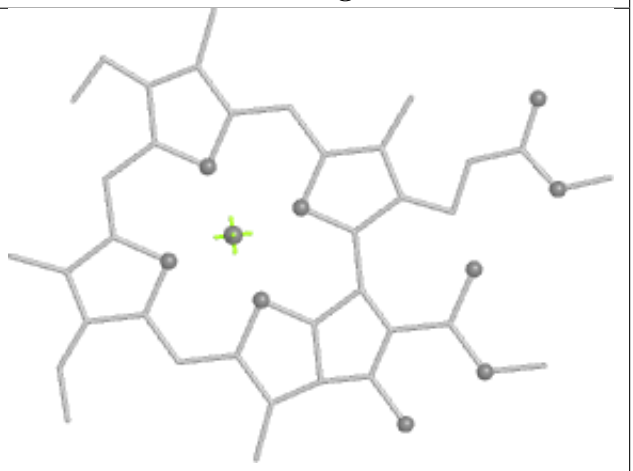
Bond lengths



Bond angles

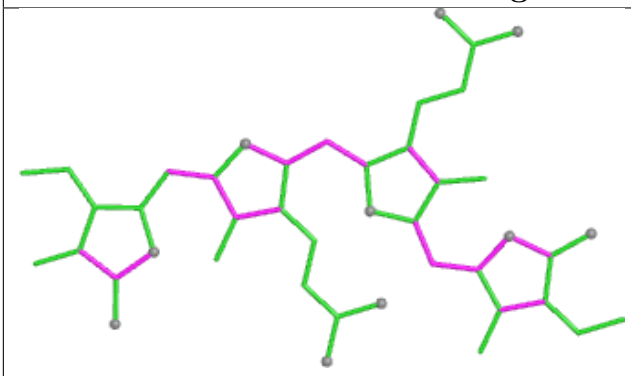


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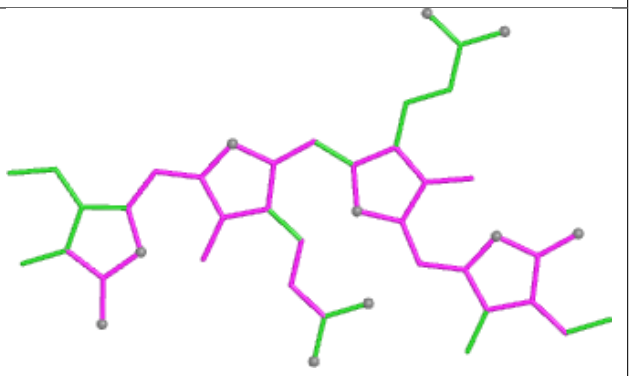


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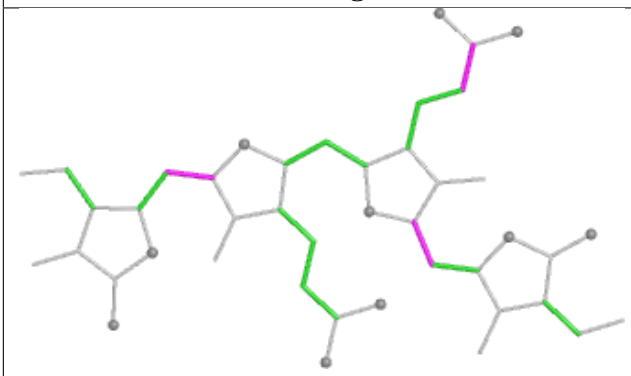
Ligand CYC NL 201



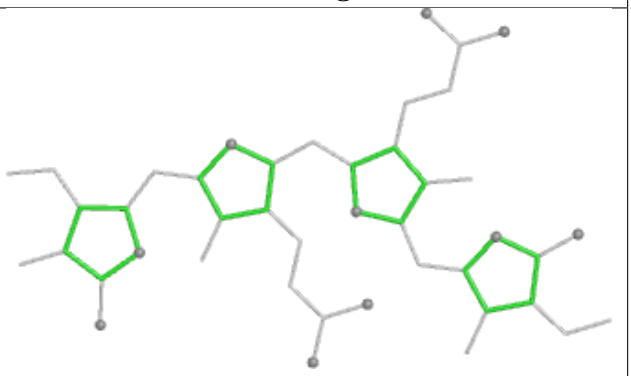
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Bond angles

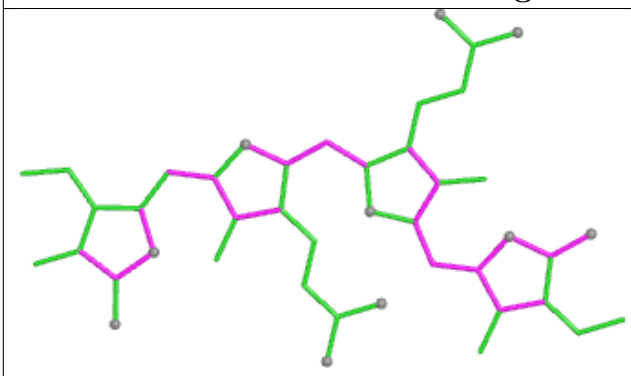


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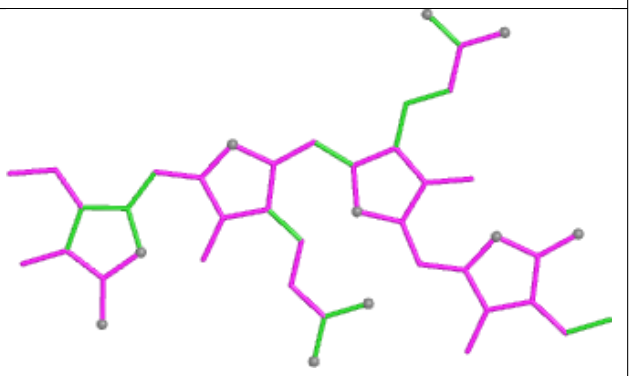


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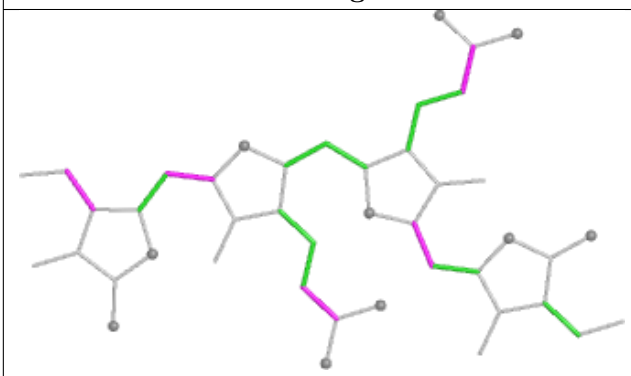
Ligand CYC IK 201



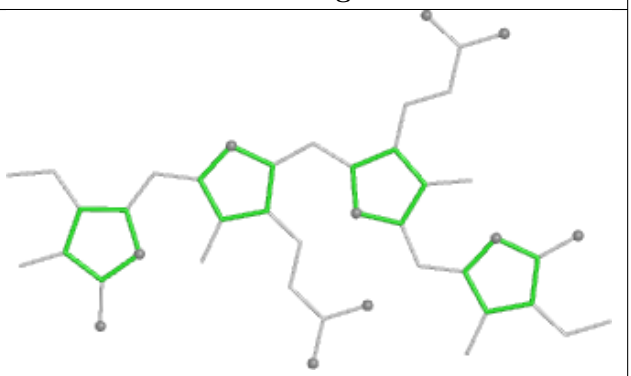
Bond lengths



Bond angles

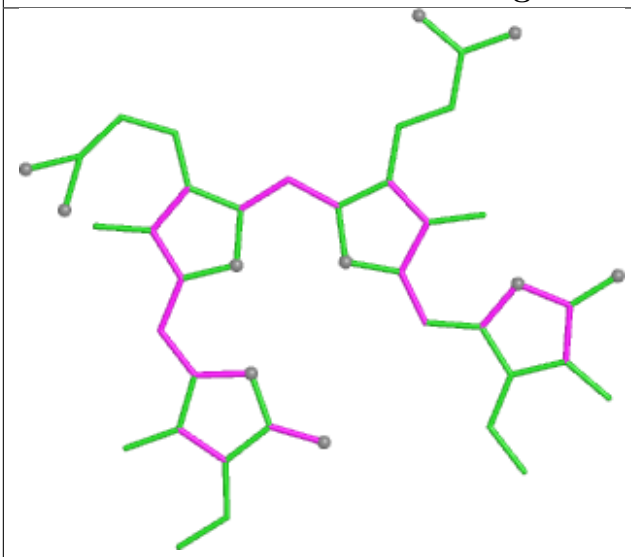


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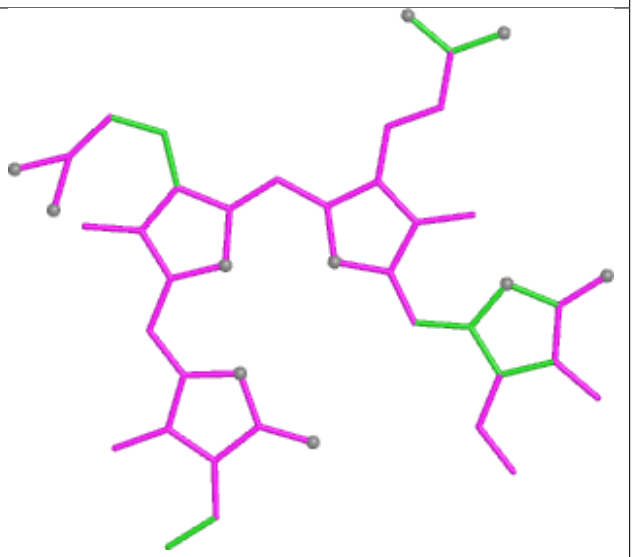


Rings

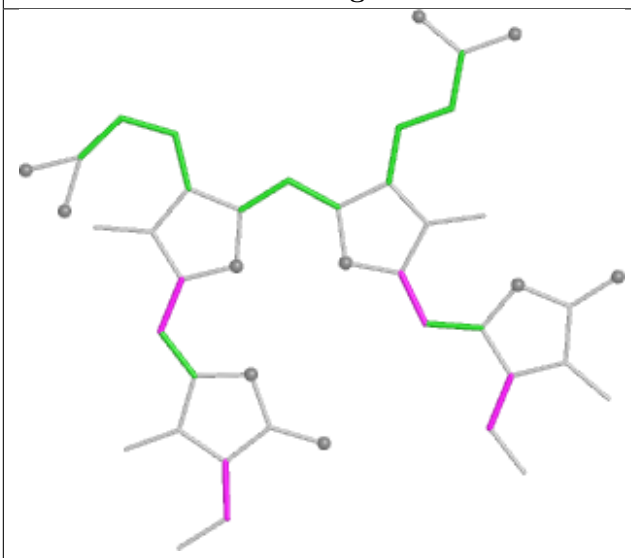
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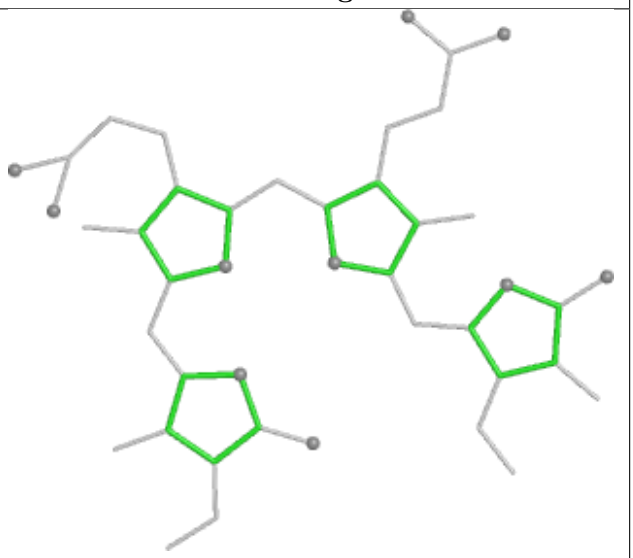
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Bond angles

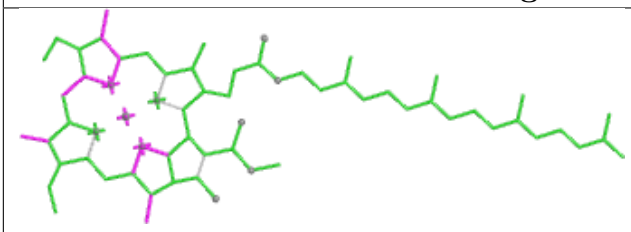


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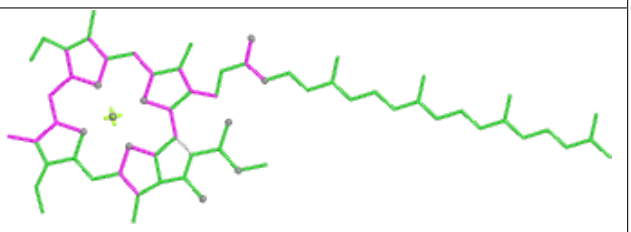


Rings

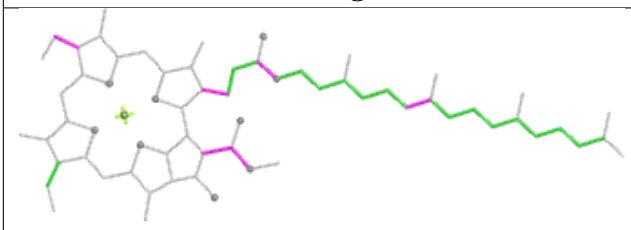
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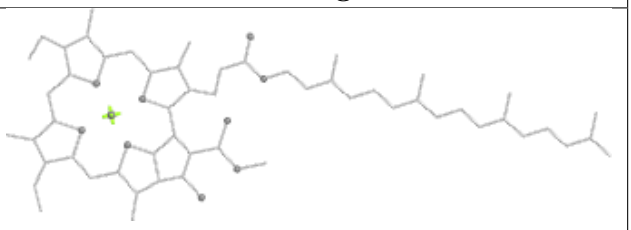
Bond lengths



Bond angles

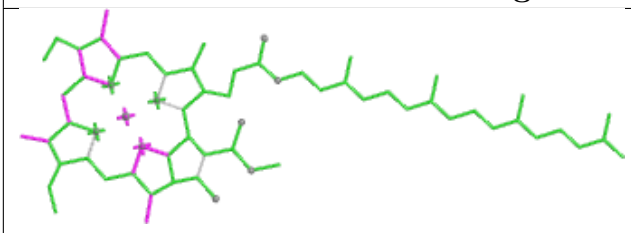


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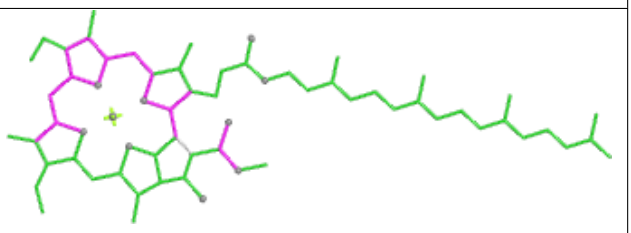


Rings

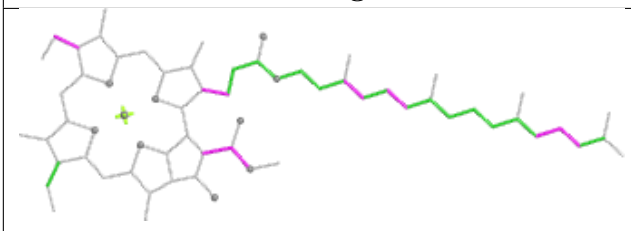
Ligand CLA hD 101



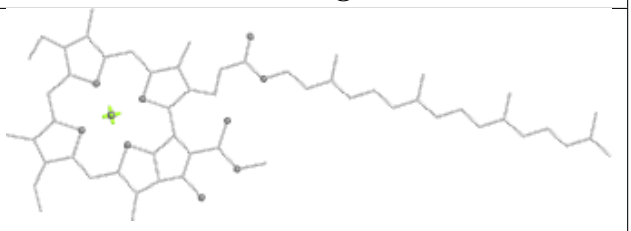
Bond lengths



Bond angles

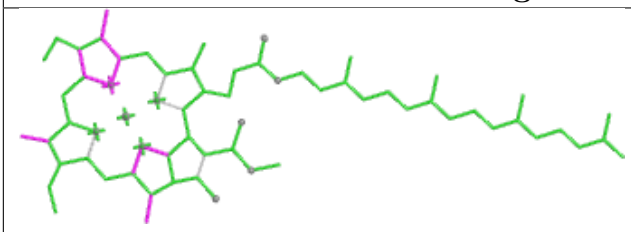


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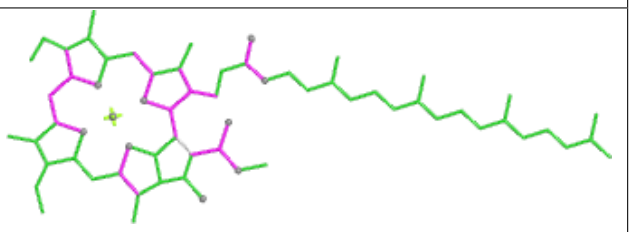


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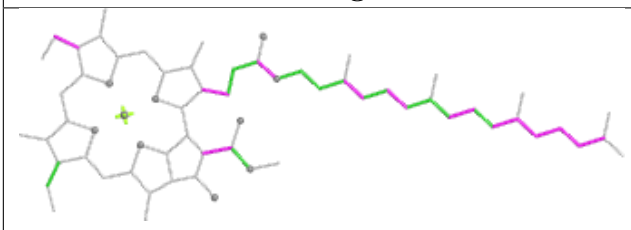
Ligand CLA bD 606



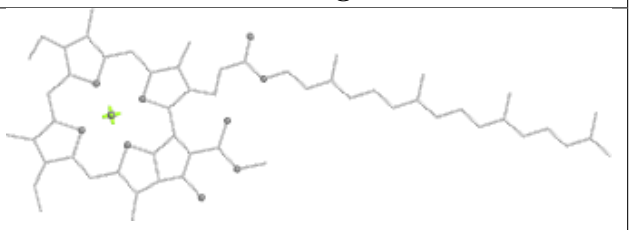
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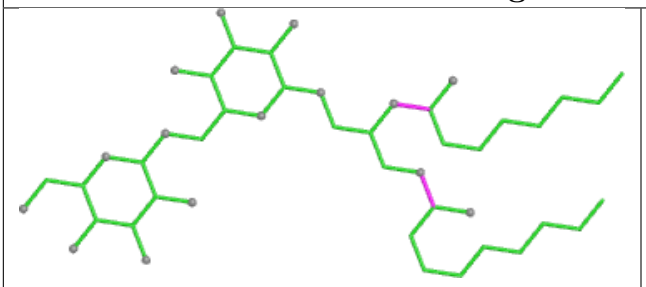


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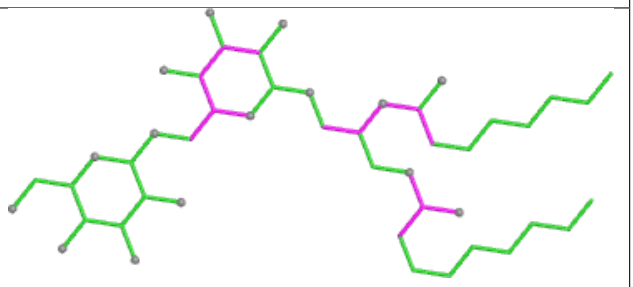


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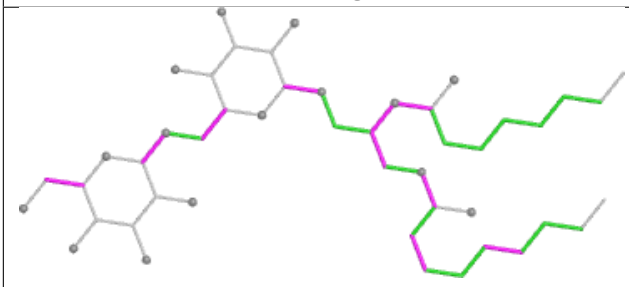
Ligand DGD CE 517



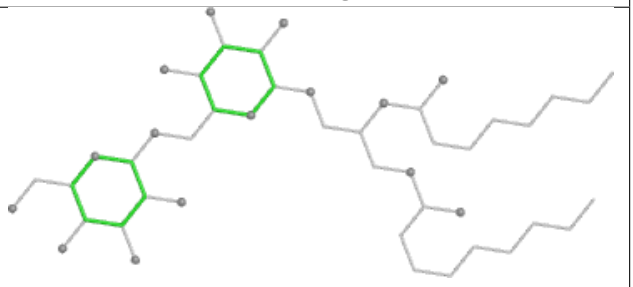
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Bond angles

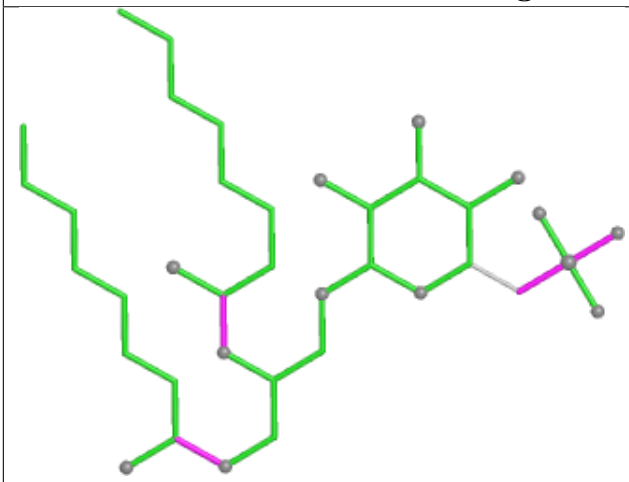


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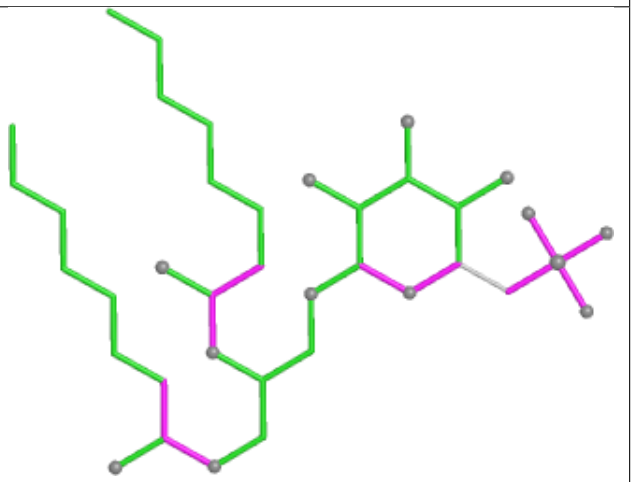


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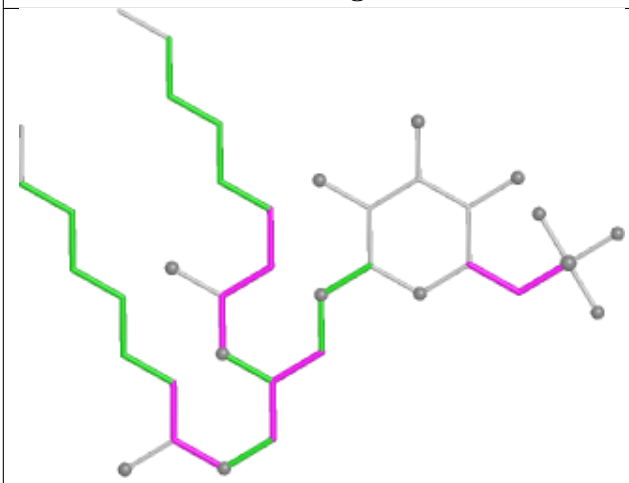
Ligand SQD B1 622



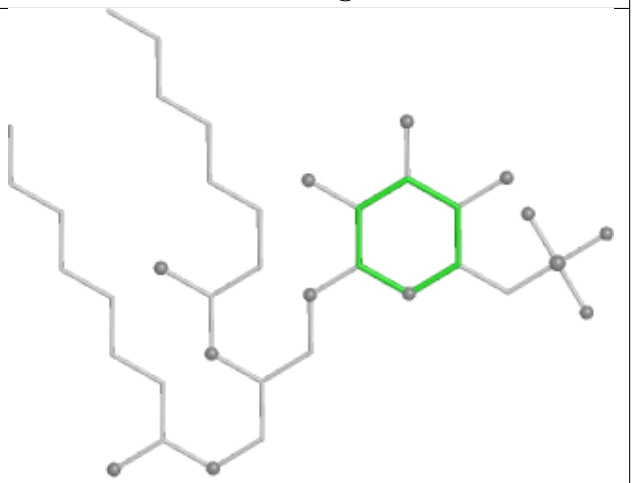
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Bond angles

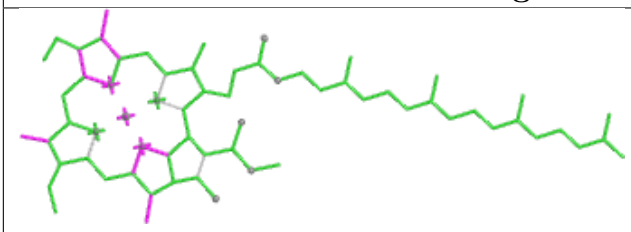


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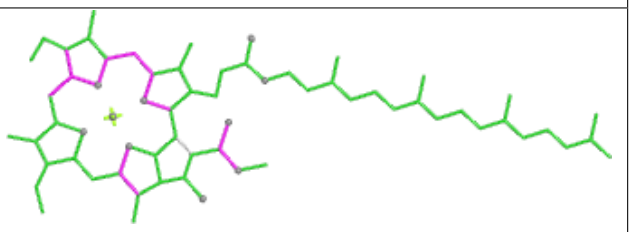


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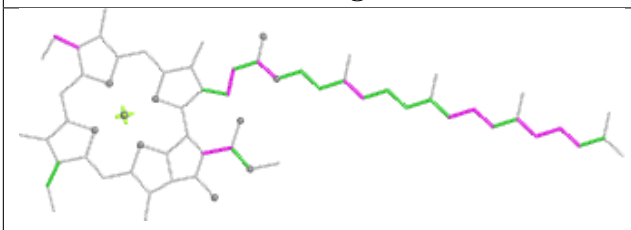
Ligand CLA BE 613



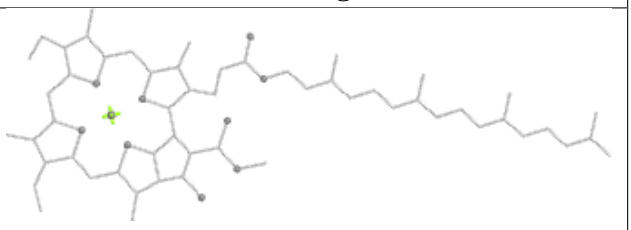
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Bond angles

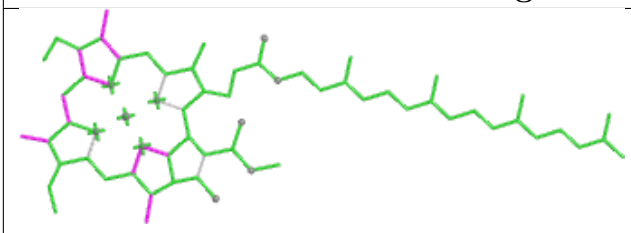


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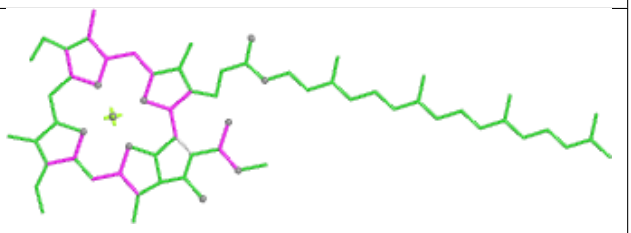


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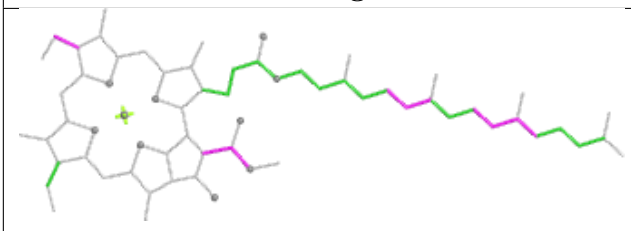
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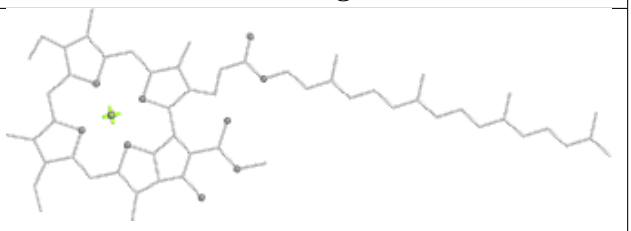
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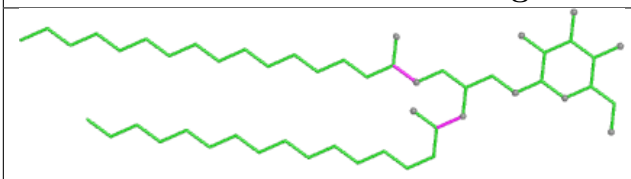


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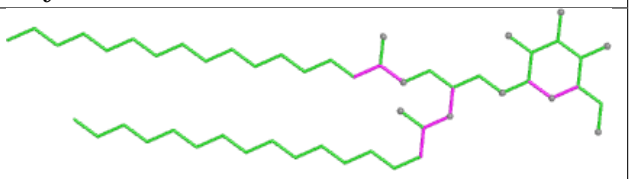


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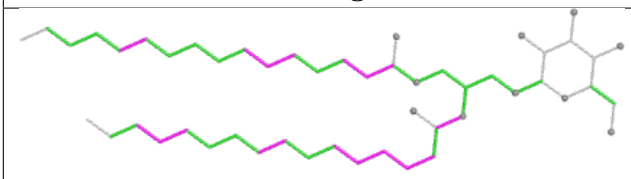
Ligand LMG yE 101



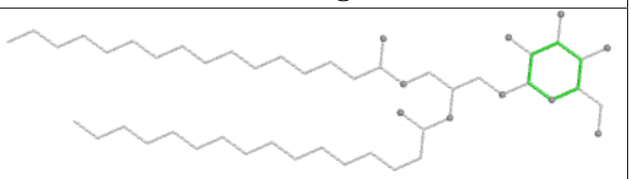
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Bond angles

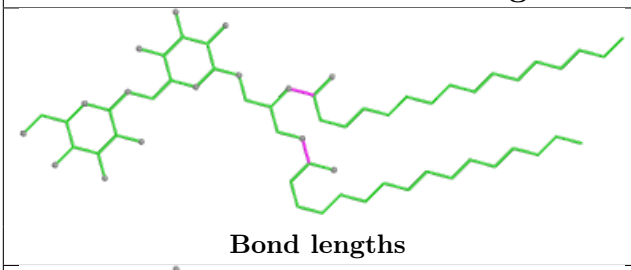


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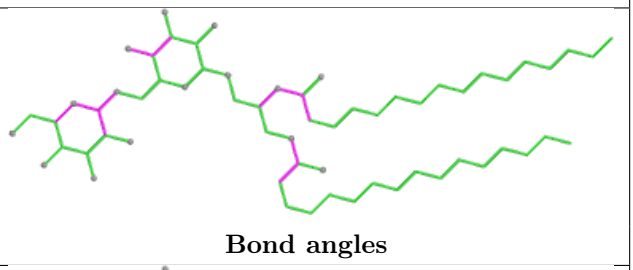


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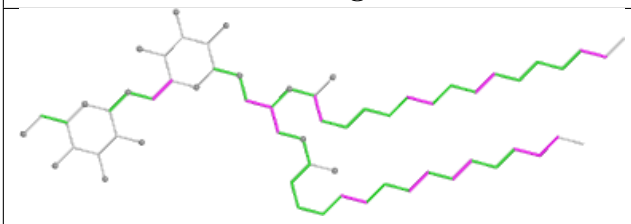
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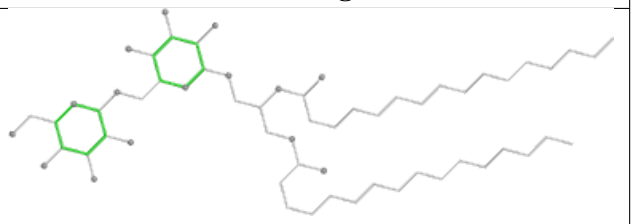
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Bond angles

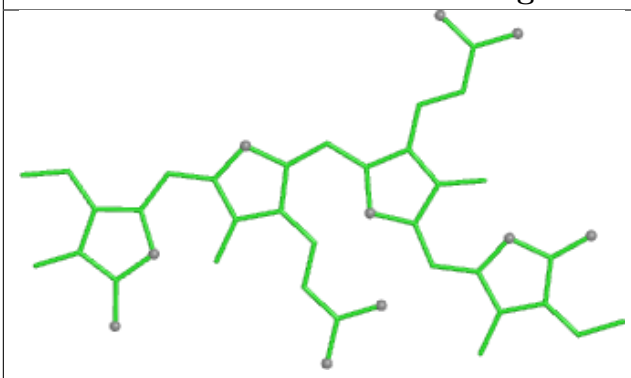


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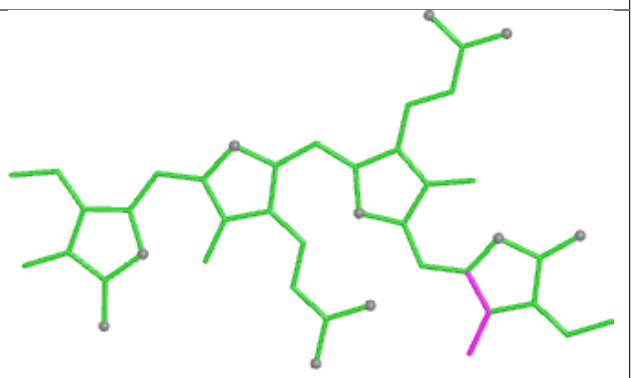


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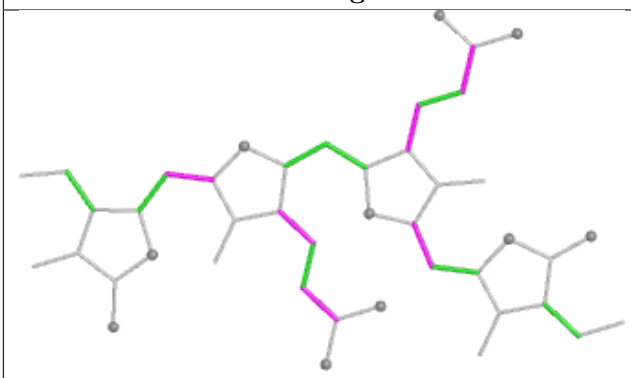
Ligand CYC iC 201



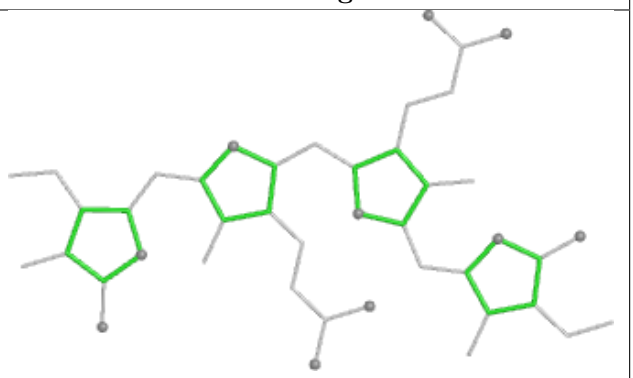
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Bond angles

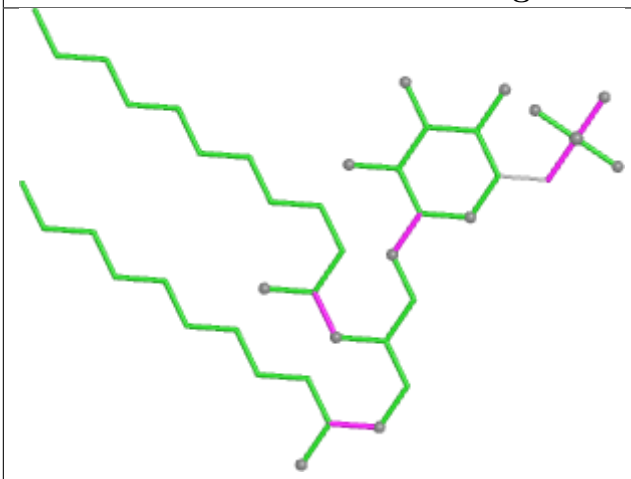


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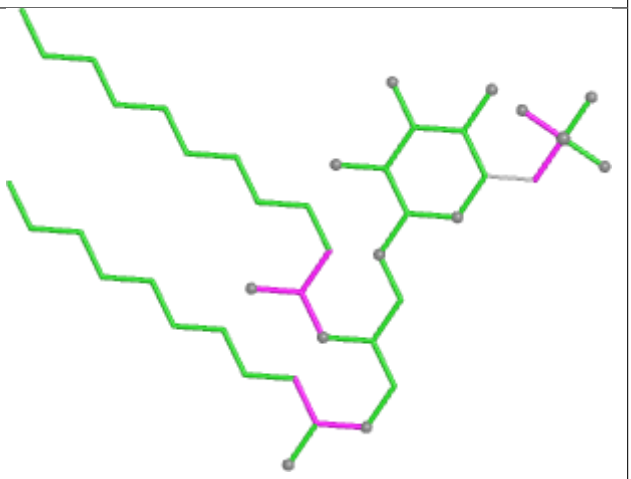


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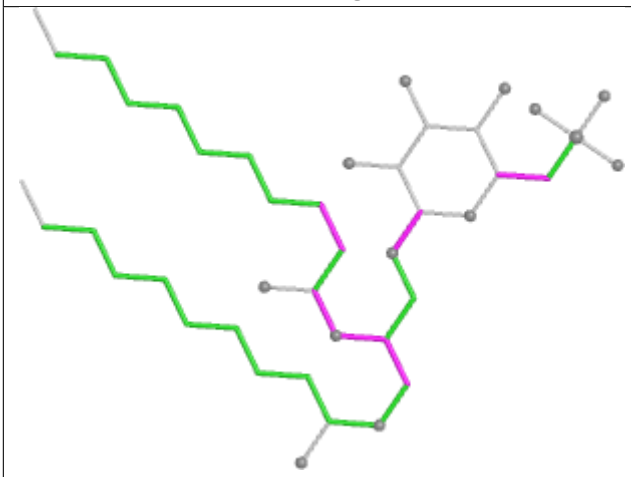
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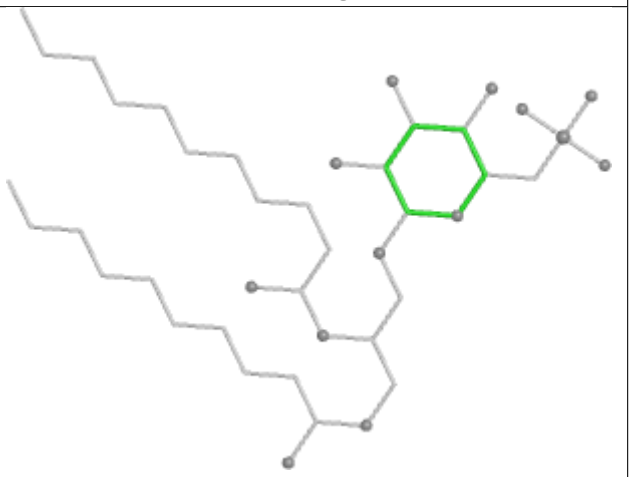
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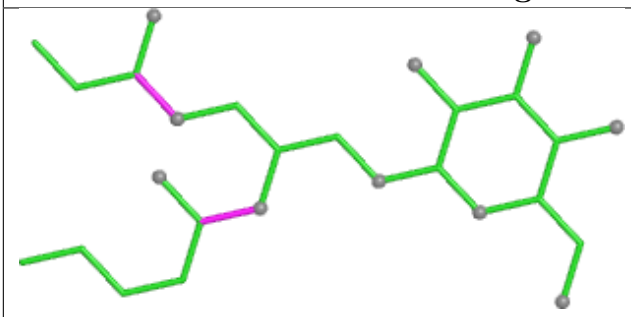


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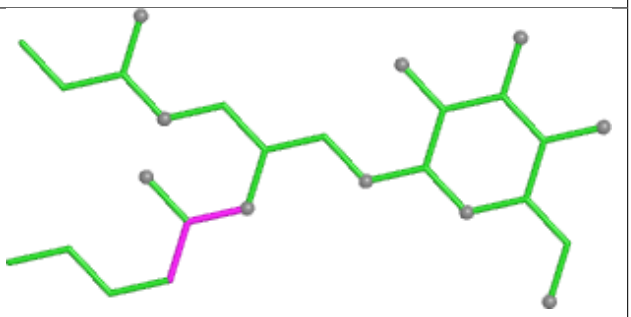


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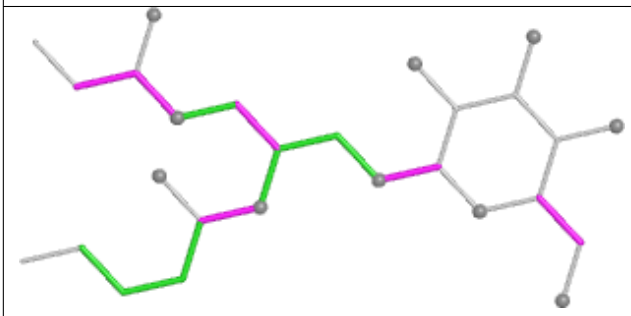
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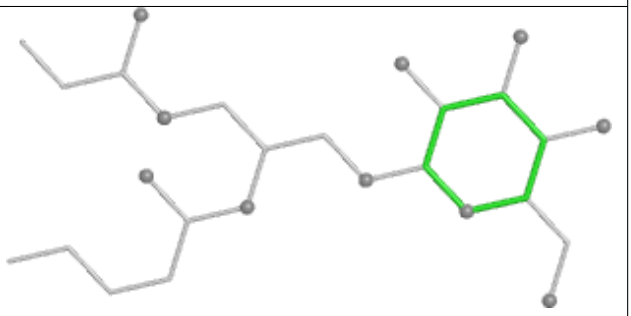
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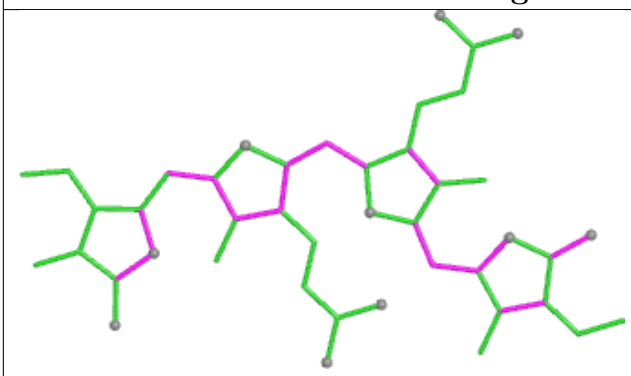


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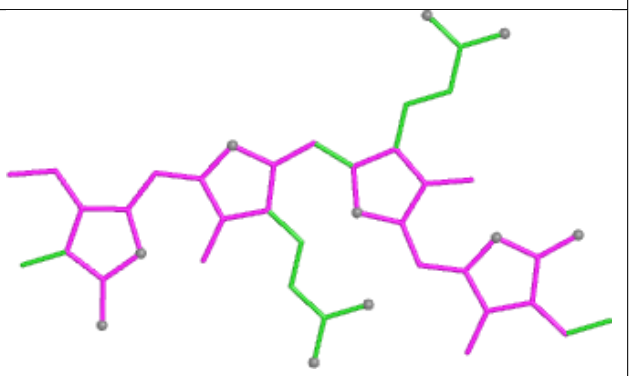


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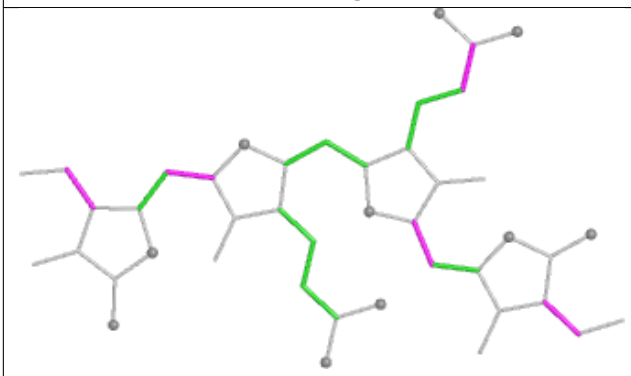
Ligand CYC RL 201



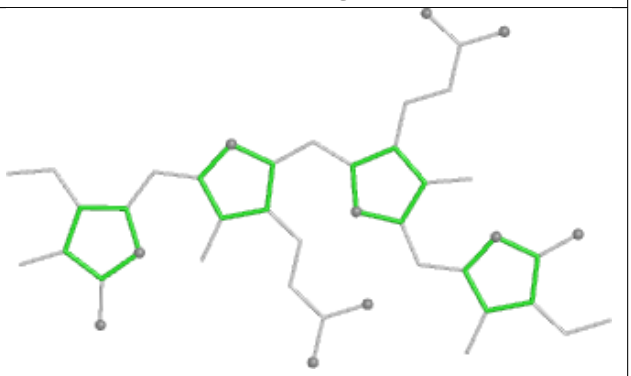
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Bond angles

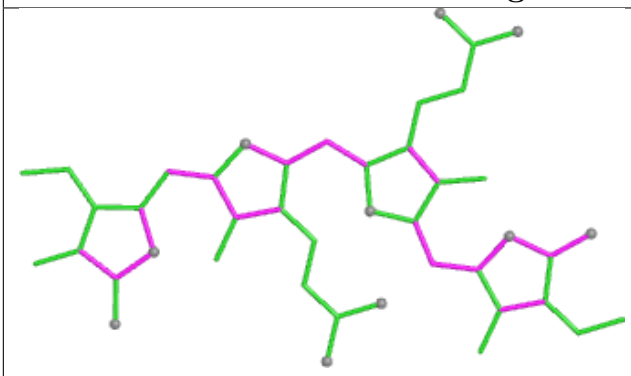


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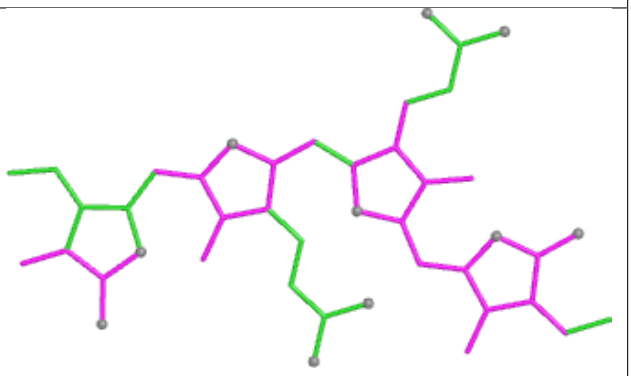


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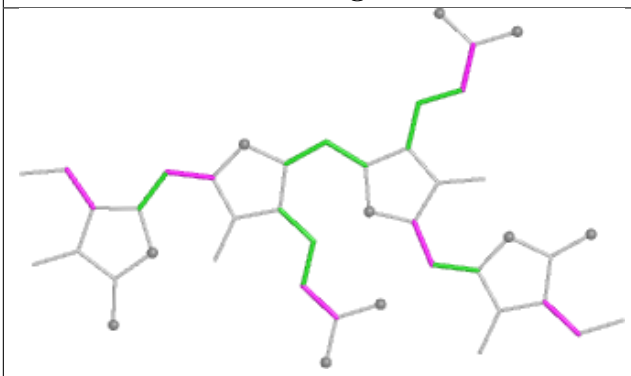
Ligand CYC XK 201



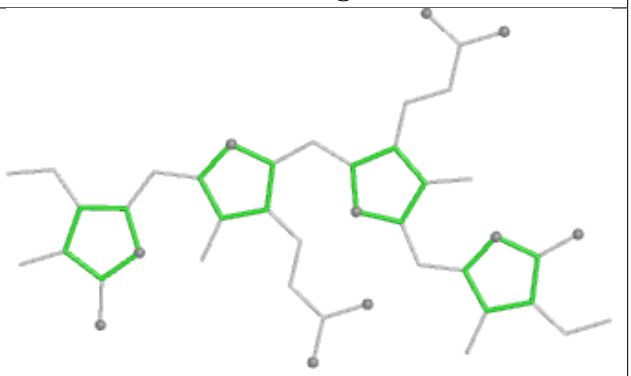
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Bond angles

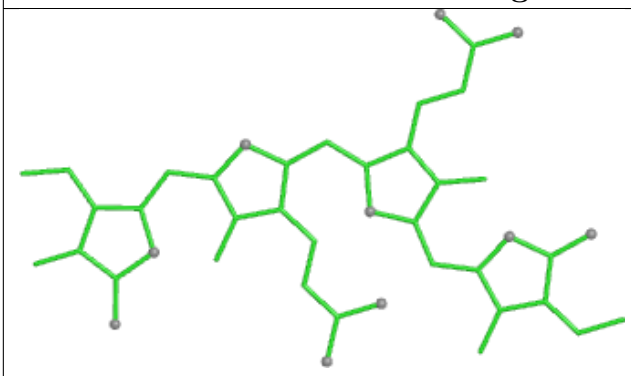


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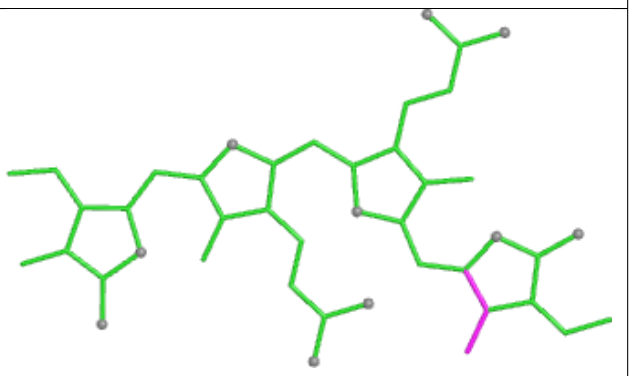


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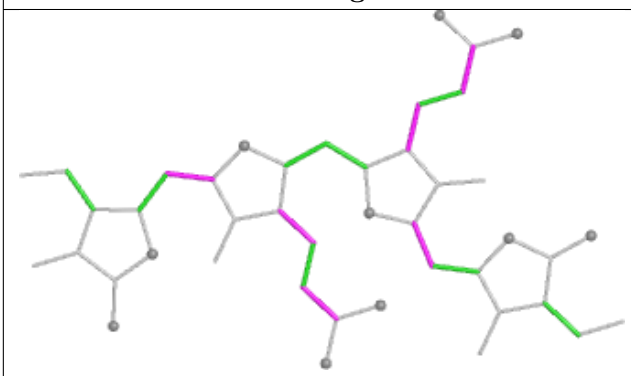
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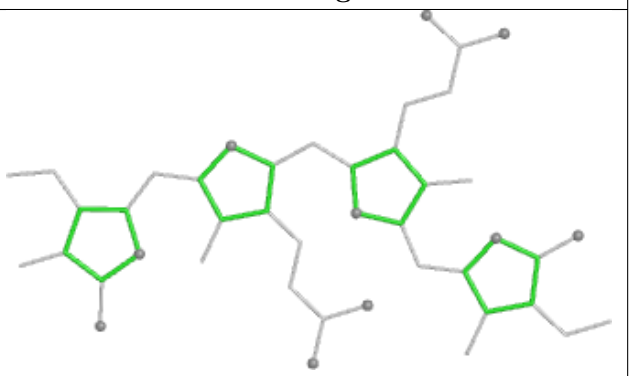
Bond lengths



