Full wwPDB EM Validation Report (i)

Mar 9, 2026 – 03:05 PM UTC

PDB ID	:	9HD7 / pdb_00009hd7
EMDB ID	:	EMD-52056
Title	:	Cryo-EM structure of photosystem II C2S2M2L2 supercomplex from the green alga Chlorella ohadii
Authors	:	Kopecny, D.; Kouril, R.; Ardhad, R.; Skalidis, I.; Kastritis, P.
Deposited on	:	2024-11-11
Resolution	:	2.95 Å(reported)
Based on initial models	:	8C29, 7OUI

This is a Full wwPDB EM Validation 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:

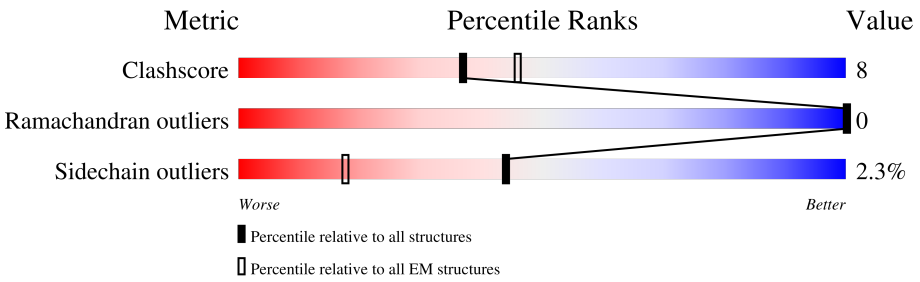
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.49

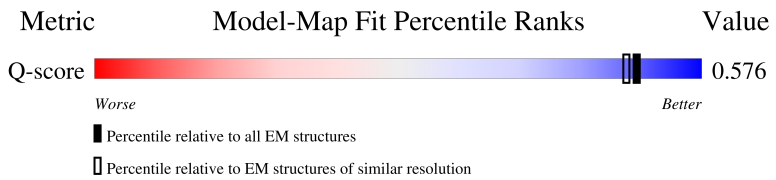
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 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	13114 (2.45 - 3.45)

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	1	249	42% 71% 16% • 12%
1	11	249	49% 67% 21% • 10%
1	14	249	48% 69% 19% • 10%
1	4	249	43% 71% 15% • 12%

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Mol	Chain	Length	Quality of chain
1	G	249	7% 78% 12% 10%
1	g	249	7% 75% 14% 10%
2	12	247	56% 50% 18% • 31%
2	15	247	57% 51% 16% • 31%
2	2	247	51% 64% 15% 21%
2	5	247	50% 64% 15% • 21%
2	N	247	8% 74% 15% 11%
2	n	247	8% 70% 18% 11%
3	3	259	5% 73% 10% 17%
3	6	259	6% 74% 9% 17%
4	7	140	23% 65% 11% 24%
4	8	140	21% 69% 7% 24%
5	13	243	12% 71% 16% • 12%
5	16	243	12% 71% 17% • 12%
6	A	353	79% 16% 5%
6	a	353	79% 15% • 5%
7	B	508	• 89% 10% •
7	b	508	• 89% 10% ••
8	C	473	81% 13% 5%
8	c	473	82% 13% 5%
9	D	352	86% 11% • •
9	d	352	84% 12% • •
10	E	83	• 84% 12% •
10	e	83	• 83% 13% •
11	F	41	• 88% • 10%

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Mol	Chain	Length	Quality of chain
11	f	41	5% 78% 12% 10%
12	H	80	• 72% 11% 16%
12	h	80	• 76% 8% 16%
13	I	38	• 87% • 11%
13	i	38	• 87% • 11%
14	J	42	5% 76% 14% 10%
14	j	42	• 79% 12% 10%
15	K	42	71% 17% 12%
15	k	42	71% 17% 12%
16	L	38	5% 79% 16% • •
16	l	38	5% 74% 21% • •
17	M	34	• 82% 6% 12%
17	m	34	• 88% 12%
18	O	305	8% 67% 10% • 22%
18	o	305	7% 66% 12% • 22%
19	P	915	• 19% • 79%
19	p	915	• 19% • 79%
20	Q	203	22% 62% 8% 29%
20	q	203	22% 63% 8% 29%
21	R	297	• 67% 11% 22%
21	r	297	• 66% 12% 22%
22	S	293	8% 73% 15% 12%
22	s	293	9% 75% 13% 12%
23	T	31	• 94% • •
23	t	31	• 90% 6% •

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Mol	Chain	Length	Quality of chain
24	U	367	8% 92%
24	u	367	7% 92%
25	V	33	21% 97%
25	v	33	21% 91% 9%
26	W	447	11% 87%
26	w	447	11% 87%
27	X	100	34% 62%
27	x	100	33% 5% 62%
28	Y	256	77% 9% 13%
28	y	256	75% 12% 13%
29	Z	62	6% 94% 6%
29	z	62	6% 94% 6%

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
30	CHL	1	601	X	-	-	-
30	CHL	1	605	X	-	-	-
30	CHL	1	606	X	-	-	-
30	CHL	1	607	X	-	-	-
30	CHL	1	608	X	-	-	-
30	CHL	1	609	X	-	-	-
30	CHL	11	601	X	-	-	-
30	CHL	11	605	X	-	-	-
30	CHL	11	606	X	-	-	-
30	CHL	11	607	X	-	-	-
30	CHL	11	608	X	-	-	-
30	CHL	11	609	X	-	-	-
30	CHL	12	601	X	-	-	-
30	CHL	12	605	X	-	-	-
30	CHL	12	606	X	-	-	-
30	CHL	12	607	X	-	-	-
30	CHL	12	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	13	601	X	-	-	-
30	CHL	13	605	X	-	-	-
30	CHL	13	606	X	-	-	-
30	CHL	13	607	X	-	-	-
30	CHL	13	608	X	-	-	-
30	CHL	13	609	X	-	-	-
30	CHL	14	601	X	-	-	-
30	CHL	14	605	X	-	-	-
30	CHL	14	606	X	-	-	-
30	CHL	14	607	X	-	-	-
30	CHL	14	608	X	-	-	-
30	CHL	14	609	X	-	-	-
30	CHL	15	601	X	-	-	-
30	CHL	15	605	X	-	-	-
30	CHL	15	606	X	-	-	-
30	CHL	15	607	X	-	-	-
30	CHL	15	608	X	-	-	-
30	CHL	16	601	X	-	-	-
30	CHL	16	605	X	-	-	-
30	CHL	16	606	X	-	-	-
30	CHL	16	607	X	-	-	-
30	CHL	16	608	X	-	-	-
30	CHL	16	609	X	-	-	-
30	CHL	2	601	X	-	-	-
30	CHL	2	605	X	-	-	-
30	CHL	2	606	X	-	-	-
30	CHL	2	607	X	-	-	-
30	CHL	2	608	X	-	-	-
30	CHL	2	609	X	-	-	-
30	CHL	3	601	X	-	-	-
30	CHL	3	605	X	-	-	-
30	CHL	3	606	X	-	-	-
30	CHL	3	607	X	-	-	-
30	CHL	3	608	X	-	-	-
30	CHL	3	609	X	-	-	-
30	CHL	4	601	X	-	-	-
30	CHL	4	605	X	-	-	-
30	CHL	4	606	X	-	-	-
30	CHL	4	607	X	-	-	-
30	CHL	4	608	X	-	-	-
30	CHL	4	609	X	-	-	-
30	CHL	5	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	5	605	X	-	-	-
30	CHL	5	606	X	-	-	-
30	CHL	5	607	X	-	-	-
30	CHL	5	608	X	-	-	-
30	CHL	5	609	X	-	-	-
30	CHL	6	601	X	-	-	-
30	CHL	6	605	X	-	-	-
30	CHL	6	606	X	-	-	-
30	CHL	6	607	X	-	-	-
30	CHL	6	608	X	-	-	-
30	CHL	6	609	X	-	-	-
30	CHL	G	601	X	-	-	-
30	CHL	G	605	X	-	-	-
30	CHL	G	606	X	-	-	-
30	CHL	G	607	X	-	-	-
30	CHL	G	608	X	-	-	-
30	CHL	G	609	X	-	-	-
30	CHL	N	601	X	-	-	-
30	CHL	N	605	X	-	-	-
30	CHL	N	606	X	-	-	-
30	CHL	N	607	X	-	-	-
30	CHL	N	608	X	-	-	-
30	CHL	N	609	X	-	-	-
30	CHL	R	605	X	-	-	-
30	CHL	R	606	X	-	-	-
30	CHL	R	607	X	-	-	-
30	CHL	S	601	X	-	-	-
30	CHL	S	606	X	-	-	-
30	CHL	S	607	X	-	-	-
30	CHL	S	608	X	-	-	-
30	CHL	Y	601	X	-	-	-
30	CHL	Y	605	X	-	-	-
30	CHL	Y	606	X	-	-	-
30	CHL	Y	607	X	-	-	-
30	CHL	Y	608	X	-	-	-
30	CHL	Y	609	X	-	-	-
30	CHL	g	601	X	-	-	-
30	CHL	g	605	X	-	-	-
30	CHL	g	606	X	-	-	-
30	CHL	g	607	X	-	-	-
30	CHL	g	608	X	-	-	-
30	CHL	g	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	n	601	X	-	-	-
30	CHL	n	605	X	-	-	-
30	CHL	n	606	X	-	-	-
30	CHL	n	607	X	-	-	-
30	CHL	n	608	X	-	-	-
30	CHL	n	609	X	-	-	-
30	CHL	r	605	X	-	-	-
30	CHL	r	606	X	-	-	-
30	CHL	r	607	X	-	-	-
30	CHL	s	601	X	-	-	-
30	CHL	s	606	X	-	-	-
30	CHL	s	607	X	-	-	-
30	CHL	s	608	X	-	-	-
30	CHL	y	601	X	-	-	-
30	CHL	y	605	X	-	-	-
30	CHL	y	606	X	-	-	-
30	CHL	y	607	X	-	-	-
30	CHL	y	608	X	-	-	-
30	CHL	y	609	X	-	-	-
31	CLA	1	602	X	-	-	-
31	CLA	1	603	X	-	-	-
31	CLA	1	604	X	-	-	-
31	CLA	1	610	X	-	-	-
31	CLA	1	611	X	-	-	-
31	CLA	1	612	X	-	-	-
31	CLA	1	613	X	-	-	-
31	CLA	1	614	X	-	-	-
31	CLA	11	602	X	-	-	-
31	CLA	11	603	X	-	-	-
31	CLA	11	604	X	-	-	-
31	CLA	11	610	X	-	-	-
31	CLA	11	611	X	-	-	-
31	CLA	11	612	X	-	-	-
31	CLA	11	613	X	-	-	-
31	CLA	11	614	X	-	-	-
31	CLA	12	602	X	-	-	-
31	CLA	12	603	X	-	-	-
31	CLA	12	604	X	-	-	-
31	CLA	12	609	X	-	-	-
31	CLA	12	610	X	-	-	-
31	CLA	12	611	X	-	-	-
31	CLA	12	612	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	12	613	X	-	-	-
31	CLA	13	602	X	-	-	-
31	CLA	13	603	X	-	-	-
31	CLA	13	604	X	-	-	-
31	CLA	13	610	X	-	-	-
31	CLA	13	611	X	-	-	-
31	CLA	13	612	X	-	-	-
31	CLA	13	613	X	-	-	-
31	CLA	13	614	X	-	-	-
31	CLA	13	615	X	-	-	-
31	CLA	14	602	X	-	-	-
31	CLA	14	603	X	-	-	-
31	CLA	14	604	X	-	-	-
31	CLA	14	610	X	-	-	-
31	CLA	14	611	X	-	-	-
31	CLA	14	612	X	-	-	-
31	CLA	14	613	X	-	-	-
31	CLA	14	614	X	-	-	-
31	CLA	15	602	X	-	-	-
31	CLA	15	603	X	-	-	-
31	CLA	15	604	X	-	-	-
31	CLA	15	609	X	-	-	-
31	CLA	15	610	X	-	-	-
31	CLA	15	611	X	-	-	-
31	CLA	15	612	X	-	-	-
31	CLA	15	613	X	-	-	-
31	CLA	16	602	X	-	-	-
31	CLA	16	603	X	-	-	-
31	CLA	16	604	X	-	-	-
31	CLA	16	610	X	-	-	-
31	CLA	16	611	X	-	-	-
31	CLA	16	612	X	-	-	-
31	CLA	16	613	X	-	-	-
31	CLA	16	614	X	-	-	-
31	CLA	16	615	X	-	-	-
31	CLA	2	602	X	-	-	-
31	CLA	2	603	X	-	-	-
31	CLA	2	604	X	-	-	-
31	CLA	2	610	X	-	-	-
31	CLA	2	611	X	-	-	-
31	CLA	2	612	X	-	-	-
31	CLA	2	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	3	602	X	-	-	-
31	CLA	3	603	X	-	-	-
31	CLA	3	604	X	-	-	-
31	CLA	3	610	X	-	-	-
31	CLA	3	611	X	-	-	-
31	CLA	3	612	X	-	-	-
31	CLA	3	613	X	-	-	-
31	CLA	3	614	X	-	-	-
31	CLA	3	615	X	-	-	-
31	CLA	4	602	X	-	-	-
31	CLA	4	603	X	-	-	-
31	CLA	4	604	X	-	-	-
31	CLA	4	610	X	-	-	-
31	CLA	4	611	X	-	-	-
31	CLA	4	612	X	-	-	-
31	CLA	4	613	X	-	-	-
31	CLA	4	614	X	-	-	-
31	CLA	5	602	X	-	-	-
31	CLA	5	603	X	-	-	-
31	CLA	5	604	X	-	-	-
31	CLA	5	610	X	-	-	-
31	CLA	5	611	X	-	-	-
31	CLA	5	612	X	-	-	-
31	CLA	5	613	X	-	-	-
31	CLA	6	602	X	-	-	-
31	CLA	6	603	X	-	-	-
31	CLA	6	604	X	-	-	-
31	CLA	6	610	X	-	-	-
31	CLA	6	611	X	-	-	-
31	CLA	6	612	X	-	-	-
31	CLA	6	613	X	-	-	-
31	CLA	6	614	X	-	-	-
31	CLA	6	615	X	-	-	-
31	CLA	A	402	X	-	-	-
31	CLA	A	403	X	-	-	-
31	CLA	A	404	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	B	601	X	-	-	-
31	CLA	B	602	X	-	-	-
31	CLA	B	603	X	-	-	-
31	CLA	B	604	X	-	-	-
31	CLA	B	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	B	606	X	-	-	-
31	CLA	B	607	X	-	-	-
31	CLA	B	608	X	-	-	-
31	CLA	B	609	X	-	-	-
31	CLA	B	610	X	-	-	-
31	CLA	B	611	X	-	-	-
31	CLA	B	612	X	-	-	-
31	CLA	B	613	X	-	-	-
31	CLA	B	614	X	-	-	-
31	CLA	B	615	X	-	-	-
31	CLA	B	616	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-
31	CLA	C	506	X	-	-	-
31	CLA	C	507	X	-	-	-
31	CLA	C	508	X	-	-	-
31	CLA	C	509	X	-	-	-
31	CLA	C	510	X	-	-	-
31	CLA	C	511	X	-	-	-
31	CLA	C	512	X	-	-	-
31	CLA	C	513	X	-	-	-
31	CLA	C	514	X	-	-	-
31	CLA	D	404	X	-	-	-
31	CLA	D	405	X	-	-	-
31	CLA	G	602	X	-	-	-
31	CLA	G	603	X	-	-	-
31	CLA	G	604	X	-	-	-
31	CLA	G	610	X	-	-	-
31	CLA	G	611	X	-	-	-
31	CLA	G	612	X	-	-	-
31	CLA	G	613	X	-	-	-
31	CLA	G	614	X	-	-	-
31	CLA	N	602	X	-	-	-
31	CLA	N	603	X	-	-	-
31	CLA	N	604	X	-	-	-
31	CLA	N	610	X	-	-	-
31	CLA	N	611	X	-	-	-
31	CLA	N	612	X	-	-	-
31	CLA	N	613	X	-	-	-
31	CLA	N	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	N	615	X	-	-	-
31	CLA	R	601	X	-	-	-
31	CLA	R	602	X	-	-	-
31	CLA	R	603	X	-	-	-
31	CLA	R	604	X	-	-	-
31	CLA	R	608	X	-	-	-
31	CLA	R	609	X	-	-	-
31	CLA	R	610	X	-	-	-
31	CLA	R	611	X	-	-	-
31	CLA	R	612	X	-	-	-
31	CLA	R	613	X	-	-	-
31	CLA	R	614	X	-	-	-
31	CLA	S	602	X	-	-	-
31	CLA	S	603	X	-	-	-
31	CLA	S	604	X	-	-	-
31	CLA	S	605	X	-	-	-
31	CLA	S	609	X	-	-	-
31	CLA	S	610	X	-	-	-
31	CLA	S	611	X	-	-	-
31	CLA	S	612	X	-	-	-
31	CLA	S	613	X	-	-	-
31	CLA	S	614	X	-	-	-
31	CLA	S	615	X	-	-	-
31	CLA	Y	602	X	-	-	-
31	CLA	Y	603	X	-	-	-
31	CLA	Y	604	X	-	-	-
31	CLA	Y	610	X	-	-	-
31	CLA	Y	611	X	-	-	-
31	CLA	Y	612	X	-	-	-
31	CLA	Y	613	X	-	-	-
31	CLA	Y	614	X	-	-	-
31	CLA	Y	615	X	-	-	-
31	CLA	a	403	X	-	-	-
31	CLA	a	404	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	b	601	X	-	-	-
31	CLA	b	602	X	-	-	-
31	CLA	b	603	X	-	-	-
31	CLA	b	604	X	-	-	-
31	CLA	b	605	X	-	-	-
31	CLA	b	606	X	-	-	-
31	CLA	b	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	610	X	-	-	-
31	CLA	b	611	X	-	-	-
31	CLA	b	612	X	-	-	-
31	CLA	b	613	X	-	-	-
31	CLA	b	614	X	-	-	-
31	CLA	b	615	X	-	-	-
31	CLA	b	616	X	-	-	-
31	CLA	c	502	X	-	-	-
31	CLA	c	503	X	-	-	-
31	CLA	c	504	X	-	-	-
31	CLA	c	505	X	-	-	-
31	CLA	c	506	X	-	-	-
31	CLA	c	507	X	-	-	-
31	CLA	c	508	X	-	-	-
31	CLA	c	509	X	-	-	-
31	CLA	c	510	X	-	-	-
31	CLA	c	511	X	-	-	-
31	CLA	c	512	X	-	-	-
31	CLA	c	513	X	-	-	-
31	CLA	c	514	X	-	-	-
31	CLA	d	402	X	-	-	-
31	CLA	d	404	X	-	-	-
31	CLA	d	405	X	-	-	-
31	CLA	g	602	X	-	-	-
31	CLA	g	603	X	-	-	-
31	CLA	g	604	X	-	-	-
31	CLA	g	610	X	-	-	-
31	CLA	g	611	X	-	-	-
31	CLA	g	612	X	-	-	-
31	CLA	g	613	X	-	-	-
31	CLA	g	614	X	-	-	-
31	CLA	n	602	X	-	-	-
31	CLA	n	603	X	-	-	-
31	CLA	n	604	X	-	-	-
31	CLA	n	610	X	-	-	-
31	CLA	n	611	X	-	-	-
31	CLA	n	612	X	-	-	-
31	CLA	n	613	X	-	-	-
31	CLA	n	614	X	-	-	-
31	CLA	n	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	r	601	X	-	-	-
31	CLA	r	602	X	-	-	-
31	CLA	r	603	X	-	-	-
31	CLA	r	604	X	-	-	-
31	CLA	r	608	X	-	-	-
31	CLA	r	609	X	-	-	-
31	CLA	r	610	X	-	-	-
31	CLA	r	611	X	-	-	-
31	CLA	r	612	X	-	-	-
31	CLA	r	613	X	-	-	-
31	CLA	r	614	X	-	-	-
31	CLA	s	602	X	-	-	-
31	CLA	s	603	X	-	-	-
31	CLA	s	604	X	-	-	-
31	CLA	s	605	X	-	-	-
31	CLA	s	609	X	-	-	-
31	CLA	s	610	X	-	-	-
31	CLA	s	611	X	-	-	-
31	CLA	s	612	X	-	-	-
31	CLA	s	613	X	-	-	-
31	CLA	s	614	X	-	-	-
31	CLA	s	615	X	-	-	-
31	CLA	y	602	X	-	-	-
31	CLA	y	603	X	-	-	-
31	CLA	y	604	X	-	-	-
31	CLA	y	610	X	-	-	-
31	CLA	y	611	X	-	-	-
31	CLA	y	612	X	-	-	-
31	CLA	y	613	X	-	-	-
31	CLA	y	614	X	-	-	-
31	CLA	y	615	X	-	-	-
33	LUT	12	614	-	-	X	-

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 112944 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 Chlorophyll a-b binding protein Lhcbm-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	220	1673	1084	267	317	5	0	0
1	4	220	1673	1084	267	317	5	0	0
1	11	223	1693	1094	272	322	5	0	0
1	14	223	1693	1094	272	322	5	0	0
1	G	223	1693	1094	272	322	5	0	0
1	g	223	1693	1094	272	322	5	0	0

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	196	1496	966	249	276	5	0	0
2	5	196	1496	966	249	276	5	0	0
2	12	170	1330	863	220	242	5	0	0
2	15	170	1330	863	220	242	5	0	0
2	N	220	1679	1085	278	311	5	0	0
2	n	220	1679	1085	278	311	5	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	214	1630	1056	265	304	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	214	1630	1056	265	304	5	0	0

- Molecule 4 is a protein called Chloroplast photosystem II 10 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	7	107	816	522	136	156	2	0	0
			Total	C	N	O	S		
4	8	107	816	522	136	156	2	0	0

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	13	215	1645	1064	268	308	5	0	0
			Total	C	N	O	S		
5	16	215	1645	1064	268	308	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	336	2632	1718	431	469	14	0	0
			Total	C	N	O	S		
6	a	336	2632	1718	431	469	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	505	3963	2588	669	694	12	0	0
			Total	C	N	O	S		
7	b	505	3963	2588	669	694	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C	449	3491	2284	585	607	15	0	0
			Total	C	N	O	S		
8	c	449	3491	2284	585	607	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D	342	2730	1806	449	464	11	0	0
9	d	342	2730	1806	449	464	11	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	E	80	646	420	105	121	0	0
10	e	80	646	420	105	121	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	F	37	303	206	49	47	1	0	0
11	f	37	303	206	49	47	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	67	507	336	73	95	3	0	0
12	h	67	507	336	73	95	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	34	274	187	41	45	1	0	0
13	i	34	274	187	41	45	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	J	38	270	182	42	46	0	0
14	j	38	270	182	42	46	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	K	37	295	204	43	48	0	0
15	k	37	295	204	43	48	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	L	37	303	203	48	52	0	0
16	l	37	303	203	48	52	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	M	30	228	157	33	38	0	0
17	m	30	228	157	33	38	0	0

- Molecule 18 is a protein called Chloroplast oxygen-evolving enhancer protein 1b (PsbO).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	238	1759	1106	288	357	8	0	0
18	o	238	1759	1106	288	357	8	0	0

- Molecule 19 is a protein called PWWP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	188	1443	918	245	279	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	p	188	1443	918	245	279	1	0	0

- Molecule 20 is a protein called Chloroplast oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	Q	144	1122	701	207	214	0	0
20	q	144	1122	701	207	214	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	R	231	1783	1132	303	342	6	0	0
21	r	231	1783	1132	303	342	6	0	0

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S	257	1934	1242	323	364	5	0	0
22	s	257	1934	1242	323	364	5	0	0

- Molecule 23 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	T	30	246	172	36	37	1	0	0
23	t	30	246	172	36	37	1	0	0

- Molecule 24 is a protein called Chloroplast PsbY.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	U	30	233	156	40	37	0	0
24	u	30	233	156	40	37	0	0

- Molecule 25 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	V	33	241	160	39	41	1	0	0
25	v	33	241	160	39	41	1	0	0

- Molecule 26 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	W	60	468	301	74	93	0	0
26	w	60	468	301	74	93	0	0

- Molecule 27 is a protein called Photosystem II reaction center protein X (PsbX).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	X	38	258	162	47	49	0	0
27	x	38	258	162	47	49	0	0

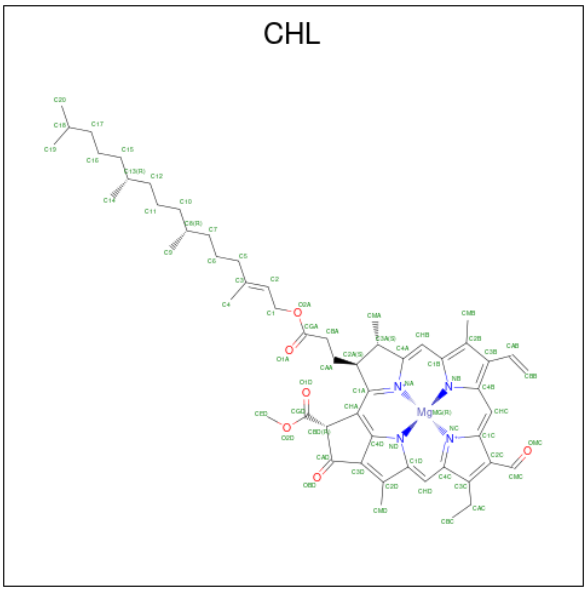
- Molecule 28 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Y	222	1694	1102	271	316	5	0	0
28	y	222	1694	1102	271	316	5	0	0

- Molecule 29 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Z	62	478	335	68	74	1	0	0
29	z	62	478	335	68	74	1	0	0

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	1	1	61	50	1	4	6	0
30	1	1	46	35	1	4	6	0
30	1	1	47	36	1	4	6	0
30	1	1	51	40	1	4	6	0
30	1	1	50	39	1	4	6	0
30	1	1	56	45	1	4	6	0
30	2	1	47	36	1	4	6	0
30	2	1	46	35	1	4	6	0
30	2	1	46	35	1	4	6	0
30	2	1	50	39	1	4	6	0
30	2	1	66	55	1	4	6	0
30	2	1	56	45	1	4	6	0
30	3	1	61	50	1	4	6	0
30	3	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	3	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	3	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	4	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	5	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	6	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	6	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	11	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	11	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
30	11	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
30	11	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	11	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	11	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	12	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	12	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	12	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	12	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	12	1	53	42	1	4	6	0
			Total	C	Mg	N	O	
30	13	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	13	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	13	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	13	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	13	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	13	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	14	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	14	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
30	14	1	47	36	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	14	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	14	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	14	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	15	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	15	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	15	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	15	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	15	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	16	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	16	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	16	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	16	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	16	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	16	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	47	36	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	52	41	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	G	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	53	42	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	N	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	R	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	R	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	R	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	S	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	S	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	S	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
30	S	1	49	38	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	Y	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
30	Y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	48	37	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	g	1	52	41	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	g	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	52	41	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	61	50	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	50	39	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	n	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	r	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	r	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	r	1	51	40	1	4	6	0
			Total	C	Mg	N	O	
30	s	1	46	35	1	4	6	0
			Total	C	Mg	N	O	
30	s	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	s	1	43	34	1	4	4	0
			Total	C	Mg	N	O	
30	s	1	49	38	1	4	6	0
			Total	C	Mg	N	O	
30	y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	y	1	56	45	1	4	6	0
			Total	C	Mg	N	O	
30	y	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
30	y	1	44	35	1	4	4	0

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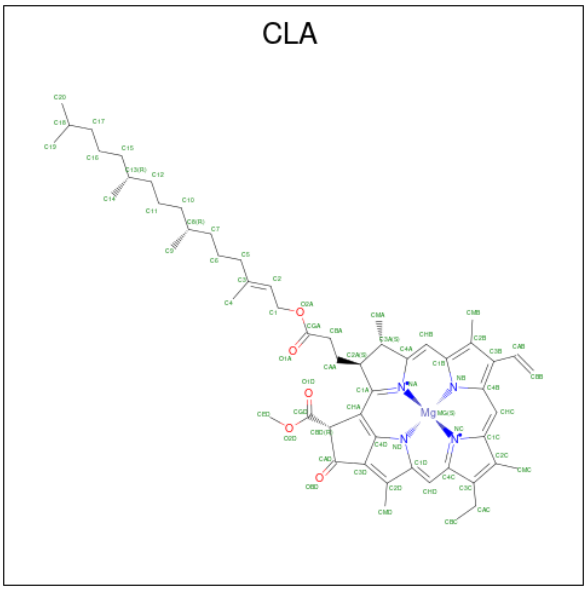
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	y	1	66	55	1	4	6	0

- Molecule 31 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	1	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	1	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
31	1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	1	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	1	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	2	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	2	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	2	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	2	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	2	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	2	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	3	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	4	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	4	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	5	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	6	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	11	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	11	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	11	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
31	11	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	11	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	11	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
31	11	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	11	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	12	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	12	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	12	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	12	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	12	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	12	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	12	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	12	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	13	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	14	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	14	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	14	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	14	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	14	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	14	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
31	14	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	14	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	15	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	15	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	15	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	15	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	15	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	15	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	15	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	15	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	16	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	16	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	16	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	16	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	16	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	16	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	16	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	16	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	16	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
31	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	G	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	N	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	R	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	R	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
31	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	S	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	Y	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	a	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	b	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
31	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	g	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	n	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	r	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	r	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	s	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	65	55	1	4	5	0

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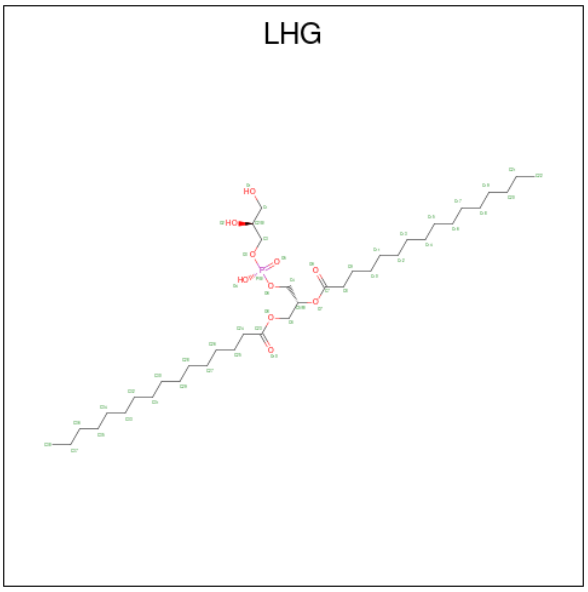
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	y	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
31	y	1	56	46	1	4	5	0

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
32	1	1	43	32	10	1	0
			Total	C	O	P	
32	3	1	44	33	10	1	0
			Total	C	O	P	
32	3	1	47	36	10	1	0
			Total	C	O	P	
32	4	1	47	36	10	1	0
			Total	C	O	P	
32	6	1	44	33	10	1	0
			Total	C	O	P	
32	6	1	47	36	10	1	0
			Total	C	O	P	
32	11	1	49	38	10	1	0
			Total	C	O	P	
32	13	1	40	29	10	1	0
			Total	C	O	P	
32	14	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
32	16	1	40	29	10	1	0
32	A	1	49	38	10	1	0
32	A	1	44	33	10	1	0
32	A	1	43	32	10	1	0
32	A	1	49	38	10	1	0
32	C	1	42	31	10	1	0
32	D	1	49	38	10	1	0
32	D	1	39	28	10	1	0
32	D	1	49	38	10	1	0
32	G	1	49	38	10	1	0
32	L	1	47	36	10	1	0
32	N	1	49	38	10	1	0
32	R	1	44	33	10	1	0
32	R	1	38	27	10	1	0
32	R	1	47	36	10	1	0
32	S	1	49	38	10	1	0
32	S	1	45	34	10	1	0
32	Y	1	47	36	10	1	0
32	Y	1	49	38	10	1	0
32	Y	1	47	36	10	1	0
32	a	1	49	38	10	1	0

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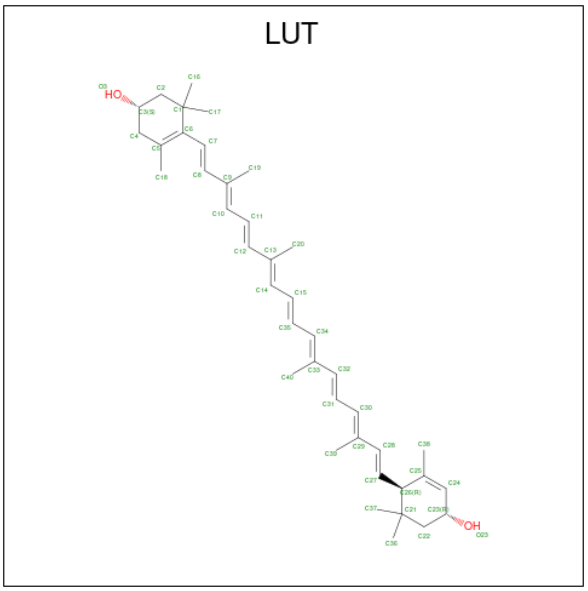
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
32	a	1	49	38	10	1	0
32	a	1	44	33	10	1	0
32	a	1	43	32	10	1	0
32	c	1	42	31	10	1	0
32	d	1	49	38	10	1	0
32	d	1	39	28	10	1	0
32	d	1	49	38	10	1	0
32	g	1	49	38	10	1	0
32	l	1	47	36	10	1	0
32	n	1	49	38	10	1	0
32	r	1	44	33	10	1	0
32	r	1	38	27	10	1	0
32	r	1	47	36	10	1	0
32	s	1	49	38	10	1	0
32	s	1	45	34	10	1	0
32	y	1	47	36	10	1	0
32	y	1	49	38	10	1	0
32	y	1	47	36	10	1	0

- Molecule 33 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	1	1	42	40	2	0
			Total	C	O	
33	1	1	42	40	2	0
			Total	C	O	
33	2	1	42	40	2	0
			Total	C	O	
33	2	1	42	40	2	0
			Total	C	O	
33	3	1	42	40	2	0
			Total	C	O	
33	3	1	42	40	2	0
			Total	C	O	
33	4	1	42	40	2	0
			Total	C	O	
33	4	1	42	40	2	0
			Total	C	O	
33	5	1	42	40	2	0
			Total	C	O	
33	5	1	42	40	2	0
			Total	C	O	
33	6	1	42	40	2	0
			Total	C	O	
33	6	1	42	40	2	0
			Total	C	O	
33	11	1	42	40	2	0
			Total	C	O	
33	11	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	12	1	42	40	2	0
			Total	C	O	
33	12	1	42	40	2	0
			Total	C	O	
33	13	1	42	40	2	0
			Total	C	O	
33	13	1	42	40	2	0
			Total	C	O	
33	14	1	42	40	2	0
			Total	C	O	
33	14	1	42	40	2	0
			Total	C	O	
33	15	1	42	40	2	0
			Total	C	O	
33	15	1	42	40	2	0
			Total	C	O	
33	16	1	42	40	2	0
			Total	C	O	
33	16	1	42	40	2	0
			Total	C	O	
33	G	1	42	40	2	0
			Total	C	O	
33	G	1	42	40	2	0
			Total	C	O	
33	N	1	42	40	2	0
			Total	C	O	
33	N	1	42	40	2	0
			Total	C	O	
33	R	1	42	40	2	0
			Total	C	O	
33	S	1	42	40	2	0
			Total	C	O	
33	S	1	42	40	2	0
			Total	C	O	
33	Y	1	42	40	2	0
			Total	C	O	
33	Y	1	42	40	2	0
			Total	C	O	
33	g	1	42	40	2	0
			Total	C	O	
33	g	1	42	40	2	0

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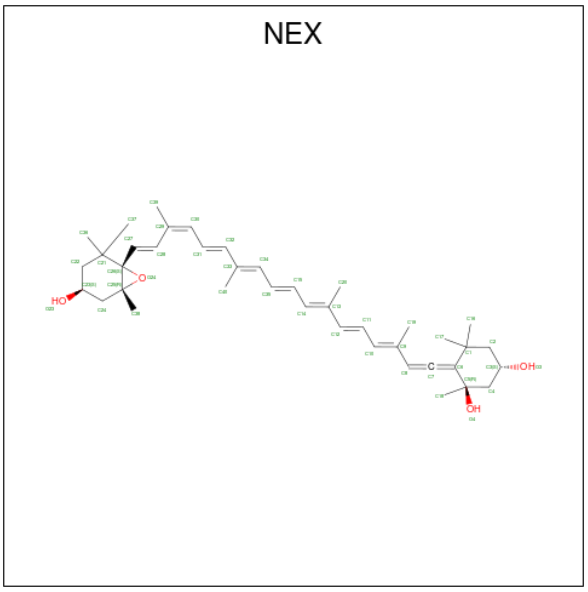
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	n	1	42	40	2	0
			Total	C	O	
33	n	1	42	40	2	0
			Total	C	O	
33	r	1	42	40	2	0
			Total	C	O	
33	s	1	42	40	2	0
			Total	C	O	
33	s	1	42	40	2	0
			Total	C	O	
33	y	1	42	40	2	0
			Total	C	O	
33	y	1	42	40	2	0

- Molecule 34 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	1	1	16	14	2	0
			Total	C	O	
34	2	1	32	30	2	0
			Total	C	O	
34	3	1	44	40	4	0

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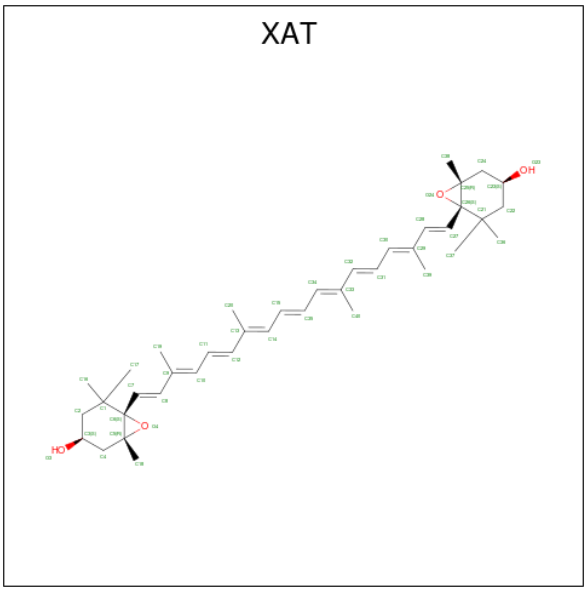
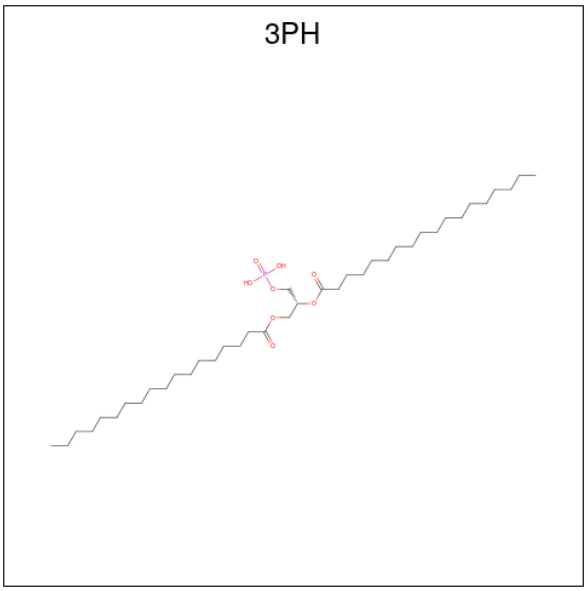
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	4	1	16	14	2	0
34	5	1	32	30	2	0
34	6	1	44	40	4	0
34	11	1	16	14	2	0
34	12	1	27	25	2	0
34	13	1	44	40	4	0
34	14	1	16	14	2	0
34	15	1	27	25	2	0
34	16	1	44	40	4	0
34	G	1	43	39	4	0
34	N	1	44	40	4	0
34	R	1	44	40	4	0
34	S	1	44	40	4	0
34	Y	1	44	40	4	0
34	g	1	44	40	4	0
34	n	1	44	40	4	0
34	r	1	44	40	4	0
34	s	1	44	40	4	0
34	y	1	44	40	4	0

- Molecule 35 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



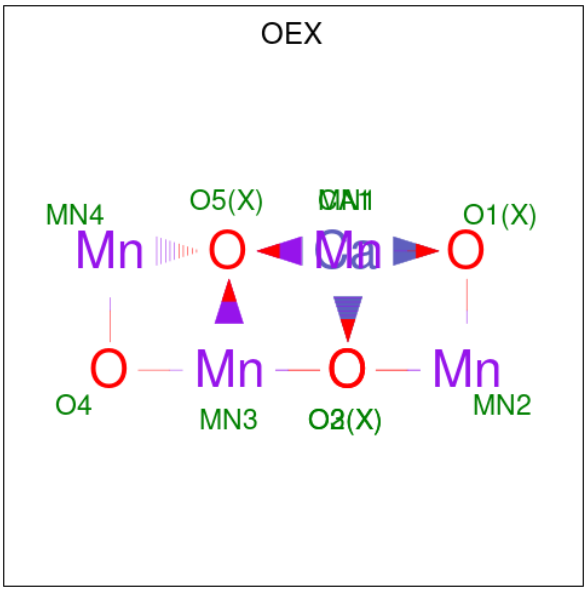
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	3	1	44	40	4	0
35	6	1	44	40	4	0
35	11	1	44	40	4	0
35	14	1	44	40	4	0
35	G	1	44	40	4	0
35	R	1	44	40	4	0
35	g	1	44	40	4	0
35	r	1	44	40	4	0

- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



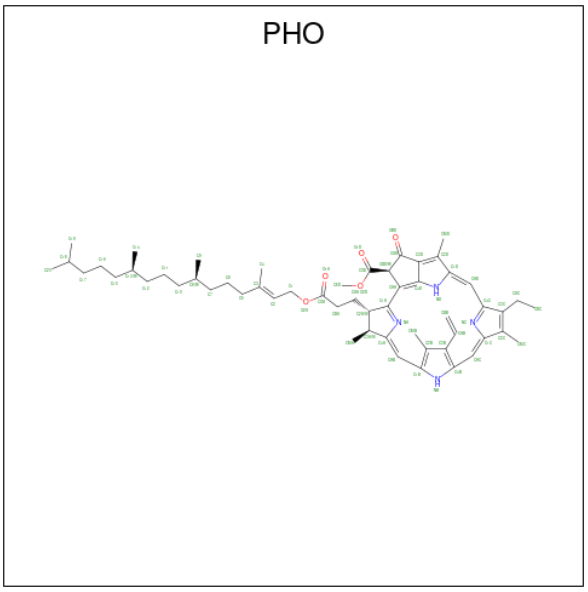
Mol	Chain	Residues	Atoms				AltConf
36	7	1	Total	C	O	P	0
			48	39	8	1	
36	8	1	Total	C	O	P	0
			48	39	8	1	
36	B	1	Total	C	O	P	0
			48	39	8	1	
36	B	1	Total	C	O	P	0
			38	29	8	1	
36	T	1	Total	C	O	P	0
			48	39	8	1	
36	b	1	Total	C	O	P	0
			39	30	8	1	

- Molecule 37 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 38 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
38	A	1	64	55	4	5	0

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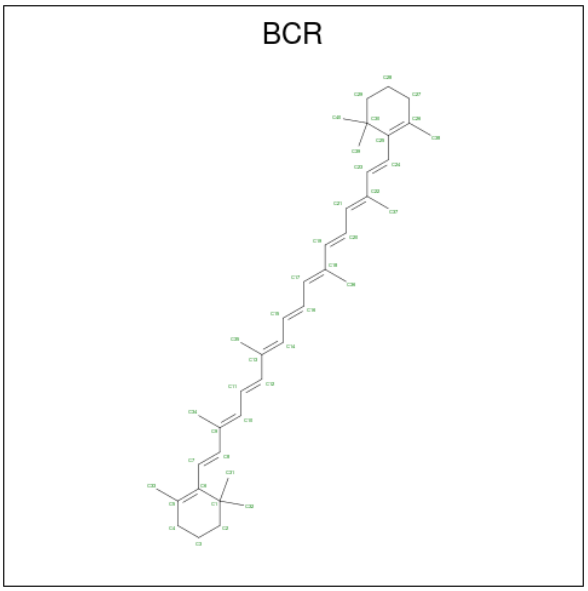
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
38	D	1	64	55	4	5	0
38	a	1	64	55	4	5	0
38	a	1	64	55	4	5	0

- Molecule 39 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
39	A	1	40	40	0
39	B	1	40	40	0
39	B	1	40	40	0
39	B	1	40	40	0
39	C	1	40	40	0
39	C	1	40	40	0
39	C	1	40	40	0
39	D	1	40	40	0

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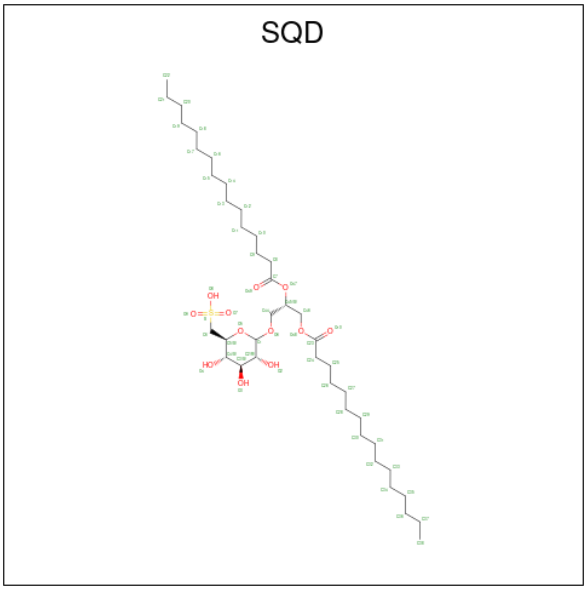
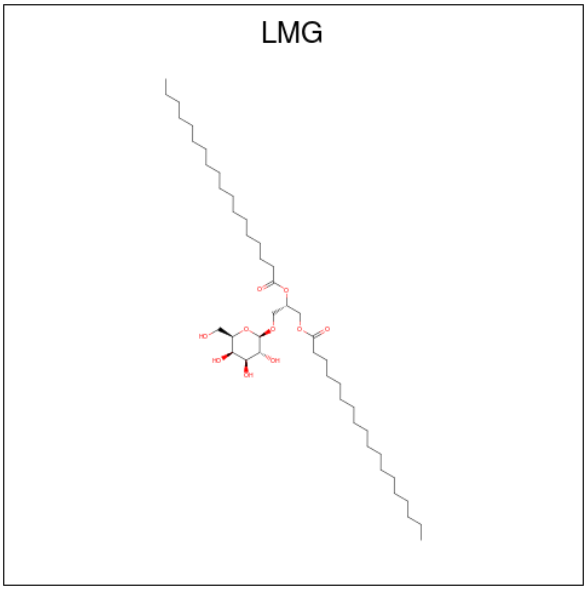
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
39	H	1	40	40	0
			Total	C	
39	J	1	40	40	0
			Total	C	
39	a	1	40	40	0
			Total	C	
39	b	1	40	40	0
			Total	C	
39	b	1	40	40	0
			Total	C	
39	b	1	40	40	0
			Total	C	
39	c	1	40	40	0
			Total	C	
39	c	1	40	40	0
			Total	C	
39	c	1	40	40	0
			Total	C	
39	d	1	40	40	0
			Total	C	
39	h	1	40	40	0
			Total	C	
39	j	1	40	40	0

- Molecule 40 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
40	A	1	Total	C	O	S	0
			51	38	12	1	
40	D	1	Total	C	O	S	0
			54	41	12	1	
40	D	1	Total	C	O	S	0
			46	33	12	1	
40	L	1	Total	C	O	S	0
			50	37	12	1	
40	a	1	Total	C	O	S	0
			51	38	12	1	
40	d	1	Total	C	O	S	0
			54	41	12	1	
40	d	1	Total	C	O	S	0
			46	33	12	1	
40	l	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 41 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
41	A	1	Total	C	O	0
			55	45	10	
41	B	1	Total	C	O	0
			49	39	10	
41	B	1	Total	C	O	0
			48	38	10	

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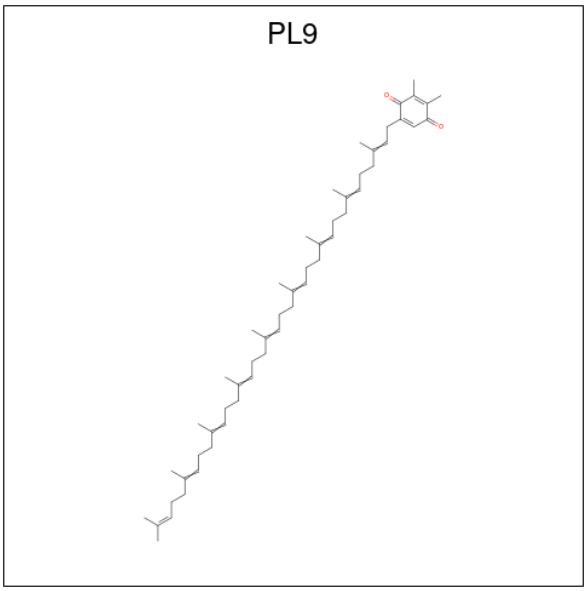
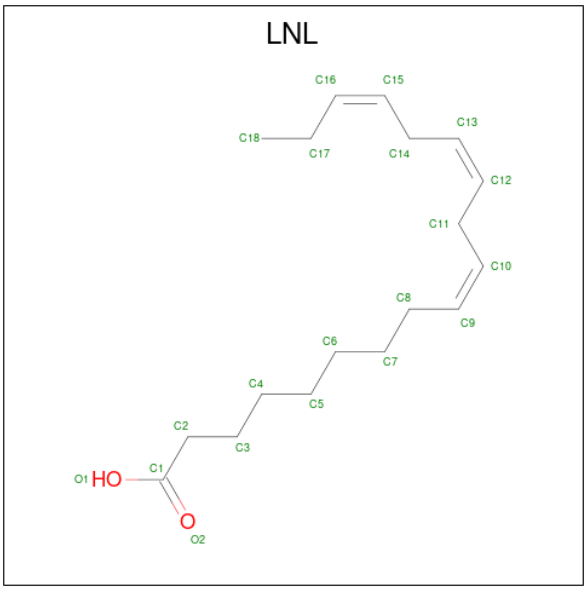
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
41	C	1	47	37	10	0
41	C	1	55	45	10	0
41	D	1	44	34	10	0
41	D	1	48	38	10	0
41	H	1	35	30	5	0
41	J	1	51	41	10	0
41	K	1	51	41	10	0
41	S	1	42	32	10	0
41	b	1	49	39	10	0
41	b	1	46	36	10	0
41	c	1	47	37	10	0
41	c	1	55	45	10	0
41	d	1	44	34	10	0
41	d	1	35	30	5	0
41	d	1	48	38	10	0
41	j	1	51	41	10	0
41	s	1	42	32	10	0
41	v	1	51	41	10	0
41	w	1	55	45	10	0

- Molecule 42 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



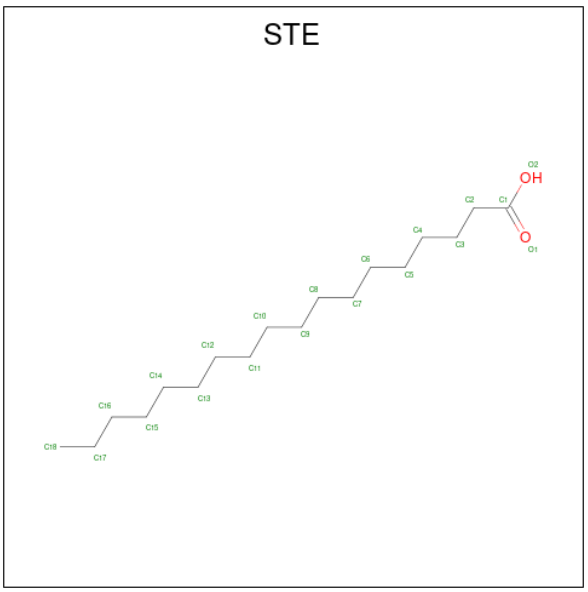
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	A	1	55	53	2	0
42	D	1	55	53	2	0
42	a	1	55	53	2	0
42	d	1	55	53	2	0

- Molecule 43 is ALPHA-LINOLENIC ACID (CCD ID: LNL) (formula: $C_{18}H_{30}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
43	A	1	20	18	2	0
43	C	1	20	18	2	0
43	C	1	20	18	2	0
43	H	1	20	18	2	0
43	I	1	20	18	2	0
43	R	1	20	18	2	0
43	W	1	20	18	2	0
43	W	1	20	18	2	0
43	X	1	20	18	2	0
43	Y	1	20	18	2	0
43	Y	1	20	18	2	0
43	a	1	20	18	2	0
43	c	1	20	18	2	0
43	c	1	20	18	2	0
43	h	1	20	18	2	0
43	i	1	20	18	2	0
43	r	1	20	18	2	0
43	w	1	20	18	2	0
43	x	1	20	18	2	0
43	y	1	20	18	2	0
43	y	1	20	18	2	0
43	y	1	20	18	2	0

- Molecule 44 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).

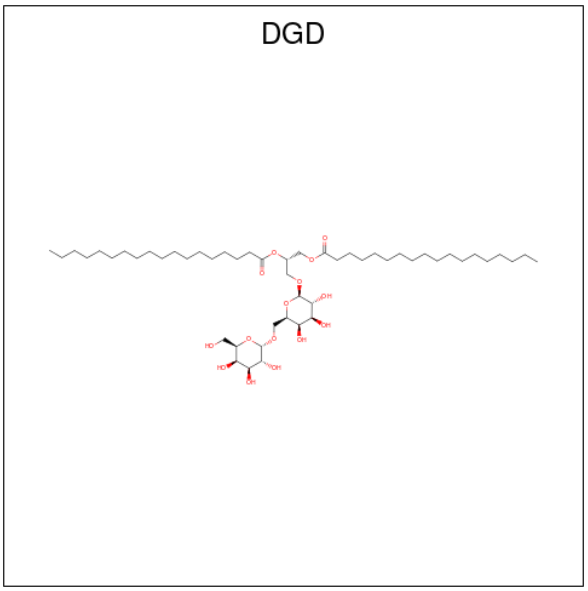


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
44	B	1	20	18	2	0
44	b	1	20	18	2	0

- Molecule 45 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
45	C	1	1	1	0
45	c	1	1	1	0

- Molecule 46 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

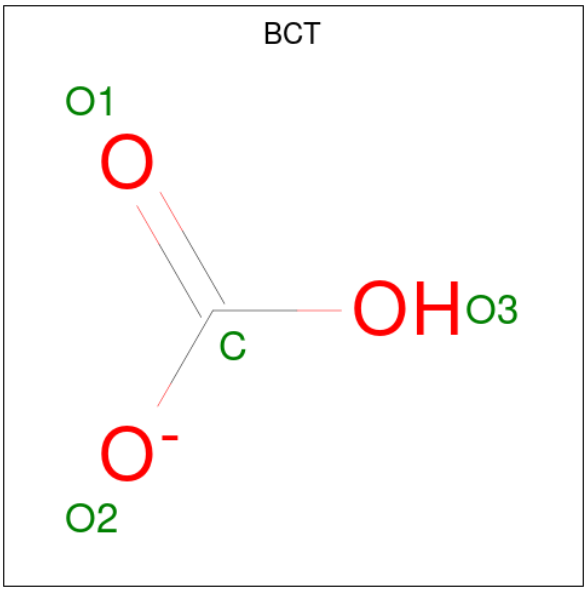


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
46	C	1	66	51	15	0
46	C	1	58	43	15	0
46	C	1	59	44	15	0
46	W	1	46	36	10	0
46	c	1	66	51	15	0
46	c	1	58	43	15	0
46	c	1	59	44	15	0
46	w	1	40	30	10	0

- Molecule 47 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

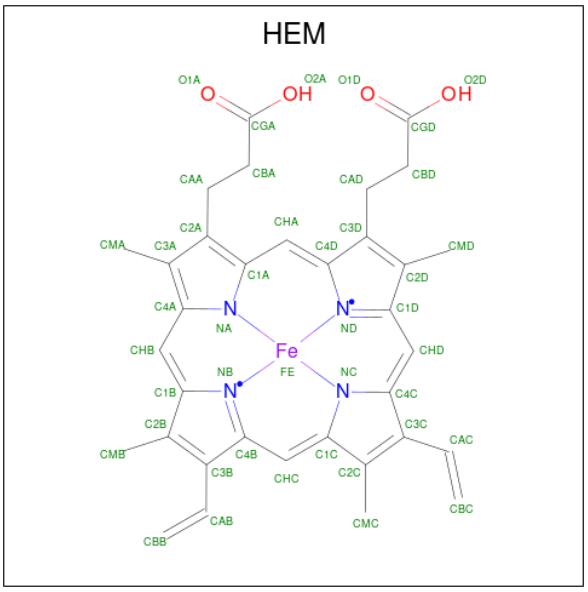
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
47	D	1	1	1	0
47	d	1	1	1	0

- Molecule 48 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				AltConf
48	D	1	Total	C	O		0
			4	1	3		
48	d	1	Total	C	O		0
			4	1	3		

- Molecule 49 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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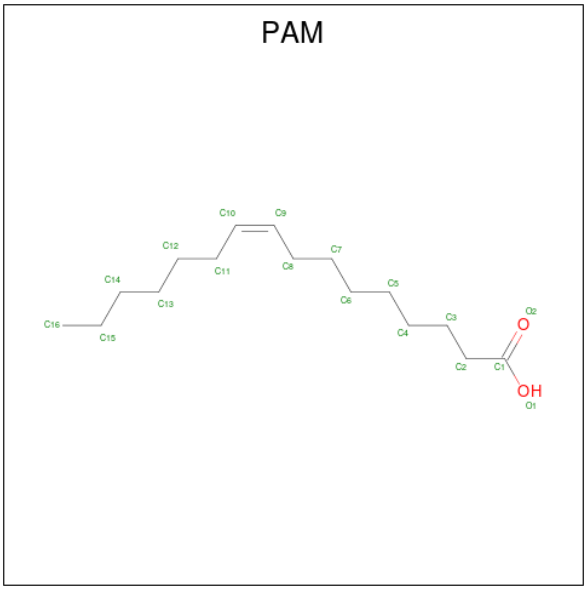
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
49	f	1	43	34	1	4	4	0

- Molecule 50 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $C_{16}H_{30}O_2$).