Bond angles

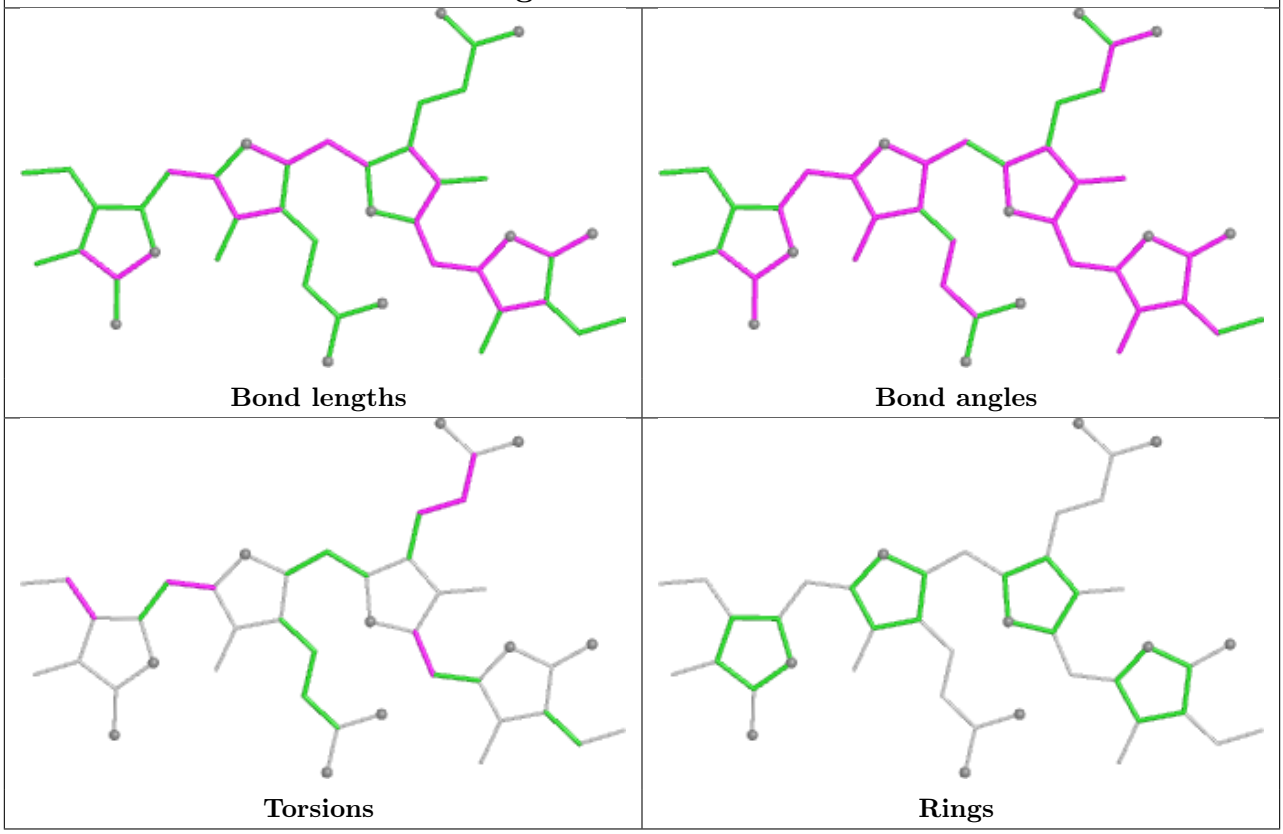


Torsions

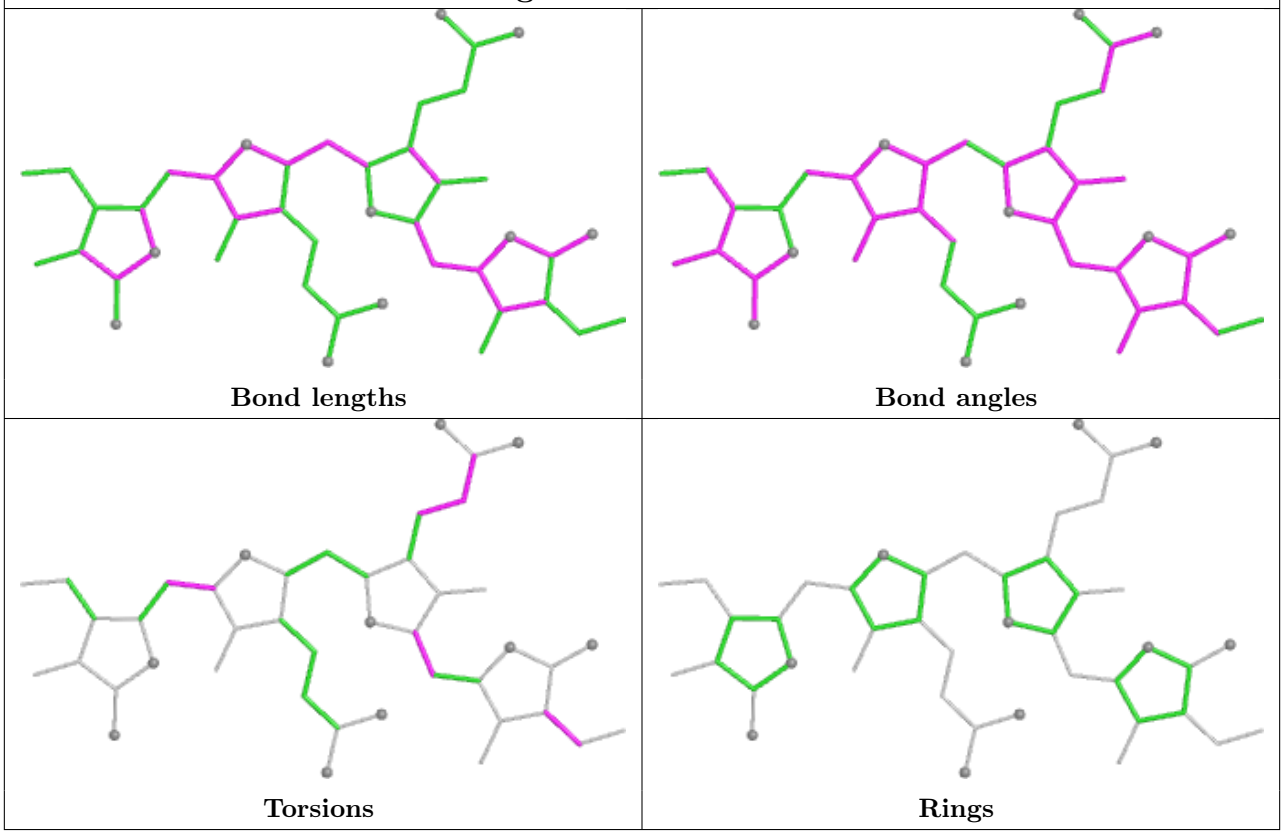


Rings

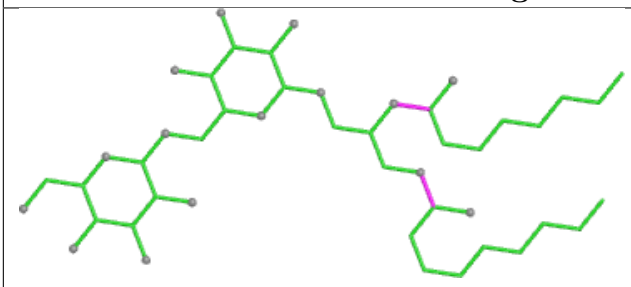
Ligand CYC 3F 101



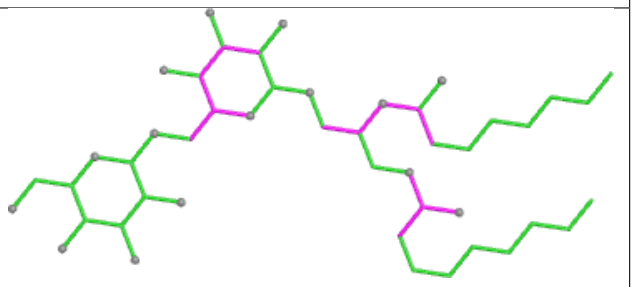
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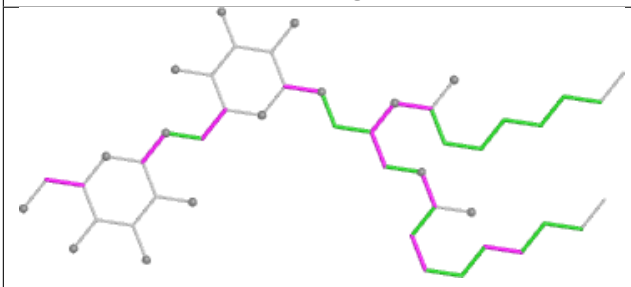
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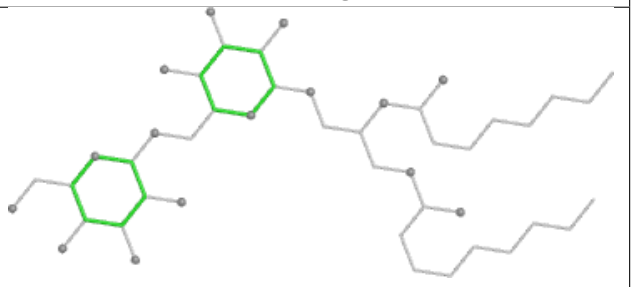
Bond lengths



Bond angles

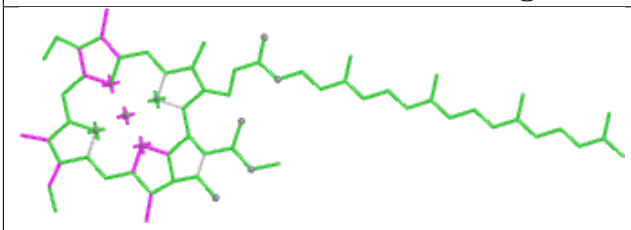


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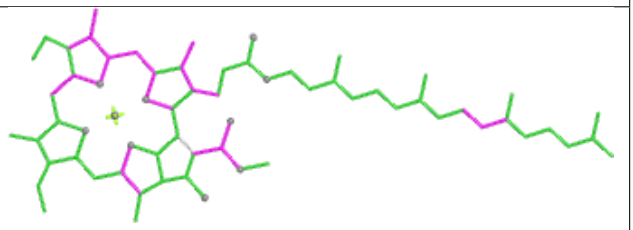


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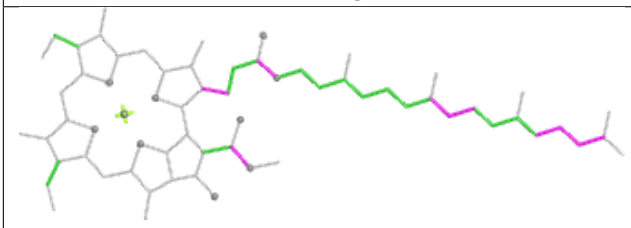
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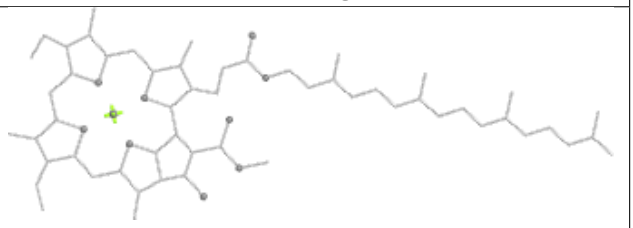
Bond lengths



Bond angles

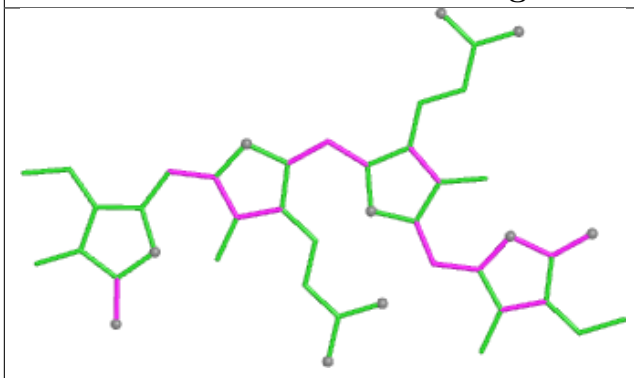


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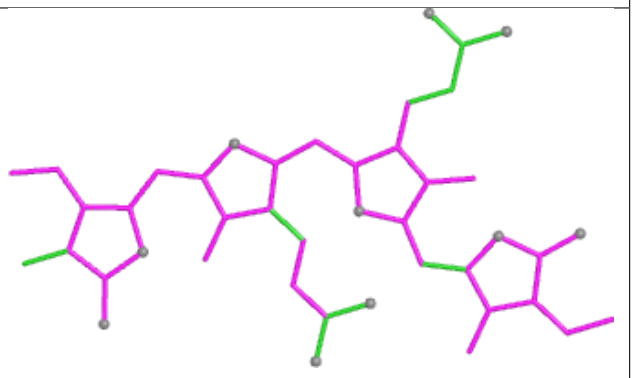


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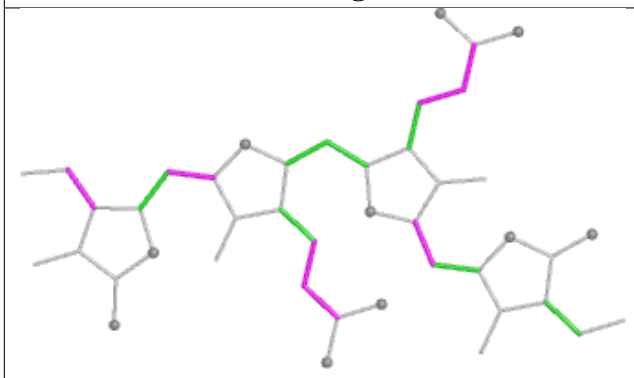
Ligand CYC VG 201



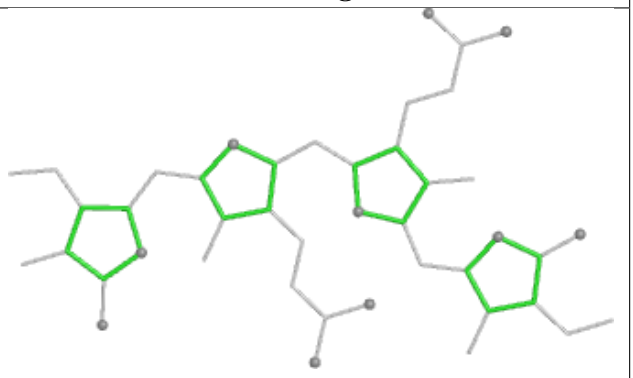
Bond lengths



Bond angles

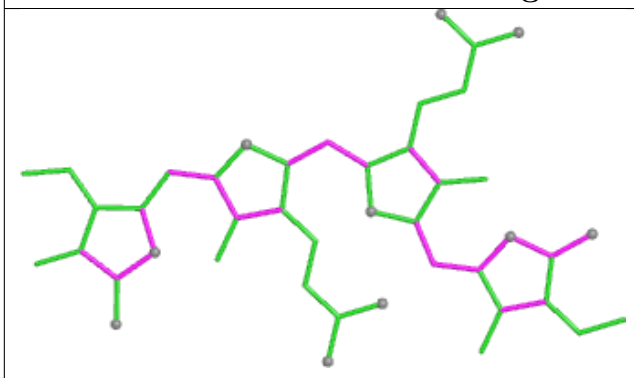


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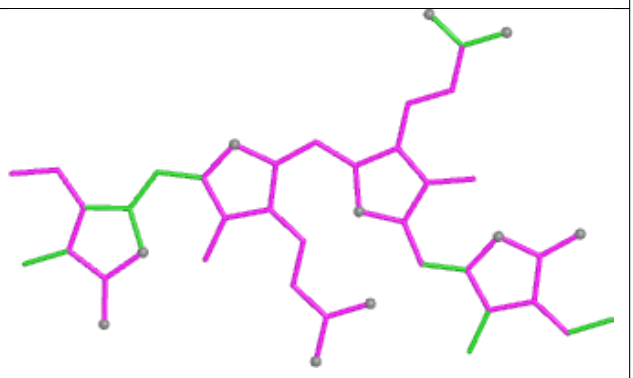


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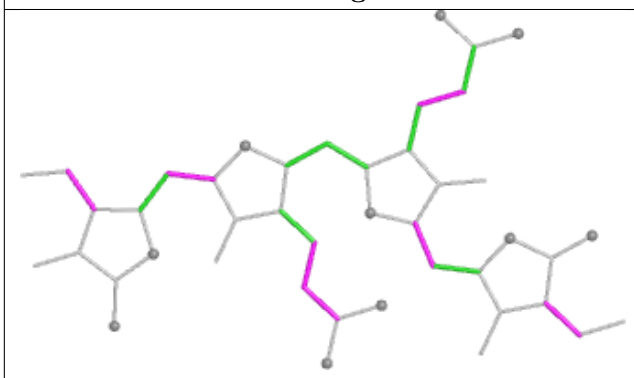
Ligand CYC f9 201



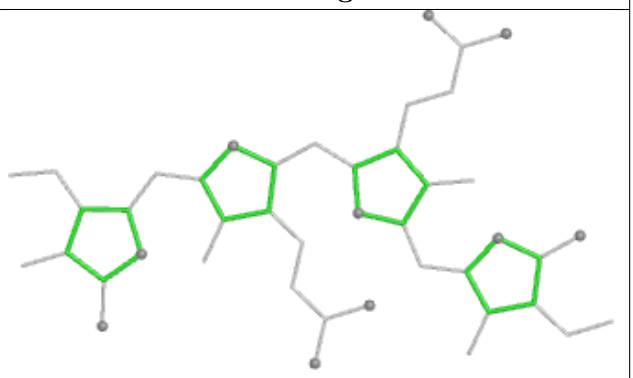
Bond lengths



Bond angles

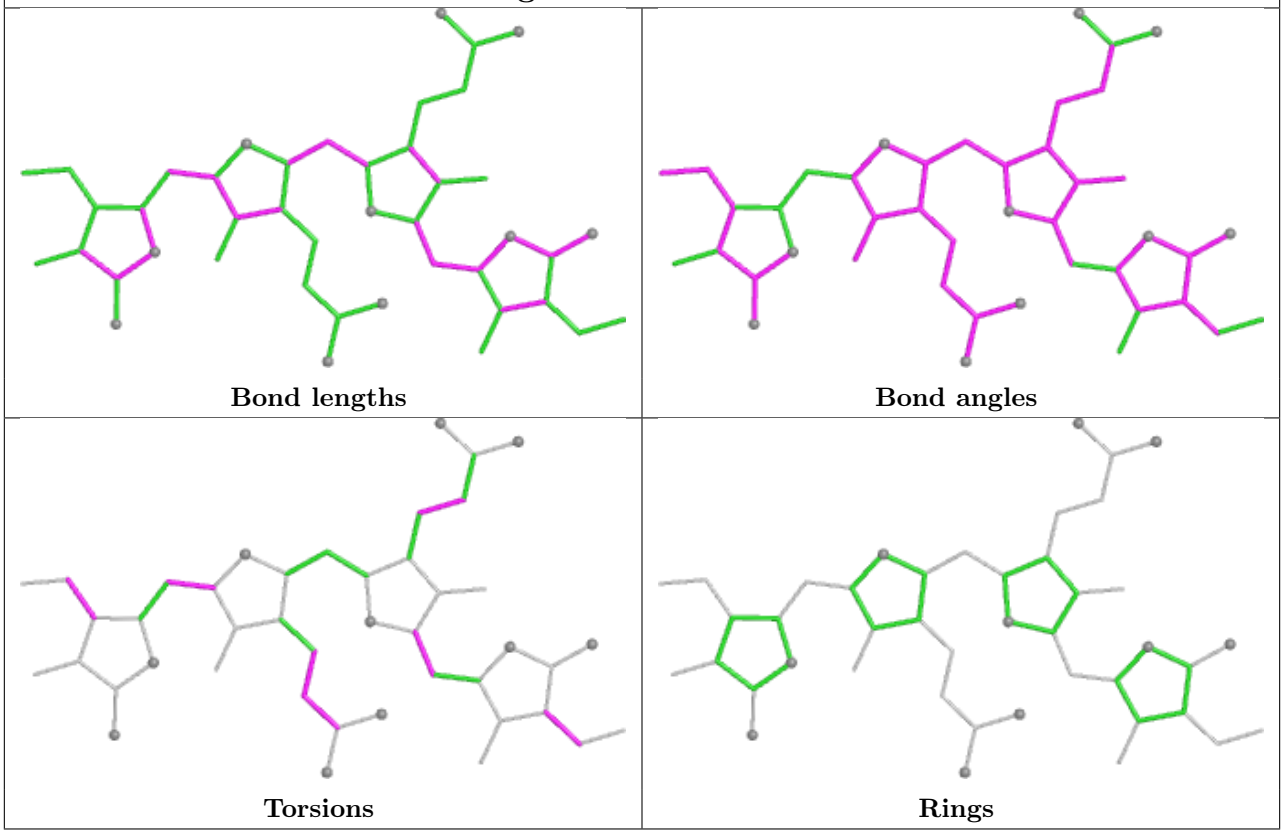


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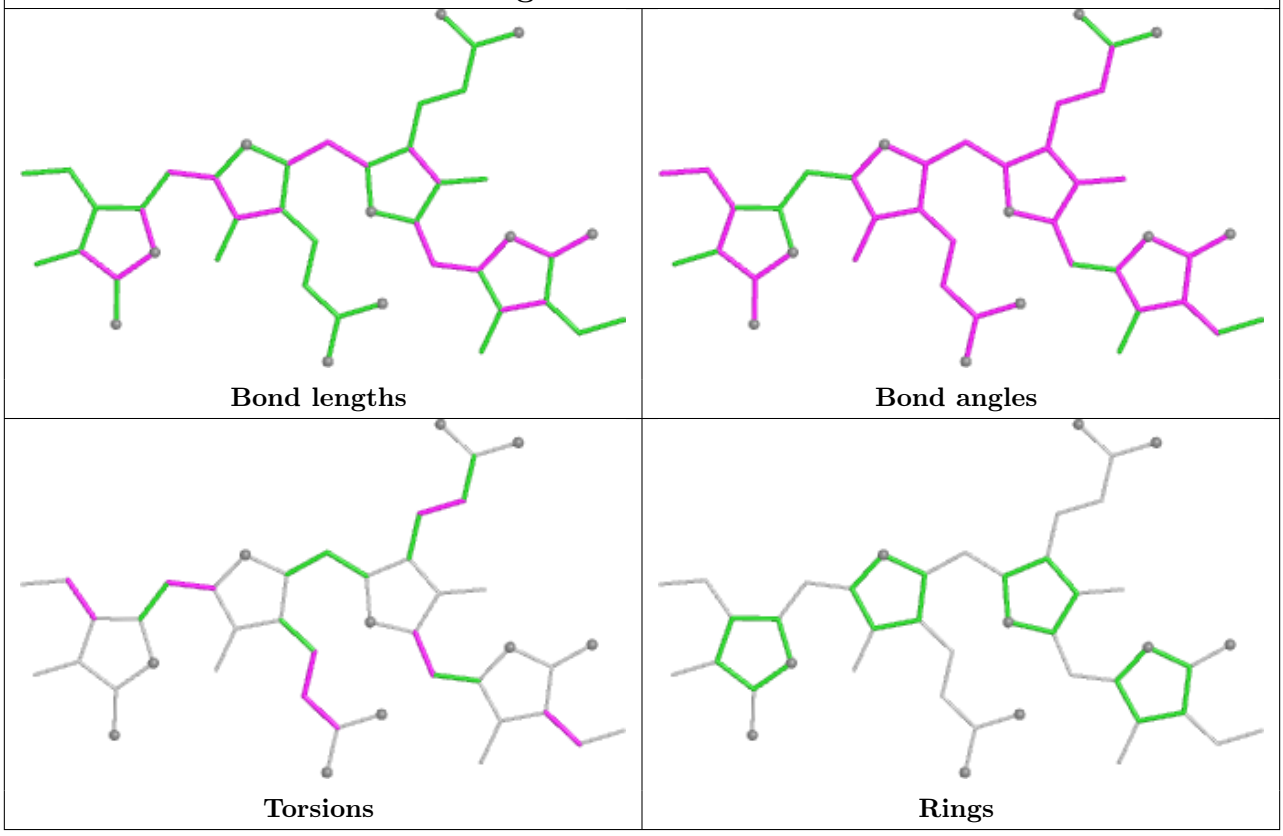


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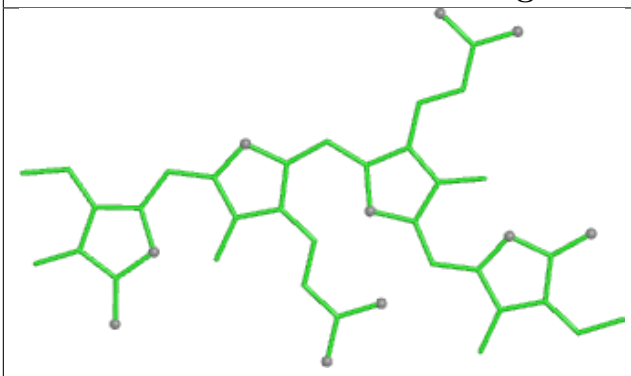
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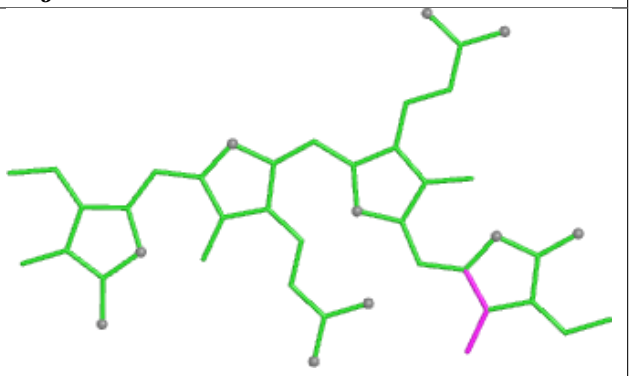
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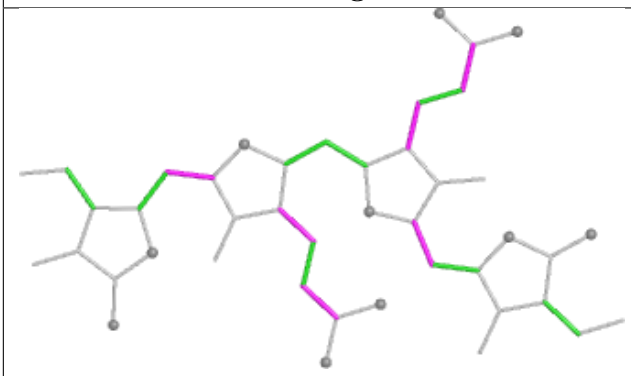
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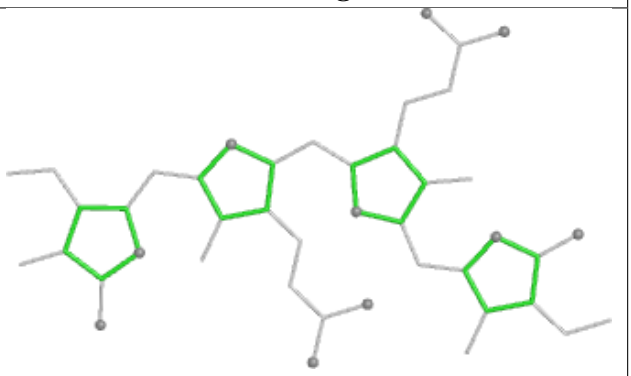
Bond lengths



Bond angles

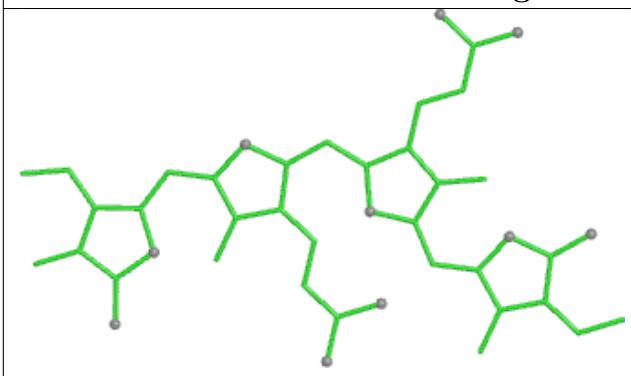


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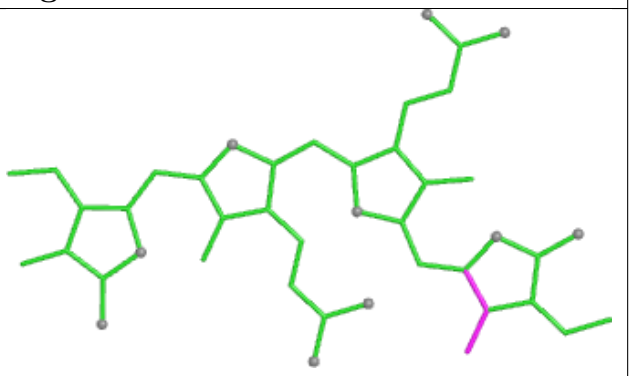


Rings

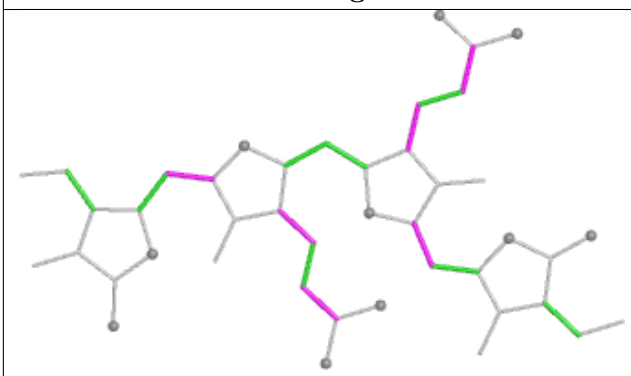
Ligand CYC gC 302



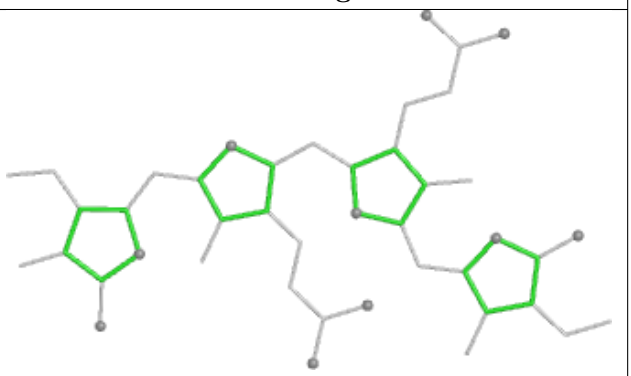
Bond lengths



Bond angles

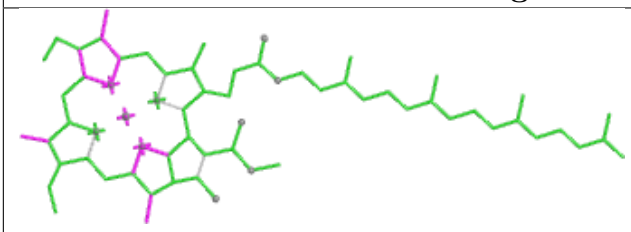


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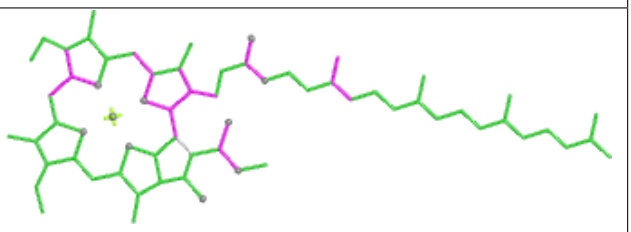


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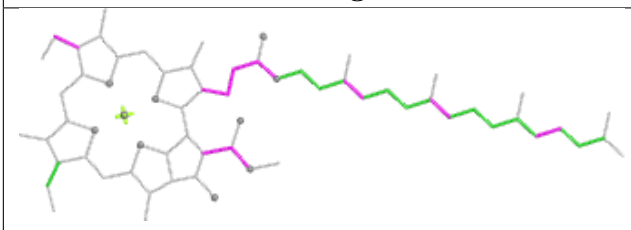
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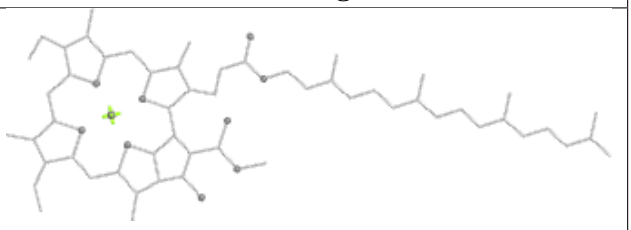
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Bond angles

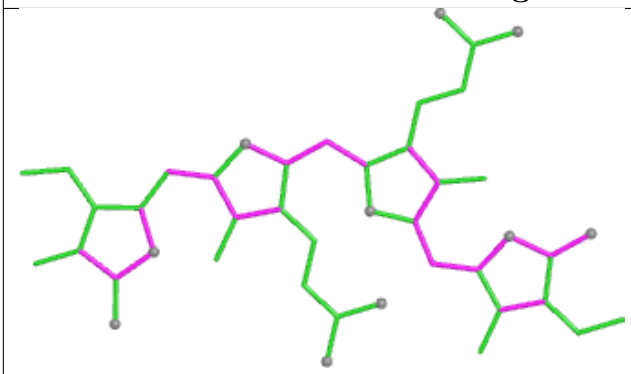


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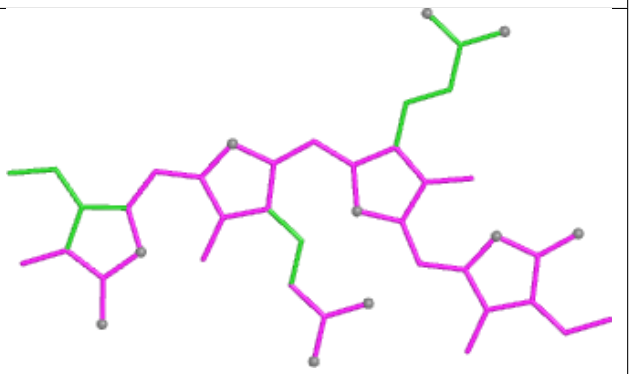


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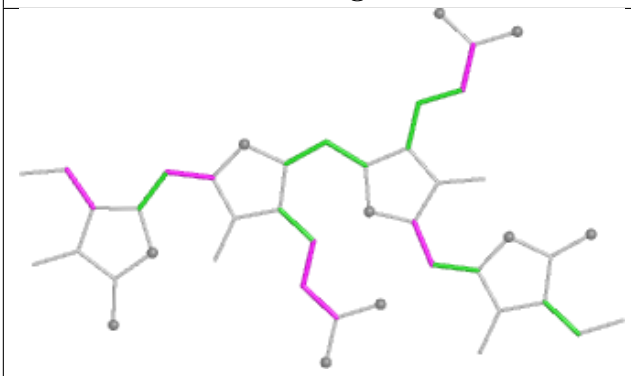
Ligand CYC 5G 201



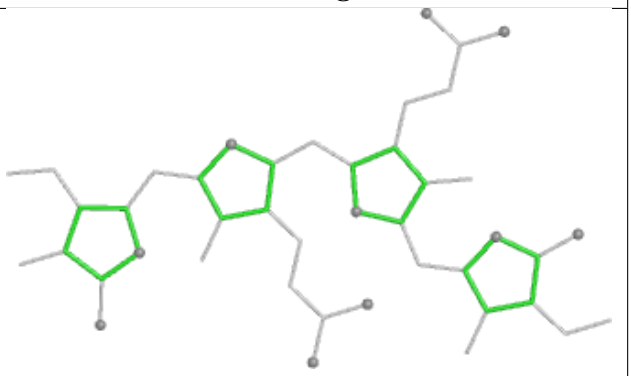
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Bond angles

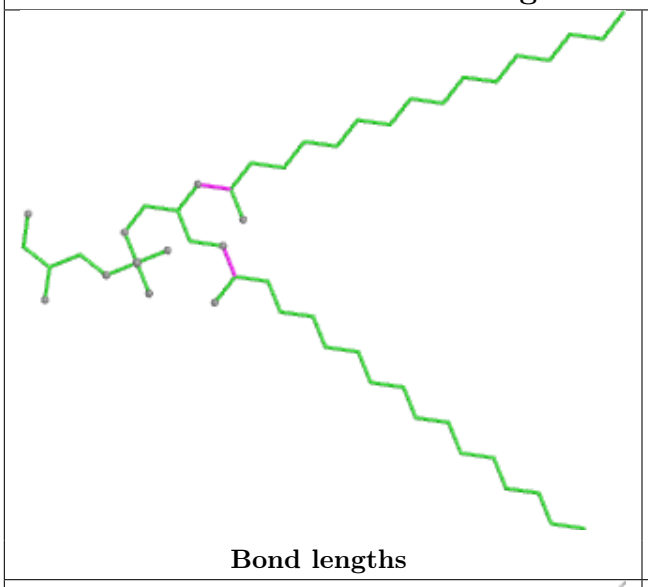


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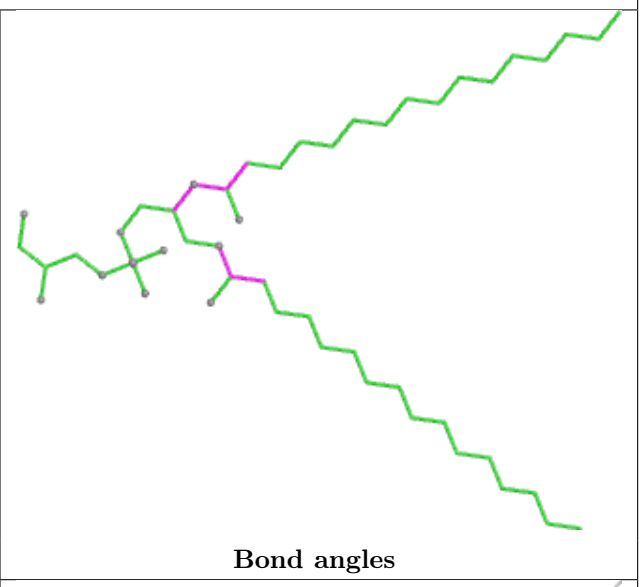


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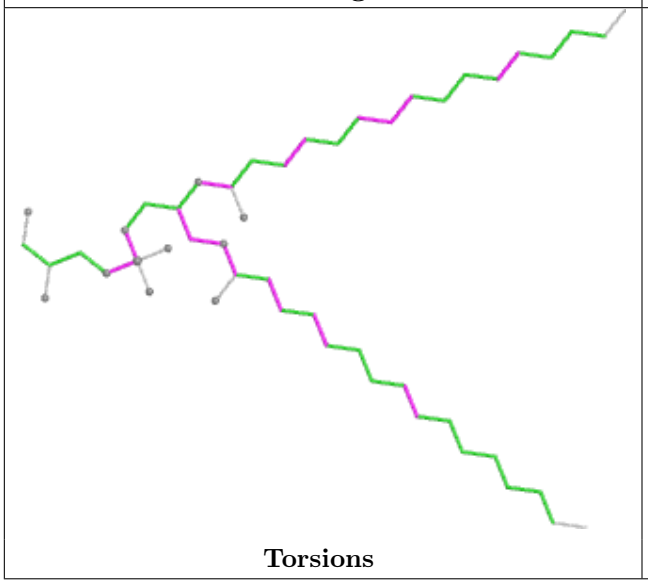
Ligand LHG lE 101



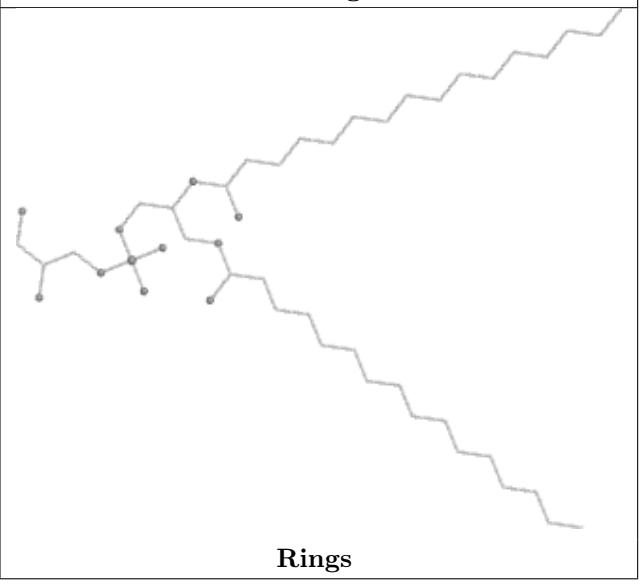
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Bond angles

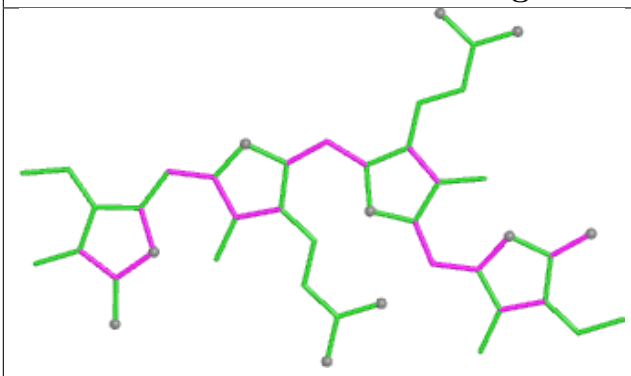


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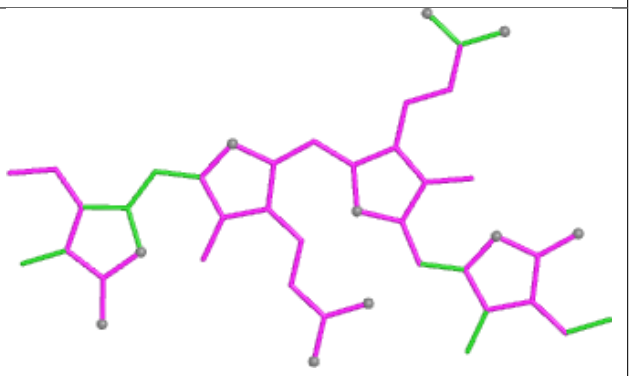


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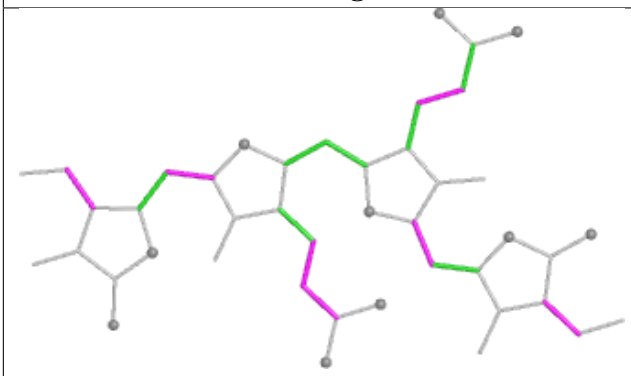
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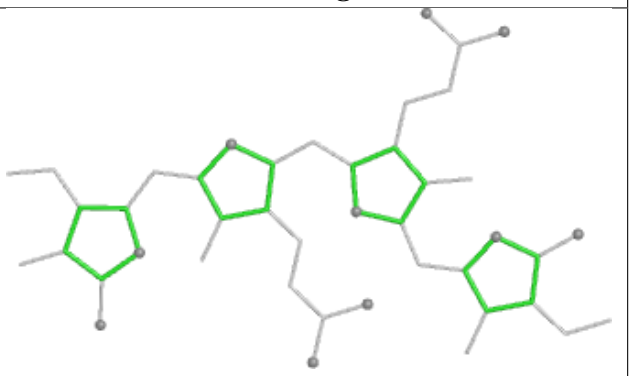
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Bond angles

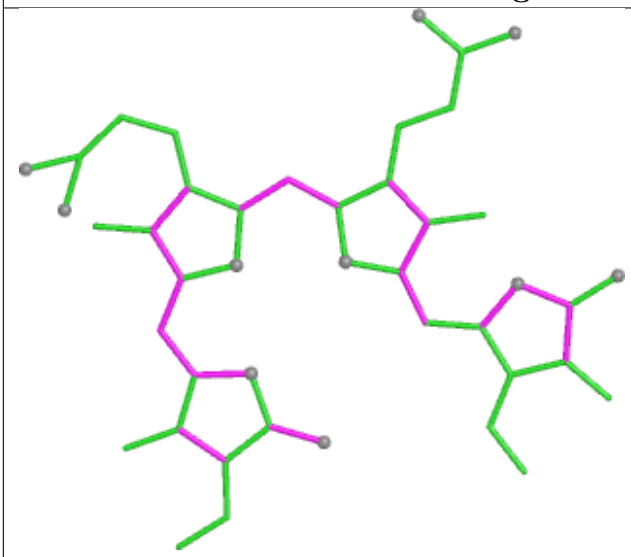


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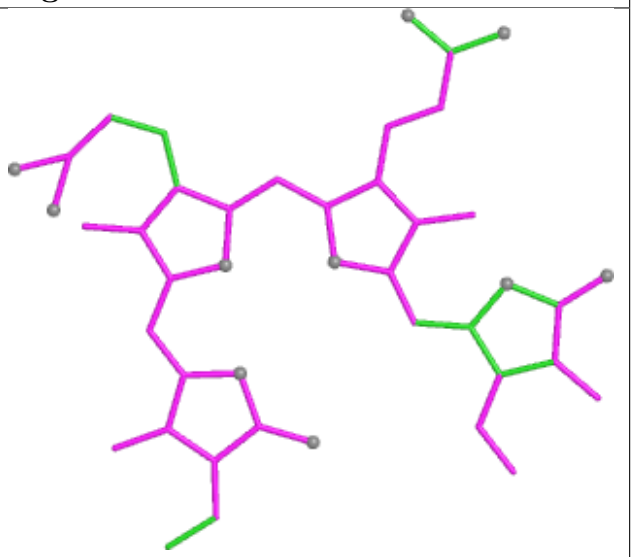


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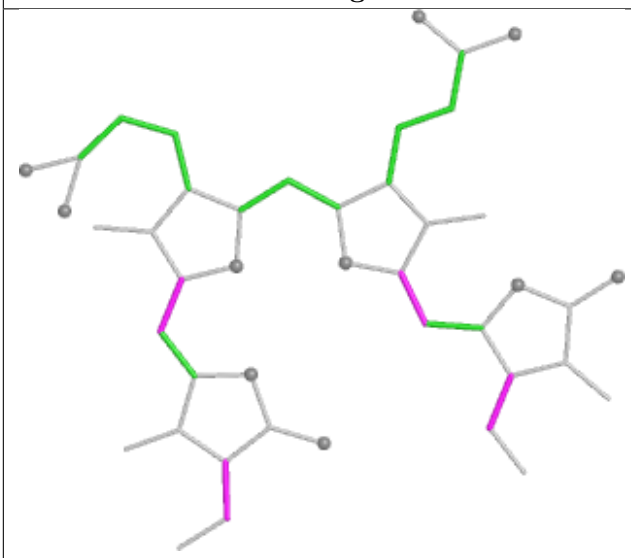
Ligand CYC gA 301



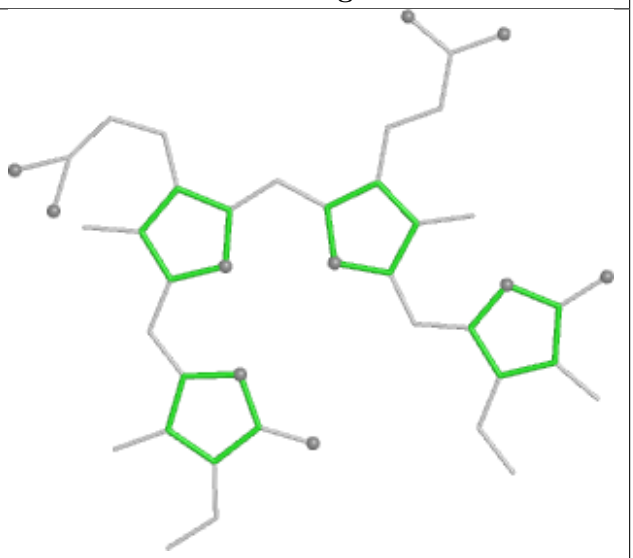
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Bond angles

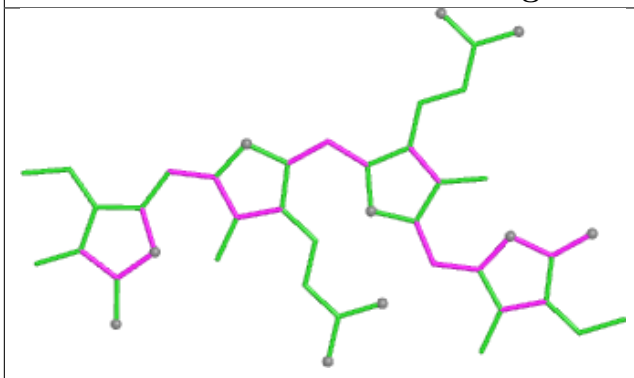


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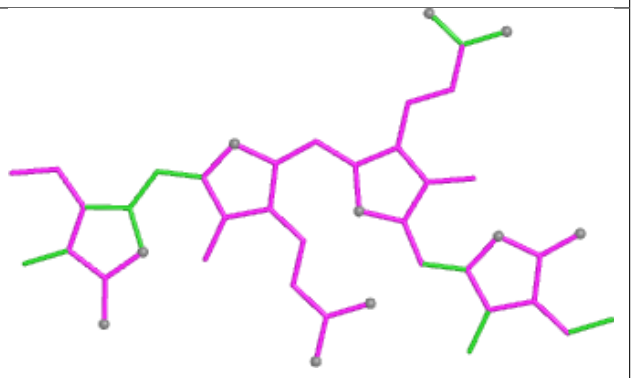


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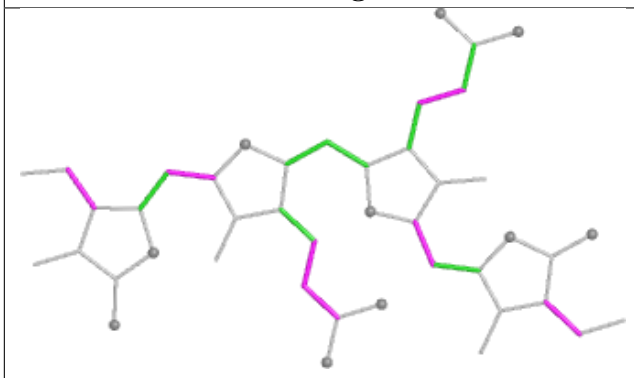
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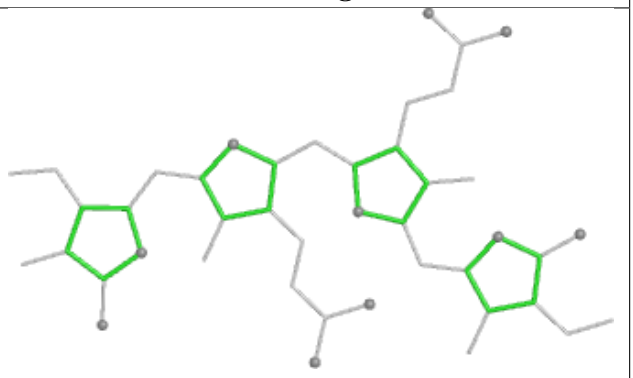
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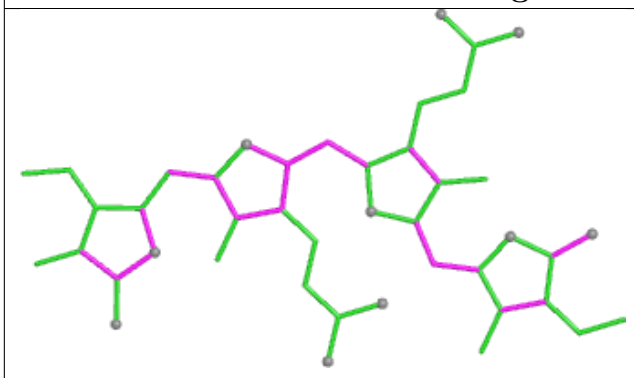


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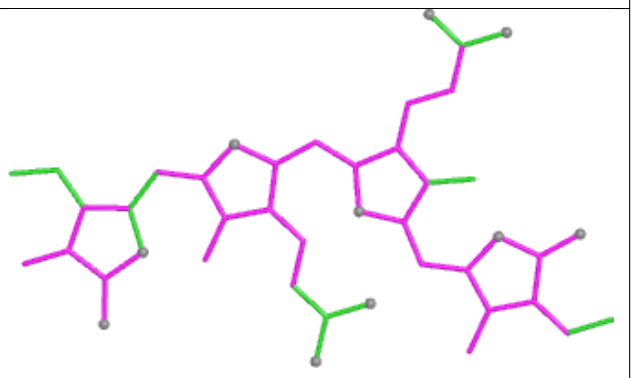


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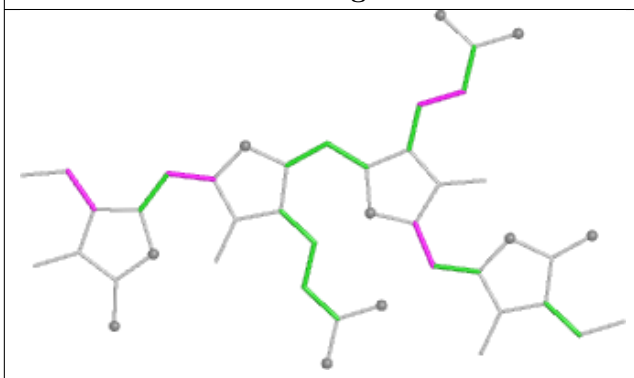
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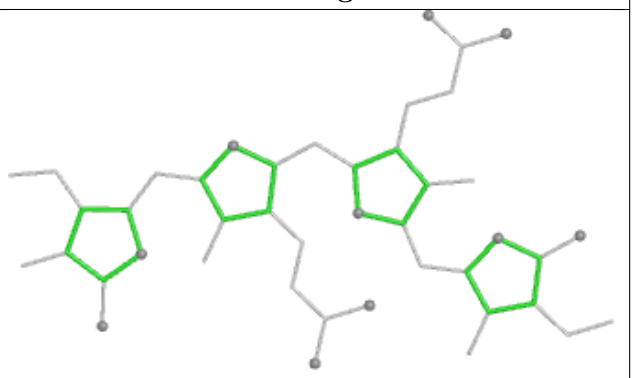
Bond lengths



Bond angles

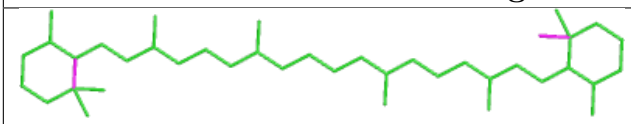


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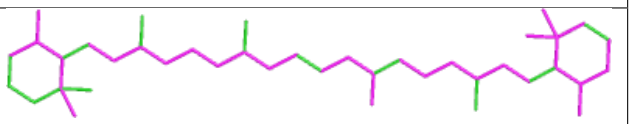


Rings

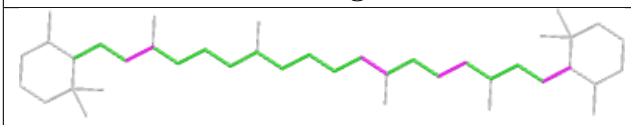
Ligand BCR XD 102



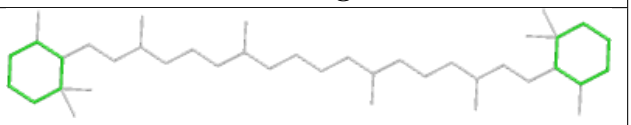
Bond lengths



Bond angles

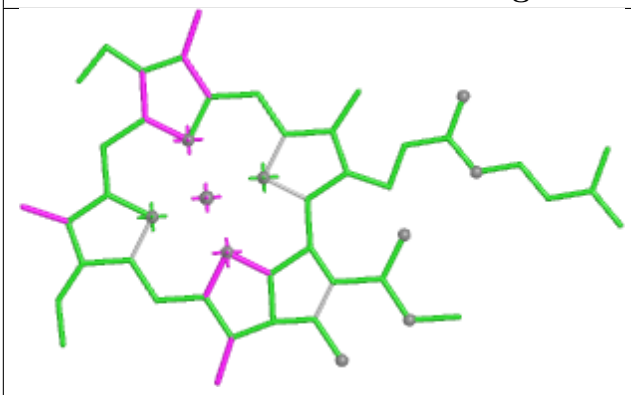


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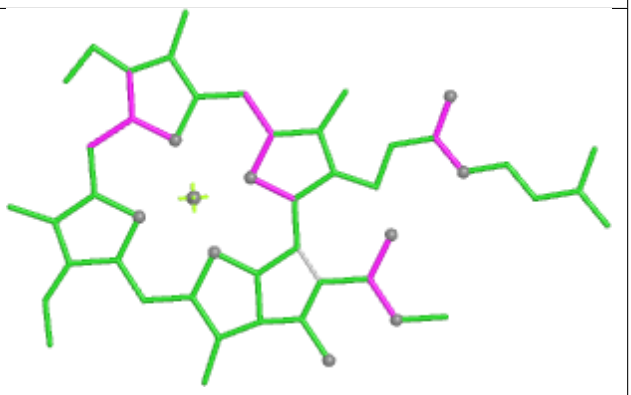


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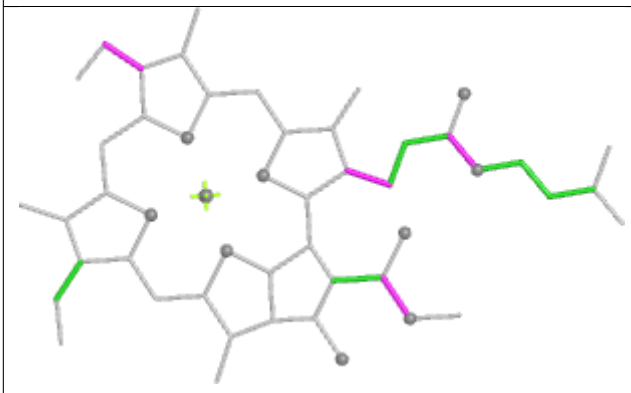
Ligand CLA CE 514



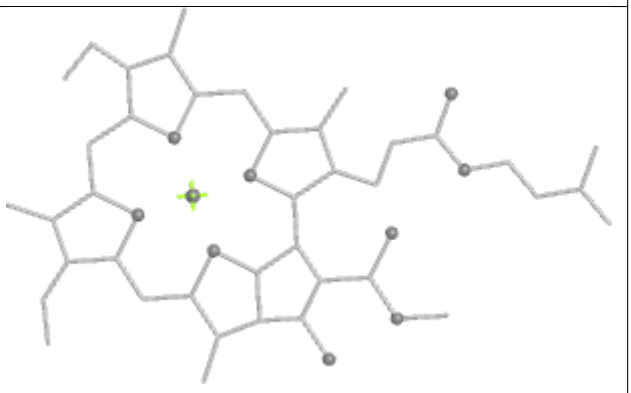
Bond lengths



Bond angles

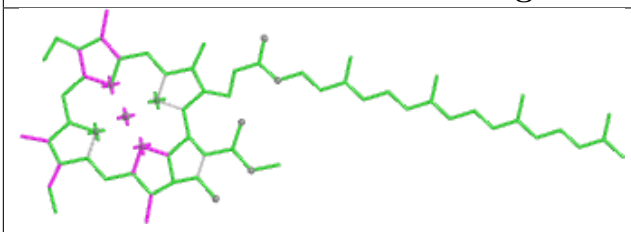


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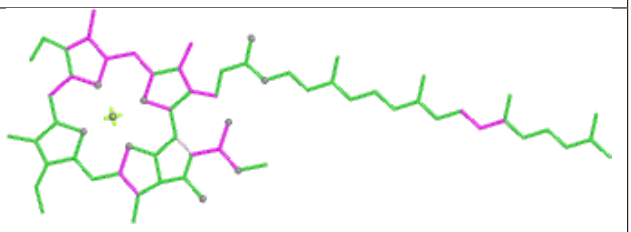


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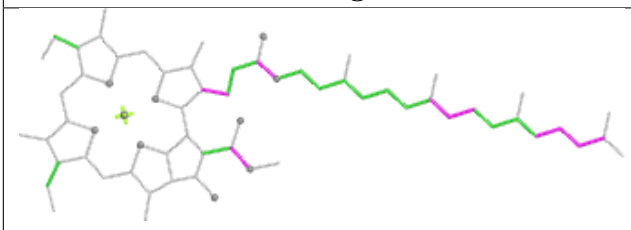
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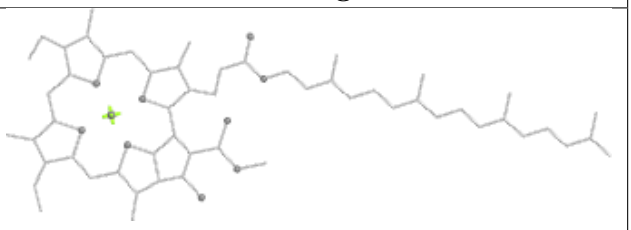
Bond lengths



Bond angles

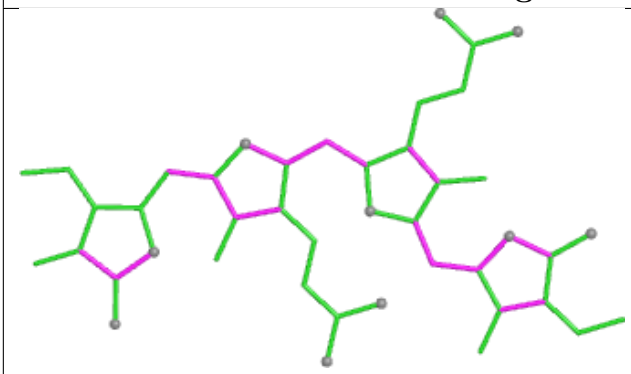


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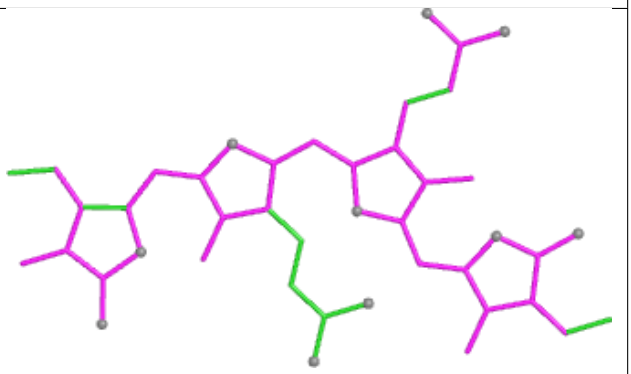


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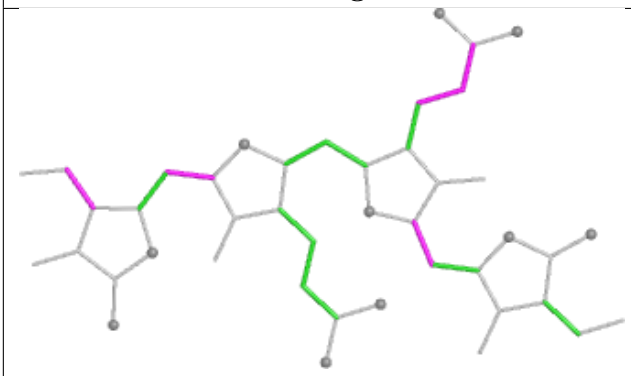
Ligand CYC 4L 201



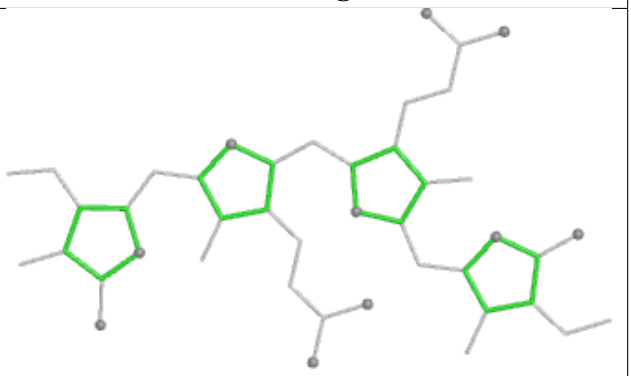
Bond lengths



Bond angles

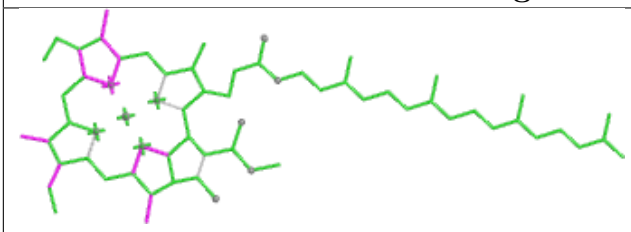


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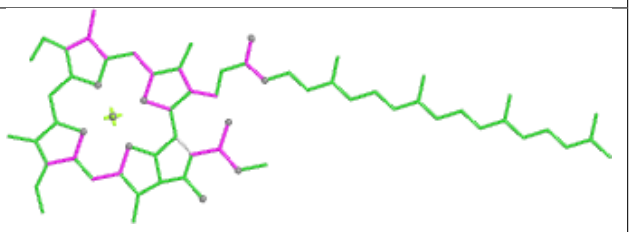


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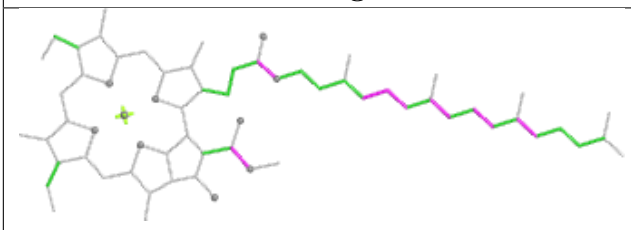
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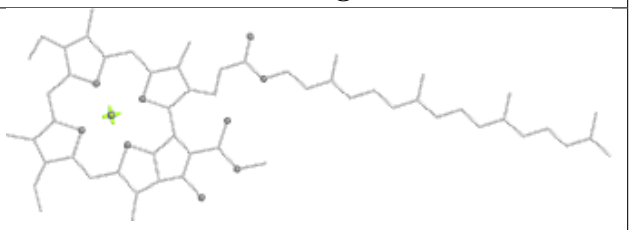
Bond lengths



Bond angles



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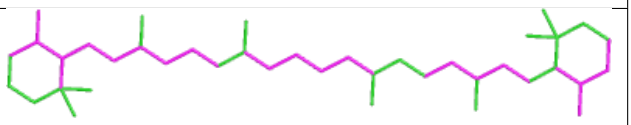


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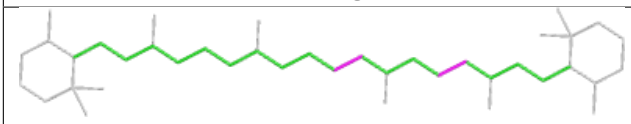
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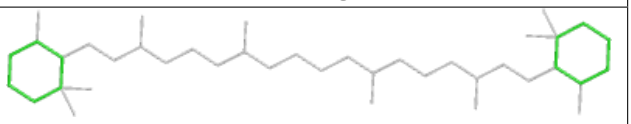
Bond lengths



Bond angles

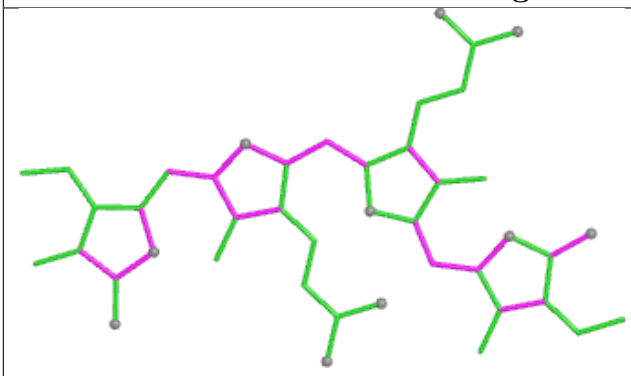


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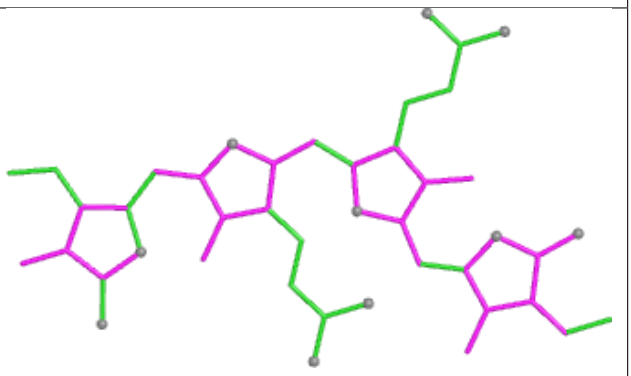


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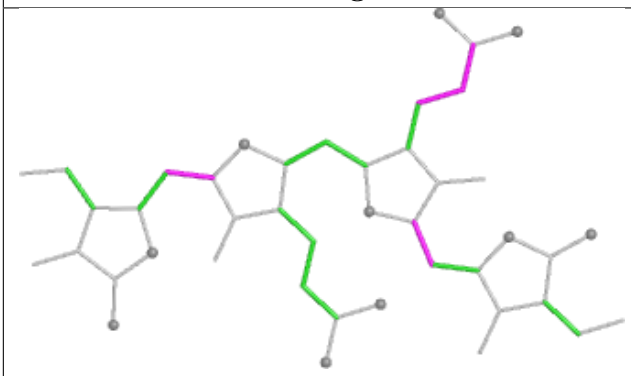
Ligand CYC 9K 201



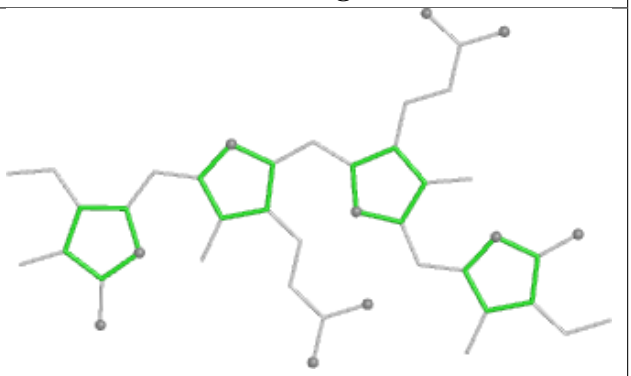
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Bond angles

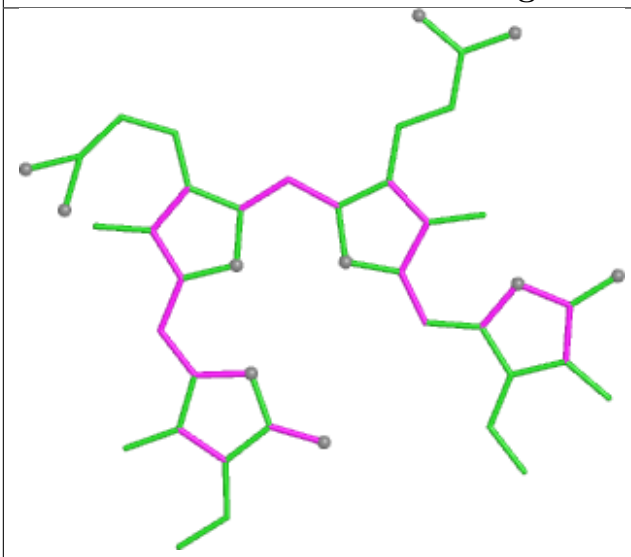


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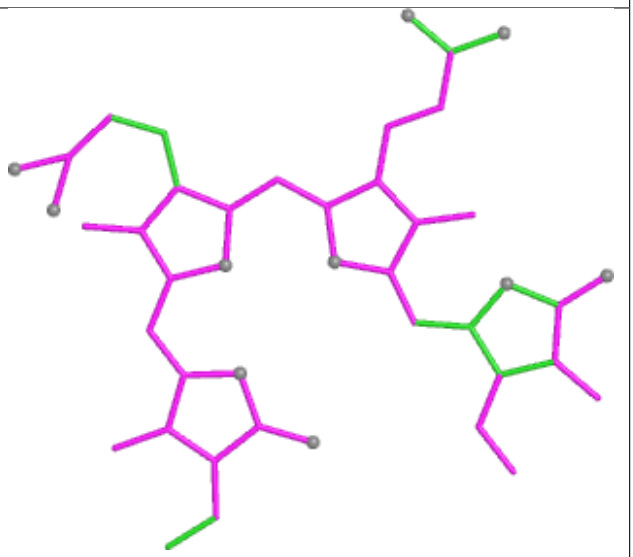


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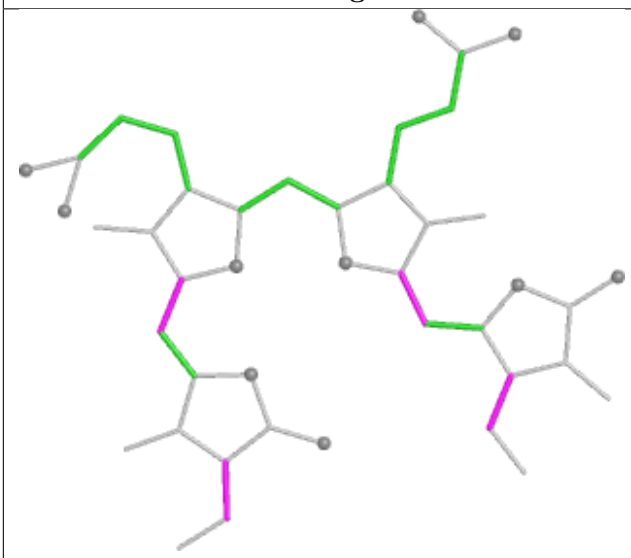
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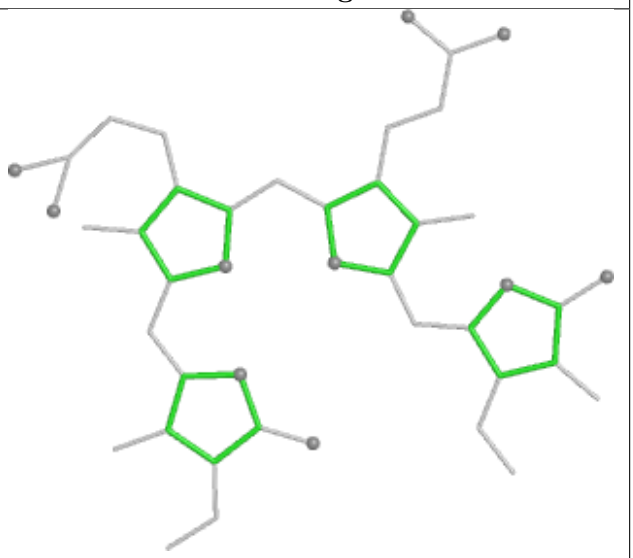
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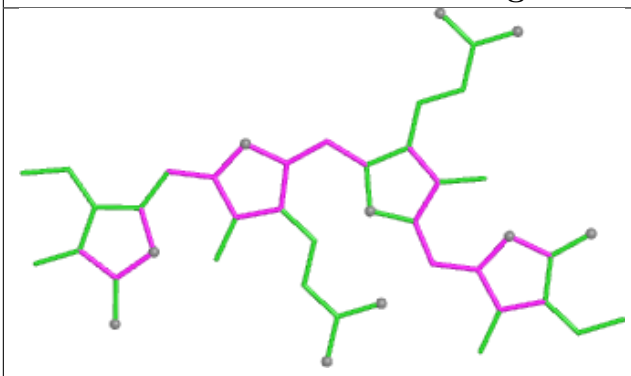


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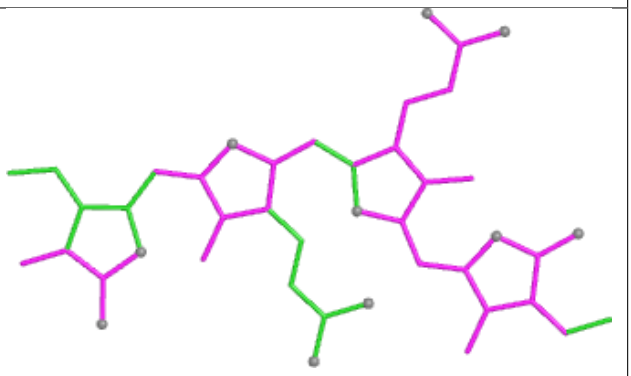


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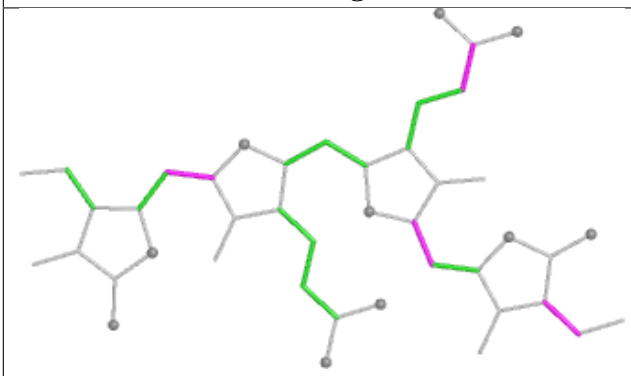
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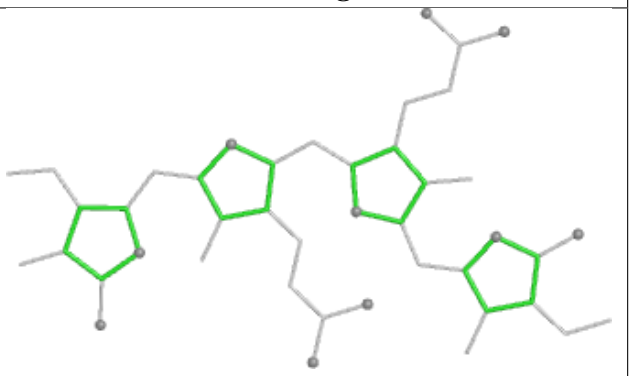
Bond lengths



Bond angles

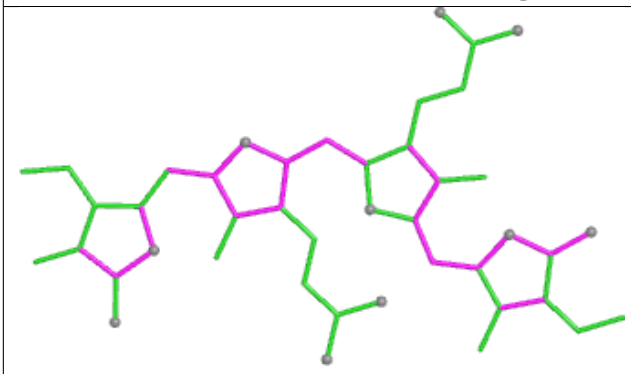


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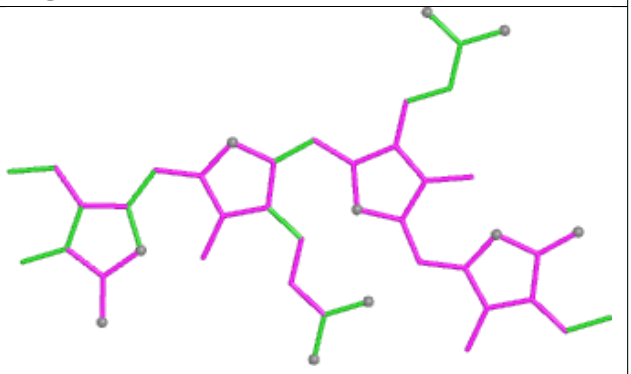


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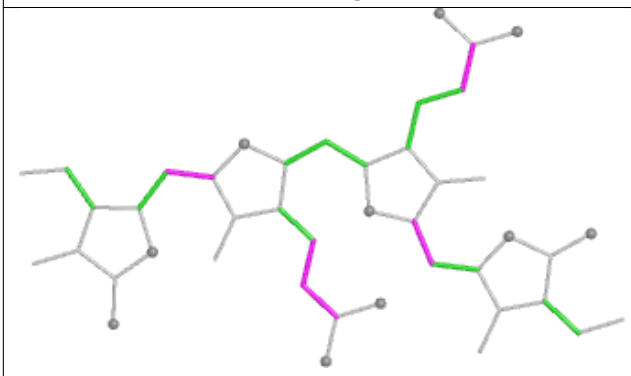
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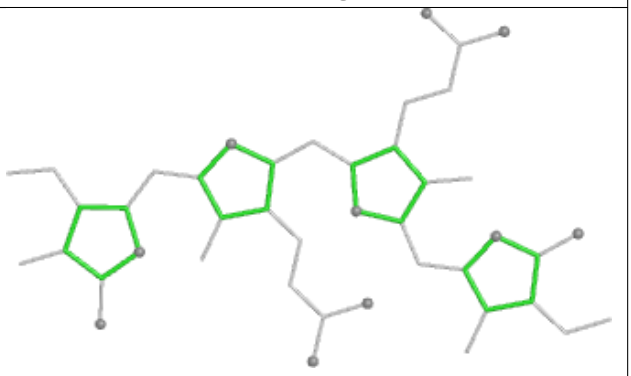
Bond lengths



Bond angles

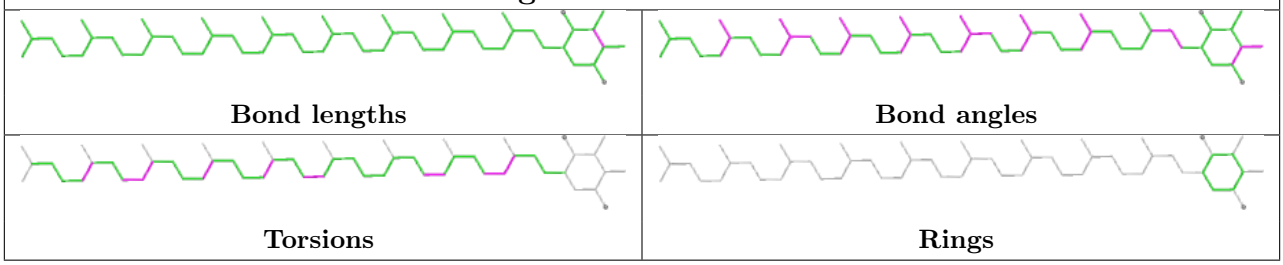


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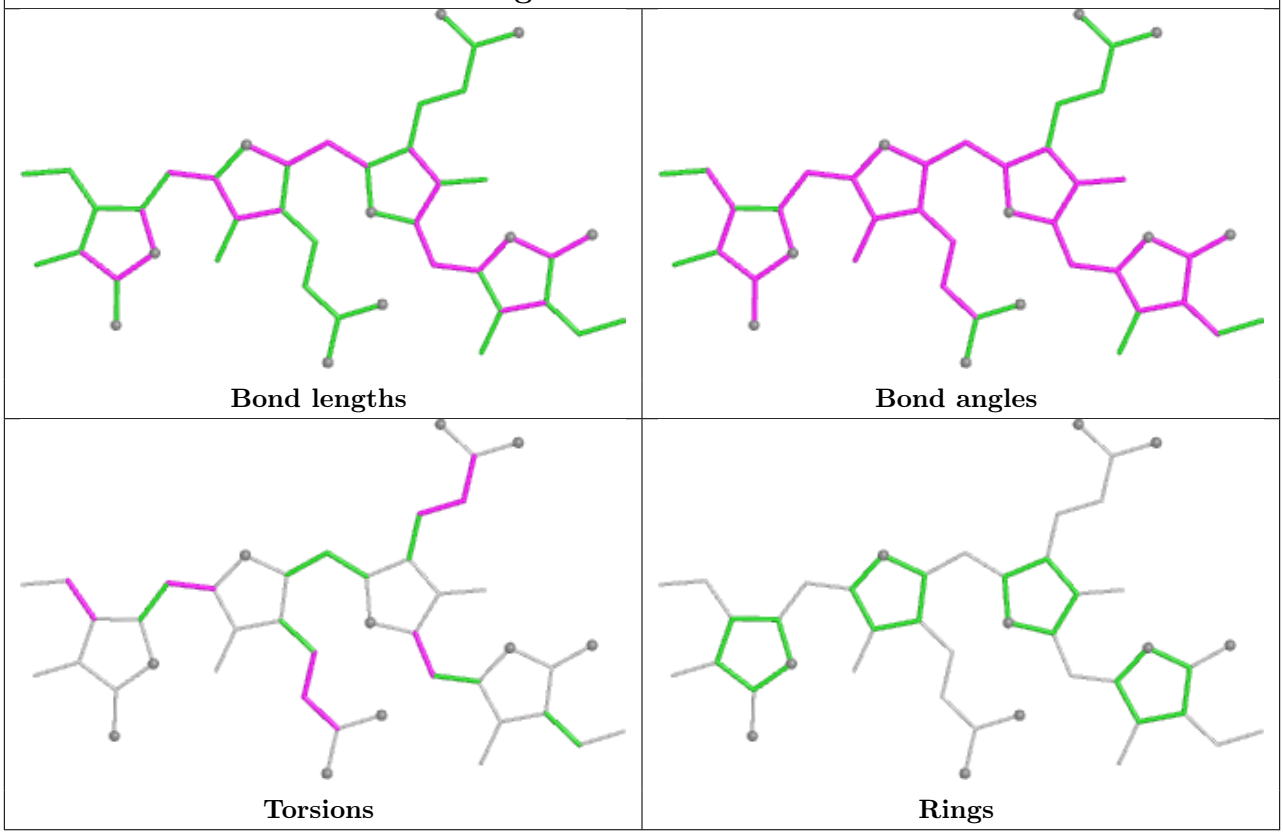


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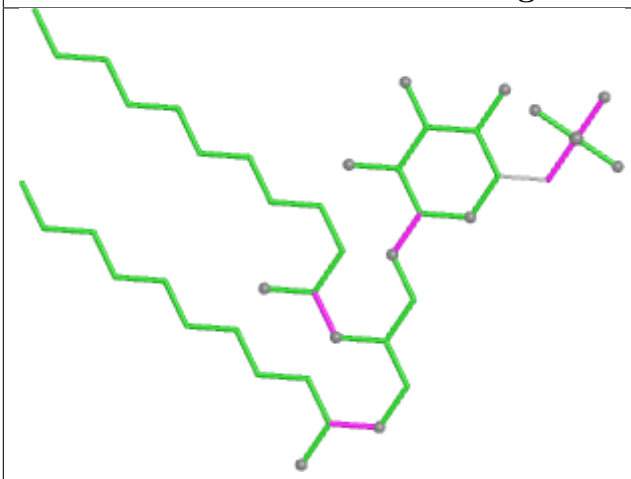
Ligand PL9 AE 406



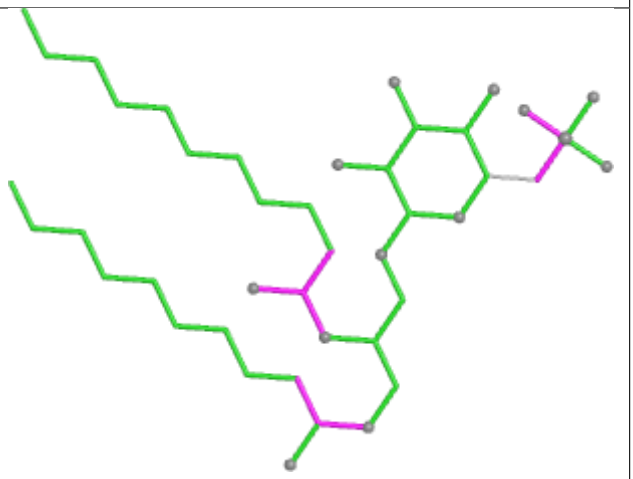
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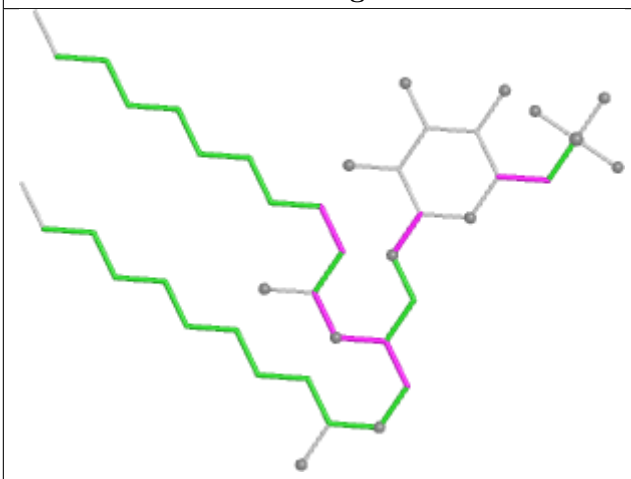
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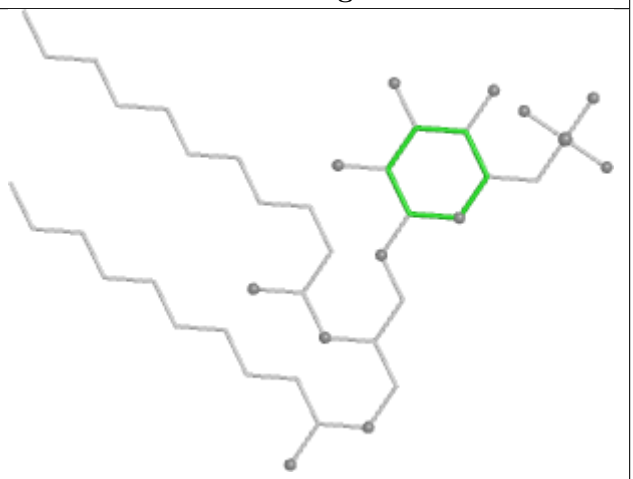
Bond lengths



Bond angles

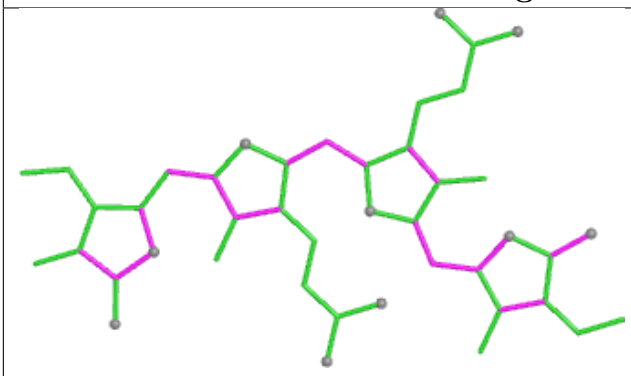


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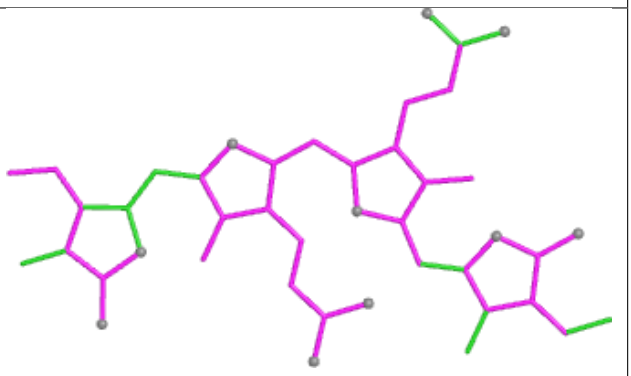


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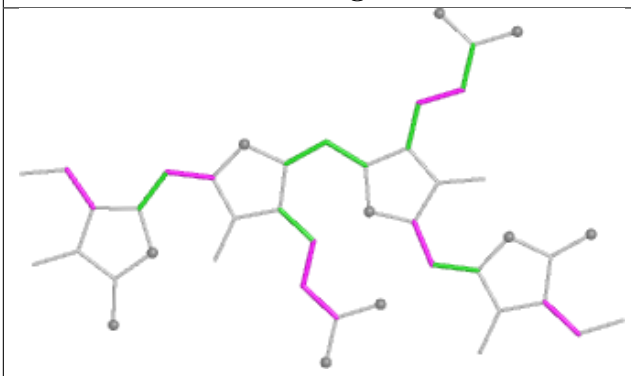
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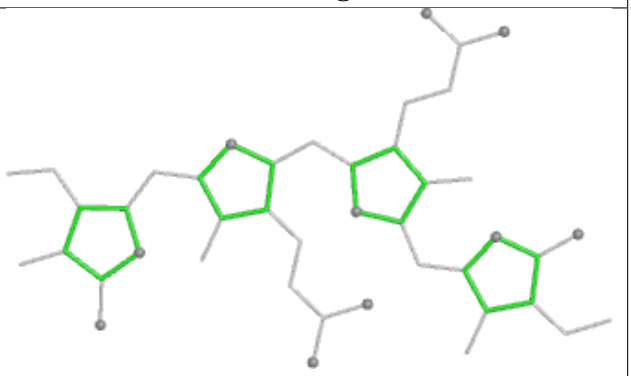
Bond lengths



Bond angles

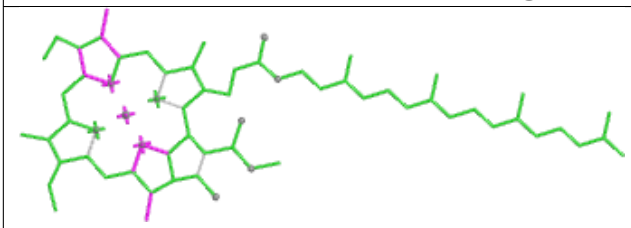


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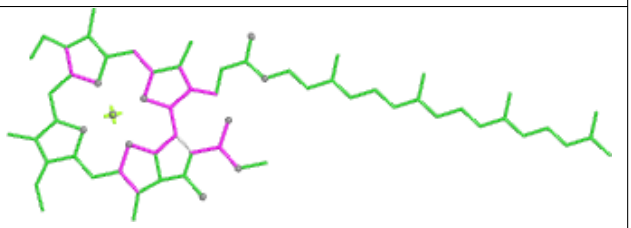


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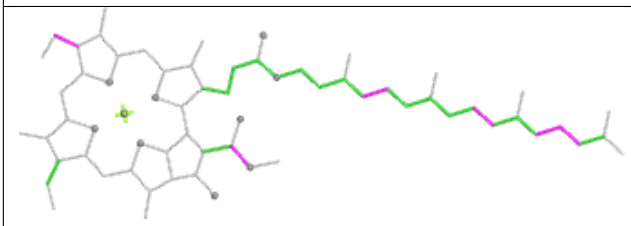
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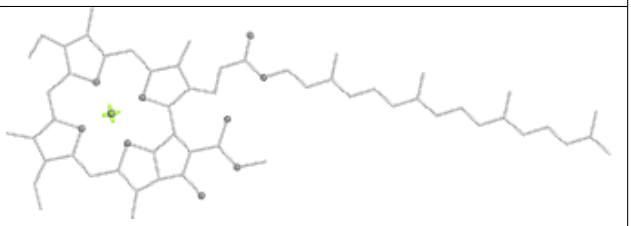
Bond lengths



Bond angles

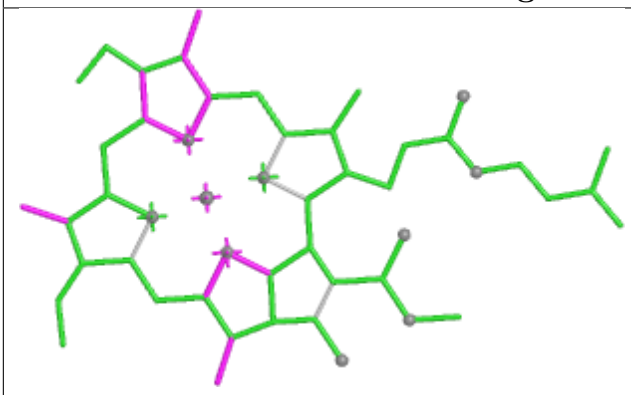


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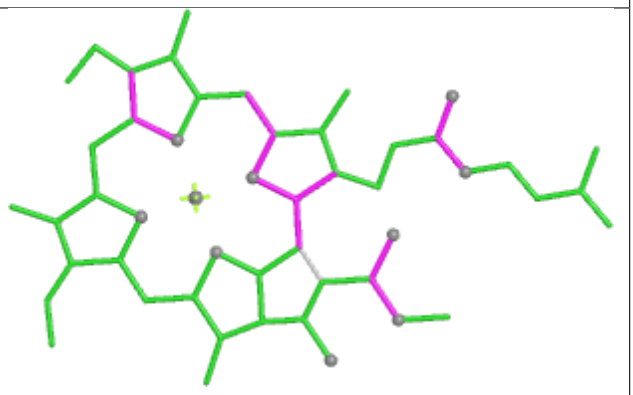


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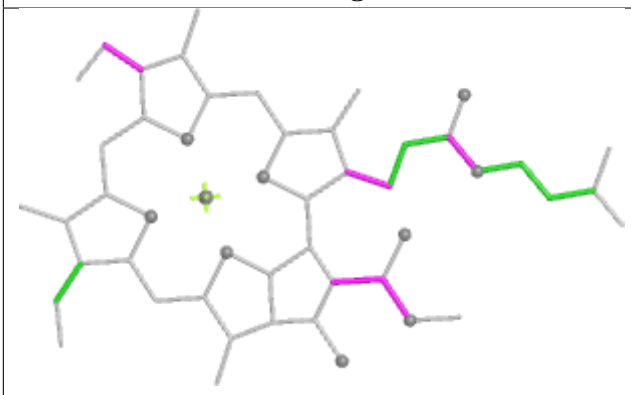
Ligand CLA cE 513



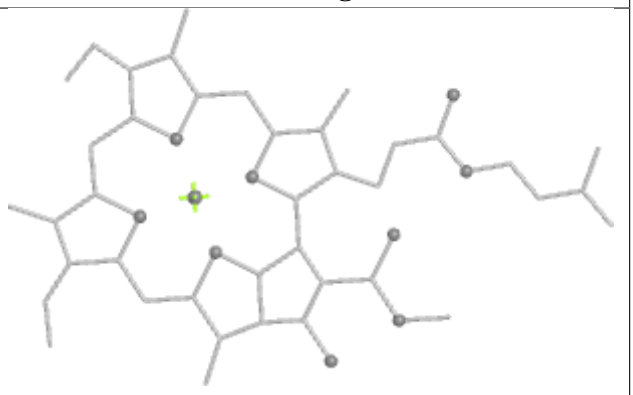
Bond lengths



Bond angles

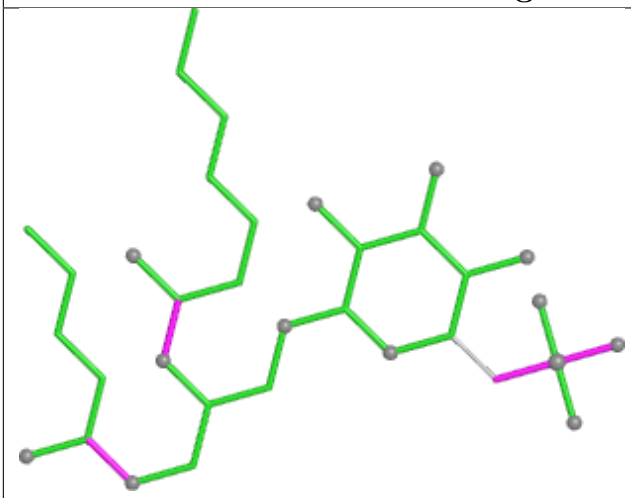


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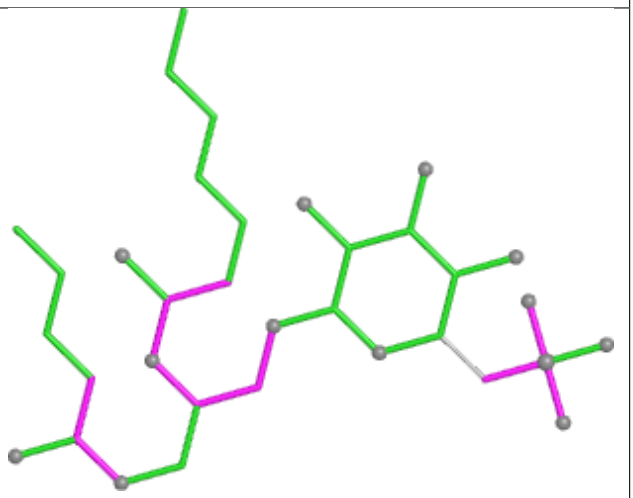


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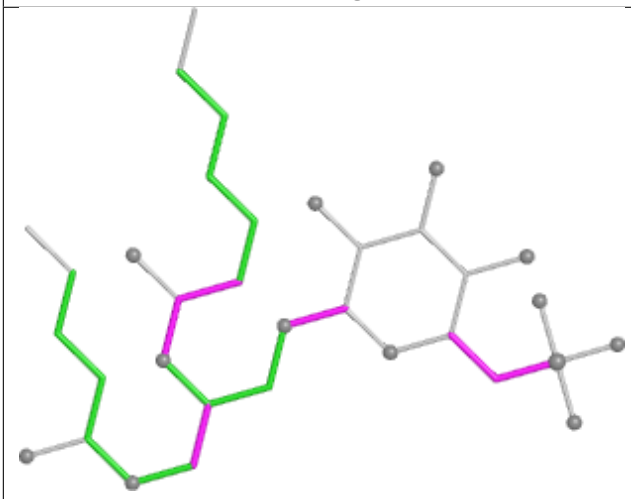
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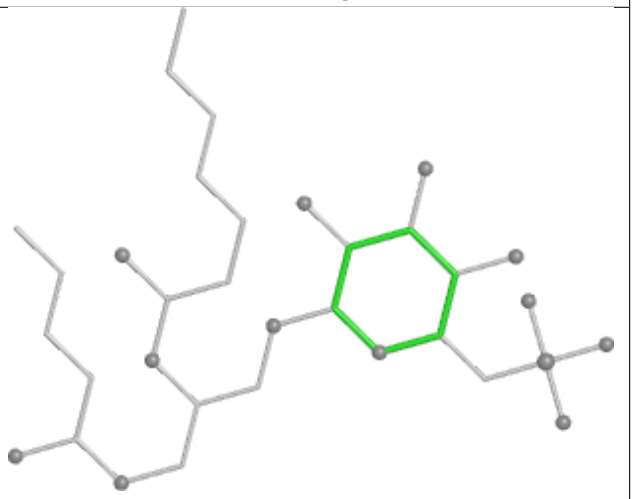
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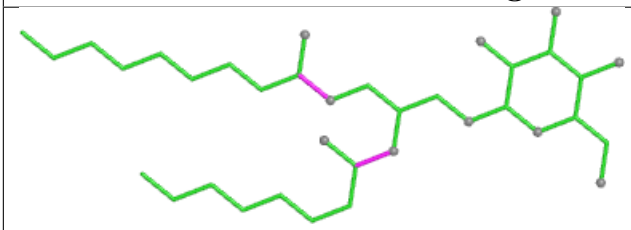


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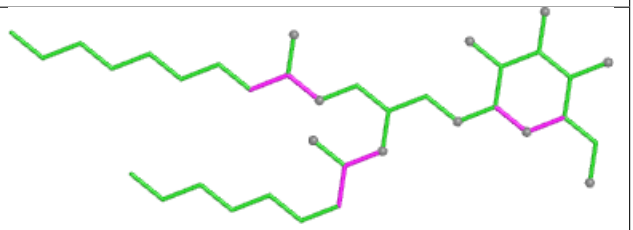


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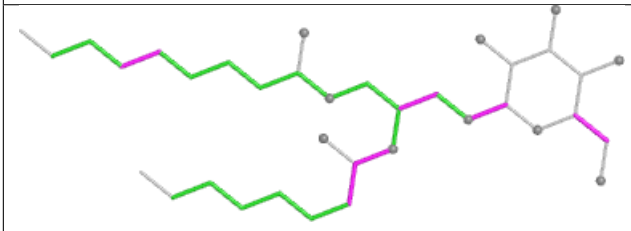
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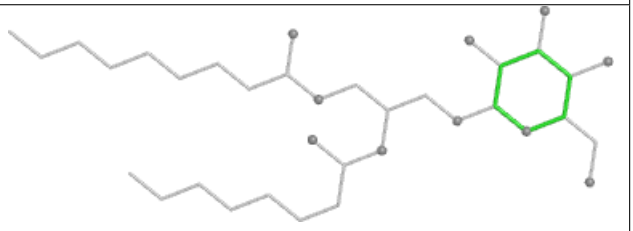
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Bond angles

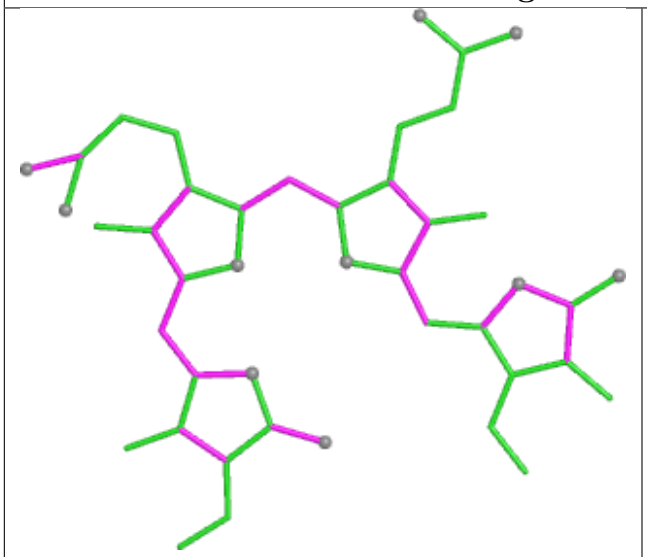


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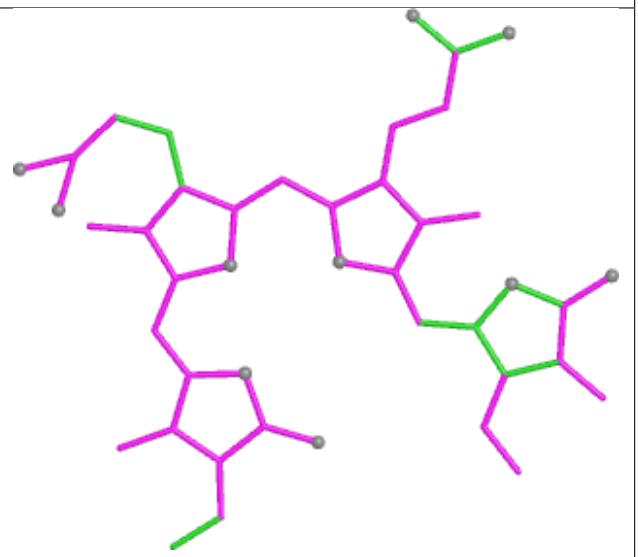


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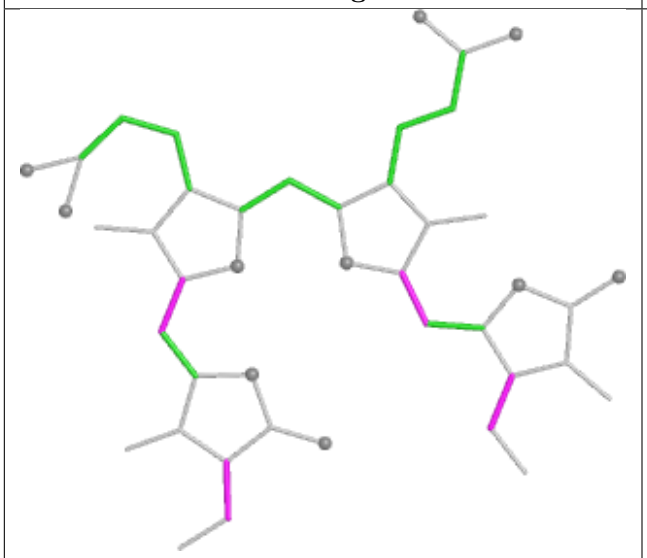
Ligand CYC k2 201