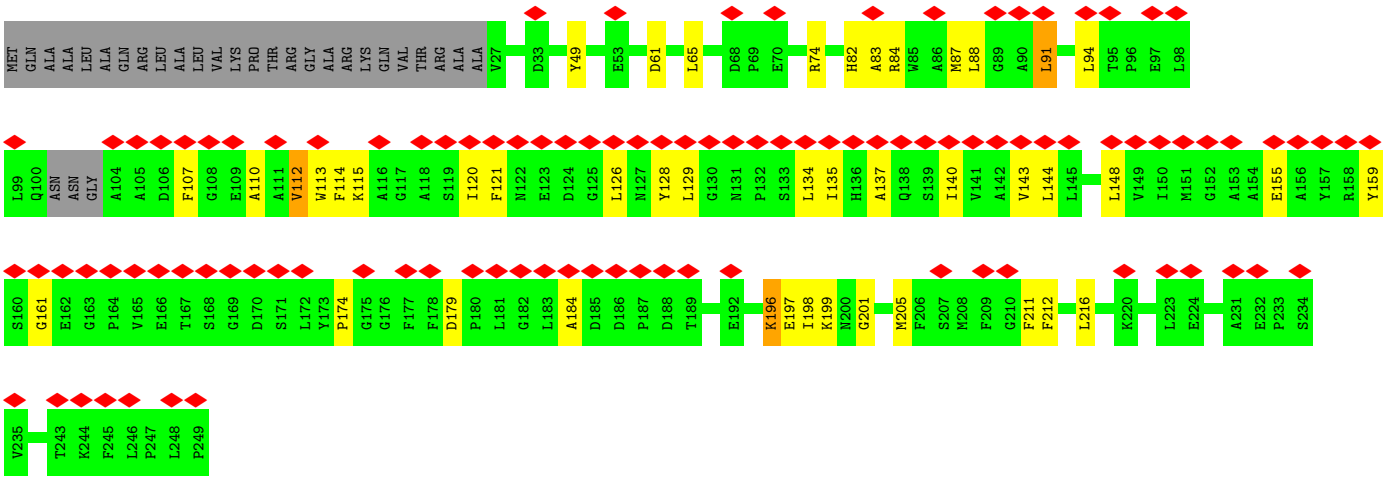
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	N	1	18	16	2	0
			Total	C	O	
50	n	1	18	16	2	0

3 Residue-property plots (i)

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

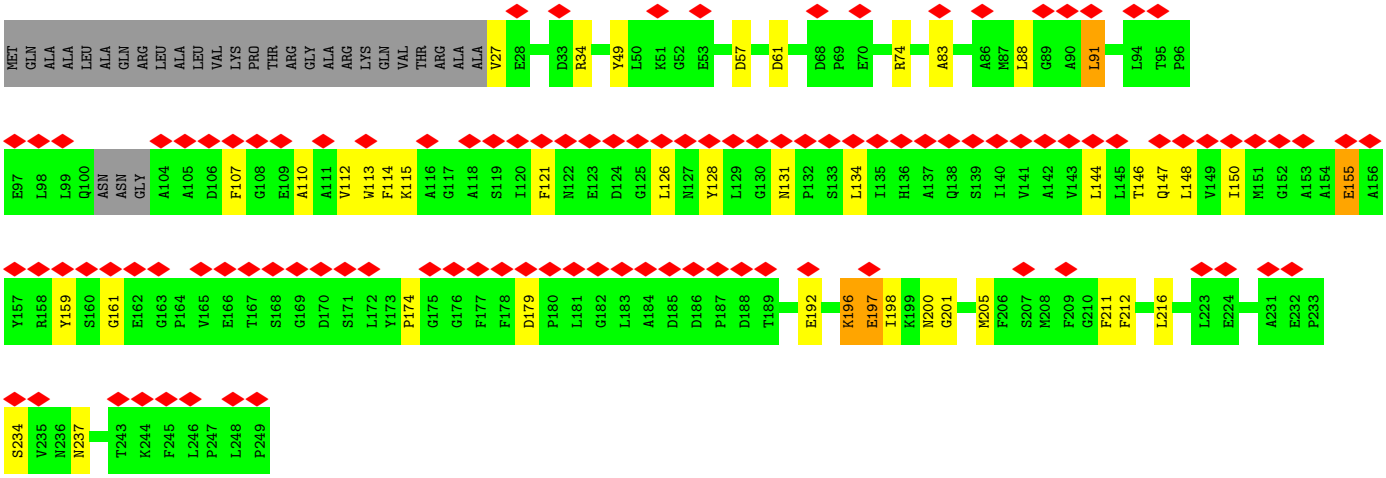
• Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

Chain 1:



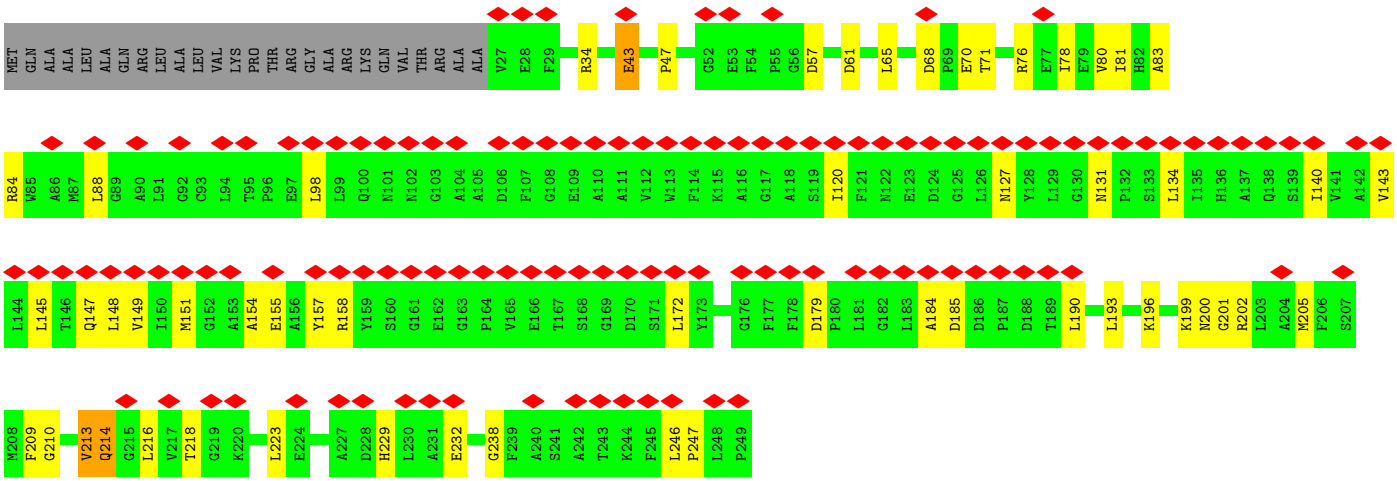
• Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

Chain 4:



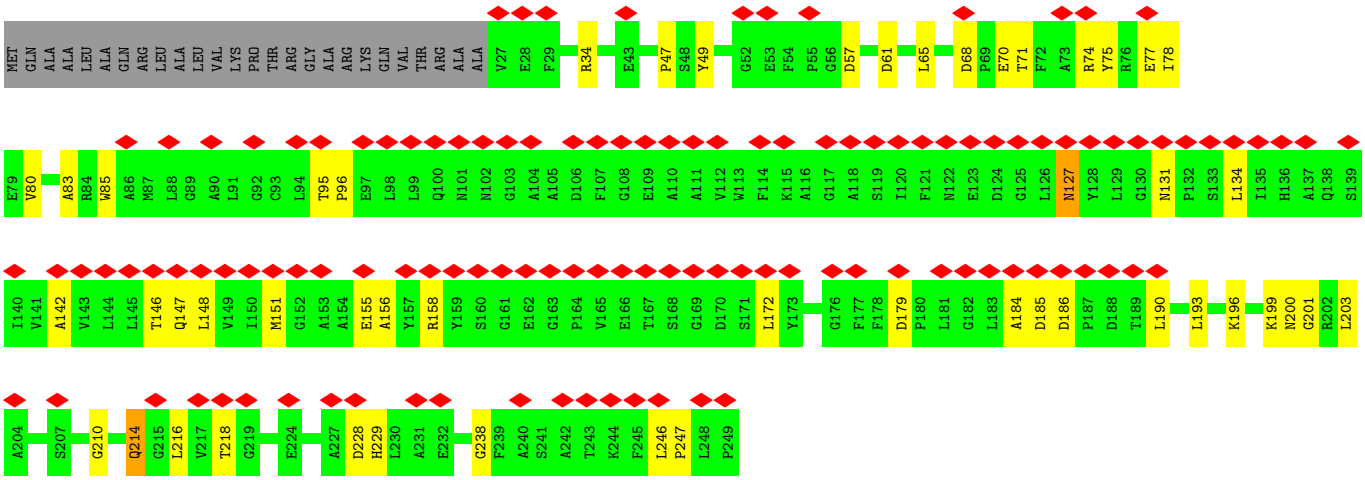
• Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

Chain 11:



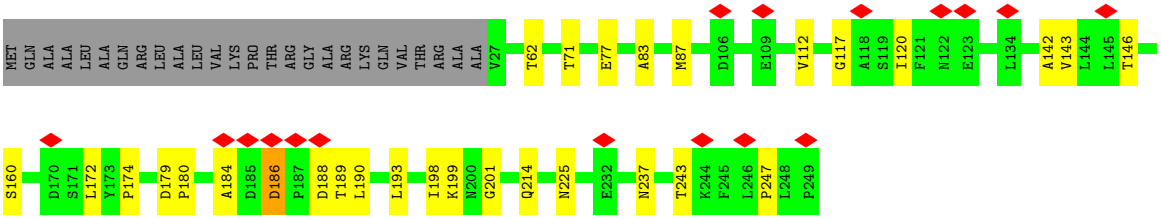
• Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

Chain 14:



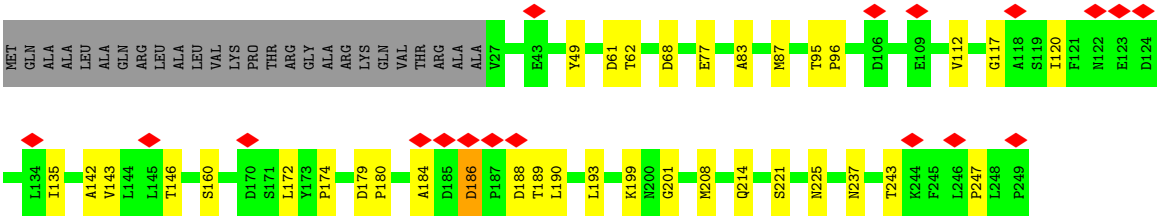
• Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

Chain G:



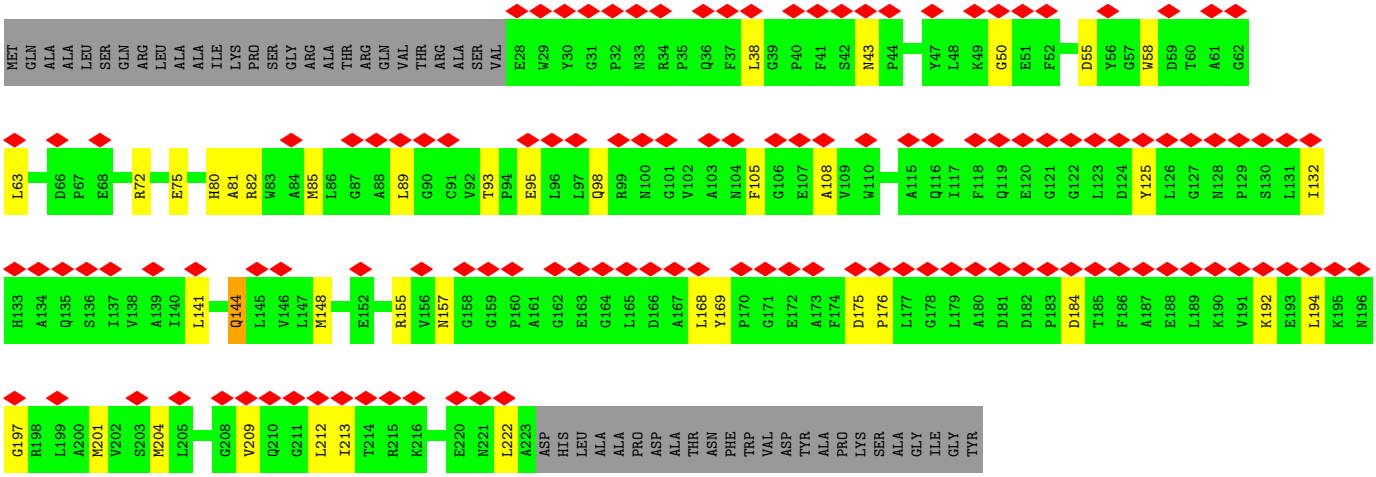
• Molecule 1: Chlorophyll a-b binding protein Lhcbm-I

Chain g:



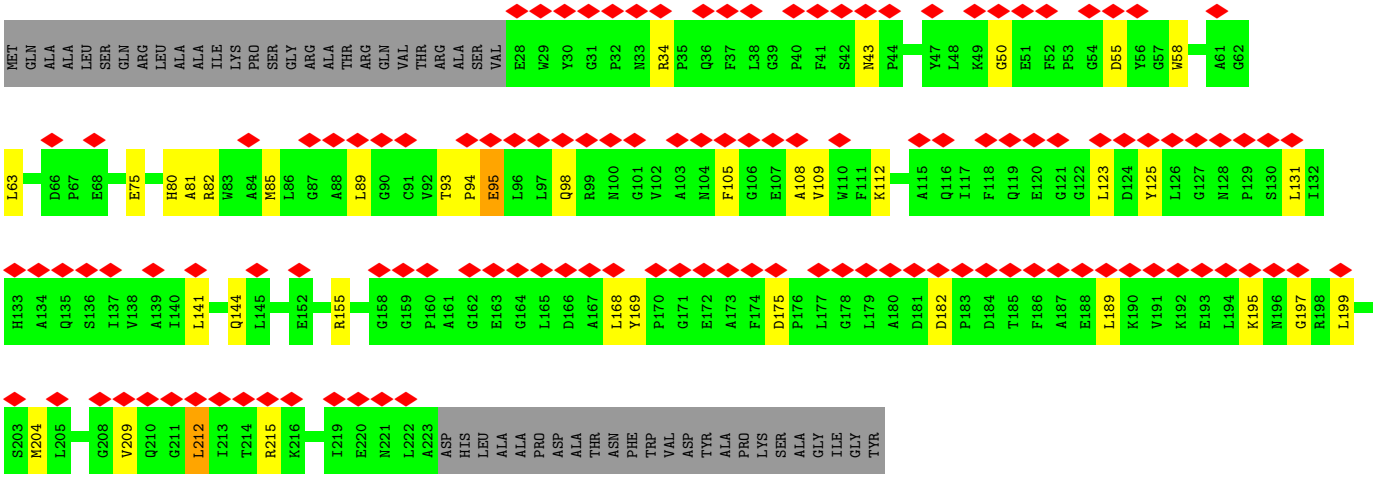
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



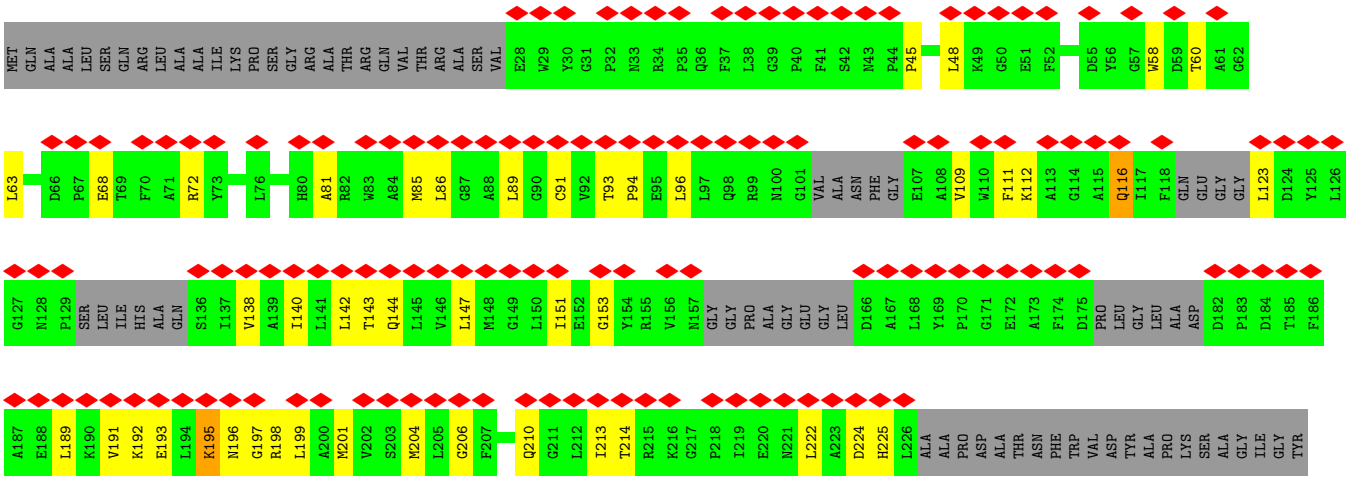
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 12:

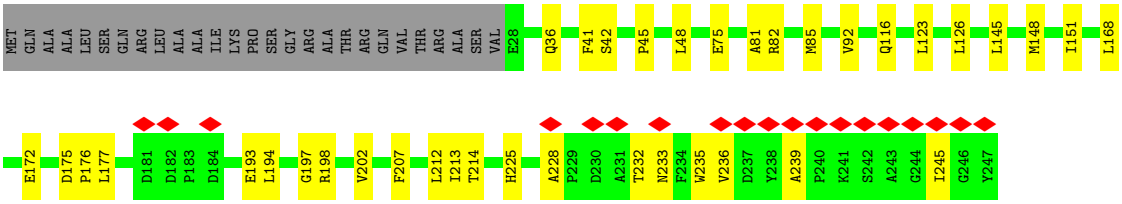


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 15:

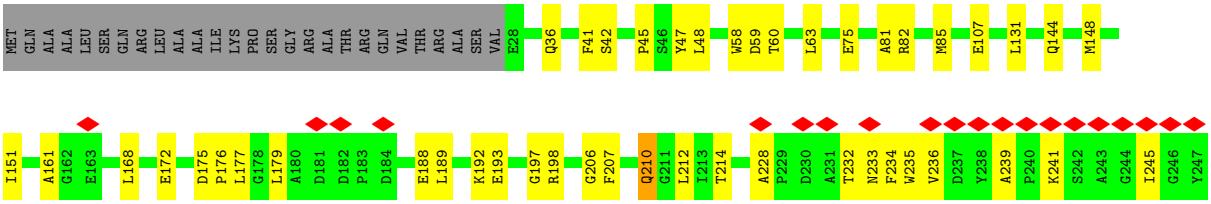
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain N:



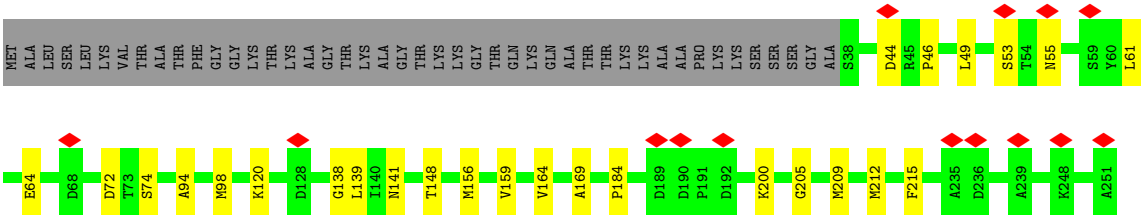
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain n:



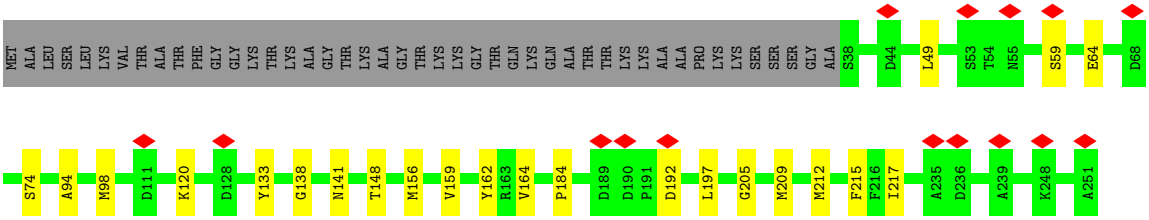
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



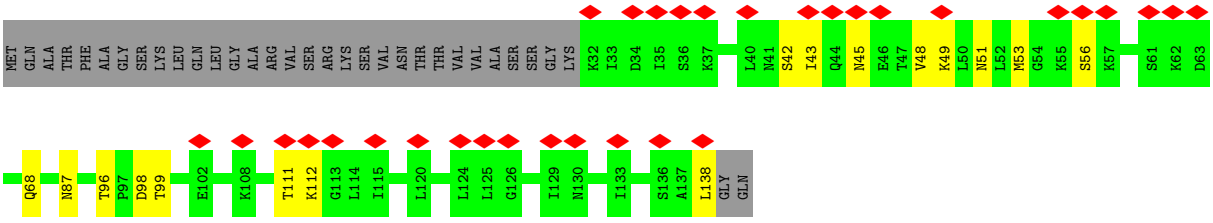
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



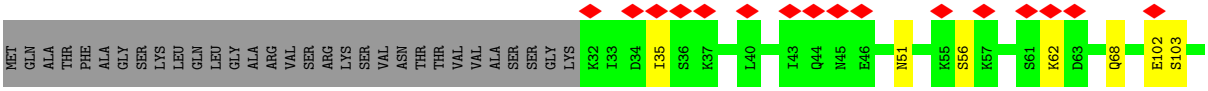
• Molecule 4: Chloroplast photosystem II 10 kDa protein

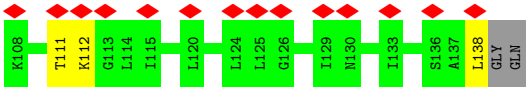
Chain 7:



• Molecule 4: Chloroplast photosystem II 10 kDa protein

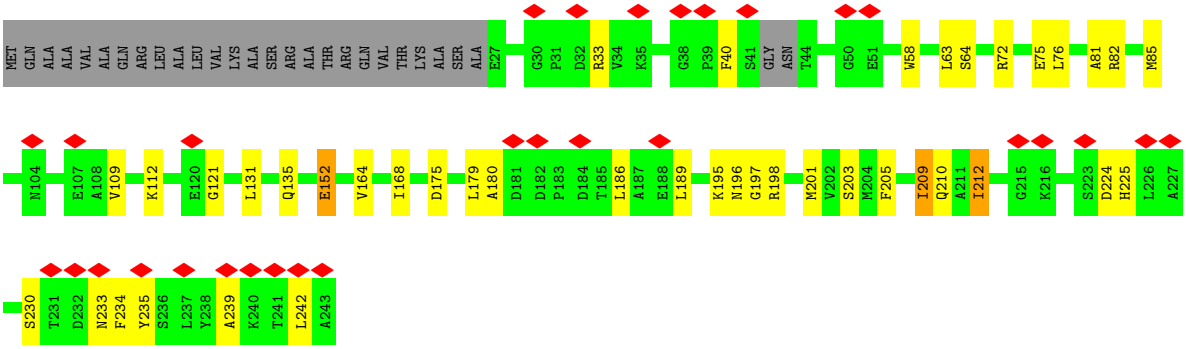
Chain 8:





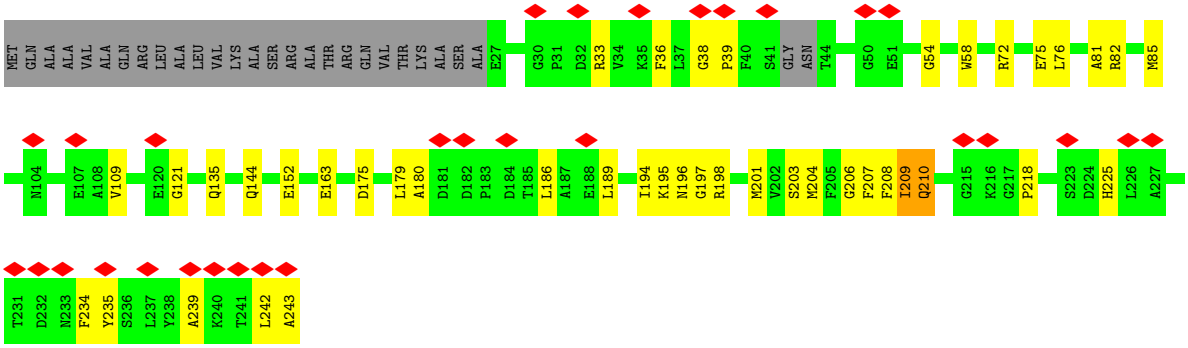
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 13:



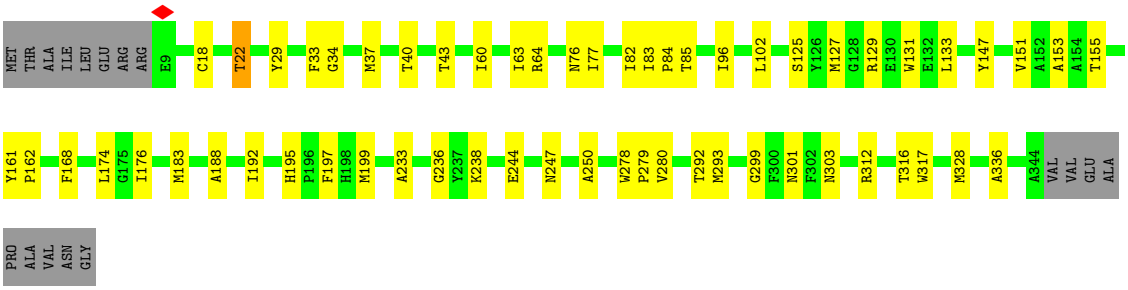
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 16:



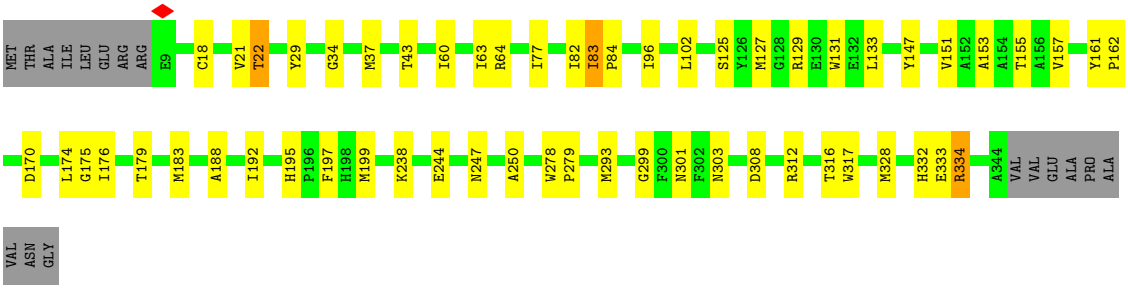
• Molecule 6: Photosystem II protein D1

Chain A:



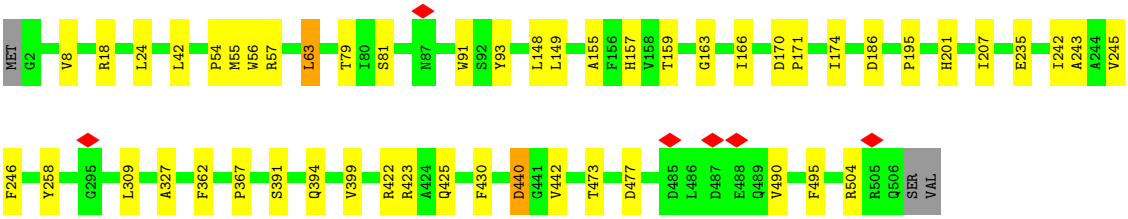
• Molecule 6: Photosystem II protein D1

Chain a:



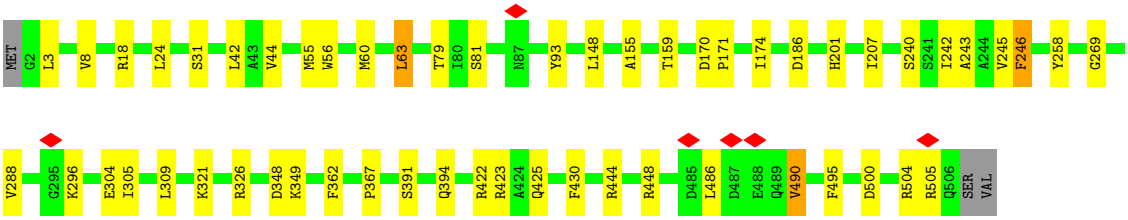
• Molecule 7: Photosystem II CP47 reaction center protein

Chain B:



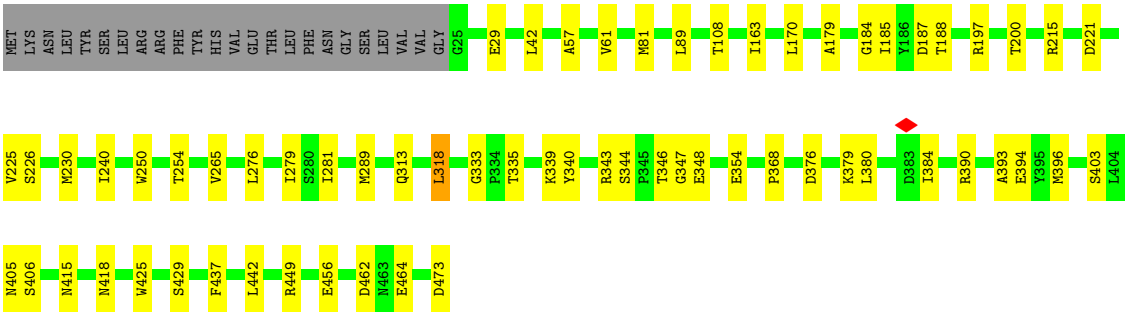
• Molecule 7: Photosystem II CP47 reaction center protein

Chain b:



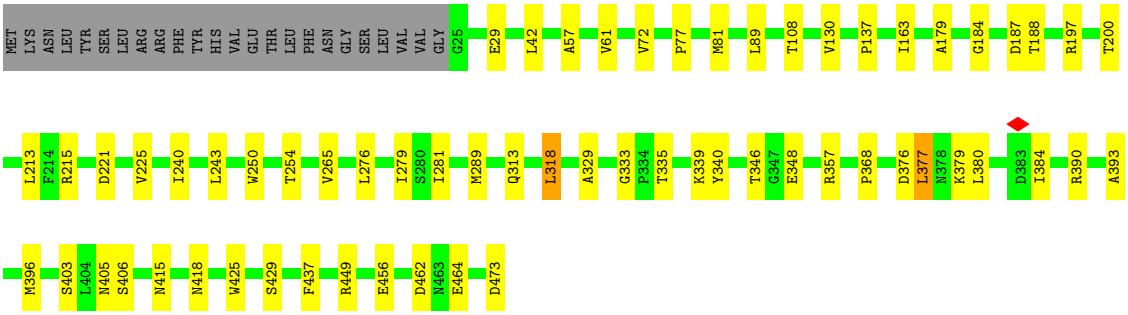
• Molecule 8: Photosystem II CP43 reaction center protein

Chain C:



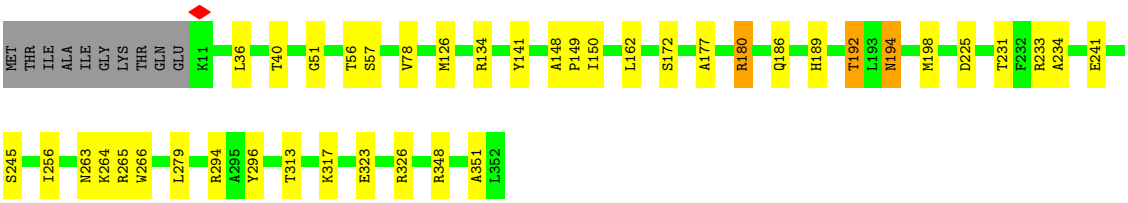
• Molecule 8: Photosystem II CP43 reaction center protein

Chain c:



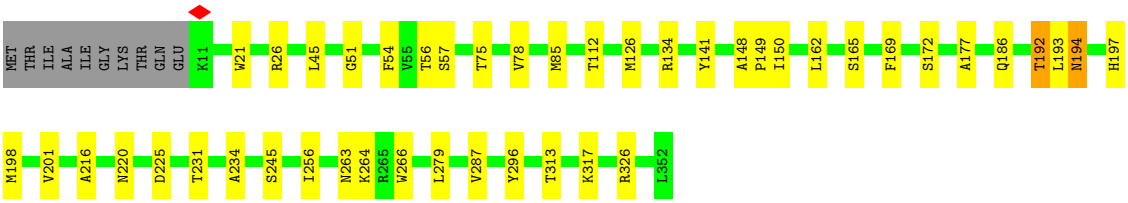
- Molecule 9: Photosystem II D2 protein

Chain D:



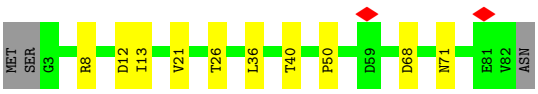
- Molecule 9: Photosystem II D2 protein

Chain d:



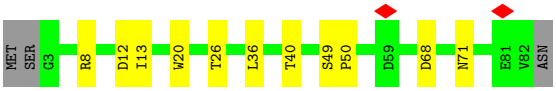
- Molecule 10: Cytochrome b559 subunit alpha

Chain E:



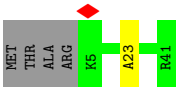
- Molecule 10: Cytochrome b559 subunit alpha

Chain e:



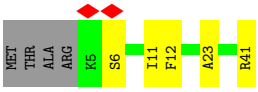
- Molecule 11: Cytochrome b559 subunit beta

Chain F:



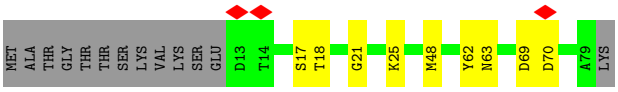
• Molecule 11: Cytochrome b559 subunit beta

Chain f:



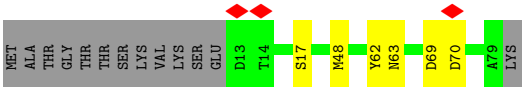
• Molecule 12: Photosystem II reaction center protein H

Chain H:



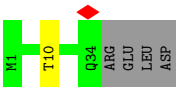
• Molecule 12: Photosystem II reaction center protein H

Chain h:



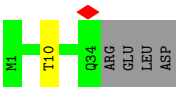
• Molecule 13: Photosystem II reaction center protein I

Chain I:



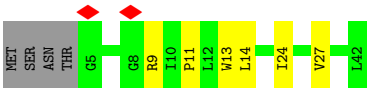
• Molecule 13: Photosystem II reaction center protein I

Chain i:



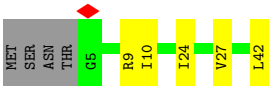
• Molecule 14: Photosystem II reaction center protein J

Chain J:



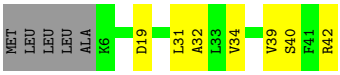
• Molecule 14: Photosystem II reaction center protein J

Chain j:



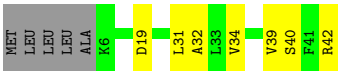
• Molecule 15: Photosystem II reaction center protein K

Chain K:



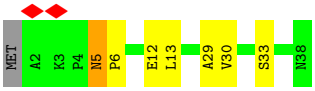
• Molecule 15: Photosystem II reaction center protein K

Chain k:



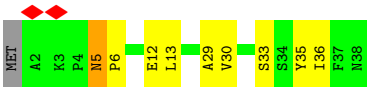
• Molecule 16: Photosystem II reaction center protein L

Chain L:



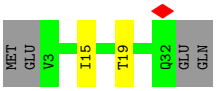
• Molecule 16: Photosystem II reaction center protein L

Chain l:



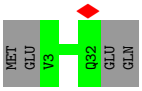
• Molecule 17: Photosystem II reaction center protein M

Chain M:



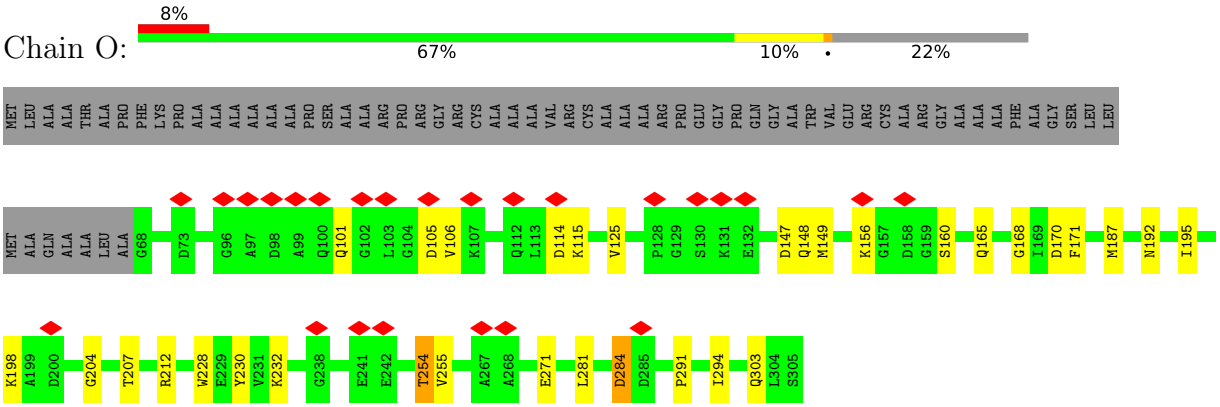
• Molecule 17: Photosystem II reaction center protein M

Chain m:



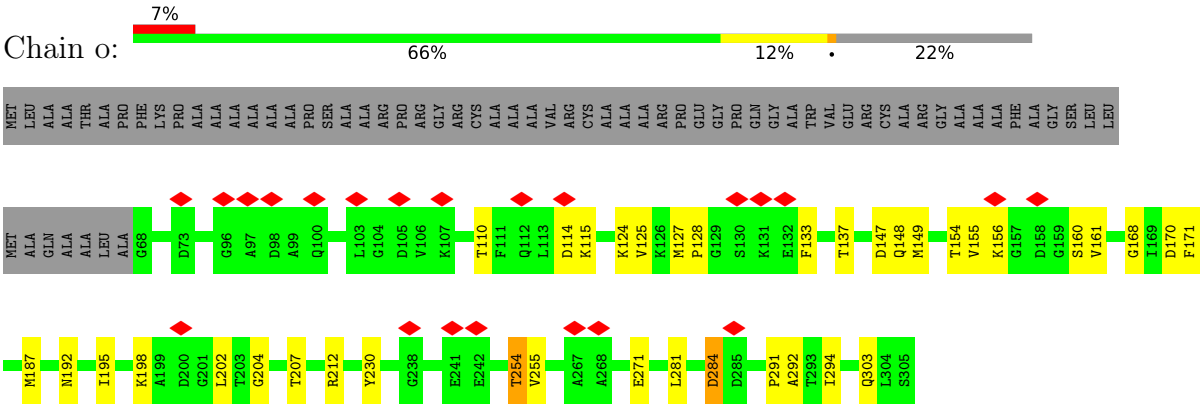
• Molecule 18: Chloroplast oxygen-evolving enhancer protein 1b (PsbO)

Chain O:



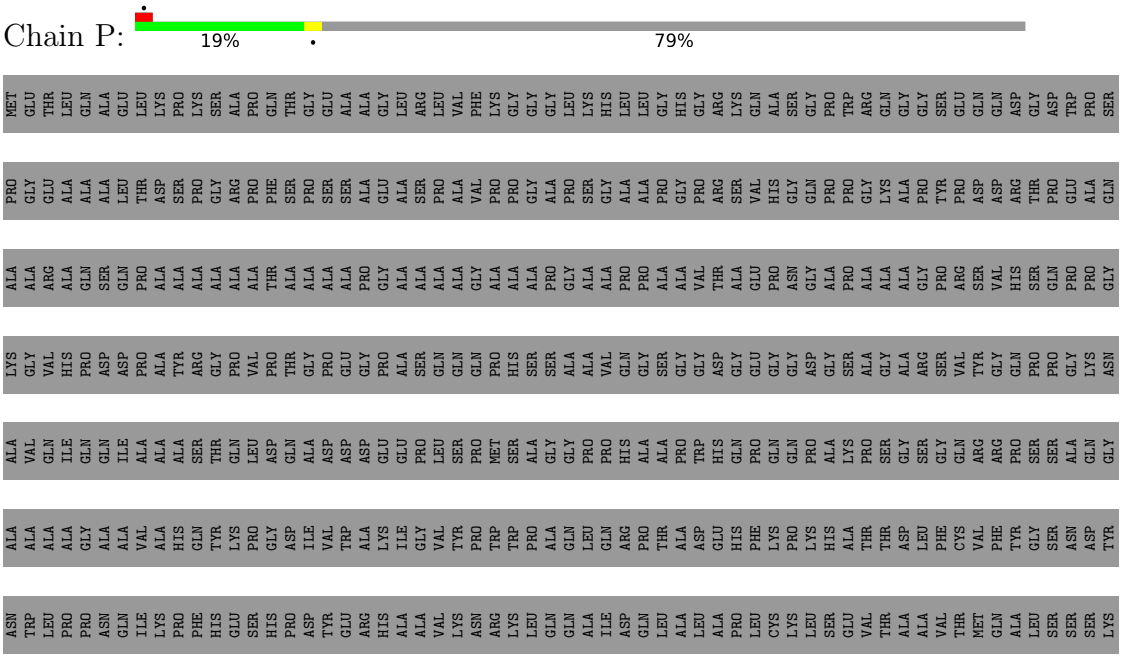
• Molecule 18: Chloroplast oxygen-evolving enhancer protein 1b (PsbO)

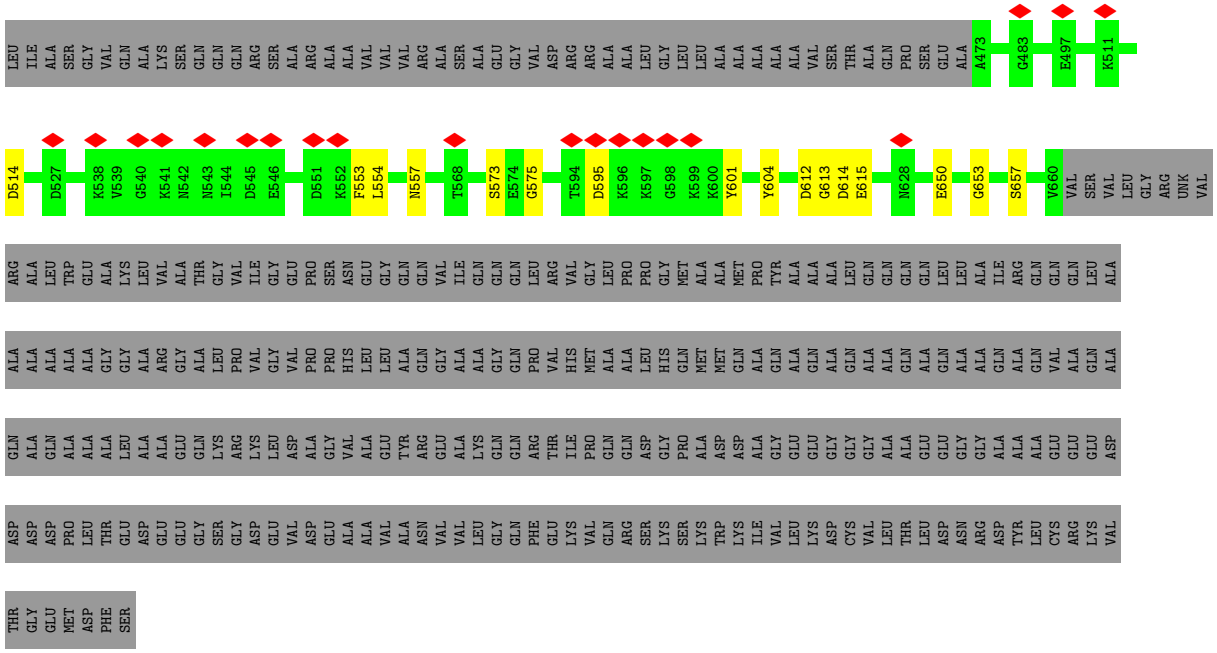
Chain o:



• Molecule 19: PWWP domain-containing protein

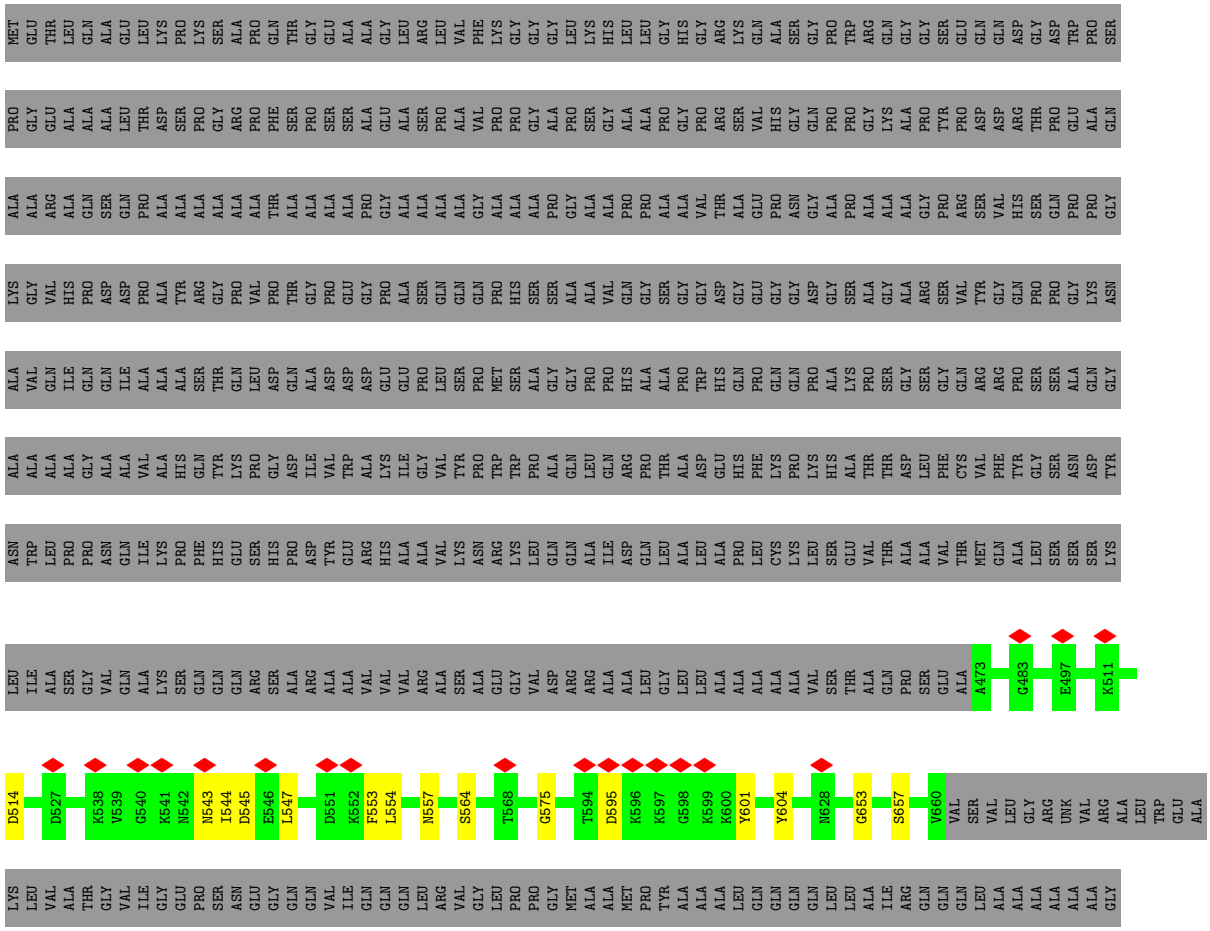
Chain P:

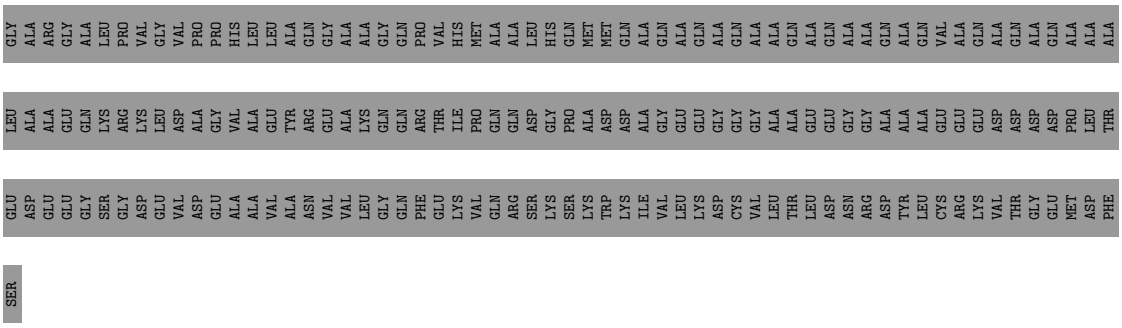




- Molecule 19: PWWP domain-containing protein

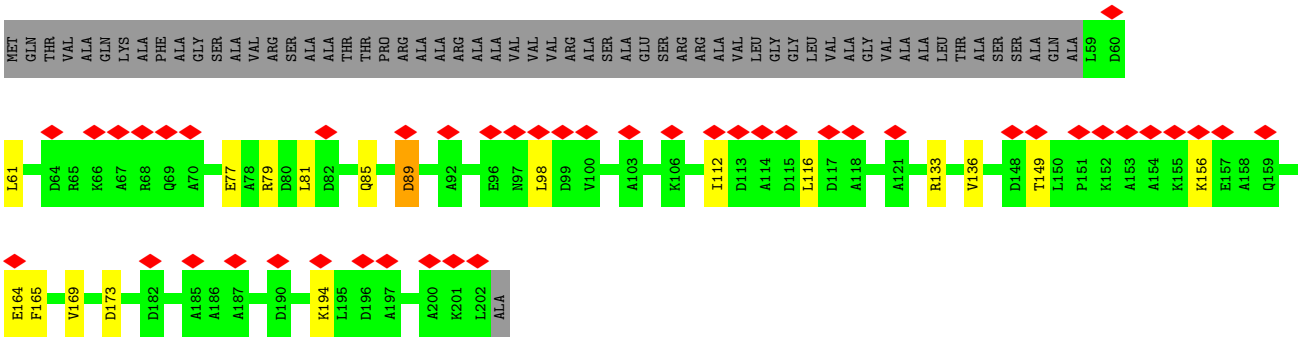
Chain p:





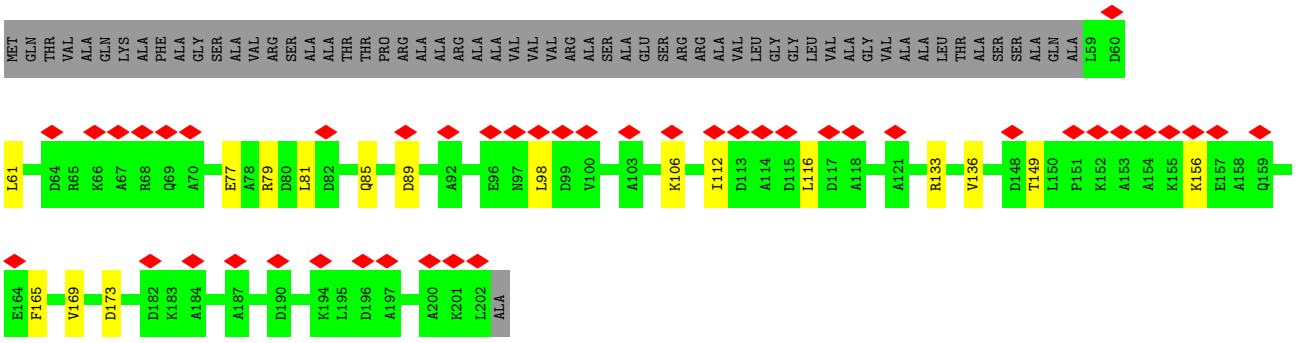
• Molecule 20: Chloroplast oxygen-evolving enhancer protein 3

Chain Q:



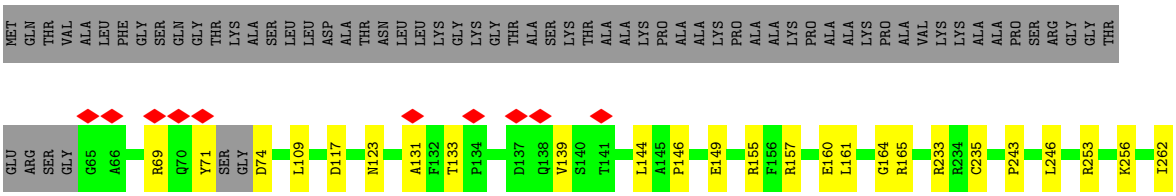
• Molecule 20: Chloroplast oxygen-evolving enhancer protein 3

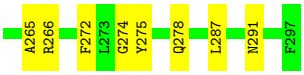
Chain q:



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

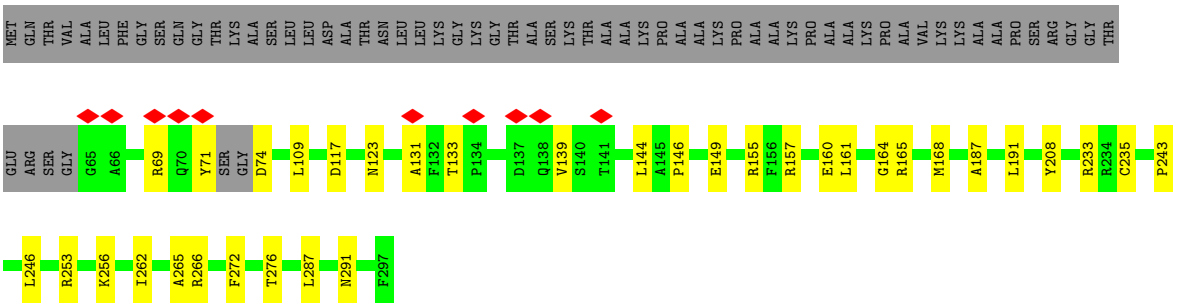
Chain R:





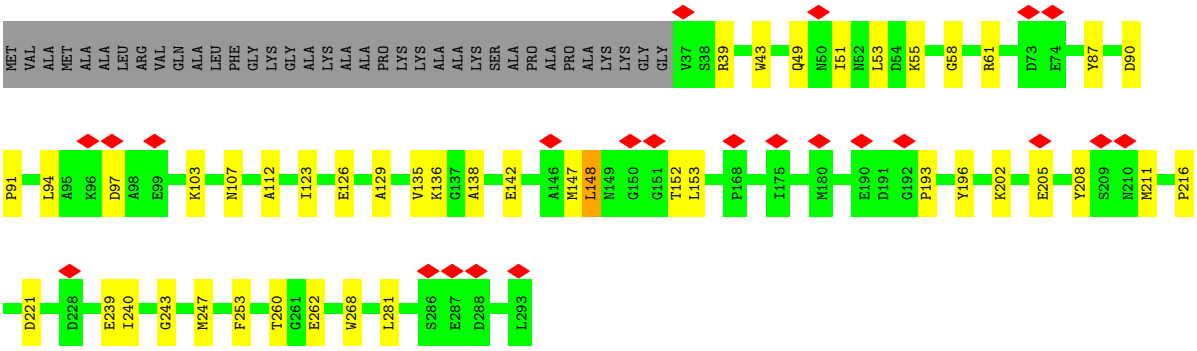
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain r:



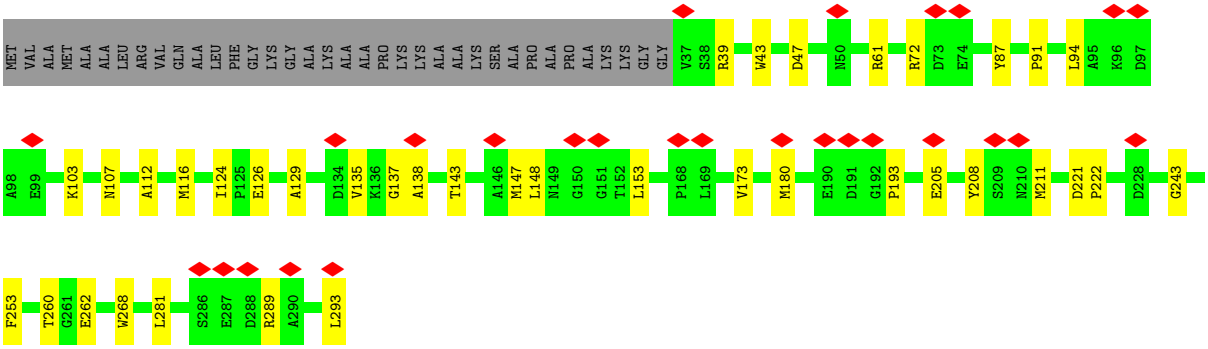
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain S:



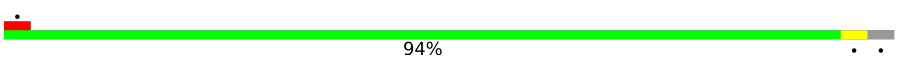
• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

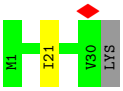
Chain s:



• Molecule 23: Photosystem II reaction center protein T

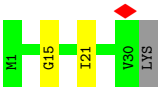
Chain T:





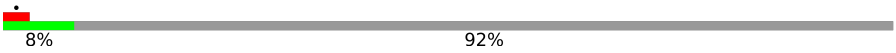
• Molecule 23: Photosystem II reaction center protein T

Chain t:



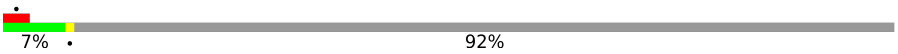
• Molecule 24: Chloroplast PsbY

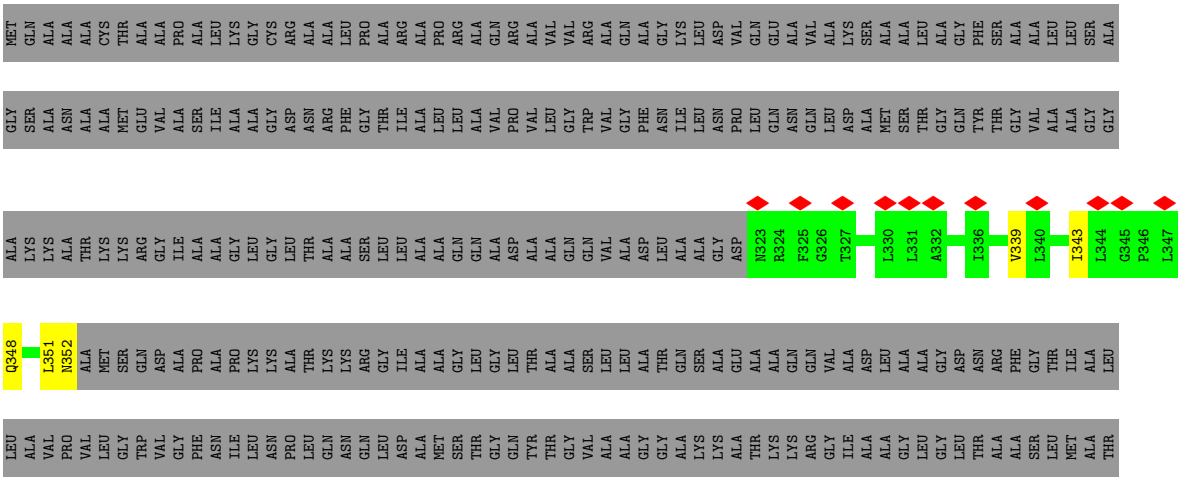
Chain U:

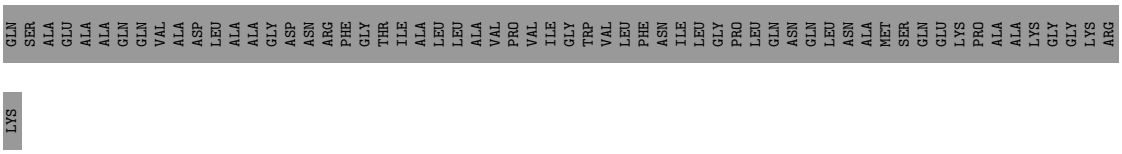


• Molecule 24: Chloroplast PsbY

Chain u:

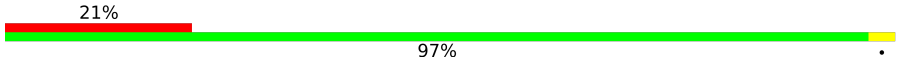


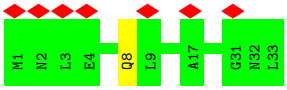




• Molecule 25: Photosystem II reaction center protein Psb30

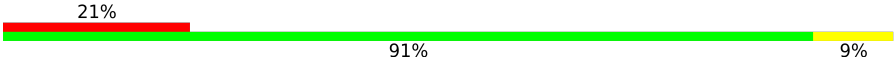
Chain V:





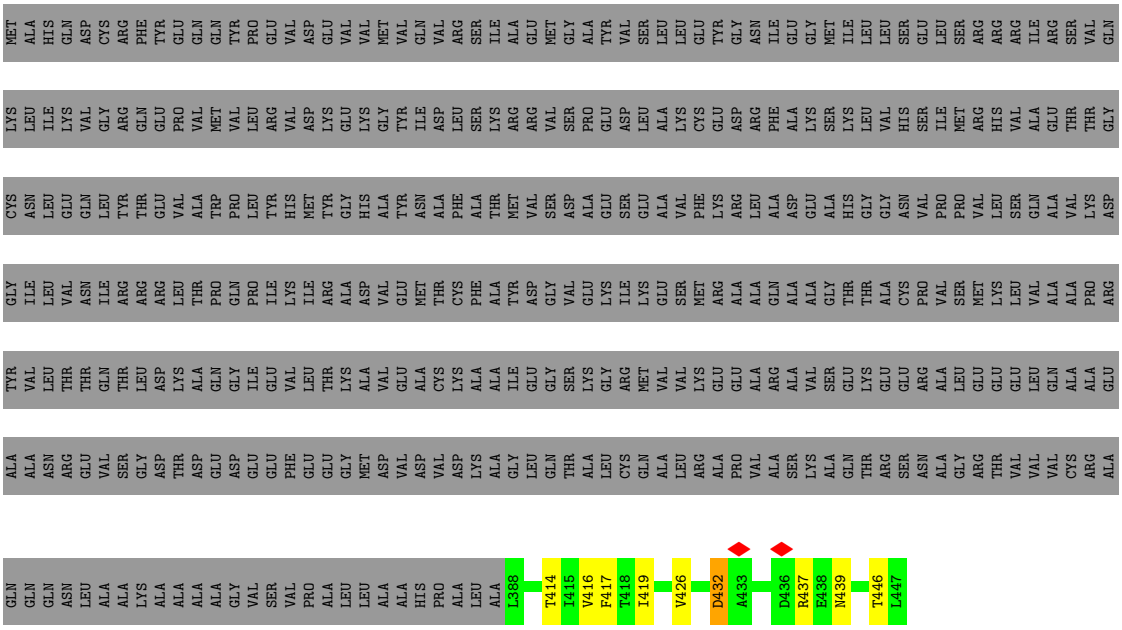
• Molecule 25: Photosystem II reaction center protein Psb30

Chain v:



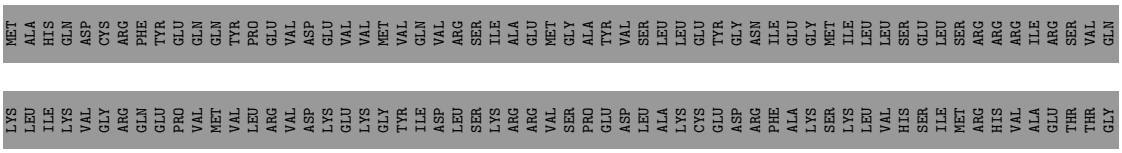
• Molecule 26: PSII 6.1 kDa protein

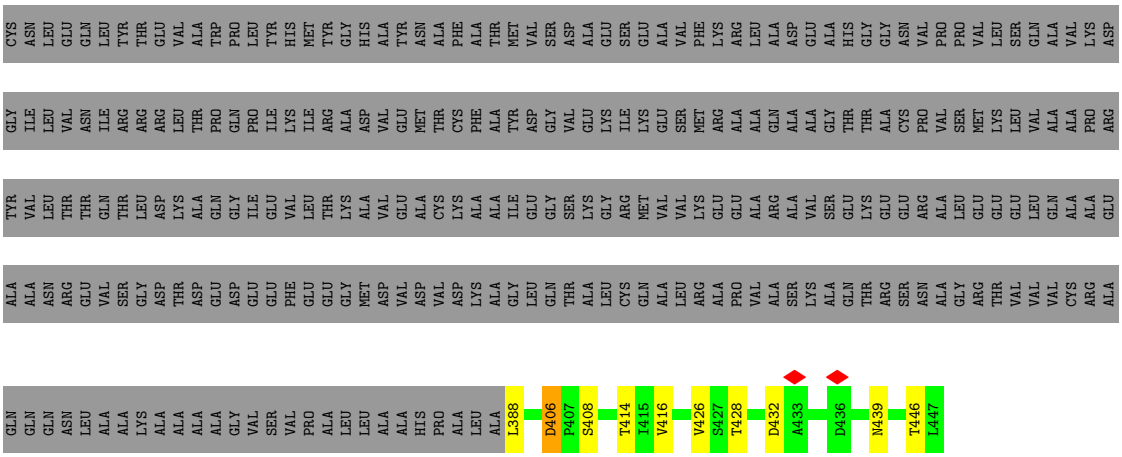
Chain W:



• Molecule 26: PSII 6.1 kDa protein

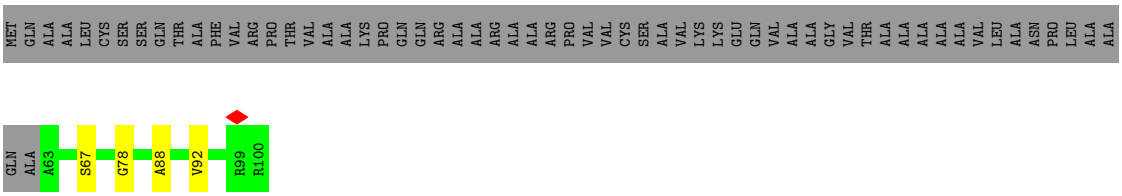
Chain w:





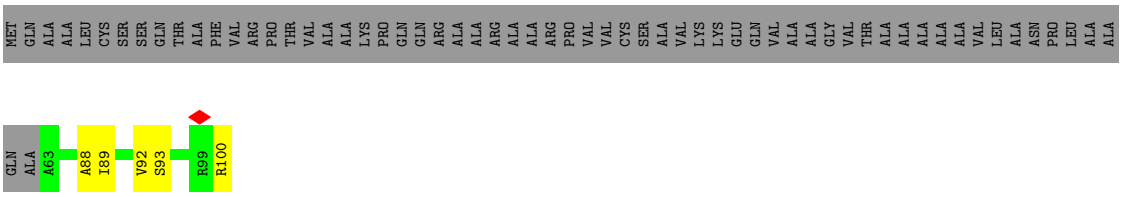
• Molecule 27: Photosystem II reaction center protein X (PsbX)

Chain X: 34% 62%



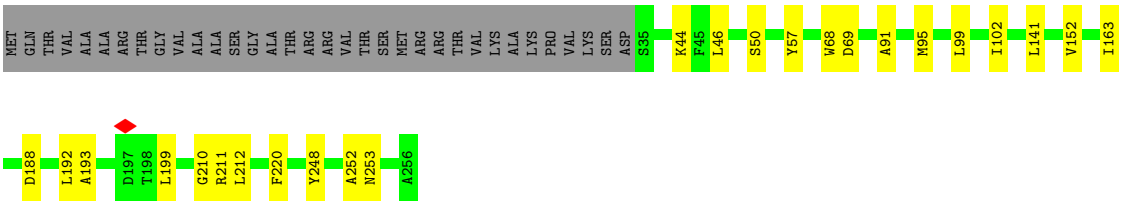
• Molecule 27: Photosystem II reaction center protein X (PsbX)

Chain x: 33% 5% 62%



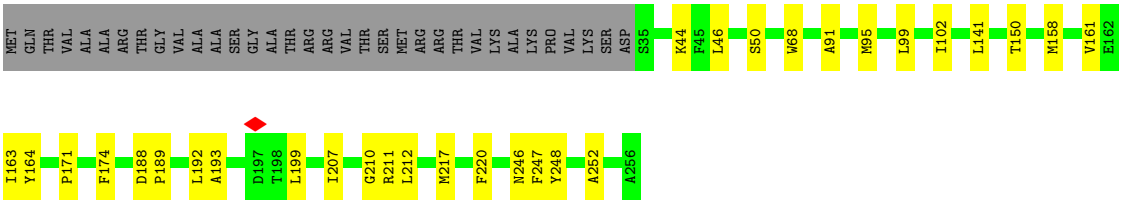
• Molecule 28: Chlorophyll a-b binding protein, chloroplastic