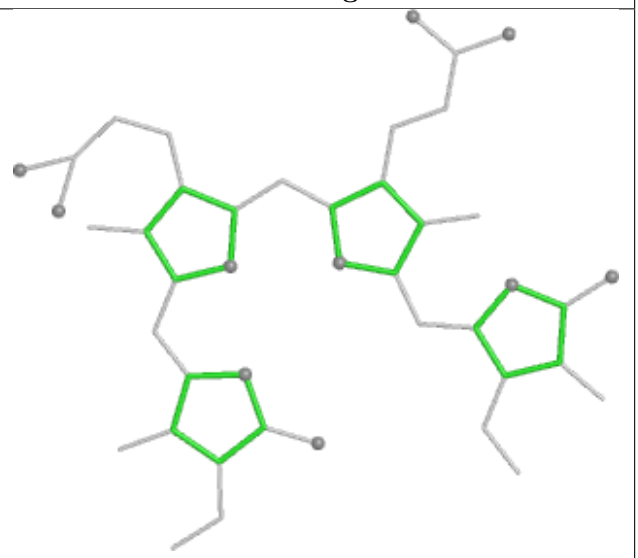
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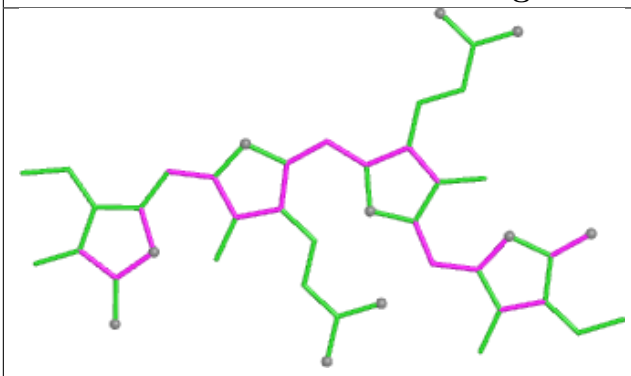


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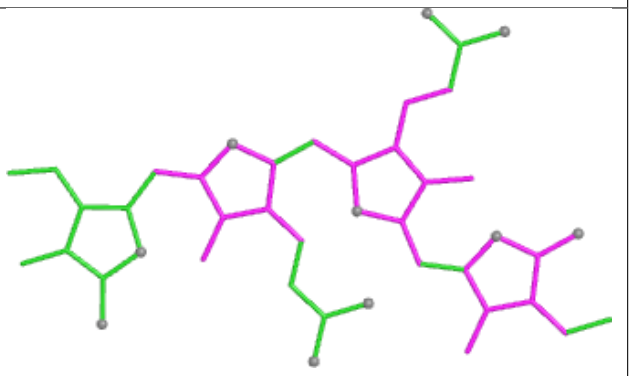


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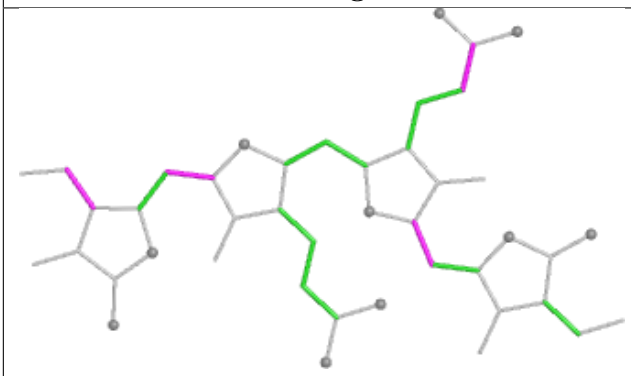
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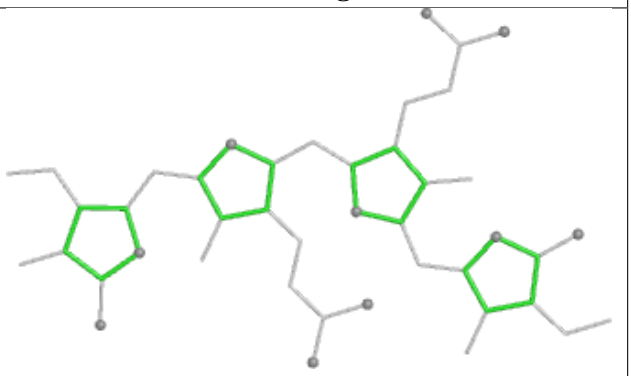
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Bond angles

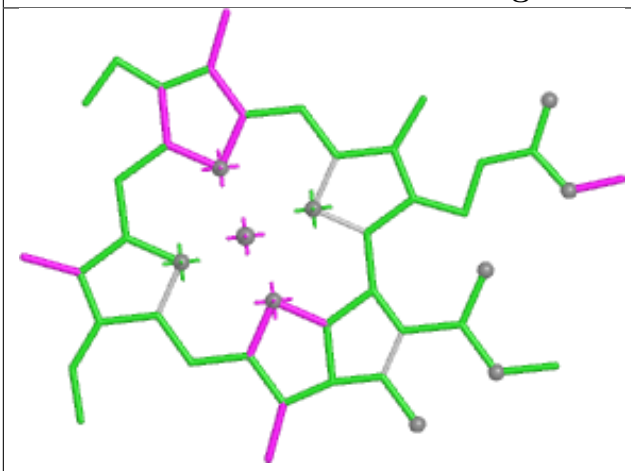


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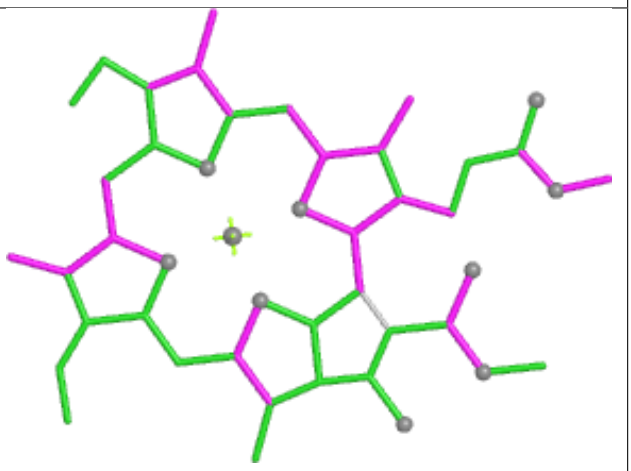


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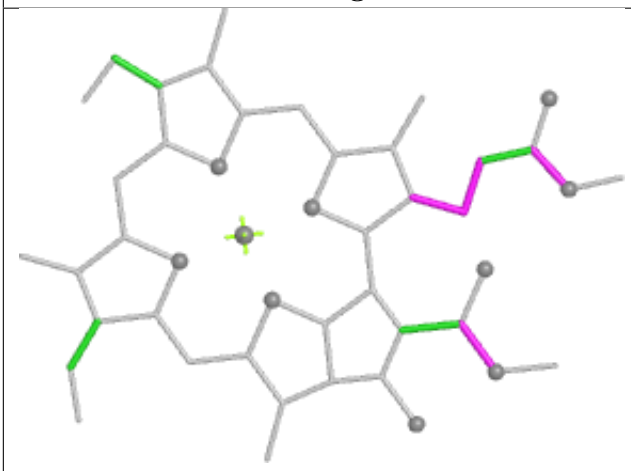
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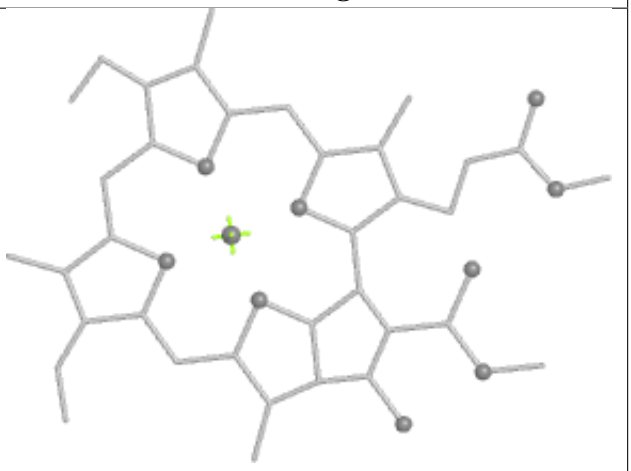
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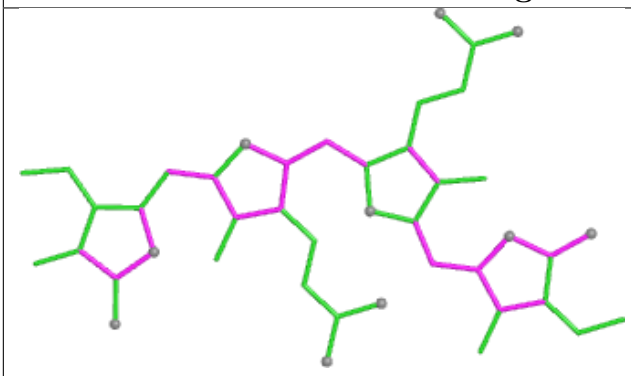


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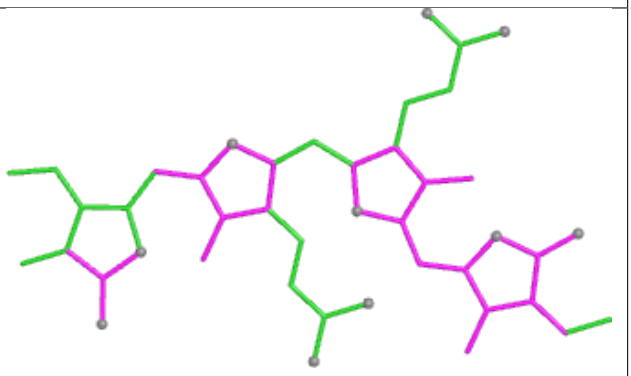


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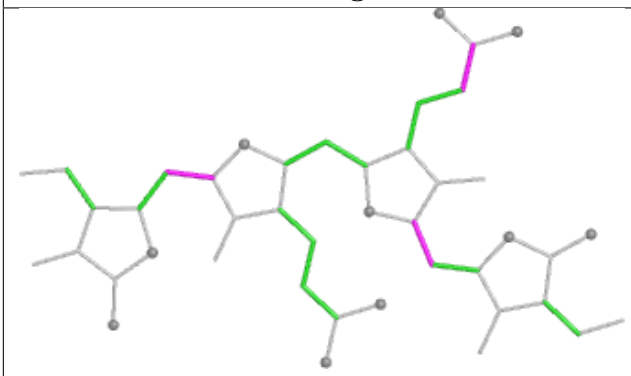
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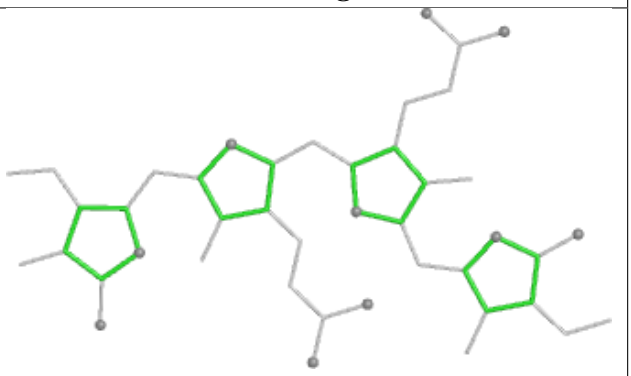
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Bond angles

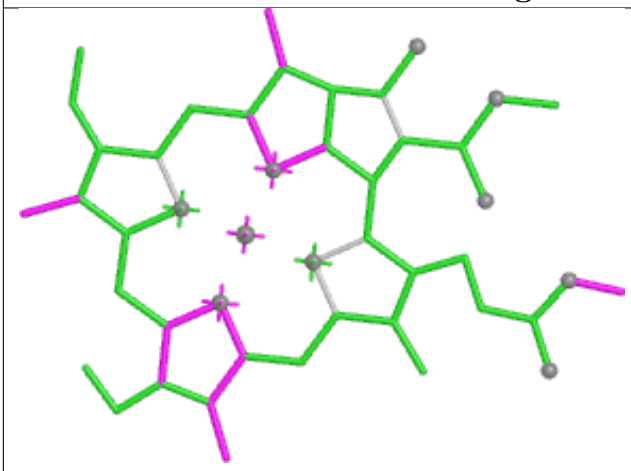


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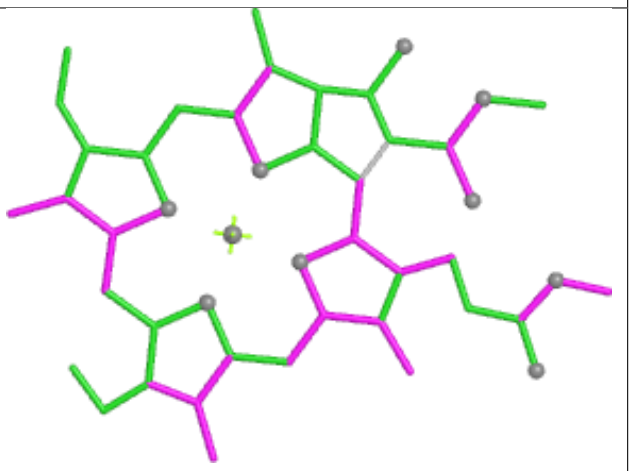


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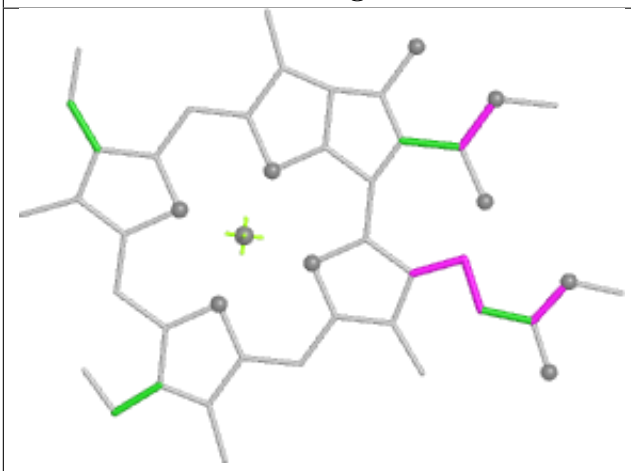
Ligand CLA A1 404



Bond lengths



Bond angles

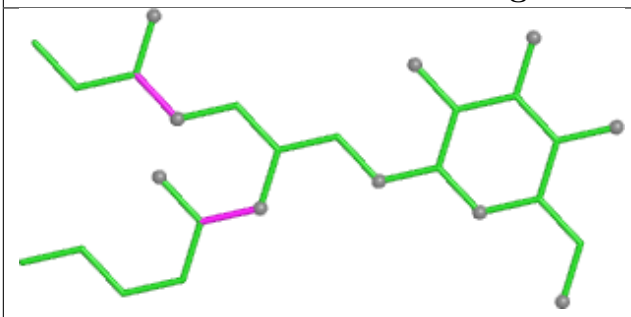


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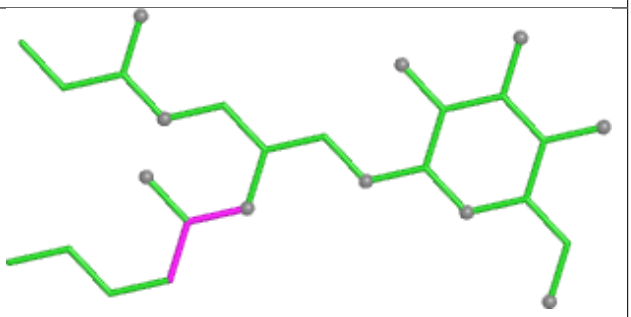


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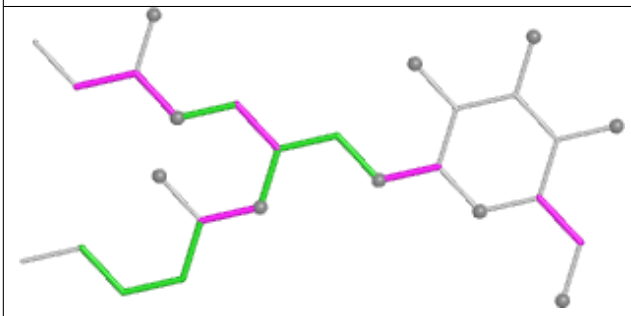
Ligand LMG JD 102



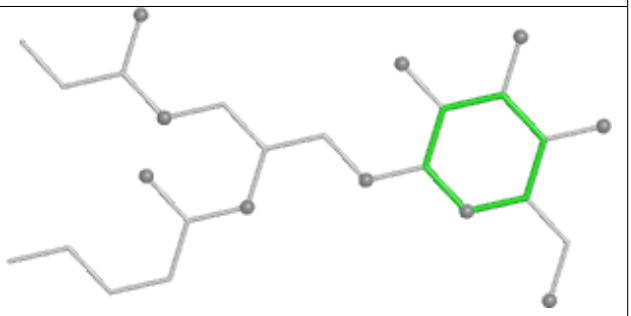
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Bond angles

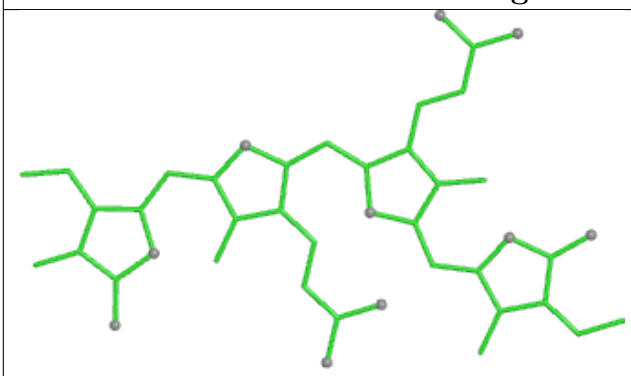


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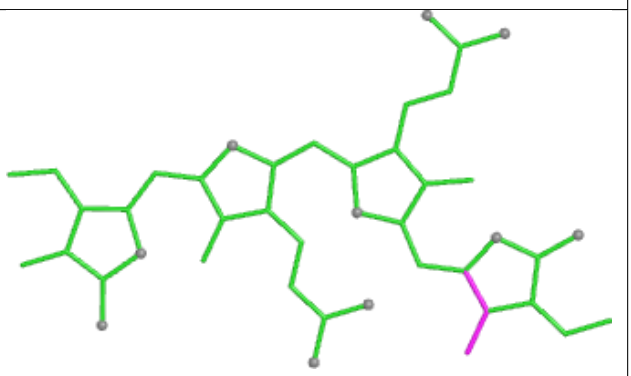


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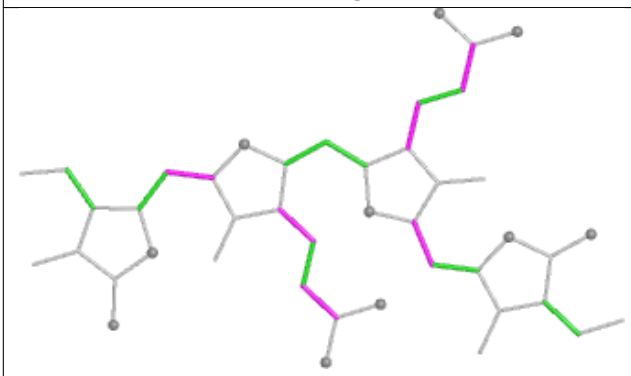
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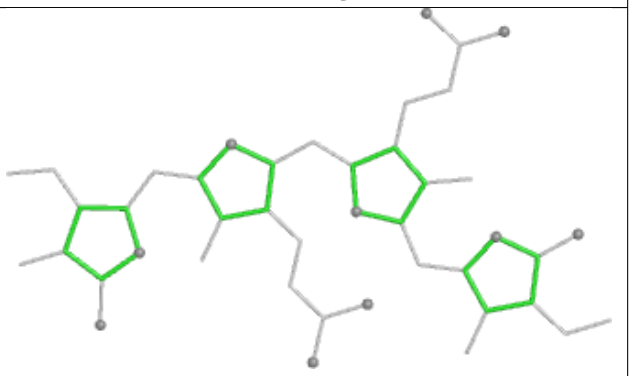
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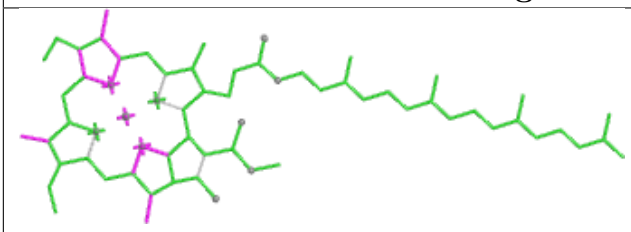


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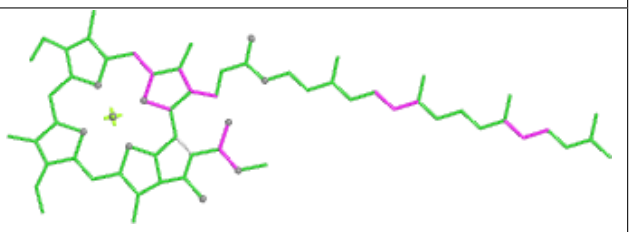


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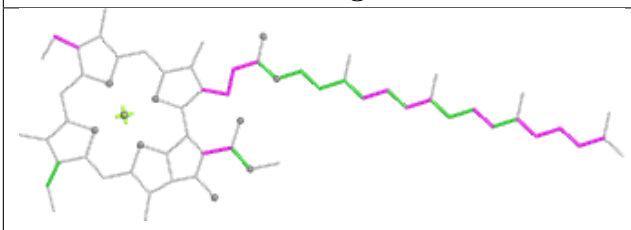
Ligand CLA bE 613



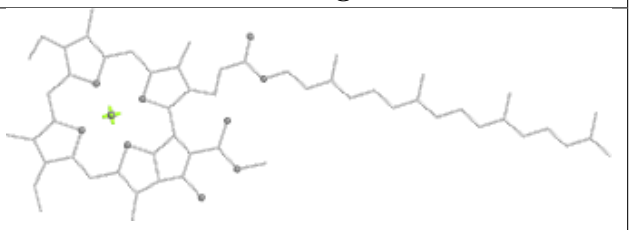
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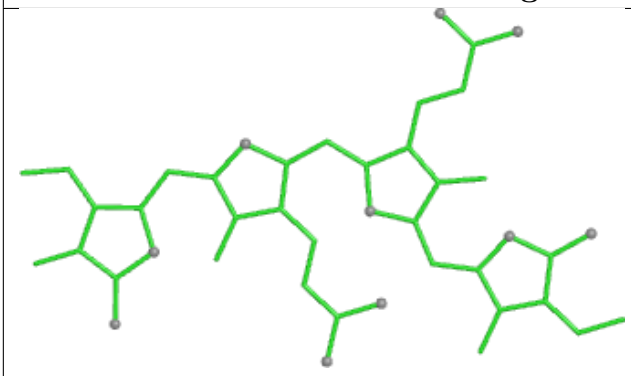


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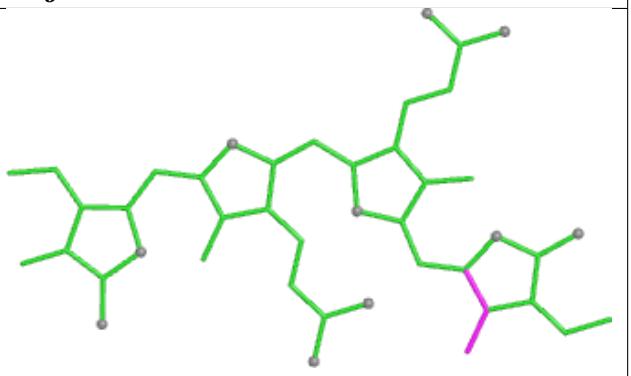


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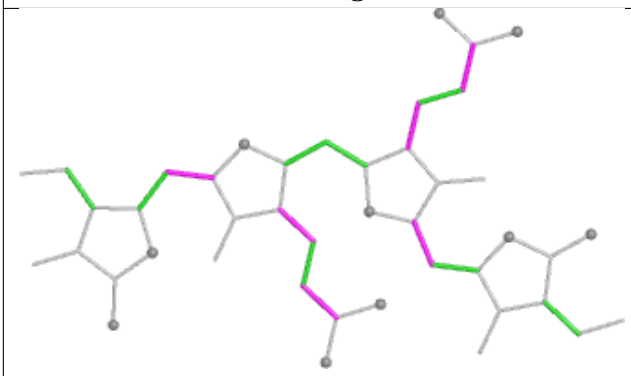
Ligand CYC j2 202



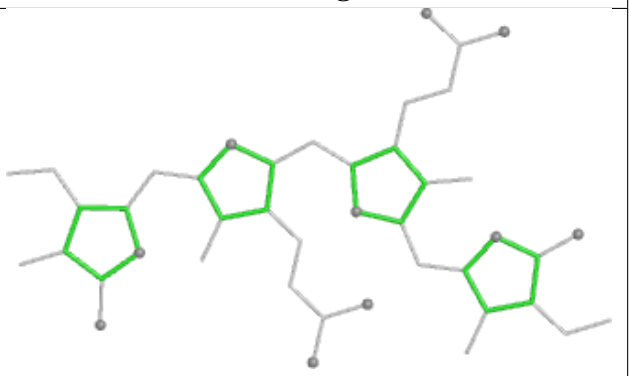
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Bond angles

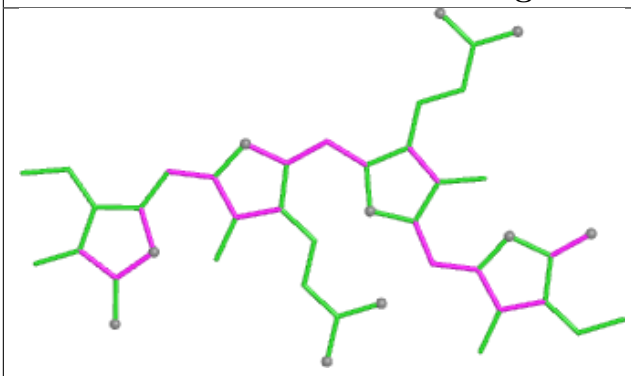


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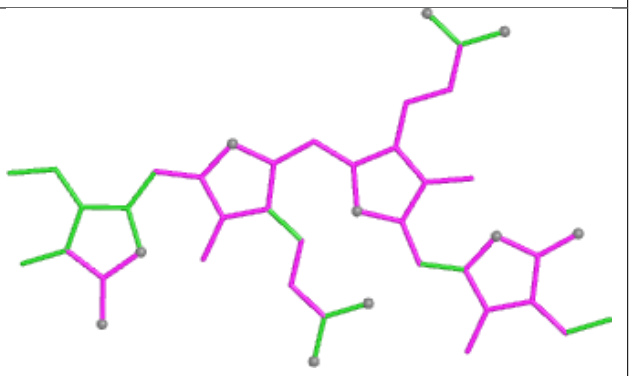


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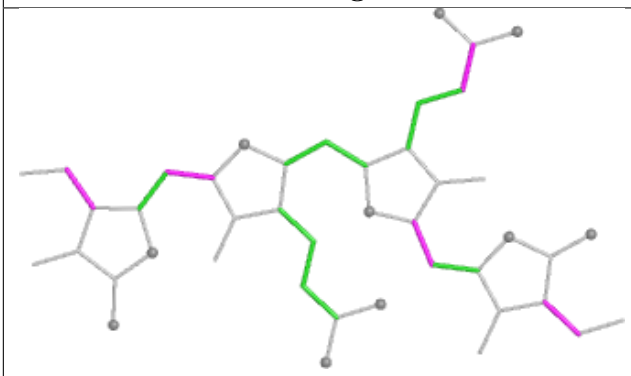
Ligand CYC aF 201



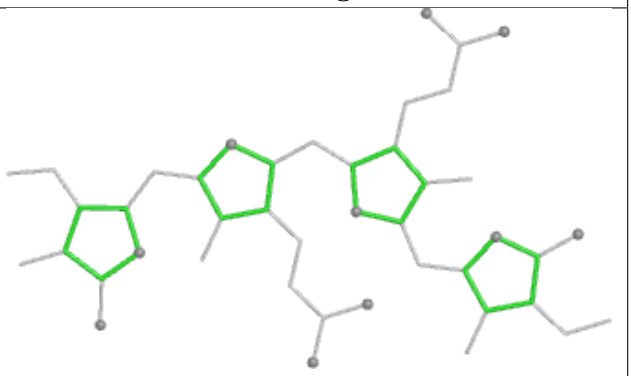
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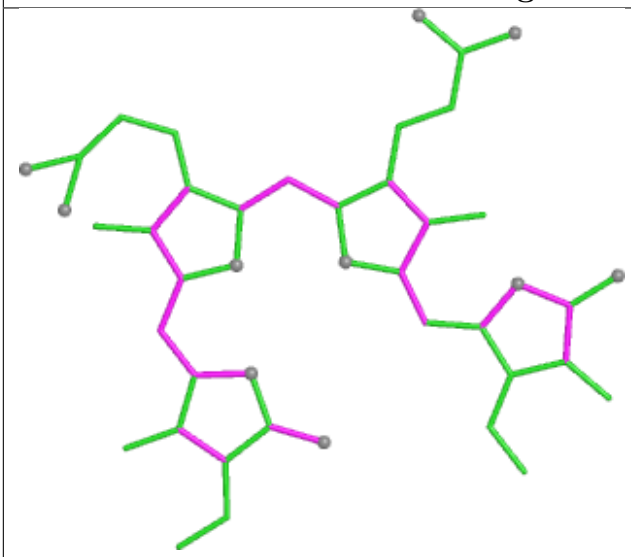


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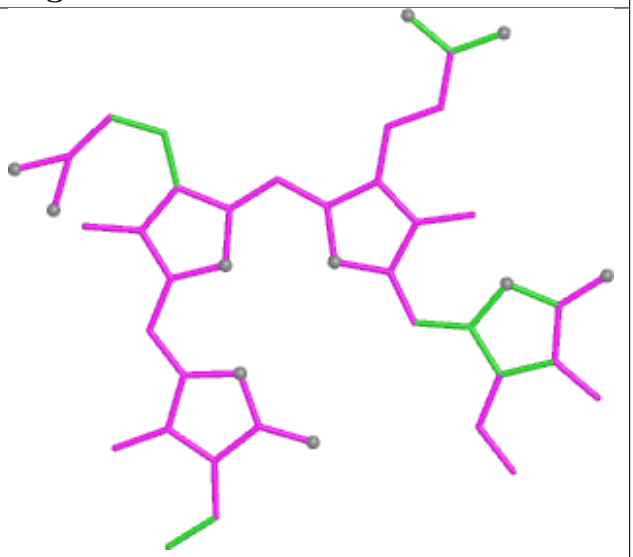


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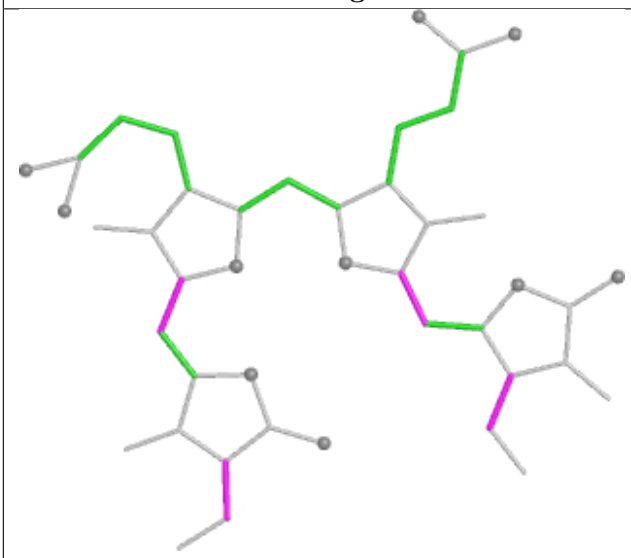
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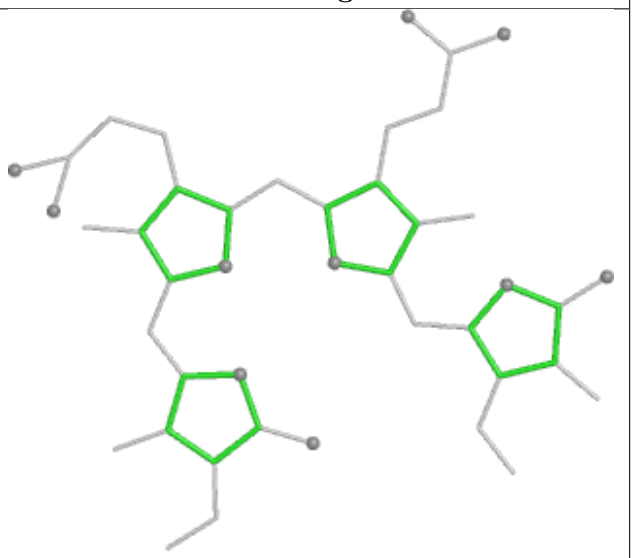
Bond lengths



Bond angles

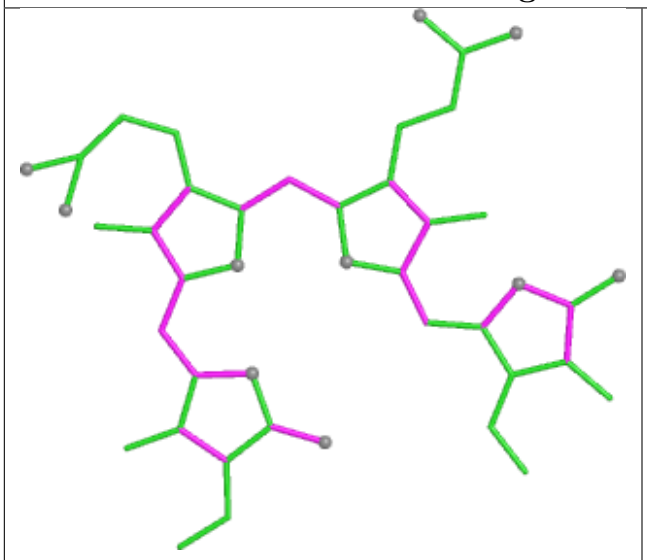


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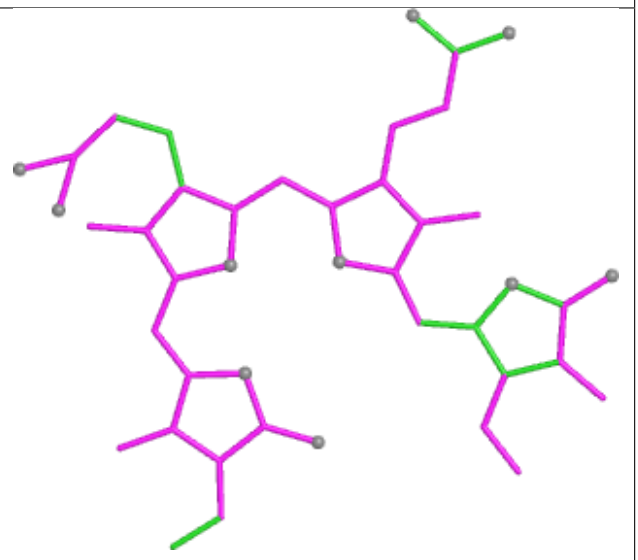


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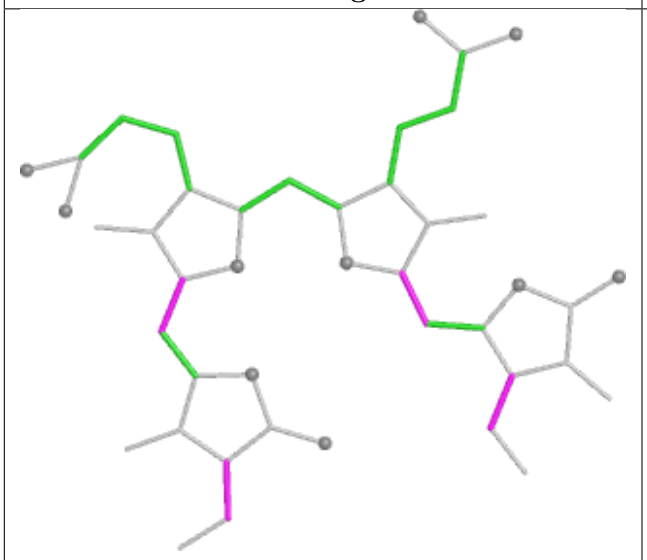
Ligand CYC eJ 201



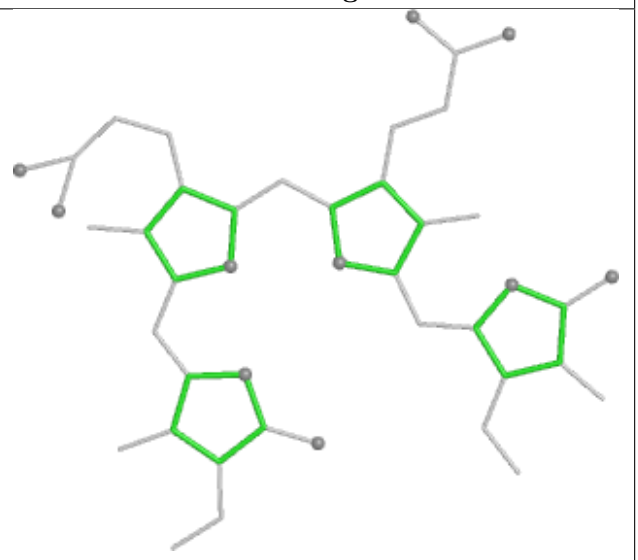
Bond lengths



Bond angles



Torsions

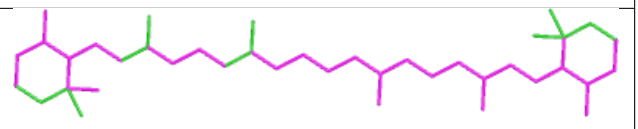


Rings

Ligand BCR Z1 101



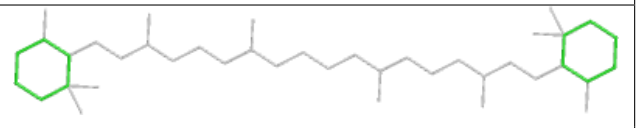
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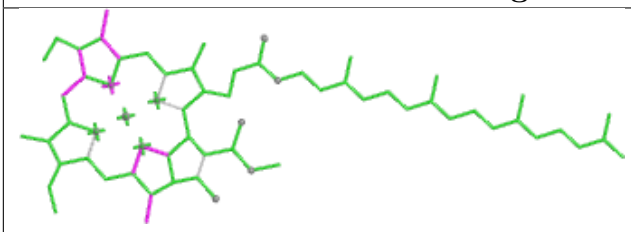
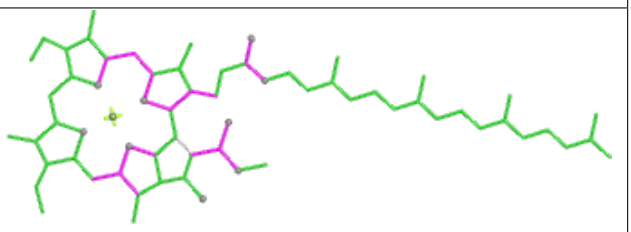
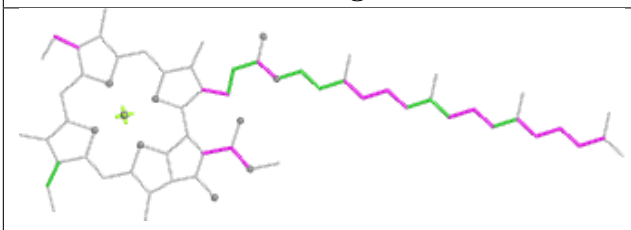
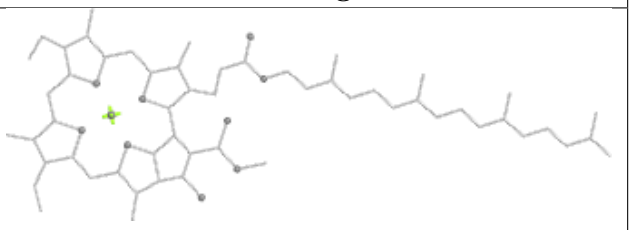
Bond angles



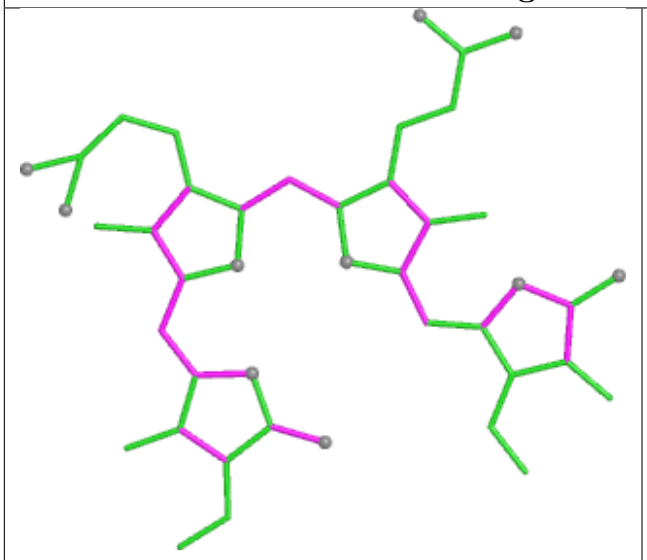
Torsions



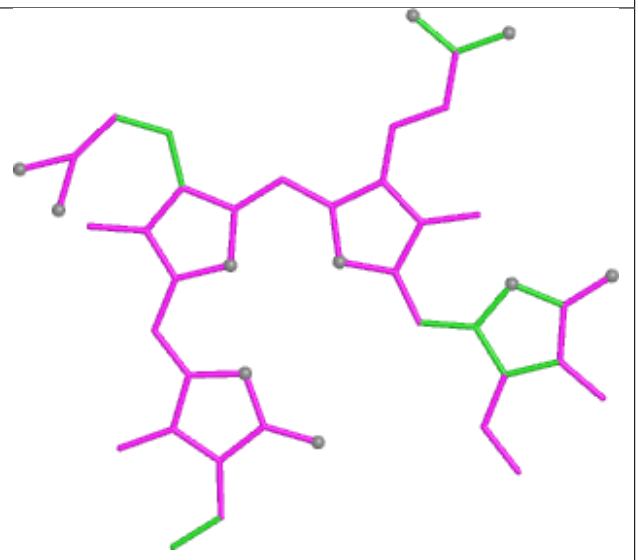
Rings

Ligand CLA CD 511	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

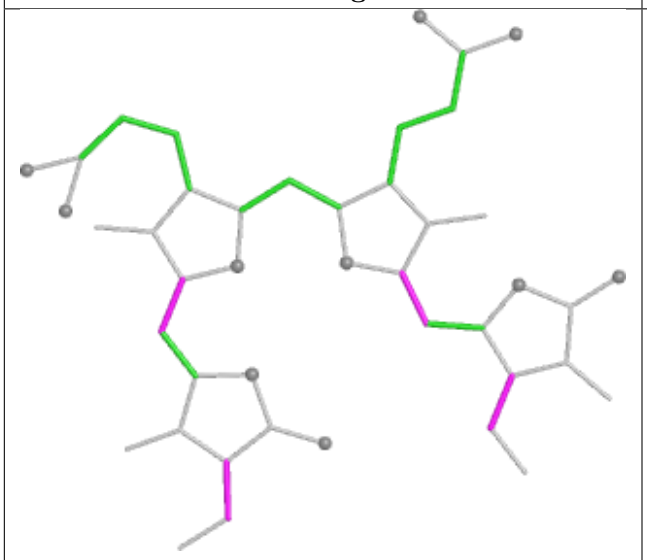
Ligand CYC iC 202



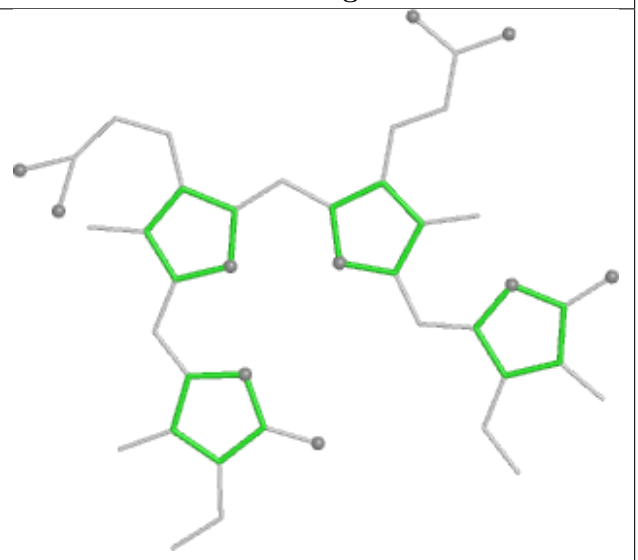
Bond lengths



Bond angles

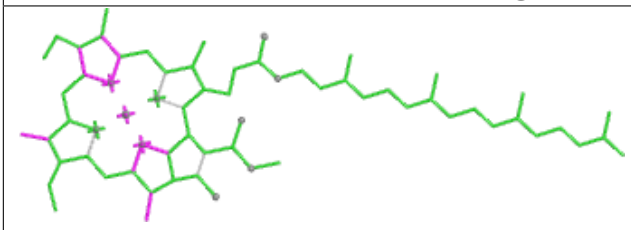


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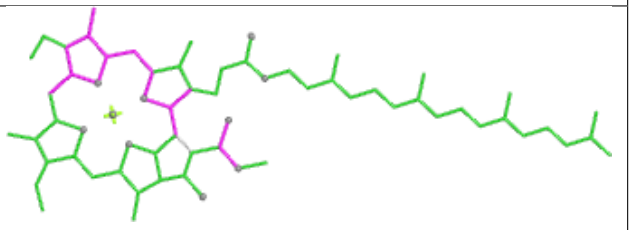


Rings

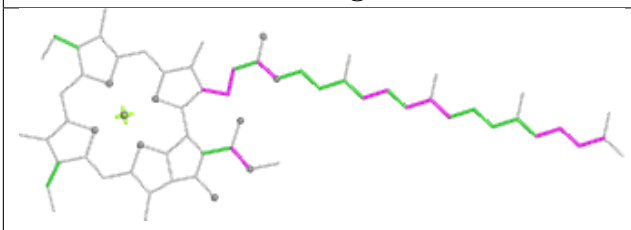
Ligand CLA CE 515



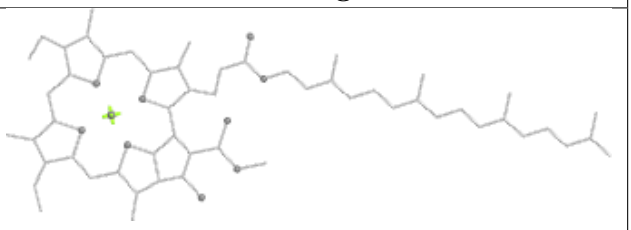
Bond lengths



Bond angles

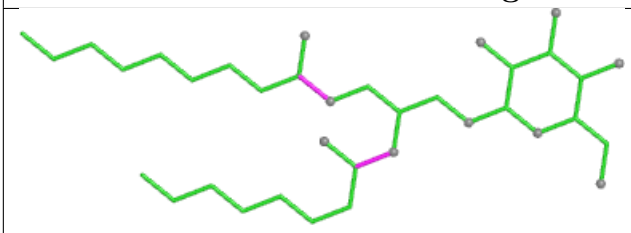


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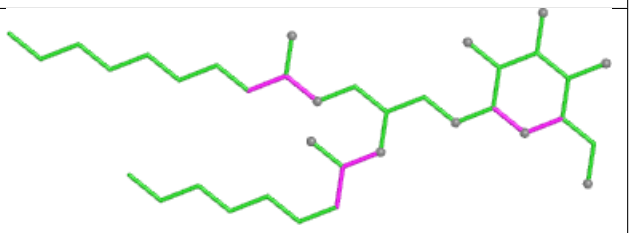


Rings

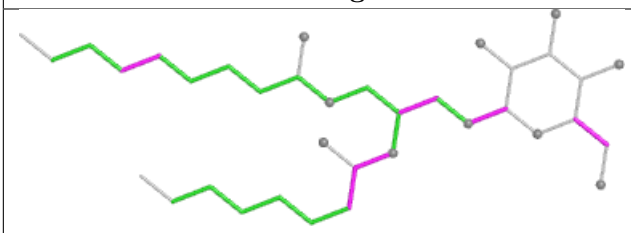
Ligand LMG MD 101



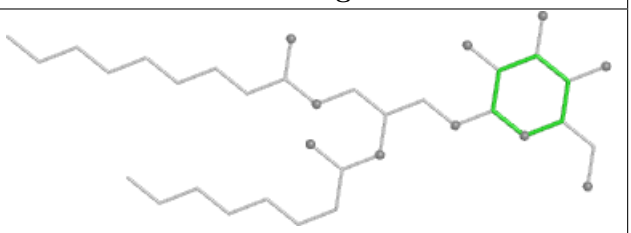
Bond lengths



Bond angles

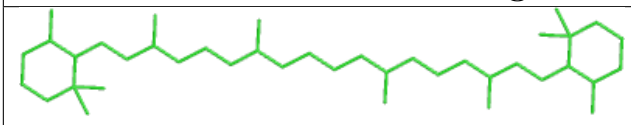


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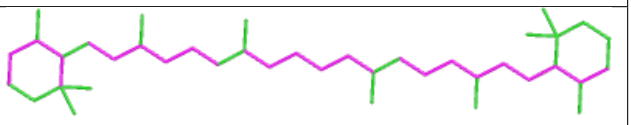


Rings

Ligand BCR CD 519



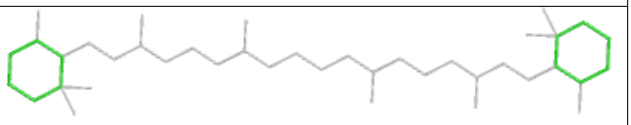
Bond lengths



Bond angles

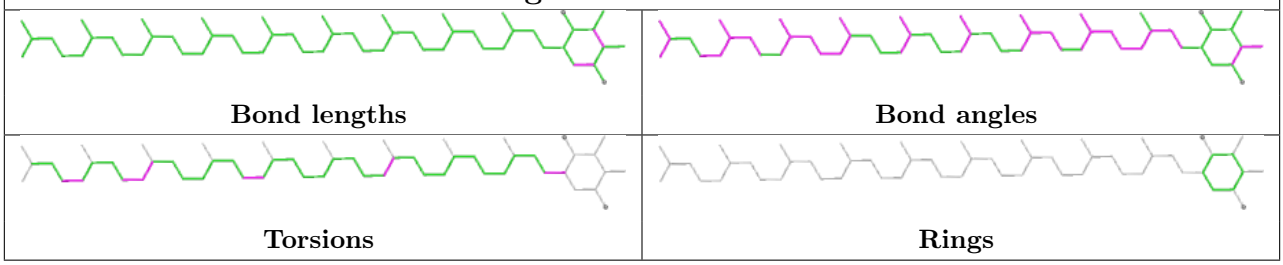


Torsions



Rings

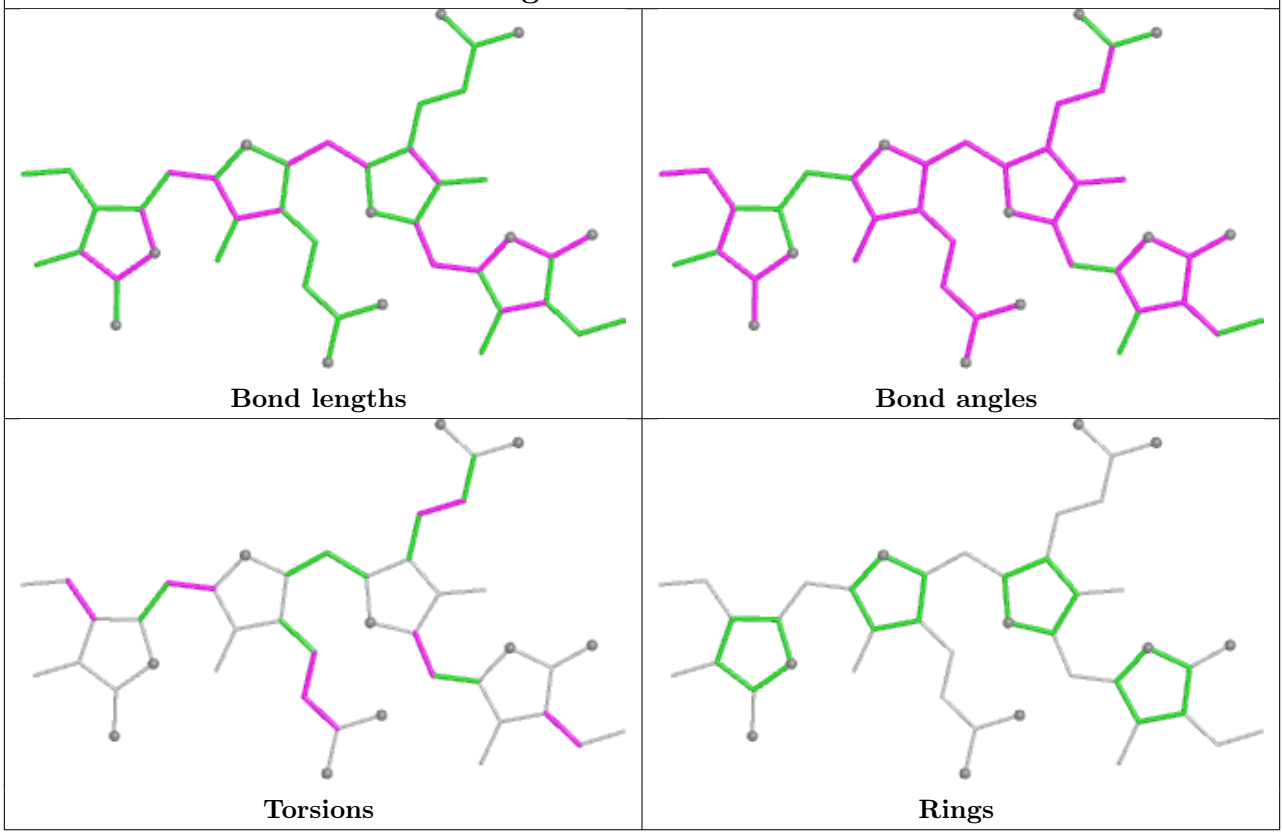
Ligand PL9 d1 408



Bond lengths | Bond angles

Torsions | Rings

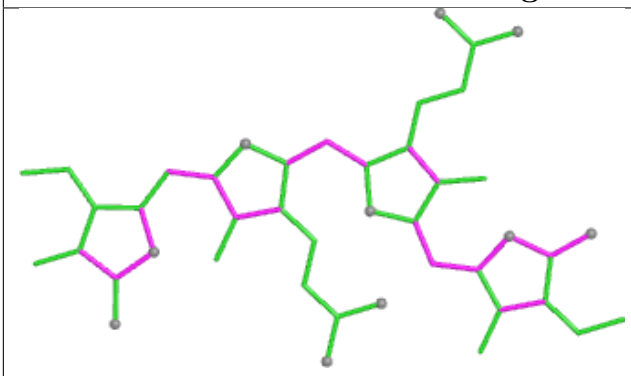
Ligand CYC f2 201



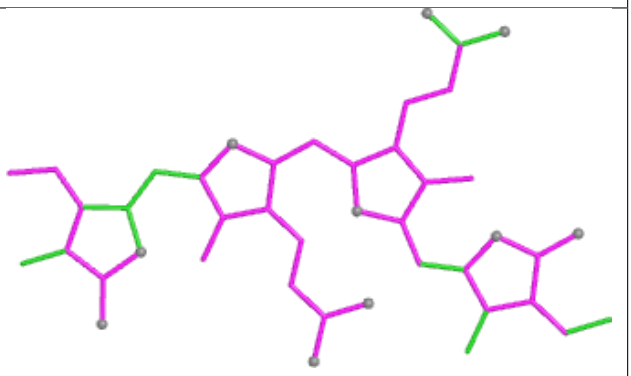
Bond lengths | Bond angles

Torsions | Rings

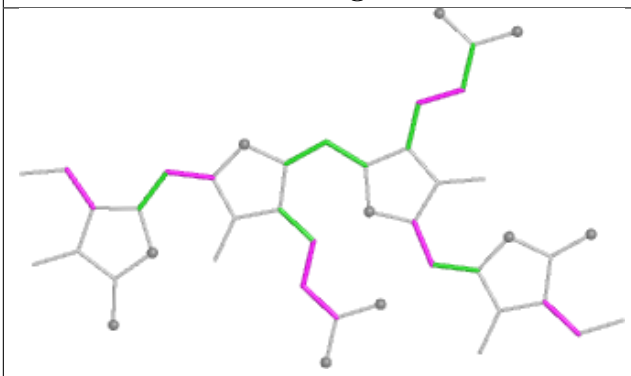
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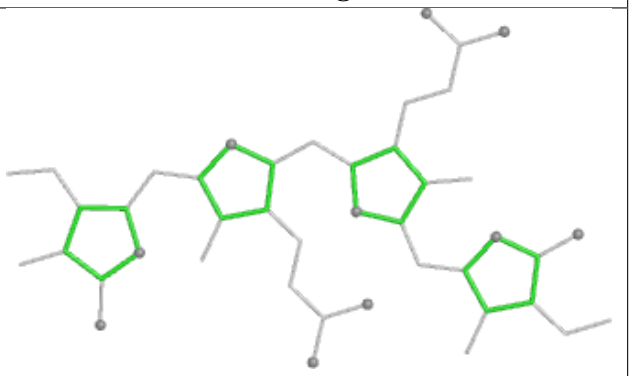
Bond lengths



Bond angles

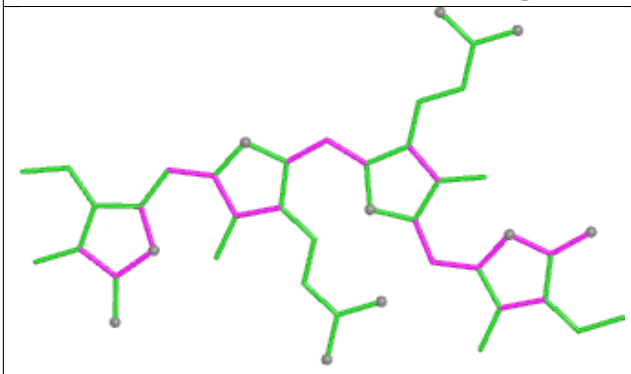


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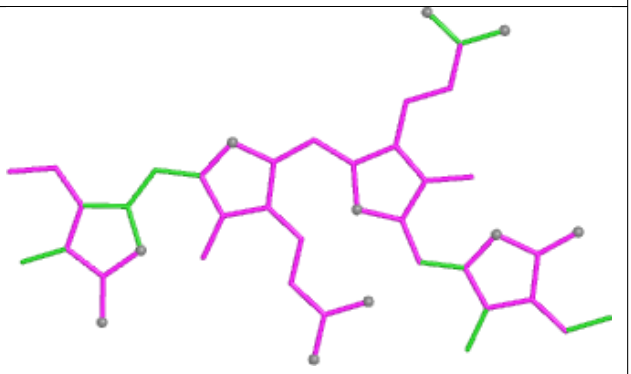


Rings

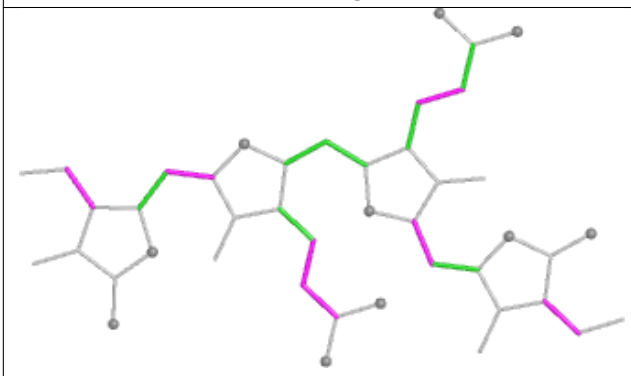
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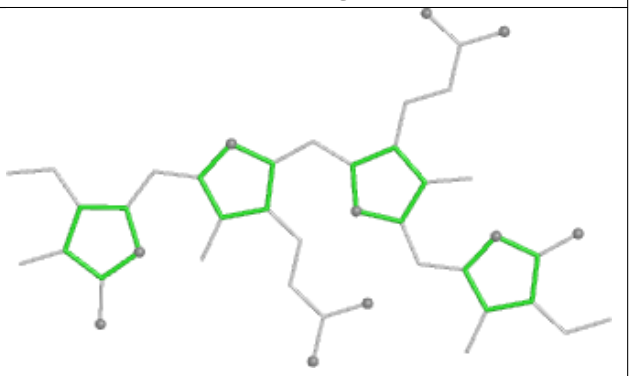
Bond lengths



Bond angles

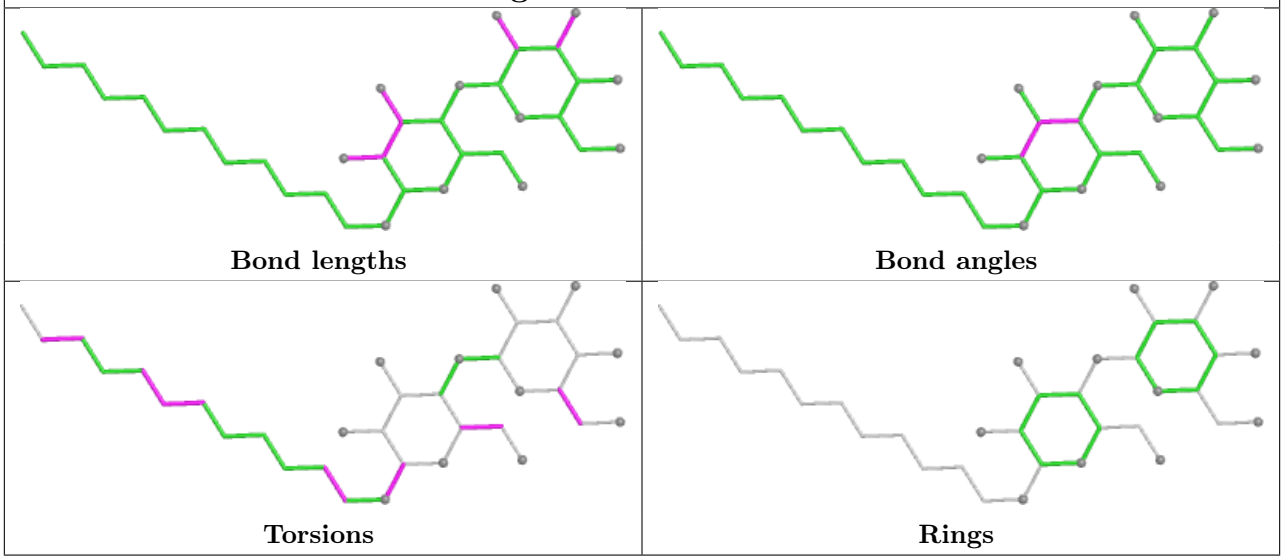


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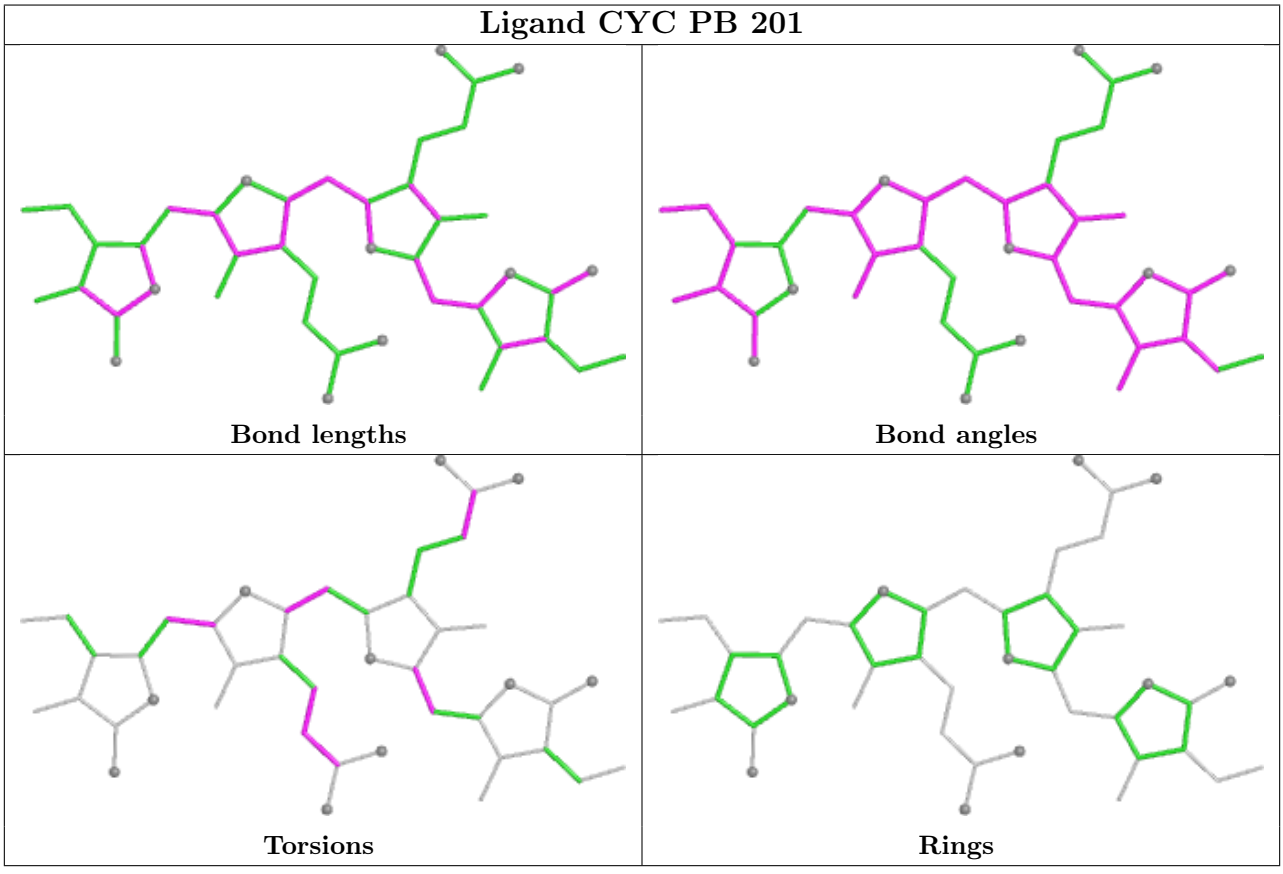


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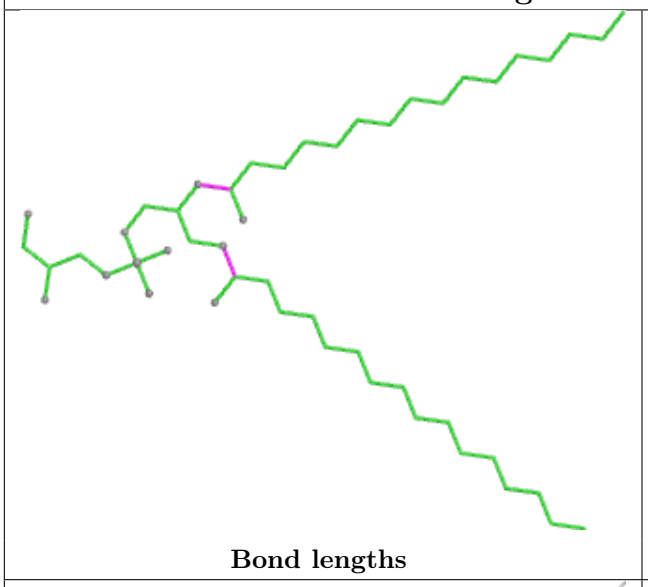
Ligand LMT BE 622



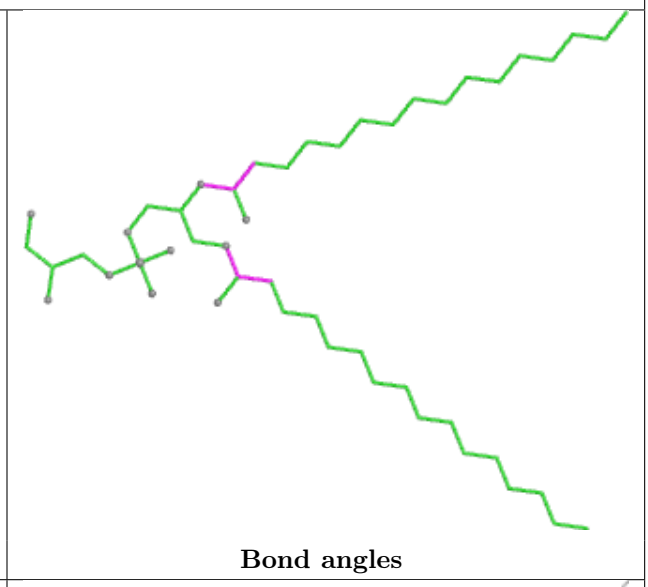
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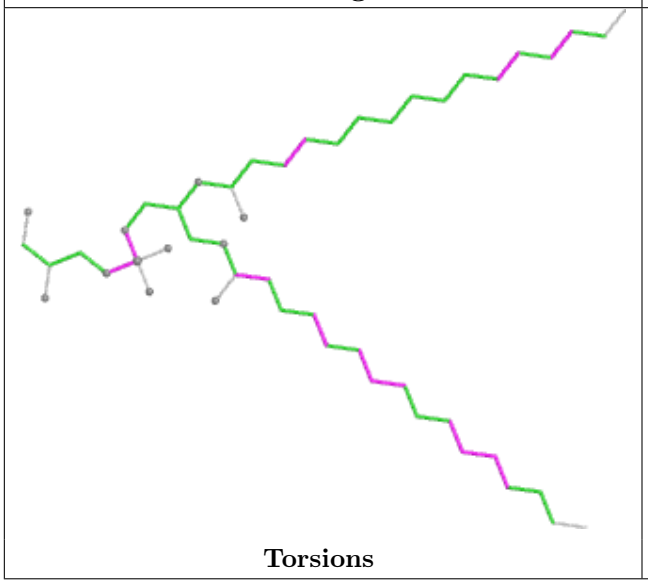
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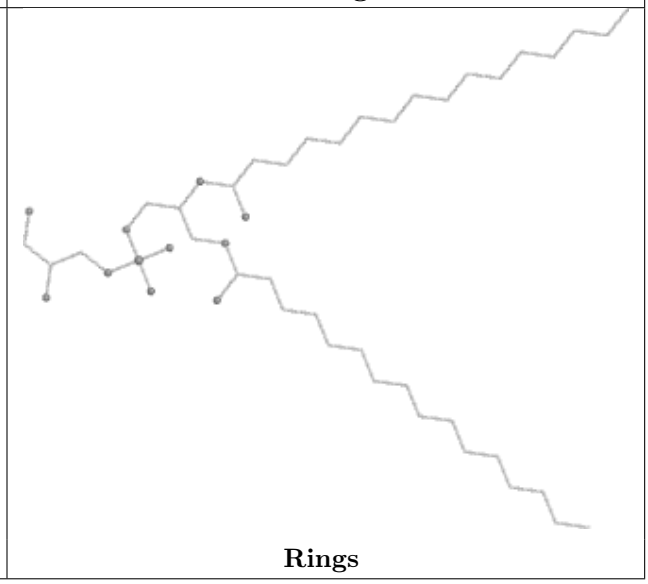
Bond lengths



Bond angles

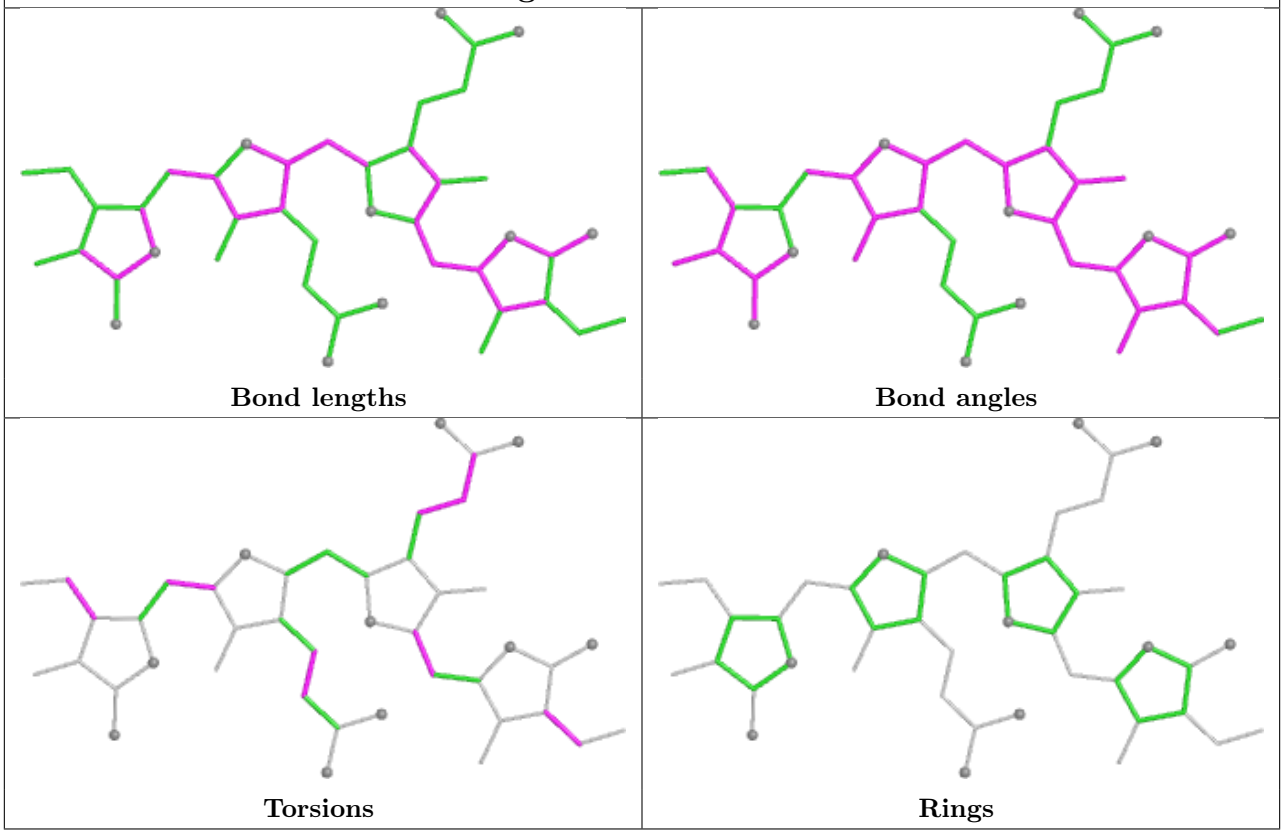


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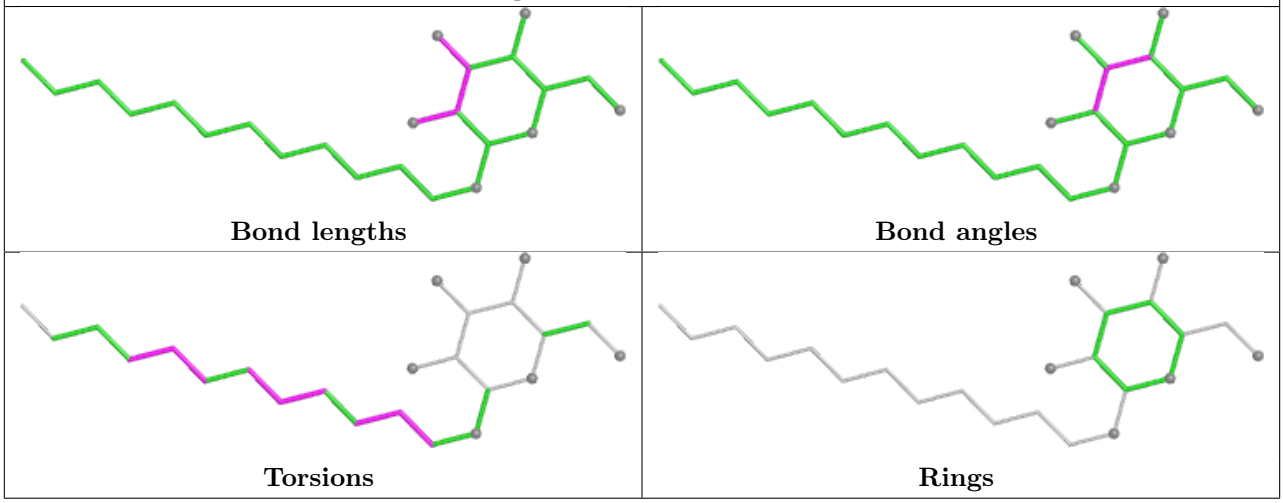


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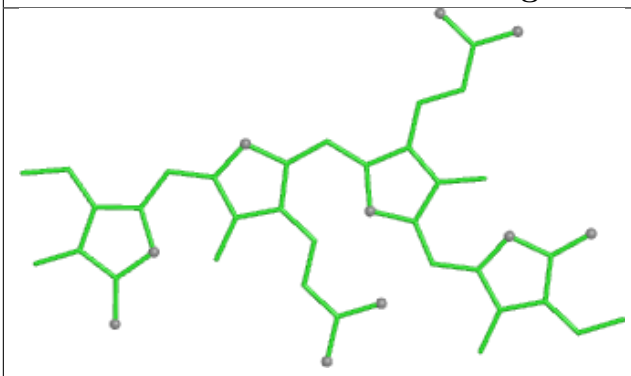
Ligand CYC o4 201



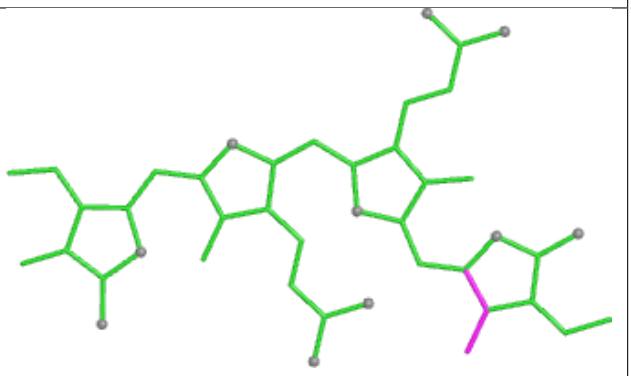
Ligand LMT BD 619



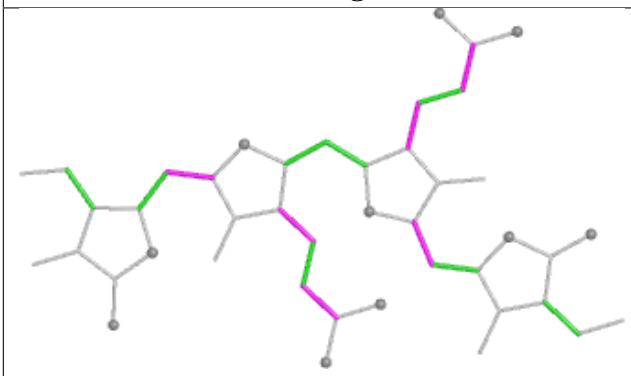
Ligand CYC i8 201



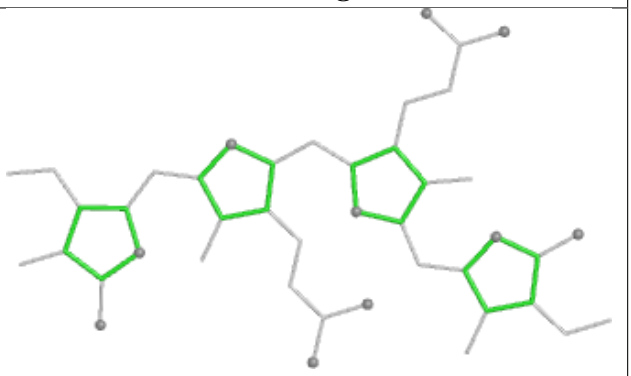
Bond lengths



Bond angles

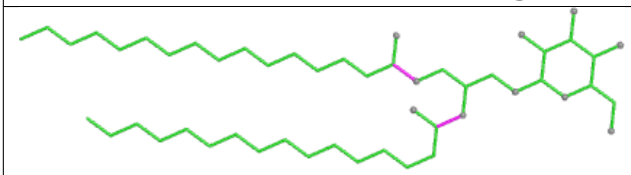


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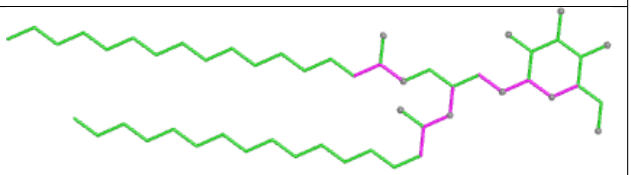


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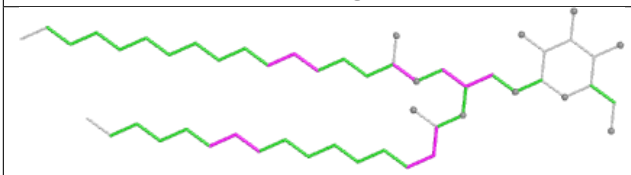
Ligand LMG C1 502



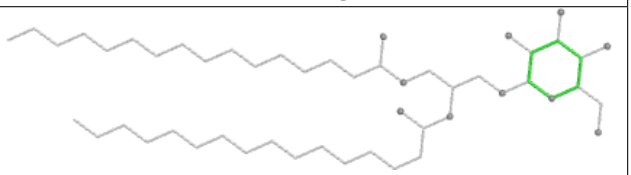
Bond lengths



Bond angles

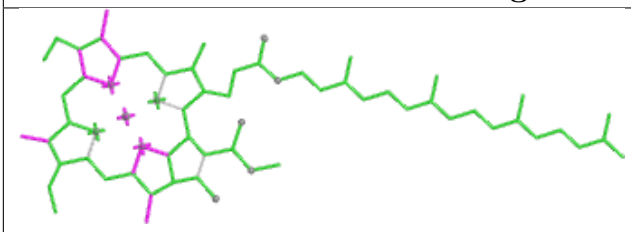


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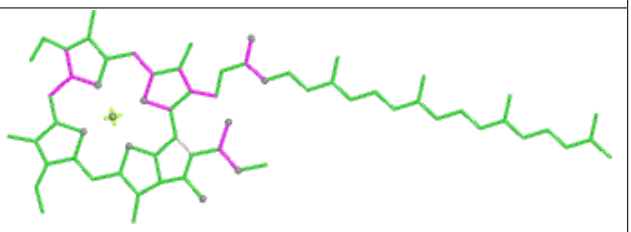


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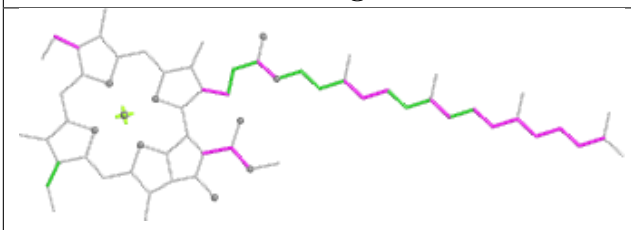
Ligand CLA XD 101



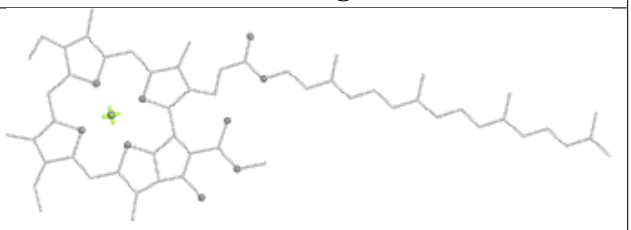
Bond lengths



Bond angles

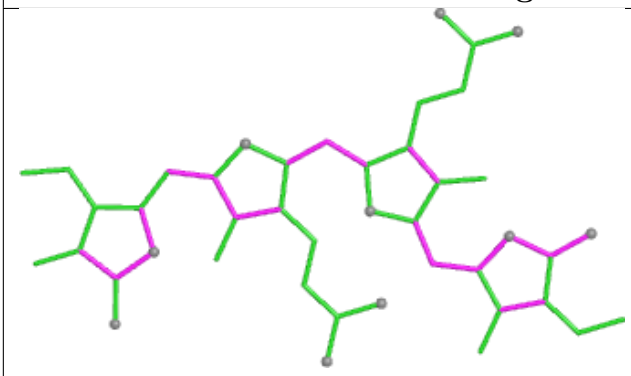


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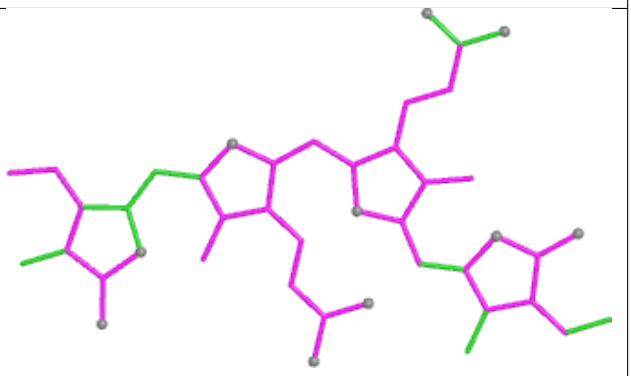


Rings

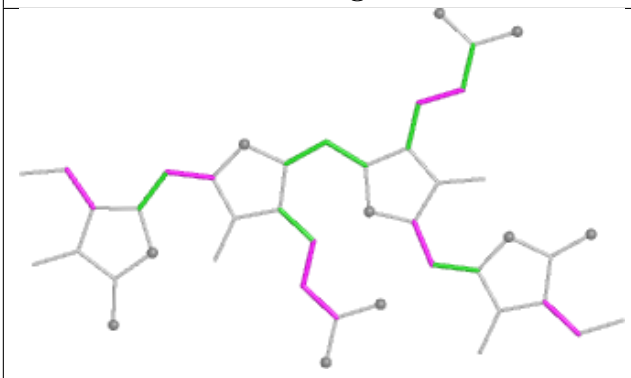
Ligand CYC fA 201



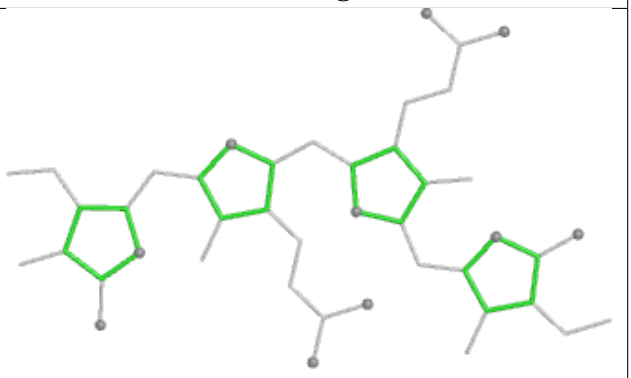
Bond lengths



Bond angles

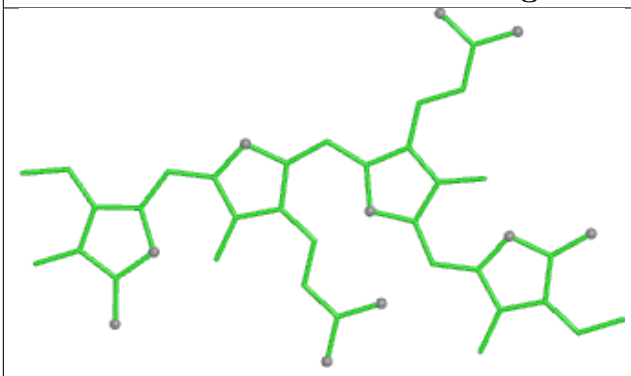


Torsions

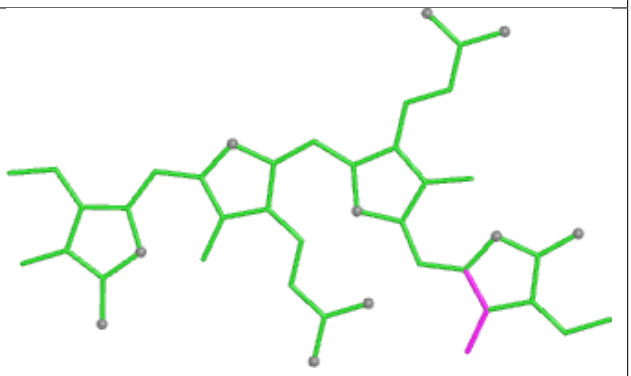


Rings

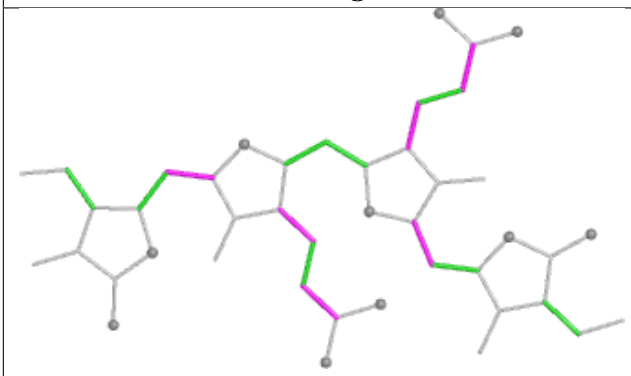
Ligand CYC iJ 201



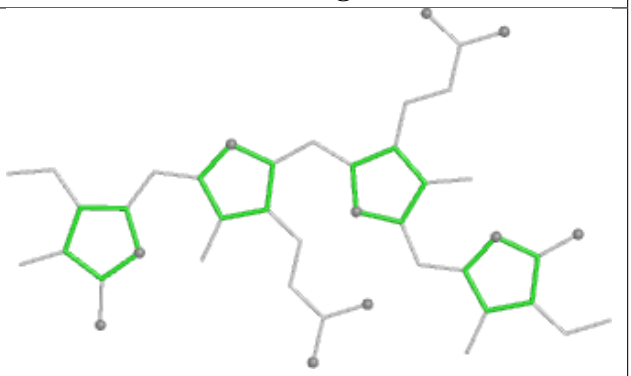
Bond lengths



Bond angles

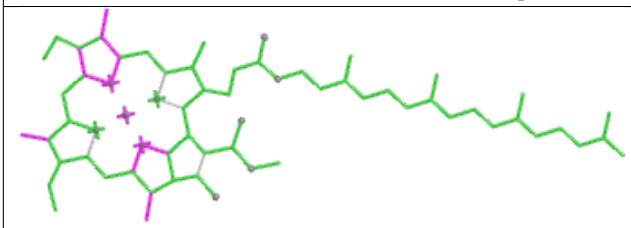


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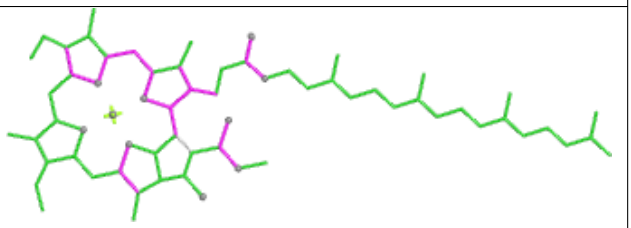


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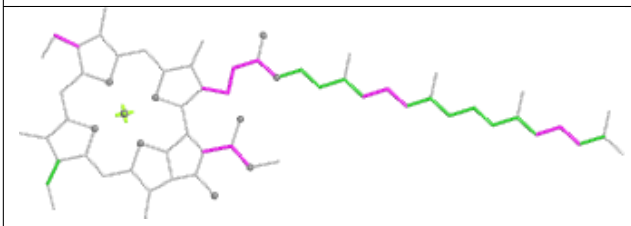
Ligand CLA CE 503



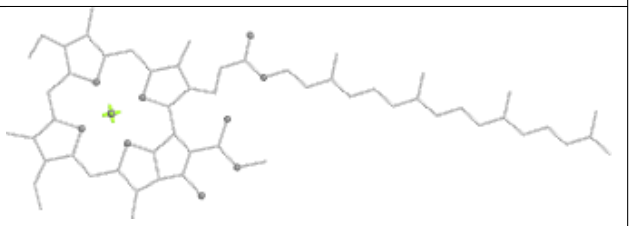
Bond lengths



Bond angles

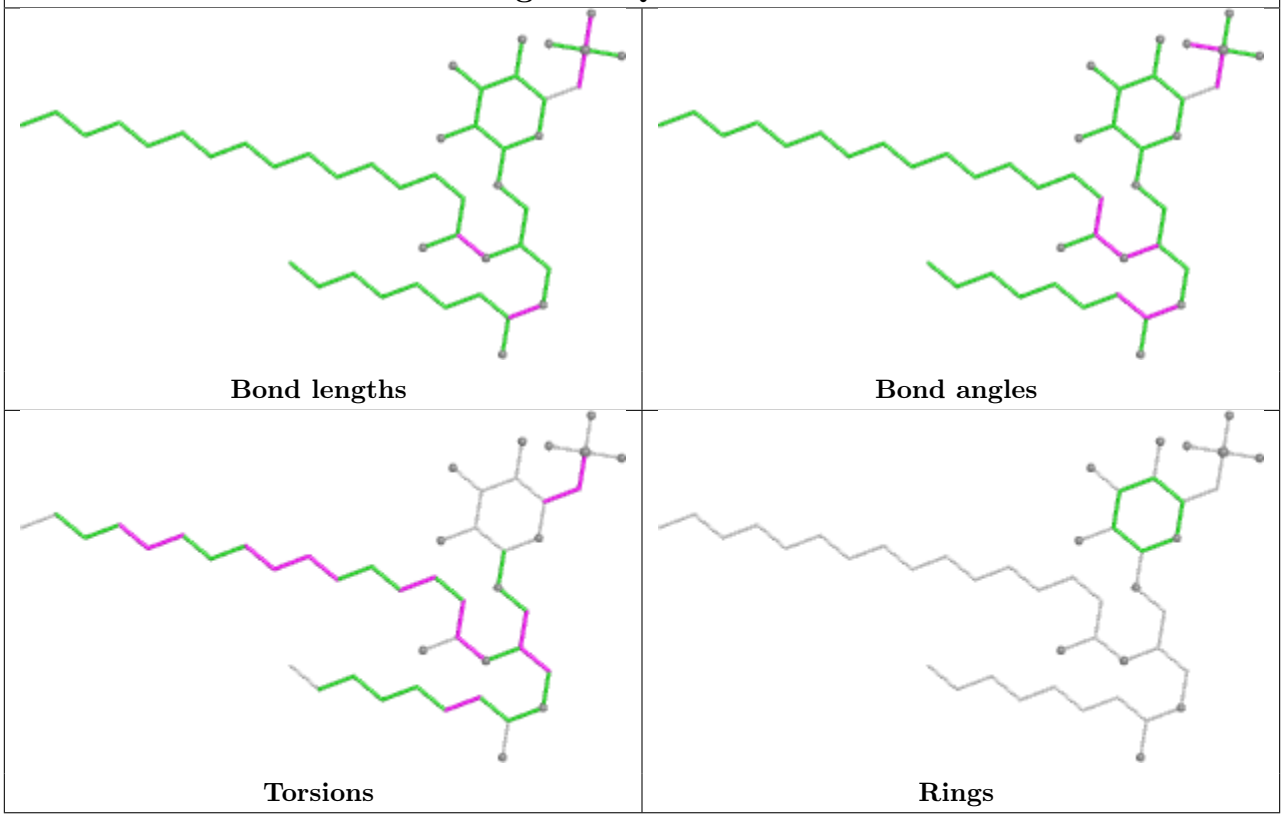


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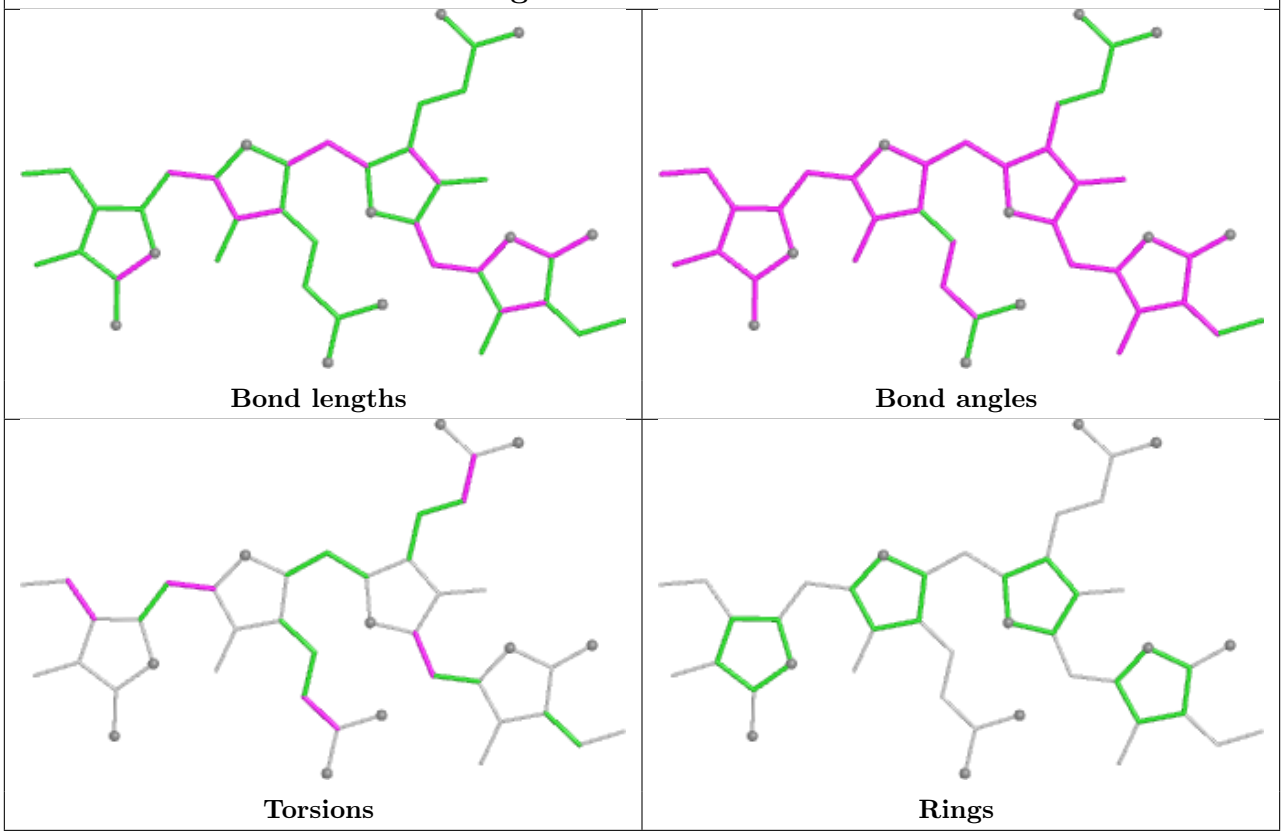


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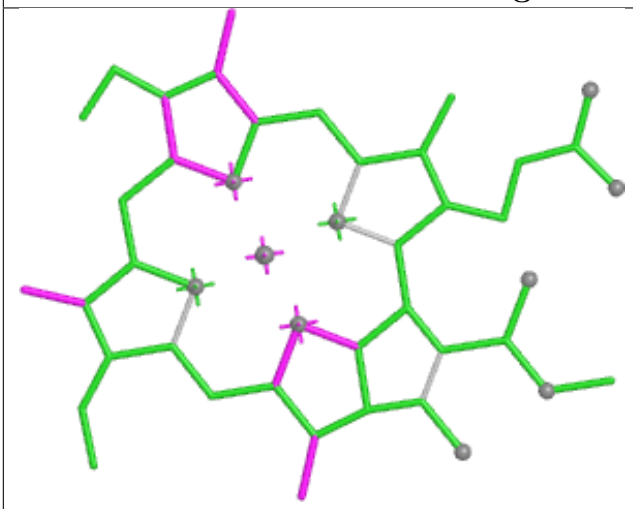
Ligand SQD A1 407



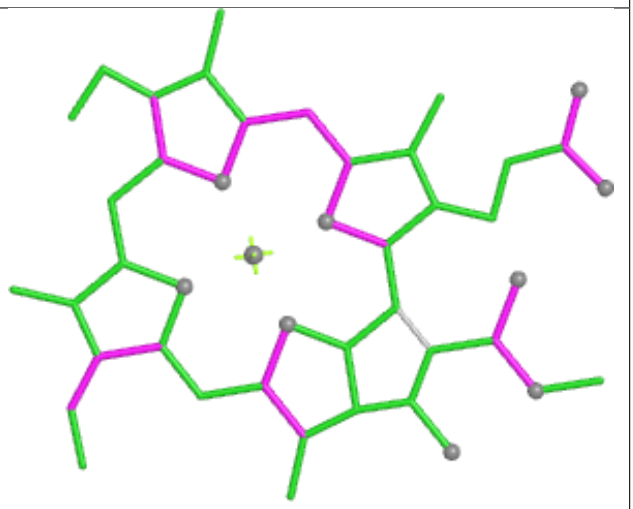
Ligand CYC KF 201



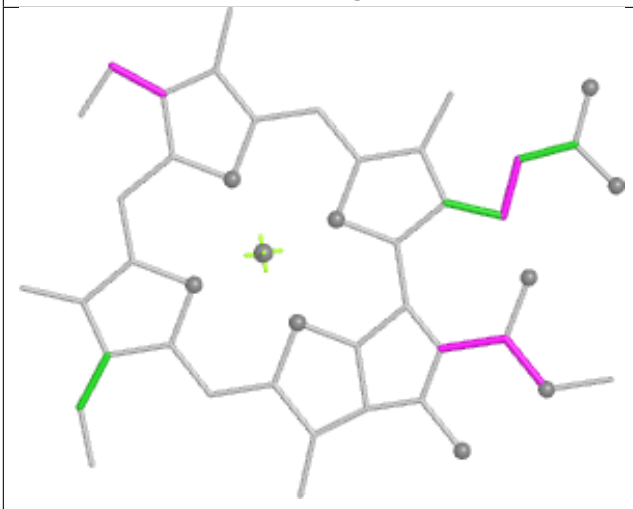
Ligand CLA bD 603



Bond lengths



Bond angles

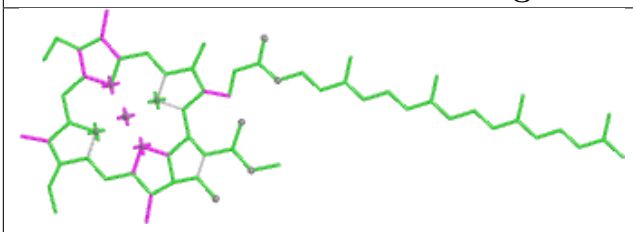


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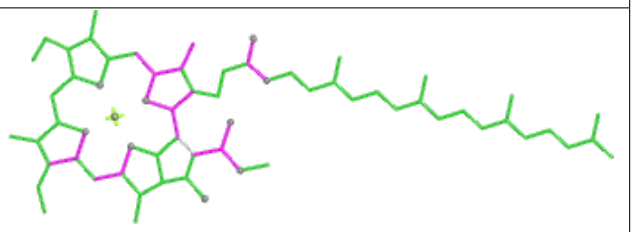


Rings

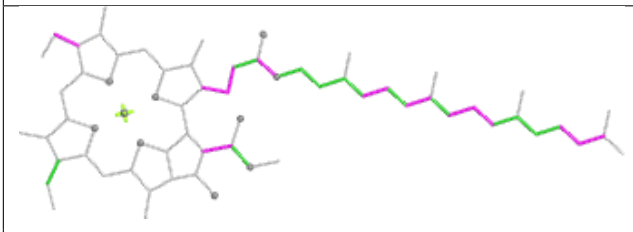
Ligand CLA bD 604



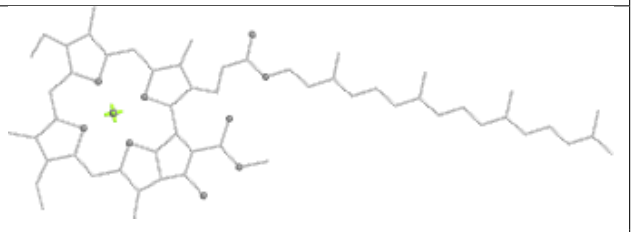
Bond lengths



Bond angles

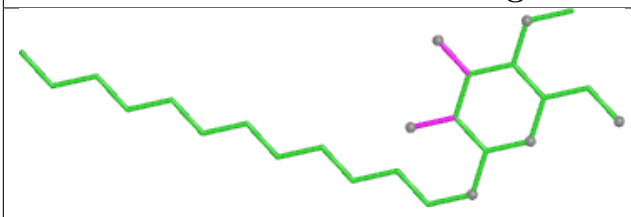


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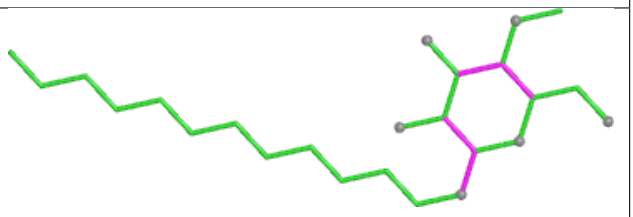


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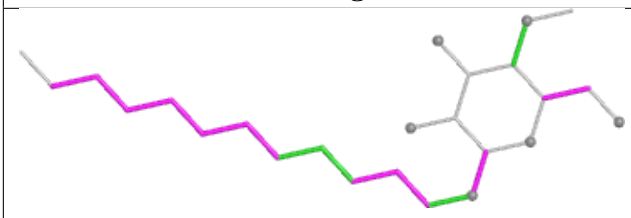
Ligand LMT DD 412