Chain Y: 77% 9% 13%



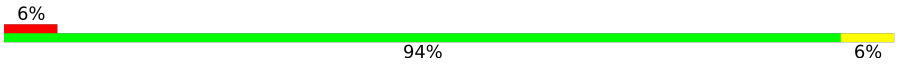
• Molecule 28: Chlorophyll a-b binding protein, chloroplastic

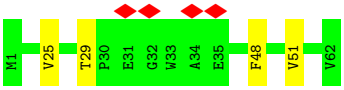
Chain y: 75% 12% 13%



• Molecule 29: Photosystem II reaction center protein Z

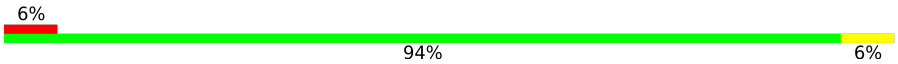
Chain Z:

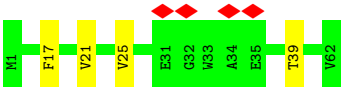




• Molecule 29: Photosystem II reaction center protein Z

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	225372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	90	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.292	Depositor
Minimum map value	-0.740	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	454.56, 454.56, 454.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94699997, 0.94699997, 0.94699997	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: XAT, LMG, CL, BCT, LUT, OEX, 3PH, CHL, STE, NEX, LHG, HEM, FE2, PAM, LNL, SQD, DGD, CLA, BCR, PL9, PHO

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	1	0.35	2/1720 (0.1%)	0.31	0/2339
1	11	0.54	5/1741 (0.3%)	0.30	0/2369
1	14	0.69	5/1741 (0.3%)	0.38	2/2369 (0.1%)
1	4	0.37	3/1720 (0.2%)	0.33	1/2339 (0.0%)
1	G	0.13	0/1741	0.25	0/2369
1	g	0.12	0/1741	0.24	0/2369
2	12	0.61	3/1362 (0.2%)	0.44	2/1844 (0.1%)
2	15	0.36	3/1362 (0.2%)	0.34	0/1844
2	2	0.15	0/1536	0.33	0/2088
2	5	0.15	0/1536	0.29	0/2088
2	N	0.14	0/1727	0.26	0/2352
2	n	0.14	0/1727	0.33	1/2352 (0.0%)
3	3	0.12	0/1675	0.24	0/2283
3	6	0.14	0/1675	0.27	0/2283
4	7	0.10	0/831	0.24	0/1122
4	8	0.10	0/831	0.24	0/1122
5	13	0.54	6/1688 (0.4%)	0.32	0/2296
5	16	0.53	5/1688 (0.3%)	0.31	0/2296
6	A	0.18	0/2714	0.34	0/3701
6	a	0.21	0/2714	0.39	1/3701 (0.0%)
7	B	0.15	0/4094	0.26	0/5576
7	b	0.15	0/4094	0.26	0/5576
8	C	0.15	0/3611	0.26	0/4921
8	c	0.15	0/3611	0.26	0/4921
9	D	0.16	0/2825	0.29	0/3849
9	d	0.17	0/2825	0.29	0/3849
10	E	0.12	0/664	0.24	0/905
10	e	0.12	0/664	0.24	0/905
11	F	0.13	0/313	0.23	0/426
11	f	0.14	0/313	0.25	0/426
12	H	0.14	0/518	0.24	0/708

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	h	0.14	0/518	0.24	0/708
13	I	0.17	0/282	0.28	0/382
13	i	0.17	0/282	0.28	0/382
14	J	0.12	0/276	0.25	0/377
14	j	0.12	0/276	0.24	0/377
15	K	0.18	0/305	0.37	0/420
15	k	0.18	0/305	0.38	0/420
16	L	0.18	0/311	0.29	0/422
16	l	0.18	0/311	0.28	0/422
17	M	0.16	0/231	0.27	0/316
17	m	0.15	0/231	0.28	0/316
18	O	0.11	0/1790	0.26	0/2420
18	o	0.10	0/1790	0.24	0/2420
19	P	0.09	0/1473	0.21	0/1991
19	p	0.09	0/1473	0.20	0/1991
20	Q	0.11	0/1132	0.23	0/1521
20	q	0.11	0/1132	0.24	0/1521
21	R	0.15	0/1820	0.27	0/2475
21	r	0.14	0/1820	0.24	0/2475
22	S	0.16	0/1985	0.32	0/2711
22	s	0.12	0/1985	0.28	0/2711
23	T	0.14	0/253	0.20	0/343
23	t	0.14	0/253	0.20	0/343
24	U	0.12	0/238	0.24	0/326
24	u	0.15	0/238	0.30	0/326
25	V	0.08	0/242	0.19	0/329
25	v	0.08	0/242	0.19	0/329
26	W	0.14	0/477	0.23	0/650
26	w	0.15	0/477	0.25	0/650
27	X	0.11	0/259	0.18	0/353
27	x	0.11	0/259	0.19	0/353
28	Y	0.15	0/1741	0.25	0/2367
28	y	0.15	0/1741	0.24	0/2367
29	Z	0.11	0/491	0.24	0/672
29	z	0.10	0/491	0.24	0/672
All	All	0.24	32/84132 (0.0%)	0.28	7/114446 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	a	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14	229	HIS	C-N	19.06	1.59	1.33
1	14	214	GLN	C-N	16.36	1.53	1.33
1	11	214	GLN	C-N	14.82	1.53	1.33
2	12	224	ASP	C-N	14.44	1.51	1.33
2	12	196	ASN	C-N	12.55	1.50	1.33
5	13	196	ASN	C-N	12.38	1.48	1.33
5	16	152	GLU	C-N	11.78	1.49	1.33
5	16	196	ASN	C-N	11.40	1.47	1.33
5	13	225	HIS	C-N	10.71	1.48	1.34
1	1	155	GLU	C-N	10.06	1.47	1.33
1	4	197	GLU	C-N	9.11	1.45	1.34
1	11	229	HIS	C-N	9.06	1.46	1.33
1	11	200	ASN	C-N	8.75	1.44	1.33
5	16	210	GLN	C-N	8.43	1.45	1.33
1	4	155	GLU	C-N	8.25	1.44	1.33
1	1	196	LYS	C-N	8.22	1.45	1.33
1	14	200	ASN	C-N	8.19	1.43	1.33
5	13	152	GLU	C-N	7.72	1.44	1.33
2	15	196	ASN	C-N	7.70	1.44	1.33
1	4	196	LYS	C-N	7.57	1.45	1.33
5	13	210	GLN	C-N	7.45	1.43	1.33
2	12	195	LYS	C-N	7.16	1.43	1.33
1	14	228	ASP	C-N	-6.20	1.26	1.33
1	14	199	LYS	C-N	5.96	1.42	1.34
1	11	213	VAL	C-N	-5.88	1.26	1.33
2	15	192	LYS	C-N	5.74	1.41	1.33
5	16	225	HIS	C-N	5.74	1.41	1.34
1	11	199	LYS	C-N	5.65	1.41	1.34
5	16	208	PHE	C-N	-5.38	1.27	1.33
5	13	224	ASP	C-N	5.34	1.41	1.33
5	13	205	PHE	C-N	-5.20	1.26	1.33
2	15	224	ASP	C-N	-5.17	1.27	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	12	225	HIS	O-C-N	6.57	128.93	122.09
6	a	332	HIS	CA-CB-CG	6.53	120.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	n	210	GLN	CA-CB-CG	5.64	125.37	114.10
2	12	224	ASP	O-C-N	-5.61	116.17	122.12
1	14	228	ASP	CA-C-N	-5.42	113.22	120.54
1	14	228	ASP	C-N-CA	-5.42	113.22	120.54
1	4	197	GLU	CA-CB-CG	5.32	124.73	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	a	334	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1673	0	1609	34	0
1	11	1693	0	1625	34	0
1	14	1693	0	1625	33	0
1	4	1673	0	1609	26	0
1	G	1693	0	1625	19	0
1	g	1693	0	1625	25	0
2	12	1330	0	1299	37	0
2	15	1330	0	1299	40	0
2	2	1496	0	1463	33	0
2	5	1496	0	1463	27	0
2	N	1679	0	1626	24	0
2	n	1679	0	1626	36	0
3	3	1630	0	1583	18	0
3	6	1630	0	1583	18	0
4	7	816	0	831	11	0
4	8	816	0	831	5	0
5	13	1645	0	1602	29	0
5	16	1645	0	1602	31	0
6	A	2632	0	2532	43	0
6	a	2632	0	2532	37	0
7	B	3963	0	3831	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	b	3963	0	3831	35	0
8	C	3491	0	3379	42	0
8	c	3491	0	3379	43	0
9	D	2730	0	2630	33	0
9	d	2730	0	2630	30	0
10	E	646	0	631	6	0
10	e	646	0	631	8	0
11	F	303	0	311	1	0
11	f	303	0	311	5	0
12	H	507	0	520	7	0
12	h	507	0	520	5	0
13	I	274	0	280	1	0
13	i	274	0	280	1	0
14	J	270	0	282	5	0
14	j	270	0	282	5	0
15	K	295	0	311	6	0
15	k	295	0	311	6	0
16	L	303	0	311	5	0
16	l	303	0	311	7	0
17	M	228	0	257	1	0
17	m	228	0	257	0	0
18	O	1759	0	1714	20	0
18	o	1759	0	1714	21	0
19	P	1443	0	1408	10	0
19	p	1443	0	1408	9	0
20	Q	1122	0	1151	12	0
20	q	1122	0	1151	11	0
21	R	1783	0	1705	21	0
21	r	1783	0	1705	24	0
22	S	1934	0	1878	33	0
22	s	1934	0	1878	31	0
23	T	246	0	262	2	0
23	t	246	0	262	3	0
24	U	233	0	246	0	0
24	u	233	0	246	5	0
25	V	241	0	275	1	0
25	v	241	0	275	2	0
26	W	468	0	450	7	0
26	w	468	0	450	5	0
27	X	258	0	273	2	0
27	x	258	0	273	5	0
28	Y	1694	0	1641	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	y	1694	0	1641	26	0
29	Z	478	0	513	2	0
29	z	478	0	513	2	0
30	1	311	0	240	14	0
30	11	314	0	249	9	0
30	12	250	0	183	8	0
30	13	345	0	302	14	0
30	14	318	0	255	7	0
30	15	258	0	199	16	0
30	16	345	0	302	11	0
30	2	311	0	247	13	0
30	3	365	0	351	11	0
30	4	321	0	263	19	0
30	5	315	0	253	8	0
30	6	365	0	351	15	0
30	G	329	0	280	11	0
30	N	357	0	332	19	0
30	R	173	0	154	12	0
30	S	204	0	164	8	0
30	Y	364	0	358	10	0
30	g	332	0	286	13	0
30	n	356	0	330	18	0
30	r	173	0	154	6	0
30	s	204	0	164	11	0
30	y	364	0	358	9	0
31	1	409	0	336	18	0
31	11	413	0	350	20	0
31	12	410	0	344	58	0
31	13	495	0	462	25	0
31	14	442	0	409	27	0
31	15	410	0	344	41	0
31	16	495	0	462	23	0
31	2	349	0	277	17	0
31	3	521	0	504	12	0
31	4	427	0	373	10	0
31	5	352	0	281	14	0
31	6	515	0	487	14	0
31	A	250	0	265	8	0
31	B	1025	0	1116	31	0
31	C	820	0	877	24	0
31	D	130	0	144	6	0
31	G	457	0	448	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	N	492	0	448	12	0
31	R	631	0	608	21	0
31	S	613	0	586	19	0
31	Y	545	0	558	23	0
31	a	185	0	193	5	0
31	b	1025	0	1116	39	0
31	c	820	0	877	26	0
31	d	195	0	216	10	0
31	g	457	0	448	10	0
31	n	492	0	448	22	0
31	r	636	0	621	25	0
31	s	613	0	586	24	0
31	y	540	0	545	23	0
32	1	43	0	59	1	0
32	11	49	0	74	3	0
32	13	40	0	53	3	0
32	14	49	0	74	3	0
32	16	40	0	53	3	0
32	3	91	0	125	3	0
32	4	47	0	67	2	0
32	6	91	0	125	5	0
32	A	185	0	268	11	0
32	C	42	0	57	4	0
32	D	137	0	196	5	0
32	G	49	0	74	2	0
32	L	47	0	67	4	0
32	N	49	0	74	2	0
32	R	129	0	174	9	0
32	S	94	0	137	7	0
32	Y	143	0	208	9	0
32	a	185	0	268	8	0
32	c	42	0	57	3	0
32	d	137	0	196	5	0
32	g	49	0	74	5	0
32	l	47	0	67	4	0
32	n	49	0	74	5	0
32	r	129	0	174	11	0
32	s	94	0	137	7	0
32	y	143	0	208	7	0
33	1	84	0	112	6	0
33	11	84	0	112	7	0
33	12	84	0	112	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	13	84	0	112	3	0
33	14	84	0	112	5	0
33	15	84	0	112	13	0
33	16	84	0	112	6	0
33	2	84	0	112	9	0
33	3	84	0	112	3	0
33	4	84	0	112	7	0
33	5	84	0	112	3	0
33	6	84	0	112	4	0
33	G	84	0	112	3	0
33	N	84	0	112	6	0
33	R	42	0	56	1	0
33	S	84	0	112	8	0
33	Y	84	0	112	4	0
33	g	84	0	112	4	0
33	n	84	0	112	8	0
33	r	42	0	56	4	0
33	s	84	0	112	10	0
33	y	84	0	112	6	0
34	1	16	0	20	0	0
34	11	16	0	20	0	0
34	12	27	0	33	2	0
34	13	44	0	56	0	0
34	14	16	0	20	0	0
34	15	27	0	33	3	0
34	16	44	0	56	0	0
34	2	32	0	39	0	0
34	3	44	0	56	3	0
34	4	16	0	20	0	0
34	5	32	0	39	0	0
34	6	44	0	56	4	0
34	G	43	0	53	1	0
34	N	44	0	56	1	0
34	R	44	0	56	1	0
34	S	44	0	56	1	0
34	Y	44	0	56	1	0
34	g	44	0	56	0	0
34	n	44	0	56	1	0
34	r	44	0	56	1	0
34	s	44	0	56	1	0
34	y	44	0	56	0	0
35	11	44	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	14	44	0	56	1	0
35	3	44	0	56	3	0
35	6	44	0	56	4	0
35	G	44	0	56	1	0
35	R	44	0	56	2	0
35	g	44	0	56	2	0
35	r	44	0	56	1	0
36	7	48	0	75	1	0
36	8	48	0	75	2	0
36	B	86	0	127	7	0
36	T	48	0	75	4	0
36	b	39	0	54	1	0
37	A	10	0	0	0	0
37	a	10	0	0	0	0
38	A	64	0	74	0	0
38	D	64	0	74	4	0
38	a	128	0	148	1	0
39	A	40	0	56	2	0
39	B	120	0	168	7	0
39	C	120	0	168	5	0
39	D	40	0	56	2	0
39	H	40	0	56	3	0
39	J	40	0	56	3	0
39	a	40	0	56	1	0
39	b	120	0	168	5	0
39	c	120	0	168	4	0
39	d	40	0	56	1	0
39	h	40	0	56	4	0
39	j	40	0	56	3	0
40	A	51	0	68	0	0
40	D	100	0	136	2	0
40	L	50	0	64	3	0
40	a	51	0	68	0	0
40	d	100	0	136	7	0
40	l	50	0	64	2	0
41	A	55	0	86	1	0
41	B	97	0	137	3	0
41	C	102	0	153	2	0
41	D	92	0	124	2	0
41	H	35	0	51	0	0
41	J	51	0	75	5	0
41	K	51	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	S	42	0	54	3	0
41	b	95	0	130	2	0
41	c	102	0	153	2	0
41	d	127	0	175	4	0
41	j	51	0	75	5	0
41	s	42	0	54	2	0
41	v	51	0	72	1	0
41	w	55	0	86	3	0
42	A	55	0	80	2	0
42	D	55	0	80	2	0
42	a	55	0	80	4	0
42	d	55	0	80	2	0
43	A	20	0	29	0	0
43	C	40	0	58	1	0
43	H	20	0	29	4	0
43	I	20	0	29	0	0
43	R	20	0	29	0	0
43	W	40	0	58	2	0
43	X	20	0	29	1	0
43	Y	40	0	58	2	0
43	a	20	0	29	0	0
43	c	40	0	58	1	0
43	h	20	0	29	2	0
43	i	20	0	29	0	0
43	r	20	0	29	0	0
43	w	20	0	29	1	0
43	x	20	0	29	1	0
43	y	60	0	87	4	0
44	B	20	0	35	1	0
44	b	20	0	35	0	0
45	C	1	0	0	0	0
45	c	1	0	0	0	0
46	C	183	0	246	9	0
46	W	46	0	64	4	0
46	c	183	0	246	8	0
46	w	40	0	52	2	0
47	D	1	0	0	0	0
47	d	1	0	0	0	0
48	D	4	0	1	0	0
48	d	4	0	0	0	0
49	F	43	0	30	2	0
49	f	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	N	18	0	29	1	0
50	n	18	0	29	1	0
All	All	112944	0	113167	1728	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 8.

All (1728) 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)
31:12:612:CLA:C3B	33:12:614:LUT:H183	1.22	1.54
31:12:612:CLA:CAB	33:12:614:LUT:H183	1.53	1.36
31:12:612:CLA:C3B	33:12:614:LUT:C18	2.18	1.21
31:12:612:CLA:CAB	33:12:614:LUT:C18	2.22	1.17
1:11:210:GLY:O	1:11:214:GLN:HG3	1.44	1.17
31:15:603:CLA:HED1	30:15:608:CHL:C9	1.78	1.13
31:12:612:CLA:CBB	33:12:614:LUT:C18	2.26	1.13
31:15:603:CLA:HED1	30:15:608:CHL:H92	1.38	1.03
31:15:612:CLA:C3B	33:15:614:LUT:H183	1.88	1.03
31:12:612:CLA:CBB	33:12:614:LUT:H181	1.97	0.92
1:14:210:GLY:O	1:14:214:GLN:HG3	1.71	0.90
31:15:603:CLA:HED1	30:15:608:CHL:H91	1.53	0.88
31:12:612:CLA:CHB	33:12:614:LUT:H3	2.04	0.86
1:1:197:GLU:HG3	31:1:610:CLA:NB	1.92	0.84
31:12:612:CLA:C1B	33:12:614:LUT:H42	2.08	0.83
30:4:606:CHL:HBB1	33:4:617:LUT:H161	1.61	0.83
31:12:612:CLA:C4B	33:12:614:LUT:H183	2.09	0.81
31:5:604:CLA:HBD	31:5:604:CLA:HBA1	1.62	0.80
5:16:243:ALA:HB1	31:16:615:CLA:HBB1	1.63	0.80
31:12:612:CLA:C2B	33:12:614:LUT:H183	2.07	0.79
31:12:612:CLA:HBB1	33:12:614:LUT:C18	2.12	0.79
43:H:101:LNL:H16	32:R:619:LHG:H162	1.63	0.79
31:12:612:CLA:NB	33:12:614:LUT:H42	1.98	0.79
31:5:611:CLA:HED3	31:5:611:CLA:H2A	1.64	0.78
31:12:612:CLA:CBB	33:12:614:LUT:H183	1.97	0.78
9:D:186:GLN:HB2	31:D:404:CLA:HBC1	1.64	0.78
9:d:186:GLN:HB2	31:d:404:CLA:HBC1	1.64	0.78
31:4:613:CLA:HBD	31:4:613:CLA:HBA1	1.66	0.77
31:n:615:CLA:HBA1	31:n:615:CLA:HBD	1.65	0.77
3:3:212:MET:HE2	33:3:619:LUT:H10	1.65	0.77
2:n:198:ARG:HB3	31:n:602:CLA:HBC3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:197:GLU:HG3	31:1:610:CLA:C4B	2.16	0.75
2:n:206:GLY:O	2:n:210:GLN:HB3	1.86	0.75
9:D:126:MET:HE2	9:D:150:ILE:HD12	1.70	0.74
28:y:150:THR:HG22	30:y:605:CHL:HAC1	1.68	0.74
1:14:80:VAL:HG21	1:14:172:LEU:HD21	1.70	0.74
3:6:212:MET:HE2	33:6:619:LUT:H10	1.70	0.73
30:N:606:CHL:HBA1	34:N:619:NEX:H403	1.70	0.73
16:L:5:ASN:HD22	16:L:6:PRO:HD2	1.54	0.73
31:N:615:CLA:HBA1	31:N:615:CLA:HBD	1.68	0.73
2:12:206:GLY:O	2:12:210:GLN:HG3	1.88	0.73
21:R:266:ARG:HB3	31:R:602:CLA:HBC2	1.69	0.73
2:5:81:ALA:HB1	2:5:197:GLY:HA3	1.70	0.73
31:14:603:CLA:HED3	33:15:615:LUT:H372	1.71	0.73
21:r:266:ARG:HB3	31:r:602:CLA:HBC2	1.71	0.73
9:d:126:MET:HE2	9:d:150:ILE:HD12	1.71	0.72
30:n:606:CHL:HBA1	34:n:619:NEX:H403	1.70	0.72
31:15:612:CLA:CAB	33:15:614:LUT:H183	2.18	0.72
30:4:608:CHL:H2	33:4:616:LUT:H383	1.70	0.72
28:Y:211:ARG:HB3	31:Y:602:CLA:HBC3	1.72	0.72
16:l:5:ASN:HD22	16:l:6:PRO:HD2	1.54	0.72
2:2:81:ALA:HB1	2:2:197:GLY:HA3	1.72	0.72
28:y:211:ARG:HB3	31:y:602:CLA:HBC3	1.72	0.71
2:15:226:LEU:CD2	31:15:613:CLA:HHC	2.21	0.71
30:g:608:CHL:HBD	30:g:608:CHL:HBA1	1.72	0.71
2:n:36:GLN:HG3	2:n:42:SER:HB2	1.72	0.71
21:R:164:GLY:HA3	21:R:265:ALA:HB1	1.73	0.71
2:12:192:LYS:HD2	31:12:611:CLA:HBD	1.71	0.70
30:6:606:CHL:HBA1	34:6:621:NEX:H403	1.73	0.70
5:13:81:ALA:HB1	5:13:197:GLY:HA3	1.73	0.70
30:G:608:CHL:HBD	30:G:608:CHL:HBA1	1.73	0.70
43:h:101:LNL:H16	32:r:619:LHG:H162	1.73	0.70
8:C:185:ILE:HD12	8:C:230:MET:HE3	1.74	0.70
1:4:126:LEU:HD22	30:4:606:CHL:HMD2	1.74	0.70
2:15:192:LYS:HD2	31:15:611:CLA:HBD	1.73	0.70
1:1:161:GLY:HA2	30:1:608:CHL:HAC1	1.72	0.69
5:16:81:ALA:HB1	5:16:197:GLY:HA3	1.73	0.69
6:A:77:ILE:HD13	16:L:30:VAL:HG13	1.74	0.69
2:15:226:LEU:HD23	31:15:613:CLA:HHC	1.74	0.69
2:n:81:ALA:O	2:n:85:MET:HG3	1.93	0.69
2:5:204:MET:HE2	33:5:615:LUT:H10	1.73	0.69
30:1:608:CHL:H2	33:1:616:LUT:H383	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:36:GLN:HG3	2:N:42:SER:HB2	1.74	0.69
21:r:164:GLY:HA3	21:r:265:ALA:HB1	1.74	0.69
1:4:161:GLY:HA2	30:4:608:CHL:HAC1	1.74	0.69
31:11:602:CLA:H91	31:13:603:CLA:H71	1.74	0.69
2:2:204:MET:HE2	33:2:615:LUT:H10	1.75	0.69
5:13:152:GLU:HG3	30:13:609:CHL:NB	2.08	0.69
32:Y:618:LHG:H351	31:Y:613:CLA:H151	1.75	0.69
10:e:12:ASP:OD1	14:j:9:ARG:NH2	2.26	0.69
1:11:83:ALA:HB1	1:11:201:GLY:HA3	1.73	0.69
2:15:81:ALA:HB1	2:15:197:GLY:HA3	1.75	0.68
8:c:81:MET:HE2	8:c:89:LEU:HB3	1.76	0.68
3:6:94:ALA:HB1	3:6:205:GLY:HA3	1.76	0.68
2:12:144:GLN:NE2	30:12:606:CHL:OMC	2.26	0.68
2:N:198:ARG:HB3	31:N:602:CLA:HBC3	1.75	0.68
10:E:12:ASP:OD1	14:J:9:ARG:NH2	2.26	0.68
32:a:414:LHG:HC41	26:w:426:VAL:HG21	1.76	0.68
30:13:608:CHL:H12	33:13:617:LUT:H383	1.76	0.67
35:3:620:XAT:H22	30:3:607:CHL:HAA2	1.76	0.67
1:4:83:ALA:HB1	1:4:201:GLY:HA3	1.76	0.67
6:a:77:ILE:HD13	16:l:30:VAL:HG13	1.74	0.67
31:c:507:CLA:H71	41:w:501:LMG:H441	1.75	0.67
20:q:85:GLN:NE2	20:q:89:ASP:OD2	2.27	0.67
1:11:184:ALA:HB1	1:11:190:LEU:HD13	1.76	0.67
1:14:83:ALA:HB1	1:14:201:GLY:HA3	1.75	0.67
30:16:608:CHL:H12	33:16:617:LUT:H383	1.75	0.67
30:3:606:CHL:HBA1	34:3:621:NEX:H403	1.75	0.67
9:D:192:THR:HG23	31:D:404:CLA:HBC2	1.77	0.67
8:C:81:MET:HE2	8:C:89:LEU:HB3	1.77	0.67
18:O:147:ASP:OD1	18:O:148:GLN:N	2.28	0.67
20:Q:112:ILE:O	20:Q:116:LEU:HB2	1.94	0.67
7:b:55:MET:HE2	7:b:63:LEU:HD23	1.76	0.67
31:15:603:CLA:CED	30:15:608:CHL:H91	2.23	0.66
31:2:613:CLA:H2A	31:2:613:CLA:HED2	1.77	0.66
32:3:616:LHG:H281	32:3:616:LHG:HC81	1.77	0.66
9:d:192:THR:HG23	31:d:404:CLA:HBC2	1.76	0.66
22:S:193:PRO:HD2	30:S:608:CHL:HBB2	1.76	0.66
32:6:616:LHG:HC81	32:6:616:LHG:H281	1.76	0.66
2:12:192:LYS:HD2	31:12:611:CLA:CBD	2.25	0.66
24:u:348:GLN:O	24:u:352:ASN:ND2	2.29	0.66
2:12:189:LEU:HD13	31:12:609:CLA:H12	1.78	0.66
1:14:155:GLU:OE1	1:14:158:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:81:ALA:HB1	2:N:197:GLY:HA3	1.78	0.66
1:g:83:ALA:HB1	1:g:201:GLY:HA3	1.76	0.66
31:6:615:CLA:HBD	31:6:615:CLA:HBA1	1.78	0.66
31:12:612:CLA:C1B	33:12:614:LUT:C4	2.74	0.66
32:A:413:LHG:HC92	32:L:102:LHG:HC81	1.77	0.65
46:c:518:DGD:HA72	46:c:519:DGD:HB72	1.78	0.65
28:y:91:ALA:HB1	28:y:210:GLY:HA3	1.79	0.65
2:12:81:ALA:HB1	2:12:197:GLY:HA3	1.77	0.65
32:a:413:LHG:HC92	32:l:102:LHG:HC81	1.78	0.65
1:1:196:LYS:HD2	31:1:612:CLA:HBA2	1.78	0.65
35:6:620:XAT:H22	30:6:607:CHL:HAA2	1.79	0.65
2:15:192:LYS:HD2	31:15:611:CLA:CBD	2.26	0.65
5:16:180:ALA:HB1	5:16:186:LEU:HD13	1.78	0.65
22:s:193:PRO:HD2	30:s:608:CHL:HBB2	1.77	0.65
5:16:198:ARG:HB3	31:16:602:CLA:HBC3	1.77	0.65
30:S:606:CHL:H201	34:S:620:NEX:H371	1.79	0.64
30:4:609:CHL:H141	30:4:609:CHL:H193	1.79	0.64
2:12:116:GLN:HB2	2:12:123:LEU:HD12	1.79	0.64
31:5:613:CLA:H2A	31:5:613:CLA:HED2	1.79	0.64
39:B:618:BCR:H391	32:a:401:LHG:H181	1.80	0.64
7:b:269:GLY:O	7:b:448:ARG:NH1	2.29	0.64
20:Q:85:GLN:NE2	20:Q:89:ASP:OD2	2.29	0.64
1:14:184:ALA:HB1	1:14:190:LEU:HD13	1.80	0.64
30:14:601:CHL:HAC1	32:14:615:LHG:HC11	1.79	0.64
28:Y:91:ALA:HB1	28:Y:210:GLY:HA3	1.79	0.64
20:q:112:ILE:O	20:q:116:LEU:HB2	1.97	0.64
1:1:174:PRO:HB3	30:1:608:CHL:HBC2	1.79	0.64
31:12:612:CLA:CAB	33:12:614:LUT:H181	2.17	0.64
30:13:607:CHL:HBB1	33:13:618:LUT:H171	1.80	0.64
46:W:501:DGD:HB21	31:Y:611:CLA:H11	1.80	0.64
6:a:29:TYR:O	6:a:129:ARG:NH1	2.30	0.64
46:C:518:DGD:HA72	46:C:519:DGD:HB72	1.80	0.63
1:G:83:ALA:HB1	1:G:201:GLY:HA3	1.79	0.63
30:n:605:CHL:H91	33:s:618:LUT:H172	1.81	0.63
1:1:83:ALA:HB1	1:1:201:GLY:HA3	1.80	0.63
2:12:147:LEU:O	2:12:151:ILE:HG12	1.99	0.63
3:3:148:THR:HG22	30:3:605:CHL:HAC1	1.81	0.63
22:s:112:ALA:HB1	22:s:243:GLY:HA3	1.81	0.63
2:15:63:LEU:HB3	31:15:602:CLA:H11	1.81	0.63
31:s:604:CLA:H51	30:s:606:CHL:HBA1	1.80	0.63
2:12:138:VAL:O	2:12:142:LEU:HG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:J:101:BCR:H403	39:J:101:BCR:H23C	1.81	0.62
39:j:101:BCR:H403	39:j:101:BCR:H23C	1.82	0.62
31:y:613:CLA:H72	32:y:616:LHG:H182	1.80	0.62
2:2:81:ALA:O	2:2:85:MET:HG3	1.99	0.62
31:15:603:CLA:CED	30:15:608:CHL:C9	2.65	0.62
1:11:213:VAL:HG21	31:11:613:CLA:HAC2	1.81	0.62
31:B:608:CLA:HBA1	31:B:608:CLA:HBD	1.82	0.62
2:15:34:ARG:HH22	2:15:50:GLY:HA2	1.65	0.62
43:H:101:LNL:H15	32:R:619:LHG:H141	1.82	0.62
6:A:131:TRP:HZ2	8:C:449:ARG:HG2	1.65	0.62
7:b:391:SER:HB3	7:b:394:GLN:HG3	1.82	0.62
19:p:553:PHE:O	19:p:557:ASN:ND2	2.32	0.62
5:13:64:SER:OG	31:13:602:CLA:O1A	2.16	0.62
2:15:147:LEU:O	2:15:151:ILE:HG12	1.99	0.62
2:15:191:VAL:O	2:15:195:LYS:HG2	2.00	0.62
1:G:142:ALA:O	1:G:146:THR:HG23	2.00	0.62
31:b:608:CLA:HBA1	31:b:608:CLA:HBD	1.82	0.62
9:d:172:SER:HB2	9:d:177:ALA:HB1	1.81	0.62
18:o:147:ASP:OD1	18:o:148:GLN:N	2.33	0.62
5:16:204:MET:HA	5:16:204:MET:HE2	1.81	0.61
31:16:602:CLA:H52	33:16:618:LUT:H28	1.81	0.61
32:A:415:LHG:H181	39:b:618:BCR:H391	1.81	0.61
30:3:605:CHL:HHC	30:3:605:CHL:HBB1	1.83	0.61
2:5:155:ARG:NH2	30:5:609:CHL:O1D	2.31	0.61
2:2:89:LEU:O	2:2:93:THR:HG23	1.99	0.61
32:6:617:LHG:H301	34:6:621:NEX:H402	1.82	0.61
31:11:613:CLA:H11	35:11:619:XAT:H203	1.81	0.61
28:Y:193:ALA:HB1	28:Y:199:LEU:HD13	1.82	0.61
31:12:612:CLA:CHB	33:12:614:LUT:C3	2.76	0.61
1:g:142:ALA:O	1:g:146:THR:HG23	2.01	0.61
30:6:607:CHL:H141	30:6:609:CHL:H112	1.83	0.61
6:a:131:TRP:HZ2	8:c:449:ARG:HG2	1.65	0.61
2:12:191:VAL:O	2:12:195:LYS:HG2	2.00	0.61
2:15:111:PHE:CG	31:16:615:CLA:HBB2	2.35	0.61
6:A:29:TYR:O	6:A:129:ARG:NH1	2.32	0.61
8:c:215:ARG:HG2	8:c:221:ASP:HB3	1.82	0.61
3:3:94:ALA:HB1	3:3:205:GLY:HA3	1.83	0.60
30:15:607:CHL:H12	33:15:614:LUT:H383	1.82	0.60
31:12:603:CLA:H12	5:13:63:LEU:HD11	1.82	0.60
22:s:91:PRO:HD2	33:s:619:LUT:H23	1.83	0.60
27:x:88:ALA:O	27:x:92:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:y:46:LEU:HB2	28:y:50:SER:HB3	1.82	0.60
28:y:193:ALA:HB1	28:y:199:LEU:HD13	1.81	0.60
10:E:68:ASP:OD2	10:E:71:ASN:ND2	2.34	0.60
18:O:105:ASP:N	18:O:105:ASP:OD1	2.34	0.60
31:g:604:CLA:HMB2	30:g:606:CHL:HBB1	1.81	0.60
31:6:613:CLA:HBD	31:6:613:CLA:HAA1	1.82	0.60
2:15:199:LEU:HB3	33:15:614:LUT:H202	1.83	0.60
31:n:604:CLA:HMB1	30:n:606:CHL:HBB1	1.82	0.60
2:2:157:ASN:OD1	3:3:55:ASN:ND2	2.34	0.60
31:2:604:CLA:HBD	31:2:604:CLA:HBA1	1.83	0.60
1:14:193:LEU:HB3	31:14:610:CLA:H3A	1.83	0.60
7:B:391:SER:HB3	7:B:394:GLN:HG3	1.82	0.60
38:D:402:PHO:HBA2	31:D:404:CLA:H142	1.83	0.60
1:4:128:TYR:HB3	1:4:134:LEU:HD12	1.82	0.60
31:3:614:CLA:HBD	31:3:614:CLA:HBA1	1.84	0.60
30:12:607:CHL:H12	33:12:614:LUT:H383	1.84	0.60
5:13:180:ALA:HB1	5:13:186:LEU:HD13	1.82	0.60
22:S:126:GLU:HA	22:S:138:ALA:HB1	1.84	0.60
46:w:502:DGD:HB21	31:y:611:CLA:H11	1.83	0.60
8:C:215:ARG:HG2	8:C:221:ASP:HB3	1.83	0.60
19:P:553:PHE:O	19:P:557:ASN:ND2	2.32	0.60
1:11:80:VAL:HG21	1:11:172:LEU:HD21	1.83	0.59
4:8:51:ASN:ND2	15:k:42:ARG:OXT	2.35	0.59
1:11:131:ASN:HB2	1:11:134:LEU:HD23	1.84	0.59
31:12:612:CLA:C4B	33:12:614:LUT:H42	2.31	0.59
2:15:182:ASP:OD2	2:15:182:ASP:N	2.34	0.59
30:Y:606:CHL:H151	34:Y:623:NEX:H8	1.84	0.59
5:13:76:LEU:HD22	31:13:603:CLA:HAA2	1.84	0.59
8:c:179:ALA:HA	8:c:184:GLY:HA2	1.85	0.59
18:o:281:LEU:HD23	18:o:291:PRO:HB2	1.83	0.59
34:3:621:NEX:O3	21:R:69:ARG:O	2.21	0.59
30:R:606:CHL:H102	32:R:619:LHG:H342	1.83	0.59
30:n:608:CHL:H12	33:n:617:LUT:H383	1.84	0.59
22:s:61:ARG:O	22:s:72:ARG:NH2	2.32	0.59
32:L:102:LHG:O3	32:L:102:LHG:O1	2.19	0.59
30:1:606:CHL:HBA2	30:1:606:CHL:HBD	1.83	0.59
3:6:148:THR:HG22	30:6:605:CHL:HAC1	1.83	0.59
31:12:612:CLA:HMB3	33:12:614:LUT:H162	1.83	0.59
30:G:608:CHL:H12	33:G:616:LUT:H383	1.85	0.59
7:B:207:ILE:HD13	30:R:606:CHL:H11	1.85	0.59
7:B:235:GLU:HB3	7:B:473:THR:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:D:414:LMG:O10	12:H:63:ASN:ND2	2.36	0.59
22:S:112:ALA:HB1	22:S:243:GLY:HA3	1.84	0.59
41:d:415:LMG:O10	12:h:63:ASN:ND2	2.36	0.59
31:12:612:CLA:HHB	33:12:614:LUT:H3	1.83	0.59
7:B:24:LEU:HD21	31:B:616:CLA:HBB1	1.85	0.59
32:d:408:LHG:H321	23:t:21:ILE:HD11	1.85	0.59
9:D:279:LEU:HD22	38:D:402:PHO:HBC3	1.85	0.59
30:n:607:CHL:H71	32:y:616:LHG:H202	1.85	0.59
30:2:608:CHL:HHC	30:2:608:CHL:HBB1	1.85	0.59
1:11:145:LEU:O	1:11:149:VAL:HG23	2.02	0.59
15:K:40:SER:O	15:K:40:SER:OG	2.21	0.59
2:5:34:ARG:HE	2:5:50:GLY:HA3	1.68	0.58
2:5:81:ALA:O	2:5:85:MET:HG3	2.03	0.58
2:15:138:VAL:O	2:15:142:LEU:HG	2.03	0.58
21:R:155:ARG:NH2	31:R:603:CLA:O1A	2.36	0.58
4:7:51:ASN:ND2	15:K:42:ARG:OXT	2.35	0.58
27:X:88:ALA:O	27:X:92:VAL:HG23	2.04	0.58
7:b:79:THR:HG22	7:b:81:SER:H	1.69	0.58
22:s:126:GLU:HA	22:s:138:ALA:HB1	1.85	0.58
1:11:193:LEU:HB3	31:11:610:CLA:H3A	1.84	0.58
32:y:618:LHG:H351	31:y:613:CLA:H151	1.85	0.58
1:14:147:GLN:O	1:14:151:MET:HG2	2.03	0.58
8:C:200:THR:O	41:C:522:LMG:O3	2.22	0.58
2:2:75:GLU:HA	2:2:168:LEU:HD21	1.85	0.58
1:4:83:ALA:HB2	1:4:205:MET:HE2	1.85	0.58
3:6:133:TYR:HH	34:6:621:NEX:H1	1.44	0.58
18:o:161:VAL:HG23	18:o:202:LEU:HD21	1.85	0.58
4:7:43:ILE:HD12	4:7:49:LYS:HG3	1.84	0.58
8:c:329:ALA:HB2	8:c:377:LEU:HD11	1.86	0.58
32:l:102:LHG:O3	32:l:102:LHG:O1	2.19	0.58
2:2:155:ARG:NH2	30:2:609:CHL:O1D	2.37	0.58
1:g:193:LEU:HD22	31:g:610:CLA:H11	1.85	0.58
1:11:179:ASP:OD1	33:11:616:LUT:O23	2.20	0.58
22:S:91:PRO:HD2	33:S:619:LUT:H23	1.86	0.58
22:S:208:TYR:CD1	30:S:608:CHL:HMC	2.38	0.58
30:6:605:CHL:HHC	30:6:605:CHL:HBB1	1.85	0.58
31:12:604:CLA:HMA2	30:12:605:CHL:HBC3	1.85	0.58
31:14:602:CLA:H71	31:14:603:CLA:H3A	1.86	0.58
21:r:157:ARG:NH1	21:r:160:GLU:OE1	2.37	0.58
31:14:602:CLA:H91	31:16:603:CLA:H71	1.85	0.58
10:E:26:THR:HB	49:F:101:HEM:HAB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:202:VAL:HG11	32:N:616:LHG:H302	1.85	0.58
31:11:610:CLA:H62	33:11:616:LUT:H30	1.85	0.57
6:A:133:LEU:HD23	9:D:256:ILE:HG12	1.86	0.57
38:a:406:PHO:HBC3	9:d:279:LEU:HD22	1.85	0.57
7:b:186:ASP:OD1	7:b:186:ASP:N	2.34	0.57
2:n:81:ALA:HB1	2:n:197:GLY:HA3	1.86	0.57
21:r:155:ARG:NH2	31:r:603:CLA:O1A	2.36	0.57
2:5:95:GLU:HA	2:5:108:ALA:HB1	1.86	0.57
36:B:620:3PH:H2E2	40:L:101:SQD:H332	1.86	0.57
9:D:172:SER:HB2	9:D:177:ALA:HB1	1.87	0.57
30:11:607:CHL:HBB1	33:11:617:LUT:H171	1.86	0.57
2:15:144:GLN:NE2	30:15:606:CHL:OMC	2.37	0.57
31:s:604:CLA:HBA1	31:s:604:CLA:HBD	1.87	0.57
6:a:133:LEU:HD23	9:d:256:ILE:HG12	1.86	0.57
8:c:200:THR:O	41:c:522:LMG:O3	2.21	0.57
22:s:208:TYR:CD1	30:s:608:CHL:HMC	2.40	0.57
31:s:604:CLA:H193	31:s:615:CLA:H3A	1.87	0.57
2:2:175:ASP:OD1	33:2:614:LUT:O23	2.21	0.57
2:2:209:VAL:HG11	31:2:613:CLA:HAC2	1.87	0.57
31:12:612:CLA:C2B	33:12:614:LUT:C5	2.82	0.57
7:b:24:LEU:HD21	31:b:616:CLA:HBB1	1.85	0.57
1:g:87:MET:SD	31:g:610:CLA:HBB1	2.45	0.57
18:o:127:MET:HG3	18:o:128:PRO:HD2	1.85	0.57
31:N:604:CLA:HMB1	30:N:606:CHL:HBB1	1.86	0.57
15:k:19:ASP:OD2	25:v:8:GLN:NE2	2.38	0.57
1:1:179:ASP:OD1	33:1:616:LUT:O23	2.19	0.57
34:6:621:NEX:O3	21:r:69:ARG:O	2.21	0.57
7:B:79:THR:HG22	7:B:81:SER:H	1.69	0.57
9:D:296:TYR:OH	9:D:326:ARG:NH1	2.30	0.57
8:c:464:GLU:OE2	9:d:245:SER:OG	2.23	0.57
1:4:146:THR:O	1:4:150:ILE:HG22	2.05	0.57
31:14:603:CLA:HED3	33:15:615:LUT:C37	2.34	0.57
31:A:404:CLA:H142	32:A:411:LHG:H151	1.87	0.57
21:R:157:ARG:NH1	21:R:160:GLU:OE1	2.37	0.57
10:e:26:THR:HB	49:f:101:HEM:HAB	1.85	0.57
24:u:339:VAL:O	24:u:343:ILE:HG22	2.05	0.57
31:C:507:CLA:H41	46:W:501:DGD:HA51	1.86	0.56
1:11:70:GLU:OE2	1:11:70:GLU:N	2.35	0.56
5:16:121:GLY:O	5:16:135:GLN:NE2	2.39	0.56
31:b:615:CLA:H143	31:b:616:CLA:HMA3	1.86	0.56
30:g:608:CHL:H12	33:g:616:LUT:H383	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:r:610:CLA:HBC3	32:r:618:LHG:H242	1.87	0.56
5:13:121:GLY:O	5:13:135:GLN:NE2	2.38	0.56
31:C:511:CLA:H203	41:K:102:LMG:H392	1.86	0.56
32:D:408:LHG:H321	23:T:21:ILE:HD11	1.88	0.56
1:G:193:LEU:HD22	31:G:610:CLA:H11	1.87	0.56
8:C:179:ALA:HA	8:C:184:GLY:HA2	1.88	0.56
32:D:408:LHG:H302	23:T:21:ILE:HD11	1.86	0.56
40:d:414:SQD:H272	27:x:92:VAL:HG22	1.87	0.56
24:u:343:ILE:HG13	24:u:343:ILE:O	2.05	0.56
2:5:75:GLU:HG2	2:5:168:LEU:HD21	1.87	0.56
5:13:198:ARG:HB3	31:13:602:CLA:HBC3	1.87	0.56
1:14:68:ASP:O	1:14:71:THR:OG1	2.20	0.56
15:K:19:ASP:OD2	25:V:8:GLN:NE2	2.38	0.56
31:6:610:CLA:H12	33:6:618:LUT:H26	1.87	0.56
5:13:135:GLN:HG3	30:13:605:CHL:HAB	1.87	0.56
38:D:402:PHO:H52	31:D:404:CLA:H13	1.88	0.56
20:q:165:PHE:O	20:q:169:VAL:HG23	2.05	0.56
21:R:117:ASP:O	21:R:123:ASN:ND2	2.36	0.56
21:r:117:ASP:O	21:r:123:ASN:ND2	2.35	0.56
22:s:289:ARG:NH1	32:s:621:LHG:O5	2.38	0.56
30:3:605:CHL:H52	31:R:612:CLA:H12	1.87	0.56
5:13:198:ARG:HA	5:13:201:MET:HE3	1.87	0.56
20:Q:165:PHE:O	20:Q:169:VAL:HG23	2.05	0.56
1:1:65:LEU:HD13	31:1:602:CLA:H42	1.88	0.56
1:11:147:GLN:O	1:11:151:MET:HG2	2.05	0.56
2:12:45:PRO:HG2	2:12:48:LEU:HD12	1.88	0.56
1:14:196:LYS:NZ	31:14:612:CLA:HED3	2.20	0.56
30:Y:606:CHL:H52	43:Y:619:LNL:H16	1.88	0.56
6:a:244:GLU:OE2	9:d:264:LYS:NZ	2.37	0.56
31:2:613:CLA:HBA1	31:2:613:CLA:HBD	1.87	0.55
1:14:142:ALA:O	1:14:146:THR:HG23	2.05	0.55
31:14:610:CLA:H52	33:14:616:LUT:H30	1.87	0.55
31:C:512:CLA:H202	39:C:526:BCR:H17C	1.87	0.55
18:O:281:LEU:HD23	18:O:291:PRO:HB2	1.88	0.55
22:S:253:PHE:HE1	33:S:618:LUT:H41	1.71	0.55
7:b:155:ALA:O	7:b:159:THR:OG1	2.24	0.55
1:1:212:PHE:O	1:1:216:LEU:HD12	2.06	0.55
5:13:76:LEU:CD2	31:13:603:CLA:HAA2	2.37	0.55
8:C:406:SER:O	8:C:418:ASN:ND2	2.39	0.55
10:e:68:ASP:OD2	10:e:71:ASN:ND2	2.36	0.55
32:r:621:LHG:H112	32:r:621:LHG:H241	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:12:604:CLA:H42	34:12:616:NEX:H373	1.88	0.55
21:R:253:ARG:HG3	21:R:253:ARG:HH11	1.71	0.55
1:1:128:TYR:HB3	1:1:134:LEU:HD12	1.88	0.55
31:12:612:CLA:C1B	33:12:614:LUT:H3	2.37	0.55
31:14:613:CLA:H11	35:14:619:XAT:H203	1.87	0.55
6:A:301:ASN:OD1	6:A:303:ASN:ND2	2.40	0.55
32:y:616:LHG:O3	32:y:616:LHG:O1	2.20	0.55
31:11:604:CLA:HBD	31:11:604:CLA:HBA2	1.89	0.55
5:13:233:ASN:ND2	31:13:614:CLA:O2D	2.40	0.55
31:B:614:CLA:H8	39:B:617:BCR:H362	1.89	0.55
1:14:179:ASP:OD1	33:14:616:LUT:O23	2.23	0.55
6:A:188:ALA:HB2	6:A:328:MET:HG3	1.88	0.55
39:C:526:BCR:H391	15:K:32:ALA:HB2	1.89	0.55
1:G:180:PRO:HD2	33:G:616:LUT:H23	1.88	0.55
18:O:192:ASN:HB2	18:O:207:THR:HG22	1.89	0.55
31:b:607:CLA:H193	16:l:29:ALA:HA	1.88	0.55
31:3:613:CLA:HAA1	31:3:613:CLA:HBD	1.88	0.55
1:4:49:TYR:OH	1:4:61:ASP:OD2	2.23	0.55
1:4:212:PHE:O	1:4:216:LEU:HD12	2.07	0.55
31:5:613:CLA:HBA1	31:5:613:CLA:HBD	1.88	0.55
18:O:284:ASP:OD1	18:O:284:ASP:N	2.40	0.55
32:r:621:LHG:HC91	32:r:621:LHG:HC62	1.89	0.55
31:15:603:CLA:CED	30:15:608:CHL:H92	2.26	0.55
30:15:605:CHL:HBA1	34:15:616:NEX:H403	1.89	0.55
18:o:192:ASN:HB2	18:o:207:THR:HG22	1.89	0.55
22:s:180:MET:HA	22:s:180:MET:HE3	1.89	0.55
2:2:222:LEU:HB2	33:2:614:LUT:H22	1.89	0.55
30:13:606:CHL:H92	30:13:606:CHL:H41	1.89	0.55
6:A:192:ILE:HG13	6:A:293:MET:HE1	1.88	0.55
7:B:155:ALA:O	7:B:159:THR:OG1	2.25	0.55
22:S:221:ASP:OD1	33:S:618:LUT:O23	2.25	0.55
36:T:101:3PH:H332	39:b:617:BCR:H383	1.89	0.55
8:c:137:PRO:HD3	31:c:514:CLA:HED1	1.89	0.55
31:n:613:CLA:HBD	31:n:613:CLA:HBA1	1.88	0.55
20:q:98:LEU:HD11	20:q:149:THR:HG21	1.89	0.55
1:14:131:ASN:HB2	1:14:134:LEU:HD23	1.89	0.55
2:15:204:MET:HA	2:15:204:MET:HE2	1.89	0.55
8:c:403:SER:OG	8:c:405:ASN:OD1	2.25	0.55
39:c:526:BCR:H391	15:k:32:ALA:HB2	1.89	0.55
1:g:186:ASP:HB2	1:g:189:THR:HG23	1.90	0.55
20:Q:98:LEU:HD11	20:Q:149:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:301:ASN:OD1	6:a:303:ASN:ND2	2.40	0.54
31:c:512:CLA:HAA1	31:c:512:CLA:HBD	1.88	0.54
31:r:601:CLA:HBD	32:r:618:LHG:HC42	1.89	0.54
30:s:606:CHL:H143	30:s:608:CHL:HBA1	1.89	0.54
30:5:607:CHL:HHC	30:5:607:CHL:HBB1	1.88	0.54
22:S:94:LEU:HD13	31:S:602:CLA:H42	1.88	0.54
1:g:180:PRO:HD2	33:g:616:LUT:H23	1.88	0.54
1:1:107:PHE:HB3	1:1:110:ALA:HB3	1.90	0.54
1:G:186:ASP:HB2	1:G:189:THR:HG23	1.89	0.54
31:b:614:CLA:H8	39:b:617:BCR:H362	1.88	0.54
1:g:214:GLN:HE21	1:g:225:ASN:HD22	1.55	0.54
2:12:222:LEU:HA	31:12:612:CLA:HMA2	1.89	0.54
7:B:174:ILE:HD11	7:B:309:LEU:HD13	1.89	0.54
31:Y:613:CLA:HBA1	31:Y:613:CLA:HBD	1.89	0.54
32:c:521:LHG:H272	32:s:617:LHG:H371	1.88	0.54
18:o:171:PHE:HB2	18:o:187:MET:HE3	1.89	0.54
1:11:155:GLU:OE1	1:11:158:ARG:NH2	2.39	0.54
22:S:211:MET:HE3	22:S:216:PRO:HB3	1.89	0.54
6:a:192:ILE:HG13	6:a:293:MET:HE1	1.89	0.54
21:r:253:ARG:HG3	21:r:253:ARG:HH11	1.71	0.54
28:y:95:MET:SD	31:y:610:CLA:HBB1	2.47	0.54
30:5:608:CHL:HHC	30:5:608:CHL:HBB1	1.89	0.54
21:R:74:ASP:OD1	21:R:74:ASP:N	2.41	0.54
31:Y:614:CLA:HBC1	33:Y:621:LUT:H162	1.89	0.54
8:c:368:PRO:HG3	20:q:133:ARG:HG3	1.88	0.54
1:g:179:ASP:OD1	33:g:616:LUT:O23	2.25	0.54
2:n:228:ALA:O	2:n:232:THR:OG1	2.26	0.54
32:C:521:LHG:H311	32:S:617:LHG:H101	1.90	0.54
6:a:303:ASN:O	8:c:415:ASN:ND2	2.41	0.54
8:c:77:PRO:HG3	22:s:293:LEU:HD22	1.89	0.54
31:N:611:CLA:HBC3	32:N:616:LHG:HC62	1.89	0.54
30:N:607:CHL:H191	31:Y:602:CLA:H191	1.90	0.54
31:S:615:CLA:HAA1	31:S:615:CLA:HBD	1.90	0.54
1:g:174:PRO:HB3	30:g:608:CHL:HBC2	1.89	0.54
4:8:112:LYS:H	4:8:112:LYS:HD3	1.73	0.54
31:c:505:CLA:H42	46:c:518:DGD:HB32	1.90	0.54
31:s:611:CLA:HBD	31:s:612:CLA:OBD	2.08	0.54
2:N:225:HIS:CG	31:N:613:CLA:HAA2	2.43	0.54
31:c:512:CLA:H202	39:c:526:BCR:H17C	1.88	0.54
9:D:56:THR:HG21	10:E:50:PRO:HD3	1.89	0.53
6:A:303:ASN:O	8:C:415:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:172:GLU:OE1	22:S:39:ARG:NH1	2.39	0.53
2:N:228:ALA:O	2:N:232:THR:OG1	2.26	0.53
2:2:184:ASP:N	2:2:184:ASP:OD1	2.41	0.53
31:12:609:CLA:H8	33:12:614:LUT:C30	2.38	0.53
2:15:45:PRO:HG2	2:15:48:LEU:HD12	1.90	0.53
32:Y:616:LHG:O3	32:Y:616:LHG:O1	2.20	0.53
31:G:604:CLA:HMB2	30:G:606:CHL:HBB1	1.89	0.53
28:Y:95:MET:SD	31:Y:610:CLA:HBB1	2.48	0.53
1:g:199:LYS:NZ	32:g:615:LHG:O5	2.41	0.53
30:6:608:CHL:HBA1	32:6:617:LHG:H341	1.90	0.53
31:11:612:CLA:HBB1	33:11:616:LUT:C14	2.38	0.53
1:14:95:THR:HG21	31:14:604:CLA:HBC3	1.90	0.53
5:16:207:PHE:CE1	5:16:218:PRO:HB3	2.44	0.53
35:G:619:XAT:H41	30:Y:607:CHL:HAA2	1.91	0.53
31:b:610:CLA:H142	31:b:612:CLA:H52	1.91	0.53
21:r:155:ARG:NH1	31:r:613:CLA:OBD	2.41	0.53
26:w:432:ASP:OD2	26:w:439:ASN:ND2	2.42	0.53
5:16:72:ARG:NH1	5:16:75:GLU:OE1	2.41	0.53
6:A:40:THR:HG23	31:A:406:CLA:HBB1	1.91	0.53
7:B:423:ARG:NH2	7:B:430:PHE:O	2.42	0.53
22:S:90:ASP:OD1	33:S:619:LUT:O23	2.26	0.53
4:7:112:LYS:H	4:7:112:LYS:HD3	1.74	0.53
32:A:414:LHG:O9	32:A:414:LHG:O1	2.24	0.53
2:N:81:ALA:O	2:N:85:MET:HG3	2.08	0.53
31:4:604:CLA:HBA1	31:4:604:CLA:HBD	1.91	0.53
1:14:78:ILE:HG21	31:14:603:CLA:HAA2	1.91	0.53
22:S:268:TRP:HB2	33:S:618:LUT:H22	1.90	0.53
32:r:621:LHG:H292	31:r:602:CLA:H193	1.90	0.53
32:r:619:LHG:HC82	32:r:619:LHG:H261	1.91	0.53
31:y:614:CLA:HBC1	33:y:622:LUT:H162	1.91	0.53
32:A:414:LHG:HC62	26:W:426:VAL:HG21	1.89	0.53
31:R:601:CLA:HBD	32:R:618:LHG:HC42	1.92	0.53
31:r:610:CLA:HBC3	32:r:618:LHG:HC62	1.91	0.53
28:y:99:LEU:HD13	31:y:612:CLA:HBB2	1.90	0.53
2:12:143:THR:O	2:12:147:LEU:HD23	2.09	0.52
2:12:213:ILE:HG23	2:12:214:THR:HG23	1.92	0.52
1:14:214:GLN:O	1:14:218:THR:HB	2.09	0.52
8:C:393:ALA:HB1	20:Q:79:ARG:HG3	1.91	0.52
8:c:376:ASP:HB3	8:c:379:LYS:HB2	1.91	0.52
32:d:408:LHG:H302	23:t:21:ILE:HD11	1.90	0.52
11:f:11:ILE:HD13	24:u:343:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:12:193:GLU:HB2	31:12:609:CLA:C2B	2.40	0.52
7:B:166:ILE:HD11	7:B:195:PRO:HB3	1.92	0.52
8:C:250:TRP:O	8:C:254:THR:OG1	2.25	0.52
8:C:403:SER:OG	8:C:405:ASN:OD1	2.25	0.52
20:Q:133:ARG:NH2	20:Q:173:ASP:OD2	2.42	0.52
9:d:197:HIS:O	9:d:201:VAL:HG12	2.08	0.52
1:4:196:LYS:O	1:4:200:ASN:ND2	2.43	0.52
31:C:512:CLA:HAA1	31:C:512:CLA:HBD	1.90	0.52
31:S:611:CLA:HBD	31:S:612:CLA:OBD	2.09	0.52
28:Y:99:LEU:HD13	31:Y:612:CLA:HBB2	1.90	0.52
30:y:607:CHL:H91	30:y:609:CHL:H172	1.90	0.52
5:16:36:PHE:CG	5:16:58:TRP:HB2	2.44	0.52
7:B:186:ASP:OD1	7:B:186:ASP:N	2.34	0.52
7:b:423:ARG:NH2	7:b:430:PHE:O	2.42	0.52
2:5:195:LYS:NZ	31:5:611:CLA:O1D	2.32	0.52
30:12:605:CHL:HBA1	34:12:616:NEX:H403	1.91	0.52
2:15:197:GLY:O	2:15:201:MET:HG3	2.10	0.52
31:R:608:CLA:H43	31:R:613:CLA:H51	1.91	0.52
22:S:97:ASP:OD1	22:S:97:ASP:N	2.43	0.52
18:o:284:ASP:OD1	18:o:284:ASP:N	2.40	0.52
2:12:189:LEU:CD1	31:12:609:CLA:H12	2.39	0.52
32:13:616:LHG:O1	32:13:616:LHG:O3	2.28	0.52
31:B:610:CLA:H142	31:B:612:CLA:H52	1.91	0.52
46:C:518:DGD:HA41	41:K:102:LMG:H342	1.90	0.52
22:S:43:TRP:HZ2	41:S:616:LMG:HC71	1.74	0.52
28:Y:152:VAL:HG22	43:Y:620:LNL:H16	1.92	0.52
7:b:258:TYR:OH	9:d:162:LEU:O	2.23	0.52
31:c:502:CLA:C3D	31:c:504:CLA:H2	2.40	0.52
32:3:617:LHG:H301	34:3:621:NEX:H402	1.90	0.52
31:4:610:CLA:H12	33:4:616:LUT:H26	1.91	0.52
1:14:34:ARG:NH2	1:14:57:ASP:OD1	2.39	0.52
1:14:70:GLU:OE1	1:14:70:GLU:N	2.42	0.52
31:11:602:CLA:H71	31:11:603:CLA:H3A	1.91	0.52
31:R:603:CLA:HMC3	31:R:608:CLA:H172	1.92	0.52
21:r:74:ASP:OD1	21:r:74:ASP:N	2.40	0.52
31:s:614:CLA:HBC1	33:s:618:LUT:H162	1.92	0.52
4:7:56:SER:HB2	8:C:29:GLU:HG2	1.92	0.52
30:Y:607:CHL:H91	30:Y:609:CHL:H172	1.91	0.52
7:b:326:ARG:HB3	7:b:444:ARG:HD3	1.91	0.52
2:n:235:TRP:O	2:n:239:ALA:HB3	2.10	0.52
43:H:101:LNL:H71	32:R:621:LHG:HC81	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:g:619:XAT:H41	30:y:607:CHL:HAA2	1.91	0.52
2:n:75:GLU:HA	2:n:168:LEU:HD11	1.92	0.52
8:c:393:ALA:HB1	20:q:79:ARG:HG3	1.91	0.51
18:o:254:THR:HG22	18:o:255:VAL:H	1.76	0.51
20:q:133:ARG:NH2	20:q:173:ASP:OD2	2.42	0.51
2:12:199:LEU:HB3	33:12:614:LUT:H202	1.91	0.51
5:13:152:GLU:HG3	30:13:609:CHL:C1B	2.39	0.51
31:13:615:CLA:H2A	31:13:615:CLA:HED2	1.91	0.51
39:D:406:BCR:H393	41:D:410:LMG:H161	1.92	0.51
18:O:254:THR:HG22	18:O:255:VAL:H	1.76	0.51
7:b:207:ILE:HD13	30:r:606:CHL:H11	1.90	0.51
31:12:612:CLA:C1B	33:12:614:LUT:C3	2.88	0.51
5:13:72:ARG:NH1	5:13:75:GLU:OE1	2.43	0.51
2:15:192:LYS:HZ2	31:15:611:CLA:HED2	1.75	0.51
32:a:413:LHG:O4	9:d:141:TYR:OH	2.21	0.51
8:c:318:LEU:HD12	8:c:340:TYR:HB3	1.92	0.51
32:c:521:LHG:H312	32:s:617:LHG:H111	1.91	0.51
2:2:95:GLU:HA	2:2:108:ALA:HB1	1.92	0.51
30:14:606:CHL:HBB2	30:14:607:CHL:HBB1	1.93	0.51
31:15:612:CLA:CBB	33:15:614:LUT:H183	2.39	0.51
31:c:514:CLA:H203	32:s:621:LHG:H382	1.92	0.51
9:d:56:THR:HG21	10:e:50:PRO:HD3	1.90	0.51
30:s:608:CHL:H12	33:s:618:LUT:H383	1.91	0.51
6:A:233:ALA:O	6:A:236:GLY:N	2.43	0.51
30:N:608:CHL:H12	33:N:617:LUT:H383	1.92	0.51
31:n:614:CLA:HBA1	31:n:614:CLA:HBD	1.93	0.51
2:15:198:ARG:HB3	31:15:602:CLA:HBC3	1.92	0.51
8:C:376:ASP:HB3	8:C:379:LYS:HB2	1.93	0.51
40:D:411:SQD:O49	40:D:411:SQD:O2	2.28	0.51
41:j:102:LMG:H361	41:v:101:LMG:H232	1.92	0.51
4:7:68:GLN:NE2	8:C:456:GLU:OE2	2.44	0.51
2:12:63:LEU:HD23	31:12:602:CLA:H42	1.92	0.51
30:14:601:CHL:HED2	32:14:615:LHG:H142	1.92	0.51
31:C:502:CLA:C3D	31:C:504:CLA:H2	2.39	0.51
31:C:514:CLA:H61	32:C:521:LHG:H262	1.93	0.51
2:n:172:GLU:OE1	22:s:39:ARG:NH1	2.40	0.51
30:1:601:CHL:H141	35:3:620:XAT:H161	1.92	0.51
2:5:189:LEU:HD22	31:5:610:CLA:H11	1.92	0.51
2:12:197:GLY:O	2:12:201:MET:HG3	2.10	0.51
5:16:235:TYR:HA	5:16:239:ALA:HB2	1.93	0.51
5:16:235:TYR:HD2	31:16:614:CLA:HED3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:176:ILE:HD13	31:A:403:CLA:HED3	1.93	0.51
31:G:613:CLA:HBD	31:G:613:CLA:HAA1	1.93	0.51
21:R:155:ARG:NH1	31:R:613:CLA:OBD	2.42	0.51
31:r:602:CLA:H202	31:r:603:CLA:H151	1.93	0.51
2:n:210:GLN:O	2:n:214:THR:OG1	2.25	0.51
1:11:196:LYS:HD3	31:11:612:CLA:HBA2	1.93	0.51
5:16:235:TYR:CD2	31:16:614:CLA:HED3	2.46	0.51
8:C:318:LEU:HD12	8:C:340:TYR:HB3	1.92	0.51
8:C:464:GLU:OE2	9:D:245:SER:OG	2.24	0.51
43:H:101:LNL:H9	39:H:103:BCR:H402	1.92	0.51
32:R:621:LHG:H241	32:R:621:LHG:H112	1.93	0.51
18:o:195:ILE:HG22	18:o:204:GLY:HA3	1.93	0.51
30:6:605:CHL:H191	31:r:602:CLA:H141	1.93	0.50
2:15:192:LYS:NZ	31:15:611:CLA:HED2	2.26	0.50
6:A:96:ILE:HD11	6:A:102:LEU:HD21	1.92	0.50
8:C:368:PRO:HG3	20:Q:133:ARG:HG3	1.91	0.50
31:C:502:CLA:HBC1	31:C:513:CLA:H43	1.92	0.50
2:N:75:GLU:HA	2:N:168:LEU:HD11	1.93	0.50
28:Y:46:LEU:HB2	28:Y:50:SER:HB3	1.93	0.50
31:y:613:CLA:HBA1	31:y:613:CLA:HBD	1.92	0.50
1:4:179:ASP:OD1	33:4:616:LUT:O23	2.18	0.50
4:7:49:LYS:O	4:7:53:MET:HG3	2.11	0.50
2:12:189:LEU:HD13	31:12:609:CLA:C1	2.40	0.50
9:D:351:ALA:HA	19:P:614:ASP:HA	1.93	0.50
31:S:610:CLA:HBB2	31:S:612:CLA:CHB	2.41	0.50
26:W:414:THR:HG23	46:W:501:DGD:HBF2	1.94	0.50
21:r:276:THR:HG21	31:r:608:CLA:H203	1.93	0.50
4:7:49:LYS:HG2	4:7:53:MET:HE3	1.94	0.50
31:13:604:CLA:HMB2	30:13:606:CHL:HBB1	1.94	0.50
30:16:607:CHL:HBB1	33:16:618:LUT:H171	1.93	0.50
11:F:23:ALA:HB1	49:F:101:HEM:HAC	1.93	0.50
30:1:607:CHL:HBB1	33:1:617:LUT:H171	1.93	0.50
31:12:612:CLA:C2B	33:12:614:LUT:C18	2.79	0.50
1:14:65:LEU:HD13	31:14:602:CLA:H42	1.92	0.50
31:15:604:CLA:H42	34:15:616:NEX:H373	1.93	0.50
31:16:615:CLA:H2A	31:16:615:CLA:HED3	1.93	0.50
30:N:607:CHL:H172	32:Y:616:LHG:H162	1.92	0.50
6:a:96:ILE:HD11	6:a:102:LEU:HD21	1.92	0.50
7:b:174:ILE:HD11	7:b:309:LEU:HD13	1.92	0.50
31:g:613:CLA:H111	32:g:615:LHG:H342	1.93	0.50
1:4:174:PRO:HB3	30:4:608:CHL:HBC2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5:603:CLA:O1A	3:6:74:SER:OG	2.30	0.50
31:13:614:CLA:H2A	31:13:614:CLA:HED2	1.94	0.50
6:A:233:ALA:HB1	9:D:265:ARG:HH11	1.76	0.50
32:a:401:LHG:H182	32:a:401:LHG:H372	1.94	0.50
31:15:604:CLA:HMA2	30:15:605:CHL:HBC3	1.92	0.50
6:A:37:MET:HB2	6:A:125:SER:HB2	1.94	0.50
7:B:440:ASP:N	7:B:440:ASP:OD1	2.45	0.50
32:C:521:LHG:H282	32:S:617:LHG:HC91	1.92	0.50
1:G:77:GLU:HG3	1:G:172:LEU:HD13	1.94	0.50
2:N:148:MET:HA	2:N:151:ILE:HG12	1.94	0.50
8:c:250:TRP:O	8:c:254:THR:OG1	2.24	0.50
11:f:23:ALA:HB1	49:f:101:HEM:HAC	1.93	0.50
14:j:27:VAL:HG11	41:j:102:LMG:H391	1.92	0.50
1:1:128:TYR:HE2	31:1:604:CLA:H2	1.77	0.50
30:11:601:CHL:OBD	32:11:615:LHG:H272	2.12	0.50
2:15:226:LEU:HD21	31:15:613:CLA:HHC	1.93	0.50
31:15:603:CLA:HMA2	31:15:603:CLA:H52	1.94	0.50
31:C:504:CLA:HMA1	32:S:621:LHG:H281	1.93	0.50
31:C:506:CLA:HAA1	31:C:506:CLA:HBD	1.94	0.50
21:R:287:LEU:O	21:R:291:ASN:ND2	2.44	0.50
2:12:204:MET:HE2	2:12:204:MET:HA	1.93	0.50
31:C:514:CLA:HBD	31:C:514:CLA:HBA1	1.93	0.50
31:R:603:CLA:H18	30:R:606:CHL:H121	1.94	0.50
6:a:37:MET:HB2	6:a:125:SER:HB2	1.94	0.50
31:b:601:CLA:HBB2	39:h:102:BCR:H363	1.92	0.50
32:n:616:LHG:O3	32:n:616:LHG:O1	2.23	0.50
31:s:604:CLA:HMB2	30:s:606:CHL:HBB1	1.94	0.50
32:4:615:LHG:HC91	35:6:620:XAT:H371	1.94	0.50
2:5:98:GLN:OE1	2:5:105:PHE:N	2.39	0.50
2:N:116:GLN:HB2	2:N:123:LEU:HD12	1.93	0.50
43:W:503:LNL:H111	28:Y:192:LEU:HD13	1.94	0.50
7:b:148:LEU:HD23	31:b:604:CLA:H201	1.93	0.50
31:b:610:CLA:H122	31:b:615:CLA:HAA1	1.93	0.50
8:c:346:THR:OG1	8:c:348:GLU:OE1	2.30	0.50
2:N:175:ASP:OD1	33:N:617:LUT:O23	2.24	0.49
31:R:613:CLA:H52	31:R:614:CLA:H43	1.94	0.49
41:d:411:LMG:H162	40:d:412:SQD:H251	1.93	0.49
31:g:613:CLA:HAA1	31:g:613:CLA:HBD	1.94	0.49
22:s:137:GLY:O	22:s:143:THR:HG22	2.12	0.49
28:y:192:LEU:HD13	43:y:621:LNL:H111	1.93	0.49
3:6:138:GLY:H	3:6:141:ASN:HD21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:14:203:LEU:HD13	31:14:611:CLA:HBC1	1.94	0.49
1:G:117:GLY:HA3	30:G:607:CHL:CAD	2.42	0.49
1:G:179:ASP:OD1	33:G:616:LUT:O23	2.23	0.49
1:G:214:GLN:HE21	1:G:225:ASN:HD22	1.60	0.49
2:N:207:PHE:HE1	33:N:617:LUT:H41	1.77	0.49
21:R:243:PRO:HD2	33:R:615:LUT:H23	1.94	0.49
8:c:406:SER:O	8:c:418:ASN:ND2	2.39	0.49
9:d:296:TYR:OH	9:d:326:ARG:NH1	2.33	0.49
2:n:207:PHE:HE1	33:n:617:LUT:H41	1.76	0.49
3:6:162:TYR:CD2	30:6:608:CHL:HBB1	2.47	0.49
1:11:65:LEU:HD21	31:13:603:CLA:H11	1.94	0.49
14:J:27:VAL:HG11	41:J:102:LMG:H391	1.93	0.49
19:P:595:ASP:HB2	19:P:601:TYR:HE2	1.76	0.49
19:p:653:GLY:O	19:p:657:SER:OG	2.22	0.49
2:15:111:PHE:CD1	2:15:112:LYS:HG3	2.47	0.49
31:A:402:CLA:HBD	31:A:403:CLA:HAC2	1.94	0.49
1:G:117:GLY:HA2	1:G:120:ILE:HG22	1.95	0.49
22:s:222:PRO:HD2	33:s:618:LUT:H23	1.95	0.49
2:5:209:VAL:HG11	31:5:613:CLA:HAC2	1.94	0.49
33:11:617:LUT:H372	31:13:603:CLA:HED2	1.94	0.49
6:A:18:CYS:O	6:A:22:THR:OG1	2.31	0.49
7:B:201:HIS:HB2	31:B:602:CLA:CHB	2.42	0.49
1:g:117:GLY:HA3	30:g:607:CHL:CAD	2.42	0.49
31:g:603:CLA:H72	31:n:603:CLA:H92	1.93	0.49
31:6:614:CLA:HAA1	31:6:614:CLA:HBD	1.94	0.49
4:7:96:THR:OG1	4:7:99:THR:OG1	2.30	0.49
32:A:414:LHG:HC41	26:W:426:VAL:HG11	1.93	0.49
46:c:518:DGD:HA42	41:j:102:LMG:H381	1.93	0.49
19:p:595:ASP:HB2	19:p:601:TYR:HE2	1.76	0.49
31:s:615:CLA:HBD	31:s:615:CLA:HAA1	1.93	0.49
2:5:175:ASP:OD1	33:5:614:LUT:O23	2.30	0.49
6:A:33:PHE:HE1	31:C:506:CLA:H92	1.78	0.49
6:A:244:GLU:OE2	9:D:264:LYS:NZ	2.38	0.49
7:B:55:MET:SD	7:B:63:LEU:HD23	2.53	0.49
31:C:509:CLA:HBC3	31:C:509:CLA:HHD	1.95	0.49
9:D:263:ASN:HB3	9:D:266:TRP:HB3	1.93	0.49
30:G:601:CHL:HMB3	28:Y:163:ILE:HD11	1.95	0.49
9:d:134:ARG:HG2	40:d:412:SQD:H1	1.93	0.49
21:r:287:LEU:O	21:r:291:ASN:ND2	2.45	0.49
5:16:54:GLY:O	5:16:198:ARG:NH2	2.36	0.49
41:J:102:LMG:H361	41:K:102:LMG:H232	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:281:LEU:HD12	32:S:621:LHG:HC92	1.95	0.49
31:c:509:CLA:HBC3	31:c:509:CLA:HHD	1.95	0.49
9:d:54:PHE:O	10:e:49:SER:OG	2.29	0.49
28:y:188:ASP:OD1	33:y:622:LUT:O23	2.27	0.49
1:11:68:ASP:O	1:11:71:THR:OG1	2.23	0.49
31:15:603:CLA:HED3	33:16:618:LUT:H372	1.95	0.49
7:B:367:PRO:O	7:B:425:GLN:NE2	2.46	0.49
2:N:82:ARG:NH1	30:N:608:CHL:OBD	2.40	0.49
29:Z:25:VAL:O	29:Z:29:THR:HG23	2.13	0.49
31:y:603:CLA:H61	31:y:603:CLA:H41	1.57	0.49
30:4:606:CHL:HBB2	30:4:607:CHL:HBB1	1.93	0.49
30:11:605:CHL:HHC	30:11:605:CHL:HBB1	1.95	0.49
32:A:413:LHG:O4	9:D:141:TYR:OH	2.23	0.49
30:R:605:CHL:HBA1	34:R:617:NEX:H403	1.94	0.49
6:a:188:ALA:HB2	6:a:328:MET:HG3	1.94	0.49
31:b:612:CLA:H102	31:b:612:CLA:H162	1.93	0.49
31:12:603:CLA:H71	31:13:602:CLA:H91	1.95	0.48
7:B:56:TRP:H	7:B:56:TRP:CD1	2.31	0.48
7:B:477:ASP:OD1	7:B:477:ASP:N	2.40	0.48
32:C:521:LHG:O9	32:C:521:LHG:O2	2.23	0.48
22:S:196:TYR:HB2	22:S:202:LYS:HG2	1.95	0.48
6:a:278:TRP:HB3	6:a:279:PRO:HD3	1.94	0.48
43:h:101:LNL:H9	39:h:102:BCR:H323	1.95	0.48
21:r:243:PRO:HD2	33:r:615:LUT:H23	1.94	0.48
28:y:246:ASN:OD1	28:y:246:ASN:N	2.46	0.48
2:2:169:TYR:HB3	31:2:610:CLA:O1D	2.13	0.48
2:2:222:LEU:HD22	33:2:614:LUT:H172	1.94	0.48
3:3:138:GLY:H	3:3:141:ASN:HD21	1.60	0.48
4:8:68:GLN:NE2	8:c:456:GLU:OE2	2.46	0.48
30:15:605:CHL:HBB2	33:15:615:LUT:H7	1.94	0.48
26:W:432:ASP:OD2	26:W:439:ASN:ND2	2.46	0.48
1:1:197:GLU:HG3	31:1:610:CLA:C1B	2.42	0.48
8:C:390:ARG:NH2	20:Q:77:GLU:OE1	2.46	0.48
30:G:607:CHL:CHA	30:G:607:CHL:HBA1	2.43	0.48
2:N:193:GLU:HB2	31:N:610:CLA:C1B	2.44	0.48
31:c:504:CLA:HMA1	32:s:621:LHG:H281	1.95	0.48
26:w:406:ASP:OD2	26:w:408:SER:OG	2.30	0.48
1:4:196:LYS:HD3	31:4:612:CLA:HBD	1.96	0.48
33:4:617:LUT:H372	31:6:603:CLA:HED3	1.95	0.48
31:G:611:CLA:HBC3	32:G:615:LHG:HC61	1.94	0.48
18:O:149:MET:HA	18:O:168:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:MET:SD	31:G:610:CLA:HBB1	2.54	0.48
6:a:308:ASP:OD1	6:a:312:ARG:N	2.46	0.48
31:c:506:CLA:H18	41:w:501:LMG:H272	1.96	0.48
13:i:10:THR:HG23	26:w:416:VAL:HG21	1.94	0.48
39:j:101:BCR:H15C	15:k:31:LEU:HB2	1.95	0.48
22:s:129:ALA:HB2	22:s:135:VAL:HB	1.96	0.48
1:4:112:VAL:HB	1:4:115:LYS:HB2	1.96	0.48
5:13:189:LEU:HB3	31:13:610:CLA:H3A	1.94	0.48
2:15:34:ARG:NH2	2:15:50:GLY:HA2	2.28	0.48
30:16:605:CHL:HBA1	30:16:605:CHL:H3A	1.73	0.48
19:p:554:LEU:HG	20:q:61:LEU:HD21	1.96	0.48
2:5:212:LEU:O	2:5:215:ARG:NH1	2.41	0.48
5:16:195:LYS:HG2	32:16:616:LHG:H242	1.96	0.48
5:16:198:ARG:HA	5:16:201:MET:HE3	1.94	0.48
32:A:415:LHG:H372	32:A:415:LHG:H182	1.94	0.48
31:B:615:CLA:H162	31:B:615:CLA:H192	1.73	0.48
6:a:18:CYS:O	6:a:22:THR:OG1	2.31	0.48
6:a:155:THR:HG21	46:c:517:DGD:HBH2	1.95	0.48
8:c:339:LYS:HD3	19:p:575:GLY:HA3	1.95	0.48
9:d:225:ASP:HB2	9:d:234:ALA:HB1	1.94	0.48
16:l:29:ALA:O	16:l:33:SER:HB3	2.13	0.48
2:n:210:GLN:NE2	31:n:613:CLA:NA	2.61	0.48
31:r:611:CLA:HBB1	33:r:615:LUT:C35	2.44	0.48
2:2:192:LYS:HD3	31:2:612:CLA:HAA2	1.95	0.48
2:15:68:GLU:O	2:15:72:ARG:HG2	2.14	0.48
36:B:620:3PH:H2G2	23:t:15:GLY:HA3	1.95	0.48
1:G:143:VAL:HG22	30:G:605:CHL:HAC1	1.96	0.48
31:R:604:CLA:HMB2	30:R:605:CHL:HBB1	1.96	0.48
7:b:367:PRO:O	7:b:425:GLN:NE2	2.46	0.48
8:c:425:TRP:O	8:c:429:SER:OG	2.30	0.48
30:n:607:CHL:H2	28:y:247:PHE:HE2	1.78	0.48
31:y:613:CLA:H52	32:y:616:LHG:H201	1.95	0.48
2:2:82:ARG:NH1	30:2:608:CHL:OBD	2.47	0.48
2:15:213:ILE:HG23	2:15:214:THR:HG23	1.95	0.48
31:c:502:CLA:HBC1	31:c:513:CLA:H43	1.95	0.48
2:n:148:MET:HA	2:n:151:ILE:HG12	1.96	0.48
30:1:601:CHL:HBA1	30:1:601:CHL:H3A	1.63	0.48
30:1:605:CHL:H3A	30:1:605:CHL:HBA2	1.62	0.48
31:1:611:CLA:HBD	31:1:611:CLA:HBA1	1.95	0.48
1:4:144:LEU:O	1:4:148:LEU:HG	2.14	0.48
2:12:68:GLU:O	2:12:72:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:13:608:CHL:H3A	30:13:608:CHL:HBA2	1.50	0.48
1:14:95:THR:HG22	1:14:96:PRO:HD3	1.96	0.48
5:16:58:TRP:CZ2	30:16:601:CHL:HBA1	2.48	0.48
30:16:608:CHL:HBA2	30:16:608:CHL:H3A	1.51	0.48
39:J:101:BCR:H15C	15:K:31:LEU:HB2	1.94	0.48
21:r:256:LYS:HE2	21:r:256:LYS:HB3	1.54	0.48
30:4:608:CHL:H3A	30:4:608:CHL:HBA2	1.58	0.47
31:13:613:CLA:HAA1	31:13:613:CLA:HBD	1.95	0.47
5:16:179:LEU:HD12	31:16:610:CLA:H11	1.96	0.47
6:A:278:TRP:HB3	6:A:279:PRO:HD3	1.96	0.47
30:N:608:CHL:H3A	30:N:608:CHL:HBA2	1.41	0.47
32:a:414:LHG:H371	31:y:611:CLA:H202	1.96	0.47
31:c:506:CLA:HAA1	31:c:506:CLA:HBD	1.95	0.47
30:g:607:CHL:HBA1	30:g:607:CHL:CHA	2.43	0.47
22:s:221:ASP:OD1	33:s:618:LUT:O23	2.31	0.47
31:14:602:CLA:H2A	31:14:602:CLA:HED2	1.96	0.47
31:B:610:CLA:H122	31:B:615:CLA:HAA1	1.95	0.47
9:D:225:ASP:HB2	9:D:234:ALA:HB1	1.95	0.47
31:Y:615:CLA:H92	31:Y:615:CLA:H61	1.75	0.47
6:a:176:ILE:HD13	31:d:402:CLA:HED3	1.96	0.47
41:d:411:LMG:H371	32:d:413:LHG:H131	1.96	0.47
10:e:8:ARG:HB3	10:e:13:ILE:HD11	1.95	0.47
11:f:41:ARG:NH2	14:j:42:LEU:O	2.39	0.47
31:5:602:CLA:HBA2	31:5:602:CLA:H3A	1.61	0.47
5:16:189:LEU:HB3	31:16:610:CLA:H3A	1.96	0.47
18:O:271:GLU:HG2	18:O:303:GLN:HG2	1.97	0.47
31:a:403:CLA:HBD	31:d:402:CLA:HAC2	1.96	0.47
2:n:85:MET:HE2	33:n:617:LUT:C34	2.44	0.47
19:p:564:SER:O	19:p:564:SER:OG	2.29	0.47
31:r:601:CLA:O1A	31:r:610:CLA:HBB1	2.15	0.47
2:5:34:ARG:HD2	2:5:55:ASP:O	2.14	0.47
31:5:604:CLA:HBA1	31:5:604:CLA:CBD	2.39	0.47
1:11:34:ARG:NH2	1:11:57:ASP:OD1	2.44	0.47
1:14:74:ARG:NH1	1:14:77:GLU:OE1	2.46	0.47
6:A:162:PRO:HB3	6:A:168:PHE:HA	1.97	0.47
6:a:63:ILE:HB	8:c:335:THR:HG21	1.97	0.47
1:g:117:GLY:HA2	1:g:120:ILE:HG22	1.96	0.47
2:n:45:PRO:HD2	2:n:48:LEU:HD12	1.95	0.47
25:v:26:LEU:HD21	29:z:25:VAL:HA	1.95	0.47
1:1:112:VAL:HB	1:1:115:LYS:HB2	1.95	0.47
1:1:144:LEU:O	1:1:148:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:14:49:TYR:OH	1:14:61:ASP:OD2	2.27	0.47
31:16:604:CLA:HMB2	30:16:606:CHL:HBB1	1.96	0.47
30:16:609:CHL:H41	30:16:609:CHL:H62	1.69	0.47
31:B:612:CLA:H102	31:B:612:CLA:H162	1.96	0.47
8:C:108:THR:HG22	8:C:108:THR:O	2.14	0.47
10:E:8:ARG:HB3	10:E:13:ILE:HD11	1.95	0.47
31:R:610:CLA:HBC3	32:R:618:LHG:HC62	1.96	0.47
22:S:123:ILE:HG21	31:S:611:CLA:H203	1.96	0.47
8:c:163:ILE:HG23	43:c:523:LNL:H141	1.96	0.47
46:c:518:DGD:HA42	41:j:102:LMG:H351	1.96	0.47
12:h:70:ASP:OD1	12:h:70:ASP:N	2.39	0.47
31:s:603:CLA:HBB1	33:s:619:LUT:C34	2.44	0.47
30:4:601:CHL:H141	35:6:620:XAT:H161	1.97	0.47
31:13:602:CLA:H41	31:13:602:CLA:H61	1.53	0.47
6:A:131:TRP:CH2	31:C:506:CLA:HAA2	2.50	0.47
26:w:414:THR:HG23	46:w:502:DGD:HBH1	1.95	0.47
31:y:614:CLA:HBD	31:y:614:CLA:HAA1	1.96	0.47
1:1:49:TYR:OH	1:1:61:ASP:OD2	2.28	0.47
1:1:211:PHE:HE1	33:1:616:LUT:H41	1.79	0.47
31:1:610:CLA:CBB	33:1:616:LUT:H32	2.44	0.47
2:2:93:THR:HG21	31:2:604:CLA:HBC3	1.97	0.47
30:4:609:CHL:H62	30:4:609:CHL:H41	1.55	0.47
30:5:608:CHL:HBA2	30:5:608:CHL:H3A	1.61	0.47
5:13:209:ILE:O	5:13:212:ILE:HG22	2.14	0.47
5:16:175:ASP:OD1	33:16:617:LUT:O23	2.29	0.47
7:B:24:LEU:CD2	31:B:616:CLA:HBB1	2.45	0.47
31:B:614:CLA:H62	31:B:614:CLA:H41	1.56	0.47
44:B:623:STE:H183	44:B:623:STE:H151	1.74	0.47
46:C:518:DGD:HA42	41:J:102:LMG:H351	1.96	0.47
9:D:266:TRP:HH2	32:L:102:LHG:H102	1.80	0.47
31:D:405:CLA:H41	31:D:405:CLA:H61	1.51	0.47
18:O:125:VAL:HG22	18:O:294:ILE:HG12	1.97	0.47
19:P:554:LEU:HG	20:Q:61:LEU:HD21	1.95	0.47
7:b:288:VAL:HG23	7:b:305:ILE:HD11	1.95	0.47
2:n:47:TYR:OH	2:n:59:ASP:OD2	2.27	0.47
30:3:608:CHL:HBA2	30:3:608:CHL:H3A	1.42	0.47
2:5:125:TYR:HB3	2:5:131:LEU:HD23	1.97	0.47
31:15:603:CLA:OBD	30:15:608:CHL:H11	2.14	0.47
12:H:18:THR:HG22	12:H:21:GLY:H	1.80	0.47
2:N:85:MET:SD	31:N:610:CLA:HBB1	2.54	0.47
18:O:170:ASP:OD1	18:O:170:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:57:ALA:O	8:c:61:VAL:HG23	2.14	0.47
30:n:605:CHL:H102	31:s:611:CLA:H171	1.96	0.47
30:1:608:CHL:H3A	30:1:608:CHL:HBA2	1.56	0.47
31:3:610:CLA:H92	31:3:610:CLA:H61	1.74	0.47
2:5:82:ARG:NH1	30:5:608:CHL:OBD	2.47	0.47
5:13:235:TYR:HA	5:13:239:ALA:HB2	1.96	0.47
6:A:63:ILE:HB	8:C:335:THR:HG21	1.96	0.47
30:N:607:CHL:H71	32:Y:616:LHG:H223	1.96	0.47
31:b:610:CLA:H202	31:b:610:CLA:H161	1.68	0.47
21:r:233:ARG:HG3	21:r:233:ARG:HH11	1.80	0.47
7:B:54:PRO:HD2	7:B:57:ARG:HG3	1.96	0.47
7:B:243:ALA:HA	7:B:246:PHE:CD2	2.50	0.47
31:C:512:CLA:H92	31:C:512:CLA:H62	1.77	0.47
30:N:607:CHL:H41	30:N:607:CHL:H62	1.58	0.47
28:Y:57:TYR:OH	28:Y:69:ASP:OD2	2.24	0.47
1:g:77:GLU:HG3	1:g:172:LEU:HD13	1.97	0.47
1:g:143:VAL:HG22	30:g:605:CHL:HAC1	1.97	0.47
1:14:238:GLY:N	31:14:613:CLA:O1A	2.44	0.46
7:B:495:PHE:HD1	7:B:504:ARG:HA	1.80	0.46
1:G:199:LYS:NZ	32:G:615:LHG:O5	2.48	0.46
30:N:608:CHL:HBA1	41:S:616:LMG:H222	1.96	0.46
36:T:101:3PH:H2F1	36:T:101:3PH:H3A2	1.97	0.46
22:s:268:TRP:HB2	33:s:618:LUT:H22	1.95	0.46
31:s:604:CLA:H92	31:s:604:CLA:H62	1.76	0.46
31:2:602:CLA:H52	33:2:615:LUT:H28	1.97	0.46
2:5:112:LYS:HB3	2:5:112:LYS:HE2	1.63	0.46
6:A:151:VAL:HG12	46:C:517:DGD:HBV2	1.97	0.46
46:C:518:DGD:HA42	41:J:102:LMG:H381	1.95	0.46
7:b:201:HIS:HB2	31:b:602:CLA:CHB	2.45	0.46
7:b:495:PHE:HD1	7:b:504:ARG:HA	1.81	0.46
8:c:380:LEU:HA	8:c:384:ILE:HG13	1.97	0.46
9:d:51:GLY:HA3	9:d:78:VAL:HG22	1.98	0.46
9:d:263:ASN:HB3	9:d:266:TRP:HB3	1.97	0.46
40:d:414:SQD:H441	11:f:12:PHE:O	2.15	0.46
21:r:109:LEU:HD23	21:r:131:ALA:HA	1.97	0.46
31:r:602:CLA:HBC3	31:r:602:CLA:HHD	1.96	0.46
2:2:155:ARG:HG3	30:2:608:CHL:C1D	2.45	0.46
2:2:222:LEU:HD13	33:2:614:LUT:H163	1.97	0.46
31:11:602:CLA:H61	31:11:602:CLA:H41	1.58	0.46
31:15:612:CLA:CBB	33:15:614:LUT:C18	2.93	0.46
1:G:184:ALA:HB1	1:G:190:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:T:101:3PH:H2E1	40:l:101:SQD:H341	1.97	0.46
1:1:84:ARG:HA	1:1:87:MET:HE3	1.98	0.46
3:3:215:PHE:HE1	33:3:618:LUT:H41	1.81	0.46
17:M:15:ILE:O	17:M:19:THR:OG1	2.31	0.46
31:d:405:CLA:H193	31:d:405:CLA:H162	1.76	0.46
1:g:184:ALA:HB1	1:g:190:LEU:HD13	1.98	0.46
30:n:605:CHL:H51	30:n:605:CHL:H8	1.80	0.46
18:o:149:MET:HA	18:o:168:GLY:HA3	1.98	0.46
31:r:608:CLA:H202	31:r:608:CLA:H161	1.74	0.46
1:1:184:ALA:HB2	31:1:610:CLA:HAA2	1.98	0.46
2:2:80:HIS:HB3	2:2:201:MET:HE3	1.98	0.46
30:2:609:CHL:H142	30:2:609:CHL:H111	1.83	0.46
3:6:94:ALA:O	3:6:98:MET:HG3	2.14	0.46
8:C:346:THR:OG1	8:C:348:GLU:OE1	2.33	0.46
9:D:194:ASN:O	9:D:198:MET:HG3	2.16	0.46
30:G:608:CHL:HBA1	30:G:608:CHL:CBD	2.43	0.46
21:R:233:ARG:HG3	21:R:233:ARG:HH11	1.80	0.46
31:S:603:CLA:HBB1	33:S:619:LUT:C33	2.46	0.46
7:b:243:ALA:HA	7:b:246:PHE:CD2	2.50	0.46
30:g:608:CHL:HBA1	30:g:608:CHL:CBD	2.43	0.46
1:14:85:TRP:CD1	30:14:609:CHL:HMD3	2.50	0.46
33:15:614:LUT:H12	33:15:614:LUT:H191	1.98	0.46
22:S:142:GLU:HA	30:S:607:CHL:HED1	1.96	0.46
2:n:85:MET:HE1	31:n:610:CLA:CBB	2.46	0.46
3:6:205:GLY:O	3:6:209:MET:HG3	2.16	0.46
43:W:502:LNL:H171	28:Y:102:ILE:HG21	1.98	0.46
2:n:131:LEU:HD23	2:n:131:LEU:HA	1.79	0.46
18:o:127:MET:HE3	18:o:292:ALA:HB2	1.98	0.46
30:r:605:CHL:H41	30:r:605:CHL:H61	1.62	0.46
22:s:153:LEU:HD23	31:s:604:CLA:HBA2	1.98	0.46
3:3:98:MET:HE3	3:3:205:GLY:N	2.31	0.46
1:4:74:ARG:HA	1:4:74:ARG:HD3	1.69	0.46
2:5:212:LEU:HD21	31:6:615:CLA:H11	1.98	0.46
5:13:195:LYS:HG2	32:13:616:LHG:H242	1.98	0.46
31:G:610:CLA:H92	31:G:610:CLA:H62	1.79	0.46
30:N:607:CHL:H92	30:N:607:CHL:H61	1.75	0.46
1:1:88:LEU:HD11	31:1:610:CLA:HAC1	1.98	0.46
1:4:34:ARG:NH2	1:4:57:ASP:OD1	2.47	0.46
31:4:603:CLA:H42	2:5:63:LEU:HD11	1.98	0.46
2:5:169:TYR:HB3	31:5:610:CLA:O1D	2.15	0.46
1:11:47:PRO:HG2	1:11:61:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:13:131:LEU:HD23	5:13:131:LEU:HA	1.72	0.46
31:15:602:CLA:H61	31:15:602:CLA:H41	1.55	0.46
31:16:613:CLA:HAA1	31:16:613:CLA:HBD	1.98	0.46
8:C:380:LEU:HA	8:C:384:ILE:HG13	1.97	0.46
31:D:405:CLA:H193	31:D:405:CLA:H162	1.73	0.46
30:N:607:CHL:H201	31:Y:602:CLA:H201	1.98	0.46
28:Y:188:ASP:OD1	33:Y:621:LUT:O23	2.27	0.46
6:a:183:MET:HB3	31:a:403:CLA:HBC2	1.98	0.46
6:a:247:ASN:HB3	6:a:250:ALA:HB3	1.98	0.46
7:b:24:LEU:CD2	31:b:616:CLA:HBB1	2.45	0.46
31:d:402:CLA:H202	31:d:402:CLA:H161	1.73	0.46
32:6:617:LHG:H261	31:r:610:CLA:H11	1.98	0.45
1:11:80:VAL:HG23	1:11:81:ILE:HD12	1.98	0.45
31:B:602:CLA:H12	12:H:62:TYR:CD2	2.51	0.45
39:B:617:BCR:H383	36:B:620:3PH:H352	1.97	0.45
32:Y:618:LHG:H121	32:Y:618:LHG:H291	1.97	0.45
31:b:613:CLA:H41	31:b:613:CLA:H62	1.65	0.45
8:c:281:ILE:HG12	41:w:501:LMG:H251	1.98	0.45
31:c:514:CLA:HBD	31:c:514:CLA:HBA1	1.98	0.45
39:c:515:BCR:H24C	39:c:515:BCR:H371	1.84	0.45
9:d:21:TRP:O	9:d:26:ARG:NH2	2.47	0.45
30:n:607:CHL:H91	30:n:607:CHL:H112	1.66	0.45
22:s:87:TYR:OH	32:s:617:LHG:O5	2.32	0.45
43:w:503:LNL:H171	28:y:102:ILE:HG21	1.98	0.45
1:1:82:HIS:HB3	1:1:205:MET:HE3	1.98	0.45
1:1:159:TYR:CE2	2:2:43:ASN:HB2	2.51	0.45
32:1:615:LHG:O1	35:3:620:XAT:O23	2.28	0.45
3:3:44:ASP:OD1	3:3:44:ASP:N	2.43	0.45
30:4:605:CHL:H3A	30:4:605:CHL:HBA2	1.60	0.45
31:6:611:CLA:HAC1	32:6:616:LHG:H301	1.99	0.45
42:D:407:PL9:H221	42:D:407:PL9:H201	1.82	0.45
21:R:109:LEU:HD23	21:R:131:ALA:HA	1.97	0.45
31:S:613:CLA:H2A	31:S:613:CLA:HED3	1.98	0.45
36:T:101:3PH:H321	36:T:101:3PH:H32	1.43	0.45
6:a:131:TRP:CH2	31:c:506:CLA:HAA2	2.52	0.45
22:s:43:TRP:HZ2	41:s:616:LMG:HC71	1.81	0.45
22:s:116:MET:HE3	22:s:243:GLY:CA	2.46	0.45
31:y:612:CLA:H193	31:y:612:CLA:H161	1.77	0.45
33:15:614:LUT:H191	33:15:614:LUT:C12	2.46	0.45
31:16:603:CLA:H92	31:16:603:CLA:H61	1.79	0.45
2:N:45:PRO:HD2	2:N:48:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:262:ILE:HD12	21:R:262:ILE:HA	1.86	0.45
22:S:87:TYR:OH	32:S:617:LHG:O5	2.35	0.45
22:S:129:ALA:HB2	22:S:135:VAL:HB	1.98	0.45
28:Y:248:TYR:HA	28:Y:252:ALA:HB2	1.99	0.45
31:Y:614:CLA:HAA1	31:Y:614:CLA:HBD	1.98	0.45
31:b:605:CLA:H41	31:b:605:CLA:H61	1.81	0.45
31:c:507:CLA:H202	31:c:507:CLA:H161	1.65	0.45
40:d:412:SQD:O49	40:d:412:SQD:O2	2.34	0.45
30:n:609:CHL:H62	30:n:609:CHL:H41	1.67	0.45
31:r:611:CLA:HBB1	33:r:615:LUT:C15	2.46	0.45
31:s:602:CLA:CBB	33:s:619:LUT:H32	2.46	0.45
2:2:176:PRO:HD2	33:2:614:LUT:H23	1.97	0.45
1:11:84:ARG:NH1	30:11:608:CHL:OBD	2.49	0.45
1:11:157:TYR:CD2	30:11:608:CHL:HBB1	2.51	0.45
31:11:603:CLA:H11	31:11:603:CLA:HBA1	1.78	0.45
2:12:193:GLU:HB2	31:12:609:CLA:C1B	2.45	0.45
31:12:609:CLA:H8	33:12:614:LUT:C29	2.46	0.45
30:14:601:CHL:H62	30:14:601:CHL:H2	1.63	0.45
16:L:29:ALA:O	16:L:33:SER:HB3	2.15	0.45
27:X:78:GLY:HA2	43:X:201:LNL:H142	1.99	0.45
8:c:187:ASP:OD2	8:c:197:ARG:NH1	2.49	0.45
39:j:101:BCR:H382	15:k:34:VAL:HG22	1.97	0.45
15:k:40:SER:O	15:k:40:SER:OG	2.22	0.45
31:1:610:CLA:HMB1	31:1:610:CLA:H12	1.98	0.45
3:3:49:LEU:HB2	3:3:53:SER:HB3	1.99	0.45
31:3:604:CLA:H41	31:3:604:CLA:H61	1.52	0.45
1:4:159:TYR:CE2	2:5:43:ASN:HB2	2.52	0.45
30:4:601:CHL:H41	30:4:601:CHL:H62	1.75	0.45
3:6:217:ILE:HG21	31:6:613:CLA:HAC2	1.99	0.45
31:11:612:CLA:HBB1	33:11:616:LUT:C15	2.47	0.45
31:12:612:CLA:C2B	33:12:614:LUT:C4	2.94	0.45
31:13:610:CLA:H62	31:13:610:CLA:H41	1.72	0.45
5:16:206:GLY:O	5:16:210:GLN:HG3	2.17	0.45
6:A:34:GLY:HA2	6:A:37:MET:HB3	1.98	0.45
6:A:197:PHE:HE1	46:C:519:DGD:HBW2	1.81	0.45
7:B:327:ALA:HB1	41:B:621:LMG:HC8	1.99	0.45
8:c:313:GLN:HG3	8:c:396:MET:HE3	1.99	0.45
9:d:266:TRP:HH2	32:l:102:LHG:H102	1.81	0.45
31:r:603:CLA:HBB1	31:r:608:CLA:H18	1.98	0.45
31:s:610:CLA:H3A	31:s:610:CLA:HBA2	1.59	0.45
43:y:619:LNL:H10	43:y:619:LNL:H13	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:609:CHL:HBA2	30:1:609:CHL:H3A	1.29	0.45
31:3:602:CLA:H3A	31:3:602:CLA:HBA2	1.62	0.45
1:4:107:PHE:HB3	1:4:110:ALA:HB3	1.98	0.45
30:12:608:CHL:HBA2	30:12:608:CHL:H3A	1.61	0.45
30:13:601:CHL:NA	32:13:616:LHG:H102	2.32	0.45
5:16:76:LEU:CD2	31:16:603:CLA:HBD	2.47	0.45
31:B:607:CLA:H2	41:B:621:LMG:H152	1.99	0.45
1:G:198:ILE:HD12	1:G:198:ILE:HA	1.82	0.45
32:R:621:LHG:H292	31:R:602:CLA:H193	1.99	0.45
7:b:42:LEU:HD11	7:b:93:TYR:HB3	1.98	0.45
9:d:193:LEU:O	16:l:35:TYR:OH	2.23	0.45
31:s:609:CLA:H41	31:s:609:CLA:H62	1.66	0.45
31:4:610:CLA:CBB	33:4:616:LUT:H32	2.47	0.45
31:4:613:CLA:H92	31:4:613:CLA:H61	1.78	0.45
5:13:179:LEU:HD12	31:13:610:CLA:H11	1.99	0.45
6:A:183:MET:HB3	31:A:402:CLA:HBC2	1.98	0.45
31:S:603:CLA:HBB1	33:S:619:LUT:C34	2.47	0.45
40:d:414:SQD:H241	40:d:414:SQD:H282	1.99	0.45
1:1:198:ILE:HD12	1:1:198:ILE:HA	1.83	0.45
36:8:201:3PH:H2	36:8:201:3PH:H221	1.63	0.45
12:H:70:ASP:OD1	12:H:70:ASP:N	2.35	0.45
2:N:145:LEU:HD21	32:Y:616:LHG:H161	1.98	0.45
30:N:605:CHL:H2A	30:N:605:CHL:O1D	2.17	0.45
30:N:607:CHL:H91	30:N:607:CHL:H112	1.67	0.45
31:b:602:CLA:H12	12:h:62:TYR:CD2	2.51	0.45
18:o:160:SER:OG	18:o:198:LYS:NZ	2.50	0.45
22:s:260:THR:HG22	22:s:262:GLU:HG2	1.99	0.45
22:s:281:LEU:HD12	32:s:621:LHG:HC92	1.99	0.45
31:1:613:CLA:HBD	31:1:613:CLA:HAA1	1.99	0.45
3:3:205:GLY:O	3:3:209:MET:HG3	2.16	0.45
30:3:607:CHL:HBB2	30:3:609:CHL:HBC1	1.99	0.45
30:12:607:CHL:H3A	30:12:607:CHL:HBA2	1.37	0.45
5:13:82:ARG:HA	5:13:85:MET:HE3	1.99	0.45
5:16:76:LEU:HD21	31:16:603:CLA:HBD	1.99	0.45
7:B:157:HIS:HA	7:B:163:GLY:HA3	1.99	0.45
8:C:425:TRP:O	8:C:429:SER:OG	2.31	0.45
22:S:55:LYS:NZ	32:S:617:LHG:O1	2.41	0.45
30:3:606:CHL:H61	30:3:606:CHL:H41	1.66	0.45
33:12:614:LUT:H191	33:12:614:LUT:C12	2.47	0.45
30:13:605:CHL:HBA1	30:13:605:CHL:H3A	1.68	0.45
31:14:610:CLA:H152	31:14:610:CLA:H18	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:247:ASN:HB3	6:A:250:ALA:HB3	1.99	0.45
31:S:604:CLA:H111	31:S:604:CLA:H71	1.68	0.45
31:b:604:CLA:H92	31:b:604:CLA:H61	1.81	0.45
31:d:404:CLA:H192	31:d:404:CLA:H162	1.77	0.45
31:s:604:CLA:H121	30:s:606:CHL:H152	1.99	0.45
2:2:50:GLY:HA2	2:2:55:ASP:HB3	1.99	0.44
1:4:234:SER:O	1:4:237:ASN:ND2	2.50	0.44
6:A:102:LEU:HD23	6:A:102:LEU:HA	1.85	0.44
8:C:240:ILE:HG12	31:C:502:CLA:HBB1	2.00	0.44
9:D:189:HIS:HA	9:D:294:ARG:HD2	1.99	0.44
2:N:235:TRP:O	2:N:239:ALA:HB3	2.17	0.44
31:S:610:CLA:HBB1	31:S:610:CLA:H51	1.99	0.44
42:a:410:PL9:H322	42:a:410:PL9:H301	1.76	0.44
9:d:194:ASN:O	9:d:198:MET:HG3	2.17	0.44
1:g:112:VAL:HG13	1:g:221:SER:HB3	1.99	0.44
31:1:610:CLA:H3A	31:1:610:CLA:HBA2	1.68	0.44
1:G:174:PRO:HB3	30:G:608:CHL:HBC2	1.99	0.44
2:n:161:ALA:HB2	41:s:616:LMG:H111	2.00	0.44
2:n:193:GLU:HB2	31:n:610:CLA:C1B	2.47	0.44
2:5:58:TRP:HZ3	31:5:602:CLA:HBC2	1.82	0.44
32:A:414:LHG:H272	26:W:419:ILE:HG12	2.00	0.44
31:B:602:CLA:H12	12:H:62:TYR:HD2	1.83	0.44
8:C:187:ASP:OD2	8:C:197:ARG:NH1	2.51	0.44
39:C:515:BCR:H24C	39:C:515:BCR:H371	1.83	0.44
9:D:348:ARG:NH2	19:P:615:GLU:OE2	2.51	0.44
39:J:101:BCR:H382	15:K:34:VAL:HG22	1.99	0.44
18:O:160:SER:OG	18:O:198:LYS:NZ	2.51	0.44
30:R:606:CHL:H91	30:R:606:CHL:H112	1.72	0.44
31:c:503:CLA:H111	31:c:504:CLA:HMB2	1.98	0.44
31:d:405:CLA:H51	43:x:201:LNL:H182	2.00	0.44
2:n:85:MET:HE2	33:n:617:LUT:H34	1.99	0.44
30:n:607:CHL:H41	30:n:607:CHL:H61	1.63	0.44
18:o:170:ASP:OD1	18:o:170:ASP:N	2.46	0.44
2:2:80:HIS:CE1	31:2:603:CLA:ND	2.85	0.44
30:2:609:CHL:H62	30:2:609:CHL:H41	1.52	0.44
31:6:604:CLA:H61	31:6:604:CLA:H41	1.53	0.44
30:6:605:CHL:H51	31:r:612:CLA:H2	2.00	0.44
4:7:45:ASN:HB3	4:7:48:VAL:HB	1.99	0.44
36:8:201:3PH:H351	36:8:201:3PH:H242	2.00	0.44
31:13:603:CLA:H92	31:13:603:CLA:H61	1.72	0.44
31:14:602:CLA:H41	31:14:602:CLA:H61	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:201:HIS:HE2	31:B:603:CLA:C1B	2.31	0.44
19:P:612:ASP:OD1	19:P:613:GLY:N	2.51	0.44
6:a:34:GLY:HA2	6:a:37:MET:HB3	1.98	0.44
2:n:175:ASP:OD1	33:n:617:LUT:O23	2.27	0.44
2:n:176:PRO:HD2	33:n:617:LUT:H23	2.00	0.44
2:n:192:LYS:HE2	31:n:612:CLA:HBD	1.97	0.44
31:y:610:CLA:H102	31:y:610:CLA:H62	1.75	0.44
5:13:58:TRP:CZ2	30:13:601:CHL:HBA1	2.52	0.44
38:D:402:PHO:HBA2	38:D:402:PHO:H3A	1.67	0.44
18:O:195:ILE:HG22	18:O:204:GLY:HA3	1.98	0.44
31:R:610:CLA:H102	31:R:610:CLA:H62	1.57	0.44
30:Y:605:CHL:HHC	30:Y:605:CHL:HBB1	2.00	0.44
6:a:161:TYR:HB3	6:a:162:PRO:HD3	2.00	0.44
31:b:615:CLA:H192	31:b:615:CLA:H162	1.74	0.44
31:2:610:CLA:H3A	31:2:610:CLA:HBA2	1.76	0.44
3:6:215:PHE:HE1	33:6:618:LUT:H41	1.82	0.44
31:6:610:CLA:H62	31:6:610:CLA:H41	1.80	0.44
2:12:198:ARG:HB3	31:12:602:CLA:HBC3	1.99	0.44
31:12:603:CLA:H61	31:12:603:CLA:H92	1.72	0.44
30:15:608:CHL:H52	30:16:601:CHL:H71	1.99	0.44
31:B:606:CLA:H62	39:B:619:BCR:H342	1.99	0.44
8:C:343:ARG:NH1	8:C:347:GLY:O	2.49	0.44
18:O:114:ASP:OD1	18:O:115:LYS:N	2.50	0.44
20:Q:156:LYS:HE2	20:Q:156:LYS:HB3	1.75	0.44
22:S:260:THR:HG22	22:S:262:GLU:HG2	1.99	0.44
31:Y:602:CLA:HMC1	33:Y:622:LUT:C31	2.48	0.44
7:b:500:ASP:OD2	27:x:100:ARG:NH1	2.46	0.44
30:n:601:CHL:HBA1	30:n:601:CHL:H3A	1.55	0.44
30:n:607:CHL:H2	28:y:247:PHE:CE2	2.53	0.44
28:y:247:PHE:HB2	31:y:613:CLA:CAD	2.48	0.44
1:11:246:LEU:HD12	1:11:247:PRO:HD2	1.99	0.44
2:12:93:THR:HG21	31:12:604:CLA:HAC2	1.99	0.44
6:A:195:HIS:O	6:A:199:MET:HG3	2.17	0.44
9:D:148:ALA:HB3	9:D:149:PRO:HD3	2.00	0.44
22:S:148:LEU:HD23	22:S:148:LEU:HA	1.79	0.44
8:c:243:LEU:HD21	32:y:618:LHG:H172	1.98	0.44
19:p:544:ILE:HD12	19:p:547:LEU:HD13	2.00	0.44
21:r:262:ILE:HD12	21:r:262:ILE:HA	1.87	0.44
28:y:217:MET:HE2	33:y:623:LUT:H10	2.00	0.44
31:12:602:CLA:H41	31:12:602:CLA:H61	1.75	0.44
30:12:605:CHL:HBB2	33:12:615:LUT:H7	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:13:234:PHE:HB2	31:13:613:CLA:CAD	2.47	0.44
5:16:82:ARG:HA	5:16:85:MET:HE3	2.00	0.44
5:16:234:PHE:HB2	31:16:613:CLA:CAD	2.48	0.44
9:D:231:THR:OG1	32:D:409:LHG:O4	2.35	0.44
14:J:11:PRO:HB2	14:J:14:LEU:HB2	2.00	0.44
31:S:610:CLA:CBB	33:S:618:LUT:H32	2.48	0.44
28:Y:212:LEU:HD13	31:Y:611:CLA:HBC1	1.99	0.44
31:Y:603:CLA:H51	31:Y:603:CLA:HMA2	1.98	0.44
31:b:602:CLA:H12	12:h:62:TYR:HD2	1.82	0.44
8:c:130:VAL:HG21	31:c:512:CLA:H161	2.00	0.44
28:y:158:MET:HA	28:y:161:VAL:HG22	2.00	0.44
31:14:610:CLA:H2	33:14:616:LUT:H28	2.00	0.44
6:A:299:GLY:O	8:C:403:SER:HB2	2.18	0.44
13:I:10:THR:HG23	26:W:416:VAL:HG21	2.00	0.44
22:S:49:GLN:HG2	22:S:51:ILE:HG12	1.99	0.44
31:Y:602:CLA:H62	31:Y:602:CLA:H41	1.85	0.44
31:Y:613:CLA:H192	31:Y:613:CLA:H162	1.78	0.44
6:a:127:MET:HB2	6:a:147:TYR:HD2	1.83	0.44
7:b:201:HIS:HB2	31:b:602:CLA:C1B	2.47	0.44
2:12:192:LYS:HB2	2:12:192:LYS:HE2	1.81	0.43
1:14:127:ASN:N	1:14:127:ASN:OD1	2.49	0.43
32:A:414:LHG:H371	31:Y:611:CLA:H202	2.00	0.43
31:R:603:CLA:H162	30:R:606:CHL:H72	1.99	0.43
8:c:240:ILE:HG12	31:c:502:CLA:HBB1	1.99	0.43
40:d:414:SQD:H82	27:x:92:VAL:HG11	2.00	0.43
30:g:609:CHL:H43	30:n:601:CHL:H43	1.99	0.43
2:n:189:LEU:HB3	31:n:610:CLA:H3A	1.99	0.43
31:n:611:CLA:HMA3	32:n:616:LHG:HC32	1.99	0.43
28:y:68:TRP:CZ2	30:y:601:CHL:HBA1	2.53	0.43
28:y:164:TYR:CZ	28:y:171:PRO:HG3	2.53	0.43
31:2:602:CLA:H3A	31:2:602:CLA:HBA2	1.66	0.43
30:5:609:CHL:H142	30:5:609:CHL:H111	1.87	0.43
2:12:86:LEU:HB3	31:12:604:CLA:CBB	2.47	0.43
2:12:198:ARG:HB3	31:12:602:CLA:CBC	2.48	0.43
31:12:609:CLA:C10	31:12:611:CLA:HMB3	2.49	0.43
31:13:603:CLA:O2D	31:13:603:CLA:H2A	2.18	0.43
31:15:604:CLA:H92	31:15:604:CLA:H62	1.79	0.43
31:B:601:CLA:HBB2	39:H:103:BCR:H351	1.99	0.43
8:C:276:LEU:HD21	31:C:509:CLA:HBB1	2.00	0.43
31:C:512:CLA:H202	31:C:512:CLA:H162	1.82	0.43
30:G:609:CHL:H91	30:G:609:CHL:H111	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N:610:CLA:H62	31:N:610:CLA:H41	1.92	0.43
18:O:165:GLN:NE2	18:O:170:ASP:OD2	2.40	0.43
31:R:602:CLA:H61	31:R:602:CLA:H41	1.85	0.43
31:R:603:CLA:H61	31:R:603:CLA:H41	1.67	0.43
22:S:205:GLU:H	22:S:205:GLU:CD	2.26	0.43
7:b:148:LEU:HD11	36:b:623:3PH:H2H2	1.98	0.43
31:b:605:CLA:H61	31:b:605:CLA:H92	1.90	0.43
18:o:125:VAL:HG22	18:o:294:ILE:HG12	2.00	0.43
21:r:165:ARG:NH1	30:r:607:CHL:OBD	2.50	0.43
31:s:610:CLA:H62	31:s:610:CLA:H41	1.87	0.43
31:2:603:CLA:H72	31:3:602:CLA:H91	2.00	0.43
30:4:601:CHL:HBA1	30:4:601:CHL:H3A	1.63	0.43
32:11:615:LHG:H162	32:11:615:LHG:H132	1.85	0.43
7:B:91:TRP:HE1	41:B:622:LMG:HC72	1.83	0.43
30:R:605:CHL:H61	30:R:605:CHL:H41	1.77	0.43
6:a:195:HIS:O	6:a:199:MET:HG3	2.17	0.43
7:b:170:ASP:HB2	7:b:171:PRO:HD2	2.00	0.43
31:b:610:CLA:H102	31:b:610:CLA:H62	1.76	0.43
39:b:619:BCR:H24C	39:b:619:BCR:H371	1.85	0.43
8:c:390:ARG:NH2	20:q:77:GLU:OE1	2.51	0.43
8:c:473:ASP:N	8:c:473:ASP:OD1	2.52	0.43
9:d:85:MET:HE3	9:d:85:MET:HB3	1.89	0.43
31:n:604:CLA:H62	31:n:604:CLA:H41	1.70	0.43
22:s:205:GLU:H	22:s:205:GLU:CD	2.26	0.43
43:y:619:LNL:H15	43:y:619:LNL:H12	1.75	0.43
2:5:89:LEU:HB2	33:5:614:LUT:H401	2.00	0.43
4:8:56:SER:HB2	8:c:29:GLU:HG2	1.99	0.43
10:E:36:LEU:O	10:E:40:THR:OG1	2.22	0.43
12:H:25:LYS:HA	12:H:25:LYS:HD2	1.85	0.43
21:R:256:LYS:HB3	21:R:256:LYS:HE2	1.65	0.43
6:a:299:GLY:O	8:c:403:SER:HB2	2.18	0.43
6:a:316:THR:HG22	6:a:317:TRP:N	2.33	0.43
31:b:607:CLA:H2	41:b:620:LMG:H152	2.00	0.43
9:d:231:THR:OG1	32:d:409:LHG:O4	2.36	0.43
2:n:241:LYS:HE2	2:n:241:LYS:HB2	1.86	0.43
31:s:604:CLA:H142	30:s:606:CHL:H13	2.00	0.43
1:1:126:LEU:HB2	1:1:137:ALA:HB3	2.00	0.43
1:11:78:ILE:HG21	31:11:603:CLA:HAA2	2.00	0.43
30:13:607:CHL:H142	30:13:609:CHL:H102	2.00	0.43
1:14:75:TYR:HE1	31:14:603:CLA:O2A	2.01	0.43
5:16:54:GLY:HA3	5:16:194:ILE:HG21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:A:410:PL9:H322	42:A:410:PL9:H301	1.76	0.43
30:N:605:CHL:H111	31:S:611:CLA:H162	2.00	0.43
19:P:653:GLY:O	19:P:657:SER:OG	2.23	0.43
31:R:603:CLA:HBB1	35:R:616:XAT:C33	2.48	0.43
26:W:417:PHE:HZ	46:W:501:DGD:HA61	1.83	0.43
31:Y:612:CLA:H193	31:Y:612:CLA:H161	1.78	0.43
31:b:601:CLA:HAC1	39:h:102:BCR:H331	1.99	0.43
8:c:265:VAL:HG21	8:c:449:ARG:HD3	2.01	0.43
9:d:148:ALA:HB3	9:d:149:PRO:HD3	2.00	0.43
28:y:212:LEU:HD13	31:y:611:CLA:HBC1	2.00	0.43
31:y:612:CLA:H91	31:y:612:CLA:H112	1.88	0.43
30:5:605:CHL:H3A	30:5:605:CHL:HBA2	1.51	0.43
30:6:608:CHL:H3A	30:6:608:CHL:HBA2	1.55	0.43
36:B:620:3PH:H2G1	40:L:101:SQD:H352	2.00	0.43
8:C:313:GLN:HG3	8:C:396:MET:HE3	2.01	0.43
31:S:604:CLA:H13	30:S:606:CHL:H152	2.00	0.43
32:a:414:LHG:H262	31:y:612:CLA:H71	2.00	0.43
30:r:606:CHL:H91	32:r:619:LHG:H172	1.99	0.43
30:r:606:CHL:H111	32:r:619:LHG:H351	2.00	0.43
22:s:147:MET:SD	22:s:153:LEU:HB2	2.58	0.43
30:1:609:CHL:H41	30:1:609:CHL:H61	1.56	0.43
30:6:605:CHL:H101	30:6:605:CHL:H61	1.62	0.43
2:15:63:LEU:HD23	31:15:602:CLA:C2	2.49	0.43
31:15:612:CLA:C4B	33:15:614:LUT:H183	2.46	0.43
31:B:609:CLA:C2	31:B:610:CLA:HBB2	2.49	0.43
31:C:503:CLA:H111	31:C:504:CLA:HMB2	2.01	0.43
14:J:24:ILE:HG21	41:J:102:LMG:H261	2.01	0.43
31:S:604:CLA:HBA1	31:S:604:CLA:HBD	2.01	0.43
30:S:608:CHL:HBA2	30:S:608:CHL:H3A	1.71	0.43
6:a:60:ILE:HB	6:a:83:ILE:HG22	2.00	0.43
31:c:510:CLA:HBA1	31:c:510:CLA:H3A	1.71	0.43
14:j:24:ILE:HG21	41:j:102:LMG:H261	2.01	0.43
31:r:614:CLA:H92	31:r:614:CLA:H62	1.79	0.43
31:y:602:CLA:HMC1	33:y:623:LUT:C31	2.49	0.43
3:3:120:LYS:HA	30:3:607:CHL:HED1	1.99	0.43
3:6:162:TYR:HD2	30:6:608:CHL:HBB1	1.84	0.43
5:13:233:ASN:HD22	31:13:614:CLA:CGD	2.32	0.43
7:B:258:TYR:OH	9:D:162:LEU:O	2.22	0.43
1:G:160:SER:HB3	2:N:41:PHE:HB3	2.01	0.43
30:G:609:CHL:HBA1	30:N:601:CHL:O1A	2.19	0.43
41:b:621:LMG:O10	21:r:208:TYR:OH	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:276:LEU:HD21	31:c:509:CLA:HBB1	1.99	0.43
34:r:617:NEX:H403	30:r:605:CHL:HBA1	2.00	0.43
22:s:253:PHE:HE1	33:s:618:LUT:H41	1.82	0.43
30:2:609:CHL:H3A	30:2:609:CHL:HBA2	1.33	0.43
2:5:182:ASP:OD2	2:5:182:ASP:C	2.61	0.43
3:6:120:LYS:HA	30:6:607:CHL:HED1	1.99	0.43
1:11:127:ASN:OD1	1:11:127:ASN:N	2.52	0.43
30:11:609:CHL:HED1	2:12:60:THR:HB	2.01	0.43
31:14:611:CLA:C4C	32:14:615:LHG:HC61	2.49	0.43
31:15:602:CLA:H61	31:15:602:CLA:H92	1.74	0.43
7:B:170:ASP:HB2	7:B:171:PRO:HD2	2.01	0.43
31:B:609:CLA:H61	31:B:609:CLA:H92	1.70	0.43
39:D:406:BCR:H20C	39:D:406:BCR:H361	1.92	0.43
31:S:609:CLA:H92	31:S:609:CLA:H61	1.82	0.43
8:c:225:VAL:HG22	8:c:289:MET:HG2	2.00	0.43
41:c:520:LMG:HC1	31:y:611:CLA:HBA1	2.01	0.43
42:d:407:PL9:H221	42:d:407:PL9:H201	1.82	0.43
1:1:94:LEU:HD23	1:1:94:LEU:HA	1.87	0.43
1:1:113:TRP:CE2	1:1:114:PHE:HD2	2.36	0.43
30:15:608:CHL:H72	30:15:608:CHL:H112	1.63	0.43
8:C:163:ILE:HG23	43:C:523:LNL:H141	2.00	0.43
8:C:225:VAL:HG22	8:C:289:MET:HG2	2.01	0.43
7:b:18:ARG:NH1	16:l:5:ASN:OD1	2.52	0.43
31:b:604:CLA:C2C	31:b:613:CLA:HAB	2.49	0.43
31:b:611:CLA:H202	31:b:611:CLA:H161	1.73	0.43
8:c:333:GLY:HA2	8:c:339:LYS:HG3	2.01	0.43
32:g:615:LHG:H361	35:g:619:XAT:H371	2.00	0.43
31:n:613:CLA:H93	32:n:616:LHG:H151	2.01	0.43
31:r:609:CLA:H62	31:r:609:CLA:H41	1.89	0.43
1:4:192:GLU:HG2	1:4:196:LYS:HE3	2.01	0.42
1:11:78:ILE:HG12	30:11:609:CHL:HED2	2.01	0.42
31:11:602:CLA:HBA2	31:11:602:CLA:H3A	1.79	0.42
2:12:91:CYS:SG	33:12:615:LUT:H41	2.59	0.42
5:13:175:ASP:OD1	33:13:617:LUT:O23	2.27	0.42
1:14:47:PRO:HG2	1:14:61:ASP:HB3	2.01	0.42
1:14:75:TYR:CE1	31:14:602:CLA:H43	2.54	0.42
1:14:246:LEU:HD12	1:14:247:PRO:HD2	2.00	0.42
5:16:209:ILE:HD12	31:16:613:CLA:HBC1	2.01	0.42
30:16:605:CHL:H8	32:r:621:LHG:H161	2.00	0.42
31:B:601:CLA:H8	31:B:601:CLA:H52	1.72	0.42
8:C:226:SER:O	8:C:226:SER:OG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:C:520:LMG:HC1	31:Y:611:CLA:HBA1	2.00	0.42
7:b:242:ILE:HA	7:b:245:VAL:HG22	2.01	0.42
31:c:502:CLA:H152	31:c:508:CLA:H72	2.01	0.42
31:n:611:CLA:H12	31:n:611:CLA:HBA1	1.69	0.42
31:2:603:CLA:O1A	3:3:74:SER:OG	2.37	0.42
31:4:604:CLA:H12	30:4:606:CHL:HBD	2.01	0.42
30:4:608:CHL:HHC	30:4:608:CHL:HBB1	2.01	0.42
31:6:613:CLA:H62	31:6:613:CLA:H2	1.76	0.42
1:11:202:ARG:HA	1:11:205:MET:HE3	2.01	0.42
31:12:609:CLA:H3A	31:12:609:CLA:HBA2	1.60	0.42
2:15:210:GLN:OE1	31:15:612:CLA:ND	2.52	0.42
6:A:153:ALA:HB1	31:A:402:CLA:HED1	2.01	0.42
6:A:155:THR:HG21	46:C:517:DGD:HBH2	2.01	0.42
31:G:602:CLA:H18	31:G:602:CLA:H152	1.74	0.42
21:R:272:PHE:CE2	35:R:616:XAT:H10	2.55	0.42
28:Y:46:LEU:HD23	28:Y:46:LEU:HA	1.87	0.42
28:Y:141:LEU:HD23	28:Y:141:LEU:HA	1.82	0.42
6:a:175:GLY:O	6:a:179:THR:OG1	2.23	0.42
31:c:506:CLA:H161	31:c:506:CLA:H202	1.77	0.42
1:g:160:SER:HB3	2:n:41:PHE:HB3	2.01	0.42
31:s:604:CLA:HAB	34:s:620:NEX:C39	2.49	0.42
30:s:606:CHL:H112	30:s:606:CHL:H71	1.91	0.42
1:1:114:PHE:HD1	30:1:607:CHL:H11	1.84	0.42
30:4:609:CHL:HBA2	30:4:609:CHL:H3A	1.29	0.42
31:6:615:CLA:HBA1	31:6:615:CLA:CBD	2.48	0.42
31:12:609:CLA:C2B	31:12:609:CLA:H42	2.48	0.42
31:14:603:CLA:HBA1	31:14:603:CLA:H11	1.78	0.42
2:15:226:LEU:HA	31:15:613:CLA:HBB1	2.01	0.42
31:B:615:CLA:HBA1	31:B:615:CLA:H3A	1.81	0.42
8:C:473:ASP:N	8:C:473:ASP:OD1	2.52	0.42
31:G:610:CLA:H203	34:G:618:NEX:H363	2.01	0.42
30:Y:606:CHL:H61	30:Y:606:CHL:H41	1.84	0.42
31:a:403:CLA:H72	31:d:402:CLA:HAB	2.01	0.42
31:b:609:CLA:H92	31:b:609:CLA:H61	1.70	0.42
39:c:526:BCR:H24C	39:c:526:BCR:H371	1.84	0.42
30:2:608:CHL:HBA1	30:2:608:CHL:H12	1.79	0.42
3:6:197:LEU:HD13	31:6:610:CLA:HBA2	2.01	0.42
31:15:603:CLA:H92	31:15:603:CLA:H41	2.00	0.42
31:15:612:CLA:HBA1	31:15:612:CLA:CHA	2.49	0.42
5:16:38:GLY:HA3	5:16:39:PRO:HD3	1.91	0.42
6:A:60:ILE:HD12	6:A:84:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:161:TYR:HB3	6:A:162:PRO:HD3	2.00	0.42
7:B:42:LEU:HD11	7:B:93:TYR:HB3	2.00	0.42
31:B:611:CLA:H203	31:B:613:CLA:H8	2.02	0.42
8:C:265:VAL:HG21	8:C:449:ARG:HD3	2.02	0.42
9:D:134:ARG:HG2	40:D:411:SQD:H1	2.01	0.42
2:N:176:PRO:HD2	33:N:617:LUT:H23	2.01	0.42
7:b:3:LEU:HD23	7:b:3:LEU:HA	1.94	0.42
18:o:124:LYS:HB3	18:o:133:PHE:HB3	2.01	0.42
21:r:246:LEU:HB2	31:r:609:CLA:HBA1	2.01	0.42
22:s:148:LEU:HA	22:s:148:LEU:HD23	1.76	0.42
28:y:248:TYR:HA	28:y:252:ALA:HB2	2.00	0.42
1:4:211:PHE:HE1	33:4:616:LUT:H41	1.85	0.42
31:6:610:CLA:H61	31:6:610:CLA:H92	1.75	0.42
1:14:156:ALA:HB1	2:15:41:PHE:CE1	2.54	0.42
30:14:609:CHL:H41	30:14:609:CHL:H61	1.49	0.42
2:15:86:LEU:HB3	31:15:604:CLA:CBB	2.50	0.42
39:B:617:BCR:H15C	36:B:620:3PH:H3E1	2.00	0.42
31:C:510:CLA:HBA1	31:C:510:CLA:H3A	1.71	0.42
21:R:165:ARG:NH1	30:R:607:CHL:OBD	2.50	0.42
22:s:103:LYS:NZ	22:s:107:ASN:OD1	2.51	0.42
31:s:613:CLA:H2A	31:s:613:CLA:HED3	2.01	0.42
31:y:615:CLA:H92	31:y:615:CLA:H61	1.80	0.42
2:5:93:THR:OG1	2:5:94:PRO:HD3	2.20	0.42
36:7:201:3PH:H232	14:J:13:TRP:HB3	2.00	0.42
31:12:612:CLA:C2B	33:12:614:LUT:H42	2.49	0.42
5:16:144:GLN:OE1	30:16:607:CHL:HMC	2.20	0.42
31:A:402:CLA:H201	32:D:408:LHG:H312	2.00	0.42
31:B:604:CLA:C2C	31:B:613:CLA:HAB	2.49	0.42
31:C:505:CLA:HAA1	31:C:505:CLA:HBD	2.02	0.42
6:a:82:ILE:HB	6:a:174:LEU:HB2	2.02	0.42
31:a:403:CLA:H201	32:d:408:LHG:H312	2.00	0.42
42:a:410:PL9:H472	42:a:410:PL9:H451	1.85	0.42
7:b:348:ASP:OD1	7:b:349:LYS:N	2.53	0.42
31:g:602:CLA:H152	31:g:602:CLA:H18	1.72	0.42
2:n:82:ARG:NH1	30:n:608:CHL:OBD	2.47	0.42
2:n:188:GLU:O	2:n:192:LYS:HG3	2.19	0.42
50:n:620:PAM:H52	31:y:615:CLA:CAD	2.49	0.42
18:o:155:VAL:HG22	18:o:161:VAL:HG12	2.01	0.42
18:o:271:GLU:HG2	18:o:303:GLN:HG2	2.01	0.42
20:q:156:LYS:HE2	20:q:156:LYS:HB3	1.75	0.42
21:r:164:GLY:O	21:r:168:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:605:CHL:H3A	30:2:605:CHL:HBA2	1.54	0.42
1:4:91:LEU:HD22	1:4:91:LEU:HA	1.90	0.42
31:4:602:CLA:H92	31:4:602:CLA:H62	1.67	0.42
32:4:615:LHG:H131	35:6:620:XAT:H403	2.02	0.42
3:6:156:MET:HA	3:6:159:VAL:HG22	2.01	0.42
31:14:611:CLA:H41	31:14:611:CLA:H61	1.66	0.42
31:16:611:CLA:HAA1	31:16:611:CLA:HBD	2.02	0.42
41:A:409:LMG:H251	8:C:281:ILE:HG12	2.00	0.42
39:B:618:BCR:H371	39:B:618:BCR:H24C	1.85	0.42
16:L:13:LEU:HA	32:L:102:LHG:HC11	2.01	0.42
50:N:621:PAM:H41	31:Y:615:CLA:CAD	2.50	0.42
31:Y:610:CLA:H102	31:Y:610:CLA:H62	1.80	0.42
6:a:60:ILE:HD12	6:a:84:PRO:HD2	2.01	0.42
6:a:238:LYS:HA	6:a:238:LYS:HD3	1.90	0.42
39:b:617:BCR:H24C	39:b:617:BCR:H371	1.88	0.42
33:12:614:LUT:H191	33:12:614:LUT:H12	2.01	0.42
31:15:603:CLA:CAD	30:15:608:CHL:H11	2.50	0.42
8:C:333:GLY:HA2	8:C:339:LYS:HG3	2.02	0.42
9:D:323:GLU:OE1	18:O:232:LYS:HE3	2.20	0.42
2:N:233:ASN:HD21	2:N:236:VAL:HB	1.84	0.42
21:R:246:LEU:HB2	31:R:609:CLA:HBA1	2.02	0.42
30:R:607:CHL:H3A	30:R:607:CHL:HBA2	1.70	0.42
31:R:614:CLA:H92	31:R:614:CLA:H62	1.75	0.42
7:b:321:LYS:HB3	7:b:321:LYS:HE3	1.75	0.42
7:b:422:ARG:HD3	18:o:230:TYR:CE2	2.55	0.42
2:n:144:GLN:OE1	30:n:607:CHL:HMC	2.20	0.42
31:r:614:CLA:H62	31:r:614:CLA:H41	1.68	0.42
28:y:220:PHE:HE1	33:y:622:LUT:H41	1.84	0.42
30:y:601:CHL:H62	30:y:601:CHL:H41	1.66	0.42
4:8:102:GLU:OE2	11:f:6:SER:HA	2.19	0.42
31:11:602:CLA:HBD	31:11:602:CLA:HAA1	2.02	0.42
31:G:604:CLA:HAA1	31:G:604:CLA:HBD	2.02	0.42
9:d:56:THR:OG1	9:d:57:SER:N	2.52	0.42
31:g:613:CLA:H101	32:g:615:LHG:H131	2.02	0.42
22:s:94:LEU:HD13	31:s:602:CLA:H42	2.02	0.42
22:s:173:VAL:HG12	30:s:607:CHL:HBC1	2.02	0.42
22:s:211:MET:HE3	22:s:211:MET:HB3	1.88	0.42
1:1:74:ARG:HA	1:1:74:ARG:HD3	1.67	0.42
1:1:199:LYS:HB3	1:1:199:LYS:HE2	1.84	0.42
30:1:601:CHL:HHC	30:1:601:CHL:HBB1	2.02	0.42
3:3:46:PRO:HB3	30:3:601:CHL:HBC1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:612:CLA:HBA1	31:3:612:CLA:H3A	1.83	0.42
30:4:601:CHL:HHC	30:4:601:CHL:HBB1	2.02	0.42
30:5:605:CHL:HHC	30:5:605:CHL:HBB1	2.02	0.42
5:13:112:LYS:HA	30:13:607:CHL:HED1	2.02	0.42
31:14:602:CLA:HAA1	31:14:602:CLA:HBD	2.02	0.42
42:A:410:PL9:H303	32:A:411:LHG:H372	2.01	0.42
31:B:604:CLA:H92	31:B:604:CLA:H61	1.71	0.42
8:C:57:ALA:O	8:C:61:VAL:HG23	2.20	0.42
9:D:241:GLU:CD	9:D:241:GLU:H	2.27	0.42
30:N:609:CHL:H111	30:N:609:CHL:H71	1.92	0.42
6:a:197:PHE:HE1	46:c:519:DGD:HBW2	1.84	0.42
31:b:611:CLA:H112	31:b:611:CLA:H72	1.76	0.42
2:n:63:LEU:HD13	31:n:602:CLA:H42	2.01	0.42
31:r:609:CLA:H3A	31:r:609:CLA:HBA2	1.66	0.42
1:4:155:GLU:HG3	30:4:609:CHL:C4B	2.50	0.41
2:5:80:HIS:CE1	31:5:603:CLA:ND	2.87	0.41
4:7:87:ASN:ND2	9:D:233:ARG:O	2.45	0.41
31:12:609:CLA:H2A	31:12:609:CLA:HED3	2.02	0.41
2:15:91:CYS:SG	33:15:615:LUT:H41	2.59	0.41
2:15:111:PHE:CD1	31:16:615:CLA:HBB2	2.55	0.41
2:15:123:LEU:HD21	31:15:604:CLA:HBA1	2.02	0.41
2:15:198:ARG:HB3	31:15:602:CLA:CBC	2.50	0.41
31:16:602:CLA:HBC3	32:16:616:LHG:H261	2.01	0.41
6:A:280:VAL:HG11	32:D:409:LHG:H282	2.02	0.41
6:A:316:THR:HG22	6:A:317:TRP:N	2.34	0.41
6:A:336:ALA:O	8:C:354:GLU:HG3	2.20	0.41
31:B:605:CLA:HBC3	31:B:612:CLA:H42	2.01	0.41
31:C:505:CLA:H62	31:C:505:CLA:H41	1.87	0.41
9:D:51:GLY:HA3	9:D:78:VAL:HG22	2.02	0.41
9:D:56:THR:OG1	9:D:57:SER:N	2.53	0.41
1:G:243:THR:HG23	30:Y:607:CHL:HED1	2.02	0.41
1:G:247:PRO:HD3	30:Y:607:CHL:H12	2.02	0.41
18:O:171:PHE:CD2	18:O:187:MET:HE1	2.55	0.41
22:S:53:LEU:HD23	22:S:53:LEU:HA	1.92	0.41
31:Y:612:CLA:H91	31:Y:612:CLA:H112	1.86	0.41
7:b:44:VAL:HG23	7:b:60:MET:HE1	2.02	0.41
7:b:56:TRP:CD1	7:b:56:TRP:H	2.36	0.41
31:b:604:CLA:HAA1	31:b:604:CLA:HBD	2.02	0.41
10:e:20:TRP:CD1	14:j:10:ILE:HD12	2.54	0.41
1:g:95:THR:HB	1:g:96:PRO:HD3	2.02	0.41
31:n:602:CLA:H41	31:n:602:CLA:H61	1.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:351:LEU:HD23	24:u:351:LEU:HA	1.85	0.41
31:1:603:CLA:H11	2:2:63:LEU:HD21	2.02	0.41
3:6:184:PRO:HD2	33:6:618:LUT:H23	2.02	0.41
1:11:120:ILE:HG12	1:11:140:ILE:HG22	2.01	0.41
2:12:58:TRP:HE3	31:12:602:CLA:HMD1	1.84	0.41
2:15:93:THR:OG1	2:15:94:PRO:HD3	2.20	0.41
46:C:518:DGD:HA21	46:C:519:DGD:HB31	2.02	0.41
31:G:602:CLA:H62	31:G:602:CLA:H41	1.96	0.41
29:Z:48:PHE:O	29:Z:51:VAL:HG12	2.20	0.41
31:c:503:CLA:H92	31:c:513:CLA:H51	2.03	0.41
12:h:48:MET:HG2	39:h:102:BCR:H393	2.02	0.41
31:n:602:CLA:H92	31:n:602:CLA:H62	1.72	0.41
21:r:161:LEU:HD12	21:r:235:CYS:HB3	2.01	0.41
30:1:606:CHL:HBB2	30:1:607:CHL:CBB	2.51	0.41
30:2:608:CHL:HBA2	30:2:608:CHL:H3A	1.71	0.41
31:3:614:CLA:HBA1	31:3:614:CLA:CBD	2.49	0.41
1:4:113:TRP:CE2	1:4:114:PHE:HD2	2.39	0.41
1:11:76:ARG:O	1:11:80:VAL:HG22	2.20	0.41
31:12:604:CLA:H12	30:12:605:CHL:HBD	2.01	0.41
30:14:608:CHL:CHA	30:14:608:CHL:HBA1	2.51	0.41
5:16:58:TRP:CZ3	33:16:618:LUT:H383	2.55	0.41
39:A:407:BCR:H20C	39:A:407:BCR:H361	1.91	0.41
7:B:18:ARG:NH1	16:L:5:ASN:OD1	2.53	0.41
7:B:422:ARG:HD3	18:O:230:TYR:CE2	2.54	0.41
36:B:624:3PH:H272	30:R:606:CHL:HAA2	2.02	0.41
8:C:339:LYS:HD3	19:P:575:GLY:HA3	2.01	0.41
31:R:602:CLA:HBC3	31:R:602:CLA:HHD	2.02	0.41
30:R:606:CHL:H8	32:R:619:LHG:H151	2.03	0.41
31:Y:612:CLA:HBC2	31:Y:612:CLA:HHD	2.02	0.41
6:a:43:THR:HG23	39:a:408:BCR:H362	2.02	0.41
6:a:153:ALA:HB1	31:a:403:CLA:HED1	2.02	0.41
7:b:504:ARG:NH1	7:b:504:ARG:HG3	2.35	0.41
31:b:610:CLA:HHC	31:b:610:CLA:HBB1	2.02	0.41
31:c:511:CLA:H112	31:c:511:CLA:H151	1.94	0.41
30:n:607:CHL:H193	32:y:616:LHG:H181	2.02	0.41
18:o:110:THR:HA	18:o:154:THR:HA	2.03	0.41
22:s:107:ASN:ND2	31:s:609:CLA:OBD	2.53	0.41
31:3:612:CLA:H192	31:3:612:CLA:H161	1.87	0.41
1:4:198:ILE:HD12	1:4:198:ILE:HA	1.83	0.41
31:12:609:CLA:H61	31:12:611:CLA:H3A	2.02	0.41
31:13:603:CLA:H12	31:13:603:CLA:H72	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:14:214:GLN:HE21	1:14:214:GLN:HB3	1.66	0.41
2:15:76:LEU:HD13	31:15:603:CLA:HAA2	2.01	0.41
31:16:611:CLA:H202	31:16:611:CLA:H162	1.75	0.41
39:C:526:BCR:H24C	39:C:526:BCR:H371	1.84	0.41
31:N:613:CLA:H62	31:N:613:CLA:H41	1.74	0.41
18:O:101:GLN:C	18:O:101:GLN:OE1	2.63	0.41
31:c:505:CLA:HBD	31:c:505:CLA:HAA1	2.03	0.41
10:e:36:LEU:O	10:e:40:THR:OG1	2.23	0.41
1:g:208:MET:HE2	33:g:617:LUT:H10	2.02	0.41
30:g:609:CHL:H111	30:g:609:CHL:H91	1.82	0.41
16:l:13:LEU:HA	32:l:102:LHG:HC11	2.02	0.41
19:p:554:LEU:HD22	19:p:604:TYR:CD1	2.55	0.41
21:r:187:ALA:O	21:r:191:LEU:HD23	2.20	0.41
31:s:611:CLA:HBD	31:s:611:CLA:HAA1	2.02	0.41
31:1:603:CLA:HED3	33:2:615:LUT:H372	2.01	0.41
1:4:147:GLN:HE22	30:4:607:CHL:HBC2	1.86	0.41
1:11:209:PHE:O	1:11:213:VAL:HG22	2.19	0.41
2:12:93:THR:OG1	2:12:94:PRO:HD3	2.20	0.41
31:13:602:CLA:HAA1	31:13:602:CLA:HBD	2.02	0.41
2:15:93:THR:HG21	31:15:604:CLA:HAC2	2.02	0.41
31:15:604:CLA:HAB	34:15:616:NEX:H393	2.02	0.41
31:16:610:CLA:H41	31:16:610:CLA:H62	1.73	0.41
6:A:127:MET:HB2	6:A:147:TYR:HD2	1.85	0.41
6:A:317:TRP:CZ3	9:D:180:ARG:HD2	2.56	0.41
8:C:170:LEU:HD23	8:C:170:LEU:HA	1.91	0.41
31:C:511:CLA:H151	31:C:511:CLA:H112	1.93	0.41
9:D:323:GLU:OE2	18:O:228:TRP:NE1	2.52	0.41
40:L:101:SQD:H251	40:L:101:SQD:H282	1.87	0.41
19:P:554:LEU:HD22	19:P:604:TYR:CD1	2.55	0.41
30:S:606:CHL:H93	30:S:606:CHL:H111	1.86	0.41
6:a:64:ARG:O	18:o:212:ARG:NH2	2.47	0.41
42:a:410:PL9:H352	32:a:411:LHG:H321	2.03	0.41
9:d:45:LEU:HD23	9:d:45:LEU:HA	1.93	0.41
9:d:165:SER:HB2	9:d:169:PHE:CD2	2.56	0.41
1:g:49:TYR:OH	1:g:61:ASP:OD2	2.26	0.41
31:n:610:CLA:H61	31:n:610:CLA:H92	1.79	0.41
19:p:543:ASN:HB3	19:p:545:ASP:OD1	2.19	0.41
21:r:272:PHE:CE2	35:r:616:XAT:H10	2.55	0.41
28:y:189:PRO:HD2	33:y:622:LUT:H23	2.02	0.41
30:y:601:CHL:H91	30:y:601:CHL:H111	1.87	0.41
2:2:38:LEU:HD23	2:2:38:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:609:CHL:H162	30:2:609:CHL:H121	1.94	0.41
31:4:610:CLA:HBA2	31:4:610:CLA:H3A	1.71	0.41
3:6:192:ASP:OD1	3:6:192:ASP:N	2.53	0.41
5:13:33:ARG:H	5:13:33:ARG:HG3	1.51	0.41
5:16:194:ILE:HD12	5:16:194:ILE:HA	1.82	0.41
6:A:43:THR:HG23	39:A:407:BCR:H362	2.02	0.41
31:C:505:CLA:H42	46:C:518:DGD:HB32	2.02	0.41
39:C:515:BCR:H20C	39:C:515:BCR:H361	1.91	0.41
2:N:213:ILE:HG22	2:N:214:THR:HG23	2.03	0.41
19:P:650:GLU:H	19:P:650:GLU:HG2	1.60	0.41
28:Y:68:TRP:CZ2	30:Y:601:CHL:HBA1	2.55	0.41
6:a:170:ASP:OD1	8:c:357:ARG:NH2	2.51	0.41
42:a:410:PL9:HC2	42:a:410:PL9:HC8	1.77	0.41
1:g:243:THR:HG23	30:y:607:CHL:HED1	2.03	0.41
2:n:233:ASN:HD21	2:n:236:VAL:HB	1.85	0.41
31:s:610:CLA:H92	31:s:610:CLA:H61	1.74	0.41
28:y:207:ILE:HD12	28:y:207:ILE:HA	1.87	0.41
1:1:91:LEU:HD22	1:1:91:LEU:HA	1.91	0.41
2:2:98:GLN:OE1	2:2:105:PHE:N	2.43	0.41
31:2:603:CLA:HBB1	30:2:609:CHL:H162	2.03	0.41
3:3:200:LYS:NZ	31:3:612:CLA:O1D	2.53	0.41
31:12:602:CLA:H62	31:12:602:CLA:H92	1.77	0.41
31:15:612:CLA:C1D	31:15:612:CLA:H2	2.51	0.41
6:A:64:ARG:O	18:O:212:ARG:NH2	2.50	0.41
31:B:610:CLA:HHC	31:B:610:CLA:HBB1	2.02	0.41
12:H:48:MET:HG2	39:H:103:BCR:H312	2.02	0.41
30:S:606:CHL:H171	30:S:608:CHL:HBA1	2.02	0.41
31:S:614:CLA:H192	31:S:614:CLA:H162	1.83	0.41
32:Y:618:LHG:HC31	32:Y:618:LHG:HC62	2.03	0.41
18:o:114:ASP:OD1	18:o:115:LYS:N	2.53	0.41
31:r:613:CLA:H8	31:r:614:CLA:H2	2.03	0.41
2:2:72:ARG:NH1	2:2:75:GLU:OE1	2.51	0.41
3:3:156:MET:HA	3:3:159:VAL:HG22	2.01	0.41
1:14:196:LYS:HZ3	31:14:612:CLA:HED3	1.83	0.41
7:B:91:TRP:CH2	31:B:606:CLA:H12	2.56	0.41
8:C:394:GLU:OE2	20:Q:85:GLN:NE2	2.44	0.41
9:D:294:ARG:H	9:D:294:ARG:HG2	1.63	0.41
22:S:136:LYS:NZ	22:S:152:THR:O	2.52	0.41
22:S:147:MET:HE3	22:S:153:LEU:HB2	2.02	0.41
28:Y:220:PHE:HE1	33:Y:621:LUT:H41	1.86	0.41
31:b:607:CLA:H162	31:b:607:CLA:H202	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c:213:LEU:HD22	31:c:507:CLA:H193	2.02	0.41
9:d:216:ALA:O	9:d:220:ASN:ND2	2.41	0.41
1:g:172:LEU:HD12	1:g:172:LEU:HA	1.91	0.41
30:s:606:CHL:H171	30:s:608:CHL:HAA2	2.03	0.41
31:s:611:CLA:H203	31:s:612:CLA:HBB1	2.03	0.41
30:y:605:CHL:H51	30:y:605:CHL:H8	1.70	0.41
31:y:612:CLA:HBC2	31:y:612:CLA:HHD	2.02	0.41
1:1:91:LEU:HB3	31:1:604:CLA:HMC2	2.03	0.41
1:1:128:TYR:CE2	31:1:604:CLA:H2	2.54	0.41
2:2:194:LEU:HD23	2:2:194:LEU:HA	1.88	0.41
30:3:605:CHL:H191	31:R:602:CLA:H141	2.01	0.41
2:5:85:MET:HE1	31:5:610:CLA:CBB	2.51	0.41
3:6:49:LEU:HD23	3:6:49:LEU:HA	1.93	0.41
1:11:88:LEU:HD23	1:11:88:LEU:HA	1.89	0.41
31:11:610:CLA:H62	33:11:616:LUT:C30	2.50	0.41
31:11:611:CLA:C4C	32:11:615:LHG:HC61	2.50	0.41
2:12:89:LEU:HD13	31:12:611:CLA:HBB2	2.03	0.41
2:12:96:LEU:HD23	2:12:96:LEU:HA	1.90	0.41
30:13:609:CHL:H93	30:13:609:CHL:H61	1.93	0.41
1:14:238:GLY:HA2	31:14:613:CLA:CAD	2.51	0.41
31:14:610:CLA:H112	31:14:610:CLA:H151	1.62	0.41
2:15:34:ARG:NH2	2:15:55:ASP:HB3	2.35	0.41
30:15:607:CHL:H3A	30:15:607:CHL:HBA2	1.39	0.41
6:A:238:LYS:HD3	6:A:238:LYS:HA	1.81	0.41
7:B:242:ILE:HA	7:B:245:VAL:HG22	2.03	0.41
9:D:313:THR:O	9:D:317:LYS:HG3	2.21	0.41
21:R:139:VAL:HG13	21:R:146:PRO:HB2	2.01	0.41
21:R:161:LEU:HD12	21:R:235:CYS:HB3	2.02	0.41
22:S:43:TRP:CZ2	41:S:616:LMG:HC71	2.55	0.41
22:S:103:LYS:NZ	22:S:107:ASN:OD1	2.53	0.41
22:S:239:GLU:HB2	31:S:610:CLA:C1B	2.51	0.41
32:Y:618:LHG:H331	32:Y:618:LHG:H361	1.82	0.41
6:a:151:VAL:HG12	46:c:517:DGD:HBV2	2.02	0.41
7:b:486:LEU:O	7:b:490:VAL:HG23	2.21	0.41
31:b:605:CLA:HBC3	31:b:612:CLA:H42	2.03	0.41
31:b:611:CLA:H203	31:b:613:CLA:H8	2.03	0.41
31:b:614:CLA:H62	31:b:614:CLA:H41	1.73	0.41
9:d:313:THR:O	9:d:317:LYS:HG3	2.20	0.41
31:d:402:CLA:H91	42:d:407:PL9:H402	2.02	0.41
1:g:87:MET:HE2	1:g:201:GLY:CA	2.51	0.41
40:l:101:SQD:H1	40:l:101:SQD:H45	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:58:TRP:CE3	33:n:618:LUT:H383	2.56	0.41
31:n:615:CLA:HBA1	31:n:615:CLA:CBD	2.45	0.41
32:n:616:LHG:H223	32:n:616:LHG:H191	1.92	0.41
20:q:106:LYS:HE3	20:q:106:LYS:HB2	1.93	0.41
21:r:139:VAL:HG13	21:r:146:PRO:HB2	2.02	0.41
22:s:293:LEU:HD23	22:s:293:LEU:HA	1.87	0.41
28:y:141:LEU:HA	28:y:141:LEU:HD23	1.83	0.41
1:1:120:ILE:HG12	1:1:140:ILE:HG22	2.03	0.41
31:3:614:CLA:HBA1	31:3:614:CLA:CHA	2.52	0.41
31:12:609:CLA:H41	33:12:614:LUT:H28	2.03	0.41
31:14:612:CLA:HBB1	33:14:616:LUT:C14	2.50	0.41
7:B:246:PHE:CD1	7:B:246:PHE:C	2.98	0.41
31:B:612:CLA:HAA2	31:B:612:CLA:H71	2.03	0.41
9:D:36:LEU:O	9:D:40:THR:OG1	2.34	0.41
31:N:602:CLA:CBB	33:N:618:LUT:H32	2.51	0.41
31:N:604:CLA:H41	31:N:604:CLA:H62	1.70	0.41
22:S:112:ALA:HB2	22:S:247:MET:HE2	2.03	0.41
31:S:604:CLA:H202	31:S:604:CLA:H162	1.79	0.41
31:b:609:CLA:C2	31:b:610:CLA:HBB2	2.51	0.41
8:c:240:ILE:HD12	8:c:240:ILE:HA	1.99	0.41
30:n:607:CHL:H3A	30:n:607:CHL:HBA2	1.75	0.41
31:2:603:CLA:HHD	30:2:609:CHL:HMD2	2.02	0.40
3:3:184:PRO:HD2	33:3:618:LUT:H23	2.03	0.40
4:7:42:SER:OG	4:7:98:ASP:OD1	2.38	0.40
1:11:43:GLU:OE2	1:11:43:GLU:C	2.64	0.40
31:11:604:CLA:HMB1	30:11:606:CHL:HBB1	2.03	0.40
6:A:82:ILE:HB	6:A:174:LEU:HB2	2.02	0.40
30:N:607:CHL:H161	32:Y:616:LHG:H182	2.03	0.40
20:Q:164:GLU:OE1	20:Q:194:LYS:HE2	2.21	0.40
21:R:274:GLY:O	21:R:275:TYR:C	2.64	0.40
31:b:606:CLA:H162	31:b:606:CLA:H122	1.80	0.40
31:b:615:CLA:H162	31:b:615:CLA:H122	1.87	0.40
46:c:518:DGD:HA21	46:c:519:DGD:HB31	2.03	0.40
32:c:521:LHG:O9	32:c:521:LHG:O2	2.22	0.40
2:n:207:PHE:CE1	33:n:617:LUT:H41	2.55	0.40
29:z:17:PHE:O	29:z:21:VAL:HG23	2.21	0.40
31:1:602:CLA:H142	33:1:617:LUT:H393	2.02	0.40
3:3:169:ALA:HA	32:3:617:LHG:HC5	2.03	0.40
1:11:214:GLN:O	1:11:218:THR:HG22	2.21	0.40
31:12:612:CLA:HBB1	33:12:614:LUT:H182	1.99	0.40
31:13:611:CLA:HAA1	31:13:611:CLA:HBD	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:16:616:LHG:H282	32:16:616:LHG:H311	1.87	0.40
31:A:403:CLA:H91	42:D:407:PL9:H402	2.03	0.40
31:B:606:CLA:H162	31:B:606:CLA:H122	1.84	0.40
32:g:615:LHG:H171	32:g:615:LHG:H142	1.87	0.40
31:n:611:CLA:H51	31:n:612:CLA:HED3	2.04	0.40
27:x:89:ILE:O	27:x:93:SER:OG	2.32	0.40
2:2:58:TRP:CE3	33:2:615:LUT:H383	2.57	0.40
2:2:144:GLN:O	2:2:148:MET:HB2	2.21	0.40
1:11:238:GLY:N	31:11:613:CLA:O1A	2.44	0.40
33:14:617:LUT:H372	31:16:603:CLA:HED3	2.03	0.40
5:16:135:GLN:HG3	30:16:605:CHL:HAB	2.02	0.40
22:S:58:GLY:O	22:S:61:ARG:NH1	2.47	0.40
32:S:621:LHG:H341	31:S:614:CLA:H2	2.04	0.40
39:d:406:BCR:H393	41:d:410:LMG:H171	2.03	0.40
1:g:135:ILE:HD13	1:g:135:ILE:HA	1.83	0.40
1:g:247:PRO:HD3	30:y:607:CHL:H12	2.03	0.40
31:g:603:CLA:H41	31:g:603:CLA:H62	1.90	0.40
32:n:616:LHG:H121	32:n:616:LHG:HC92	1.95	0.40
31:r:609:CLA:CBB	33:r:615:LUT:H34	2.51	0.40
28:y:174:PHE:HB2	43:y:619:LNL:H61	2.03	0.40
1:1:128:TYR:CD1	1:1:129:LEU:HG	2.57	0.40
2:2:213:ILE:HA	2:2:213:ILE:HD12	1.86	0.40
31:2:613:CLA:HBD	31:2:613:CLA:HED3	1.86	0.40
3:3:61:LEU:HD11	3:3:72:ASP:HB2	2.04	0.40
31:3:610:CLA:HBA2	31:3:610:CLA:H3A	1.51	0.40
1:11:154:ALA:HB1	30:11:608:CHL:HMA1	2.02	0.40
31:11:603:CLA:HMA2	31:11:603:CLA:H2	2.02	0.40
2:12:153:GLY:HA3	5:13:40:PHE:CD1	2.57	0.40
2:15:78:VAL:O	2:15:82:ARG:HG3	2.22	0.40
7:B:148:LEU:HD11	36:B:624:3PH:H2G2	2.02	0.40
7:B:149:LEU:HD13	31:B:604:CLA:H192	2.02	0.40
31:B:613:CLA:H41	31:B:613:CLA:H62	1.66	0.40
2:N:207:PHE:CE1	33:N:617:LUT:H41	2.56	0.40
31:N:604:CLA:CMB	30:N:606:CHL:HBB1	2.51	0.40
30:Y:606:CHL:HBA2	30:Y:606:CHL:HBD	2.04	0.40
7:b:296:LYS:NZ	7:b:304:GLU:OE1	2.41	0.40
31:b:605:CLA:HAA1	31:b:605:CLA:HBD	2.03	0.40
31:b:612:CLA:H61	31:b:612:CLA:H101	1.87	0.40
8:c:279:ILE:HD11	8:c:437:PHE:CD2	2.57	0.40
30:g:601:CHL:HMB2	28:y:163:ILE:HD11	2.03	0.40
31:g:604:CLA:CMB	30:g:606:CHL:HBB1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:125:TYR:HB2	2:2:132:ILE:HG12	2.02	0.40
31:2:604:CLA:HBA1	31:2:604:CLA:CBD	2.51	0.40
30:6:607:CHL:H92	30:6:607:CHL:H62	1.80	0.40
30:6:607:CHL:H142	30:6:607:CHL:H111	1.86	0.40
1:11:98:LEU:HD13	1:11:223:LEU:HD11	2.03	0.40
2:12:58:TRP:HE3	31:12:602:CLA:CMD	2.35	0.40
2:12:111:PHE:CD1	2:12:112:LYS:HG3	2.57	0.40
5:13:230:SER:HA	31:13:614:CLA:HMA1	2.02	0.40
2:15:54:GLY:HA3	2:15:194:LEU:HD23	2.04	0.40
6:A:312:ARG:HE	6:A:312:ARG:HB3	1.70	0.40
31:B:605:CLA:HBD	31:B:605:CLA:HAA1	2.04	0.40
39:B:618:BCR:H20C	39:B:618:BCR:H361	1.90	0.40
8:C:279:ILE:HD11	8:C:437:PHE:CD2	2.56	0.40
31:C:504:CLA:H41	31:C:504:CLA:H61	1.94	0.40
30:g:609:CHL:HAA2	2:n:60:THR:HG21	2.03	0.40
2:n:234:PHE:N	31:n:613:CLA:O1A	2.54	0.40