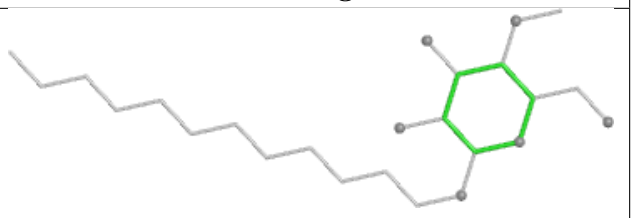
Bond lengths



Bond angles

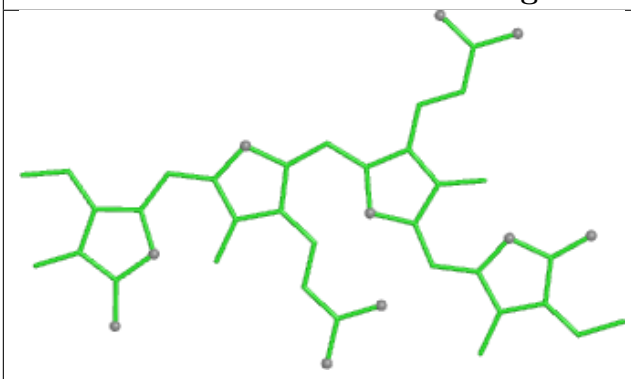


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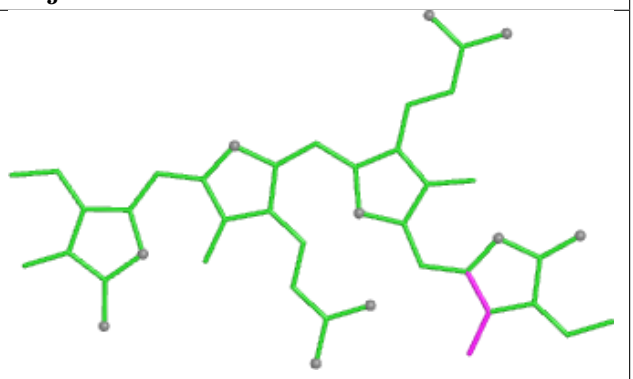


Rings

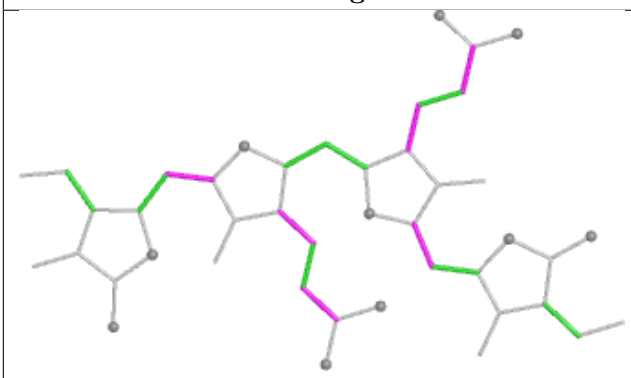
Ligand CYC j9 202



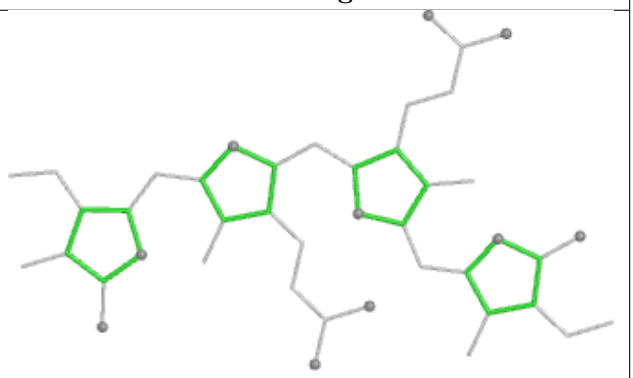
Bond lengths



Bond angles

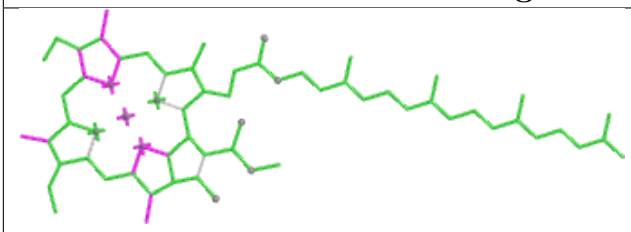


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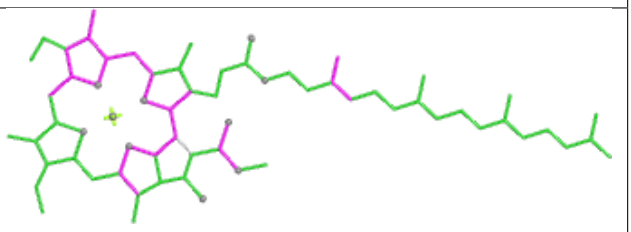


Rings

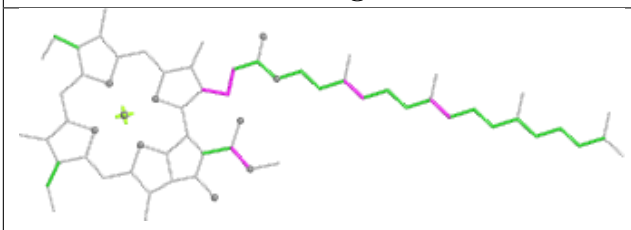
Ligand CLA cD 508



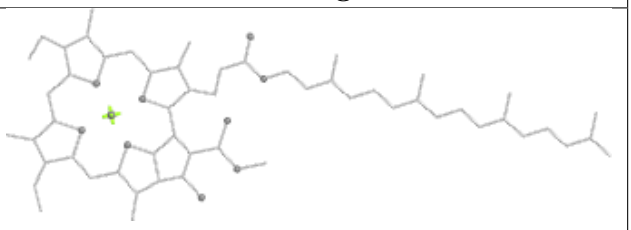
Bond lengths



Bond angles

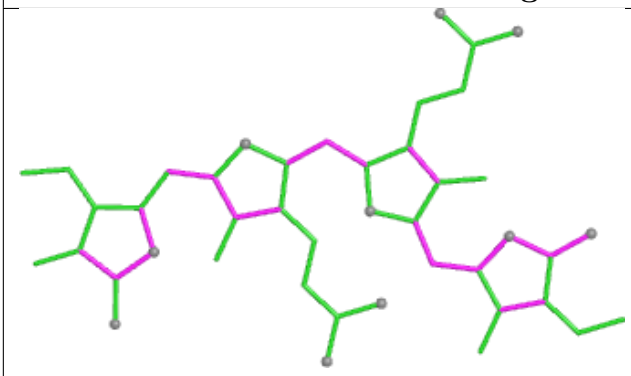


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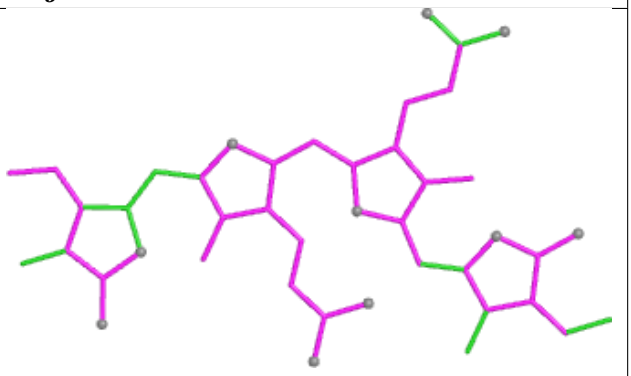


Rings

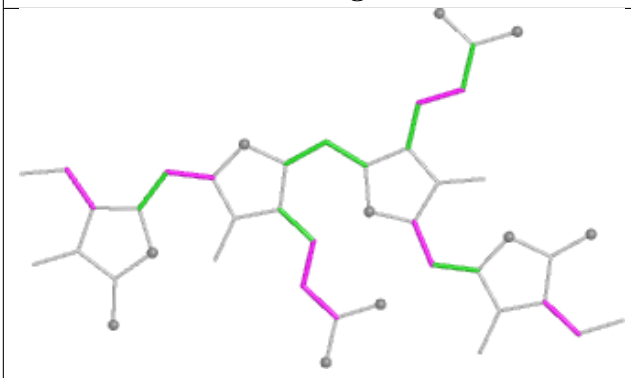
Ligand CYC j5 201



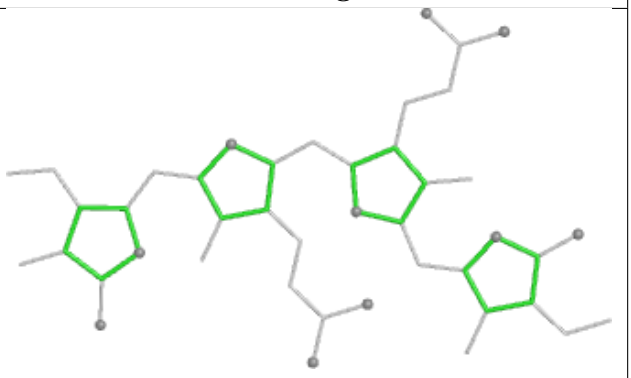
Bond lengths



Bond angles

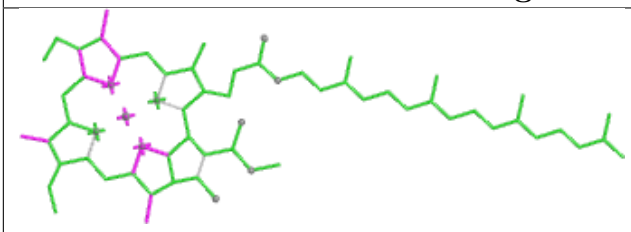


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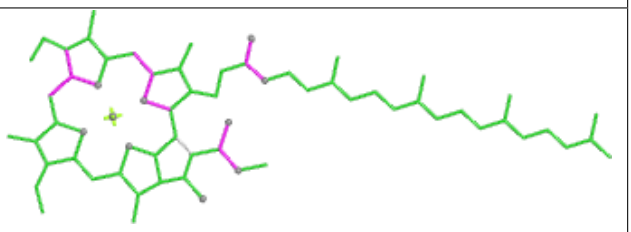


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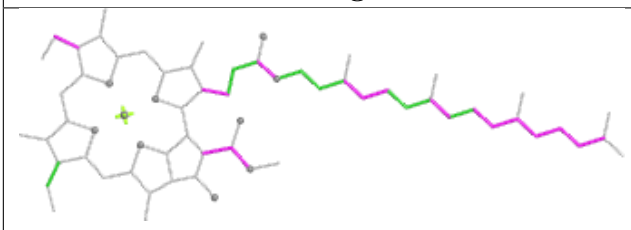
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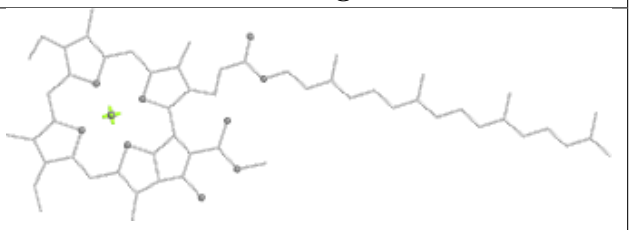
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Bond angles

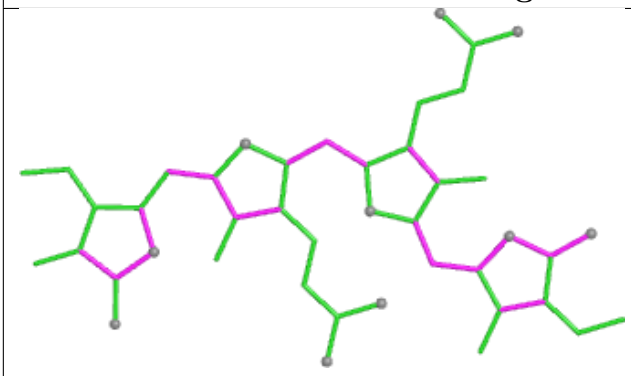


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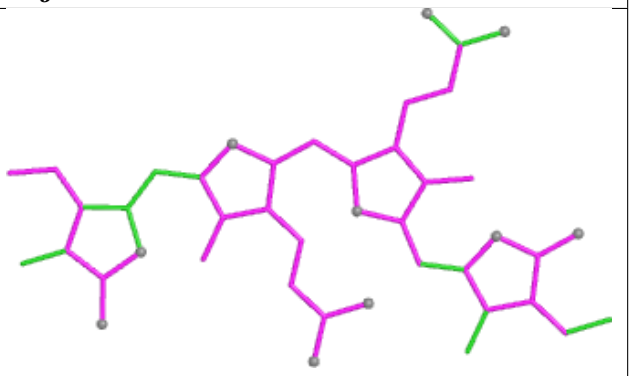


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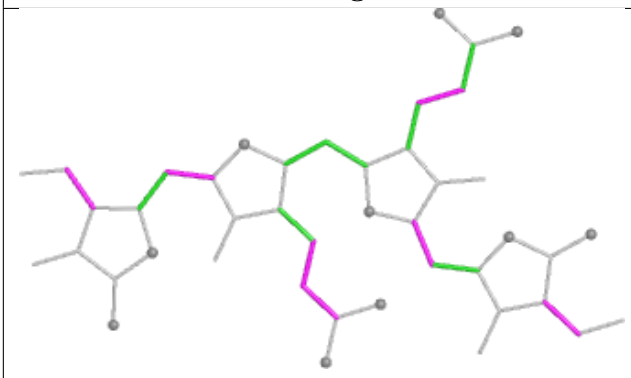
Ligand CYC jH 201



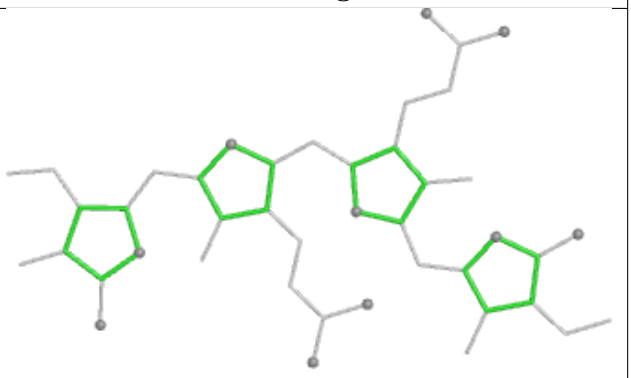
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Bond angles

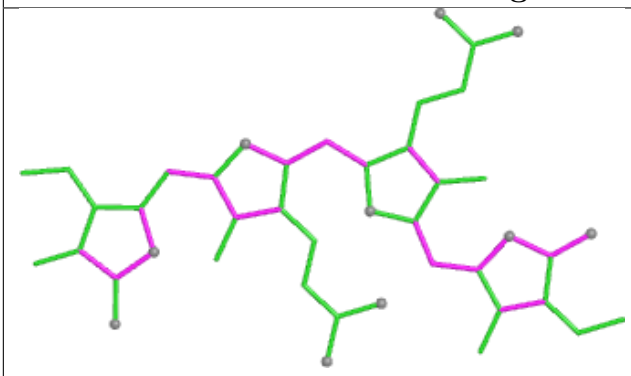


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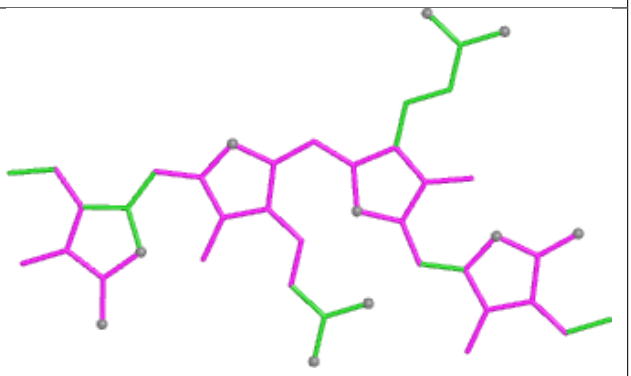


Rings

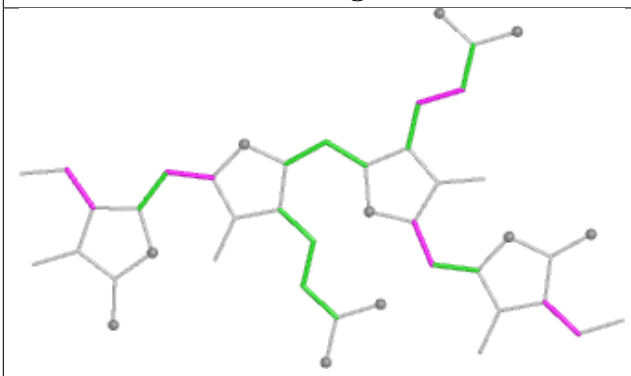
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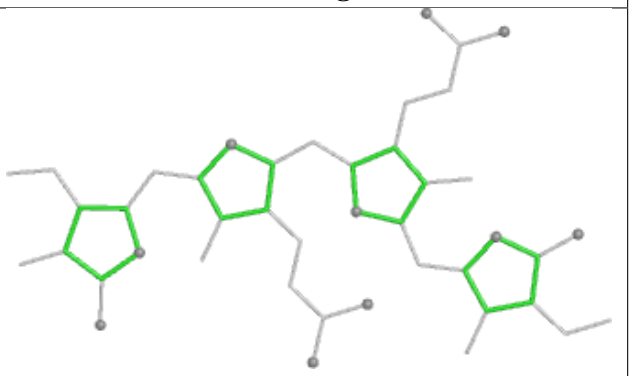
Bond lengths



Bond angles

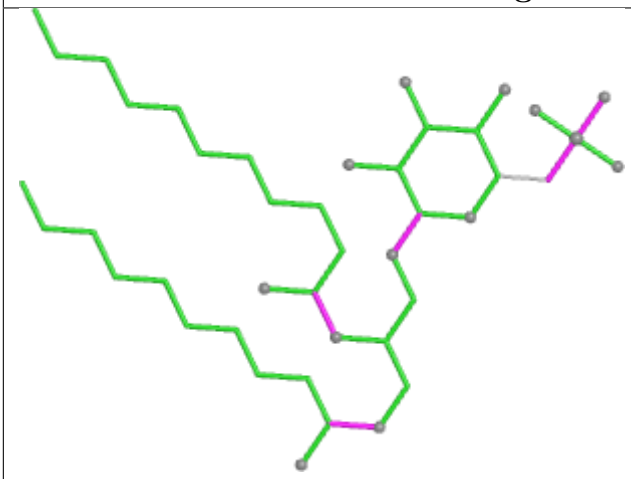


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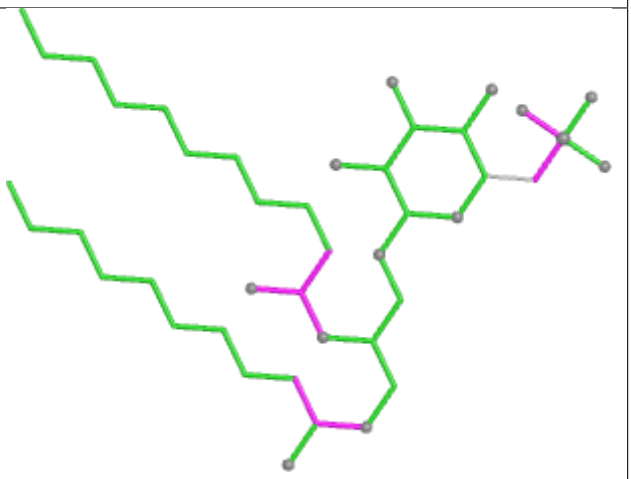


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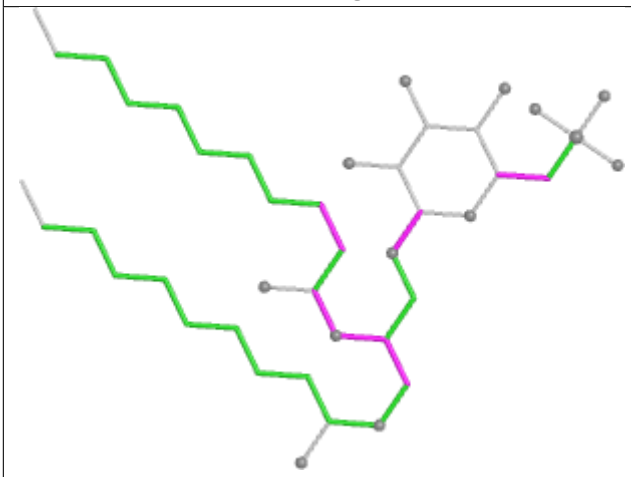
Ligand SQD LE 101



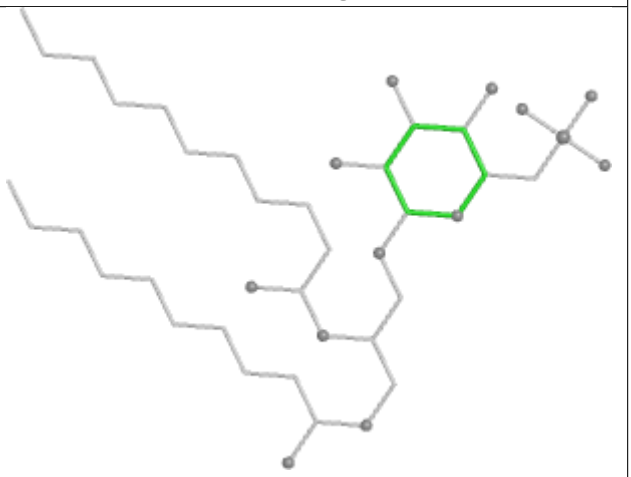
Bond lengths



Bond angles

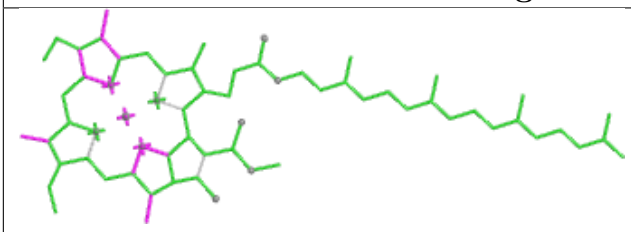


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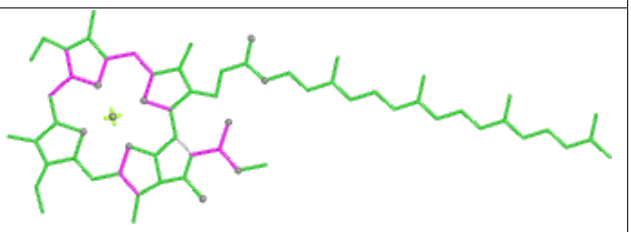


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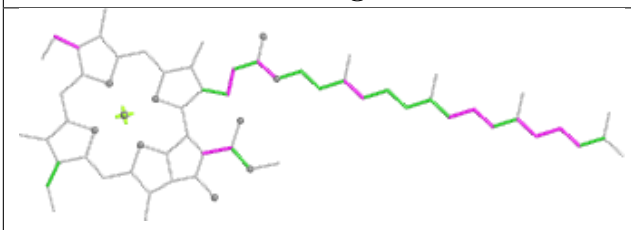
Ligand CLA B1 613



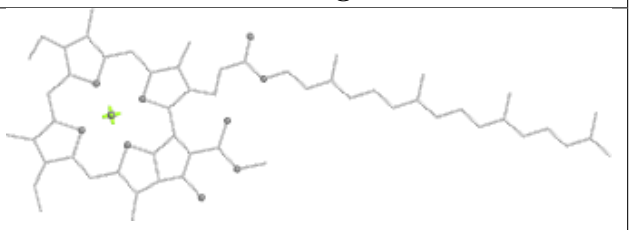
Bond lengths



Bond angles

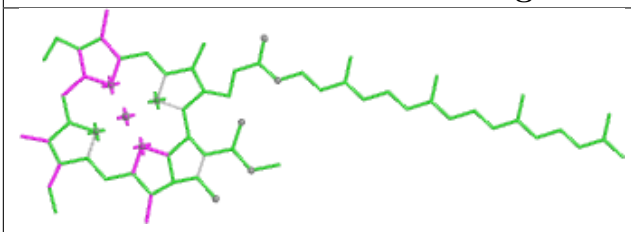


Torsions

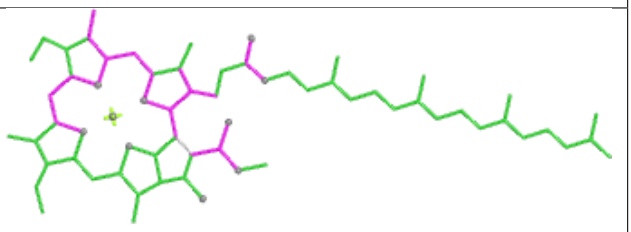


Rings

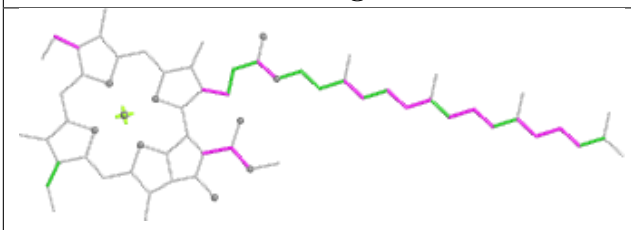
Ligand CLA B1 610



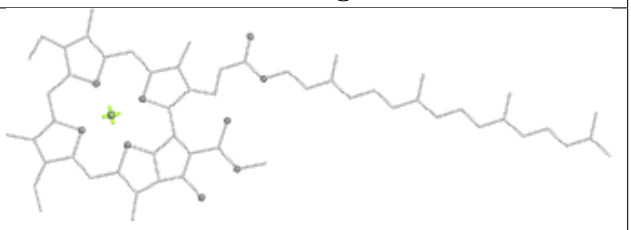
Bond lengths



Bond angles



Torsions

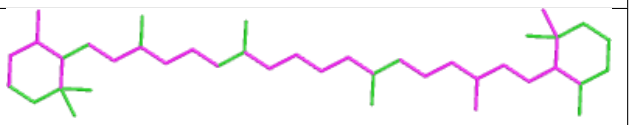


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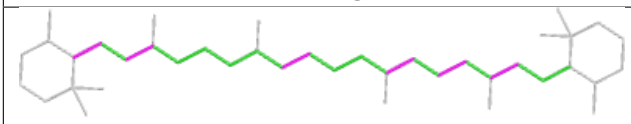
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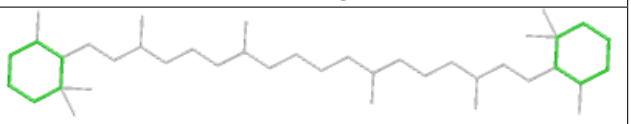
Bond lengths



Bond angles

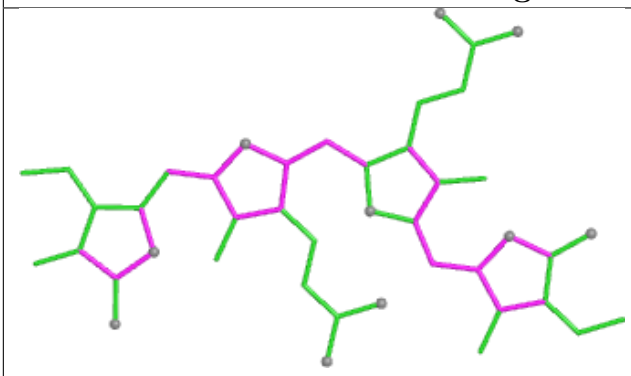


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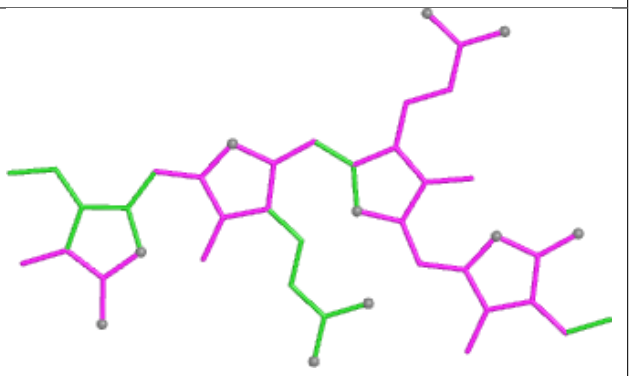


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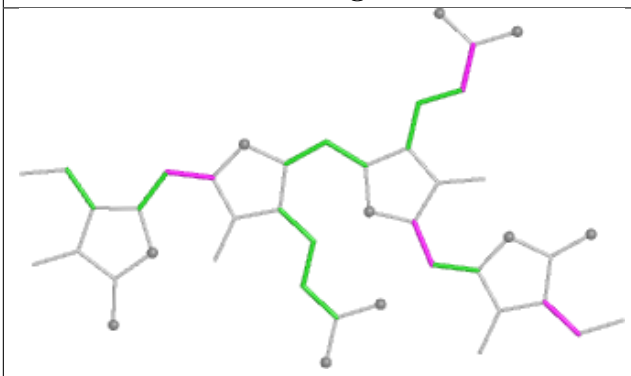
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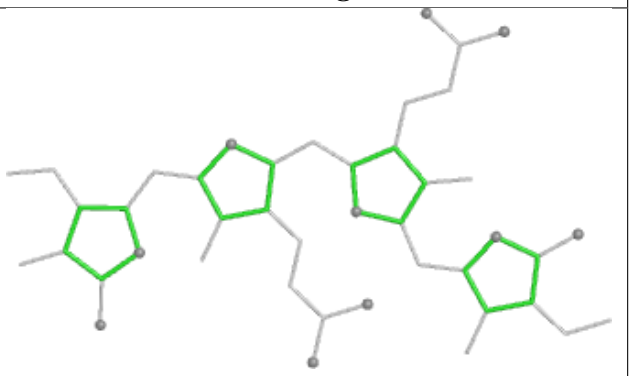
Bond lengths



Bond angles

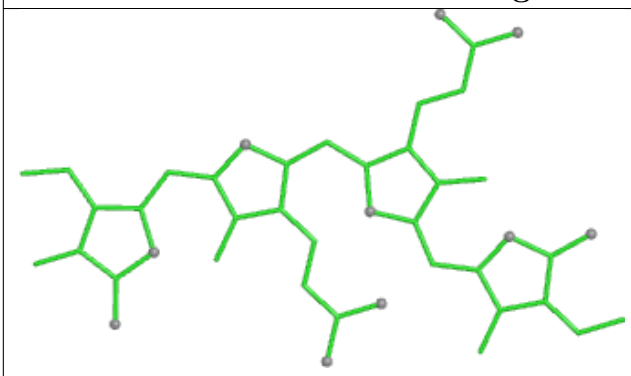


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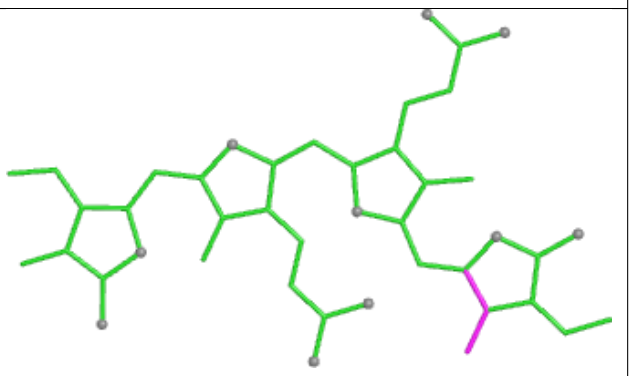


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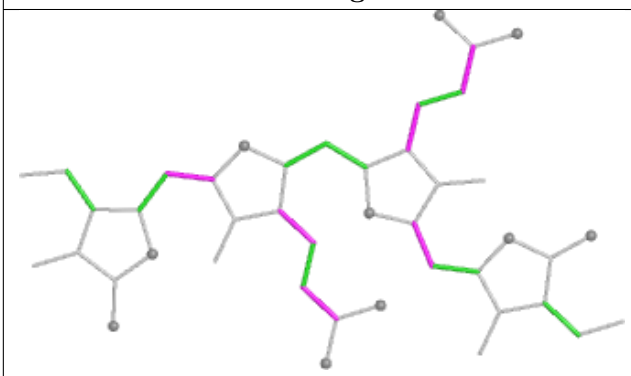
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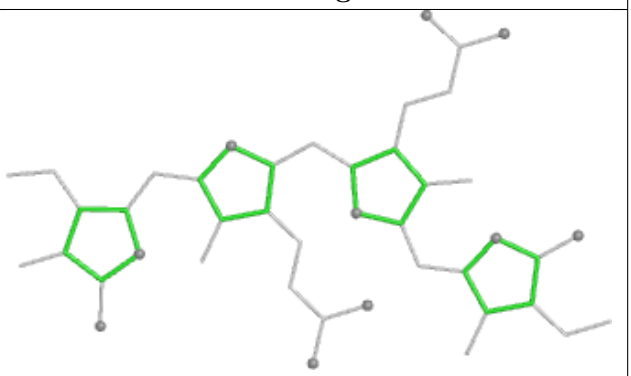
Bond lengths



Bond angles

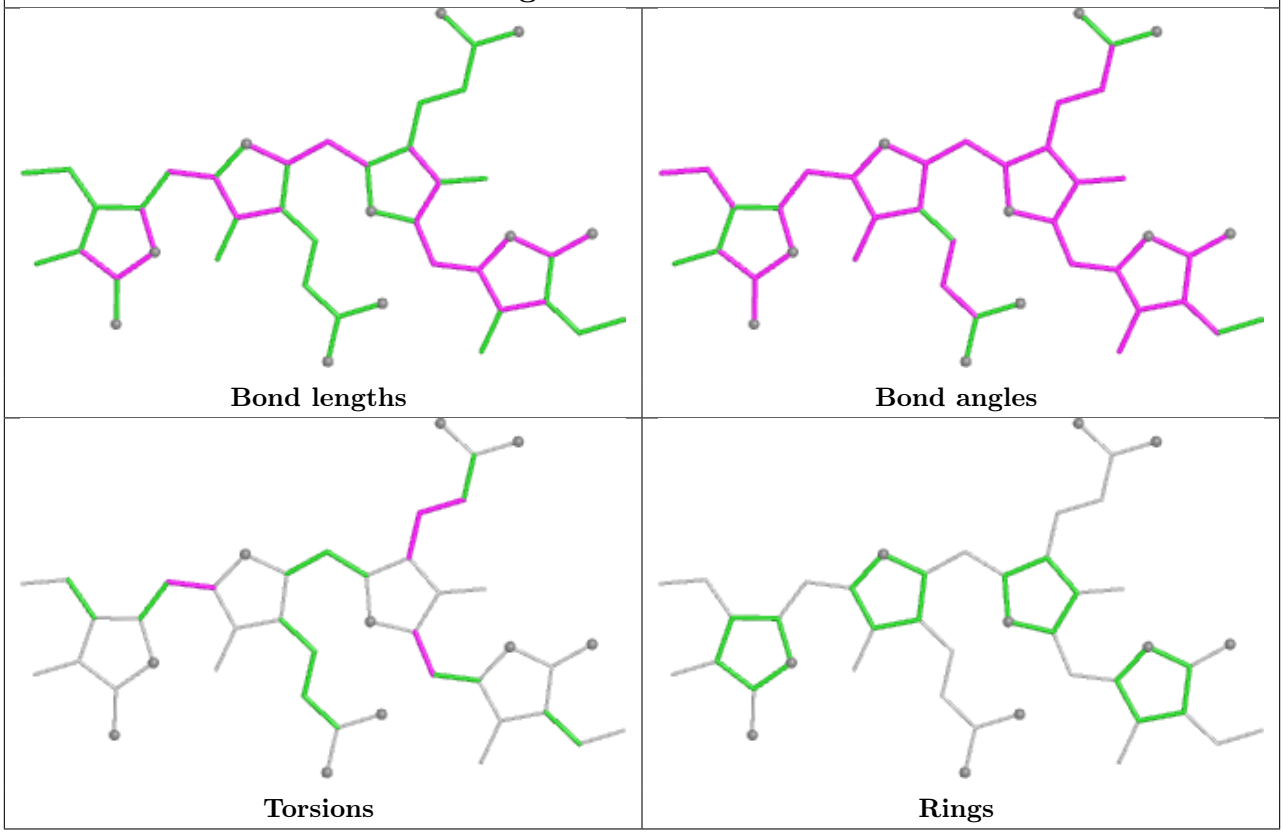


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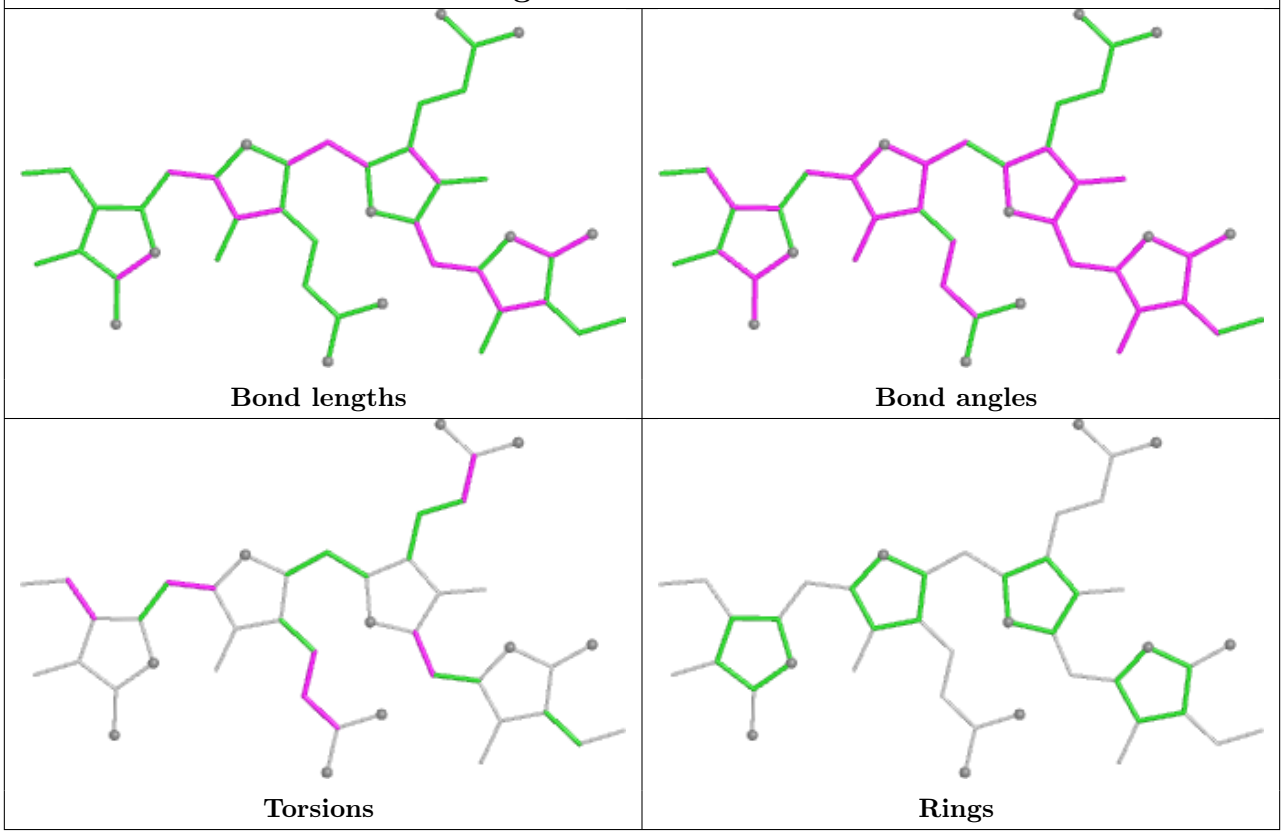


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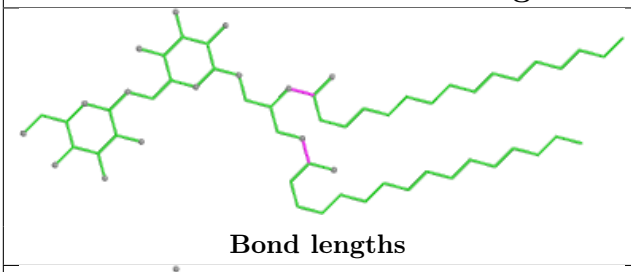
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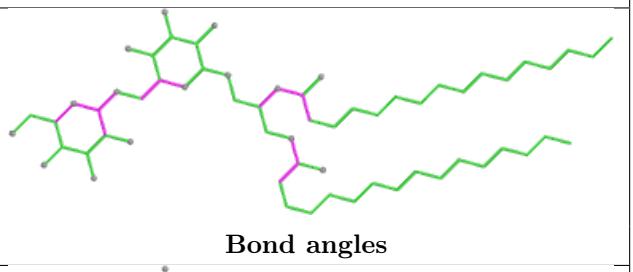
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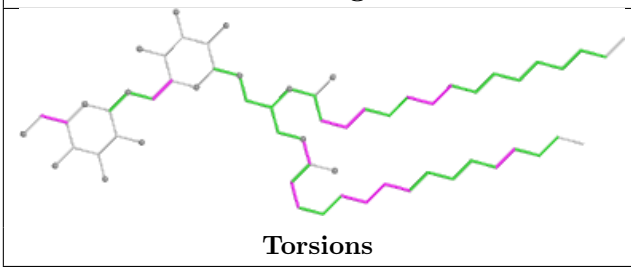
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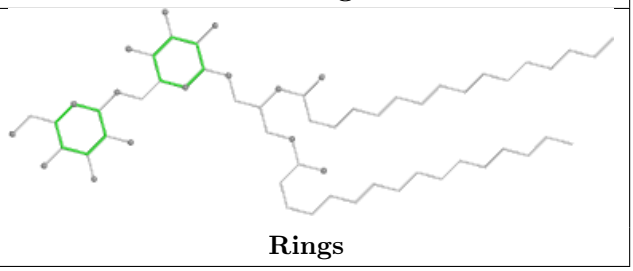
Bond lengths



Bond angles

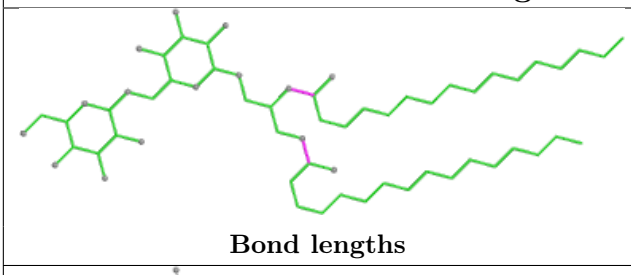


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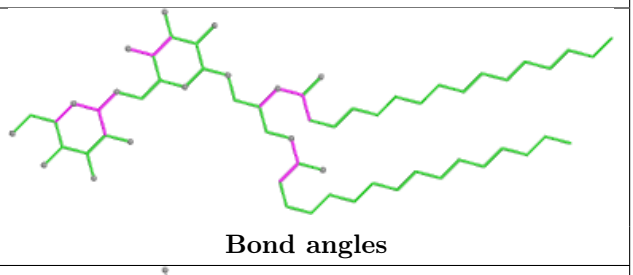


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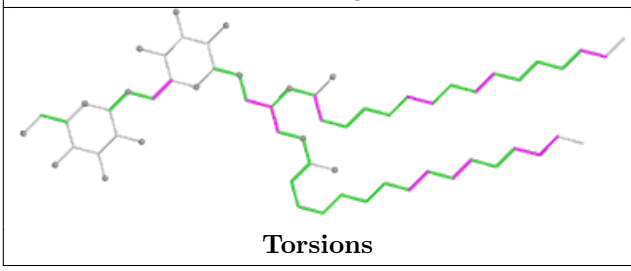
Ligand DGD h1 104



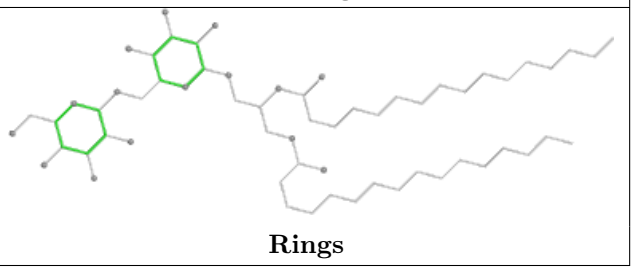
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Bond angles

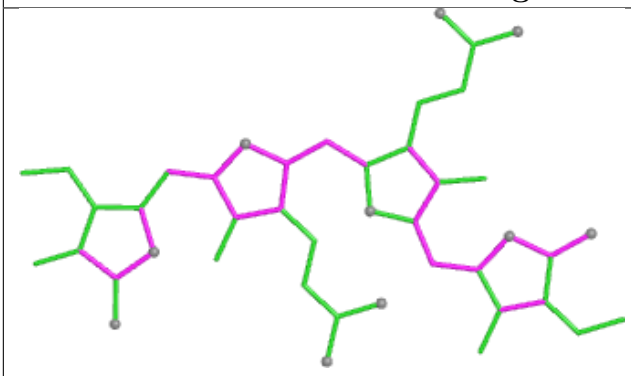


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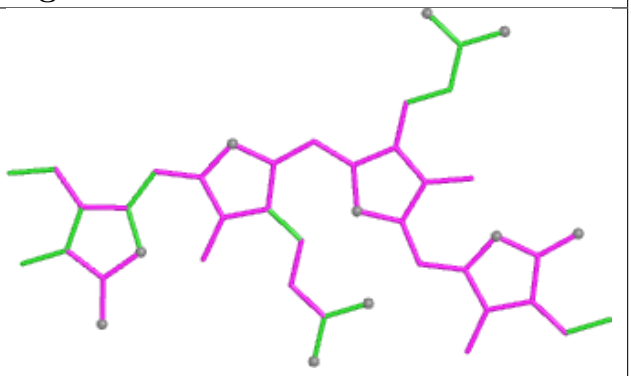


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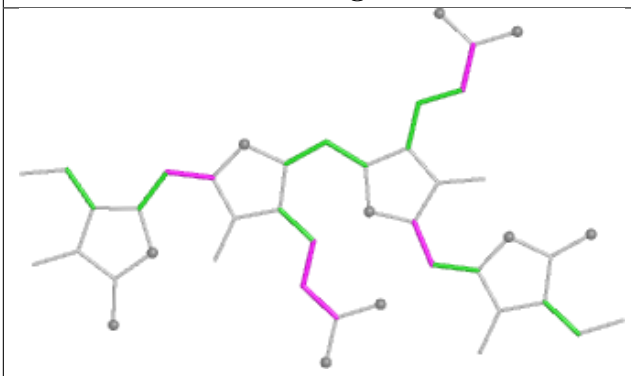
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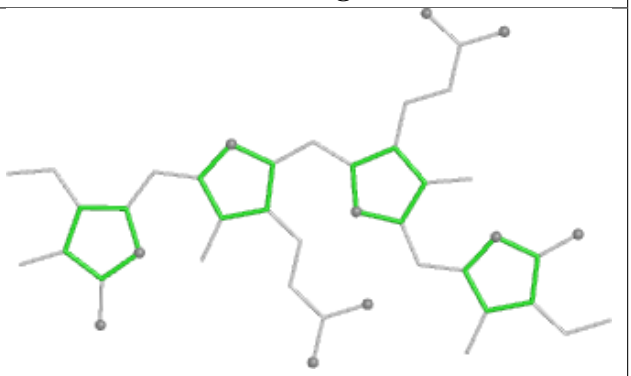
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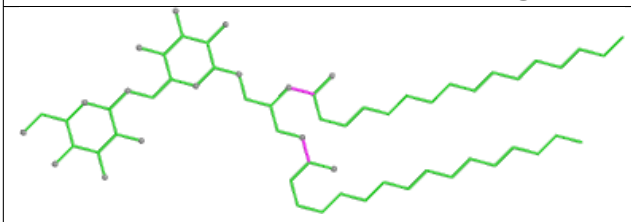


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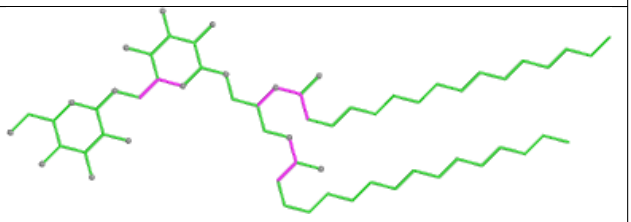


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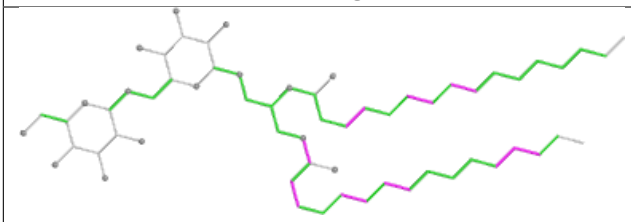
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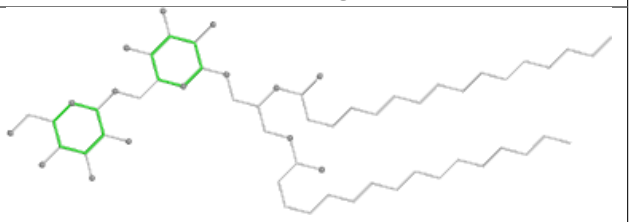
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Bond angles

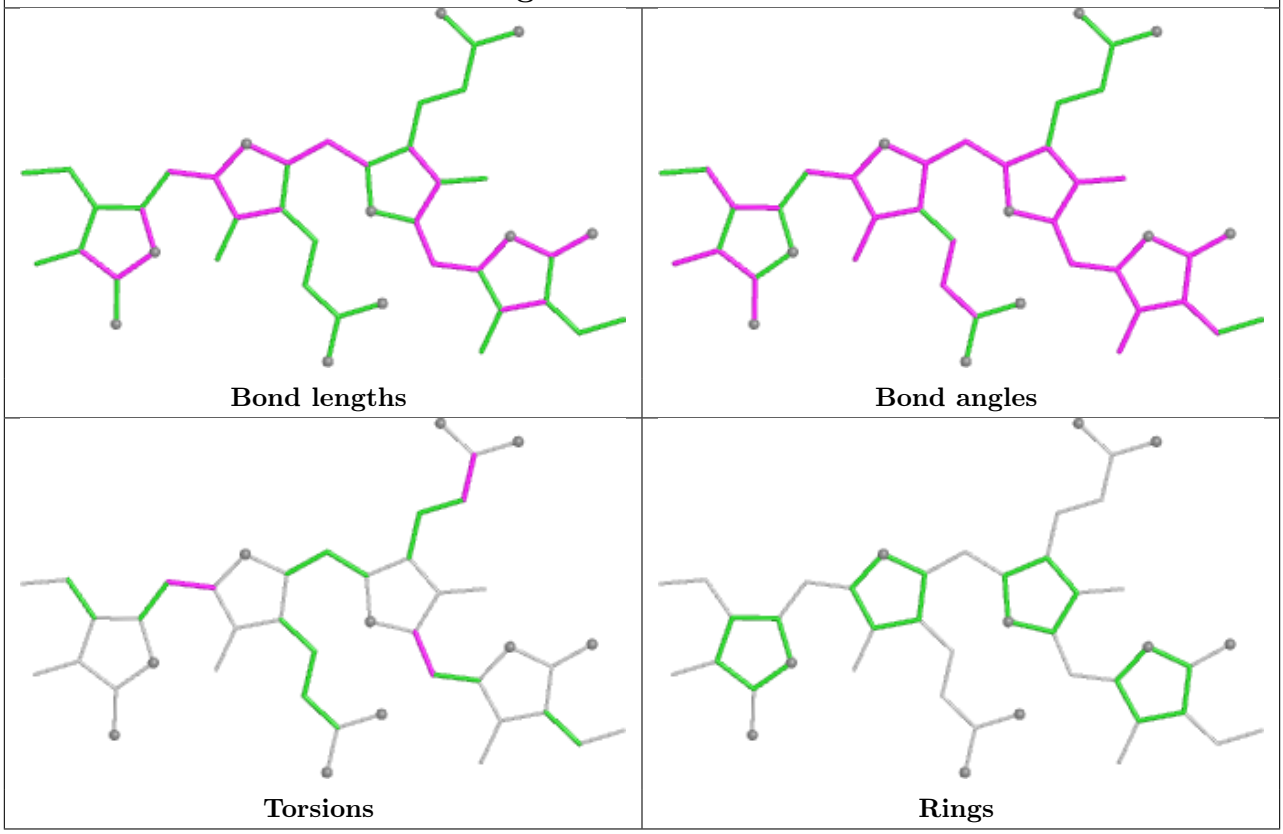


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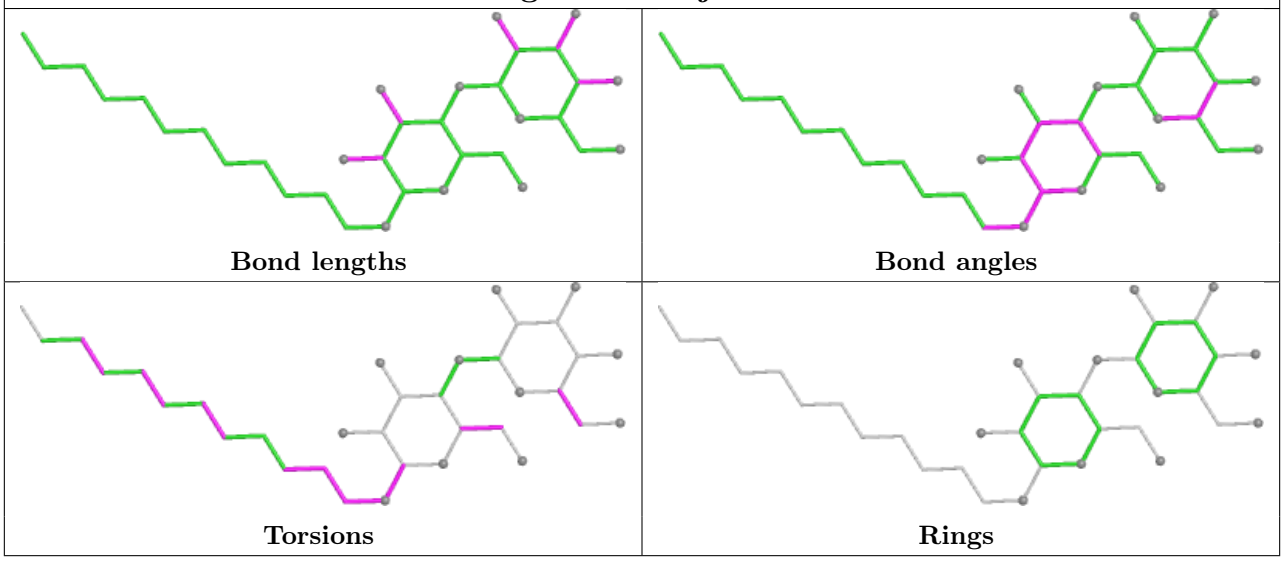