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	1	216/249 (87%)	210 (97%)	6 (3%)	0	100 100
1	11	221/249 (89%)	213 (96%)	8 (4%)	0	100 100
1	14	221/249 (89%)	213 (96%)	8 (4%)	0	100 100
1	4	216/249 (87%)	208 (96%)	8 (4%)	0	100 100
1	G	221/249 (89%)	217 (98%)	4 (2%)	0	100 100
1	g	221/249 (89%)	215 (97%)	6 (3%)	0	100 100
2	12	158/247 (64%)	154 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	15	158/247 (64%)	150 (95%)	8 (5%)	0	100	100
2	2	194/247 (78%)	187 (96%)	7 (4%)	0	100	100
2	5	194/247 (78%)	190 (98%)	4 (2%)	0	100	100
2	N	218/247 (88%)	209 (96%)	9 (4%)	0	100	100
2	n	218/247 (88%)	210 (96%)	8 (4%)	0	100	100
3	3	212/259 (82%)	204 (96%)	8 (4%)	0	100	100
3	6	212/259 (82%)	206 (97%)	6 (3%)	0	100	100
4	7	105/140 (75%)	104 (99%)	1 (1%)	0	100	100
4	8	105/140 (75%)	102 (97%)	3 (3%)	0	100	100
5	13	211/243 (87%)	205 (97%)	6 (3%)	0	100	100
5	16	211/243 (87%)	205 (97%)	6 (3%)	0	100	100
6	A	334/353 (95%)	322 (96%)	12 (4%)	0	100	100
6	a	334/353 (95%)	322 (96%)	12 (4%)	0	100	100
7	B	503/508 (99%)	488 (97%)	15 (3%)	0	100	100
7	b	503/508 (99%)	486 (97%)	17 (3%)	0	100	100
8	C	447/473 (94%)	437 (98%)	10 (2%)	0	100	100
8	c	447/473 (94%)	437 (98%)	10 (2%)	0	100	100
9	D	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
9	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
10	E	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
10	e	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
11	F	35/41 (85%)	35 (100%)	0	0	100	100
11	f	35/41 (85%)	35 (100%)	0	0	100	100
12	H	65/80 (81%)	63 (97%)	2 (3%)	0	100	100
12	h	65/80 (81%)	63 (97%)	2 (3%)	0	100	100
13	I	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
13	i	32/38 (84%)	28 (88%)	4 (12%)	0	100	100
14	J	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
14	j	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
15	K	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
15	k	35/42 (83%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	L	35/38 (92%)	35 (100%)	0	0	100	100
16	l	35/38 (92%)	35 (100%)	0	0	100	100
17	M	28/34 (82%)	28 (100%)	0	0	100	100
17	m	28/34 (82%)	28 (100%)	0	0	100	100
18	O	236/305 (77%)	230 (98%)	6 (2%)	0	100	100
18	o	236/305 (77%)	229 (97%)	7 (3%)	0	100	100
19	P	186/915 (20%)	183 (98%)	3 (2%)	0	100	100
19	p	186/915 (20%)	183 (98%)	3 (2%)	0	100	100
20	Q	142/203 (70%)	139 (98%)	3 (2%)	0	100	100
20	q	142/203 (70%)	137 (96%)	5 (4%)	0	100	100
21	R	226/297 (76%)	219 (97%)	7 (3%)	0	100	100
21	r	226/297 (76%)	220 (97%)	6 (3%)	0	100	100
22	S	255/293 (87%)	248 (97%)	7 (3%)	0	100	100
22	s	255/293 (87%)	244 (96%)	11 (4%)	0	100	100
23	T	28/31 (90%)	28 (100%)	0	0	100	100
23	t	28/31 (90%)	28 (100%)	0	0	100	100
24	U	28/367 (8%)	28 (100%)	0	0	100	100
24	u	28/367 (8%)	28 (100%)	0	0	100	100
25	V	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
25	v	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
26	W	58/447 (13%)	56 (97%)	2 (3%)	0	100	100
26	w	58/447 (13%)	56 (97%)	2 (3%)	0	100	100
27	X	36/100 (36%)	36 (100%)	0	0	100	100
27	x	36/100 (36%)	36 (100%)	0	0	100	100
28	Y	220/256 (86%)	217 (99%)	3 (1%)	0	100	100
28	y	220/256 (86%)	215 (98%)	5 (2%)	0	100	100
29	Z	60/62 (97%)	60 (100%)	0	0	100	100
29	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
All	All	10460/15046 (70%)	10166 (97%)	294 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	170/190 (90%)	165 (97%)	5 (3%)	37	61
1	11	172/190 (90%)	166 (96%)	6 (4%)	32	57
1	14	172/190 (90%)	167 (97%)	5 (3%)	37	61
1	4	170/190 (90%)	164 (96%)	6 (4%)	32	57
1	G	172/190 (90%)	166 (96%)	6 (4%)	32	57
1	g	172/190 (90%)	167 (97%)	5 (3%)	37	61
2	12	136/187 (73%)	132 (97%)	4 (3%)	37	61
2	15	136/187 (73%)	129 (95%)	7 (5%)	21	47
2	2	150/187 (80%)	147 (98%)	3 (2%)	48	71
2	5	150/187 (80%)	143 (95%)	7 (5%)	23	49
2	N	167/187 (89%)	161 (96%)	6 (4%)	31	56
2	n	167/187 (89%)	162 (97%)	5 (3%)	36	60
3	3	165/196 (84%)	162 (98%)	3 (2%)	51	72
3	6	165/196 (84%)	162 (98%)	3 (2%)	51	72
4	7	88/113 (78%)	86 (98%)	2 (2%)	44	67
4	8	88/113 (78%)	83 (94%)	5 (6%)	18	42
5	13	168/187 (90%)	161 (96%)	7 (4%)	26	53
5	16	168/187 (90%)	162 (96%)	6 (4%)	31	56
6	A	274/287 (96%)	269 (98%)	5 (2%)	51	72
6	a	274/287 (96%)	268 (98%)	6 (2%)	45	69
7	B	403/406 (99%)	396 (98%)	7 (2%)	53	73
7	b	403/406 (99%)	395 (98%)	8 (2%)	48	71
8	C	351/373 (94%)	345 (98%)	6 (2%)	53	73
8	c	351/373 (94%)	344 (98%)	7 (2%)	48	71
9	D	277/285 (97%)	274 (99%)	3 (1%)	65	80
9	d	277/285 (97%)	272 (98%)	5 (2%)	51	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	E	71/74 (96%)	70 (99%)	1 (1%)	59	77
10	e	71/74 (96%)	71 (100%)	0	100	100
11	F	31/34 (91%)	31 (100%)	0	100	100
11	f	31/34 (91%)	31 (100%)	0	100	100
12	H	57/68 (84%)	55 (96%)	2 (4%)	32	57
12	h	57/68 (84%)	55 (96%)	2 (4%)	32	57
13	I	31/35 (89%)	31 (100%)	0	100	100
13	i	31/35 (89%)	31 (100%)	0	100	100
14	J	27/31 (87%)	27 (100%)	0	100	100
14	j	27/31 (87%)	27 (100%)	0	100	100
15	K	33/37 (89%)	32 (97%)	1 (3%)	36	60
15	k	33/37 (89%)	32 (97%)	1 (3%)	36	60
16	L	34/35 (97%)	32 (94%)	2 (6%)	18	41
16	l	34/35 (97%)	31 (91%)	3 (9%)	9	24
17	M	26/30 (87%)	26 (100%)	0	100	100
17	m	26/30 (87%)	26 (100%)	0	100	100
18	O	182/217 (84%)	178 (98%)	4 (2%)	45	69
18	o	182/217 (84%)	178 (98%)	4 (2%)	45	69
19	P	147/651 (23%)	145 (99%)	2 (1%)	59	77
19	p	147/651 (23%)	146 (99%)	1 (1%)	76	87
20	Q	108/143 (76%)	105 (97%)	3 (3%)	38	62
20	q	108/143 (76%)	106 (98%)	2 (2%)	50	71
21	R	182/225 (81%)	177 (97%)	5 (3%)	39	64
21	r	182/225 (81%)	178 (98%)	4 (2%)	45	69
22	S	192/212 (91%)	190 (99%)	2 (1%)	68	82
22	s	192/212 (91%)	190 (99%)	2 (1%)	68	82
23	T	26/27 (96%)	26 (100%)	0	100	100
23	t	26/27 (96%)	26 (100%)	0	100	100
24	U	25/241 (10%)	25 (100%)	0	100	100
24	u	25/241 (10%)	25 (100%)	0	100	100
25	V	27/27 (100%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	v	27/27 (100%)	26 (96%)	1 (4%)	30	55
26	W	50/362 (14%)	47 (94%)	3 (6%)	17	40
26	w	50/362 (14%)	46 (92%)	4 (8%)	11	28
27	X	26/66 (39%)	25 (96%)	1 (4%)	29	55
27	x	26/66 (39%)	26 (100%)	0	100	100
28	Y	171/197 (87%)	169 (99%)	2 (1%)	63	79
28	y	171/197 (87%)	170 (99%)	1 (1%)	78	89
29	Z	52/52 (100%)	52 (100%)	0	100	100
29	z	52/52 (100%)	51 (98%)	1 (2%)	50	71
All	All	8382/11484 (73%)	8190 (98%)	192 (2%)	44	67

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	91	LEU
1	1	112	VAL
1	1	121	PHE
1	1	135	ILE
1	1	143	VAL
2	2	141	LEU
2	2	144	GLN
2	2	212	LEU
3	3	64	GLU
3	3	139	LEU
3	3	164	VAL
1	4	27	VAL
1	4	88	LEU
1	4	91	LEU
1	4	121	PHE
1	4	131	ASN
1	4	197	GLU
2	5	95	GLU
2	5	109	VAL
2	5	123	LEU
2	5	141	LEU
2	5	144	GLN
2	5	199	LEU
2	5	212	LEU
3	6	59	SER

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Mol	Chain	Res	Type
3	6	64	GLU
3	6	164	VAL
4	7	111	THR
4	7	138	LEU
4	8	35	ILE
4	8	62	LYS
4	8	103	SER
4	8	111	THR
4	8	138	LEU
1	11	43	GLU
1	11	143	VAL
1	11	148	LEU
1	11	185	ASP
1	11	216	LEU
1	11	232	GLU
2	12	85	MET
2	12	109	VAL
2	12	116	GLN
2	12	140	ILE
5	13	109	VAL
5	13	164	VAL
5	13	168	ILE
5	13	203	SER
5	13	209	ILE
5	13	212	ILE
5	13	242	LEU
1	14	127	ASN
1	14	148	LEU
1	14	185	ASP
1	14	186	ASP
1	14	216	LEU
2	15	63	LEU
2	15	95	GLU
2	15	109	VAL
2	15	138	VAL
2	15	174	PHE
2	15	182	ASP
2	15	210	GLN
5	16	33	ARG
5	16	109	VAL
5	16	163	GLU
5	16	203	SER

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Mol	Chain	Res	Type
5	16	209	ILE
5	16	242	LEU
6	A	22	THR
6	A	76	ASN
6	A	83	ILE
6	A	85	THR
6	A	292	THR
7	B	8	VAL
7	B	63	LEU
7	B	362	PHE
7	B	399	VAL
7	B	440	ASP
7	B	442	VAL
7	B	490	VAL
8	C	42	LEU
8	C	188	THR
8	C	318	LEU
8	C	344	SER
8	C	442	LEU
8	C	462	ASP
9	D	180	ARG
9	D	192	THR
9	D	194	ASN
10	E	21	VAL
1	G	62	THR
1	G	71	THR
1	G	112	VAL
1	G	186	ASP
1	G	188	ASP
1	G	237	ASN
12	H	17	SER
12	H	69	ASP
15	K	39	VAL
16	L	5	ASN
16	L	12	GLU
2	N	92	VAL
2	N	126	LEU
2	N	177	LEU
2	N	194	LEU
2	N	212	LEU
2	N	245	ILE
18	O	106	VAL

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Mol	Chain	Res	Type
18	O	156	LYS
18	O	254	THR
18	O	284	ASP
19	P	514	ASP
19	P	573	SER
20	Q	81	LEU
20	Q	89	ASP
20	Q	136	VAL
21	R	71	TYR
21	R	133	THR
21	R	144	LEU
21	R	149	GLU
21	R	278	GLN
22	S	148	LEU
22	S	240	ILE
26	W	432	ASP
26	W	437	ARG
26	W	446	THR
27	X	67	SER
28	Y	44	LYS
28	Y	253	ASN
6	a	21	VAL
6	a	22	THR
6	a	83	ILE
6	a	157	VAL
6	a	333	GLU
6	a	334	ARG
7	b	8	VAL
7	b	31	SER
7	b	63	LEU
7	b	240	SER
7	b	246	PHE
7	b	362	PHE
7	b	490	VAL
7	b	505	ARG
8	c	42	LEU
8	c	72	VAL
8	c	108	THR
8	c	188	THR
8	c	318	LEU
8	c	377	LEU
8	c	462	ASP

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Mol	Chain	Res	Type
9	d	75	THR
9	d	112	THR
9	d	192	THR
9	d	194	ASN
9	d	287	VAL
1	g	62	THR
1	g	68	ASP
1	g	186	ASP
1	g	188	ASP
1	g	237	ASN
12	h	17	SER
12	h	69	ASP
15	k	39	VAL
16	l	5	ASN
16	l	12	GLU
16	l	36	ILE
2	n	107	GLU
2	n	177	LEU
2	n	179	LEU
2	n	212	LEU
2	n	245	ILE
18	o	137	THR
18	o	156	LYS
18	o	254	THR
18	o	284	ASP
19	p	514	ASP
20	q	81	LEU
20	q	136	VAL
21	r	71	TYR
21	r	133	THR
21	r	144	LEU
21	r	149	GLU
22	s	47	ASP
22	s	124	ILE
25	v	32	ASN
26	w	388	LEU
26	w	406	ASP
26	w	428	THR
26	w	446	THR
28	y	44	LYS
29	z	39	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56)

such sidechains are listed below:

Mol	Chain	Res	Type
1	1	127	ASN
1	1	131	ASN
1	1	136	HIS
3	3	152	GLN
3	3	165	ASN
1	4	131	ASN
1	4	136	HIS
3	6	218	GLN
4	7	38	GLN
4	8	38	GLN
1	11	138	GLN
1	11	236	ASN
5	13	116	GLN
1	14	237	ASN
2	15	116	GLN
5	16	210	GLN
6	A	247	ASN
6	A	267	ASN
6	A	338	ASN
8	C	322	GLN
8	C	332	GLN
8	C	385	GLN
9	D	336	HIS
12	H	63	ASN
16	L	5	ASN
16	L	7	ASN
2	N	210	GLN
18	O	76	GLN
21	R	80	ASN
21	R	189	GLN
21	R	255	GLN
24	U	352	ASN
26	W	439	ASN
28	Y	138	ASN
6	a	247	ASN
6	a	267	ASN
6	a	337	HIS
6	a	338	ASN
7	b	466	HIS
8	c	118	HIS
8	c	332	GLN
8	c	385	GLN