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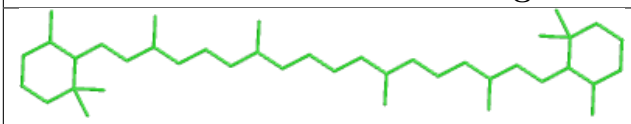
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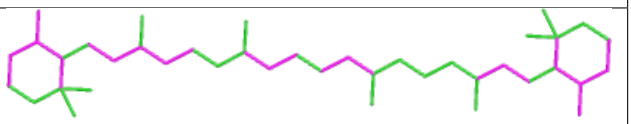
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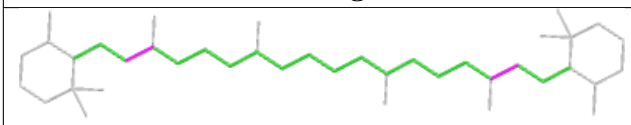
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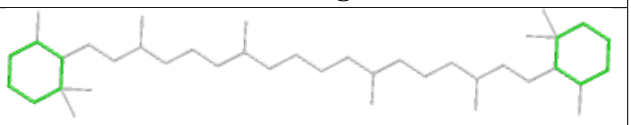
Bond lengths



Bond angles

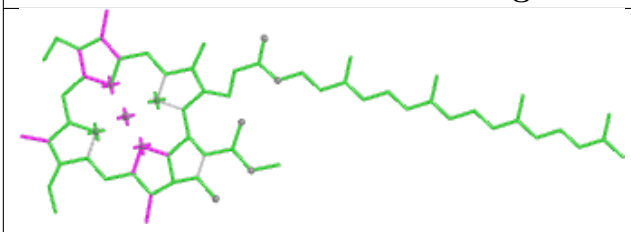


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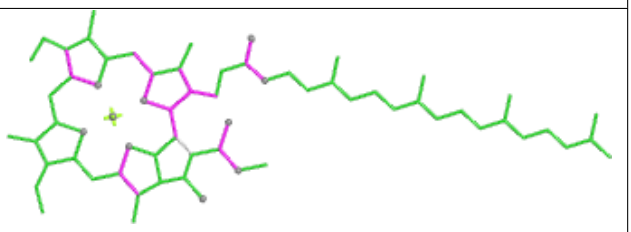


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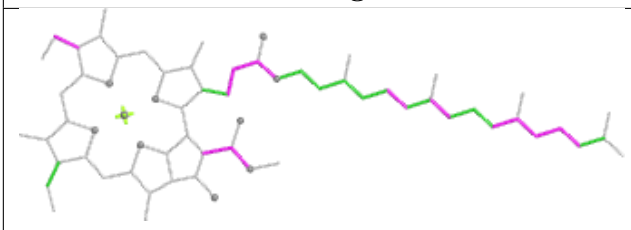
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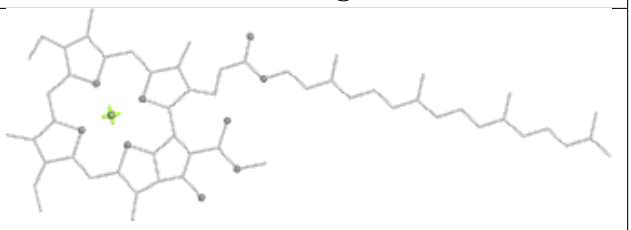
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Bond angles

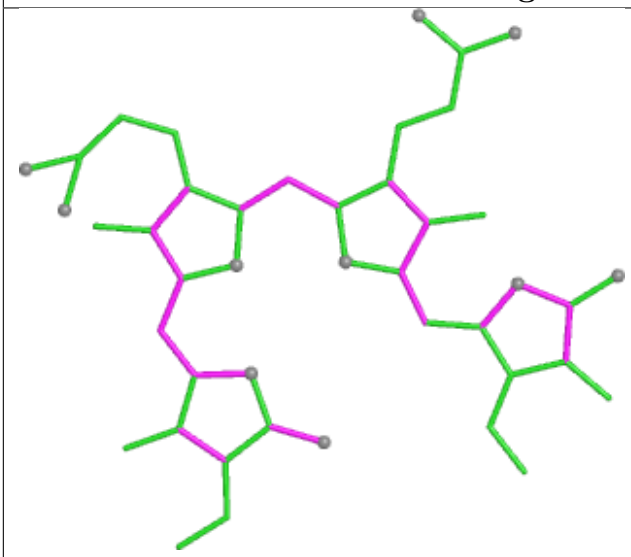


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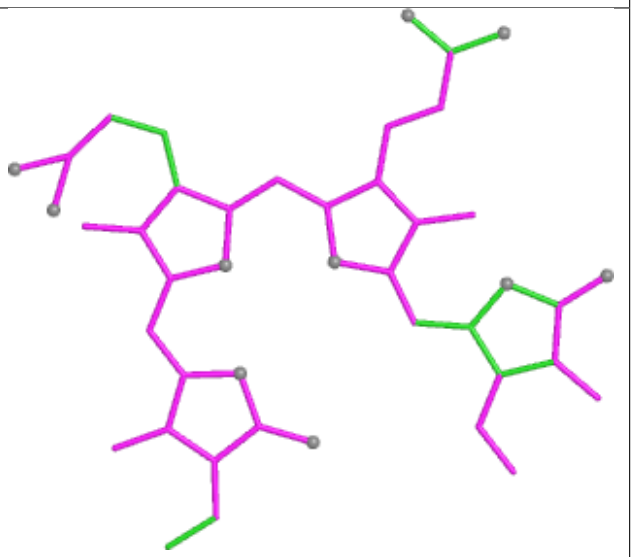


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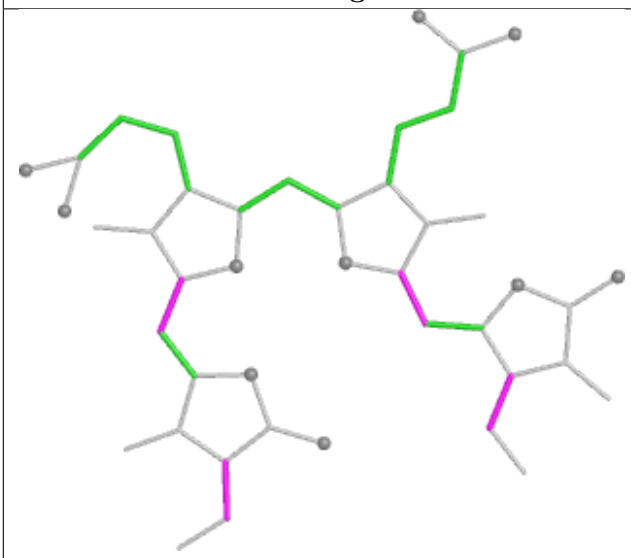
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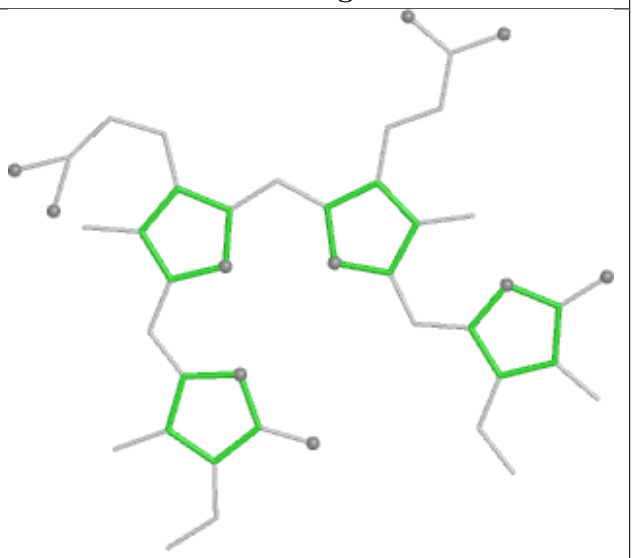
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Bond angles

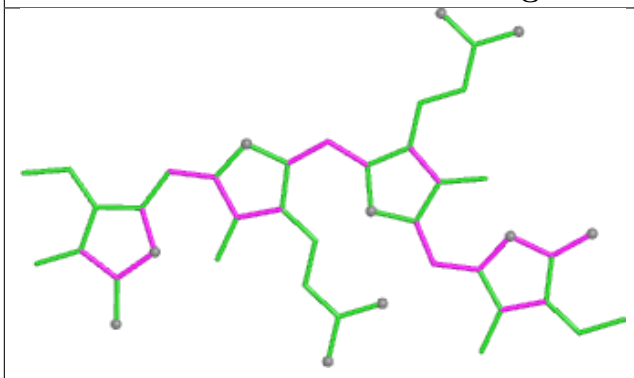


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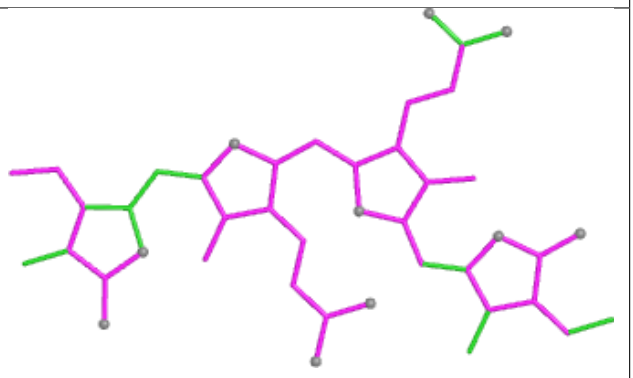


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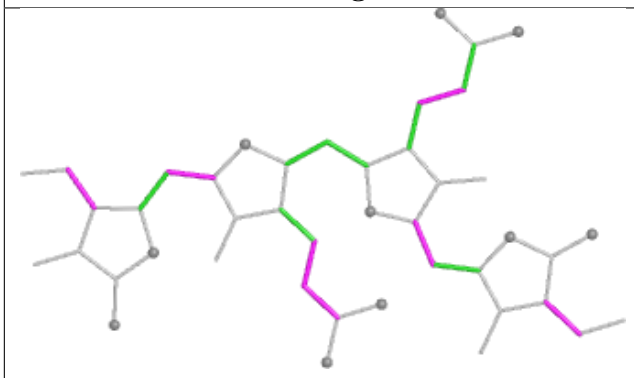
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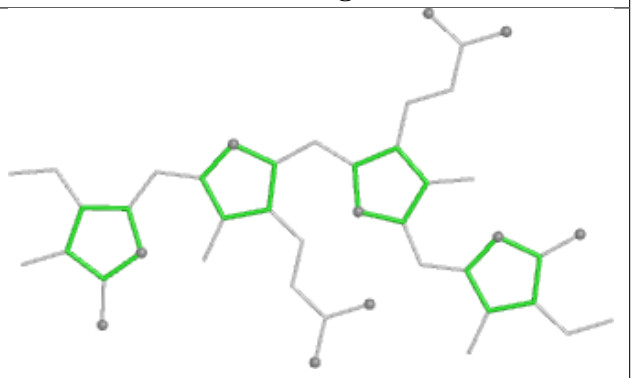
Bond lengths



Bond angles

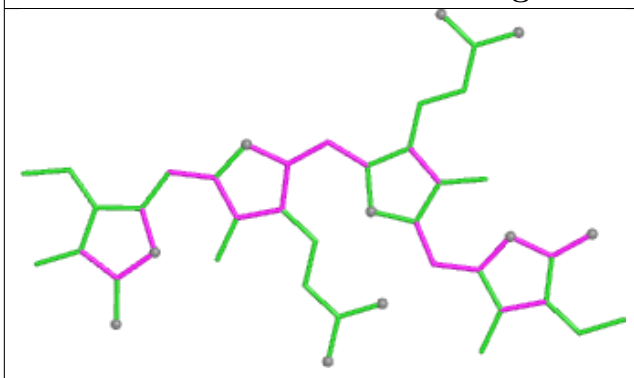


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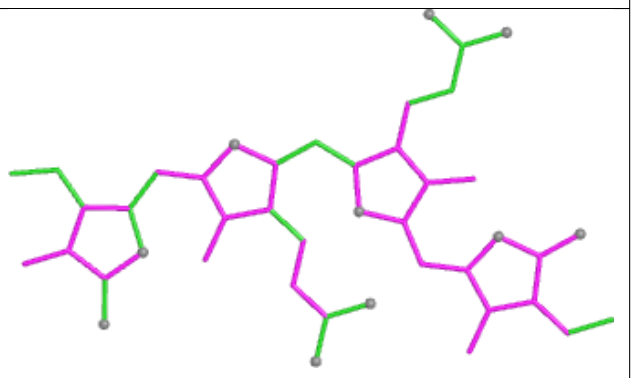


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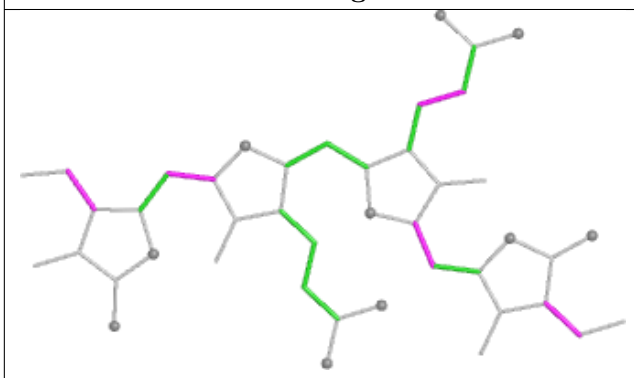
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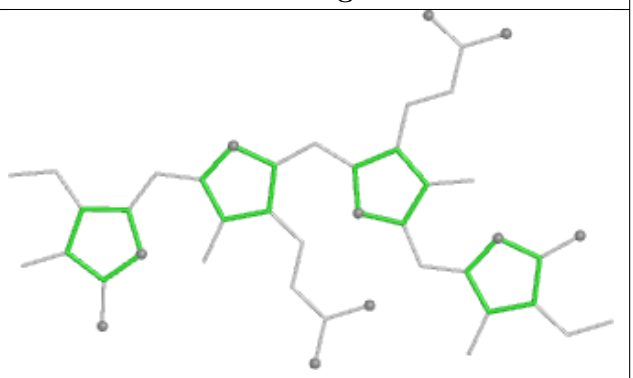
Bond lengths



Bond angles

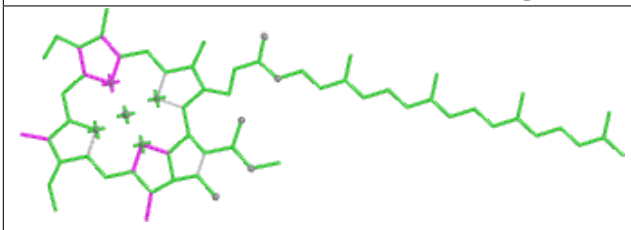


Torsions

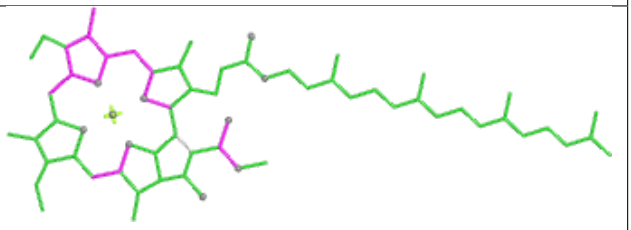


Rings

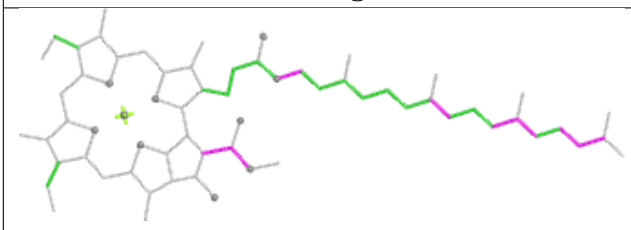
Ligand CLA d1 403



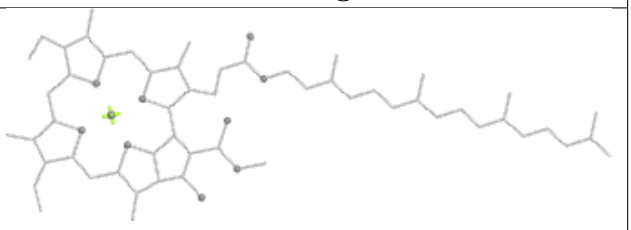
Bond lengths



Bond angles

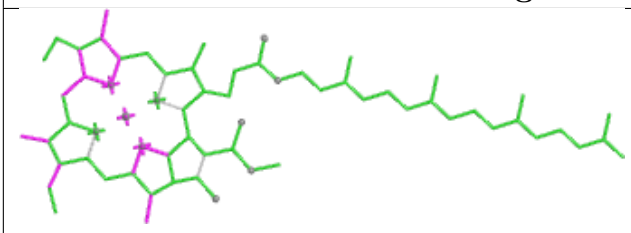


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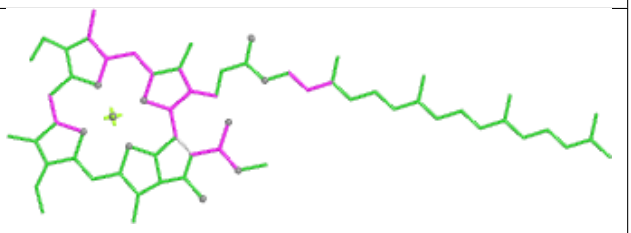


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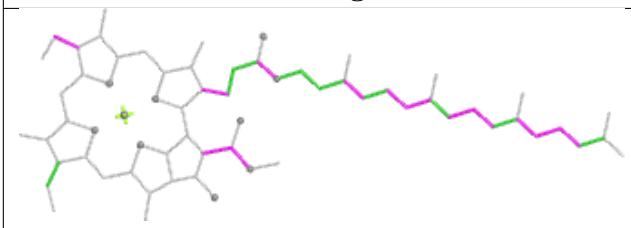
Ligand CLA bE 611



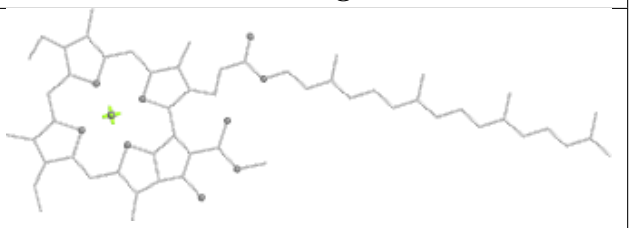
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Bond angles

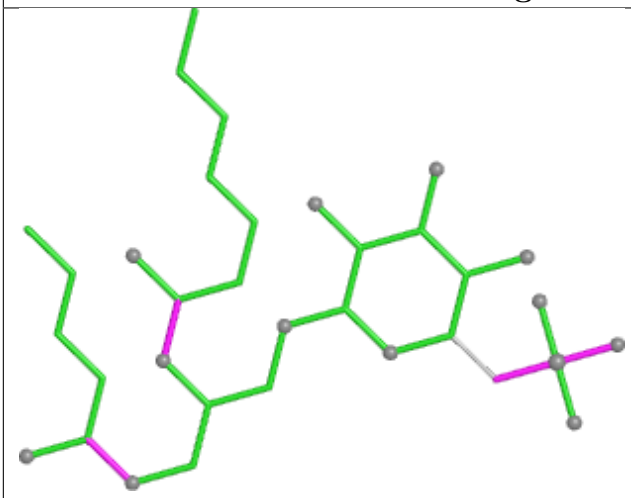


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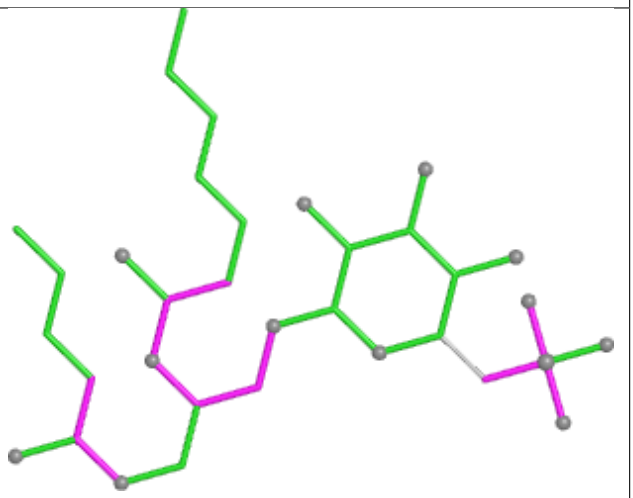


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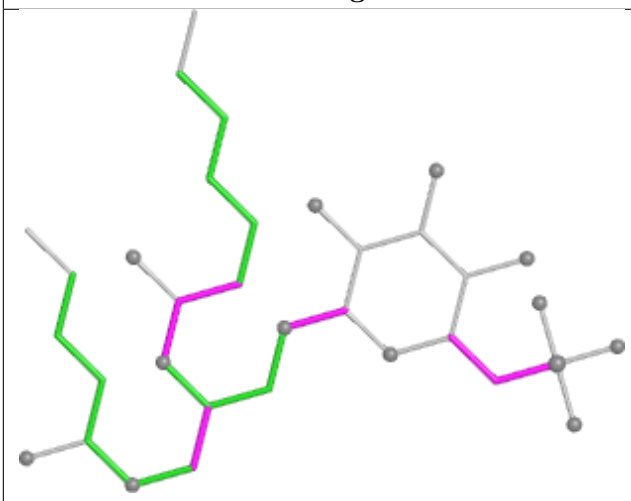
Ligand SQD D1 413



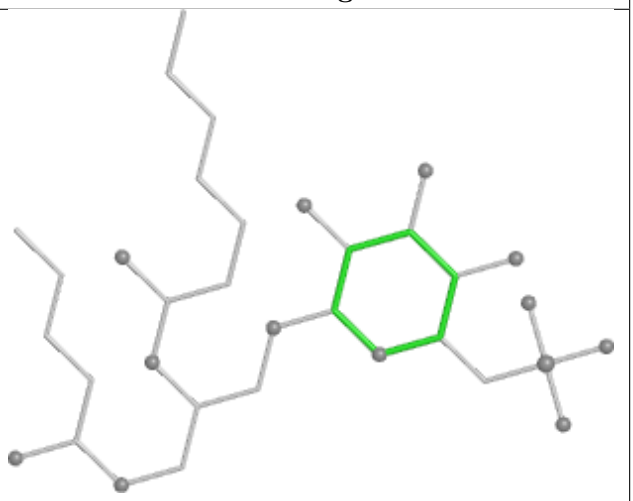
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Bond angles

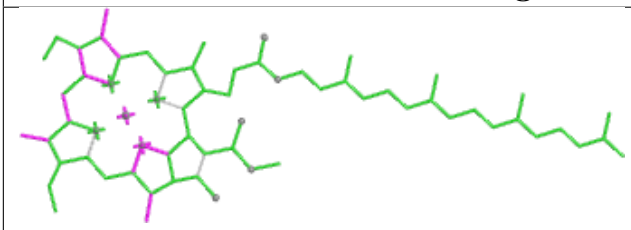


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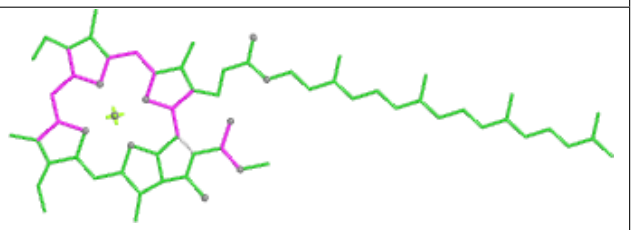


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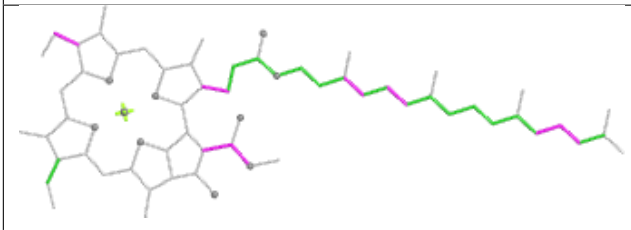
Ligand CLA H1 103



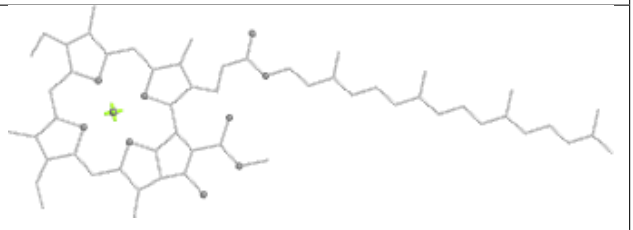
Bond lengths



Bond angles

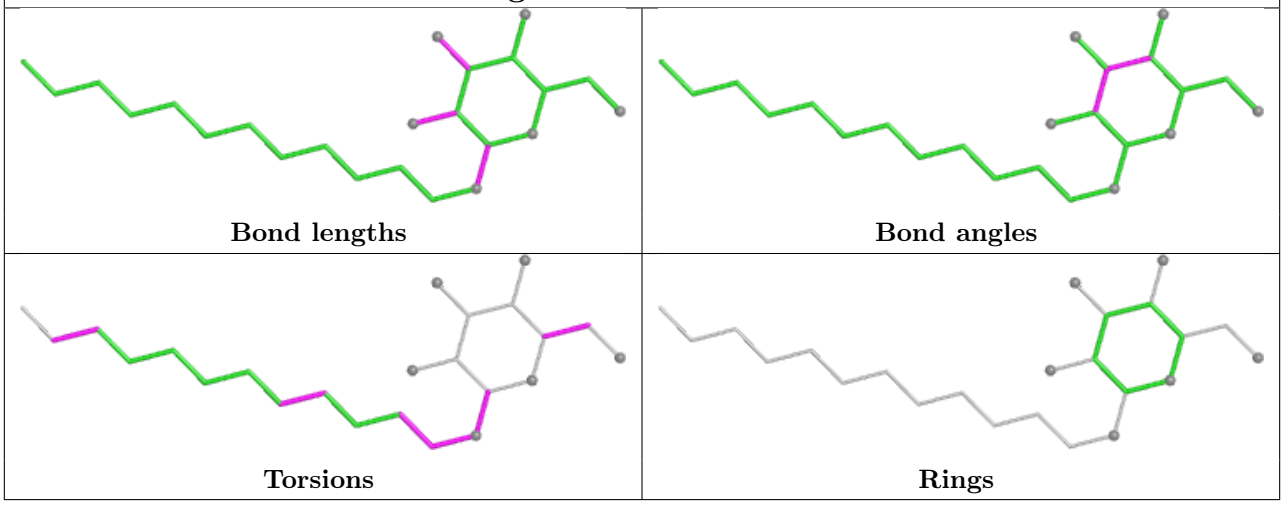


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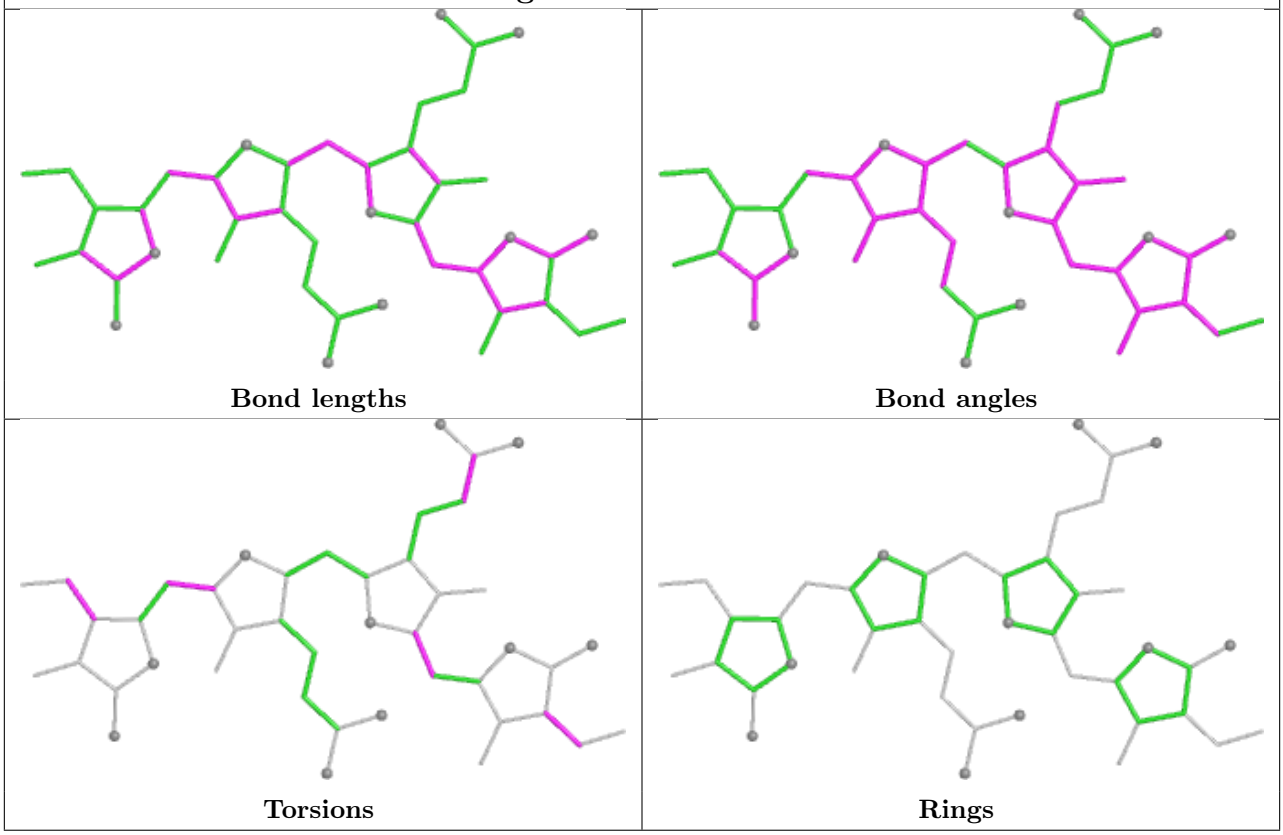


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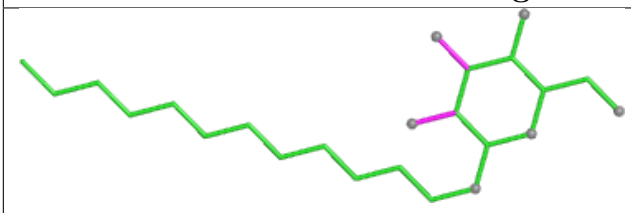
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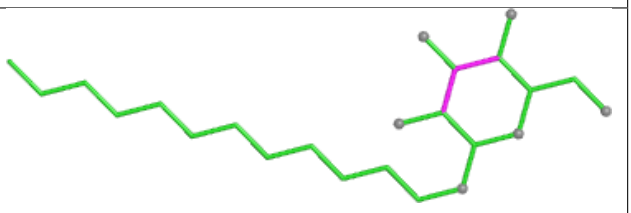
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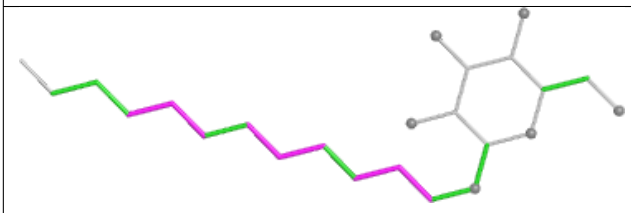
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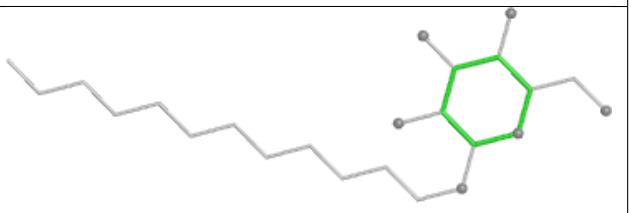
Bond lengths



Bond angles

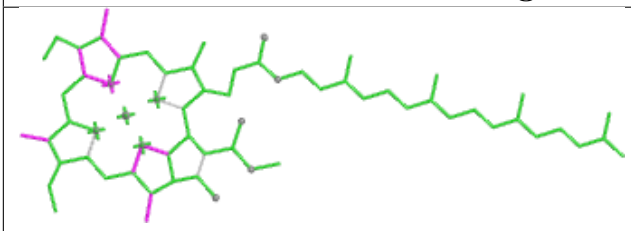


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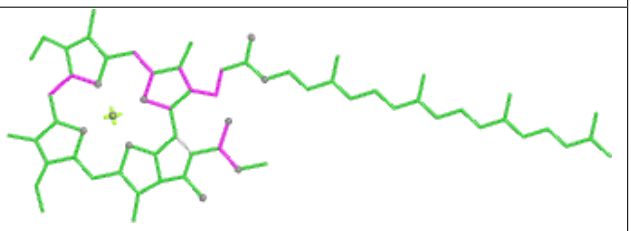


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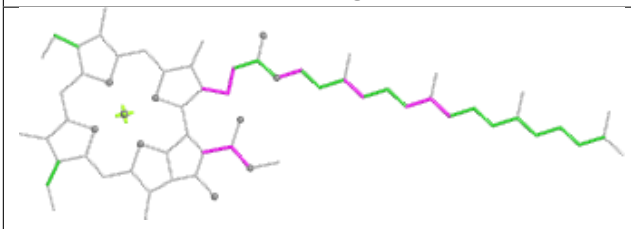
Ligand CLA cE 511



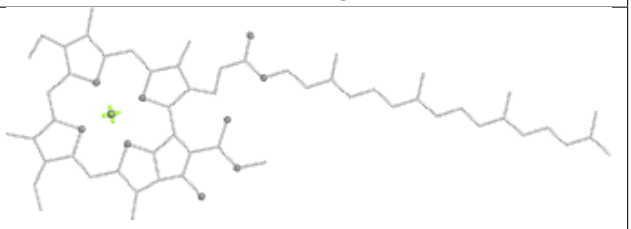
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Bond angles

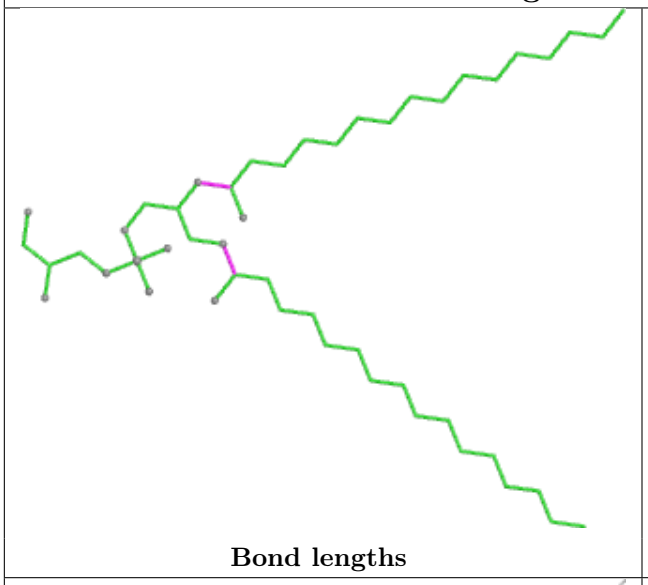


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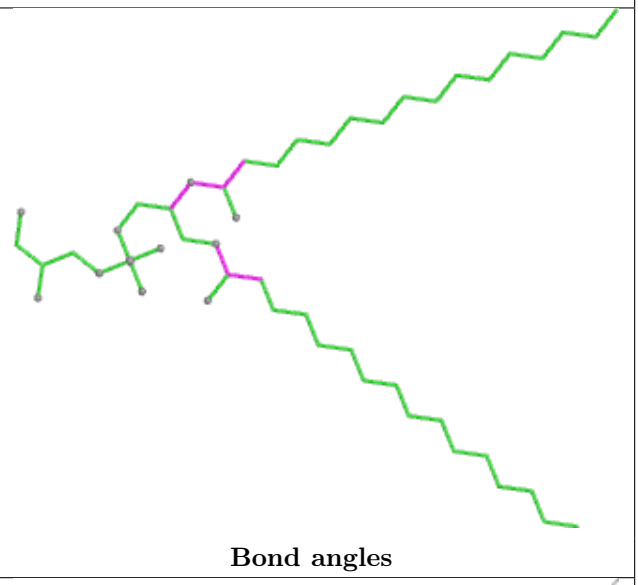


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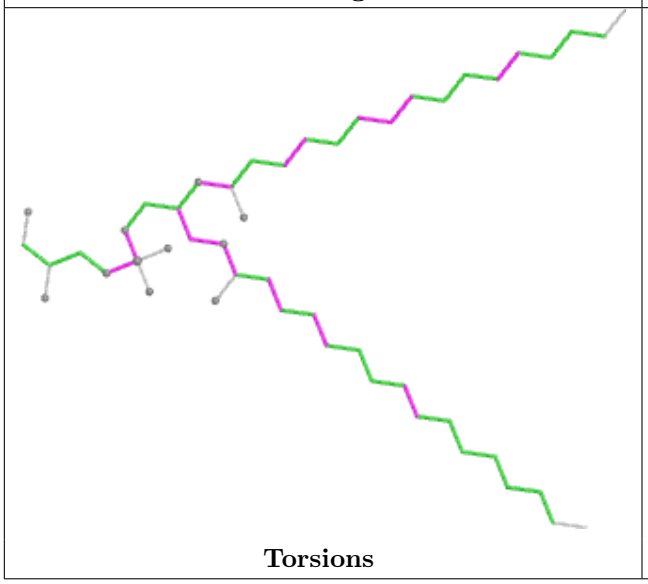
Ligand LHG l1 101



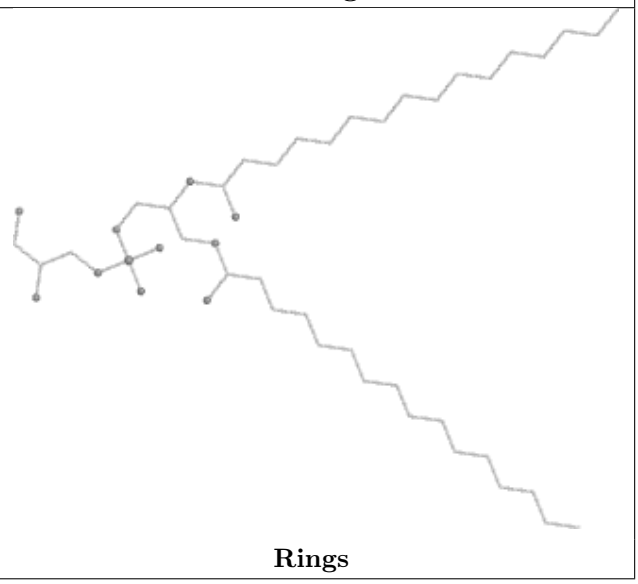
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Bond angles

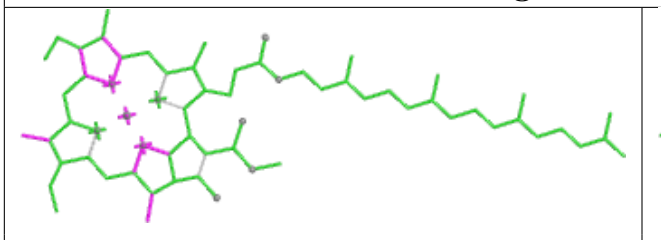


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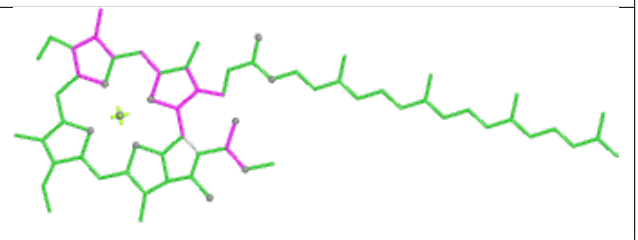


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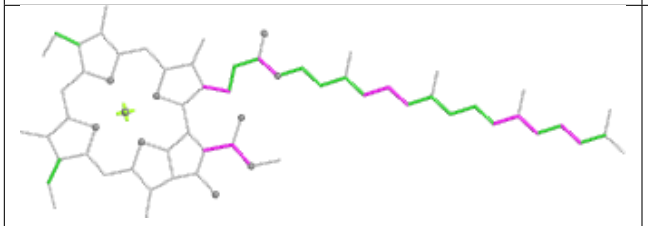
Ligand CLA CE 513



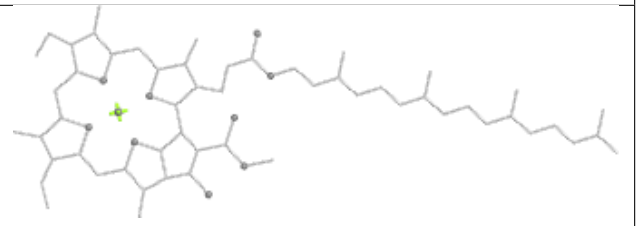
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Bond angles

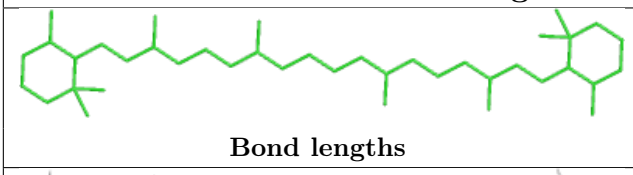


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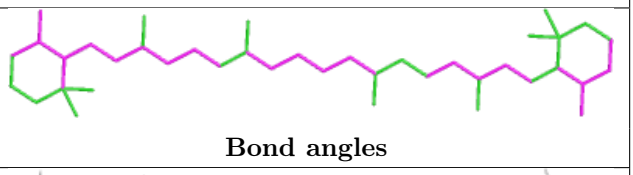


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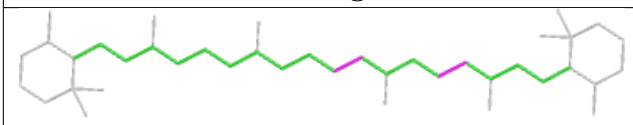
Ligand BCR BE 616



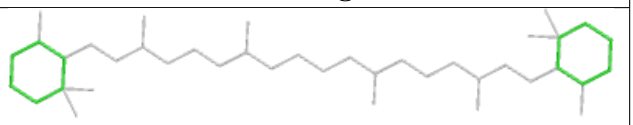
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Bond angles

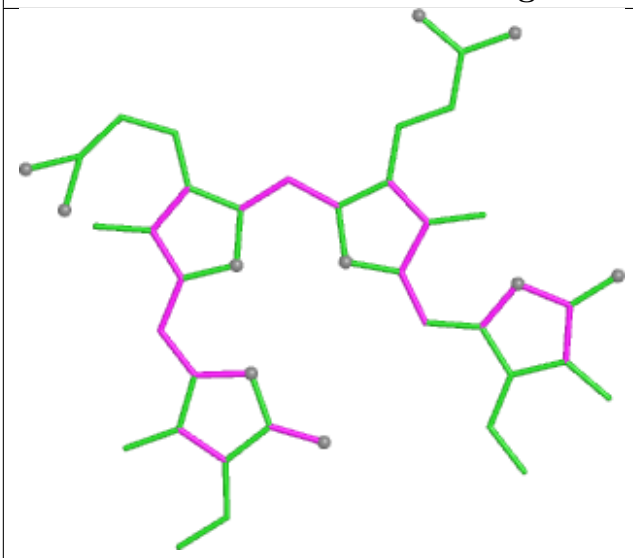


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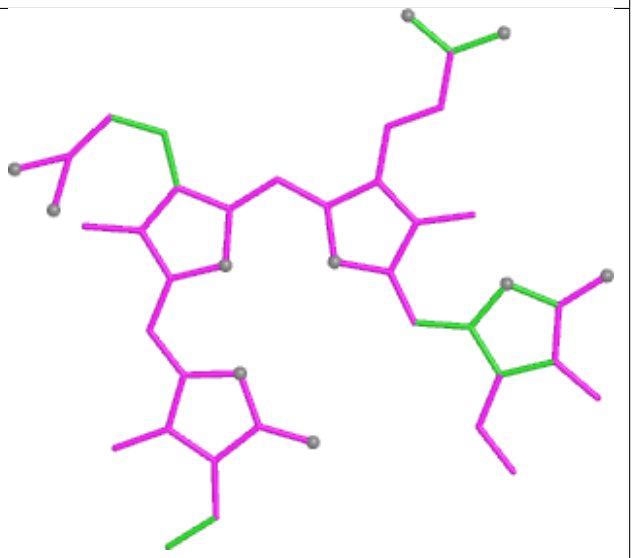


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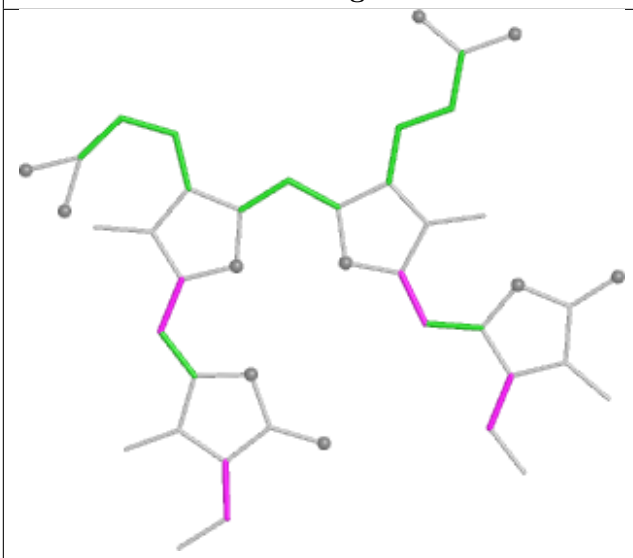
Ligand CYC c9 201



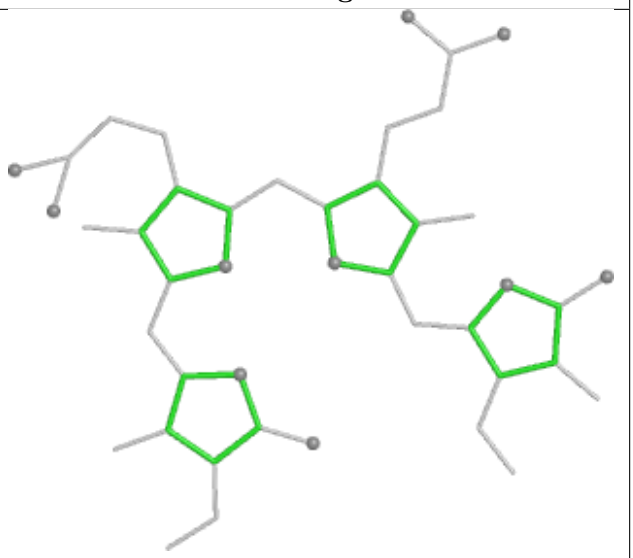
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Bond angles

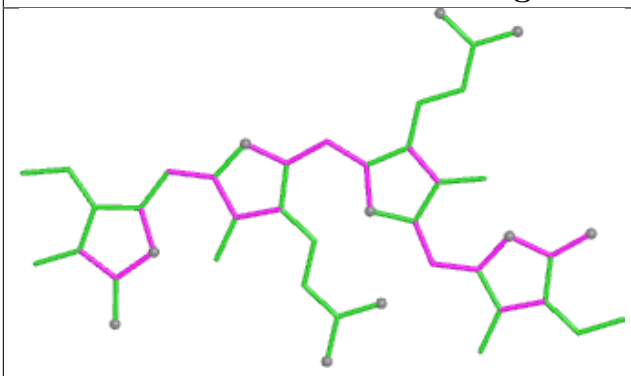


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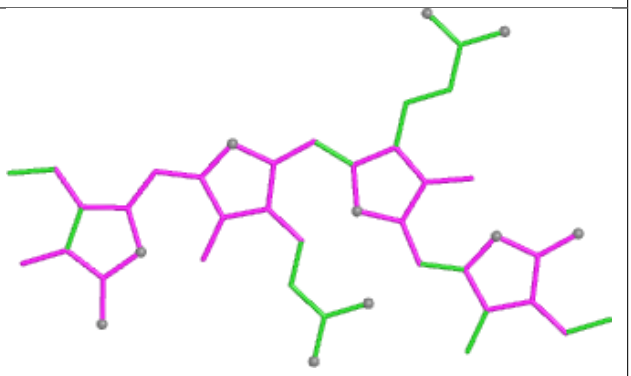


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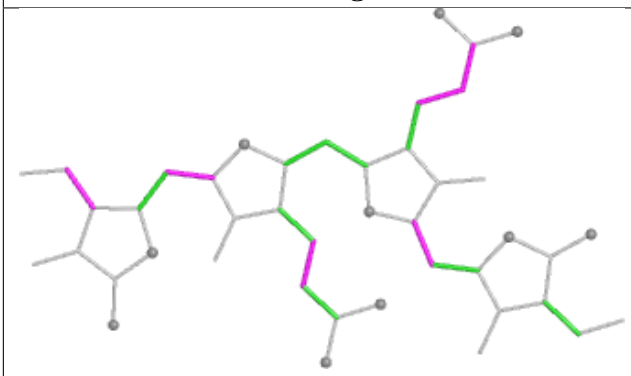
Ligand CYC bF 201



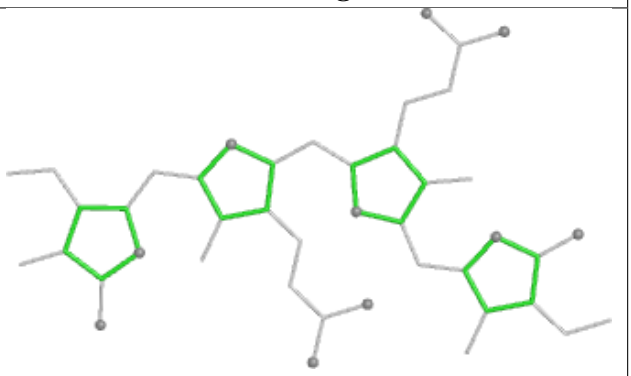
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Bond angles

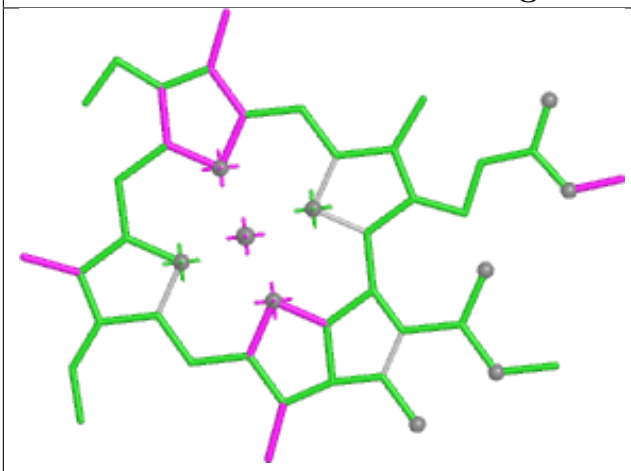


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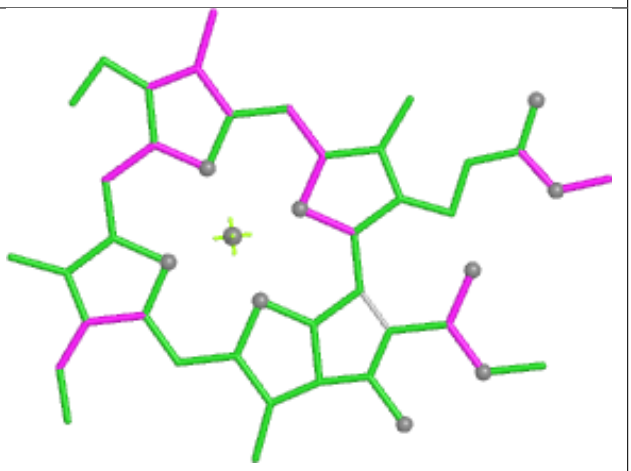


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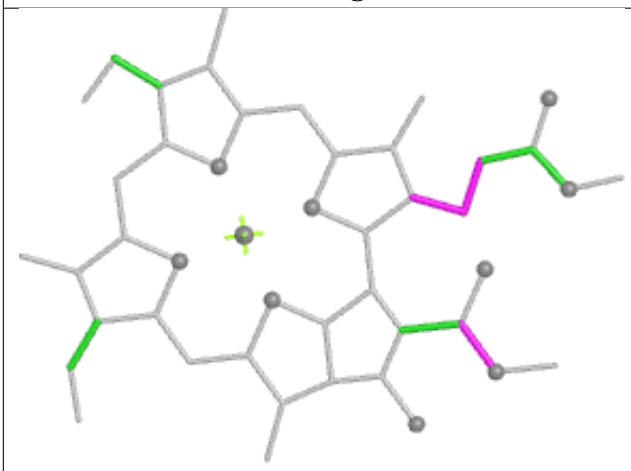
Ligand CLA a1 405



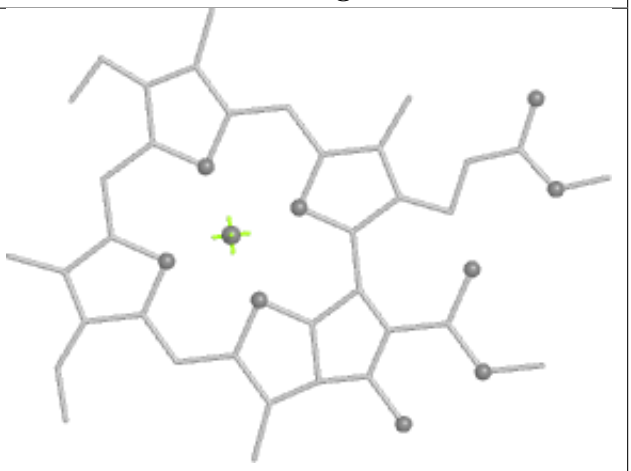
Bond lengths



Bond angles



Torsions



Rings

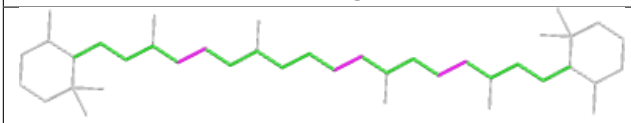
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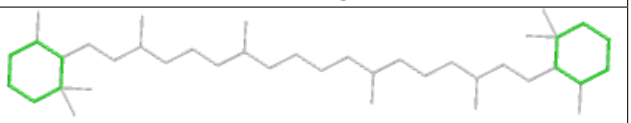
Bond lengths



Bond angles

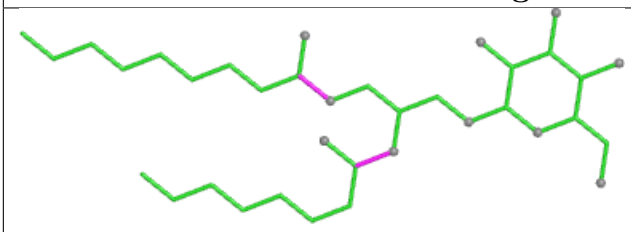


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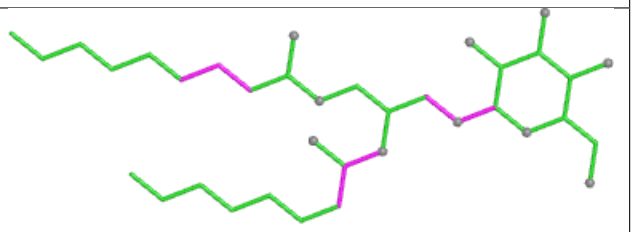


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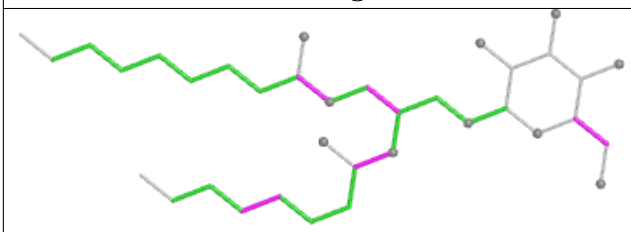
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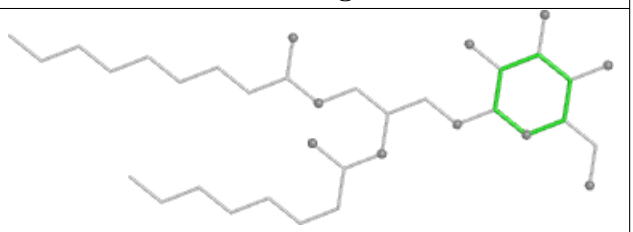
Bond lengths



Bond angles

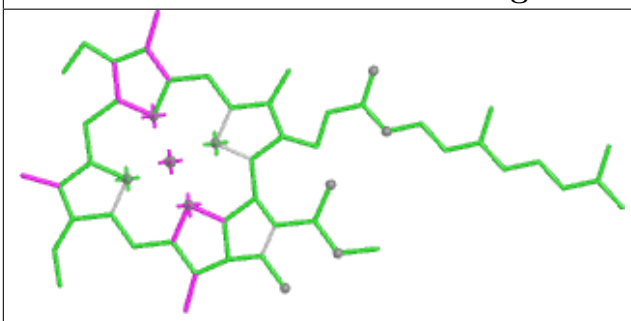


Torsions

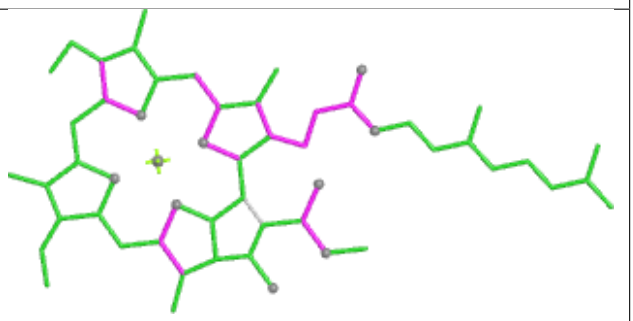


Rings

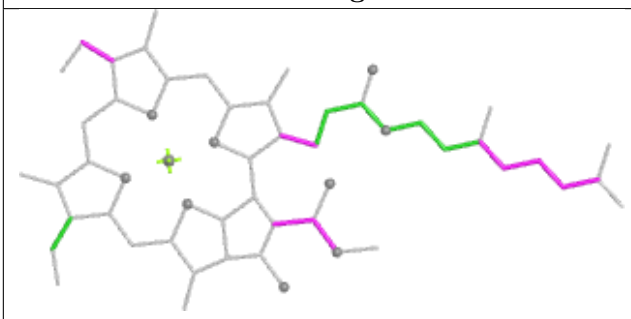
Ligand CLA CD 507



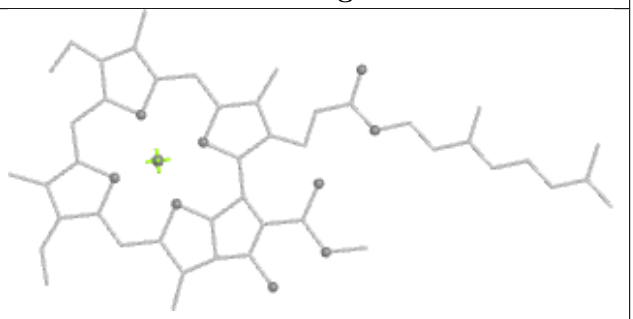
Bond lengths



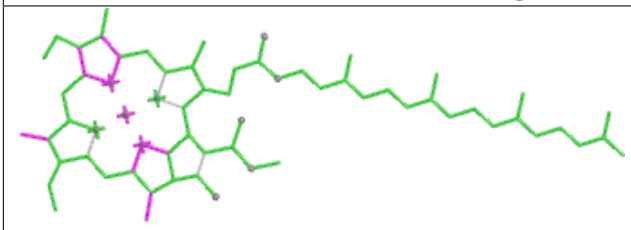
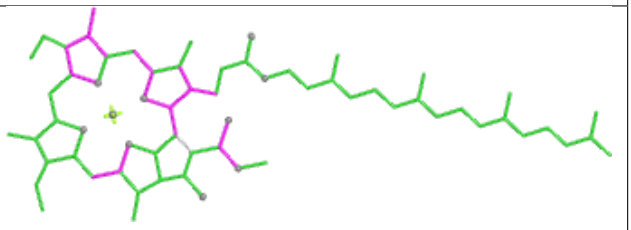
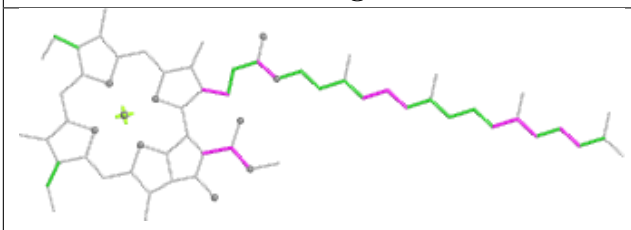
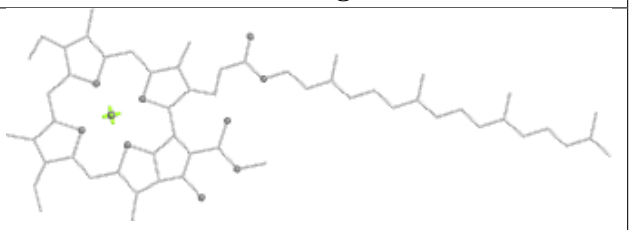
Bond angles



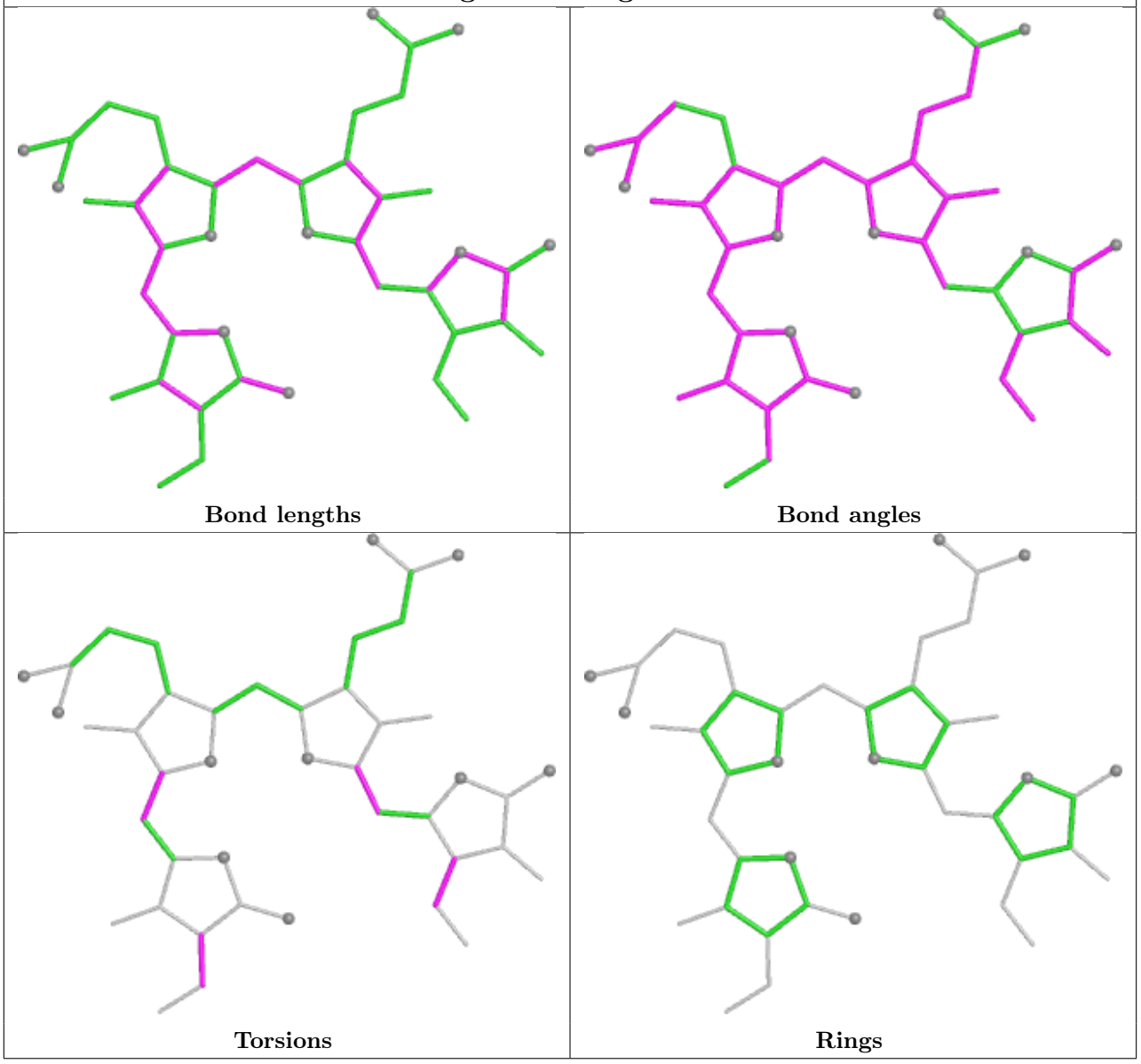
Torsions



Rings

Ligand CLA CD 513	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CYC g7 202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

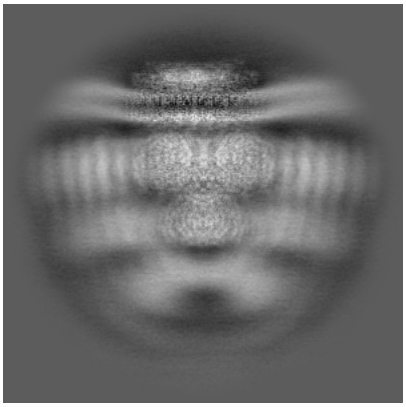
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37749. These allow visual inspection of the internal detail of the map and identification of artifacts.

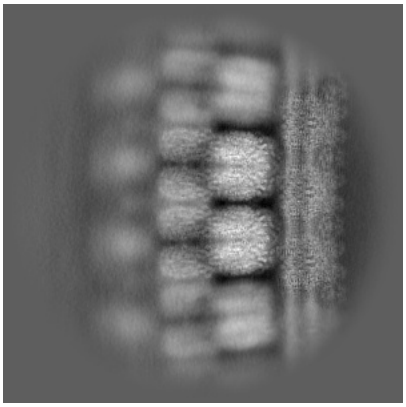
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

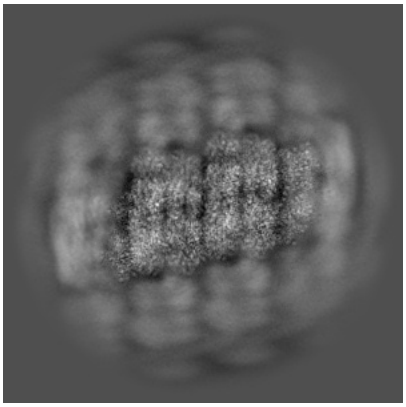
6.1.1 Primary map



X



Y

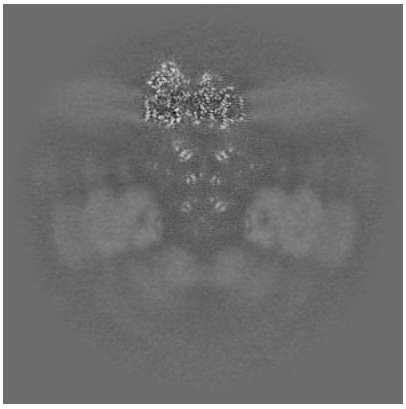


Z

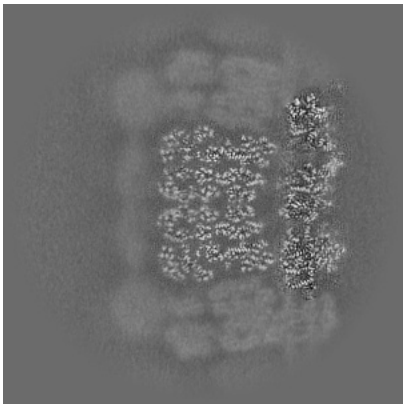
The images above show the map projected in three orthogonal directions.

6.2 Central slices

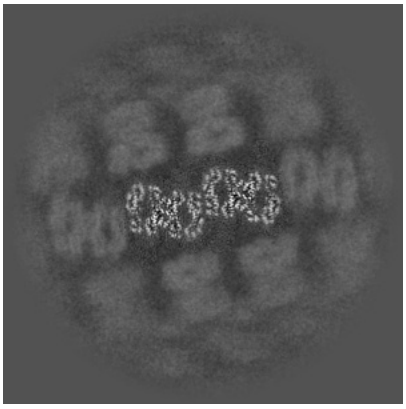
6.2.1 Primary map



X Index: 200



Y Index: 200

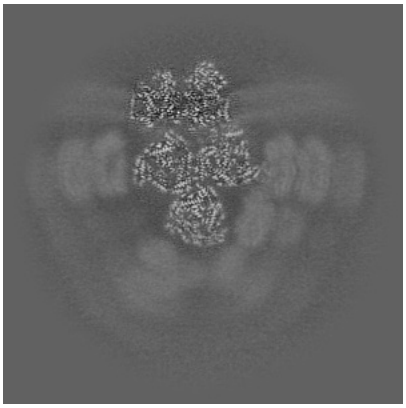


Z Index: 200

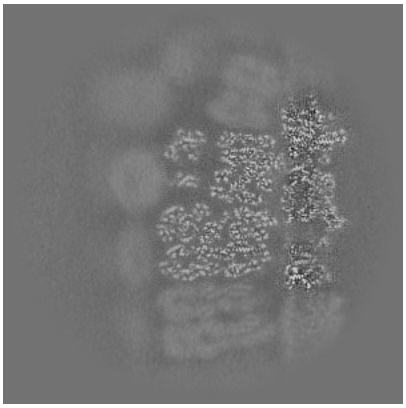
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

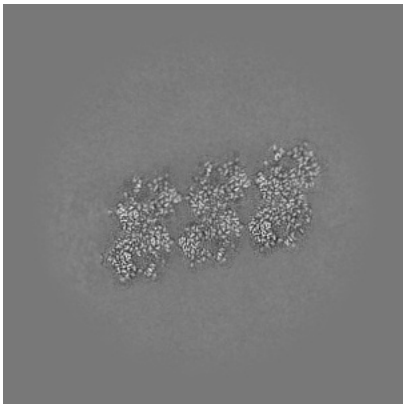
6.3.1 Primary map



X Index: 152



Y Index: 180

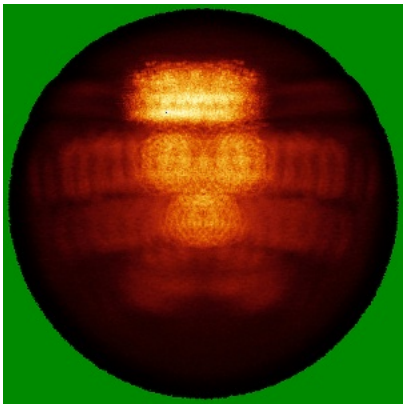


Z Index: 291

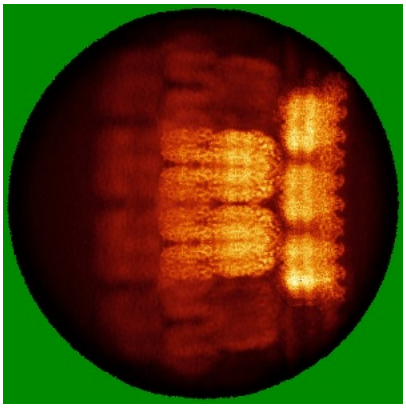
The images above show the largest variance slices of the map in three orthogonal directions.

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

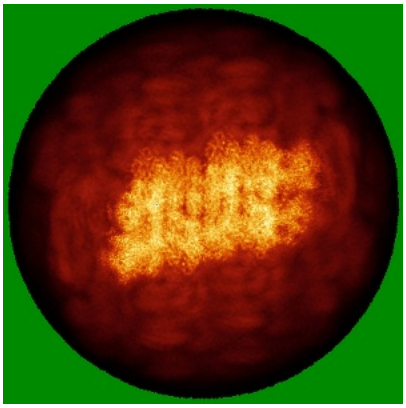
6.4.1 Primary map



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 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

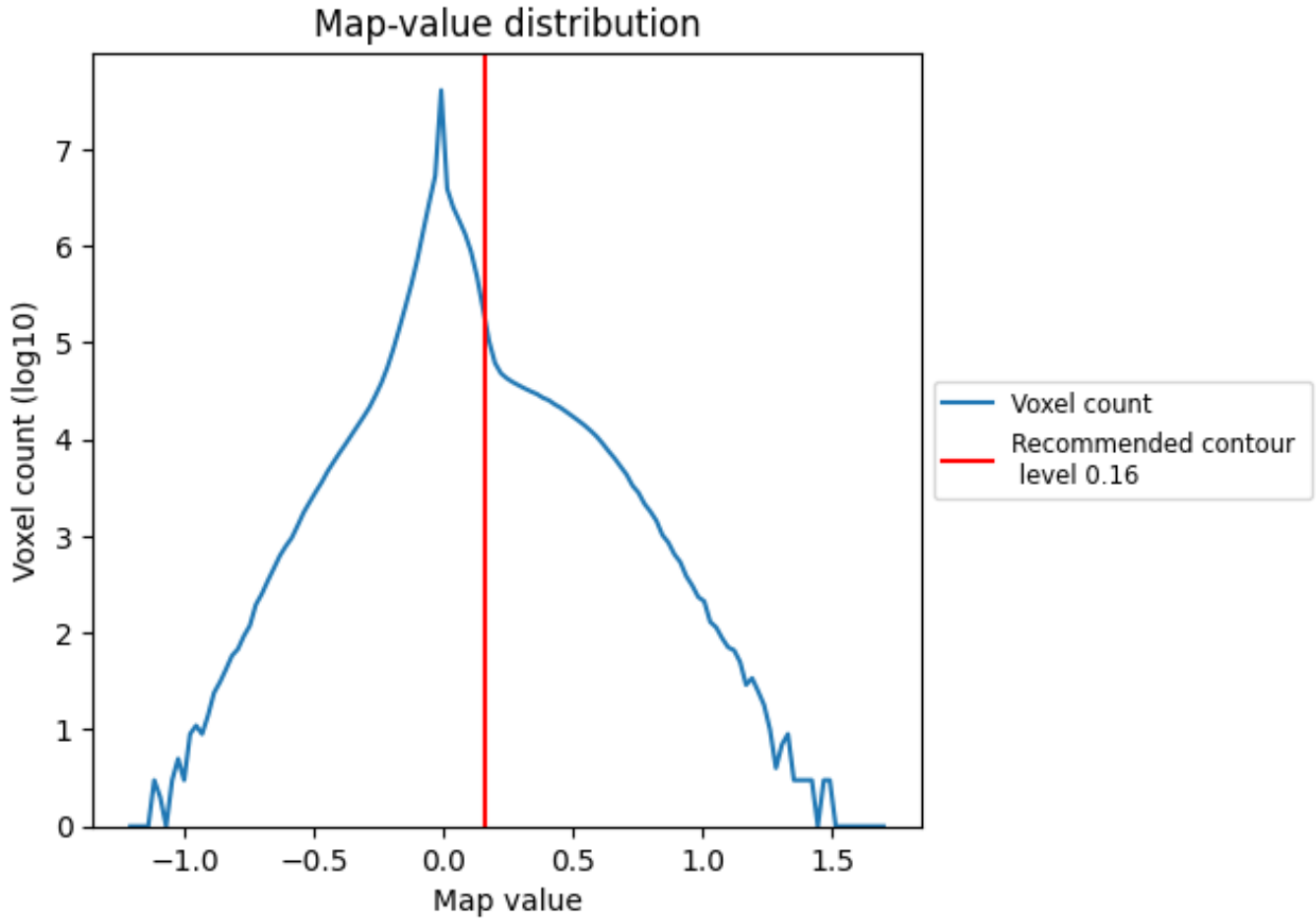
6.6 Mask visualisation (i)

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

7 Map analysis

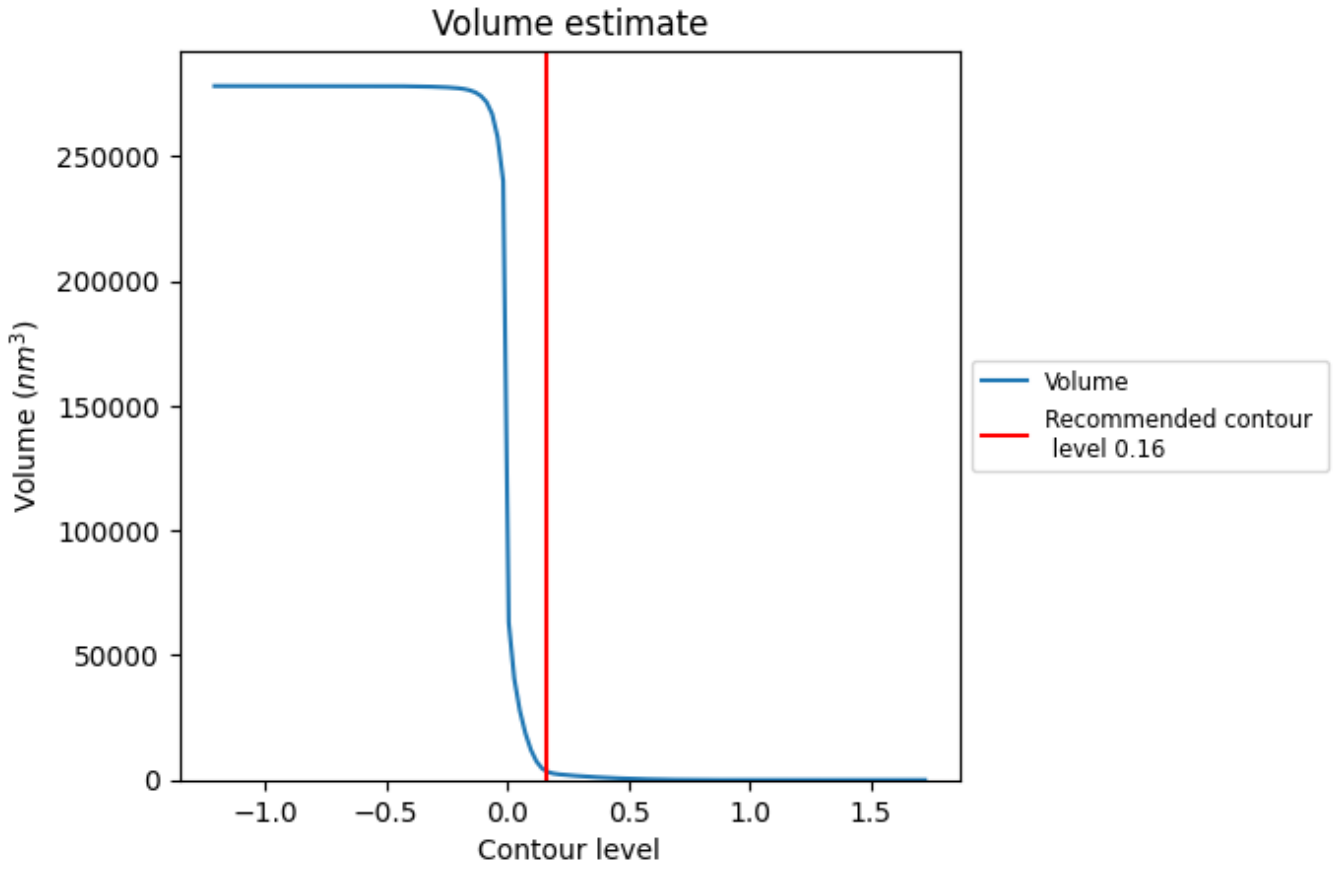
This section contains the results of statistical analysis of the map.

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.

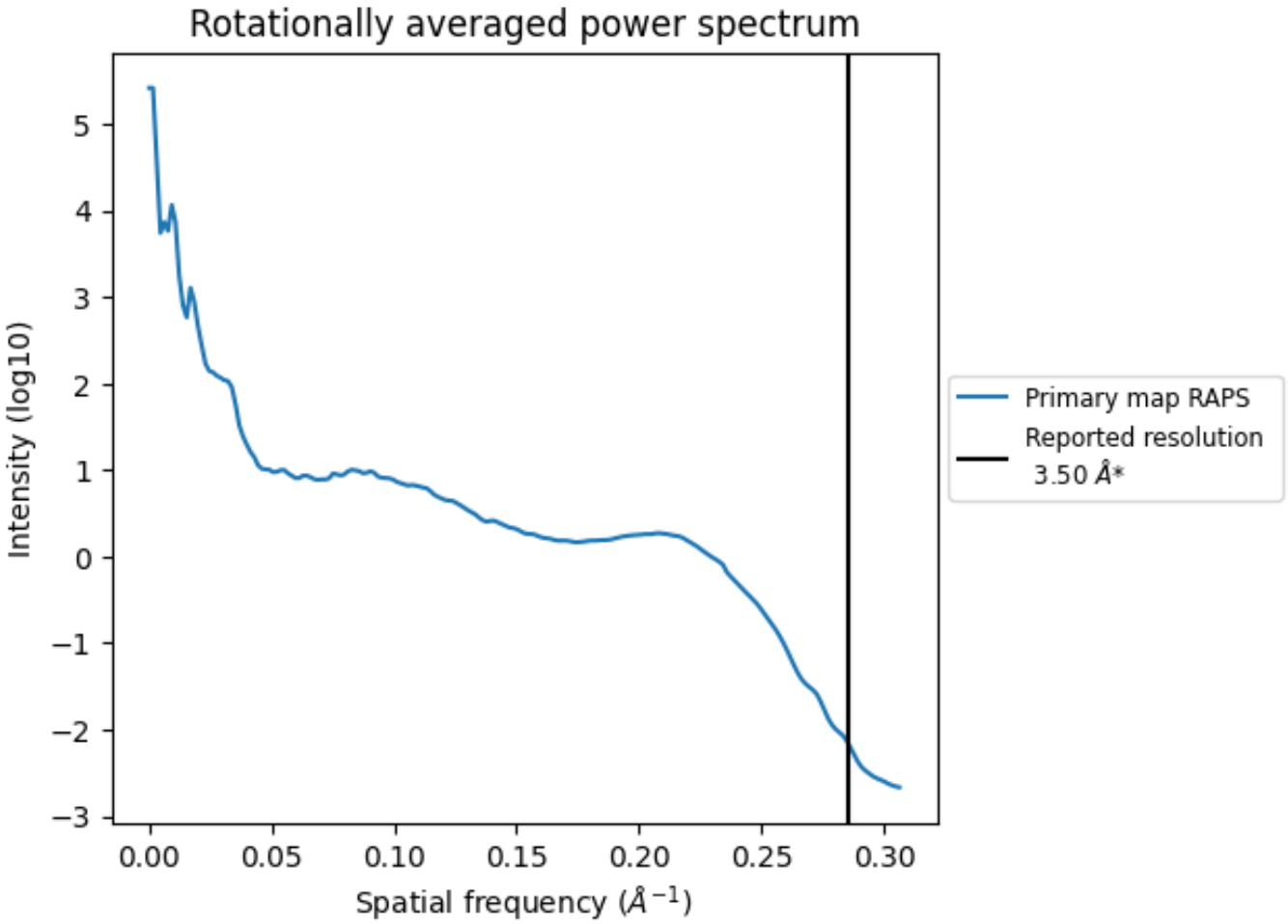
7.2 Volume estimate (i)



The volume at the recommended contour level is 3581 nm^3; this corresponds to an approximate mass of 3235 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 0.286 Å^{-1}

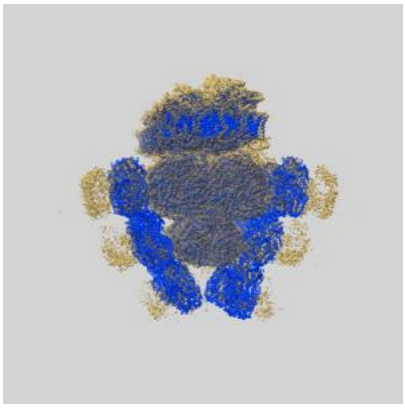
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

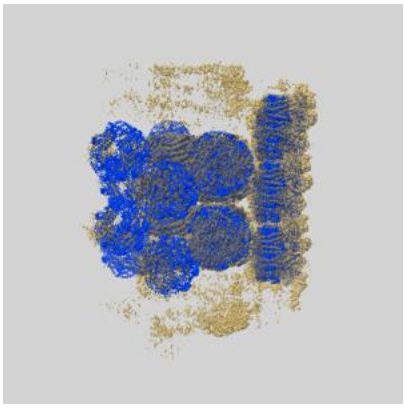
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37749 and PDB model 8WQL. Per-residue inclusion information can be found in section 3 on page 97.

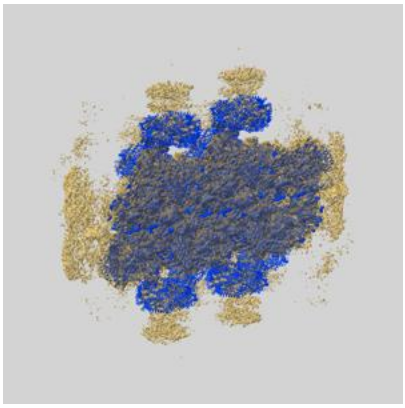
9.1 Map-model overlay



X



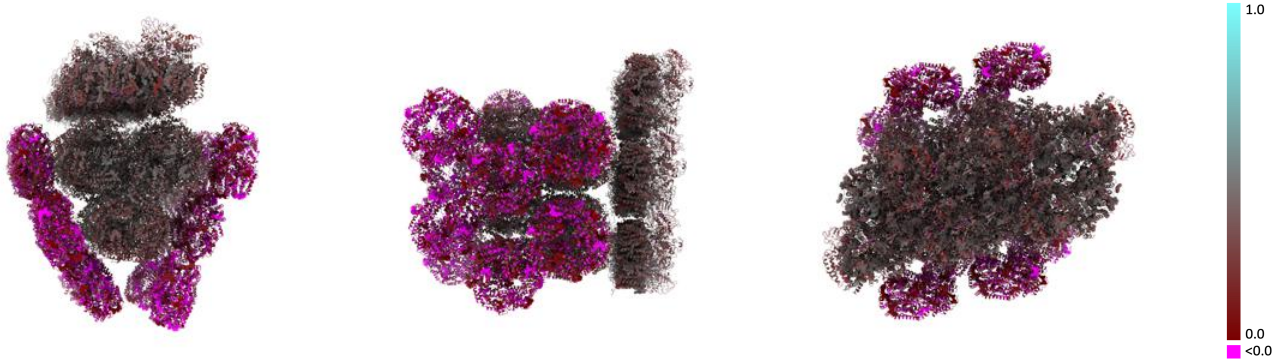
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

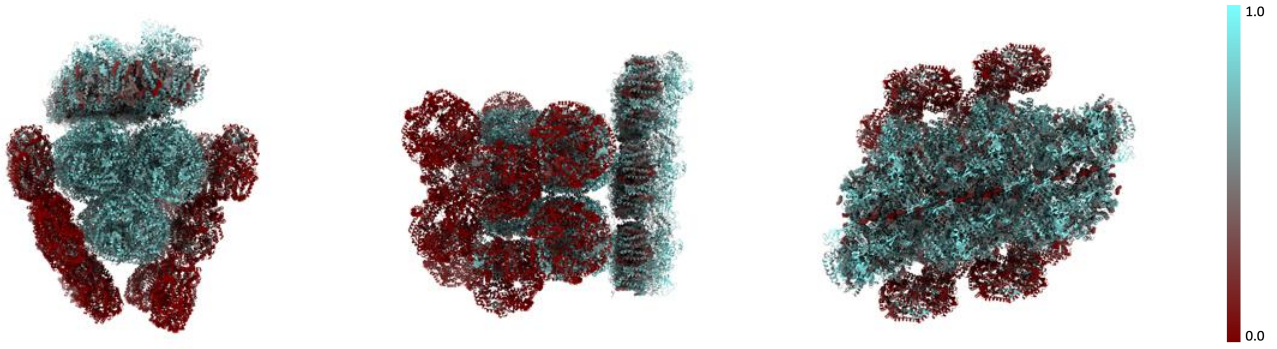
9.2 Q-score mapped to coordinate model



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.

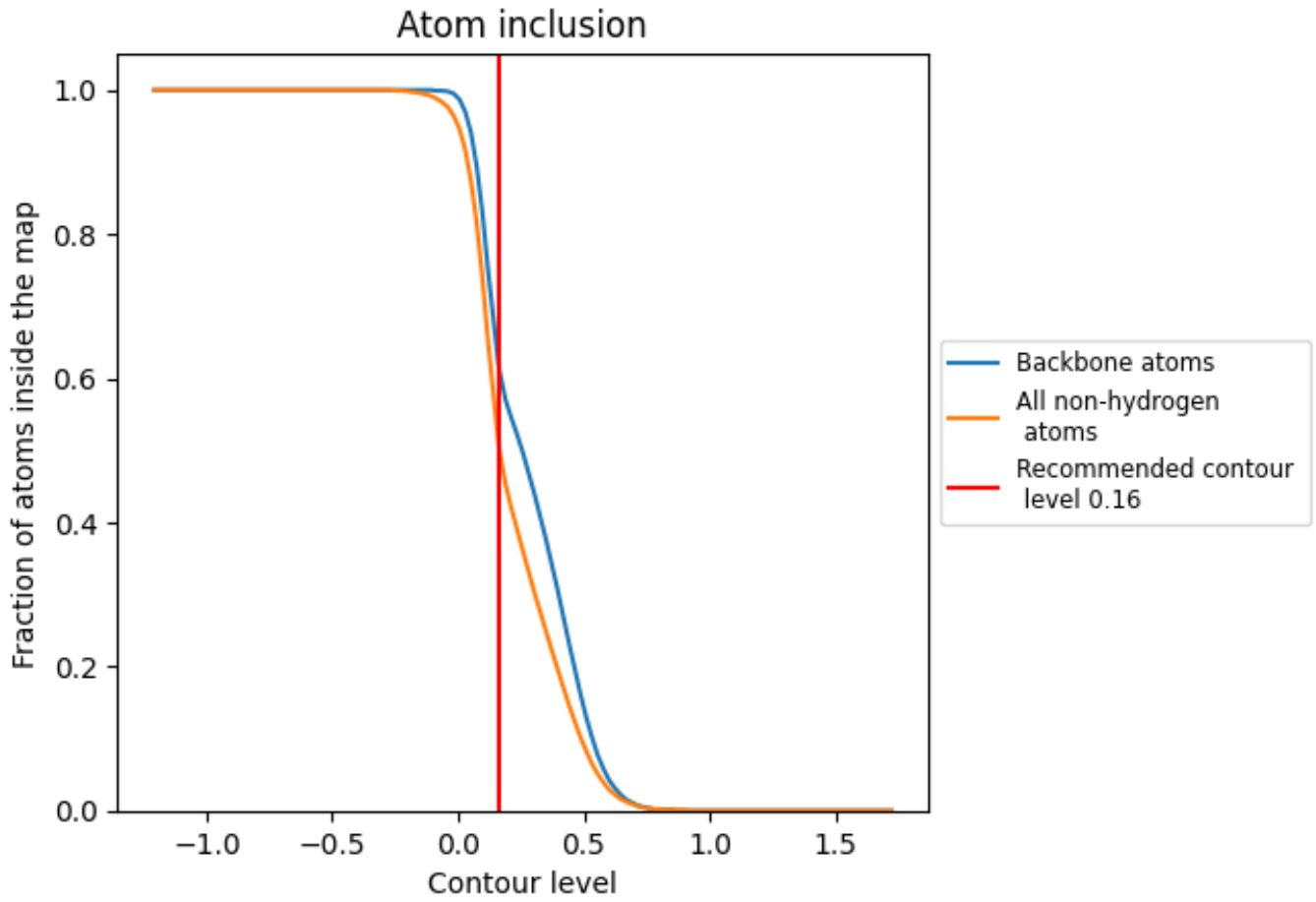
9.3 Atom inclusion mapped to coordinate model



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 (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 51% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5110	0.2640
1G	0.7400	0.3490
1L	0.7520	0.3550
2G	0.7450	0.4140
2L	0.7550	0.4180
3F	0.7640	0.4160
3K	0.7700	0.4200
4G	0.7210	0.3480
4L	0.7350	0.3610
5G	0.7590	0.3770
5L	0.7840	0.3990
6G	0.7310	0.3910
6L	0.7440	0.4080
7G	0.7730	0.3670
7L	0.7720	0.3720
8G	0.7440	0.4210
8L	0.7730	0.4300
9F	0.7650	0.3630
9K	0.7710	0.3670
A1	0.6720	0.3960
AD	0.6470	0.3870
AE	0.6800	0.3980
AG	0.7730	0.3430
AL	0.7720	0.3470
B1	0.6740	0.3850
B2	0.1440	0.0850
B3	0.1810	0.0740
B4	0.7740	0.4050
B5	0.2070	0.0720
B6	0.1120	0.0460
B7	0.1580	0.0740
B8	0.2250	0.1140
B9	0.1650	0.0990
BA	0.1700	0.0470
BB	0.7760	0.4030



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Chain	Atom inclusion	Q-score
BC	0.1510	0.0680
BD	0.6680	0.3910
BE	0.6670	0.3850
BG	0.6940	0.3580
BH	0.2280	0.1160
BI	0.1530	0.0990
BJ	0.2150	0.1020
BL	0.6650	0.3460
C1	0.6850	0.3980
C4	0.7670	0.3970
CB	0.7730	0.3990
CD	0.6720	0.3920
CE	0.6880	0.3960
D1	0.6680	0.4020
DD	0.6520	0.4000
DE	0.6580	0.4000
E1	0.7070	0.3750
ED	0.7080	0.3790
EE	0.7040	0.3680
EF	0.7200	0.4300
EK	0.6850	0.4090
F1	0.6750	0.3500
FD	0.6930	0.3490
FE	0.6970	0.3510
GG	0.7580	0.4100
GL	0.7670	0.4190
H1	0.4490	0.3060
HD	0.5490	0.3530
HE	0.5540	0.3450
HG	0.7820	0.4130
HL	0.7800	0.4220
I1	0.6410	0.4170
ID	0.6220	0.4200
IE	0.6560	0.4250
IF	0.7490	0.3590
IG	0.6930	0.3160
IK	0.7710	0.3780
IL	0.7070	0.3200
J1	0.5950	0.3900
JD	0.5750	0.3870
JE	0.5630	0.3870
JF	0.7470	0.3460

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Chain	Atom inclusion	Q-score
JG	0.8060	0.4150
JK	0.7450	0.3650
JL	0.7900	0.4020
K1	0.6320	0.3750
KD	0.6530	0.3590
KE	0.6840	0.3760
KF	0.7760	0.3870
KG	0.8000	0.3860
KK	0.7970	0.4040
KL	0.7980	0.3840
L1	0.5850	0.3930
LD	0.5750	0.3990
LE	0.6110	0.3920
LF	0.7260	0.3830
LG	0.7880	0.4270
LK	0.7520	0.4020
LL	0.7940	0.4300
M1	0.5390	0.3770
MD	0.5050	0.3690
ME	0.5420	0.3760
MF	0.7760	0.3670
MG	0.8010	0.3990
MK	0.7760	0.3780
ML	0.7920	0.3960
NF	0.7560	0.4390
NG	0.7280	0.3660
NK	0.7710	0.4450
NL	0.7500	0.3830
O1	0.7140	0.2770
O4	0.6500	0.2890
OB	0.6570	0.2970
OD	0.7170	0.2720
OE	0.7250	0.2720
OG	0.7680	0.4150
OL	0.7770	0.4260
P4	0.7040	0.3210
PB	0.7190	0.3270
PG	0.7590	0.4210
PL	0.7840	0.4270
Q1	0.6200	0.2630
Q4	0.6980	0.3240
QB	0.7050	0.3320

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Chain	Atom inclusion	Q-score
QD	0.6270	0.2670
QE	0.6320	0.2670
QG	0.8050	0.4120
QL	0.7970	0.4050
R1	0.5950	0.2720
R4	0.7450	0.3290
RB	0.7510	0.3410
RD	0.5990	0.2640
RE	0.5950	0.2730
RG	0.7180	0.3850
RL	0.7530	0.4060
S1	0.7620	0.4420
S4	0.7210	0.3530
SB	0.7450	0.3730
SD	0.7660	0.4730
SE	0.7530	0.4360
SG	0.7330	0.3460
SL	0.7420	0.3630
T1	0.6130	0.4170
T4	0.7210	0.3200
TB	0.7260	0.3280
TD	0.5660	0.4020
TE	0.6130	0.4180
TG	0.7400	0.3370
TL	0.7490	0.3410
U1	0.8120	0.3100
U4	0.7070	0.3790
UB	0.7340	0.3840
UD	0.8120	0.3070
UE	0.8150	0.3120
UG	0.8280	0.3690
UL	0.8230	0.3720
V1	0.8210	0.3480
V4	0.6450	0.2890
VB	0.6510	0.3000
VD	0.8270	0.3510
VE	0.8230	0.3480
VG	0.7860	0.3570
VL	0.7910	0.3600
W4	0.7190	0.3040
WB	0.7290	0.3100
WG	0.7680	0.3990

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Chain	Atom inclusion	Q-score
WL	0.7970	0.4150
X1	0.5700	0.3430
X4	0.6830	0.3140
XB	0.7000	0.3280
XD	0.5890	0.3420
XE	0.5380	0.3320
XF	0.7370	0.3780
XK	0.7490	0.3900
Y1	0.5950	0.3020
Y4	0.7560	0.3330
YB	0.7780	0.3460
YD	0.5950	0.3020
YE	0.6030	0.2970
YF	0.7950	0.4050
YK	0.7910	0.4040
Z1	0.6090	0.3380
Z4	0.7170	0.3480
ZB	0.7360	0.3590
ZD	0.6100	0.3260
ZE	0.6160	0.3390
ZF	0.7970	0.3880
ZK	0.7950	0.3880
a1	0.6520	0.3830
a4	0.7310	0.3170
aB	0.7460	0.3210
aD	0.6320	0.3760
aE	0.6490	0.3790
aF	0.7910	0.4360
aK	0.7950	0.4380
b1	0.7170	0.4050
b2	0.2980	0.0820
b3	0.0320	0.0320
b4	0.7050	0.3840
b5	0.3290	0.1090
b6	0.1440	0.0370
b7	0.0690	0.0160
b8	0.2240	0.1080
b9	0.2320	0.0690
bA	0.0280	0.0080
bB	0.7230	0.3910
bC	0.0890	0.0100
bD	0.6840	0.3990

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Chain	Atom inclusion	Q-score
bE	0.7240	0.4070
bF	0.7660	0.4210
bH	0.3360	0.0970
bI	0.1920	0.0620
bJ	0.2330	0.0800
bK	0.7740	0.4250
c1	0.6350	0.3730
c2	0.0840	0.1140
c3	0.0220	0.0220
c5	0.1710	0.0930
c6	0.0450	-0.0150
c7	0.0160	0.0220
c8	0.1370	0.0680
c9	0.0910	0.0990
cA	0.0710	0.0260
cC	0.0260	0.0040
cD	0.6340	0.3750
cE	0.6200	0.3690
cF	0.7960	0.4210
cH	0.1790	0.0810
cI	0.0480	0.0970
cJ	0.1920	0.0970
cK	0.7890	0.4190
d1	0.6770	0.4100
d2	0.0040	0.0360
d3	0.0350	0.0430
d5	0.1730	0.0460
d6	0.0120	0.0350
d7	0.0160	0.0020
d8	0.3140	0.0650
d9	0.0080	0.0520
dA	0.0110	0.0220
dC	0.0110	0.0250
dD	0.6460	0.4050
dE	0.6680	0.4050
dF	0.7160	0.3690
dH	0.1800	0.0580
dI	0.0000	0.0560
dJ	0.3450	0.0550
dK	0.7300	0.3760
e1	0.6770	0.3620
e2	0.0060	0.0730

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Chain	Atom inclusion	Q-score
e3	0.0310	0.0170
e5	0.0420	0.0260
e6	0.0010	0.0370
e7	0.0130	0.0200
e8	0.0680	0.0450
e9	0.0110	0.0960
eA	0.0200	0.0250
eC	0.0060	0.0170
eD	0.6570	0.3590
eE	0.6690	0.3660
eF	0.7640	0.4260
eH	0.0340	0.0280
eI	0.0020	0.0380
eJ	0.0620	0.0250
eK	0.7630	0.4250
f1	0.6960	0.3810
f2	0.0500	0.0240
f3	0.0910	0.0390
f5	0.0530	0.0170
f6	0.0220	0.0070
f7	0.0090	0.0120
f8	0.1180	0.0260
f9	0.0630	0.0270
fA	0.0520	0.0250
fC	0.0330	0.0200
fD	0.6690	0.3860
fE	0.6900	0.3830
fF	0.7490	0.4150
fH	0.1310	0.0430
fI	0.0770	0.0420
fJ	0.1320	0.0360
fK	0.7580	0.4170
g2	0.1000	0.0830
g3	0.0620	0.0140
g5	0.1900	0.0860
g6	0.0620	0.0400
g7	0.0560	0.0260
g8	0.2150	0.1120
g9	0.1020	0.0680
gA	0.0790	0.0100
gC	0.1020	0.0250
gF	0.7970	0.4170

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Chain	Atom inclusion	Q-score
gH	0.2460	0.0970
gI	0.0730	0.0640
gJ	0.2260	0.0960
gK	0.7970	0.4160
h1	0.6380	0.3710
h2	0.1390	0.0470
h3	0.0090	0.0060
h5	0.2470	0.0580
h6	0.0820	0.0440
h7	0.0120	0.0200
h8	0.1780	0.0330
h9	0.0880	0.0500
hA	0.0030	0.0130
hC	0.0120	-0.0050
hD	0.5840	0.3690
hE	0.6500	0.3820
hF	0.7990	0.4100
hH	0.2410	0.0410
hI	0.0280	0.0400
hJ	0.2420	0.0500
hK	0.7950	0.4070
i1	0.6410	0.3930
i2	0.1350	0.0610
i3	0.0140	0.0110
i5	0.1160	0.0780
i6	0.0600	0.0110
i7	0.0270	0.0220
i8	0.0730	0.0830
i9	0.1030	0.0550
iA	0.0030	0.0050
iC	0.0610	0.0300
iD	0.6140	0.4150
iE	0.5890	0.3860
iF	0.7290	0.3840
iH	0.1100	0.0860
iI	0.1050	0.0620
iJ	0.0920	0.0540
iK	0.7460	0.4010
j1	0.4480	0.3120
j2	0.1540	0.0490
j3	0.0560	0.0210
j5	0.1460	0.0780

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Chain	Atom inclusion	Q-score
j6	0.0850	0.0220
j7	0.0440	0.0110
j8	0.1580	0.0620
j9	0.1630	0.0270
jA	0.0720	0.0190
jC	0.0520	0.0140
jD	0.4540	0.3130
jE	0.4630	0.3170
jF	0.7470	0.3620
jH	0.2430	0.0500
jI	0.1630	0.0510
jJ	0.1650	0.0620
jK	0.7640	0.3730
k1	0.6110	0.3840
k2	0.0530	0.0420
k3	0.0390	-0.0050
k5	0.0350	0.0360
k6	0.0230	0.0040
k7	0.0030	0.0050
k8	0.0370	0.0420
k9	0.0730	0.0570
kA	0.0240	0.0040
kC	0.0120	0.0380
kD	0.6200	0.3920
kE	0.5980	0.3840
kF	0.7380	0.3360
kH	0.1100	0.0570
kI	0.0400	0.0220
kJ	0.0640	0.0280
kK	0.7460	0.3500
l1	0.6740	0.4040
l2	0.0200	0.0320
l3	0.0820	0.0180
l5	0.0840	0.0280
l6	0.0050	0.0340
l7	0.0160	0.0150
l8	0.1510	0.0330
l9	0.0120	0.0440
lA	0.0430	0.0140
lC	0.0170	0.0080
lD	0.6260	0.3990
lE	0.6490	0.4090

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Chain	Atom inclusion	Q-score
lF	0.8310	0.3620
lH	0.0950	0.0280
lI	0.0040	0.0300
lJ	0.1880	0.0400
lK	0.8370	0.3730
m1	0.5740	0.4010
m2	0.0410	0.0300
m3	0.0620	0.0080
m5	0.1630	0.0330
m6	0.0110	0.0080
m7	0.0190	-0.0060
m8	0.1510	0.0440
m9	0.0190	0.0450
mA	0.0480	0.0450
mC	0.0310	-0.0070
mD	0.5050	0.3970
mE	0.5200	0.3850
mF	0.7870	0.3570
mH	0.1540	0.0550
mI	0.0110	0.0290
mJ	0.2580	0.0470
mK	0.7940	0.3610
nF	0.7540	0.3840
nK	0.7770	0.4010
o1	0.7250	0.2560
o4	0.6810	0.3260
oB	0.6860	0.3230
oD	0.7190	0.2590
oE	0.7220	0.2600
p4	0.7230	0.3480
pB	0.7240	0.3430
q1	0.5990	0.2270
q4	0.7180	0.3320
qB	0.7270	0.3420
qD	0.5960	0.2120
qE	0.5880	0.2160
r1	0.6890	0.2880
r4	0.8250	0.4180
rB	0.8240	0.4220
rD	0.6380	0.2880
rE	0.6610	0.2890
s4	0.7950	0.4020

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Chain	Atom inclusion	Q-score
sB	0.8120	0.4140
t1	0.5610	0.3880
t4	0.7760	0.3830
tB	0.7760	0.3800
tD	0.5190	0.3830
tE	0.5450	0.3790
u1	0.8020	0.3030
u4	0.6660	0.3140
uB	0.6820	0.3210
uD	0.7980	0.2960
uE	0.8040	0.3060
v1	0.7800	0.3290
v4	0.7180	0.3480
vB	0.7250	0.3490
vD	0.7790	0.3190
vE	0.7720	0.3230
w4	0.7360	0.3460
wB	0.7400	0.3420
x1	0.6020	0.3240
x4	0.8150	0.4220
xB	0.8270	0.4210
xD	0.5960	0.3180
xE	0.6290	0.3330
y1	0.4900	0.3490
y4	0.7920	0.3980
yB	0.8080	0.4130
yD	0.4830	0.3580
yE	0.4930	0.3500
z1	0.5840	0.3230
z4	0.7830	0.3890
zB	0.7780	0.3860
zD	0.5820	0.3180
zE	0.5630	0.3120