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Mol	Chain	Res	Type
9	d	332	GLN
9	d	336	HIS
1	g	127	ASN
12	h	63	ASN
18	o	91	GLN
19	p	508	ASN
19	p	542	ASN
21	r	80	ASN
21	r	255	GLN
21	r	278	GLN
26	w	439	ASN
28	y	138	ASN
28	y	209	ASN
28	y	234	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 612 ligands modelled in this entry, 4 are monoatomic - leaving 608 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	$\#\|Z\| > 2$
31	CLA	2	603	2	59,63,73	1.33	6 (10%)	70,101,113	1.83	8 (11%)
31	CLA	n	613	2	59,63,73	1.38	5 (8%)	70,101,113	1.61	8 (11%)
35	XAT	r	616	-	41,47,47	0.14	0	54,74,74	0.85	2 (3%)
30	CHL	G	605	1	42,56,74	2.23	11 (26%)	36,92,114	3.14	17 (47%)
31	CLA	11	610	-	59,63,73	1.32	6 (10%)	70,101,113	1.79	9 (12%)
32	LHG	d	409	-	38,38,48	1.42	8 (21%)	41,44,54	0.80	2 (4%)
33	LUT	N	618	-	42,43,43	0.47	1 (2%)	51,60,60	0.28	0
30	CHL	3	608	-	44,58,74	2.14	11 (25%)	37,94,114	3.11	18 (48%)
30	CHL	S	606	22	60,74,74	1.91	12 (20%)	58,114,114	2.52	19 (32%)
30	CHL	y	605	28	50,64,74	2.10	12 (24%)	46,102,114	2.96	19 (41%)
38	PHO	A	405	-	58,69,69	0.94	1 (1%)	55,99,99	0.90	4 (7%)
31	CLA	n	604	-	59,63,73	1.32	6 (10%)	70,101,113	1.73	9 (12%)
31	CLA	13	615	5	49,53,73	1.39	6 (12%)	58,89,113	1.81	6 (10%)
31	CLA	Y	612	28	69,73,73	1.24	6 (8%)	82,113,113	1.61	10 (12%)
33	LUT	14	617	-	42,43,43	0.52	1 (2%)	51,60,60	0.28	0
30	CHL	15	606	-	45,59,74	2.20	12 (26%)	40,96,114	3.01	18 (45%)
31	CLA	13	604	-	59,63,73	1.32	7 (11%)	70,101,113	1.66	9 (12%)
31	CLA	A	404	-	69,73,73	1.22	7 (10%)	82,113,113	1.56	11 (13%)
39	BCR	B	619	-	41,41,41	0.12	0	56,56,56	0.24	0
32	LHG	y	616	31	48,48,48	1.30	6 (12%)	51,54,54	0.80	2 (3%)
31	CLA	c	509	8	64,68,73	1.29	7 (10%)	76,107,113	1.70	10 (13%)
30	CHL	12	601	2	44,58,74	2.18	11 (25%)	37,94,114	3.08	17 (45%)
31	CLA	b	602	7	69,73,73	1.22	7 (10%)	82,113,113	1.62	9 (10%)
31	CLA	14	604	-	59,63,73	1.33	6 (10%)	70,101,113	1.69	8 (11%)
30	CHL	5	601	2	45,59,74	2.21	13 (28%)	40,96,114	2.97	18 (45%)
34	NEX	G	618	-	40,45,46	0.75	2 (5%)	48,67,70	0.55	0
33	LUT	13	618	-	42,43,43	0.49	1 (2%)	51,60,60	0.29	0
36	3PH	b	623	-	38,38,47	0.29	0	41,43,52	0.33	0
31	CLA	B	601	-	59,63,73	1.31	7 (11%)	70,101,113	1.72	7 (10%)
31	CLA	S	615	22	51,55,73	1.38	6 (11%)	60,91,113	1.85	6 (10%)
31	CLA	Y	602	28	69,73,73	1.23	7 (10%)	82,113,113	1.64	10 (12%)
39	BCR	c	526	-	41,41,41	0.11	0	56,56,56	0.21	0
32	LHG	a	411	-	48,48,48	1.38	8 (16%)	51,54,54	0.75	2 (3%)
33	LUT	n	618	-	42,43,43	0.49	1 (2%)	51,60,60	0.27	0
37	OEX	a	402	6,8	0,15,15	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	CLA	B	602	7	69,73,73	1.22	7 (10%)	82,113,113	1.62	9 (10%)
43	LNL	h	101	-	19,19,19	0.45	0	19,19,19	0.49	0
31	CLA	S	612	22	49,53,73	1.54	8 (16%)	58,89,113	1.56	5 (8%)
31	CLA	d	402	-	69,73,73	1.22	7 (10%)	82,113,113	1.55	13 (15%)
33	LUT	S	618	-	42,43,43	0.42	1 (2%)	51,60,60	0.36	0
30	CHL	r	605	21	50,64,74	2.06	12 (24%)	46,102,114	2.89	19 (41%)
31	CLA	R	611	21	53,57,73	1.36	8 (15%)	61,93,113	1.79	4 (6%)
33	LUT	2	614	-	42,43,43	0.38	0	51,60,60	0.28	0
30	CHL	n	609	2	60,74,74	1.89	12 (20%)	58,114,114	2.59	18 (31%)
39	BCR	b	619	-	41,41,41	0.12	0	56,56,56	0.25	0
32	LHG	a	414	-	42,42,48	1.49	8 (19%)	45,48,54	0.79	2 (4%)
30	CHL	1	609	-	50,64,74	2.09	12 (24%)	46,102,114	2.78	19 (41%)
30	CHL	R	606	21	60,74,74	1.84	11 (18%)	58,114,114	2.59	19 (32%)
31	CLA	r	611	21	53,57,73	1.37	7 (13%)	61,93,113	1.80	6 (9%)
33	LUT	G	616	-	42,43,43	0.46	1 (2%)	51,60,60	0.25	0
41	LMG	w	501	-	55,55,55	0.16	0	63,63,63	0.16	0
31	CLA	5	611	-	50,54,73	1.39	6 (12%)	59,90,113	1.73	6 (10%)
31	CLA	C	503	8	69,73,73	1.21	7 (10%)	82,113,113	1.69	8 (9%)
31	CLA	S	611	32	69,73,73	1.24	6 (8%)	82,113,113	1.69	10 (12%)
31	CLA	b	601	-	59,63,73	1.31	7 (11%)	70,101,113	1.72	7 (10%)
31	CLA	b	616	7	64,68,73	1.27	7 (10%)	76,107,113	1.74	9 (11%)
30	CHL	16	606	-	55,69,74	1.99	12 (21%)	52,108,114	2.70	18 (34%)
30	CHL	Y	601	28	60,74,74	1.86	12 (20%)	58,114,114	2.57	19 (32%)
32	LHG	S	621	-	48,48,48	1.38	8 (16%)	51,54,54	0.79	2 (3%)
42	PL9	A	410	-	55,55,55	0.08	0	68,69,69	0.21	0
30	CHL	g	606	-	44,58,74	2.18	11 (25%)	37,94,114	3.15	17 (45%)
31	CLA	b	615	7	69,73,73	1.24	7 (10%)	82,113,113	1.68	11 (13%)
39	BCR	a	408	-	41,41,41	0.11	0	56,56,56	0.23	0
31	CLA	14	610	-	69,73,73	1.23	6 (8%)	82,113,113	1.68	9 (10%)
31	CLA	S	603	22	46,50,73	1.40	6 (13%)	53,85,113	1.92	5 (9%)
38	PHO	a	406	-	58,69,69	0.97	1 (1%)	55,99,99	0.93	4 (7%)
41	LMG	d	410	-	44,44,55	0.18	0	52,52,63	0.19	0
31	CLA	S	605	22	54,58,73	1.38	6 (11%)	64,95,113	1.69	7 (10%)
30	CHL	14	601	1	60,74,74	1.90	12 (20%)	58,114,114	2.55	19 (32%)
30	CHL	6	607	-	60,74,74	1.91	12 (20%)	58,114,114	2.62	19 (32%)
43	LNL	c	524	-	19,19,19	0.45	0	19,19,19	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CLA	4	614	1	50,54,73	1.39	7 (14%)	59,90,113	1.83	8 (13%)
31	CLA	B	615	7	69,73,73	1.24	7 (10%)	82,113,113	1.69	11 (13%)
30	CHL	2	609	2	60,74,74	1.93	12 (20%)	58,114,114	2.46	19 (32%)
31	CLA	R	613	21	64,68,73	1.28	6 (9%)	76,107,113	1.77	10 (13%)
31	CLA	g	612	1	47,51,73	1.40	6 (12%)	55,86,113	1.83	5 (9%)
30	CHL	3	609	3	60,74,74	1.91	12 (20%)	58,114,114	2.53	19 (32%)
30	CHL	12	607	-	44,58,74	2.21	11 (25%)	37,94,114	3.04	17 (45%)
30	CHL	s	601	22	40,54,74	2.29	12 (30%)	34,90,114	3.26	17 (50%)
31	CLA	r	610	32	64,68,73	1.28	7 (10%)	76,107,113	1.71	8 (10%)
31	CLA	2	602	2	59,63,73	1.33	8 (13%)	70,101,113	1.71	9 (12%)
33	LUT	n	617	-	42,43,43	0.43	1 (2%)	51,60,60	0.29	0
30	CHL	6	605	3	60,74,74	1.90	12 (20%)	58,114,114	2.67	18 (31%)
41	LMG	D	414	-	48,48,55	0.18	0	56,56,63	0.15	0
30	CHL	1	605	1	40,54,74	2.34	13 (32%)	34,90,114	3.23	17 (50%)
31	CLA	B	607	-	69,73,73	1.21	6 (8%)	82,113,113	1.66	8 (9%)
30	CHL	3	606	-	50,64,74	2.08	12 (24%)	46,102,114	2.83	18 (39%)
31	CLA	G	613	1	69,73,73	1.22	6 (8%)	82,113,113	1.61	8 (9%)
33	LUT	11	617	-	42,43,43	0.52	1 (2%)	51,60,60	0.28	0
31	CLA	S	602	22	69,73,73	1.23	7 (10%)	82,113,113	1.65	10 (12%)
32	LHG	D	408	-	48,48,48	1.33	7 (14%)	51,54,54	0.74	2 (3%)
31	CLA	1	612	1	50,54,73	1.40	6 (12%)	59,90,113	1.73	6 (10%)
31	CLA	c	502	8	69,73,73	1.21	7 (10%)	82,113,113	1.60	8 (9%)
39	BCR	c	516	-	41,41,41	0.11	0	56,56,56	0.32	0
31	CLA	Y	604	-	59,63,73	1.32	6 (10%)	70,101,113	1.74	8 (11%)
31	CLA	B	604	7	69,73,73	1.23	6 (8%)	82,113,113	1.67	10 (12%)
31	CLA	B	611	7	69,73,73	1.23	7 (10%)	82,113,113	1.62	9 (10%)
32	LHG	a	413	-	43,43,48	1.42	7 (16%)	46,49,54	0.84	2 (4%)
31	CLA	12	611	-	49,53,73	1.43	7 (14%)	58,89,113	1.76	6 (10%)
31	CLA	G	603	1	59,63,73	1.33	6 (10%)	70,101,113	1.78	8 (11%)
31	CLA	y	604	-	59,63,73	1.32	6 (10%)	70,101,113	1.74	8 (11%)
39	BCR	B	618	-	41,41,41	0.15	0	56,56,56	0.24	0
31	CLA	c	507	8	69,73,73	1.23	7 (10%)	82,113,113	1.60	9 (10%)
31	CLA	b	606	7	69,73,73	1.23	7 (10%)	82,113,113	1.55	10 (12%)
31	CLA	n	610	2	64,68,73	1.27	7 (10%)	76,107,113	1.70	10 (13%)
31	CLA	g	611	32	69,73,73	1.23	6 (8%)	82,113,113	1.60	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	CLA	1	611	32	54,58,73	1.40	7 (12%)	64,95,113	1.73	8 (12%)
31	CLA	12	609	2	59,63,73	1.32	6 (10%)	70,101,113	1.66	8 (11%)
31	CLA	N	603	2	64,68,73	1.27	7 (10%)	76,107,113	1.71	8 (10%)
31	CLA	C	512	8	69,73,73	1.22	7 (10%)	82,113,113	1.65	8 (9%)
33	LUT	16	617	-	42,43,43	0.44	1 (2%)	51,60,60	0.36	0
46	DGD	c	518	-	59,59,67	0.18	0	73,73,81	0.16	0
30	CHL	14	607	-	44,58,74	2.20	12 (27%)	37,94,114	3.10	16 (43%)
30	CHL	2	606	-	40,54,74	2.31	13 (32%)	34,90,114	3.25	19 (55%)
43	LNL	w	503	-	19,19,19	0.45	0	19,19,19	0.52	0
33	LUT	12	615	-	42,43,43	0.43	1 (2%)	51,60,60	0.26	0
31	CLA	4	610	1	69,73,73	1.28	8 (11%)	82,113,113	1.37	10 (12%)
30	CHL	S	601	22	40,54,74	2.29	12 (30%)	34,90,114	3.27	17 (50%)
31	CLA	15	611	-	49,53,73	1.43	7 (14%)	58,89,113	1.75	7 (12%)
32	LHG	y	618	-	46,46,48	1.44	8 (17%)	49,52,54	0.76	2 (4%)
30	CHL	16	607	-	55,69,74	1.99	12 (21%)	52,108,114	2.77	19 (36%)
34	NEX	2	616	-	30,33,46	0.50	1 (3%)	38,48,70	0.51	0
31	CLA	3	604	-	69,73,73	1.24	8 (11%)	82,113,113	1.61	11 (13%)
31	CLA	13	614	5	49,53,73	1.39	6 (12%)	58,89,113	1.79	8 (13%)
31	CLA	s	613	22	53,57,73	1.37	6 (11%)	61,93,113	1.75	7 (11%)
41	LMG	j	102	-	51,51,55	0.17	0	59,59,63	0.16	0
31	CLA	14	603	-	59,63,73	1.32	6 (10%)	70,101,113	1.67	9 (12%)
31	CLA	r	613	21	69,73,73	1.23	6 (8%)	82,113,113	1.71	9 (10%)
31	CLA	d	404	9	69,73,73	1.22	7 (10%)	82,113,113	1.64	10 (12%)
31	CLA	a	404	-	69,73,73	1.22	6 (8%)	82,113,113	1.56	10 (12%)
33	LUT	13	617	-	42,43,43	0.43	1 (2%)	51,60,60	0.36	0
30	CHL	11	607	-	40,54,74	2.32	12 (30%)	34,90,114	3.17	17 (50%)
31	CLA	12	602	2	64,68,73	1.29	7 (10%)	76,107,113	1.63	10 (13%)
31	CLA	B	613	7	69,73,73	1.21	7 (10%)	82,113,113	1.75	8 (9%)
46	DGD	C	517	-	67,67,67	0.16	0	81,81,81	0.17	0
39	BCR	h	102	-	41,41,41	0.13	0	56,56,56	0.33	0
46	DGD	C	519	-	60,60,67	0.18	0	74,74,81	0.18	0
41	LMG	H	102	-	34,34,55	0.20	0	36,36,63	0.18	0
30	CHL	14	608	-	45,59,74	2.21	12 (26%)	40,96,114	3.02	19 (47%)
31	CLA	g	602	1	69,73,73	1.23	7 (10%)	82,113,113	1.64	9 (10%)
43	LNL	W	502	-	19,19,19	0.44	0	19,19,19	0.51	0
32	LHG	s	617	31	44,44,48	1.39	7 (15%)	47,50,54	0.74	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
39	BCR	B	617	-	41,41,41	0.14	0	56,56,56	0.25	0
39	BCR	C	526	-	41,41,41	0.12	0	56,56,56	0.21	0
31	CLA	Y	614	28	53,57,73	1.36	6 (11%)	61,93,113	1.83	7 (11%)
31	CLA	15	610	-	49,53,73	1.41	6 (12%)	58,89,113	1.80	6 (10%)
34	NEX	1	618	-	14,17,46	0.39	0	19,29,70	0.53	0
31	CLA	6	611	32	69,73,73	1.22	6 (8%)	82,113,113	1.54	9 (10%)
31	CLA	Y	610	28	69,73,73	1.22	8 (11%)	82,113,113	1.65	9 (10%)
31	CLA	B	614	7	69,73,73	1.23	7 (10%)	82,113,113	1.65	10 (12%)
30	CHL	6	601	3	55,69,74	2.01	12 (21%)	52,108,114	2.69	18 (34%)
31	CLA	c	508	-	69,73,73	1.22	7 (10%)	82,113,113	1.79	9 (10%)
31	CLA	s	611	32	69,73,73	1.24	8 (11%)	82,113,113	1.70	10 (12%)
32	LHG	r	621	-	43,43,48	1.51	8 (18%)	46,49,54	0.82	2 (4%)
31	CLA	3	610	3	64,68,73	1.27	7 (10%)	76,107,113	1.65	9 (11%)
30	CHL	12	606	-	45,59,74	2.19	12 (26%)	40,96,114	3.03	17 (42%)
31	CLA	15	603	-	59,63,73	1.32	6 (10%)	70,101,113	1.80	9 (12%)
31	CLA	c	503	8	69,73,73	1.21	7 (10%)	82,113,113	1.70	8 (9%)
33	LUT	6	618	-	42,43,43	0.52	1 (2%)	51,60,60	0.30	0
31	CLA	r	609	21	69,73,73	1.23	7 (10%)	82,113,113	1.63	8 (9%)
33	LUT	1	616	-	42,43,43	0.42	1 (2%)	51,60,60	0.26	0
31	CLA	C	508	-	69,73,73	1.23	6 (8%)	82,113,113	1.48	11 (13%)
31	CLA	n	615	2	51,55,73	1.37	8 (15%)	60,91,113	1.86	9 (15%)
31	CLA	6	612	3	59,63,73	1.34	6 (10%)	70,101,113	1.74	10 (14%)
31	CLA	3	614	3	54,58,73	1.38	7 (12%)	64,95,113	1.73	7 (10%)
39	BCR	b	618	-	41,41,41	0.14	0	56,56,56	0.23	0
31	CLA	12	612	2	54,58,73	1.38	7 (12%)	64,95,113	1.74	8 (12%)
41	LMG	C	522	-	55,55,55	0.17	0	63,63,63	0.16	0
32	LHG	3	616	31	43,43,48	1.45	8 (18%)	46,49,54	0.80	2 (4%)
33	LUT	Y	621	-	42,43,43	0.47	1 (2%)	51,60,60	0.48	0
31	CLA	12	610	-	49,53,73	1.41	6 (12%)	58,89,113	1.79	6 (10%)
30	CHL	13	607	-	55,69,74	2.00	12 (21%)	52,108,114	2.79	19 (36%)
31	CLA	r	603	21	69,73,73	1.24	8 (11%)	82,113,113	1.70	9 (10%)
43	LNL	x	201	-	19,19,19	0.43	0	19,19,19	0.46	0
40	SQD	l	101	-	48,50,54	0.18	0	58,61,65	0.21	0
31	CLA	1	602	1	64,68,73	1.27	7 (10%)	76,107,113	1.68	11 (14%)
31	CLA	C	504	8	69,73,73	1.23	8 (11%)	82,113,113	1.68	11 (13%)
30	CHL	2	605	2	40,54,74	2.32	13 (32%)	34,90,114	3.15	16 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CLA	15	609	2	59,63,73	1.33	7 (11%)	70,101,113	1.74	10 (14%)
33	LUT	3	618	-	42,43,43	0.51	1 (2%)	51,60,60	0.30	0
31	CLA	13	610	-	69,73,73	1.22	6 (8%)	82,113,113	1.66	10 (12%)
41	LMG	B	621	-	49,49,55	0.19	0	57,57,63	0.18	0
31	CLA	y	613	28	69,73,73	1.22	6 (8%)	82,113,113	1.58	9 (10%)
31	CLA	s	612	22	49,53,73	1.43	8 (16%)	58,89,113	1.81	7 (12%)
31	CLA	12	603	-	59,63,73	1.32	6 (10%)	70,101,113	1.76	7 (10%)
31	CLA	R	601	21	53,57,73	1.36	6 (11%)	61,93,113	1.66	8 (13%)
31	CLA	r	612	21	54,58,73	1.37	7 (12%)	64,95,113	1.75	9 (14%)
33	LUT	12	614	-	42,43,43	0.46	1 (2%)	51,60,60	0.36	0
43	LNL	Y	619	-	19,19,19	0.44	0	19,19,19	0.50	0
31	CLA	S	614	22	69,73,73	1.22	6 (8%)	82,113,113	1.60	9 (10%)
43	LNL	c	523	-	19,19,19	0.44	0	19,19,19	0.48	0
31	CLA	C	506	8	69,73,73	1.22	6 (8%)	82,113,113	1.67	7 (8%)
30	CHL	G	601	1	60,74,74	1.86	12 (20%)	58,114,114	2.54	19 (32%)
33	LUT	G	617	-	42,43,43	0.57	1 (2%)	51,60,60	0.33	0
31	CLA	1	613	1	59,63,73	1.32	6 (10%)	70,101,113	1.71	8 (11%)
30	CHL	y	601	28	60,74,74	1.86	12 (20%)	58,114,114	2.57	19 (32%)
34	NEX	5	616	-	30,33,46	0.49	1 (3%)	38,48,70	0.51	0
32	LHG	Y	617	-	46,46,48	1.48	8 (17%)	49,52,54	0.78	2 (4%)
39	BCR	c	515	-	41,41,41	0.11	0	56,56,56	0.23	0
30	CHL	2	608	-	44,58,74	2.19	12 (27%)	37,94,114	3.12	17 (45%)
30	CHL	15	607	-	44,58,74	2.21	11 (25%)	37,94,114	3.05	18 (48%)
31	CLA	D	404	9	69,73,73	1.21	7 (10%)	82,113,113	1.67	10 (12%)
31	CLA	16	615	-	49,53,73	1.40	6 (12%)	58,89,113	1.68	9 (15%)
31	CLA	3	613	3	59,63,73	1.32	7 (11%)	70,101,113	1.71	6 (8%)
32	LHG	13	616	31	39,39,48	1.53	8 (20%)	42,45,54	0.82	2 (4%)
30	CHL	s	606	22	60,74,74	1.92	12 (20%)	58,114,114	2.55	18 (31%)
31	CLA	c	513	8	59,63,73	1.33	7 (11%)	70,101,113	1.74	8 (11%)
30	CHL	r	606	21	60,74,74	1.85	11 (18%)	58,114,114	2.56	19 (32%)
34	NEX	13	619	-	40,46,46	0.42	1 (2%)	50,70,70	0.43	0
33	LUT	3	619	-	42,43,43	0.49	1 (2%)	51,60,60	0.28	0
31	CLA	n	603	2	64,68,73	1.27	7 (10%)	76,107,113	1.77	8 (10%)
30	CHL	11	606	-	41,55,74	2.26	11 (26%)	35,91,114	3.17	17 (48%)
30	CHL	14	609	-	50,64,74	2.13	12 (24%)	46,102,114	2.75	20 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
32	LHG	G	615	31	48,48,48	1.36	7 (14%)	51,54,54	0.74	2 (3%)
44	STE	B	623	-	19,19,19	0.59	0	19,19,19	1.02	2 (10%)
31	CLA	6	602	3	64,68,73	1.27	8 (12%)	76,107,113	1.64	10 (13%)
32	LHG	r	618	31	37,37,48	1.45	7 (18%)	40,43,54	0.88	2 (5%)
40	SQD	A	408	-	49,51,54	0.18	0	59,62,65	0.27	0
41	LMG	C	520	-	47,47,55	0.19	0	55,55,63	0.16	0
44	STE	b	622	-	19,19,19	0.61	0	19,19,19	1.00	2 (10%)
31	CLA	14	602	1	64,68,73	1.28	7 (10%)	76,107,113	1.71	10 (13%)
31	CLA	n	612	2	49,53,73	1.41	6 (12%)	58,89,113	1.86	6 (10%)
31	CLA	C	507	8	69,73,73	1.23	7 (10%)	82,113,113	1.62	9 (10%)
30	CHL	N	606	-	55,69,74	1.98	12 (21%)	52,108,114	2.70	18 (34%)
30	CHL	13	609	-	55,69,74	2.00	12 (21%)	52,108,114	2.64	18 (34%)
30	CHL	G	607	-	44,58,74	2.16	11 (25%)	37,94,114	3.10	17 (45%)
37	OEX	A	401	6,8	0,15,15	-	-	-		
32	LHG	R	618	31	37,37,48	1.46	7 (18%)	40,43,54	0.87	2 (5%)
31	CLA	16	603	-	64,68,73	1.27	6 (9%)	76,107,113	1.65	8 (10%)
35	XAT	g	619	-	41,47,47	0.14	0	54,74,74	0.46	0
31	CLA	r	608	21	69,73,73	1.22	6 (8%)	82,113,113	1.59	9 (10%)
42	PL9	d	407	-	55,55,55	0.09	0	68,69,69	0.20	0
38	PHO	D	402	-	58,69,69	0.97	1 (1%)	55,99,99	0.92	4 (7%)
31	CLA	11	612	1	47,51,73	1.42	6 (12%)	55,86,113	1.73	7 (12%)
33	LUT	N	617	-	42,43,43	0.44	1 (2%)	51,60,60	0.28	0
30	CHL	n	606	-	55,69,74	1.98	12 (21%)	52,108,114	2.71	18 (34%)
43	LNL	Y	620	-	19,19,19	0.44	0	19,19,19	0.48	0
31	CLA	C	511	8	69,73,73	1.21	7 (10%)	82,113,113	1.70	9 (10%)
31	CLA	G	602	1	69,73,73	1.22	7 (10%)	82,113,113	1.55	10 (12%)
32	LHG	L	102	-	46,46,48	1.33	8 (17%)	49,52,54	0.78	2 (4%)
32	LHG	14	615	31	48,48,48	1.42	8 (16%)	51,54,54	0.75	2 (3%)
30	CHL	15	601	2	44,58,74	2.18	11 (25%)	37,94,114	3.07	18 (48%)
32	LHG	S	617	31	44,44,48	1.42	8 (18%)	47,50,54	0.79	2 (4%)
32	LHG	s	621	-	48,48,48	1.38	8 (16%)	51,54,54	0.79	2 (3%)
30	CHL	14	606	-	41,55,74	2.27	12 (29%)	35,91,114	3.11	16 (45%)
33	LUT	y	623	-	42,43,43	0.54	1 (2%)	51,60,60	0.29	0
31	CLA	13	603	-	64,68,73	1.27	6 (9%)	76,107,113	1.73	8 (10%)
31	CLA	C	510	8	69,73,73	1.22	7 (10%)	82,113,113	1.76	8 (9%)
31	CLA	Y	613	28	69,73,73	1.22	6 (8%)	82,113,113	1.57	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	CLA	5	610	2	54,58,73	1.37	7 (12%)	64,95,113	1.67	10 (15%)
31	CLA	G	610	1	69,73,73	1.22	6 (8%)	82,113,113	1.67	9 (10%)
31	CLA	c	506	8	69,73,73	1.22	6 (8%)	82,113,113	1.66	7 (8%)
31	CLA	d	405	9	69,73,73	1.23	6 (8%)	82,113,113	1.57	10 (12%)
43	LNL	H	101	-	19,19,19	0.44	0	19,19,19	0.48	0
43	LNL	X	201	-	19,19,19	0.44	0	19,19,19	0.48	0
33	LUT	s	618	-	42,43,43	0.39	0	51,60,60	0.46	0
30	CHL	5	609	2	60,74,74	1.93	12 (20%)	58,114,114	2.48	19 (32%)
31	CLA	13	612	5	49,53,73	1.44	6 (12%)	58,89,113	1.79	5 (8%)
48	BCT	d	403	47	3,3,3	0.81	0	2,3,3	3.20	2 (100%)
31	CLA	y	611	32	69,73,73	1.23	6 (8%)	82,113,113	1.62	9 (10%)
34	NEX	4	618	-	14,17,46	0.37	0	19,29,70	0.53	0
31	CLA	5	613	2	54,58,73	1.37	7 (12%)	64,95,113	1.64	7 (10%)
33	LUT	r	615	-	42,43,43	0.47	1 (2%)	51,60,60	0.31	0
30	CHL	G	606	-	41,55,74	2.25	11 (26%)	35,91,114	3.25	16 (45%)
32	LHG	a	401	-	48,48,48	1.43	8 (16%)	51,54,54	0.73	2 (3%)
39	BCR	C	516	-	41,41,41	0.11	0	56,56,56	0.31	0
33	LUT	5	615	-	42,43,43	0.45	1 (2%)	51,60,60	0.27	0
30	CHL	y	606	-	60,74,74	1.88	12 (20%)	58,114,114	2.59	18 (31%)
35	XAT	14	619	-	41,47,47	0.13	0	54,74,74	0.46	0
35	XAT	6	620	-	41,47,47	0.16	0	54,74,74	0.72	1 (1%)
32	LHG	c	521	-	41,41,48	1.49	8 (19%)	44,47,54	0.80	2 (4%)
31	CLA	r	602	21	69,73,73	1.24	8 (11%)	82,113,113	1.67	10 (12%)
33	LUT	15	614	-	42,43,43	0.46	1 (2%)	51,60,60	0.39	0
30	CHL	16	601	5	50,64,74	2.11	12 (24%)	46,102,114	2.82	18 (39%)
34	NEX	S	620	-	40,46,46	0.45	1 (2%)	50,70,70	0.48	0
31	CLA	n	614	2	49,53,73	1.41	8 (16%)	58,89,113	1.78	6 (10%)
39	BCR	C	515	-	41,41,41	0.11	0	56,56,56	0.22	0
34	NEX	Y	623	-	40,46,46	0.46	1 (2%)	50,70,70	0.43	0
31	CLA	11	602	1	64,68,73	1.28	7 (10%)	76,107,113	1.71	11 (14%)
31	CLA	11	613	1	59,63,73	1.32	6 (10%)	70,101,113	1.69	8 (11%)
30	CHL	5	607	-	50,64,74	2.09	12 (24%)	46,102,114	2.83	17 (36%)
31	CLA	b	604	7	69,73,73	1.23	7 (10%)	82,113,113	1.66	8 (9%)
31	CLA	13	611	32	69,73,73	1.23	6 (8%)	82,113,113	1.63	10 (12%)
31	CLA	14	614	1	53,57,73	1.37	7 (13%)	61,93,113	1.80	6 (9%)
31	CLA	16	612	5	49,53,73	1.43	6 (12%)	58,89,113	1.80	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	CLA	16	613	5	54,58,73	1.38	6 (11%)	64,95,113	1.84	6 (9%)
32	LHG	4	615	31	46,46,48	1.43	8 (17%)	49,52,54	0.73	2 (4%)
46	DGD	C	518	-	59,59,67	0.18	0	73,73,81	0.16	0
30	CHL	Y	609	28	60,74,74	1.90	12 (20%)	58,114,114	2.60	18 (31%)
31	CLA	2	612	-	50,54,73	1.41	7 (14%)	59,90,113	1.79	6 (10%)
30	CHL	1	601	1	55,69,74	1.96	12 (21%)	52,108,114	2.67	19 (36%)
31	CLA	G	612	1	47,51,73	1.40	6 (12%)	55,86,113	1.83	5 (9%)
31	CLA	N	614	2	49,53,73	1.40	7 (14%)	58,89,113	1.71	7 (12%)
31	CLA	2	604	-	54,58,73	1.40	9 (16%)	64,95,113	1.73	9 (14%)
31	CLA	y	612	28	69,73,73	1.25	7 (10%)	82,113,113	1.62	10 (12%)
43	LNL	W	503	-	19,19,19	0.43	0	19,19,19	0.49	0
34	NEX	3	621	-	40,46,46	0.44	1 (2%)	50,70,70	0.37	0
31	CLA	a	407	6	59,63,73	1.32	6 (10%)	70,101,113	1.69	8 (11%)
30	CHL	4	608	-	44,58,74	2.21	11 (25%)	37,94,114	3.10	17 (45%)
31	CLA	3	603	3	59,63,73	1.32	6 (10%)	70,101,113	1.77	6 (8%)
31	CLA	11	614	-	53,57,73	1.37	7 (13%)	61,93,113	1.80	6 (9%)
30	CHL	3	601	3	55,69,74	2.01	12 (21%)	52,108,114	2.66	18 (34%)
43	LNL	I	101	-	19,19,19	0.44	0	19,19,19	0.49	0
31	CLA	b	611	7	69,73,73	1.23	7 (10%)	82,113,113	1.61	9 (10%)
30	CHL	g	609	1	60,74,74	1.92	12 (20%)	58,114,114	2.51	19 (32%)
31	CLA	R	609	21	69,73,73	1.22	7 (10%)	82,113,113	1.58	7 (8%)
43	LNL	y	621	-	19,19,19	0.44	0	19,19,19	0.49	0
31	CLA	Y	611	32	69,73,73	1.23	6 (8%)	82,113,113	1.64	9 (10%)
31	CLA	16	604	-	59,63,73	1.32	7 (11%)	70,101,113	1.65	9 (12%)
30	CHL	n	605	2	55,69,74	1.99	12 (21%)	52,108,114	2.68	19 (36%)
31	CLA	3	612	3	69,73,73	1.24	6 (8%)	82,113,113	1.65	10 (12%)
43	LNL	i	101	-	19,19,19	0.45	0	19,19,19	0.49	0
31	CLA	g	604	-	54,58,73	1.38	6 (11%)	64,95,113	1.77	9 (14%)
30	CHL	N	601	2	47,61,74	2.16	13 (27%)	41,98,114	3.06	18 (43%)
42	PL9	a	410	-	55,55,55	0.09	0	68,69,69	0.20	0
30	CHL	11	609	-	50,64,74	2.14	12 (24%)	46,102,114	2.74	19 (41%)
31	CLA	N	610	2	64,68,73	1.27	7 (10%)	76,107,113	1.67	8 (10%)
41	LMG	v	101	-	51,51,55	0.18	0	59,59,63	0.15	0
32	LHG	n	616	31	48,48,48	1.35	7 (14%)	51,54,54	0.78	2 (3%)
33	LUT	15	615	-	42,43,43	0.39	0	51,60,60	0.24	0
31	CLA	1	604	-	54,58,73	1.38	7 (12%)	64,95,113	1.79	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
41	LMG	D	410	-	44,44,55	0.19	0	52,52,63	0.17	0
31	CLA	3	611	32	69,73,73	1.23	6 (8%)	82,113,113	1.55	9 (10%)
31	CLA	R	608	21	69,73,73	1.22	7 (10%)	82,113,113	1.59	9 (10%)
30	CHL	s	607	-	37,51,74	2.28	11 (29%)	30,86,114	3.44	15 (50%)
30	CHL	1	607	-	45,59,74	2.20	12 (26%)	40,96,114	3.05	18 (45%)
32	LHG	R	621	-	43,43,48	1.50	8 (18%)	46,49,54	0.80	2 (4%)
34	NEX	12	616	-	25,28,46	0.38	0	32,42,70	0.55	0
41	LMG	s	616	-	42,42,55	0.18	0	50,50,63	0.17	0
30	CHL	11	601	1	60,74,74	1.89	12 (20%)	58,114,114	2.57	19 (32%)
31	CLA	5	612	-	50,54,73	1.41	6 (12%)	59,90,113	1.79	5 (8%)
32	LHG	r	619	-	46,46,48	1.43	8 (17%)	49,52,54	0.77	2 (4%)
31	CLA	R	604	-	52,56,73	1.38	6 (11%)	61,92,113	1.75	8 (13%)
30	CHL	S	608	-	43,57,74	2.19	11 (25%)	37,93,114	3.09	16 (43%)
32	LHG	N	616	31	48,48,48	1.33	7 (14%)	51,54,54	0.79	2 (3%)
34	NEX	s	620	-	40,46,46	0.44	1 (2%)	50,70,70	0.45	0
32	LHG	D	409	-	38,38,48	1.41	7 (18%)	41,44,54	0.80	2 (4%)
35	XAT	G	619	-	41,47,47	0.13	0	54,74,74	0.45	0
30	CHL	6	609	3	60,74,74	1.90	12 (20%)	58,114,114	2.53	19 (32%)
30	CHL	r	607	-	45,59,74	2.14	11 (24%)	40,96,114	3.04	19 (47%)
31	CLA	B	610	-	69,73,73	1.21	7 (10%)	82,113,113	1.68	11 (13%)
30	CHL	R	605	21	50,64,74	2.04	12 (24%)	46,102,114	2.89	19 (41%)
31	CLA	S	613	22	53,57,73	1.37	6 (11%)	61,93,113	1.76	8 (13%)
32	LHG	11	615	31	48,48,48	1.41	8 (16%)	51,54,54	0.75	2 (3%)
39	BCR	J	101	-	41,41,41	0.22	0	56,56,56	0.48	0
31	CLA	2	611	-	50,54,73	1.39	8 (16%)	59,90,113	1.76	7 (11%)
31	CLA	C	505	-	59,63,73	1.31	7 (11%)	70,101,113	1.70	8 (11%)
40	SQD	d	414	-	44,46,54	0.18	0	54,57,65	0.24	0
38	PHO	a	405	-	58,69,69	0.94	1 (1%)	55,99,99	0.90	4 (7%)
31	CLA	B	609	7	69,73,73	1.23	7 (10%)	82,113,113	1.63	8 (9%)
33	LUT	g	616	-	42,43,43	0.45	1 (2%)	51,60,60	0.25	0
31	CLA	11	611	32	54,58,73	1.39	7 (12%)	64,95,113	1.73	6 (9%)
32	LHG	Y	616	31	48,48,48	1.31	6 (12%)	51,54,54	0.80	2 (3%)
30	CHL	13	605	5	50,64,74	2.09	12 (24%)	46,102,114	2.86	19 (41%)
30	CHL	n	601	2	46,60,74	2.17	12 (26%)	40,97,114	3.10	19 (47%)
30	CHL	Y	608	-	38,52,74	2.18	11 (28%)	31,87,114	3.32	15 (48%)
31	CLA	6	603	3	59,63,73	1.32	6 (10%)	70,101,113	1.80	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
34	NEX	n	619	-	40,46,46	0.42	1 (2%)	50,70,70	0.42	0
50	PAM	N	621	-	17,17,17	0.47	0	17,17,17	0.46	0
31	CLA	b	613	7	69,73,73	1.22	7 (10%)	82,113,113	1.75	8 (9%)
39	BCR	b	617	-	41,41,41	0.14	0	56,56,56	0.26	0
43	LNL	C	523	-	19,19,19	0.44	0	19,19,19	0.49	0
32	LHG	6	617	-	46,46,48	1.39	8 (17%)	49,52,54	0.76	2 (4%)
31	CLA	B	603	7	69,73,73	1.23	6 (8%)	82,113,113	1.65	9 (10%)
31	CLA	A	406	6	59,63,73	1.32	6 (10%)	70,101,113	1.71	7 (10%)
32	LHG	A	413	-	43,43,48	1.42	7 (16%)	46,49,54	0.85	2 (4%)
30	CHL	5	608	-	44,58,74	2.20	11 (25%)	37,94,114	3.10	16 (43%)
30	CHL	g	608	-	46,60,74	2.17	12 (26%)	40,97,114	3.05	18 (45%)
34	NEX	14	618	-	14,17,46	0.40	0	19,29,70	0.54	0
30	CHL	16	609	-	55,69,74	2.00	12 (21%)	52,108,114	2.66	18 (34%)
41	LMG	d	415	-	48,48,55	0.18	0	56,56,63	0.15	0
31	CLA	B	612	7	69,73,73	1.23	7 (10%)	82,113,113	1.75	7 (8%)
39	BCR	A	407	-	41,41,41	0.10	0	56,56,56	0.23	0
34	NEX	16	619	-	40,46,46	0.43	1 (2%)	50,70,70	0.42	0
31	CLA	R	614	-	59,63,73	1.31	7 (11%)	70,101,113	1.75	9 (12%)
30	CHL	g	607	-	44,58,74	2.16	11 (25%)	37,94,114	3.08	16 (43%)
43	LNL	C	524	-	19,19,19	0.44	0	19,19,19	0.49	0
31	CLA	b	603	7	69,73,73	1.23	6 (8%)	82,113,113	1.65	9 (10%)
31	CLA	6	604	-	69,73,73	1.24	8 (11%)	82,113,113	1.62	10 (12%)
32	LHG	16	616	31	39,39,48	1.54	8 (20%)	42,45,54	0.82	2 (4%)
43	LNL	r	620	-	19,19,19	0.45	0	19,19,19	0.50	0
31	CLA	16	614	5	49,53,73	1.39	6 (12%)	58,89,113	1.78	7 (12%)
31	CLA	4	602	1	64,68,73	1.27	7 (10%)	76,107,113	1.68	10 (13%)
31	CLA	a	403	6	69,73,73	1.23	8 (11%)	82,113,113	1.67	9 (10%)
30	CHL	N	608	-	44,58,74	2.14	11 (25%)	37,94,114	3.10	18 (48%)
32	LHG	D	412	-	48,48,48	1.47	8 (16%)	51,54,54	0.75	2 (3%)
36	3PH	8	201	-	47,47,47	0.30	0	50,52,52	0.41	0
32	LHG	y	617	-	46,46,48	1.47	8 (17%)	49,52,54	0.74	2 (4%)
30	CHL	2	607	-	50,64,74	2.07	12 (24%)	46,102,114	2.81	17 (36%)
31	CLA	G	614	1	53,57,73	1.38	6 (11%)	61,93,113	1.75	4 (6%)
31	CLA	s	610	22	69,73,73	1.22	7 (10%)	82,113,113	1.62	8 (9%)
31	CLA	N	604	-	59,63,73	1.32	6 (10%)	70,101,113	1.74	9 (12%)
49	HEM	F	101	11,10	50,50,50	0.54	0	67,82,82	0.49	0
30	CHL	4	609	-	60,74,74	1.91	12 (20%)	58,114,114	2.50	20 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
32	LHG	Y	618	-	46,46,48	1.45	8 (17%)	49,52,54	0.76	2 (4%)
30	CHL	g	605	1	42,56,74	2.25	11 (26%)	36,92,114	3.15	17 (47%)
31	CLA	G	611	32	69,73,73	1.23	6 (8%)	82,113,113	1.61	8 (9%)
40	SQD	D	411	-	52,54,54	0.17	0	62,65,65	0.21	0
32	LHG	A	414	-	42,42,48	1.49	8 (19%)	45,48,54	0.81	2 (4%)
30	CHL	4	601	1	55,69,74	1.96	12 (21%)	52,108,114	2.64	19 (36%)
39	BCR	H	103	-	41,41,41	0.13	0	56,56,56	0.33	0
31	CLA	b	608	7	69,73,73	1.22	7 (10%)	82,113,113	1.57	9 (10%)
31	CLA	5	602	2	59,63,73	1.33	7 (11%)	70,101,113	1.66	8 (11%)
31	CLA	b	609	7	69,73,73	1.23	7 (10%)	82,113,113	1.65	8 (9%)
31	CLA	C	514	8	69,73,73	1.22	6 (8%)	82,113,113	1.52	8 (9%)
36	3PH	T	101	-	47,47,47	0.27	0	50,52,52	0.28	0
41	LMG	K	102	-	51,51,55	0.19	0	59,59,63	0.15	0
31	CLA	14	612	1	47,51,73	1.42	7 (14%)	55,86,113	1.75	5 (9%)
30	CHL	1	608	-	44,58,74	2.18	11 (25%)	37,94,114	3.08	17 (45%)
39	BCR	d	406	-	41,41,41	0.13	0	56,56,56	0.22	0
43	LNL	A	412	-	19,19,19	0.45	0	19,19,19	0.48	0
31	CLA	A	403	-	69,73,73	1.21	7 (10%)	82,113,113	1.57	13 (15%)
31	CLA	B	608	7	69,73,73	1.23	7 (10%)	82,113,113	1.56	9 (10%)
31	CLA	13	613	5	54,58,73	1.37	6 (11%)	64,95,113	1.81	6 (9%)
33	LUT	2	615	-	42,43,43	0.44	1 (2%)	51,60,60	0.27	0
34	NEX	6	621	-	40,46,46	0.45	1 (2%)	50,70,70	0.38	0
31	CLA	N	615	2	51,55,73	1.37	7 (13%)	60,91,113	1.88	8 (13%)
41	LMG	S	616	-	42,42,55	0.19	0	50,50,63	0.17	0
30	CHL	y	607	-	60,74,74	1.87	12 (20%)	58,114,114	2.56	18 (31%)
30	CHL	14	605	1	42,56,74	2.25	11 (26%)	36,92,114	3.10	17 (47%)
31	CLA	c	505	-	59,63,73	1.31	7 (11%)	70,101,113	1.71	8 (11%)
31	CLA	n	611	32	64,68,73	1.30	7 (10%)	76,107,113	1.69	8 (10%)
41	LMG	d	411	-	34,34,55	0.20	0	36,36,63	0.15	0
32	LHG	A	411	-	48,48,48	1.40	8 (16%)	51,54,54	0.75	2 (3%)
30	CHL	5	606	-	40,54,74	2.30	13 (32%)	34,90,114	3.22	17 (50%)
31	CLA	11	604	-	50,54,73	1.40	7 (14%)	59,90,113	1.80	6 (10%)
41	LMG	b	621	-	46,46,55	0.17	0	54,54,63	0.16	0
31	CLA	4	604	-	54,58,73	1.38	8 (14%)	64,95,113	1.85	7 (10%)
31	CLA	6	615	3	54,58,73	1.37	6 (11%)	64,95,113	1.85	9 (14%)
31	CLA	s	609	22	59,63,73	1.34	6 (10%)	70,101,113	1.65	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
33	LUT	16	618	-	42,43,43	0.50	1 (2%)	51,60,60	0.28	0
31	CLA	4	611	32	54,58,73	1.39	6 (11%)	64,95,113	1.77	7 (10%)
31	CLA	B	616	7	64,68,73	1.26	7 (10%)	76,107,113	1.76	10 (13%)
41	LMG	b	620	-	49,49,55	0.18	0	57,57,63	0.16	0
31	CLA	N	611	32	64,68,73	1.30	7 (10%)	76,107,113	1.70	7 (9%)
31	CLA	s	615	22	51,55,73	1.38	6 (11%)	60,91,113	1.84	6 (10%)
48	BCT	D	403	47	3,3,3	0.81	0	2,3,3	3.18	2 (100%)
30	CHL	6	608	-	44,58,74	2.15	10 (22%)	37,94,114	3.13	18 (48%)
31	CLA	c	512	8	69,73,73	1.22	7 (10%)	82,113,113	1.66	8 (9%)
33	LUT	5	614	-	42,43,43	0.40	1 (2%)	51,60,60	0.34	0
46	DGD	W	501	-	46,46,67	0.19	0	54,54,81	0.31	0
31	CLA	s	603	22	46,50,73	1.41	6 (13%)	53,85,113	1.90	5 (9%)
43	LNL	a	412	-	19,19,19	0.45	0	19,19,19	0.48	0
30	CHL	12	608	2	47,61,74	2.18	12 (25%)	41,98,114	3.02	19 (46%)
31	CLA	s	602	22	69,73,73	1.24	7 (10%)	82,113,113	1.62	8 (9%)
31	CLA	15	602	2	64,68,73	1.29	7 (10%)	76,107,113	1.61	9 (11%)
31	CLA	12	604	-	59,63,73	1.32	7 (11%)	70,101,113	1.59	8 (11%)
31	CLA	15	613	-	49,53,73	1.42	8 (16%)	58,89,113	1.72	7 (12%)
31	CLA	5	604	-	54,58,73	1.40	7 (12%)	64,95,113	1.71	8 (12%)
30	CHL	Y	606	-	60,74,74	1.89	12 (20%)	58,114,114	2.58	19 (32%)
31	CLA	6	613	3	59,63,73	1.32	6 (10%)	70,101,113	1.67	7 (10%)
31	CLA	S	604	-	69,73,73	1.23	6 (8%)	82,113,113	1.55	8 (9%)
41	LMG	c	522	-	55,55,55	0.17	0	63,63,63	0.15	0
31	CLA	4	613	1	59,63,73	1.31	6 (10%)	70,101,113	1.65	7 (10%)
31	CLA	s	605	22	54,58,73	1.37	6 (11%)	64,95,113	1.71	7 (10%)
34	NEX	r	617	-	40,46,46	0.39	1 (2%)	50,70,70	0.47	0
30	CHL	Y	605	28	50,64,74	2.07	12 (24%)	46,102,114	2.87	18 (39%)
31	CLA	c	514	8	69,73,73	1.22	6 (8%)	82,113,113	1.56	8 (9%)
33	LUT	6	619	-	42,43,43	0.50	1 (2%)	51,60,60	0.27	0
31	CLA	14	611	32	64,68,73	1.29	6 (9%)	76,107,113	1.67	8 (10%)
46	DGD	c	519	-	60,60,67	0.17	0	74,74,81	0.18	0
31	CLA	15	604	-	59,63,73	1.33	6 (10%)	70,101,113	1.61	7 (10%)
43	LNL	y	619	-	19,19,19	0.44	0	19,19,19	0.49	0
31	CLA	R	610	32	64,68,73	1.27	6 (9%)	76,107,113	1.62	9 (11%)
31	CLA	N	602	2	69,73,73	1.22	8 (11%)	82,113,113	1.66	9 (10%)
31	CLA	N	613	2	59,63,73	1.32	7 (11%)	70,101,113	1.74	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
32	LHG	6	616	31	43,43,48	1.46	8 (18%)	46,49,54	0.80	2 (4%)
31	CLA	3	602	3	64,68,73	1.28	8 (12%)	76,107,113	1.63	10 (13%)
31	CLA	B	605	7	69,73,73	1.23	6 (8%)	82,113,113	1.66	7 (8%)
30	CHL	1	606	-	41,55,74	2.29	12 (29%)	35,91,114	3.21	16 (45%)
43	LNL	y	620	-	19,19,19	0.43	0	19,19,19	0.48	0
31	CLA	16	602	5	69,73,73	1.24	8 (11%)	82,113,113	1.68	9 (10%)
41	LMG	J	102	-	51,51,55	0.17	0	59,59,63	0.16	0
31	CLA	g	603	1	59,63,73	1.32	6 (10%)	70,101,113	1.79	8 (11%)
32	LHG	d	413	-	48,48,48	1.46	8 (16%)	51,54,54	0.76	2 (3%)
30	CHL	15	605	-	40,54,74	2.34	12 (30%)	34,90,114	3.10	16 (47%)
31	CLA	B	606	7	69,73,73	1.22	6 (8%)	82,113,113	1.54	10 (12%)
39	BCR	j	101	-	41,41,41	0.21	0	56,56,56	0.47	0
33	LUT	11	616	-	42,43,43	0.39	1 (2%)	51,60,60	0.31	0
30	CHL	16	608	-	44,58,74	2.16	11 (25%)	37,94,114	3.07	18 (48%)
32	LHG	A	415	-	48,48,48	1.43	8 (16%)	51,54,54	0.76	2 (3%)
31	CLA	s	614	22	69,73,73	1.23	6 (8%)	82,113,113	1.59	10 (12%)
33	LUT	4	616	-	42,43,43	0.48	1 (2%)	51,60,60	0.28	0
41	LMG	B	622	-	48,48,55	0.17	0	56,56,63	0.20	0
30	CHL	G	609	1	60,74,74	1.91	12 (20%)	58,114,114	2.50	20 (34%)
31	CLA	n	602	2	69,73,73	1.24	8 (11%)	82,113,113	1.66	9 (10%)
31	CLA	1	603	1	51,55,73	1.37	6 (11%)	60,91,113	1.85	7 (11%)
41	LMG	A	409	-	55,55,55	0.16	0	63,63,63	0.15	0
30	CHL	y	609	28	60,74,74	1.89	12 (20%)	58,114,114	2.60	19 (32%)
33	LUT	1	617	-	42,43,43	0.44	1 (2%)	51,60,60	0.25	0
30	CHL	11	608	-	45,59,74	2.23	13 (28%)	40,96,114	2.94	20 (50%)
36	3PH	B	620	-	47,47,47	0.27	0	50,52,52	0.29	0
31	CLA	r	614	-	59,63,73	1.31	6 (10%)	70,101,113	1.70	8 (11%)
40	SQD	D	413	-	44,46,54	0.19	0	54,57,65	0.22	0
34	NEX	N	619	-	40,46,46	0.41	1 (2%)	50,70,70	0.42	0
31	CLA	R	603	21	69,73,73	1.23	7 (10%)	82,113,113	1.71	9 (10%)
30	CHL	s	608	-	43,57,74	2.18	11 (25%)	37,93,114	3.12	17 (45%)
31	CLA	C	513	8	59,63,73	1.32	7 (11%)	70,101,113	1.74	9 (12%)
31	CLA	4	612	1	50,54,73	1.44	6 (12%)	59,90,113	1.63	7 (11%)
30	CHL	16	605	5	50,64,74	2.08	12 (24%)	46,102,114	2.85	19 (41%)
30	CHL	R	607	-	45,59,74	2.14	12 (26%)	40,96,114	3.05	19 (47%)
31	CLA	b	605	7	69,73,73	1.22	6 (8%)	82,113,113	1.67	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	CLA	N	612	2	49,53,73	1.41	6 (12%)	58,89,113	1.87	6 (10%)
40	SQD	L	101	-	48,50,54	0.18	0	58,61,65	0.22	0
41	LMG	c	520	-	47,47,55	0.19	0	55,55,63	0.16	0
31	CLA	R	612	21	54,58,73	1.40	6 (11%)	64,95,113	1.60	7 (10%)
30	CHL	n	607	-	60,74,74	1.87	12 (20%)	58,114,114	2.51	19 (32%)
30	CHL	12	605	-	40,54,74	2.34	12 (30%)	34,90,114	3.11	16 (47%)
30	CHL	13	601	5	50,64,74	2.12	12 (24%)	46,102,114	2.81	18 (39%)
30	CHL	5	605	2	40,54,74	2.32	13 (32%)	34,90,114	3.16	16 (47%)
32	LHG	1	615	31	42,42,48	1.47	8 (19%)	45,48,54	0.78	2 (4%)
31	CLA	y	603	28	64,68,73	1.27	7 (10%)	76,107,113	1.74	10 (13%)
31	CLA	c	504	8	69,73,73	1.23	7 (10%)	82,113,113	1.68	11 (13%)
33	LUT	14	616	-	42,43,43	0.34	0	51,60,60	0.27	0
34	NEX	y	624	-	40,46,46	0.44	1 (2%)	50,70,70	0.68	1 (2%)
30	CHL	4	606	-	41,55,74	2.29	12 (29%)	35,91,114	3.25	16 (45%)
31	CLA	A	402	6	69,73,73	1.23	8 (11%)	82,113,113	1.66	9 (10%)
34	NEX	15	616	-	25,28,46	0.39	0	32,42,70	0.56	0
30	CHL	15	608	2	55,69,74	2.02	12 (21%)	52,108,114	2.67	19 (36%)
46	DGD	w	502	-	40,40,67	0.20	0	48,48,81	0.21	0
39	BCR	D	406	-	41,41,41	0.12	0	56,56,56	0.21	0
31	CLA	S	610	22	69,73,73	1.22	6 (8%)	82,113,113	1.61	10 (12%)
36	3PH	7	201	-	47,47,47	0.27	0	50,52,52	0.30	0
30	CHL	11	605	-	42,56,74	2.28	11 (26%)	36,92,114	3.14	17 (47%)
31	CLA	y	610	28	69,73,73	1.22	7 (10%)	82,113,113	1.66	9 (10%)
30	CHL	3	607	-	60,74,74	1.90	12 (20%)	58,114,114	2.61	19 (32%)
30	CHL	4	605	1	40,54,74	2.35	12 (30%)	34,90,114	3.25	17 (50%)
40	SQD	a	409	-	49,51,54	0.19	0	59,62,65	0.26	0
33	LUT	R	615	-	42,43,43	0.45	1 (2%)	51,60,60	0.33	0
32	LHG	R	619	-	46,46,48	1.42	8 (17%)	49,52,54	0.79	2 (4%)
42	PL9	D	407	-	55,55,55	0.09	0	68,69,69	0.20	0
30	CHL	n	608	-	44,58,74	2.13	11 (25%)	37,94,114	3.17	18 (48%)
31	CLA	14	613	1	59,63,73	1.32	7 (11%)	70,101,113	1.69	9 (12%)
32	LHG	3	617	-	46,46,48	1.42	8 (17%)	49,52,54	0.77	2 (4%)
31	CLA	12	613	-	49,53,73	1.41	7 (14%)	58,89,113	1.77	6 (10%)
30	CHL	N	605	2	55,69,74	1.99	12 (21%)	52,108,114	2.64	18 (34%)
30	CHL	13	608	-	44,58,74	2.15	11 (25%)	37,94,114	3.09	18 (48%)
31	CLA	b	614	7	69,73,73	1.23	6 (8%)	82,113,113	1.65	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	CLA	r	601	21	53,57,73	1.36	6 (11%)	61,93,113	1.68	7 (11%)
31	CLA	16	611	32	69,73,73	1.23	7 (10%)	82,113,113	1.61	9 (10%)
30	CHL	6	606	-	50,64,74	2.08	12 (24%)	46,102,114	2.84	18 (39%)
31	CLA	g	614	1	53,57,73	1.37	6 (11%)	61,93,113	1.74	5 (8%)
31	CLA	1	614	1	50,54,73	1.39	7 (14%)	59,90,113	1.84	8 (13%)
32	LHG	g	615	31	48,48,48	1.33	6 (12%)	51,54,54	0.71	2 (3%)
50	PAM	n	620	-	17,17,17	0.46	0	17,17,17	0.50	0
33	LUT	S	619	-	42,43,43	0.41	1 (2%)	51,60,60	0.25	0
31	CLA	b	607	-	69,73,73	1.21	7 (10%)	82,113,113	1.65	8 (9%)
30	CHL	g	601	1	60,74,74	1.86	12 (20%)	58,114,114	2.54	19 (32%)
31	CLA	1	610	1	59,63,73	1.32	6 (10%)	70,101,113	1.60	9 (12%)
31	CLA	b	612	7	69,73,73	1.24	7 (10%)	82,113,113	1.74	7 (8%)
31	CLA	y	615	-	60,64,73	1.31	7 (11%)	71,102,113	1.71	8 (11%)
33	LUT	g	617	-	42,43,43	0.57	1 (2%)	51,60,60	0.33	0
31	CLA	S	609	22	59,63,73	1.33	7 (11%)	70,101,113	1.75	8 (11%)
31	CLA	b	610	-	69,73,73	1.21	7 (10%)	82,113,113	1.67	10 (12%)
34	NEX	R	617	-	40,46,46	0.41	1 (2%)	50,70,70	0.47	0
31	CLA	2	613	2	51,55,73	1.37	7 (13%)	60,91,113	1.64	7 (11%)
46	DGD	c	517	-	67,67,67	0.17	0	81,81,81	0.17	0
35	XAT	11	619	-	41,47,47	0.14	0	54,74,74	0.48	0
43	LNL	R	620	-	19,19,19	0.45	0	19,19,19	0.51	0
30	CHL	S	607	-	37,51,74	2.26	10 (27%)	30,86,114	3.43	15 (50%)
31	CLA	y	602	28	64,68,73	1.28	8 (12%)	76,107,113	1.67	9 (11%)
31	CLA	G	604	-	54,58,73	1.38	6 (11%)	64,95,113	1.76	7 (10%)
31	CLA	16	610	-	69,73,73	1.22	7 (10%)	82,113,113	1.67	10 (12%)
32	LHG	C	521	-	41,41,48	1.48	8 (19%)	44,47,54	0.79	2 (4%)
30	CHL	3	605	3	60,74,74	1.91	12 (20%)	58,114,114	2.64	19 (32%)
36	3PH	B	624	-	37,37,47	0.29	0	40,42,52	0.33	0
40	SQD	d	412	-	52,54,54	0.17	0	62,65,65	0.22	0
30	CHL	2	601	2	41,55,74	2.27	12 (29%)	35,91,114	3.25	17 (48%)
32	LHG	d	408	-	48,48,48	1.31	7 (14%)	51,54,54	0.74	2 (3%)
32	LHG	l	102	-	46,46,48	1.33	8 (17%)	49,52,54	0.78	2 (4%)
31	CLA	Y	603	28	64,68,73	1.27	7 (10%)	76,107,113	1.75	9 (11%)
31	CLA	13	602	5	69,73,73	1.24	7 (10%)	82,113,113	1.63	10 (12%)
31	CLA	6	614	3	54,58,73	1.39	6 (11%)	64,95,113	1.78	7 (10%)
31	CLA	g	610	1	69,73,73	1.22	7 (10%)	82,113,113	1.64	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	CLA	y	614	28	53,57,73	1.37	6 (11%)	61,93,113	1.84	7 (11%)
31	CLA	c	510	8	69,73,73	1.22	6 (8%)	82,113,113	1.76	8 (9%)
31	CLA	g	613	1	69,73,73	1.23	6 (8%)	82,113,113	1.61	7 (8%)
49	HEM	f	101	11,10	50,50,50	0.54	0	67,82,82	0.50	0
34	NEX	11	618	-	14,17,46	0.39	0	19,29,70	0.54	0
30	CHL	Y	607	-	60,74,74	1.86	12 (20%)	58,114,114	2.56	18 (31%)
31	CLA	Y	615	-	60,64,73	1.32	7 (11%)	71,102,113	1.71	9 (12%)
33	LUT	s	619	-	42,43,43	0.38	0	51,60,60	0.25	0
31	CLA	5	603	2	59,63,73	1.32	6 (10%)	70,101,113	1.81	7 (10%)
31	CLA	D	405	9	69,73,73	1.22	6 (8%)	82,113,113	1.56	10 (12%)
31	CLA	s	604	-	69,73,73	1.22	6 (8%)	82,113,113	1.55	8 (9%)
31	CLA	r	604	-	52,56,73	1.38	6 (11%)	61,92,113	1.76	8 (13%)
30	CHL	N	609	2	60,74,74	1.89	12 (20%)	58,114,114	2.59	19 (32%)
31	CLA	R	602	21	69,73,73	1.25	7 (10%)	82,113,113	1.65	10 (12%)
35	XAT	3	620	-	41,47,47	0.16	0	54,74,74	0.71	1 (1%)
31	CLA	C	502	8	69,73,73	1.21	7 (10%)	82,113,113	1.60	7 (8%)
30	CHL	G	608	-	46,60,74	2.17	12 (26%)	40,97,114	3.06	18 (45%)
30	CHL	13	606	-	55,69,74	1.99	12 (21%)	52,108,114	2.70	18 (34%)
34	NEX	g	618	-	40,46,46	0.38	1 (2%)	50,70,70	0.49	0
31	CLA	c	511	8	69,73,73	1.21	7 (10%)	82,113,113	1.71	9 (10%)
30	CHL	y	608	-	38,52,74	2.20	10 (26%)	31,87,114	3.33	15 (48%)
33	LUT	Y	622	-	42,43,43	0.53	1 (2%)	51,60,60	0.29	0
31	CLA	11	603	-	59,63,73	1.32	6 (10%)	70,101,113	1.66	8 (11%)
30	CHL	4	607	-	45,59,74	2.19	12 (26%)	40,96,114	3.07	19 (47%)
31	CLA	4	603	1	59,63,73	1.32	6 (10%)	70,101,113	1.76	9 (12%)
31	CLA	C	509	8	64,68,73	1.30	7 (10%)	76,107,113	1.70	10 (13%)
33	LUT	y	622	-	42,43,43	0.47	1 (2%)	51,60,60	0.45	0
33	LUT	4	617	-	42,43,43	0.44	1 (2%)	51,60,60	0.25	0
35	XAT	R	616	-	41,47,47	0.15	0	54,74,74	0.84	2 (3%)
31	CLA	2	610	2	54,58,73	1.37	7 (12%)	64,95,113	1.74	8 (12%)
31	CLA	3	615	3	50,54,73	1.39	8 (16%)	59,90,113	1.85	7 (11%)
31	CLA	15	612	-	54,58,73	1.39	7 (12%)	64,95,113	1.72	9 (14%)
30	CHL	N	607	-	60,74,74	1.87	12 (20%)	58,114,114	2.51	19 (32%)
31	CLA	6	610	3	64,68,73	1.28	6 (9%)	76,107,113	1.62	11 (14%)

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
31	CLA	2	603	2	1/1/13/20	9/27/103/115	-
31	CLA	n	613	2	1/1/13/20	9/27/103/115	-
35	XAT	r	616	-	-	0/31/93/93	0/4/4/4
30	CHL	G	605	1	3/3/16/26	9/18/116/137	-
31	CLA	11	610	-	1/1/13/20	10/27/103/115	-
32	LHG	d	409	-	-	16/43/43/53	-
33	LUT	N	618	-	-	0/29/67/67	0/2/2/2
30	CHL	3	608	-	3/3/16/26	7/20/118/137	-
30	CHL	S	606	22	3/3/20/26	19/39/137/137	-
30	CHL	y	605	28	3/3/18/26	7/27/125/137	-
38	PHO	A	405	-	-	7/37/103/103	0/5/6/6
31	CLA	n	604	-	1/1/13/20	14/27/103/115	-
31	CLA	13	615	5	1/1/11/20	3/15/91/115	-
31	CLA	Y	612	28	1/1/15/20	14/39/115/115	-
33	LUT	14	617	-	-	0/29/67/67	0/2/2/2
30	CHL	15	606	-	3/3/17/26	6/21/119/137	-
31	CLA	13	604	-	1/1/13/20	10/27/103/115	-
31	CLA	A	404	-	1/1/15/20	15/39/115/115	-
39	BCR	B	619	-	-	0/29/63/63	0/2/2/2
32	LHG	y	616	31	-	15/53/53/53	-
31	CLA	c	509	8	1/1/14/20	13/33/109/115	-
30	CHL	12	601	2	3/3/16/26	6/20/118/137	-
31	CLA	b	602	7	1/1/15/20	8/39/115/115	-
31	CLA	14	604	-	1/1/13/20	13/27/103/115	-
30	CHL	5	601	2	3/3/17/26	8/21/119/137	-
34	NEX	G	618	-	-	2/27/79/83	0/3/3/3
33	LUT	13	618	-	-	0/29/67/67	0/2/2/2
36	3PH	b	623	-	-	5/40/40/49	-
31	CLA	B	601	-	1/1/13/20	11/27/103/115	-
31	CLA	S	615	22	1/1/11/20	7/18/94/115	-
31	CLA	Y	602	28	1/1/15/20	15/39/115/115	-
39	BCR	c	526	-	-	0/29/63/63	0/2/2/2
32	LHG	a	411	-	-	16/53/53/53	-
33	LUT	n	618	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	602	7	1/1/15/20	8/39/115/115	-
43	LNL	h	101	-	-	3/17/17/17	-
31	CLA	S	612	22	1/1/11/20	7/15/91/115	-
31	CLA	d	402	-	1/1/15/20	16/39/115/115	-
33	LUT	S	618	-	-	0/29/67/67	0/2/2/2
30	CHL	r	605	21	3/3/18/26	12/27/125/137	-
31	CLA	R	611	21	1/1/11/20	8/20/96/115	-
33	LUT	2	614	-	-	0/29/67/67	0/2/2/2
30	CHL	n	609	2	3/3/20/26	16/39/137/137	-
39	BCR	b	619	-	-	0/29/63/63	0/2/2/2
32	LHG	a	414	-	-	20/47/47/53	-
30	CHL	1	609	-	3/3/18/26	15/27/125/137	-
30	CHL	R	606	21	3/3/20/26	19/39/137/137	-
31	CLA	r	611	21	1/1/11/20	9/20/96/115	-
33	LUT	G	616	-	-	0/29/67/67	0/2/2/2
41	LMG	w	501	-	-	6/50/70/70	0/1/1/1
31	CLA	5	611	-	1/1/11/20	5/17/93/115	-
31	CLA	C	503	8	1/1/15/20	5/39/115/115	-
31	CLA	S	611	32	1/1/15/20	13/39/115/115	-
31	CLA	b	601	-	1/1/13/20	9/27/103/115	-
31	CLA	b	616	7	1/1/14/20	15/33/109/115	-
30	CHL	16	606	-	3/3/19/26	16/33/131/137	-
30	CHL	Y	601	28	3/3/20/26	11/39/137/137	-
32	LHG	S	621	-	-	21/53/53/53	-
42	PL9	A	410	-	-	10/53/73/73	0/1/1/1
30	CHL	g	606	-	3/3/16/26	5/20/118/137	-
31	CLA	b	615	7	1/1/15/20	10/39/115/115	-
39	BCR	a	408	-	-	0/29/63/63	0/2/2/2
31	CLA	14	610	-	1/1/15/20	19/39/115/115	-
31	CLA	S	603	22	1/1/10/20	8/12/88/115	-
38	PHO	a	406	-	-	5/37/103/103	0/5/6/6
41	LMG	d	410	-	-	8/39/59/70	0/1/1/1
31	CLA	S	605	22	1/1/12/20	9/21/97/115	-
30	CHL	14	601	1	3/3/20/26	18/39/137/137	-
30	CHL	6	607	-	3/3/20/26	20/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	LNL	c	524	-	-	5/17/17/17	-
31	CLA	4	614	1	1/1/11/20	6/17/93/115	-
31	CLA	B	615	7	1/1/15/20	10/39/115/115	-
30	CHL	2	609	2	3/3/20/26	25/39/137/137	-
31	CLA	R	613	21	1/1/14/20	9/33/109/115	-
31	CLA	g	612	1	1/1/10/20	2/13/89/115	-
30	CHL	3	609	3	3/3/20/26	16/39/137/137	-
30	CHL	12	607	-	3/3/16/26	10/20/118/137	-
30	CHL	s	601	22	3/3/16/26	6/15/113/137	-
31	CLA	r	610	32	1/1/14/20	9/33/109/115	-
31	CLA	2	602	2	1/1/13/20	16/27/103/115	-
33	LUT	n	617	-	-	0/29/67/67	0/2/2/2
30	CHL	6	605	3	3/3/20/26	17/39/137/137	-
41	LMG	D	414	-	-	12/43/63/70	0/1/1/1
30	CHL	1	605	1	3/3/16/26	5/15/113/137	-
31	CLA	B	607	-	1/1/15/20	10/39/115/115	-
30	CHL	3	606	-	3/3/18/26	6/27/125/137	-
31	CLA	G	613	1	1/1/15/20	13/39/115/115	-
33	LUT	11	617	-	-	0/29/67/67	0/2/2/2
31	CLA	S	602	22	1/1/15/20	14/39/115/115	-
32	LHG	D	408	-	-	14/53/53/53	-
31	CLA	1	612	1	1/1/11/20	7/17/93/115	-
31	CLA	c	502	8	1/1/15/20	14/39/115/115	-
39	BCR	c	516	-	-	3/29/63/63	0/2/2/2
31	CLA	Y	604	-	1/1/13/20	10/27/103/115	-
31	CLA	B	604	7	1/1/15/20	10/39/115/115	-
31	CLA	B	611	7	1/1/15/20	13/39/115/115	-
32	LHG	a	413	-	-	13/48/48/53	-
31	CLA	12	611	-	1/1/11/20	6/15/91/115	-
31	CLA	G	603	1	1/1/13/20	12/27/103/115	-
31	CLA	y	604	-	1/1/13/20	8/27/103/115	-
39	BCR	B	618	-	-	0/29/63/63	0/2/2/2
31	CLA	c	507	8	1/1/15/20	20/39/115/115	-
31	CLA	b	606	7	1/1/15/20	14/39/115/115	-
31	CLA	n	610	2	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	g	611	32	1/1/15/20	13/39/115/115	-
31	CLA	1	611	32	1/1/12/20	8/21/97/115	-
31	CLA	12	609	2	1/1/13/20	15/27/103/115	-
31	CLA	N	603	2	1/1/14/20	13/33/109/115	-
31	CLA	C	512	8	1/1/15/20	16/39/115/115	-
33	LUT	16	617	-	-	0/29/67/67	0/2/2/2
46	DGD	c	518	-	-	5/47/87/95	0/2/2/2
30	CHL	14	607	-	3/3/16/26	9/20/118/137	-
30	CHL	2	606	-	3/3/16/26	8/15/113/137	-
43	LNL	w	503	-	-	4/17/17/17	-
33	LUT	12	615	-	-	0/29/67/67	0/2/2/2
31	CLA	4	610	1	1/1/15/20	15/39/115/115	-
30	CHL	S	601	22	3/3/16/26	6/15/113/137	-
31	CLA	15	611	-	1/1/11/20	6/15/91/115	-
32	LHG	y	618	-	-	28/51/51/53	-
30	CHL	16	607	-	3/3/19/26	14/33/131/137	-
34	NEX	2	616	-	-	2/25/56/83	0/2/2/3
31	CLA	3	604	-	1/1/15/20	20/39/115/115	-
31	CLA	13	614	5	1/1/11/20	7/15/91/115	-
31	CLA	s	613	22	1/1/11/20	6/20/96/115	-
41	LMG	j	102	-	-	10/46/66/70	0/1/1/1
31	CLA	14	603	-	1/1/13/20	10/27/103/115	-
31	CLA	r	613	21	1/1/15/20	9/39/115/115	-
31	CLA	d	404	9	1/1/15/20	16/39/115/115	-
31	CLA	a	404	-	1/1/15/20	16/39/115/115	-
33	LUT	13	617	-	-	0/29/67/67	0/2/2/2
30	CHL	11	607	-	3/3/16/26	10/15/113/137	-
31	CLA	12	602	2	1/1/14/20	15/33/109/115	-
31	CLA	B	613	7	1/1/15/20	22/39/115/115	-
46	DGD	C	517	-	-	17/55/95/95	0/2/2/2
39	BCR	h	102	-	-	2/29/63/63	0/2/2/2
46	DGD	C	519	-	-	8/48/88/95	0/2/2/2
41	LMG	H	102	-	-	2/36/36/70	-
30	CHL	14	608	-	3/3/17/26	13/21/119/137	-
31	CLA	g	602	1	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	LNL	W	502	-	-	4/17/17/17	-
32	LHG	s	617	31	-	21/49/49/53	-
39	BCR	B	617	-	-	2/29/63/63	0/2/2/2
39	BCR	C	526	-	-	0/29/63/63	0/2/2/2
31	CLA	Y	614	28	1/1/11/20	4/20/96/115	-
31	CLA	15	610	-	1/1/11/20	3/15/91/115	-
34	NEX	1	618	-	-	0/6/37/83	0/2/2/3
31	CLA	6	611	32	1/1/15/20	13/39/115/115	-
31	CLA	Y	610	28	1/1/15/20	8/39/115/115	-
31	CLA	B	614	7	1/1/15/20	18/39/115/115	-
30	CHL	6	601	3	3/3/19/26	14/33/131/137	-
31	CLA	c	508	-	1/1/15/20	18/39/115/115	-
31	CLA	s	611	32	1/1/15/20	12/39/115/115	-
32	LHG	r	621	-	-	18/48/48/53	-
31	CLA	3	610	3	1/1/14/20	20/33/109/115	-
30	CHL	12	606	-	3/3/17/26	5/21/119/137	-
31	CLA	15	603	-	1/1/13/20	8/27/103/115	-
31	CLA	c	503	8	1/1/15/20	8/39/115/115	-
33	LUT	6	618	-	-	0/29/67/67	0/2/2/2
31	CLA	r	609	21	1/1/15/20	18/39/115/115	-
33	LUT	1	616	-	-	0/29/67/67	0/2/2/2
31	CLA	C	508	-	1/1/15/20	18/39/115/115	-
31	CLA	n	615	2	1/1/11/20	5/18/94/115	-
31	CLA	6	612	3	1/1/13/20	9/27/103/115	-
31	CLA	3	614	3	1/1/12/20	9/21/97/115	-
39	BCR	b	618	-	-	0/29/63/63	0/2/2/2
31	CLA	12	612	2	1/1/12/20	12/21/97/115	-
41	LMG	C	522	-	-	7/50/70/70	0/1/1/1
32	LHG	3	616	31	-	11/48/48/53	-
33	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
31	CLA	12	610	-	1/1/11/20	4/15/91/115	-
30	CHL	13	607	-	3/3/19/26	13/33/131/137	-
31	CLA	r	603	21	1/1/15/20	14/39/115/115	-
43	LNL	x	201	-	-	6/17/17/17	-
40	SQD	l	101	-	-	9/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	1	602	1	1/1/14/20	14/33/109/115	-
31	CLA	C	504	8	1/1/15/20	9/39/115/115	-
30	CHL	2	605	2	3/3/16/26	7/15/113/137	-
31	CLA	15	609	2	1/1/13/20	12/27/103/115	-
33	LUT	3	618	-	-	0/29/67/67	0/2/2/2
31	CLA	13	610	-	1/1/15/20	11/39/115/115	-
41	LMG	B	621	-	-	7/44/64/70	0/1/1/1
31	CLA	y	613	28	1/1/15/20	12/39/115/115	-
31	CLA	s	612	22	1/1/11/20	3/15/91/115	-
31	CLA	12	603	-	1/1/13/20	11/27/103/115	-
31	CLA	R	601	21	1/1/11/20	5/20/96/115	-
31	CLA	r	612	21	1/1/12/20	6/21/97/115	-
33	LUT	12	614	-	-	5/29/67/67	0/2/2/2
43	LNL	Y	619	-	-	3/17/17/17	-
31	CLA	S	614	22	1/1/15/20	13/39/115/115	-
43	LNL	c	523	-	-	3/17/17/17	-
31	CLA	C	506	8	1/1/15/20	9/39/115/115	-
30	CHL	G	601	1	3/3/20/26	12/39/137/137	-
33	LUT	G	617	-	-	0/29/67/67	0/2/2/2
31	CLA	1	613	1	1/1/13/20	9/27/103/115	-
30	CHL	y	601	28	3/3/20/26	11/39/137/137	-
34	NEX	5	616	-	-	2/25/56/83	0/2/2/3
32	LHG	Y	617	-	-	24/51/51/53	-
39	BCR	c	515	-	-	2/29/63/63	0/2/2/2
30	CHL	2	608	-	3/3/16/26	6/20/118/137	-
30	CHL	15	607	-	3/3/16/26	9/20/118/137	-
31	CLA	D	404	9	1/1/15/20	15/39/115/115	-
31	CLA	16	615	-	1/1/11/20	5/15/91/115	-
31	CLA	3	613	3	1/1/13/20	10/27/103/115	-
32	LHG	13	616	31	-	25/44/44/53	-
30	CHL	s	606	22	3/3/20/26	22/39/137/137	-
31	CLA	c	513	8	1/1/13/20	8/27/103/115	-
30	CHL	r	606	21	3/3/20/26	19/39/137/137	-
34	NEX	13	619	-	-	2/27/83/83	0/3/3/3
33	LUT	3	619	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	n	603	2	1/1/14/20	14/33/109/115	-
30	CHL	11	606	-	3/3/16/26	7/17/115/137	-
30	CHL	14	609	-	3/3/18/26	16/27/125/137	-
32	LHG	G	615	31	-	20/53/53/53	-
44	STE	B	623	-	-	6/17/17/17	-
31	CLA	6	602	3	1/1/14/20	10/33/109/115	-
32	LHG	r	618	31	-	16/42/42/53	-
40	SQD	A	408	-	-	7/46/66/69	0/1/1/1
41	LMG	C	520	-	-	10/42/62/70	0/1/1/1
44	STE	b	622	-	-	9/17/17/17	-
31	CLA	14	602	1	1/1/14/20	12/33/109/115	-
31	CLA	n	612	2	1/1/11/20	7/15/91/115	-
31	CLA	C	507	8	1/1/15/20	20/39/115/115	-
30	CHL	N	606	-	3/3/19/26	13/33/131/137	-
30	CHL	13	609	-	3/3/19/26	16/33/131/137	-
30	CHL	G	607	-	3/3/16/26	6/20/118/137	-
32	LHG	R	618	31	-	14/42/42/53	-
31	CLA	16	603	-	1/1/14/20	12/33/109/115	-
35	XAT	g	619	-	-	0/31/93/93	0/4/4/4
31	CLA	r	608	21	1/1/15/20	7/39/115/115	-
42	PL9	d	407	-	-	12/53/73/73	0/1/1/1
38	PHO	D	402	-	-	9/37/103/103	0/5/6/6
31	CLA	11	612	1	1/1/10/20	7/13/89/115	-
33	LUT	N	617	-	-	0/29/67/67	0/2/2/2
30	CHL	n	606	-	3/3/19/26	15/33/131/137	-
43	LNL	Y	620	-	-	5/17/17/17	-
31	CLA	C	511	8	1/1/15/20	12/39/115/115	-
31	CLA	G	602	1	1/1/15/20	16/39/115/115	-
32	LHG	L	102	-	-	21/51/51/53	-
32	LHG	14	615	31	-	23/53/53/53	-
30	CHL	15	601	2	3/3/16/26	6/20/118/137	-
32	LHG	S	617	31	-	23/49/49/53	-
32	LHG	s	621	-	-	17/53/53/53	-
30	CHL	14	606	-	3/3/16/26	5/17/115/137	-
33	LUT	y	623	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	13	603	-	1/1/14/20	13/33/109/115	-
31	CLA	C	510	8	1/1/15/20	11/39/115/115	-
31	CLA	Y	613	28	1/1/15/20	11/39/115/115	-
31	CLA	5	610	2	1/1/12/20	11/21/97/115	-
31	CLA	G	610	1	1/1/15/20	7/39/115/115	-
31	CLA	c	506	8	1/1/15/20	10/39/115/115	-
31	CLA	d	405	9	1/1/15/20	15/39/115/115	-
43	LNL	H	101	-	-	3/17/17/17	-
43	LNL	X	201	-	-	4/17/17/17	-
33	LUT	s	618	-	-	2/29/67/67	0/2/2/2
30	CHL	5	609	2	3/3/20/26	16/39/137/137	-
31	CLA	13	612	5	1/1/11/20	2/15/91/115	-
31	CLA	y	611	32	1/1/15/20	9/39/115/115	-
34	NEX	4	618	-	-	0/6/37/83	0/2/2/3
31	CLA	5	613	2	1/1/12/20	7/21/97/115	-
33	LUT	r	615	-	-	0/29/67/67	0/2/2/2
30	CHL	G	606	-	3/3/16/26	4/17/115/137	-
32	LHG	a	401	-	-	11/53/53/53	-
39	BCR	C	516	-	-	2/29/63/63	0/2/2/2
33	LUT	5	615	-	-	0/29/67/67	0/2/2/2
30	CHL	y	606	-	3/3/20/26	14/39/137/137	-
35	XAT	14	619	-	-	0/31/93/93	0/4/4/4
35	XAT	6	620	-	-	1/31/93/93	0/4/4/4
32	LHG	c	521	-	-	19/46/46/53	-
31	CLA	r	602	21	1/1/15/20	11/39/115/115	-
33	LUT	15	614	-	-	3/29/67/67	0/2/2/2
30	CHL	16	601	5	3/3/18/26	16/27/125/137	-
34	NEX	S	620	-	-	2/27/83/83	0/3/3/3
31	CLA	n	614	2	1/1/11/20	9/15/91/115	-
39	BCR	C	515	-	-	2/29/63/63	0/2/2/2
34	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
31	CLA	11	602	1	1/1/14/20	14/33/109/115	-
31	CLA	11	613	1	1/1/13/20	11/27/103/115	-
30	CHL	5	607	-	3/3/18/26	7/27/125/137	-
31	CLA	b	604	7	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	13	611	32	1/1/15/20	12/39/115/115	-
31	CLA	14	614	1	1/1/11/20	9/20/96/115	-
31	CLA	16	612	5	1/1/11/20	3/15/91/115	-
31	CLA	16	613	5	1/1/12/20	9/21/97/115	-
32	LHG	4	615	31	-	13/51/51/53	-
46	DGD	C	518	-	-	5/47/87/95	0/2/2/2
30	CHL	Y	609	28	3/3/20/26	17/39/137/137	-
31	CLA	2	612	-	1/1/11/20	6/17/93/115	-
30	CHL	1	601	1	3/3/19/26	11/33/131/137	-
31	CLA	G	612	1	1/1/10/20	2/13/89/115	-
31	CLA	N	614	2	1/1/11/20	5/15/91/115	-
31	CLA	2	604	-	1/1/12/20	9/21/97/115	-
31	CLA	y	612	28	1/1/15/20	16/39/115/115	-
43	LNL	W	503	-	-	3/17/17/17	-
34	NEX	3	621	-	-	2/27/83/83	0/3/3/3
31	CLA	a	407	6	1/1/13/20	10/27/103/115	-
30	CHL	4	608	-	3/3/16/26	12/20/118/137	-
31	CLA	3	603	3	1/1/13/20	10/27/103/115	-
31	CLA	11	614	-	1/1/11/20	11/20/96/115	-
30	CHL	3	601	3	3/3/19/26	12/33/131/137	-
43	LNL	I	101	-	-	4/17/17/17	-
31	CLA	b	611	7	1/1/15/20	13/39/115/115	-
30	CHL	g	609	1	3/3/20/26	16/39/137/137	-
31	CLA	R	609	21	1/1/15/20	20/39/115/115	-
43	LNL	y	621	-	-	3/17/17/17	-
31	CLA	Y	611	32	1/1/15/20	10/39/115/115	-
31	CLA	16	604	-	1/1/13/20	7/27/103/115	-
30	CHL	n	605	2	3/3/19/26	15/33/131/137	-
31	CLA	3	612	3	1/1/15/20	14/39/115/115	-
43	LNL	i	101	-	-	4/17/17/17	-
31	CLA	g	604	-	1/1/12/20	9/21/97/115	-
30	CHL	N	601	2	3/3/17/26	13/24/122/137	-
42	PL9	a	410	-	-	11/53/73/73	0/1/1/1
30	CHL	11	609	-	3/3/18/26	18/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	N	610	2	1/1/14/20	5/33/109/115	-
41	LMG	v	101	-	-	11/46/66/70	0/1/1/1
32	LHG	n	616	31	-	28/53/53/53	-
33	LUT	15	615	-	-	0/29/67/67	0/2/2/2
31	CLA	1	604	-	1/1/12/20	8/21/97/115	-
41	LMG	D	410	-	-	7/39/59/70	0/1/1/1
31	CLA	3	611	32	1/1/15/20	11/39/115/115	-
31	CLA	R	608	21	1/1/15/20	9/39/115/115	-
30	CHL	s	607	-	3/3/15/26	7/12/110/137	-
30	CHL	1	607	-	3/3/17/26	6/21/119/137	-
32	LHG	R	621	-	-	14/48/48/53	-
34	NEX	12	616	-	-	2/19/50/83	0/2/2/3
41	LMG	s	616	-	-	9/37/57/70	0/1/1/1
30	CHL	11	601	1	3/3/20/26	13/39/137/137	-
31	CLA	5	612	-	1/1/11/20	9/17/93/115	-
32	LHG	r	619	-	-	18/51/51/53	-
31	CLA	R	604	-	1/1/11/20	4/19/95/115	-
30	CHL	S	608	-	3/3/16/26	10/19/117/137	-
32	LHG	N	616	31	-	23/53/53/53	-
34	NEX	s	620	-	-	2/27/83/83	0/3/3/3
32	LHG	D	409	-	-	11/43/43/53	-
35	XAT	G	619	-	-	0/31/93/93	0/4/4/4
30	CHL	6	609	3	3/3/20/26	15/39/137/137	-
30	CHL	r	607	-	3/3/17/26	5/21/119/137	-
31	CLA	B	610	-	1/1/15/20	14/39/115/115	-
30	CHL	R	605	21	3/3/18/26	9/27/125/137	-
31	CLA	S	613	22	1/1/11/20	7/20/96/115	-
32	LHG	11	615	31	-	17/53/53/53	-
39	BCR	J	101	-	-	6/29/63/63	0/2/2/2
31	CLA	2	611	-	1/1/11/20	8/17/93/115	-
31	CLA	C	505	-	1/1/13/20	6/27/103/115	-
40	SQD	d	414	-	-	7/41/61/69	0/1/1/1
38	PHO	a	405	-	-	6/37/103/103	0/5/6/6
31	CLA	B	609	7	1/1/15/20	17/39/115/115	-
33	LUT	g	616	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	11	611	32	1/1/12/20	7/21/97/115	-
32	LHG	Y	616	31	-	14/53/53/53	-
30	CHL	13	605	5	3/3/18/26	9/27/125/137	-
30	CHL	n	601	2	3/3/17/26	12/23/121/137	-
30	CHL	Y	608	-	3/3/15/26	3/13/111/137	-
31	CLA	6	603	3	1/1/13/20	8/27/103/115	-
34	NEX	n	619	-	-	2/27/83/83	0/3/3/3
50	PAM	N	621	-	-	3/15/15/15	-
31	CLA	b	613	7	1/1/15/20	20/39/115/115	-
39	BCR	b	617	-	-	2/29/63/63	0/2/2/2
43	LNL	C	523	-	-	3/17/17/17	-
32	LHG	6	617	-	-	26/51/51/53	-
31	CLA	B	603	7	1/1/15/20	14/39/115/115	-
31	CLA	A	406	6	1/1/13/20	9/27/103/115	-
32	LHG	A	413	-	-	12/48/48/53	-
30	CHL	5	608	-	3/3/16/26	8/20/118/137	-
30	CHL	g	608	-	3/3/17/26	8/23/121/137	-
34	NEX	14	618	-	-	0/6/37/83	0/2/2/3
30	CHL	16	609	-	3/3/19/26	12/33/131/137	-
41	LMG	d	415	-	-	12/43/63/70	0/1/1/1
31	CLA	B	612	7	1/1/15/20	15/39/115/115	-
39	BCR	A	407	-	-	0/29/63/63	0/2/2/2
34	NEX	16	619	-	-	2/27/83/83	0/3/3/3
31	CLA	R	614	-	1/1/13/20	11/27/103/115	-
30	CHL	g	607	-	3/3/16/26	7/20/118/137	-
43	LNL	C	524	-	-	5/17/17/17	-
31	CLA	b	603	7	1/1/15/20	14/39/115/115	-
31	CLA	6	604	-	1/1/15/20	21/39/115/115	-
32	LHG	16	616	31	-	25/44/44/53	-
43	LNL	r	620	-	-	8/17/17/17	-
31	CLA	16	614	5	1/1/11/20	6/15/91/115	-
31	CLA	4	602	1	1/1/14/20	12/33/109/115	-
31	CLA	a	403	6	1/1/15/20	12/39/115/115	-
30	CHL	N	608	-	3/3/16/26	10/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	D	412	-	-	19/53/53/53	-
36	3PH	8	201	-	-	6/49/49/49	-
32	LHG	y	617	-	-	24/51/51/53	-
30	CHL	2	607	-	3/3/18/26	8/27/125/137	-
31	CLA	G	614	1	1/1/11/20	5/20/96/115	-
31	CLA	s	610	22	1/1/15/20	15/39/115/115	-
31	CLA	N	604	-	1/1/13/20	13/27/103/115	-
49	HEM	F	101	11,10	-	6/14/54/54	-
30	CHL	4	609	-	3/3/20/26	24/39/137/137	-
32	LHG	Y	618	-	-	30/51/51/53	-
30	CHL	g	605	1	3/3/16/26	9/18/116/137	-
31	CLA	G	611	32	1/1/15/20	11/39/115/115	-
40	SQD	D	411	-	-	10/49/69/69	0/1/1/1
32	LHG	A	414	-	-	21/47/47/53	-
30	CHL	4	601	1	3/3/19/26	11/33/131/137	-
39	BCR	H	103	-	-	2/29/63/63	0/2/2/2
31	CLA	b	608	7	1/1/15/20	15/39/115/115	-
31	CLA	5	602	2	1/1/13/20	16/27/103/115	-
31	CLA	b	609	7	1/1/15/20	19/39/115/115	-
31	CLA	C	514	8	1/1/15/20	16/39/115/115	-
36	3PH	T	101	-	-	10/49/49/49	-
41	LMG	K	102	-	-	12/46/66/70	0/1/1/1
31	CLA	14	612	1	1/1/10/20	5/13/89/115	-
30	CHL	1	608	-	3/3/16/26	14/20/118/137	-
39	BCR	d	406	-	-	3/29/63/63	0/2/2/2
43	LNL	A	412	-	-	0/17/17/17	-
31	CLA	A	403	-	1/1/15/20	16/39/115/115	-
31	CLA	B	608	7	1/1/15/20	14/39/115/115	-
31	CLA	13	613	5	1/1/12/20	7/21/97/115	-
33	LUT	2	615	-	-	0/29/67/67	0/2/2/2
34	NEX	6	621	-	-	2/27/83/83	0/3/3/3
31	CLA	N	615	2	1/1/11/20	5/18/94/115	-
41	LMG	S	616	-	-	6/37/57/70	0/1/1/1
30	CHL	y	607	-	3/3/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	14	605	1	3/3/16/26	10/18/116/137	-
31	CLA	c	505	-	1/1/13/20	8/27/103/115	-
31	CLA	n	611	32	1/1/14/20	11/33/109/115	-
41	LMG	d	411	-	-	4/36/36/70	-
32	LHG	A	411	-	-	20/53/53/53	-
30	CHL	5	606	-	3/3/16/26	8/15/113/137	-
31	CLA	11	604	-	1/1/11/20	9/17/93/115	-
41	LMG	b	621	-	-	7/41/61/70	0/1/1/1
31	CLA	4	604	-	1/1/12/20	9/21/97/115	-
31	CLA	6	615	3	1/1/12/20	11/21/97/115	-
31	CLA	s	609	22	1/1/13/20	9/27/103/115	-
33	LUT	16	618	-	-	0/29/67/67	0/2/2/2
31	CLA	4	611	32	1/1/12/20	4/21/97/115	-
31	CLA	B	616	7	1/1/14/20	15/33/109/115	-
41	LMG	b	620	-	-	4/44/64/70	0/1/1/1
31	CLA	N	611	32	1/1/14/20	10/33/109/115	-
31	CLA	s	615	22	1/1/11/20	8/18/94/115	-
30	CHL	6	608	-	3/3/16/26	9/20/118/137	-
31	CLA	c	512	8	1/1/15/20	16/39/115/115	-
33	LUT	5	614	-	-	2/29/67/67	0/2/2/2
46	DGD	W	501	-	-	10/41/61/95	0/1/1/2
31	CLA	s	603	22	1/1/10/20	7/12/88/115	-
43	LNL	a	412	-	-	5/17/17/17	-
30	CHL	12	608	2	3/3/17/26	13/24/122/137	-
31	CLA	s	602	22	1/1/15/20	10/39/115/115	-
31	CLA	15	602	2	1/1/14/20	18/33/109/115	-
31	CLA	12	604	-	1/1/13/20	9/27/103/115	-
31	CLA	15	613	-	1/1/11/20	6/15/91/115	-
31	CLA	5	604	-	1/1/12/20	10/21/97/115	-
30	CHL	Y	606	-	3/3/20/26	15/39/137/137	-
31	CLA	6	613	3	1/1/13/20	10/27/103/115	-
31	CLA	S	604	-	1/1/15/20	21/39/115/115	-
41	LMG	c	522	-	-	6/50/70/70	0/1/1/1
31	CLA	4	613	1	1/1/13/20	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	s	605	22	1/1/12/20	7/21/97/115	-
34	NEX	r	617	-	-	3/27/83/83	0/3/3/3
30	CHL	Y	605	28	3/3/18/26	12/27/125/137	-
31	CLA	c	514	8	1/1/15/20	16/39/115/115	-
33	LUT	6	619	-	-	0/29/67/67	0/2/2/2
31	CLA	14	611	32	1/1/14/20	11/33/109/115	-
46	DGD	c	519	-	-	8/48/88/95	0/2/2/2
31	CLA	15	604	-	1/1/13/20	5/27/103/115	-
43	LNL	y	619	-	-	5/17/17/17	-
31	CLA	R	610	32	1/1/14/20	18/33/109/115	-
31	CLA	N	602	2	1/1/15/20	18/39/115/115	-
31	CLA	N	613	2	1/1/13/20	15/27/103/115	-
32	LHG	6	616	31	-	15/48/48/53	-
31	CLA	3	602	3	1/1/14/20	13/33/109/115	-
31	CLA	B	605	7	1/1/15/20	11/39/115/115	-
30	CHL	1	606	-	3/3/16/26	7/17/115/137	-
43	LNL	y	620	-	-	5/17/17/17	-
31	CLA	16	602	5	1/1/15/20	16/39/115/115	-
41	LMG	J	102	-	-	10/46/66/70	0/1/1/1
31	CLA	g	603	1	1/1/13/20	13/27/103/115	-
32	LHG	d	413	-	-	16/53/53/53	-
30	CHL	15	605	-	3/3/16/26	7/15/113/137	-
31	CLA	B	606	7	1/1/15/20	15/39/115/115	-
39	BCR	j	101	-	-	6/29/63/63	0/2/2/2
33	LUT	11	616	-	-	0/29/67/67	0/2/2/2
30	CHL	16	608	-	3/3/16/26	8/20/118/137	-
32	LHG	A	415	-	-	13/53/53/53	-
31	CLA	s	614	22	1/1/15/20	18/39/115/115	-
33	LUT	4	616	-	-	0/29/67/67	0/2/2/2
41	LMG	B	622	-	-	6/43/63/70	0/1/1/1
30	CHL	G	609	1	3/3/20/26	15/39/137/137	-
31	CLA	n	602	2	1/1/15/20	18/39/115/115	-
31	CLA	1	603	1	1/1/11/20	2/18/94/115	-
41	LMG	A	409	-	-	5/50/70/70	0/1/1/1
30	CHL	y	609	28	3/3/20/26	17/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LUT	1	617	-	-	0/29/67/67	0/2/2/2
30	CHL	11	608	-	3/3/17/26	11/21/119/137	-
36	3PH	B	620	-	-	12/49/49/49	-
31	CLA	r	614	-	1/1/13/20	12/27/103/115	-
40	SQD	D	413	-	-	8/41/61/69	0/1/1/1
34	NEX	N	619	-	-	2/27/83/83	0/3/3/3
31	CLA	R	603	21	1/1/15/20	18/39/115/115	-
30	CHL	s	608	-	3/3/16/26	8/19/117/137	-
31	CLA	C	513	8	1/1/13/20	8/27/103/115	-
31	CLA	4	612	1	1/1/11/20	7/17/93/115	-
30	CHL	16	605	5	3/3/18/26	7/27/125/137	-
30	CHL	R	607	-	3/3/17/26	9/21/119/137	-
31	CLA	b	605	7	1/1/15/20	11/39/115/115	-
31	CLA	N	612	2	1/1/11/20	8/15/91/115	-
40	SQD	L	101	-	-	13/45/65/69	0/1/1/1
41	LMG	c	520	-	-	10/42/62/70	0/1/1/1
31	CLA	R	612	21	1/1/12/20	8/21/97/115	-
30	CHL	n	607	-	3/3/20/26	17/39/137/137	-
30	CHL	12	605	-	3/3/16/26	7/15/113/137	-
30	CHL	13	601	5	3/3/18/26	17/27/125/137	-
30	CHL	5	605	2	3/3/16/26	8/15/113/137	-
32	LHG	1	615	31	-	14/47/47/53	-
31	CLA	y	603	28	1/1/14/20	12/33/109/115	-
31	CLA	c	504	8	1/1/15/20	10/39/115/115	-
33	LUT	14	616	-	-	0/29/67/67	0/2/2/2
34	NEX	y	624	-	-	4/27/83/83	0/3/3/3
30	CHL	4	606	-	2/2/16/26	6/17/115/137	-
31	CLA	A	402	6	1/1/15/20	12/39/115/115	-
34	NEX	15	616	-	-	2/19/50/83	0/2/2/3
30	CHL	15	608	2	3/3/19/26	12/33/131/137	-
46	DGD	w	502	-	-	10/35/55/95	0/1/1/2
39	BCR	D	406	-	-	3/29/63/63	0/2/2/2
31	CLA	S	610	22	1/1/15/20	17/39/115/115	-
36	3PH	7	201	-	-	5/49/49/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	11	605	-	2/2/16/26	8/18/116/137	-
31	CLA	y	610	28	1/1/15/20	8/39/115/115	-
30	CHL	3	607	-	3/3/20/26	20/39/137/137	-
30	CHL	4	605	1	3/3/16/26	3/15/113/137	-
40	SQD	a	409	-	-	7/46/66/69	0/1/1/1
33	LUT	R	615	-	-	0/29/67/67	0/2/2/2
32	LHG	R	619	-	-	11/51/51/53	-
42	PL9	D	407	-	-	12/53/73/73	0/1/1/1
30	CHL	n	608	-	3/3/16/26	10/20/118/137	-
31	CLA	14	613	1	1/1/13/20	11/27/103/115	-
32	LHG	3	617	-	-	30/51/51/53	-
31	CLA	12	613	-	1/1/11/20	7/15/91/115	-
30	CHL	N	605	2	3/3/19/26	16/33/131/137	-
30	CHL	13	608	-	3/3/16/26	8/20/118/137	-
31	CLA	b	614	7	1/1/15/20	16/39/115/115	-
31	CLA	r	601	21	1/1/11/20	8/20/96/115	-
31	CLA	16	611	32	1/1/15/20	12/39/115/115	-
30	CHL	6	606	-	3/3/18/26	10/27/125/137	-
31	CLA	g	614	1	1/1/11/20	5/20/96/115	-
31	CLA	1	614	1	1/1/11/20	6/17/93/115	-
32	LHG	g	615	31	-	22/53/53/53	-
50	PAM	n	620	-	-	2/15/15/15	-
33	LUT	S	619	-	-	0/29/67/67	0/2/2/2
31	CLA	b	607	-	1/1/15/20	16/39/115/115	-
30	CHL	g	601	1	3/3/20/26	14/39/137/137	-
31	CLA	1	610	1	1/1/13/20	8/27/103/115	-
31	CLA	b	612	7	1/1/15/20	17/39/115/115	-
31	CLA	y	615	-	1/1/13/20	16/29/105/115	-
33	LUT	g	617	-	-	0/29/67/67	0/2/2/2
31	CLA	S	609	22	1/1/13/20	5/27/103/115	-
31	CLA	b	610	-	1/1/15/20	14/39/115/115	-
34	NEX	R	617	-	-	3/27/83/83	0/3/3/3
31	CLA	2	613	2	1/1/11/20	6/18/94/115	-
46	DGD	c	517	-	-	17/55/95/95	0/2/2/2
35	XAT	11	619	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	LNL	R	620	-	-	6/17/17/17	-
30	CHL	S	607	-	3/3/15/26	4/12/110/137	-
31	CLA	y	602	28	1/1/14/20	12/33/109/115	-
31	CLA	G	604	-	1/1/12/20	7/21/97/115	-
31	CLA	16	610	-	1/1/15/20	11/39/115/115	-
32	LHG	C	521	-	-	18/46/46/53	-
30	CHL	3	605	3	3/3/20/26	18/39/137/137	-
36	3PH	B	624	-	-	6/39/39/49	-
40	SQD	d	412	-	-	14/49/69/69	0/1/1/1
30	CHL	2	601	2	2/2/16/26	4/17/115/137	-
32	LHG	d	408	-	-	18/53/53/53	-
32	LHG	l	102	-	-	22/51/51/53	-
31	CLA	Y	603	28	1/1/14/20	9/33/109/115	-
31	CLA	13	602	5	1/1/15/20	21/39/115/115	-
31	CLA	6	614	3	1/1/12/20	11/21/97/115	-
31	CLA	g	610	1	1/1/15/20	9/39/115/115	-
31	CLA	y	614	28	1/1/11/20	5/20/96/115	-
31	CLA	c	510	8	1/1/15/20	12/39/115/115	-
31	CLA	g	613	1	1/1/15/20	10/39/115/115	-
49	HEM	f	101	11,10	-	6/14/54/54	-
34	NEX	11	618	-	-	0/6/37/83	0/2/2/3
30	CHL	Y	607	-	3/3/20/26	15/39/137/137	-
31	CLA	Y	615	-	1/1/13/20	15/29/105/115	-
33	LUT	s	619	-	-	0/29/67/67	0/2/2/2
31	CLA	5	603	2	1/1/13/20	9/27/103/115	-
31	CLA	D	405	9	1/1/15/20	16/39/115/115	-
31	CLA	s	604	-	1/1/15/20	18/39/115/115	-
31	CLA	r	604	-	1/1/11/20	4/19/95/115	-
30	CHL	N	609	2	3/3/20/26	19/39/137/137	-
31	CLA	R	602	21	1/1/15/20	14/39/115/115	-
35	XAT	3	620	-	-	1/31/93/93	0/4/4/4
31	CLA	C	502	8	1/1/15/20	11/39/115/115	-
30	CHL	G	608	-	3/3/17/26	11/23/121/137	-
30	CHL	13	606	-	3/3/19/26	13/33/131/137	-
34	NEX	g	618	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	c	511	8	1/1/15/20	13/39/115/115	-
30	CHL	y	608	-	3/3/15/26	5/13/111/137	-
33	LUT	Y	622	-	-	0/29/67/67	0/2/2/2
31	CLA	11	603	-	1/1/13/20	8/27/103/115	-
30	CHL	4	607	-	3/3/17/26	7/21/119/137	-
31	CLA	4	603	1	1/1/13/20	4/27/103/115	-
31	CLA	C	509	8	1/1/14/20	13/33/109/115	-
33	LUT	y	622	-	-	2/29/67/67	0/2/2/2
33	LUT	4	617	-	-	0/29/67/67	0/2/2/2
35	XAT	R	616	-	-	0/31/93/93	0/4/4/4
31	CLA	2	610	2	1/1/12/20	7/21/97/115	-
31	CLA	3	615	3	1/1/11/20	5/17/93/115	-
31	CLA	15	612	-	1/1/12/20	10/21/97/115	-
30	CHL	N	607	-	3/3/20/26	16/39/137/137	-
31	CLA	6	610	3	1/1/14/20	15/33/109/115	-

All (3595) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	605	CHL	C3B-C4B	5.88	1.47	1.41
38	a	406	PHO	C1D-C2D	5.86	1.46	1.39
30	5	606	CHL	C3B-C4B	5.86	1.47	1.41
30	12	605	CHL	C3B-C4B	5.85	1.47	1.41
30	2	606	CHL	C3B-C4B	5.82	1.47	1.41
30	11	605	CHL	C3B-C4B	5.82	1.47	1.41
30	5	607	CHL	C3B-C4B	5.78	1.47	1.41
30	13	601	CHL	CMC-C2C	5.77	1.56	1.44
38	A	405	PHO	C1D-C2D	5.76	1.45	1.39
38	D	402	PHO	C1D-C2D	5.76	1.45	1.39
30	y	605	CHL	C3B-C4B	5.75	1.47	1.41
30	N	605	CHL	C3B-C4B	5.75	1.47	1.41
30	4	608	CHL	CMC-C2C	5.75	1.56	1.44
30	16	601	CHL	CMC-C2C	5.75	1.56	1.44
30	3	609	CHL	CMC-C2C	5.75	1.56	1.44
38	a	405	PHO	C1D-C2D	5.74	1.45	1.39
30	14	609	CHL	CMC-C2C	5.74	1.56	1.44
30	4	608	CHL	C3B-C4B	5.74	1.47	1.41
30	3	601	CHL	C3B-C4B	5.73	1.47	1.41
30	11	609	CHL	CMC-C2C	5.73	1.56	1.44
30	14	606	CHL	CMC-C2C	5.73	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	605	CHL	CMC-C2C	5.73	1.56	1.44
30	6	609	CHL	CMC-C2C	5.72	1.56	1.44
30	S	606	CHL	C3B-C4B	5.72	1.47	1.41
30	1	605	CHL	CMC-C2C	5.71	1.56	1.44
30	1	608	CHL	CMC-C2C	5.71	1.56	1.44
30	12	605	CHL	CMC-C2C	5.71	1.56	1.44
30	15	608	CHL	CMC-C2C	5.71	1.56	1.44
30	g	605	CHL	C3B-C4B	5.71	1.46	1.41
30	5	609	CHL	CMC-C2C	5.71	1.56	1.44
30	6	601	CHL	C3B-C4B	5.71	1.46	1.41
30	15	606	CHL	CMC-C2C	5.71	1.56	1.44
30	11	605	CHL	CMC-C2C	5.70	1.56	1.44
30	4	605	CHL	CMC-C2C	5.70	1.56	1.44
30	2	609	CHL	CMC-C2C	5.69	1.56	1.44
30	12	606	CHL	CMC-C2C	5.69	1.56	1.44
30	1	606	CHL	CMC-C2C	5.69	1.56	1.44
30	4	606	CHL	CMC-C2C	5.69	1.56	1.44
30	G	608	CHL	CMC-C2C	5.69	1.56	1.44
30	g	606	CHL	CMC-C2C	5.69	1.56	1.44
30	G	606	CHL	CMC-C2C	5.68	1.56	1.44
30	12	607	CHL	CMC-C2C	5.68	1.56	1.44
30	14	607	CHL	CMC-C2C	5.68	1.56	1.44
30	Y	606	CHL	C3B-C4B	5.68	1.46	1.41
30	14	605	CHL	C3B-C4B	5.68	1.46	1.41
30	G	609	CHL	CMC-C2C	5.68	1.56	1.44
30	S	606	CHL	CMC-C2C	5.68	1.56	1.44
30	2	608	CHL	C3B-C4B	5.68	1.46	1.41
30	11	608	CHL	CMC-C2C	5.68	1.56	1.44
30	g	609	CHL	CMC-C2C	5.67	1.56	1.44
30	4	605	CHL	C3B-C4B	5.67	1.46	1.41
30	s	606	CHL	CMC-C2C	5.67	1.56	1.44
30	1	601	CHL	CMC-C2C	5.67	1.56	1.44
30	n	605	CHL	C3B-C4B	5.67	1.46	1.41
30	1	607	CHL	CMC-C2C	5.67	1.56	1.44
30	16	609	CHL	CMC-C2C	5.67	1.56	1.44
30	14	605	CHL	CMC-C2C	5.66	1.56	1.44
30	15	607	CHL	CMC-C2C	5.66	1.56	1.44
30	5	608	CHL	CMC-C2C	5.66	1.56	1.44
30	14	601	CHL	C3B-C4B	5.66	1.46	1.41
30	s	606	CHL	C3B-C4B	5.66	1.46	1.41
30	6	601	CHL	CMC-C2C	5.65	1.56	1.44
30	g	607	CHL	CMC-C2C	5.65	1.56	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	y	606	CHL	C3B-C4B	5.65	1.46	1.41
30	4	606	CHL	C3B-C4B	5.65	1.46	1.41
30	5	601	CHL	CMC-C2C	5.65	1.56	1.44
30	4	601	CHL	CMC-C2C	5.65	1.56	1.44
30	12	608	CHL	C3B-C4B	5.65	1.46	1.41
30	13	609	CHL	CMC-C2C	5.64	1.56	1.44
30	g	608	CHL	CMC-C2C	5.64	1.56	1.44
30	G	605	CHL	CMC-C2C	5.64	1.56	1.44
30	2	605	CHL	CMC-C2C	5.64	1.56	1.44
30	4	607	CHL	CMC-C2C	5.64	1.56	1.44
30	11	606	CHL	CMC-C2C	5.64	1.56	1.44
30	y	601	CHL	CMC-C2C	5.64	1.56	1.44
30	6	606	CHL	CMC-C2C	5.64	1.56	1.44
30	2	606	CHL	CMC-C2C	5.63	1.56	1.44
30	n	609	CHL	CMC-C2C	5.63	1.56	1.44
30	g	601	CHL	C3B-C4B	5.63	1.46	1.41
30	5	605	CHL	CMC-C2C	5.63	1.56	1.44
30	N	606	CHL	C3B-C4B	5.63	1.46	1.41
30	n	605	CHL	CMC-C2C	5.63	1.56	1.44
30	14	608	CHL	CMC-C2C	5.63	1.56	1.44
30	1	605	CHL	C3B-C4B	5.63	1.46	1.41
30	2	601	CHL	CMC-C2C	5.63	1.56	1.44
30	n	606	CHL	C3B-C4B	5.63	1.46	1.41
30	2	608	CHL	CMC-C2C	5.63	1.56	1.44
30	g	605	CHL	CMC-C2C	5.63	1.56	1.44
30	12	608	CHL	CMC-C2C	5.63	1.56	1.44
30	G	601	CHL	CMC-C2C	5.62	1.56	1.44
30	1	601	CHL	C3B-C4B	5.62	1.46	1.41
30	14	606	CHL	C3B-C4B	5.62	1.46	1.41
30	11	601	CHL	CMC-C2C	5.62	1.56	1.44
30	5	601	CHL	C3B-C4B	5.62	1.46	1.41
30	14	601	CHL	CMC-C2C	5.62	1.56	1.44
30	Y	601	CHL	CMC-C2C	5.62	1.56	1.44
30	4	609	CHL	CMC-C2C	5.62	1.56	1.44
30	16	605	CHL	C3B-C4B	5.62	1.46	1.41
30	6	608	CHL	C3B-C4B	5.62	1.46	1.41
30	11	607	CHL	CMC-C2C	5.62	1.56	1.44
30	3	601	CHL	CMC-C2C	5.62	1.56	1.44
30	N	609	CHL	CMC-C2C	5.61	1.56	1.44
30	13	606	CHL	CMC-C2C	5.61	1.56	1.44
30	N	605	CHL	CMC-C2C	5.61	1.56	1.44
30	15	607	CHL	C3B-C4B	5.61	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	609	CHL	CMC-C2C	5.61	1.56	1.44
30	S	607	CHL	CMC-C2C	5.61	1.56	1.44
30	N	601	CHL	CMC-C2C	5.61	1.56	1.44
30	5	608	CHL	C3B-C4B	5.60	1.46	1.41
30	4	601	CHL	C3B-C4B	5.60	1.46	1.41
30	12	601	CHL	CMC-C2C	5.60	1.56	1.44
30	S	601	CHL	CMC-C2C	5.60	1.56	1.44
30	3	606	CHL	CMC-C2C	5.60	1.56	1.44
30	y	609	CHL	CMC-C2C	5.60	1.56	1.44
30	2	609	CHL	C3B-C4B	5.60	1.46	1.41
30	14	609	CHL	C3B-C4B	5.60	1.46	1.41
30	3	605	CHL	C3B-C4B	5.59	1.46	1.41
30	15	606	CHL	C3B-C4B	5.59	1.46	1.41
30	6	605	CHL	CMC-C2C	5.59	1.56	1.44
30	n	601	CHL	CMC-C2C	5.59	1.56	1.44
30	15	601	CHL	CMC-C2C	5.59	1.56	1.44
30	N	606	CHL	CMC-C2C	5.59	1.56	1.44
30	2	605	CHL	C3B-C4B	5.59	1.46	1.41
30	G	605	CHL	C3B-C4B	5.58	1.46	1.41
30	12	607	CHL	C3B-C4B	5.58	1.46	1.41
30	s	607	CHL	CMC-C2C	5.58	1.56	1.44
30	5	606	CHL	CMC-C2C	5.58	1.56	1.44
30	G	607	CHL	CMC-C2C	5.58	1.56	1.44
30	g	601	CHL	CMC-C2C	5.58	1.56	1.44
30	5	609	CHL	C3B-C4B	5.58	1.46	1.41
30	11	608	CHL	C3B-C4B	5.58	1.46	1.41
30	13	607	CHL	C3B-C4B	5.58	1.46	1.41
30	s	601	CHL	CMC-C2C	5.57	1.56	1.44
30	13	605	CHL	C3B-C4B	5.57	1.46	1.41
30	Y	609	CHL	CMC-C2C	5.56	1.56	1.44
30	11	606	CHL	C3B-C4B	5.56	1.46	1.41
30	n	606	CHL	CMC-C2C	5.56	1.56	1.44
30	r	607	CHL	CMC-C2C	5.56	1.56	1.44
30	n	607	CHL	CMC-C2C	5.56	1.56	1.44
30	16	605	CHL	CMC-C2C	5.56	1.56	1.44
30	3	605	CHL	CMC-C2C	5.56	1.56	1.44
30	16	606	CHL	CMC-C2C	5.56	1.56	1.44
30	S	608	CHL	CMC-C2C	5.56	1.56	1.44
30	6	608	CHL	CMC-C2C	5.55	1.56	1.44
30	16	608	CHL	CMC-C2C	5.55	1.56	1.44
30	5	605	CHL	C3B-C4B	5.55	1.46	1.41
30	15	608	CHL	C3B-C4B	5.55	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	607	CHL	CMC-C2C	5.55	1.56	1.44
30	2	601	CHL	C3B-C4B	5.55	1.46	1.41
30	16	607	CHL	CMC-C2C	5.55	1.56	1.44
30	N	608	CHL	CMC-C2C	5.55	1.56	1.44
30	13	608	CHL	CMC-C2C	5.55	1.56	1.44
30	3	606	CHL	C3B-C4B	5.55	1.46	1.41
30	13	605	CHL	CMC-C2C	5.55	1.56	1.44
30	N	607	CHL	CMC-C2C	5.55	1.56	1.44
30	11	601	CHL	C3B-C4B	5.55	1.46	1.41
30	G	601	CHL	C3B-C4B	5.55	1.46	1.41
30	Y	605	CHL	C3B-C4B	5.55	1.46	1.41
30	6	607	CHL	CMC-C2C	5.54	1.56	1.44
30	S	601	CHL	C3B-C4B	5.54	1.46	1.41
30	11	607	CHL	C3B-C4B	5.54	1.46	1.41
30	y	607	CHL	CMC-C2C	5.54	1.56	1.44
30	2	607	CHL	CMC-C2C	5.54	1.56	1.44
30	4	609	CHL	C3B-C4B	5.54	1.46	1.41
30	13	606	CHL	C3B-C4B	5.53	1.46	1.41
30	3	608	CHL	CMC-C2C	5.53	1.56	1.44
30	y	605	CHL	CMC-C2C	5.53	1.56	1.44
30	3	609	CHL	C3B-C4B	5.53	1.46	1.41
30	13	608	CHL	C3B-C4B	5.53	1.46	1.41
30	y	608	CHL	CMC-C2C	5.53	1.56	1.44
30	3	607	CHL	CMC-C2C	5.53	1.56	1.44
30	s	608	CHL	CMC-C2C	5.53	1.56	1.44
30	13	609	CHL	C3B-C4B	5.52	1.46	1.41
30	13	607	CHL	CMC-C2C	5.52	1.56	1.44
30	6	609	CHL	C3B-C4B	5.52	1.46	1.41
30	R	607	CHL	CMC-C2C	5.52	1.56	1.44
30	Y	607	CHL	CMC-C2C	5.52	1.56	1.44
30	16	607	CHL	C3B-C4B	5.52	1.46	1.41
30	r	606	CHL	C3B-C4B	5.52	1.46	1.41
30	6	607	CHL	C3B-C4B	5.51	1.46	1.41
30	Y	606	CHL	CMC-C2C	5.51	1.56	1.44
30	y	601	CHL	C3B-C4B	5.51	1.46	1.41
31	4	610	CLA	MG-NA	5.50	2.19	2.06
30	1	607	CHL	C3B-C4B	5.50	1.46	1.41
30	6	605	CHL	C3B-C4B	5.50	1.46	1.41
30	16	608	CHL	C3B-C4B	5.50	1.46	1.41
30	1	609	CHL	C3B-C4B	5.50	1.46	1.41
30	n	608	CHL	C3B-C4B	5.49	1.46	1.41
30	r	605	CHL	C3B-C4B	5.49	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	n	608	CHL	CMC-C2C	5.49	1.56	1.44
30	y	606	CHL	CMC-C2C	5.49	1.56	1.44
30	Y	601	CHL	C3B-C4B	5.49	1.46	1.41
30	11	609	CHL	C3B-C4B	5.48	1.46	1.41
30	s	601	CHL	C3B-C4B	5.48	1.46	1.41
30	12	601	CHL	C3B-C4B	5.48	1.46	1.41
30	Y	608	CHL	CMC-C2C	5.48	1.56	1.44
30	r	605	CHL	CMC-C2C	5.48	1.56	1.44
30	15	601	CHL	C3B-C4B	5.47	1.46	1.41
30	16	606	CHL	C3B-C4B	5.47	1.46	1.41
30	14	608	CHL	C3B-C4B	5.47	1.46	1.41
30	6	606	CHL	C3B-C4B	5.47	1.46	1.41
30	Y	605	CHL	CMC-C2C	5.46	1.56	1.44
30	14	607	CHL	C3B-C4B	5.46	1.46	1.41
30	N	608	CHL	C3B-C4B	5.46	1.46	1.41
30	N	609	CHL	C3B-C4B	5.46	1.46	1.41
30	n	609	CHL	C3B-C4B	5.46	1.46	1.41
30	n	601	CHL	C3B-C4B	5.46	1.46	1.41
30	N	601	CHL	C3B-C4B	5.45	1.46	1.41
30	16	601	CHL	C3B-C4B	5.44	1.46	1.41
30	S	608	CHL	C3B-C4B	5.44	1.46	1.41
30	G	606	CHL	C3B-C4B	5.44	1.46	1.41
30	13	601	CHL	C3B-C4B	5.44	1.46	1.41
30	1	606	CHL	C3B-C4B	5.44	1.46	1.41
30	Y	608	CHL	C3B-C4B	5.44	1.46	1.41
30	3	607	CHL	C3B-C4B	5.43	1.46	1.41
30	R	606	CHL	CMC-C2C	5.43	1.56	1.44
30	G	607	CHL	C3B-C4B	5.43	1.46	1.41
30	R	605	CHL	CMC-C2C	5.42	1.56	1.44
31	S	612	CLA	MG-NA	5.42	2.19	2.06
30	r	607	CHL	C3B-C4B	5.42	1.46	1.41
30	y	609	CHL	C3B-C4B	5.42	1.46	1.41
30	R	607	CHL	C3B-C4B	5.42	1.46	1.41
30	r	606	CHL	CMC-C2C	5.41	1.56	1.44
30	N	607	CHL	C3B-C4B	5.41	1.46	1.41
30	3	608	CHL	C3B-C4B	5.40	1.46	1.41
30	n	607	CHL	C3B-C4B	5.40	1.46	1.41
30	g	609	CHL	C3B-C4B	5.39	1.46	1.41
30	s	608	CHL	C3B-C4B	5.39	1.46	1.41
30	G	608	CHL	C3B-C4B	5.39	1.46	1.41
30	Y	607	CHL	C3B-C4B	5.39	1.46	1.41
30	y	607	CHL	C3B-C4B	5.39	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	607	CHL	C3B-C4B	5.39	1.46	1.41
30	G	609	CHL	C3B-C4B	5.39	1.46	1.41
30	R	605	CHL	C3B-C4B	5.39	1.46	1.41
30	g	608	CHL	C3B-C4B	5.38	1.46	1.41
30	g	606	CHL	C3B-C4B	5.38	1.46	1.41
30	s	607	CHL	C3B-C4B	5.37	1.46	1.41
30	2	607	CHL	C3B-C4B	5.37	1.46	1.41
30	y	608	CHL	C3B-C4B	5.36	1.46	1.41
30	16	609	CHL	C3B-C4B	5.35	1.46	1.41
30	12	606	CHL	C3B-C4B	5.35	1.46	1.41
31	4	612	CLA	MG-NA	5.34	2.19	2.06
30	R	606	CHL	C3B-C4B	5.34	1.46	1.41
30	4	607	CHL	C3B-C4B	5.32	1.46	1.41
30	Y	609	CHL	C3B-C4B	5.30	1.46	1.41
30	1	608	CHL	C3B-C4B	5.28	1.46	1.41
30	14	609	CHL	C1D-C2D	5.25	1.45	1.39
30	11	609	CHL	C1D-C2D	5.24	1.45	1.39
30	13	601	CHL	C1D-C2D	5.22	1.45	1.39
30	1	606	CHL	C1D-C2D	5.21	1.45	1.39
30	S	607	CHL	C3B-C4B	5.19	1.46	1.41
31	16	612	CLA	MG-NA	5.18	2.18	2.06
31	14	612	CLA	MG-NA	5.18	2.18	2.06
31	Y	612	CLA	MG-NA	5.17	2.18	2.06
30	14	607	CHL	C1D-C2D	5.17	1.45	1.39
31	11	612	CLA	MG-NA	5.16	2.18	2.06
31	13	612	CLA	MG-NA	5.16	2.18	2.06
31	N	611	CLA	MG-NA	5.15	2.18	2.06
31	15	611	CLA	MG-NA	5.15	2.18	2.06
31	y	612	CLA	MG-NA	5.14	2.18	2.06
30	16	601	CHL	C1D-C2D	5.13	1.45	1.39
31	12	611	CLA	MG-NA	5.13	2.18	2.06
31	g	612	CLA	MG-NA	5.13	2.18	2.06
30	16	609	CHL	C1D-C2D	5.12	1.45	1.39
31	s	612	CLA	MG-NA	5.12	2.18	2.06
31	G	612	CLA	MG-NA	5.11	2.18	2.06
30	4	608	CHL	C1D-C2D	5.11	1.45	1.39
30	13	608	CHL	C1D-C2D	5.11	1.45	1.39
30	2	601	CHL	C1D-C2D	5.11	1.45	1.39
31	n	611	CLA	MG-NA	5.10	2.18	2.06
31	1	612	CLA	MG-NA	5.10	2.18	2.06
31	6	612	CLA	MG-NA	5.10	2.18	2.06
30	12	608	CHL	C1D-C2D	5.10	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	606	CHL	C1D-C2D	5.10	1.45	1.39
30	3	601	CHL	C1D-C2D	5.09	1.45	1.39
30	5	605	CHL	C1D-C2D	5.09	1.45	1.39
30	2	606	CHL	C1D-C2D	5.09	1.45	1.39
30	15	608	CHL	C1D-C2D	5.09	1.45	1.39
30	14	606	CHL	C1D-C2D	5.08	1.45	1.39
30	16	608	CHL	C1D-C2D	5.08	1.45	1.39
30	14	608	CHL	C1D-C2D	5.08	1.45	1.39
30	15	607	CHL	C1D-C2D	5.08	1.45	1.39
30	5	609	CHL	C1D-C2D	5.07	1.45	1.39
30	6	601	CHL	C1D-C2D	5.07	1.45	1.39
31	b	615	CLA	MG-NA	5.07	2.18	2.06
30	13	606	CHL	C1D-C2D	5.06	1.45	1.39
31	s	603	CLA	MG-NA	5.06	2.18	2.06
31	2	612	CLA	MG-NA	5.06	2.18	2.06
31	N	612	CLA	MG-NA	5.06	2.18	2.06
30	5	608	CHL	C1D-C2D	5.06	1.45	1.39
30	15	605	CHL	C1D-C2D	5.06	1.45	1.39
30	Y	609	CHL	C1D-C2D	5.06	1.45	1.39
30	1	608	CHL	C1D-C2D	5.05	1.45	1.39
31	B	615	CLA	MG-NA	5.05	2.18	2.06
31	3	612	CLA	MG-NA	5.05	2.18	2.06
31	1	610	CLA	MG-NA	5.05	2.18	2.06
30	2	605	CHL	C1D-C2D	5.05	1.45	1.39
31	n	612	CLA	MG-NA	5.05	2.18	2.06
30	12	605	CHL	C1D-C2D	5.05	1.45	1.39
30	16	606	CHL	C1D-C2D	5.05	1.45	1.39
30	11	605	CHL	C1D-C2D	5.04	1.45	1.39
30	g	609	CHL	C1D-C2D	5.04	1.45	1.39
30	13	609	CHL	C1D-C2D	5.03	1.45	1.39
31	c	513	CLA	MG-NA	5.03	2.18	2.06
31	5	612	CLA	MG-NA	5.03	2.18	2.06
30	5	601	CHL	C1D-C2D	5.03	1.45	1.39
31	13	615	CLA	MG-NA	5.03	2.18	2.06
31	C	513	CLA	MG-NA	5.03	2.18	2.06
31	1	611	CLA	MG-NA	5.03	2.18	2.06
30	11	608	CHL	C1D-C2D	5.03	1.45	1.39
30	12	607	CHL	C1D-C2D	5.03	1.45	1.39
30	4	609	CHL	C1D-C2D	5.02	1.45	1.39
31	16	602	CLA	MG-NA	5.02	2.18	2.06
30	11	607	CHL	C1D-C2D	5.02	1.45	1.39
30	1	609	CHL	C1D-C2D	5.02	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	G	609	CHL	C1D-C2D	5.02	1.45	1.39
30	5	606	CHL	C1D-C2D	5.02	1.45	1.39
31	r	613	CLA	MG-NA	5.02	2.18	2.06
31	G	603	CLA	MG-NA	5.01	2.18	2.06
31	G	604	CLA	MG-NA	5.01	2.18	2.06
31	g	603	CLA	MG-NA	5.01	2.18	2.06
31	14	611	CLA	MG-NA	5.01	2.18	2.06
30	14	605	CHL	C1D-C2D	5.01	1.45	1.39
30	2	609	CHL	C1D-C2D	5.00	1.45	1.39
31	y	614	CLA	MG-NA	5.00	2.18	2.06
31	S	603	CLA	MG-NA	5.00	2.18	2.06
31	S	611	CLA	MG-NA	5.00	2.18	2.06
30	N	605	CHL	C1D-C2D	5.00	1.45	1.39
31	13	602	CLA	MG-NA	5.00	2.18	2.06
31	B	604	CLA	MG-NA	5.00	2.18	2.06
30	2	608	CHL	C1D-C2D	5.00	1.45	1.39
30	n	609	CHL	C1D-C2D	5.00	1.45	1.39
31	2	604	CLA	MG-NA	4.99	2.18	2.06
31	g	611	CLA	MG-NA	4.99	2.18	2.06
31	S	602	CLA	MG-NA	4.99	2.18	2.06
30	13	605	CHL	C1D-C2D	4.99	1.45	1.39
31	N	613	CLA	MG-NA	4.99	2.18	2.06
31	Y	614	CLA	MG-NA	4.99	2.18	2.06
31	G	614	CLA	MG-NA	4.99	2.18	2.06
31	n	614	CLA	MG-NA	4.99	2.18	2.06
31	R	612	CLA	MG-NA	4.99	2.18	2.06
30	1	606	CHL	C1B-C2B	4.99	1.45	1.39
31	6	610	CLA	MG-NA	4.99	2.18	2.06
31	C	509	CLA	MG-NA	4.99	2.18	2.06
31	R	613	CLA	MG-NA	4.99	2.18	2.06
30	3	609	CHL	C1D-C2D	4.98	1.45	1.39
31	y	604	CLA	MG-NA	4.98	2.18	2.06
31	1	614	CLA	MG-NA	4.98	2.18	2.06
31	c	509	CLA	MG-NA	4.98	2.18	2.06
31	s	602	CLA	MG-NA	4.98	2.18	2.06
30	16	605	CHL	C1D-C2D	4.98	1.45	1.39
31	14	614	CLA	MG-NA	4.98	2.18	2.06
31	4	611	CLA	MG-NA	4.98	2.18	2.06
31	5	603	CLA	MG-NA	4.98	2.18	2.06
31	b	604	CLA	MG-NA	4.98	2.18	2.06
31	11	611	CLA	MG-NA	4.98	2.18	2.06
31	5	604	CLA	MG-NA	4.98	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	601	CHL	C1D-C2D	4.98	1.45	1.39
31	16	613	CLA	MG-NA	4.98	2.18	2.06
30	4	607	CHL	C1D-C2D	4.98	1.45	1.39
30	S	606	CHL	C1D-C2D	4.98	1.45	1.39
31	B	603	CLA	MG-NA	4.98	2.18	2.06
31	14	604	CLA	MG-NA	4.97	2.18	2.06
31	Y	611	CLA	MG-NA	4.97	2.18	2.06
31	6	614	CLA	MG-NA	4.97	2.18	2.06
31	S	613	CLA	MG-NA	4.97	2.18	2.06
30	16	607	CHL	C1D-C2D	4.97	1.45	1.39
31	4	614	CLA	MG-NA	4.97	2.18	2.06
30	6	609	CHL	C1D-C2D	4.97	1.45	1.39
31	2	602	CLA	MG-NA	4.97	2.18	2.06
31	G	611	CLA	MG-NA	4.97	2.18	2.06
31	11	604	CLA	MG-NA	4.97	2.18	2.06
31	11	614	CLA	MG-NA	4.97	2.18	2.06
31	15	610	CLA	MG-NA	4.97	2.18	2.06
31	S	615	CLA	MG-NA	4.97	2.18	2.06
30	S	608	CHL	C1D-C2D	4.97	1.45	1.39
30	g	605	CHL	C1D-C2D	4.97	1.45	1.39
31	s	611	CLA	MG-NA	4.97	2.18	2.06
31	s	613	CLA	MG-NA	4.97	2.18	2.06
31	B	605	CLA	MG-NA	4.97	2.18	2.06
31	s	615	CLA	MG-NA	4.97	2.18	2.06
30	s	606	CHL	C1D-C2D	4.96	1.45	1.39
31	16	611	CLA	MG-NA	4.96	2.18	2.06
30	G	607	CHL	C1D-C2D	4.96	1.45	1.39
31	5	611	CLA	MG-NA	4.96	2.18	2.06
31	11	602	CLA	MG-NA	4.96	2.18	2.06
31	b	605	CLA	MG-NA	4.96	2.18	2.06
31	12	610	CLA	MG-NA	4.96	2.18	2.06
31	B	609	CLA	MG-NA	4.96	2.18	2.06
31	g	614	CLA	MG-NA	4.96	2.18	2.06
31	15	609	CLA	MG-NA	4.96	2.18	2.06
31	3	603	CLA	MG-NA	4.96	2.18	2.06
31	12	603	CLA	MG-NA	4.96	2.18	2.06
31	C	506	CLA	MG-NA	4.96	2.18	2.06
31	g	604	CLA	MG-NA	4.96	2.18	2.06
30	3	605	CHL	C1D-C2D	4.96	1.45	1.39
31	B	611	CLA	MG-NA	4.96	2.18	2.06
31	6	603	CLA	MG-NA	4.96	2.18	2.06
31	14	602	CLA	MG-NA	4.96	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	13	611	CLA	MG-NA	4.95	2.18	2.06
30	n	605	CHL	C1D-C2D	4.95	1.45	1.39
31	4	603	CLA	MG-NA	4.95	2.18	2.06
31	Y	604	CLA	MG-NA	4.95	2.18	2.06
31	1	603	CLA	MG-NA	4.95	2.18	2.06
31	N	604	CLA	MG-NA	4.95	2.18	2.06
31	n	602	CLA	MG-NA	4.95	2.18	2.06
31	S	609	CLA	MG-NA	4.95	2.18	2.06
31	n	613	CLA	MG-NA	4.95	2.18	2.06
31	5	602	CLA	MG-NA	4.95	2.18	2.06
31	g	613	CLA	MG-NA	4.95	2.18	2.06
30	1	605	CHL	C1D-C2D	4.95	1.45	1.39
31	c	504	CLA	MG-NA	4.95	2.18	2.06
31	r	610	CLA	MG-NA	4.95	2.18	2.06
30	1	605	CHL	C1B-C2B	4.95	1.45	1.39
31	c	508	CLA	MG-NA	4.95	2.18	2.06
31	13	613	CLA	MG-NA	4.95	2.18	2.06
31	15	613	CLA	MG-NA	4.95	2.18	2.06
31	R	603	CLA	MG-NA	4.95	2.18	2.06
31	r	611	CLA	MG-NA	4.95	2.18	2.06
31	3	613	CLA	MG-NA	4.94	2.18	2.06
31	16	603	CLA	MG-NA	4.94	2.18	2.06
31	C	507	CLA	MG-NA	4.94	2.18	2.06
31	b	609	CLA	MG-NA	4.94	2.18	2.06
31	12	609	CLA	MG-NA	4.94	2.18	2.06
31	b	611	CLA	MG-NA	4.94	2.18	2.06
30	N	606	CHL	C1D-C2D	4.94	1.45	1.39
31	12	613	CLA	MG-NA	4.94	2.18	2.06
31	G	613	CLA	MG-NA	4.94	2.18	2.06
31	14	603	CLA	MG-NA	4.94	2.18	2.06
30	S	607	CHL	C1D-C2D	4.94	1.45	1.39
30	n	601	CHL	C1D-C2D	4.94	1.45	1.39
31	1	613	CLA	MG-NA	4.94	2.18	2.06
30	4	605	CHL	C1D-C2D	4.93	1.45	1.39
30	6	605	CHL	C1D-C2D	4.93	1.45	1.39
31	R	602	CLA	MG-NA	4.93	2.18	2.06
31	C	504	CLA	MG-NA	4.93	2.18	2.06
30	1	607	CHL	C1D-C2D	4.93	1.45	1.39
30	N	601	CHL	C1D-C2D	4.93	1.45	1.39
31	n	604	CLA	MG-NA	4.93	2.18	2.06
31	2	603	CLA	MG-NA	4.93	2.18	2.06
31	11	603	CLA	MG-NA	4.93	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	609	CLA	MG-NA	4.93	2.18	2.06
31	y	611	CLA	MG-NA	4.93	2.18	2.06
31	3	614	CLA	MG-NA	4.93	2.18	2.06
31	6	613	CLA	MG-NA	4.93	2.18	2.06
31	b	606	CLA	MG-NA	4.92	2.18	2.06
31	s	614	CLA	MG-NA	4.92	2.18	2.06
31	b	614	CLA	MG-NA	4.92	2.18	2.06
30	G	605	CHL	C1D-C2D	4.92	1.45	1.39
31	12	602	CLA	MG-NA	4.92	2.18	2.06
31	Y	602	CLA	MG-NA	4.92	2.18	2.06
31	r	603	CLA	MG-NA	4.92	2.18	2.06
30	S	601	CHL	C1D-C2D	4.92	1.45	1.39
31	13	603	CLA	MG-NA	4.92	2.18	2.06
31	b	616	CLA	MG-NA	4.92	2.18	2.06
31	c	507	CLA	MG-NA	4.92	2.18	2.06
30	11	606	CHL	C1D-C2D	4.92	1.45	1.39
31	a	407	CLA	MG-NA	4.92	2.18	2.06
31	c	506	CLA	MG-NA	4.92	2.18	2.06
31	3	602	CLA	MG-NA	4.92	2.17	2.06
30	n	606	CHL	C1D-C2D	4.92	1.45	1.39
31	14	613	CLA	MG-NA	4.92	2.17	2.06
31	15	603	CLA	MG-NA	4.92	2.17	2.06
31	15	602	CLA	MG-NA	4.92	2.17	2.06
30	G	608	CHL	C1D-C2D	4.91	1.45	1.39
30	g	606	CHL	C1D-C2D	4.91	1.45	1.39
31	16	615	CLA	MG-NA	4.91	2.17	2.06
30	13	607	CHL	C1D-C2D	4.91	1.45	1.39
31	3	611	CLA	MG-NA	4.91	2.17	2.06
31	R	610	CLA	MG-NA	4.91	2.17	2.06
31	6	602	CLA	MG-NA	4.91	2.17	2.06
31	r	602	CLA	MG-NA	4.91	2.17	2.06
30	2	607	CHL	C1D-C2D	4.91	1.45	1.39
30	12	601	CHL	C1D-C2D	4.91	1.45	1.39
31	R	604	CLA	MG-NA	4.91	2.17	2.06
30	4	605	CHL	C1B-C2B	4.91	1.45	1.39
30	s	601	CHL	C1D-C2D	4.90	1.45	1.39
30	14	601	CHL	C1D-C2D	4.90	1.45	1.39
31	b	603	CLA	MG-NA	4.90	2.17	2.06
31	A	406	CLA	MG-NA	4.90	2.17	2.06
31	4	602	CLA	MG-NA	4.90	2.17	2.06
31	16	614	CLA	MG-NA	4.90	2.17	2.06
30	5	607	CHL	C1D-C2D	4.90	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	608	CHL	C1D-C2D	4.90	1.45	1.39
31	r	604	CLA	MG-NA	4.90	2.17	2.06
30	g	607	CHL	C1D-C2D	4.90	1.45	1.39
31	R	614	CLA	MG-NA	4.90	2.17	2.06
31	n	603	CLA	MG-NA	4.90	2.17	2.06
30	11	601	CHL	C1D-C2D	4.89	1.45	1.39
30	s	608	CHL	C1D-C2D	4.89	1.45	1.39
31	B	614	CLA	MG-NA	4.89	2.17	2.06
31	11	613	CLA	MG-NA	4.89	2.17	2.06
31	13	614	CLA	MG-NA	4.89	2.17	2.06
31	C	511	CLA	MG-NA	4.89	2.17	2.06
31	s	605	CLA	MG-NA	4.89	2.17	2.06
31	15	612	CLA	MG-NA	4.89	2.17	2.06
31	B	616	CLA	MG-NA	4.89	2.17	2.06
31	c	511	CLA	MG-NA	4.89	2.17	2.06
31	r	614	CLA	MG-NA	4.89	2.17	2.06
30	12	606	CHL	C1B-C2B	4.89	1.45	1.39
31	16	604	CLA	MG-NA	4.89	2.17	2.06
31	b	613	CLA	MG-NA	4.89	2.17	2.06
31	R	611	CLA	MG-NA	4.88	2.17	2.06
31	2	611	CLA	MG-NA	4.88	2.17	2.06
30	Y	605	CHL	C1D-C2D	4.88	1.45	1.39
31	y	602	CLA	MG-NA	4.88	2.17	2.06
31	15	604	CLA	MG-NA	4.88	2.17	2.06
31	r	601	CLA	MG-NA	4.88	2.17	2.06
31	S	605	CLA	MG-NA	4.88	2.17	2.06
31	c	514	CLA	MG-NA	4.88	2.17	2.06
31	4	604	CLA	MG-NA	4.88	2.17	2.06
31	B	606	CLA	MG-NA	4.88	2.17	2.06
31	g	602	CLA	MG-NA	4.88	2.17	2.06
31	c	505	CLA	MG-NA	4.87	2.17	2.06
30	y	609	CHL	C1D-C2D	4.87	1.45	1.39
30	G	606	CHL	C1D-C2D	4.87	1.45	1.39
31	b	607	CLA	MG-NA	4.87	2.17	2.06
31	3	610	CLA	MG-NA	4.87	2.17	2.06
31	13	604	CLA	MG-NA	4.87	2.17	2.06
31	N	603	CLA	MG-NA	4.87	2.17	2.06
31	B	607	CLA	MG-NA	4.87	2.17	2.06
31	N	614	CLA	MG-NA	4.86	2.17	2.06
31	C	505	CLA	MG-NA	4.86	2.17	2.06
31	S	614	CLA	MG-NA	4.86	2.17	2.06
31	N	610	CLA	MG-NA	4.86	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	613	CLA	MG-NA	4.86	2.17	2.06
31	Y	603	CLA	MG-NA	4.86	2.17	2.06
31	S	604	CLA	MG-NA	4.86	2.17	2.06
31	6	604	CLA	MG-NA	4.86	2.17	2.06
30	G	601	CHL	C1D-C2D	4.86	1.45	1.39
30	r	605	CHL	C1D-C2D	4.86	1.45	1.39
31	1	602	CLA	MG-NA	4.86	2.17	2.06
31	s	604	CLA	MG-NA	4.86	2.17	2.06
30	y	601	CHL	C1D-C2D	4.86	1.45	1.39
31	6	611	CLA	MG-NA	4.85	2.17	2.06
30	R	605	CHL	C1D-C2D	4.85	1.45	1.39
31	d	405	CLA	MG-NA	4.85	2.17	2.06
31	R	601	CLA	MG-NA	4.85	2.17	2.06
30	3	606	CHL	C1D-C2D	4.85	1.45	1.39
31	y	603	CLA	MG-NA	4.85	2.17	2.06
31	r	609	CLA	MG-NA	4.85	2.17	2.06
31	C	514	CLA	MG-NA	4.85	2.17	2.06
30	4	601	CHL	C1D-C2D	4.85	1.45	1.39
30	11	605	CHL	C1B-C2B	4.85	1.45	1.39
31	B	612	CLA	MG-NA	4.85	2.17	2.06
31	S	610	CLA	MG-NA	4.85	2.17	2.06
31	y	615	CLA	MG-NA	4.85	2.17	2.06
31	b	601	CLA	MG-NA	4.84	2.17	2.06
30	4	606	CHL	C1B-C2B	4.84	1.45	1.39
30	y	605	CHL	C1D-C2D	4.84	1.45	1.39
30	1	601	CHL	C1D-C2D	4.84	1.45	1.39
30	g	601	CHL	C1D-C2D	4.84	1.45	1.39
31	A	402	CLA	MG-NA	4.84	2.17	2.06
31	Y	615	CLA	MG-NA	4.84	2.17	2.06
31	C	503	CLA	MG-NA	4.84	2.17	2.06
31	c	503	CLA	MG-NA	4.84	2.17	2.06
30	N	609	CHL	C1D-C2D	4.84	1.45	1.39
31	c	512	CLA	MG-NA	4.84	2.17	2.06
31	3	615	CLA	MG-NA	4.84	2.17	2.06
31	B	613	CLA	MG-NA	4.84	2.17	2.06
31	12	612	CLA	MG-NA	4.84	2.17	2.06
31	B	601	CLA	MG-NA	4.84	2.17	2.06
31	a	403	CLA	MG-NA	4.84	2.17	2.06
31	n	610	CLA	MG-NA	4.84	2.17	2.06
30	n	608	CHL	C1D-C2D	4.84	1.45	1.39
30	14	608	CHL	C1B-C2B	4.83	1.45	1.39
31	b	610	CLA	MG-NA	4.83	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	608	CHL	C1D-C2D	4.83	1.45	1.39
31	5	613	CLA	MG-NA	4.83	2.17	2.06
31	C	502	CLA	MG-NA	4.83	2.17	2.06
31	N	602	CLA	MG-NA	4.83	2.17	2.06
31	N	615	CLA	MG-NA	4.83	2.17	2.06
31	B	608	CLA	MG-NA	4.83	2.17	2.06
31	y	613	CLA	MG-NA	4.83	2.17	2.06
31	3	604	CLA	MG-NA	4.83	2.17	2.06
30	R	607	CHL	C1D-C2D	4.83	1.45	1.39
31	R	609	CLA	MG-NA	4.83	2.17	2.06
30	6	607	CHL	C1D-C2D	4.82	1.45	1.39
30	Y	601	CHL	C1D-C2D	4.82	1.45	1.39
31	12	604	CLA	MG-NA	4.82	2.17	2.06
31	n	615	CLA	MG-NA	4.82	2.17	2.06
31	b	608	CLA	MG-NA	4.82	2.17	2.06
31	b	612	CLA	MG-NA	4.82	2.17	2.06
30	11	609	CHL	C1B-C2B	4.82	1.45	1.39
31	B	610	CLA	MG-NA	4.82	2.17	2.06
31	c	502	CLA	MG-NA	4.82	2.17	2.06
31	c	510	CLA	MG-NA	4.82	2.17	2.06
30	6	601	CHL	C1B-C2B	4.82	1.45	1.39
31	C	510	CLA	MG-NA	4.81	2.17	2.06
30	6	606	CHL	C1D-C2D	4.81	1.45	1.39
30	3	607	CHL	C1D-C2D	4.81	1.45	1.39
31	4	613	CLA	MG-NA	4.81	2.17	2.06
31	g	610	CLA	MG-NA	4.81	2.17	2.06
30	2	601	CHL	C1B-C2B	4.81	1.45	1.39
31	2	613	CLA	MG-NA	4.81	2.17	2.06
31	B	602	CLA	MG-NA	4.81	2.17	2.06
31	C	512	CLA	MG-NA	4.81	2.17	2.06
31	b	602	CLA	MG-NA	4.80	2.17	2.06
31	5	610	CLA	MG-NA	4.80	2.17	2.06
31	6	615	CLA	MG-NA	4.80	2.17	2.06
30	11	608	CHL	C1B-C2B	4.79	1.45	1.39
31	r	612	CLA	MG-NA	4.79	2.17	2.06
30	s	607	CHL	C1D-C2D	4.79	1.45	1.39
31	C	508	CLA	MG-NA	4.79	2.17	2.06
30	15	606	CHL	C1D-C2D	4.79	1.45	1.39
30	2	607	CHL	C1B-C2B	4.79	1.45	1.39
31	G	610	CLA	MG-NA	4.79	2.17	2.06
31	a	404	CLA	MG-NA	4.78	2.17	2.06
31	s	610	CLA	MG-NA	4.78	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	405	CLA	MG-NA	4.77	2.17	2.06
31	R	608	CLA	MG-NA	4.77	2.17	2.06
31	r	608	CLA	MG-NA	4.77	2.17	2.06
31	1	604	CLA	MG-NA	4.77	2.17	2.06
31	A	404	CLA	MG-NA	4.77	2.17	2.06
30	12	601	CHL	C1B-C2B	4.77	1.45	1.39
30	r	607	CHL	C1D-C2D	4.77	1.45	1.39
30	y	607	CHL	C1D-C2D	4.77	1.45	1.39
30	5	608	CHL	C1B-C2B	4.77	1.45	1.39
30	Y	606	CHL	C1D-C2D	4.77	1.45	1.39
30	Y	607	CHL	C1D-C2D	4.76	1.45	1.39
30	6	608	CHL	C1D-C2D	4.76	1.44	1.39
30	n	607	CHL	C1D-C2D	4.76	1.44	1.39
31	2	610	CLA	MG-NA	4.76	2.17	2.06
31	G	602	CLA	MG-NA	4.76	2.17	2.06
31	A	403	CLA	MG-NA	4.76	2.17	2.06
31	D	404	CLA	MG-NA	4.76	2.17	2.06
30	S	607	CHL	C1B-C2B	4.76	1.44	1.39
30	1	607	CHL	C1B-C2B	4.75	1.44	1.39
30	n	601	CHL	C1B-C2B	4.75	1.44	1.39
30	13	601	CHL	C1B-C2B	4.75	1.44	1.39
31	d	404	CLA	MG-NA	4.75	2.17	2.06
31	d	402	CLA	MG-NA	4.75	2.17	2.06
30	12	606	CHL	C1D-C2D	4.75	1.44	1.39
30	y	608	CHL	C1D-C2D	4.75	1.44	1.39
30	3	608	CHL	C1D-C2D	4.74	1.44	1.39
31	Y	610	CLA	MG-NA	4.74	2.17	2.06
30	y	606	CHL	C1D-C2D	4.74	1.44	1.39
31	y	610	CLA	MG-NA	4.73	2.17	2.06
30	15	601	CHL	C1B-C2B	4.73	1.44	1.39
30	15	606	CHL	C1B-C2B	4.73	1.44	1.39
30	11	607	CHL	C1B-C2B	4.73	1.44	1.39
30	14	605	CHL	C1B-C2B	4.73	1.44	1.39
30	2	608	CHL	C1B-C2B	4.73	1.44	1.39
31	14	610	CLA	MG-NA	4.73	2.17	2.06
30	13	607	CHL	C1B-C2B	4.72	1.44	1.39
30	g	606	CHL	C1B-C2B	4.72	1.44	1.39
30	1	608	CHL	C1B-C2B	4.72	1.44	1.39
31	11	610	CLA	MG-NA	4.72	2.17	2.06
30	15	608	CHL	C1B-C2B	4.72	1.44	1.39
30	5	601	CHL	C1B-C2B	4.71	1.44	1.39
30	12	608	CHL	C1B-C2B	4.71	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	607	CHL	C1B-C2B	4.71	1.44	1.39
30	12	607	CHL	C1B-C2B	4.71	1.44	1.39
30	5	605	CHL	C1B-C2B	4.71	1.44	1.39
30	G	606	CHL	C1B-C2B	4.71	1.44	1.39
30	s	607	CHL	C1B-C2B	4.70	1.44	1.39
30	3	601	CHL	C1B-C2B	4.70	1.44	1.39
30	4	608	CHL	C1B-C2B	4.70	1.44	1.39
30	4	607	CHL	C1B-C2B	4.69	1.44	1.39
30	11	606	CHL	C1B-C2B	4.69	1.44	1.39
30	2	605	CHL	C1B-C2B	4.69	1.44	1.39
30	14	609	CHL	C1B-C2B	4.69	1.44	1.39
30	15	605	CHL	C1B-C2B	4.68	1.44	1.39
30	N	607	CHL	C1D-C2D	4.68	1.44	1.39
30	16	606	CHL	C1B-C2B	4.68	1.44	1.39
30	14	607	CHL	C1B-C2B	4.67	1.44	1.39
31	13	610	CLA	MG-NA	4.67	2.17	2.06
30	15	607	CHL	C1B-C2B	4.66	1.44	1.39
30	3	607	CHL	C1B-C2B	4.66	1.44	1.39
30	3	608	CHL	C1B-C2B	4.66	1.44	1.39
30	16	601	CHL	C1B-C2B	4.66	1.44	1.39
30	3	606	CHL	C1B-C2B	4.65	1.44	1.39
30	2	609	CHL	C1B-C2B	4.65	1.44	1.39
30	g	605	CHL	C1B-C2B	4.65	1.44	1.39
31	16	610	CLA	MG-NA	4.65	2.17	2.06
30	N	607	CHL	C1B-C2B	4.65	1.44	1.39
30	s	601	CHL	C1B-C2B	4.64	1.44	1.39
30	Y	608	CHL	C1D-C2D	4.64	1.44	1.39
30	4	609	CHL	C1B-C2B	4.64	1.44	1.39
30	G	605	CHL	C1B-C2B	4.64	1.44	1.39
30	g	607	CHL	C1B-C2B	4.64	1.44	1.39
30	N	601	CHL	C1B-C2B	4.63	1.44	1.39
30	1	609	CHL	C1B-C2B	4.63	1.44	1.39
30	14	606	CHL	C1B-C2B	4.63	1.44	1.39
30	6	606	CHL	C1B-C2B	4.62	1.44	1.39
30	n	607	CHL	C1B-C2B	4.62	1.44	1.39
30	16	609	CHL	C1B-C2B	4.62	1.44	1.39
30	11	601	CHL	C1B-C2B	4.62	1.44	1.39
30	13	606	CHL	C1B-C2B	4.61	1.44	1.39
30	12	605	CHL	C1B-C2B	4.61	1.44	1.39
30	G	607	CHL	C1B-C2B	4.61	1.44	1.39
30	S	601	CHL	C1B-C2B	4.61	1.44	1.39
30	r	605	CHL	C1B-C2B	4.61	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	607	CHL	C1B-C2B	4.60	1.44	1.39
30	5	609	CHL	C1B-C2B	4.60	1.44	1.39
30	g	608	CHL	C1B-C2B	4.59	1.44	1.39
30	14	601	CHL	C1B-C2B	4.59	1.44	1.39
30	s	606	CHL	C1B-C2B	4.58	1.44	1.39
30	16	608	CHL	C1B-C2B	4.57	1.44	1.39
30	G	608	CHL	C1B-C2B	4.57	1.44	1.39
30	R	606	CHL	C1D-C2D	4.57	1.44	1.39
30	r	606	CHL	C1D-C2D	4.57	1.44	1.39
30	R	605	CHL	C1B-C2B	4.57	1.44	1.39
30	y	605	CHL	C1B-C2B	4.57	1.44	1.39
30	n	606	CHL	C1B-C2B	4.57	1.44	1.39
30	2	606	CHL	C1B-C2B	4.57	1.44	1.39
30	s	608	CHL	C1B-C2B	4.56	1.44	1.39
30	n	605	CHL	C1B-C2B	4.56	1.44	1.39
30	6	608	CHL	C1B-C2B	4.56	1.44	1.39
30	16	605	CHL	C1B-C2B	4.56	1.44	1.39
30	13	605	CHL	C1B-C2B	4.55	1.44	1.39
30	N	608	CHL	C1B-C2B	4.55	1.44	1.39
30	6	605	CHL	C1B-C2B	4.54	1.44	1.39
30	y	607	CHL	C1B-C2B	4.53	1.44	1.39
30	r	607	CHL	C1B-C2B	4.53	1.44	1.39
30	Y	605	CHL	C1B-C2B	4.53	1.44	1.39
30	16	607	CHL	C1B-C2B	4.53	1.44	1.39
30	S	608	CHL	C1B-C2B	4.52	1.44	1.39
30	N	606	CHL	C1B-C2B	4.52	1.44	1.39
30	R	607	CHL	C1B-C2B	4.52	1.44	1.39
30	y	608	CHL	C1B-C2B	4.51	1.44	1.39
30	3	609	CHL	C1B-C2B	4.51	1.44	1.39
30	y	601	CHL	C1B-C2B	4.51	1.44	1.39
30	13	608	CHL	C1B-C2B	4.50	1.44	1.39
30	N	605	CHL	C1B-C2B	4.50	1.44	1.39
30	G	609	CHL	C1B-C2B	4.50	1.44	1.39
30	5	606	CHL	C1B-C2B	4.49	1.44	1.39
30	6	609	CHL	C1B-C2B	4.49	1.44	1.39
30	3	605	CHL	C1B-C2B	4.48	1.44	1.39
30	n	608	CHL	C1B-C2B	4.47	1.44	1.39
30	g	609	CHL	C1B-C2B	4.47	1.44	1.39
30	S	606	CHL	C1B-C2B	4.47	1.44	1.39
30	Y	609	CHL	C1B-C2B	4.46	1.44	1.39
30	Y	608	CHL	C1B-C2B	4.45	1.44	1.39
30	Y	607	CHL	C1B-C2B	4.45	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	601	CHL	C1B-C2B	4.43	1.44	1.39
30	13	609	CHL	C1B-C2B	4.43	1.44	1.39
30	Y	601	CHL	C1B-C2B	4.43	1.44	1.39
30	R	606	CHL	C1B-C2B	4.41	1.44	1.39
30	r	606	CHL	C1B-C2B	4.41	1.44	1.39
30	y	609	CHL	C1B-C2B	4.40	1.44	1.39
30	G	601	CHL	C1B-C2B	4.39	1.44	1.39
30	Y	606	CHL	C1B-C2B	4.38	1.44	1.39
30	N	609	CHL	C1B-C2B	4.38	1.44	1.39
30	1	601	CHL	C1B-C2B	4.36	1.44	1.39
30	n	609	CHL	C1B-C2B	4.35	1.44	1.39
30	y	606	CHL	C1B-C2B	4.34	1.44	1.39
30	4	601	CHL	C1B-C2B	4.28	1.44	1.39
34	G	618	NEX	C26-C21	-3.95	1.49	1.55
30	s	607	CHL	CHA-CBD	3.92	1.56	1.51
30	N	601	CHL	CHA-CBD	3.86	1.56	1.51
30	y	605	CHL	CHA-CBD	3.82	1.56	1.51
30	11	605	CHL	CHA-CBD	3.80	1.56	1.51
30	13	607	CHL	CHA-CBD	3.74	1.56	1.51
30	4	606	CHL	CHA-CBD	3.72	1.56	1.51
30	4	605	CHL	CHA-CBD	3.72	1.56	1.51
30	S	607	CHL	CHA-CBD	3.72	1.56	1.51
30	15	607	CHL	CHA-CBD	3.72	1.56	1.51
30	12	607	CHL	CHA-CBD	3.71	1.56	1.51
30	1	605	CHL	CHA-CBD	3.70	1.56	1.51
30	13	605	CHL	CHA-CBD	3.69	1.56	1.51
30	g	605	CHL	CHA-CBD	3.69	1.56	1.51
30	g	609	CHL	C3B-C2B	-3.69	1.35	1.40
30	3	607	CHL	C3B-C2B	-3.68	1.35	1.40
30	1	607	CHL	CHA-CBD	3.68	1.56	1.51
30	1	606	CHL	CHA-CBD	3.68	1.56	1.51
30	6	608	CHL	C3B-C2B	-3.68	1.35	1.40
30	n	605	CHL	CHA-CBD	3.66	1.55	1.51
30	G	605	CHL	CHA-CBD	3.66	1.55	1.51
30	16	607	CHL	CHA-CBD	3.64	1.55	1.51
30	G	609	CHL	C3B-C2B	-3.64	1.35	1.40
30	4	607	CHL	CHA-CBD	3.64	1.55	1.51
30	Y	605	CHL	CHA-CBD	3.64	1.55	1.51
30	Y	609	CHL	C3B-C2B	-3.64	1.35	1.40
30	2	601	CHL	CHA-CBD	3.64	1.55	1.51
30	N	609	CHL	C3B-C2B	-3.63	1.35	1.40
30	4	601	CHL	C3B-C2B	-3.63	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	606	CHL	CHA-CBD	3.63	1.55	1.51
30	11	606	CHL	CHA-CBD	3.62	1.55	1.51
30	14	605	CHL	CHA-CBD	3.62	1.55	1.51
30	5	601	CHL	CHA-CBD	3.62	1.55	1.51
30	N	607	CHL	C3B-C2B	-3.62	1.35	1.40
30	S	608	CHL	C3B-C2B	-3.62	1.35	1.40
30	16	608	CHL	C3B-C2B	-3.61	1.35	1.40
30	16	609	CHL	C3B-C2B	-3.61	1.35	1.40
30	4	606	CHL	C3B-C2B	-3.61	1.35	1.40
30	r	606	CHL	C3B-C2B	-3.61	1.35	1.40
30	3	607	CHL	CHA-CBD	3.61	1.55	1.51
30	6	607	CHL	C3B-C2B	-3.60	1.35	1.40
30	14	601	CHL	C3B-C2B	-3.60	1.35	1.40
30	n	609	CHL	C3B-C2B	-3.60	1.35	1.40
30	r	605	CHL	C3B-C2B	-3.60	1.35	1.40
30	s	608	CHL	C3B-C2B	-3.60	1.35	1.40
30	g	608	CHL	CHA-CBD	3.60	1.55	1.51
30	n	601	CHL	CHA-CBD	3.60	1.55	1.51
30	g	609	CHL	CHA-CBD	3.59	1.55	1.51
30	3	608	CHL	C3B-C2B	-3.59	1.35	1.40
30	13	609	CHL	CHA-CBD	3.59	1.55	1.51
30	G	608	CHL	CHA-CBD	3.59	1.55	1.51
30	13	608	CHL	C3B-C2B	-3.59	1.35	1.40
30	6	607	CHL	CHA-CBD	3.59	1.55	1.51
30	13	609	CHL	C3B-C2B	-3.59	1.35	1.40
30	G	606	CHL	CHA-CBD	3.59	1.55	1.51
30	16	605	CHL	CHA-CBD	3.58	1.55	1.51
30	5	605	CHL	CHA-CBD	3.58	1.55	1.51
30	n	607	CHL	C3B-C2B	-3.58	1.35	1.40
30	12	601	CHL	CHA-CBD	3.57	1.55	1.51
30	11	609	CHL	CHA-CBD	3.57	1.55	1.51
30	g	606	CHL	CHA-CBD	3.57	1.55	1.51
30	S	606	CHL	C3B-C2B	-3.57	1.35	1.40
30	5	609	CHL	C3B-C2B	-3.57	1.35	1.40
30	4	608	CHL	CHA-CBD	3.57	1.55	1.51
30	y	609	CHL	C3B-C2B	-3.56	1.35	1.40
30	N	605	CHL	CHA-CBD	3.56	1.55	1.51
30	y	609	CHL	CHA-CBD	3.56	1.55	1.51
30	Y	605	CHL	C3B-C2B	-3.56	1.35	1.40
30	16	601	CHL	CHA-CBD	3.56	1.55	1.51
30	15	601	CHL	CHA-CBD	3.55	1.55	1.51
30	R	607	CHL	C3B-C2B	-3.55	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	11	607	CHL	CHA-CBD	3.55	1.55	1.51
30	6	601	CHL	C3B-C2B	-3.55	1.35	1.40
30	r	607	CHL	C3B-C2B	-3.55	1.35	1.40
30	2	605	CHL	CHA-CBD	3.55	1.55	1.51
30	1	608	CHL	CHA-CBD	3.54	1.55	1.51
30	14	605	CHL	C3B-C2B	-3.54	1.35	1.40
30	12	606	CHL	C3B-C2B	-3.54	1.35	1.40
30	n	601	CHL	C3B-C2B	-3.54	1.35	1.40
30	3	609	CHL	C3B-C2B	-3.54	1.35	1.40
30	3	601	CHL	C3B-C2B	-3.54	1.35	1.40
30	15	606	CHL	CHA-CBD	3.54	1.55	1.51
30	g	607	CHL	C3B-C2B	-3.54	1.35	1.40
30	R	606	CHL	C3B-C2B	-3.53	1.35	1.40
30	4	609	CHL	C3B-C2B	-3.53	1.35	1.40
30	G	607	CHL	C3B-C2B	-3.53	1.35	1.40
30	2	609	CHL	C3B-C2B	-3.53	1.35	1.40
30	16	605	CHL	C3B-C2B	-3.53	1.35	1.40
30	1	601	CHL	C3B-C2B	-3.53	1.35	1.40
30	y	607	CHL	CHA-CBD	3.53	1.55	1.51
30	1	609	CHL	C3B-C2B	-3.53	1.35	1.40
30	5	607	CHL	C3B-C2B	-3.53	1.35	1.40
30	2	607	CHL	C3B-C2B	-3.53	1.35	1.40
30	y	601	CHL	C3B-C2B	-3.53	1.35	1.40
30	15	605	CHL	CHA-CBD	3.52	1.55	1.51
30	Y	609	CHL	CHA-CBD	3.52	1.55	1.51
30	N	601	CHL	C3B-C2B	-3.52	1.35	1.40
30	6	605	CHL	C3B-C2B	-3.52	1.35	1.40
30	N	605	CHL	C3B-C2B	-3.52	1.35	1.40
30	14	609	CHL	CHA-CBD	3.52	1.55	1.51
30	R	605	CHL	C3B-C2B	-3.51	1.35	1.40
30	3	609	CHL	CHA-CBD	3.51	1.55	1.51
30	5	607	CHL	CHA-CBD	3.51	1.55	1.51
30	Y	601	CHL	C3B-C2B	-3.51	1.35	1.40
30	14	608	CHL	CHA-CBD	3.51	1.55	1.51
30	Y	606	CHL	CHA-CBD	3.51	1.55	1.51
30	s	606	CHL	CHA-CBD	3.51	1.55	1.51
30	N	606	CHL	C3B-C2B	-3.51	1.35	1.40
30	11	608	CHL	CHA-CBD	3.51	1.55	1.51
30	2	607	CHL	CHA-CBD	3.51	1.55	1.51
30	S	601	CHL	CHA-CBD	3.50	1.55	1.51
30	15	608	CHL	O2D-CGD	3.50	1.41	1.33
30	s	601	CHL	CHA-CBD	3.50	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	606	CHL	CHA-CBD	3.50	1.55	1.51
30	2	608	CHL	CHA-CBD	3.50	1.55	1.51
30	13	605	CHL	C3B-C2B	-3.50	1.35	1.40
30	n	605	CHL	C3B-C2B	-3.50	1.35	1.40
30	6	609	CHL	C3B-C2B	-3.50	1.35	1.40
30	12	606	CHL	CHA-CBD	3.49	1.55	1.51
30	3	605	CHL	C3B-C2B	-3.49	1.35	1.40
30	1	606	CHL	C3B-C2B	-3.49	1.35	1.40
30	G	606	CHL	C3B-C2B	-3.49	1.35	1.40
30	g	605	CHL	C3B-C2B	-3.49	1.35	1.40
30	5	608	CHL	CHA-CBD	3.49	1.55	1.51
30	g	608	CHL	C3B-C2B	-3.48	1.35	1.40
30	11	607	CHL	O2D-CGD	3.48	1.41	1.33
30	Y	606	CHL	C3B-C2B	-3.48	1.35	1.40
30	16	609	CHL	CHA-CBD	3.48	1.55	1.51
30	s	601	CHL	C3B-C2B	-3.48	1.35	1.40
30	16	601	CHL	O2D-CGD	3.48	1.41	1.33
30	n	606	CHL	C3B-C2B	-3.48	1.35	1.40
30	11	605	CHL	O2D-CGD	3.48	1.41	1.33
30	4	608	CHL	C3B-C2B	-3.47	1.35	1.40
30	13	601	CHL	CHA-CBD	3.47	1.55	1.51
30	15	606	CHL	C3B-C2B	-3.47	1.35	1.40
30	14	606	CHL	O2D-CGD	3.47	1.41	1.33
30	S	608	CHL	CHA-CBD	3.47	1.55	1.51
30	5	609	CHL	CHA-CBD	3.47	1.55	1.51
30	12	605	CHL	CHA-CBD	3.47	1.55	1.51
30	g	606	CHL	C3B-C2B	-3.47	1.35	1.40
30	12	608	CHL	O2D-CGD	3.47	1.41	1.33
30	G	609	CHL	CHA-CBD	3.47	1.55	1.51
30	15	601	CHL	O2D-CGD	3.47	1.41	1.33
30	y	606	CHL	C3B-C2B	-3.47	1.35	1.40
30	6	601	CHL	CHA-CBD	3.47	1.55	1.51
30	12	601	CHL	O2D-CGD	3.47	1.41	1.33
30	2	608	CHL	C3B-C2B	-3.47	1.35	1.40
30	13	601	CHL	C3B-C2B	-3.47	1.35	1.40
30	2	601	CHL	O2D-CGD	3.47	1.41	1.33
30	6	609	CHL	CHA-CBD	3.46	1.55	1.51
30	R	607	CHL	CHA-CBD	3.46	1.55	1.51
30	14	607	CHL	O2D-CGD	3.46	1.41	1.33
30	N	609	CHL	CHA-CBD	3.46	1.55	1.51
30	5	605	CHL	O2D-CGD	3.46	1.41	1.33
30	2	605	CHL	O2D-CGD	3.46	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	15	608	CHL	C3B-C2B	-3.46	1.35	1.40
30	12	608	CHL	C3B-C2B	-3.46	1.35	1.40
30	g	601	CHL	C3B-C2B	-3.46	1.35	1.40
30	14	605	CHL	O2D-CGD	3.46	1.41	1.33
30	15	607	CHL	O2D-CGD	3.45	1.41	1.33
30	11	606	CHL	O2D-CGD	3.45	1.41	1.33
30	N	608	CHL	CHA-CBD	3.45	1.55	1.51
30	N	608	CHL	C3B-C2B	-3.45	1.35	1.40
30	15	608	CHL	CHA-CBD	3.45	1.55	1.51
30	12	607	CHL	O2D-CGD	3.45	1.41	1.33
30	13	601	CHL	O2D-CGD	3.45	1.41	1.33
30	11	601	CHL	C3B-C2B	-3.45	1.35	1.40
30	Y	607	CHL	CHA-CBD	3.44	1.55	1.51
30	4	605	CHL	O2D-CGD	3.44	1.41	1.33
30	3	606	CHL	CHA-CBD	3.44	1.55	1.51
30	y	605	CHL	C3B-C2B	-3.44	1.35	1.40
30	4	607	CHL	C3B-C2B	-3.44	1.35	1.40
30	1	605	CHL	O2D-CGD	3.44	1.41	1.33
30	13	607	CHL	C3B-C2B	-3.44	1.35	1.40
32	Y	618	LHG	P-O3	3.44	1.72	1.59
30	s	607	CHL	C3B-C2B	-3.44	1.35	1.40
30	3	605	CHL	CHA-CBD	3.44	1.55	1.51
30	s	608	CHL	CHA-CBD	3.44	1.55	1.51
30	1	608	CHL	O2D-CGD	3.43	1.41	1.33
30	13	606	CHL	CHA-CBD	3.43	1.55	1.51
30	5	608	CHL	C3B-C2B	-3.43	1.35	1.40
30	11	609	CHL	O2D-CGD	3.43	1.41	1.33
30	11	608	CHL	O2D-CGD	3.43	1.41	1.33
30	5	601	CHL	O2D-CGD	3.43	1.41	1.33
30	6	606	CHL	CHA-CBD	3.43	1.55	1.51
30	14	606	CHL	CHA-CBD	3.43	1.55	1.51
30	1	608	CHL	C3B-C2B	-3.42	1.35	1.40
30	G	601	CHL	C3B-C2B	-3.42	1.35	1.40
30	6	608	CHL	CHA-CBD	3.42	1.55	1.51
30	12	608	CHL	CHA-CBD	3.42	1.55	1.51
30	N	607	CHL	CHA-CBD	3.42	1.55	1.51
30	S	606	CHL	CHA-CBD	3.42	1.55	1.51
30	14	608	CHL	O2D-CGD	3.42	1.41	1.33
30	G	605	CHL	C3B-C2B	-3.42	1.35	1.40
30	g	607	CHL	O2D-CGD	3.42	1.41	1.33
30	12	605	CHL	O2D-CGD	3.42	1.41	1.33
30	g	608	CHL	O2D-CGD	3.42	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	14	609	CHL	O2D-CGD	3.42	1.41	1.33
30	16	608	CHL	CHA-CBD	3.42	1.55	1.51
30	5	601	CHL	C3B-C2B	-3.42	1.35	1.40
30	11	609	CHL	C3B-C2B	-3.42	1.35	1.40
30	G	608	CHL	C3B-C2B	-3.41	1.35	1.40
30	G	605	CHL	O2D-CGD	3.41	1.41	1.33
30	15	605	CHL	O2D-CGD	3.41	1.41	1.33
30	4	607	CHL	O2D-CGD	3.41	1.41	1.33
30	3	608	CHL	CHA-CBD	3.41	1.55	1.51
30	2	609	CHL	CHA-CBD	3.41	1.55	1.51
30	s	606	CHL	C3B-C2B	-3.41	1.35	1.40
30	4	605	CHL	O2A-CGA	3.41	1.42	1.30
32	y	618	LHG	P-O3	3.41	1.72	1.59
30	s	608	CHL	O2D-CGD	3.41	1.41	1.33
30	5	606	CHL	O2D-CGD	3.41	1.41	1.33
30	S	607	CHL	C3B-C2B	-3.41	1.35	1.40
30	G	607	CHL	O2D-CGD	3.41	1.41	1.33
30	14	607	CHL	CHA-CBD	3.41	1.55	1.51
30	5	606	CHL	O2A-CGA	3.41	1.42	1.30
30	y	608	CHL	C3B-C2B	-3.40	1.35	1.40
30	12	605	CHL	O2A-CGA	3.40	1.42	1.30
30	1	609	CHL	O2D-CGD	3.40	1.41	1.33
30	16	601	CHL	C3B-C2B	-3.40	1.35	1.40
30	4	606	CHL	O2D-CGD	3.40	1.41	1.33
30	g	605	CHL	O2D-CGD	3.40	1.41	1.33
30	4	608	CHL	O2D-CGD	3.40	1.41	1.33
30	n	607	CHL	CHA-CBD	3.40	1.55	1.51
30	4	609	CHL	O2D-CGD	3.40	1.41	1.33
30	13	609	CHL	O2D-CGD	3.40	1.41	1.33
30	r	607	CHL	CHA-CBD	3.40	1.55	1.51
30	5	605	CHL	O2A-CGA	3.40	1.42	1.30
30	1	606	CHL	O2D-CGD	3.40	1.41	1.33
30	16	609	CHL	O2D-CGD	3.40	1.41	1.33
32	R	621	LHG	P-O3	3.40	1.72	1.59
30	2	606	CHL	O2D-CGD	3.40	1.41	1.33
30	S	601	CHL	O2D-CGD	3.40	1.41	1.33
30	S	608	CHL	O2D-CGD	3.40	1.41	1.33
30	2	608	CHL	O2D-CGD	3.40	1.41	1.33
30	y	606	CHL	CHA-CBD	3.39	1.55	1.51
30	5	607	CHL	O2D-CGD	3.39	1.41	1.33
30	5	605	CHL	C3B-C2B	-3.39	1.35	1.40
30	2	605	CHL	O2A-CGA	3.39	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	S	601	CHL	C3B-C2B	-3.39	1.35	1.40
30	1	607	CHL	O2D-CGD	3.39	1.41	1.33
30	15	605	CHL	O2A-CGA	3.39	1.42	1.30
30	3	606	CHL	O2D-CGD	3.39	1.41	1.33
30	15	606	CHL	O2D-CGD	3.39	1.41	1.33
30	s	601	CHL	O2D-CGD	3.39	1.41	1.33
30	16	606	CHL	CHA-CBD	3.39	1.55	1.51
30	4	605	CHL	C3B-C2B	-3.39	1.35	1.40
30	1	605	CHL	O2A-CGA	3.39	1.42	1.30
30	G	608	CHL	O2D-CGD	3.38	1.41	1.33
30	n	608	CHL	CHA-CBD	3.38	1.55	1.51
30	16	607	CHL	C3B-C2B	-3.38	1.35	1.40
30	3	601	CHL	CHA-CBD	3.38	1.55	1.51
30	2	606	CHL	O2A-CGA	3.38	1.42	1.30
30	y	607	CHL	C3B-C2B	-3.38	1.35	1.40
32	r	621	LHG	P-O3	3.38	1.72	1.59
30	S	601	CHL	O2A-CGA	3.38	1.42	1.30
30	14	609	CHL	C3B-C2B	-3.38	1.35	1.40
30	5	609	CHL	O2D-CGD	3.38	1.41	1.33
30	5	608	CHL	O2D-CGD	3.38	1.41	1.33
30	6	605	CHL	CHA-CBD	3.38	1.55	1.51
30	11	607	CHL	C3B-C2B	-3.38	1.35	1.40
30	16	606	CHL	O2D-CGD	3.38	1.41	1.33
30	n	606	CHL	O2D-CGD	3.38	1.41	1.33
30	n	609	CHL	CHA-CBD	3.38	1.55	1.51
30	1	607	CHL	C3B-C2B	-3.38	1.35	1.40
30	14	601	CHL	CHA-CBD	3.37	1.55	1.51
32	d	413	LHG	P-O3	3.37	1.72	1.59
30	2	607	CHL	O2D-CGD	3.37	1.41	1.33
30	g	606	CHL	O2D-CGD	3.37	1.41	1.33
32	D	412	LHG	P-O3	3.37	1.72	1.59
30	n	608	CHL	C3B-C2B	-3.37	1.35	1.40
30	G	607	CHL	CHA-CBD	3.37	1.55	1.51
30	11	607	CHL	O2A-CGA	3.37	1.41	1.30
30	1	605	CHL	C3B-C2B	-3.37	1.35	1.40
30	N	606	CHL	O2D-CGD	3.37	1.41	1.33
30	14	607	CHL	C3B-C2B	-3.37	1.35	1.40
30	13	606	CHL	O2D-CGD	3.37	1.41	1.33
30	6	606	CHL	O2D-CGD	3.37	1.41	1.33
30	s	606	CHL	O2D-CGD	3.37	1.41	1.33
30	15	607	CHL	C3B-C2B	-3.37	1.35	1.40
30	Y	608	CHL	C3B-C2B	-3.37	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	601	CHL	O2D-CGD	3.37	1.41	1.33
30	S	606	CHL	O2D-CGD	3.36	1.41	1.33
30	13	608	CHL	CHA-CBD	3.36	1.55	1.51
30	s	601	CHL	O2A-CGA	3.36	1.41	1.30
30	2	605	CHL	C3B-C2B	-3.36	1.35	1.40
33	G	617	LUT	C22-C23	-3.36	1.48	1.52
30	3	609	CHL	O2D-CGD	3.36	1.41	1.33
30	y	608	CHL	CHA-CBD	3.36	1.55	1.51
30	12	606	CHL	O2D-CGD	3.36	1.41	1.33
30	G	606	CHL	O2D-CGD	3.36	1.41	1.33
30	14	608	CHL	C3B-C2B	-3.36	1.35	1.40
30	14	606	CHL	C3B-C2B	-3.36	1.35	1.40
30	R	605	CHL	O2D-CGD	3.35	1.41	1.33
30	Y	601	CHL	O2D-CGD	3.35	1.41	1.33
30	g	609	CHL	O2D-CGD	3.35	1.41	1.33
30	Y	608	CHL	CHA-CBD	3.35	1.55	1.51
30	6	608	CHL	O2D-CGD	3.35	1.41	1.33
30	12	605	CHL	C3B-C2B	-3.35	1.35	1.40
30	r	605	CHL	O2D-CGD	3.35	1.41	1.33
30	S	607	CHL	O2D-CGD	3.35	1.41	1.33
30	4	609	CHL	CHA-CBD	3.35	1.55	1.51
30	Y	606	CHL	O2D-CGD	3.35	1.41	1.33
30	n	601	CHL	O2D-CGD	3.34	1.41	1.33
30	3	608	CHL	O2D-CGD	3.34	1.41	1.33
30	3	601	CHL	O2D-CGD	3.34	1.41	1.33
30	Y	608	CHL	O2D-CGD	3.34	1.41	1.33
30	6	609	CHL	O2D-CGD	3.34	1.41	1.33
30	R	606	CHL	CHA-CBD	3.34	1.55	1.51
30	2	609	CHL	O2D-CGD	3.33	1.41	1.33
30	1	609	CHL	CHA-CBD	3.33	1.55	1.51
30	g	607	CHL	CHA-CBD	3.33	1.55	1.51
33	g	617	LUT	C22-C23	-3.33	1.48	1.52
30	11	601	CHL	CHA-CBD	3.33	1.55	1.51
30	n	606	CHL	CHA-CBD	3.33	1.55	1.51
30	16	605	CHL	O2D-CGD	3.33	1.41	1.33
30	16	608	CHL	O2D-CGD	3.33	1.41	1.33
30	6	601	CHL	O2D-CGD	3.32	1.41	1.33
30	4	601	CHL	O2D-CGD	3.32	1.41	1.33
30	s	607	CHL	O2D-CGD	3.32	1.41	1.33
30	Y	607	CHL	O2D-CGD	3.32	1.41	1.33
30	N	606	CHL	CHA-CBD	3.32	1.55	1.51
30	G	609	CHL	O2D-CGD	3.32	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	y	606	CHL	O2D-CGD	3.32	1.41	1.33
30	1	601	CHL	O2D-CGD	3.32	1.41	1.33
30	11	606	CHL	C3B-C2B	-3.32	1.35	1.40
30	R	605	CHL	CHA-CBD	3.32	1.55	1.51
30	11	601	CHL	O2D-CGD	3.32	1.41	1.33
30	Y	607	CHL	C3B-C2B	-3.32	1.35	1.40
30	13	608	CHL	O2D-CGD	3.32	1.41	1.33
30	y	607	CHL	O2D-CGD	3.31	1.41	1.33
30	13	606	CHL	C3B-C2B	-3.31	1.35	1.40
30	r	606	CHL	CHA-CBD	3.31	1.55	1.51
30	y	601	CHL	O2D-CGD	3.31	1.41	1.33
30	6	607	CHL	O2D-CGD	3.31	1.41	1.33
30	R	606	CHL	O2D-CGD	3.31	1.41	1.33
30	13	605	CHL	O2D-CGD	3.31	1.41	1.33
30	1	601	CHL	CHA-CBD	3.30	1.55	1.51
30	3	607	CHL	O2D-CGD	3.30	1.41	1.33
30	4	601	CHL	CHA-CBD	3.30	1.55	1.51
30	y	608	CHL	O2D-CGD	3.30	1.41	1.33
32	Y	617	LHG	P-O3	3.30	1.72	1.59
31	n	613	CLA	MG-NC	3.30	2.14	2.06
30	n	607	CHL	O2D-CGD	3.30	1.41	1.33
30	16	607	CHL	O2D-CGD	3.30	1.41	1.33
30	y	601	CHL	CHA-CBD	3.30	1.55	1.51
32	r	619	LHG	P-O3	3.30	1.72	1.59
30	14	601	CHL	O2D-CGD	3.30	1.41	1.33
32	16	616	LHG	P-O3	3.29	1.72	1.59
32	3	617	LHG	P-O3	3.29	1.72	1.59
30	12	601	CHL	C3B-C2B	-3.29	1.35	1.40
30	15	601	CHL	C3B-C2B	-3.29	1.35	1.40
30	r	605	CHL	CHA-CBD	3.29	1.55	1.51
30	3	606	CHL	C3B-C2B	-3.29	1.35	1.40
30	6	606	CHL	C3B-C2B	-3.29	1.35	1.40
30	16	606	CHL	C3B-C2B	-3.29	1.35	1.40
30	N	607	CHL	O2D-CGD	3.29	1.41	1.33
32	y	617	LHG	P-O3	3.29	1.72	1.59
32	c	521	LHG	P-O3	3.28	1.72	1.59
30	Y	601	CHL	CHA-CBD	3.28	1.55	1.51
30	N	608	CHL	O2D-CGD	3.28	1.41	1.33
30	12	607	CHL	C3B-C2B	-3.28	1.35	1.40
30	13	607	CHL	O2D-CGD	3.28	1.41	1.33
30	15	605	CHL	C3B-C2B	-3.27	1.35	1.40
30	r	606	CHL	O2D-CGD	3.27	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	R	607	CHL	O2D-CGD	3.27	1.41	1.33
30	n	609	CHL	O2D-CGD	3.27	1.41	1.33
30	3	605	CHL	O2D-CGD	3.27	1.41	1.33
30	Y	605	CHL	O2D-CGD	3.27	1.41	1.33
30	2	601	CHL	C3B-C2B	-3.26	1.36	1.40
30	6	605	CHL	O2D-CGD	3.26	1.41	1.33
30	N	609	CHL	O2D-CGD	3.26	1.41	1.33
30	N	605	CHL	O2D-CGD	3.25	1.41	1.33
30	n	605	CHL	O2D-CGD	3.24	1.41	1.33
30	r	607	CHL	O2D-CGD	3.24	1.41	1.33
32	D	412	LHG	P-O6	3.24	1.72	1.59
32	14	615	LHG	P-O3	3.24	1.72	1.59
32	d	413	LHG	P-O6	3.24	1.72	1.59
32	R	619	LHG	P-O3	3.24	1.72	1.59
32	6	617	LHG	P-O3	3.23	1.72	1.59
30	y	605	CHL	O2D-CGD	3.23	1.41	1.33
30	G	601	CHL	CHA-CBD	3.22	1.55	1.51
30	g	601	CHL	CHA-CBD	3.22	1.55	1.51
32	C	521	LHG	P-O3	3.22	1.72	1.59
30	11	608	CHL	C3B-C2B	-3.22	1.36	1.40
30	11	605	CHL	C3B-C2B	-3.21	1.36	1.40
30	g	601	CHL	O2D-CGD	3.21	1.41	1.33
30	G	601	CHL	O2D-CGD	3.21	1.41	1.33
30	y	609	CHL	O2D-CGD	3.20	1.41	1.33
32	13	616	LHG	P-O3	3.20	1.71	1.59
30	Y	609	CHL	O2D-CGD	3.20	1.41	1.33
32	c	521	LHG	P-O6	3.19	1.71	1.59
31	S	612	CLA	MG-NC	3.19	2.13	2.06
32	a	401	LHG	P-O3	3.18	1.71	1.59
32	11	615	LHG	P-O3	3.18	1.71	1.59
32	y	617	LHG	P-O6	3.18	1.71	1.59
32	A	415	LHG	P-O6	3.18	1.71	1.59
32	s	621	LHG	P-O3	3.17	1.71	1.59
32	C	521	LHG	P-O6	3.17	1.71	1.59
32	S	621	LHG	P-O3	3.16	1.71	1.59
32	Y	617	LHG	P-O6	3.15	1.71	1.59
32	6	616	LHG	P-O3	3.15	1.71	1.59
32	a	414	LHG	P-O6	3.15	1.71	1.59
32	r	619	LHG	P-O6	3.14	1.71	1.59
32	4	615	LHG	P-O3	3.14	1.71	1.59
32	a	414	LHG	P-O3	3.14	1.71	1.59
30	y	605	CHL	C1A-CHA	3.13	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	414	LHG	P-O6	3.13	1.71	1.59
32	1	615	LHG	P-O3	3.12	1.71	1.59
33	y	623	LUT	C22-C23	-3.12	1.49	1.52
32	Y	618	LHG	P-O6	3.12	1.71	1.59
30	n	608	CHL	O2D-CGD	3.11	1.40	1.33
32	r	621	LHG	P-O6	3.11	1.71	1.59
30	13	607	CHL	C1A-CHA	3.10	1.43	1.40
32	A	413	LHG	P-O3	3.10	1.71	1.59
32	a	401	LHG	P-O6	3.10	1.71	1.59
32	A	414	LHG	P-O3	3.10	1.71	1.59
32	16	616	LHG	P-O6	3.09	1.71	1.59
32	y	617	LHG	O7-C7	3.09	1.43	1.34
32	y	618	LHG	P-O6	3.09	1.71	1.59
30	3	605	CHL	C1A-CHA	3.09	1.43	1.40
32	13	616	LHG	P-O6	3.08	1.71	1.59
30	11	605	CHL	C1A-CHA	3.08	1.43	1.40
32	R	619	LHG	O7-C7	3.07	1.43	1.34
32	R	619	LHG	P-O6	3.07	1.71	1.59
33	Y	622	LUT	C22-C23	-3.07	1.49	1.52
30	2	606	CHL	C3B-C2B	-3.07	1.36	1.40
32	3	616	LHG	P-O3	3.07	1.71	1.59
32	1	615	LHG	P-O6	3.06	1.71	1.59
32	r	621	LHG	C8-C7	3.06	1.59	1.50
32	4	615	LHG	P-O6	3.05	1.71	1.59
30	4	606	CHL	C1A-CHA	3.05	1.43	1.40
32	3	617	LHG	P-O6	3.05	1.71	1.59
30	11	608	CHL	C1A-CHA	3.05	1.43	1.40
32	A	415	LHG	P-O3	3.04	1.71	1.59
32	14	615	LHG	P-O6	3.03	1.71	1.59
32	R	621	LHG	O7-C7	3.03	1.42	1.34
32	a	413	LHG	P-O3	3.03	1.71	1.59
30	5	606	CHL	C3B-C2B	-3.03	1.36	1.40
32	r	621	LHG	O7-C7	3.02	1.42	1.34
32	A	411	LHG	O7-C7	3.02	1.42	1.34
32	s	617	LHG	P-O3	3.02	1.71	1.59
32	G	615	LHG	O7-C7	3.02	1.42	1.34
32	14	615	LHG	O7-C7	3.02	1.42	1.34
30	3	607	CHL	C1A-CHA	3.02	1.43	1.40
32	R	621	LHG	C8-C7	3.02	1.59	1.50
30	g	605	CHL	O2A-CGA	3.02	1.42	1.33
32	S	617	LHG	P-O3	3.02	1.71	1.59
32	Y	617	LHG	O7-C7	3.01	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	606	CHL	O2A-CGA	3.01	1.42	1.33
32	a	401	LHG	O7-C7	3.01	1.42	1.34
32	a	414	LHG	O7-C7	3.01	1.42	1.34
30	15	608	CHL	O2A-CGA	3.01	1.42	1.33
30	S	608	CHL	O2A-CGA	3.01	1.42	1.33
32	11	615	LHG	O7-C7	3.01	1.42	1.34
32	16	616	LHG	O7-C7	3.01	1.42	1.34
30	14	605	CHL	O2A-CGA	3.01	1.42	1.33
32	A	414	LHG	O7-C7	3.01	1.42	1.34
30	6	605	CHL	C1A-CHA	3.01	1.43	1.40
30	11	605	CHL	O2A-CGA	3.01	1.42	1.33
32	13	616	LHG	O7-C7	3.01	1.42	1.34
30	6	605	CHL	O2A-CGA	3.01	1.42	1.33
32	S	621	LHG	O7-C7	3.01	1.42	1.34
32	A	415	LHG	O7-C7	3.00	1.42	1.34
30	1	609	CHL	O2A-CGA	3.00	1.42	1.33
32	n	616	LHG	P-O3	3.00	1.71	1.59
32	s	621	LHG	O7-C7	3.00	1.42	1.34
32	G	615	LHG	P-O3	3.00	1.71	1.59
31	S	612	CLA	MG-NB	3.00	2.11	2.05
30	12	607	CHL	O2A-CGA	3.00	1.42	1.33
30	12	608	CHL	O2A-CGA	3.00	1.42	1.33
30	2	609	CHL	O2A-CGA	2.99	1.42	1.33
30	2	608	CHL	O2A-CGA	2.99	1.42	1.33
30	4	609	CHL	O2A-CGA	2.99	1.42	1.33
32	4	615	LHG	O7-C7	2.99	1.42	1.34
32	s	617	LHG	O7-C7	2.99	1.42	1.34
32	1	615	LHG	O7-C7	2.99	1.42	1.34
32	S	617	LHG	O7-C7	2.99	1.42	1.34
30	g	607	CHL	O2A-CGA	2.99	1.42	1.33
30	g	608	CHL	C1A-CHA	2.99	1.43	1.40
30	12	601	CHL	O2A-CGA	2.99	1.42	1.33
30	s	607	CHL	C1A-CHA	2.99	1.43	1.40
31	B	612	CLA	C1D-ND	-2.99	1.33	1.37
32	c	521	LHG	O7-C7	2.98	1.42	1.34
30	G	605	CHL	O2A-CGA	2.98	1.42	1.33
30	11	609	CHL	O2A-CGA	2.98	1.42	1.33
30	G	606	CHL	C1A-CHA	2.98	1.43	1.40
32	R	621	LHG	P-O6	2.98	1.71	1.59
30	4	607	CHL	O2A-CGA	2.98	1.42	1.33
30	11	608	CHL	O2A-CGA	2.98	1.42	1.33
30	1	608	CHL	O2A-CGA	2.98	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	609	CHL	O2A-CGA	2.98	1.42	1.33
30	14	608	CHL	O2A-CGA	2.98	1.42	1.33
30	Y	607	CHL	O2A-CGA	2.98	1.42	1.33
30	16	609	CHL	O2A-CGA	2.98	1.42	1.33
30	5	608	CHL	O2A-CGA	2.98	1.42	1.33
30	14	609	CHL	O2A-CGA	2.98	1.42	1.33
32	r	619	LHG	O7-C7	2.98	1.42	1.34
30	5	609	CHL	O2A-CGA	2.98	1.42	1.33
30	y	607	CHL	O2A-CGA	2.98	1.42	1.33
30	1	605	CHL	C1A-CHA	2.97	1.43	1.40
30	4	608	CHL	O2A-CGA	2.97	1.42	1.33
30	1	607	CHL	O2A-CGA	2.97	1.42	1.33
30	13	601	CHL	O2A-CGA	2.97	1.42	1.33
30	15	607	CHL	O2A-CGA	2.97	1.42	1.33
30	N	601	CHL	C1A-CHA	2.97	1.43	1.40
30	12	607	CHL	C1A-CHA	2.97	1.43	1.40
30	G	608	CHL	C1A-CHA	2.97	1.43	1.40
30	16	601	CHL	O2A-CGA	2.97	1.42	1.33
32	S	621	LHG	P-O6	2.97	1.71	1.59
30	N	601	CHL	O2A-CGA	2.97	1.42	1.33
32	A	411	LHG	P-O3	2.97	1.71	1.59
30	15	606	CHL	O2A-CGA	2.97	1.42	1.33
30	14	607	CHL	O2A-CGA	2.96	1.42	1.33
30	12	606	CHL	O2A-CGA	2.96	1.42	1.33
32	d	413	LHG	O7-C7	2.96	1.42	1.34
32	D	412	LHG	O7-C7	2.96	1.42	1.34
32	g	615	LHG	P-O3	2.96	1.71	1.59
30	3	605	CHL	O2A-CGA	2.96	1.42	1.33
30	s	608	CHL	O2A-CGA	2.96	1.42	1.33
32	a	411	LHG	O7-C7	2.96	1.42	1.34
32	s	621	LHG	P-O6	2.96	1.71	1.59
32	6	617	LHG	P-O6	2.96	1.71	1.59
30	N	609	CHL	O2A-CGA	2.95	1.42	1.33
30	2	607	CHL	O2A-CGA	2.95	1.42	1.33
30	n	608	CHL	O2A-CGA	2.95	1.42	1.33
32	a	411	LHG	P-O3	2.95	1.71	1.59
30	15	601	CHL	O2A-CGA	2.95	1.42	1.33
32	11	615	LHG	P-O6	2.95	1.70	1.59
31	b	612	CLA	C1D-ND	-2.95	1.34	1.37
30	13	607	CHL	O2A-CGA	2.95	1.41	1.33
30	3	606	CHL	O2A-CGA	2.95	1.41	1.33
30	G	609	CHL	O2A-CGA	2.95	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Y	605	CHL	O2A-CGA	2.94	1.41	1.33
30	11	601	CHL	O2A-CGA	2.94	1.41	1.33
32	C	521	LHG	O7-C7	2.94	1.42	1.34
32	n	616	LHG	O7-C7	2.94	1.42	1.34
30	G	607	CHL	O2A-CGA	2.94	1.41	1.33
33	11	617	LUT	C22-C23	-2.94	1.49	1.52
30	16	608	CHL	O2A-CGA	2.94	1.41	1.33
30	g	609	CHL	O2A-CGA	2.94	1.41	1.33
30	r	607	CHL	O2A-CGA	2.94	1.41	1.33
33	6	618	LUT	C22-C23	-2.94	1.49	1.52
30	G	606	CHL	O2A-CGA	2.94	1.42	1.33
30	3	607	CHL	O2A-CGA	2.93	1.41	1.33
30	14	601	CHL	O2A-CGA	2.93	1.41	1.33
30	y	609	CHL	O2A-CGA	2.93	1.41	1.33
30	2	601	CHL	C1A-CHA	2.93	1.43	1.40
30	g	606	CHL	C1A-CHA	2.93	1.43	1.40
30	R	605	CHL	O2A-CGA	2.93	1.41	1.33
30	5	601	CHL	O2A-CGA	2.93	1.41	1.33
30	n	601	CHL	O2A-CGA	2.93	1.41	1.33
30	r	605	CHL	O2A-CGA	2.93	1.41	1.33
30	6	607	CHL	O2A-CGA	2.93	1.41	1.33
30	13	608	CHL	O2A-CGA	2.93	1.41	1.33
30	n	609	CHL	O2A-CGA	2.93	1.41	1.33
30	y	609	CHL	C1A-CHA	2.93	1.43	1.40
30	N	608	CHL	O2A-CGA	2.92	1.41	1.33
30	Y	609	CHL	O2A-CGA	2.92	1.41	1.33
30	11	606	CHL	O2A-CGA	2.92	1.42	1.33
30	5	605	CHL	C1A-CHA	2.92	1.43	1.40
30	y	605	CHL	O2A-CGA	2.92	1.41	1.33
30	r	606	CHL	O2A-CGA	2.92	1.41	1.33
30	s	606	CHL	O2A-CGA	2.92	1.41	1.33
32	D	408	LHG	O7-C7	2.92	1.42	1.34
30	16	607	CHL	O2A-CGA	2.92	1.41	1.33
30	13	606	CHL	O2A-CGA	2.92	1.41	1.33
30	R	606	CHL	O2A-CGA	2.92	1.41	1.33
30	N	606	CHL	O2A-CGA	2.92	1.41	1.33
30	g	608	CHL	O2A-CGA	2.92	1.41	1.33
30	4	605	CHL	C1A-CHA	2.92	1.43	1.40
32	Y	618	LHG	O7-C7	2.91	1.42	1.34
30	y	606	CHL	O2A-CGA	2.91	1.41	1.33
33	14	617	LUT	C22-C23	-2.91	1.49	1.52
30	R	607	CHL	O2A-CGA	2.91	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Y	606	CHL	O2A-CGA	2.91	1.41	1.33
32	d	409	LHG	O7-C7	2.91	1.42	1.34
30	S	606	CHL	O2A-CGA	2.91	1.41	1.33
30	5	607	CHL	O2A-CGA	2.91	1.41	1.33
30	6	606	CHL	O2A-CGA	2.91	1.41	1.33
30	6	607	CHL	C1A-CHA	2.91	1.43	1.40
30	3	609	CHL	O2A-CGA	2.91	1.41	1.33
30	G	608	CHL	O2A-CGA	2.91	1.41	1.33
32	R	618	LHG	O7-C7	2.91	1.42	1.34
32	Y	616	LHG	P-O3	2.90	1.70	1.59
30	3	608	CHL	O2A-CGA	2.90	1.41	1.33
30	6	609	CHL	O2A-CGA	2.90	1.41	1.33
32	d	408	LHG	P-O3	2.90	1.70	1.59
30	y	606	CHL	C1A-CHA	2.90	1.43	1.40
32	N	616	LHG	P-O3	2.90	1.70	1.59
30	6	601	CHL	O2A-CGA	2.90	1.41	1.33
30	16	605	CHL	O2A-CGA	2.90	1.41	1.33
30	3	601	CHL	O2A-CGA	2.90	1.41	1.33
30	13	605	CHL	O2A-CGA	2.90	1.41	1.33
32	y	616	LHG	P-O3	2.89	1.70	1.59
32	g	615	LHG	O7-C7	2.89	1.42	1.34
30	Y	609	CHL	C1A-CHA	2.89	1.43	1.40
30	6	608	CHL	O2A-CGA	2.89	1.41	1.33
30	n	605	CHL	O2A-CGA	2.89	1.41	1.33
32	N	616	LHG	O7-C7	2.89	1.42	1.34
30	15	607	CHL	C1A-CHA	2.89	1.43	1.40
30	14	608	CHL	C1A-CHA	2.88	1.43	1.40
30	R	606	CHL	C1A-CHA	2.88	1.43	1.40
30	16	606	CHL	O2A-CGA	2.88	1.41	1.33
30	2	601	CHL	O2A-CGA	2.88	1.42	1.33
30	G	601	CHL	O2A-CGA	2.88	1.41	1.33
32	y	618	LHG	O7-C7	2.88	1.42	1.34
32	3	617	LHG	O7-C7	2.88	1.42	1.34
30	1	606	CHL	O2A-CGA	2.88	1.41	1.33
30	Y	606	CHL	C1A-CHA	2.88	1.43	1.40
30	N	605	CHL	O2A-CGA	2.88	1.41	1.33
30	n	606	CHL	O2A-CGA	2.88	1.41	1.33
30	4	601	CHL	O2A-CGA	2.88	1.41	1.33
30	14	606	CHL	O2A-CGA	2.88	1.41	1.33
30	12	605	CHL	C2C-C3C	2.88	1.39	1.36
32	D	409	LHG	O7-C7	2.88	1.42	1.34
32	D	408	LHG	P-O3	2.88	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	16	607	CHL	C1A-CHA	2.88	1.43	1.40
30	16	601	CHL	C1A-CHA	2.87	1.43	1.40
32	6	616	LHG	P-O6	2.87	1.70	1.59
32	r	618	LHG	O7-C7	2.87	1.42	1.34
32	r	618	LHG	P-O3	2.87	1.70	1.59
30	g	601	CHL	O2A-CGA	2.87	1.41	1.33
32	3	616	LHG	P-O6	2.87	1.70	1.59
30	11	607	CHL	C1A-CHA	2.86	1.43	1.40
30	1	601	CHL	O2A-CGA	2.86	1.41	1.33
30	s	601	CHL	C1A-CHA	2.86	1.43	1.40
30	2	605	CHL	C1A-CHA	2.86	1.43	1.40
30	12	606	CHL	C1A-CHA	2.86	1.43	1.40
30	r	606	CHL	C1A-CHA	2.86	1.43	1.40
30	4	606	CHL	O2A-CGA	2.85	1.41	1.33
32	A	415	LHG	O8-C23	2.85	1.41	1.33
32	d	408	LHG	O7-C7	2.85	1.42	1.34
30	1	606	CHL	C1A-CHA	2.85	1.43	1.40
32	n	616	LHG	P-O6	2.85	1.70	1.59
30	14	607	CHL	C1A-CHA	2.85	1.43	1.40
30	g	605	CHL	C1A-CHA	2.84	1.43	1.40
32	Y	617	LHG	O8-C23	2.84	1.41	1.33
32	11	615	LHG	O8-C23	2.84	1.41	1.33
30	S	601	CHL	C1A-CHA	2.83	1.43	1.40
32	A	411	LHG	P-O6	2.83	1.70	1.59
30	15	606	CHL	C1A-CHA	2.83	1.43	1.40
30	15	605	CHL	C2C-C3C	2.83	1.39	1.36
30	y	601	CHL	O2A-CGA	2.83	1.41	1.33
33	3	618	LUT	C22-C23	-2.83	1.49	1.52
32	6	617	LHG	O7-C7	2.83	1.42	1.34
30	N	607	CHL	O2A-CGA	2.83	1.41	1.33
30	Y	601	CHL	O2A-CGA	2.83	1.41	1.33
33	16	618	LUT	C22-C23	-2.83	1.49	1.52
30	n	607	CHL	O2A-CGA	2.83	1.41	1.33
30	6	606	CHL	C1A-CHA	2.83	1.43	1.40
30	15	605	CHL	C1A-CHA	2.82	1.43	1.40
32	a	413	LHG	O7-C7	2.82	1.42	1.34
30	S	608	CHL	C1A-CHA	2.82	1.43	1.40
32	1	615	LHG	O8-C23	2.82	1.41	1.33
32	y	617	LHG	O8-C23	2.82	1.41	1.33
32	l	102	LHG	O7-C7	2.82	1.42	1.34
32	6	616	LHG	O7-C7	2.82	1.42	1.34
30	1	607	CHL	C1A-CHA	2.81	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	n	601	CHL	C1A-CHA	2.81	1.43	1.40
30	G	605	CHL	C1A-CHA	2.81	1.43	1.40
30	11	606	CHL	C1A-CHA	2.81	1.43	1.40
32	16	616	LHG	C8-C7	2.81	1.58	1.50
32	L	102	LHG	O7-C7	2.81	1.42	1.34
30	12	605	CHL	C1A-CHA	2.81	1.43	1.40
33	6	619	LUT	C22-C23	-2.81	1.49	1.52
32	3	616	LHG	O7-C7	2.81	1.42	1.34
30	11	609	CHL	C1A-CHA	2.80	1.43	1.40
30	14	609	CHL	C1A-CHA	2.80	1.43	1.40
30	Y	607	CHL	C1A-CHA	2.80	1.43	1.40
32	a	401	LHG	O8-C23	2.80	1.41	1.33
30	4	607	CHL	C1A-CHA	2.80	1.43	1.40
32	13	616	LHG	C8-C7	2.80	1.58	1.50
32	A	413	LHG	O7-C7	2.80	1.42	1.34
30	11	609	CHL	C2C-C3C	2.80	1.39	1.36
34	Y	623	NEX	C1-C6	-2.80	1.49	1.54
32	14	615	LHG	O8-C23	2.80	1.41	1.33
33	3	619	LUT	C22-C23	-2.80	1.49	1.52
31	C	510	CLA	C1D-ND	-2.80	1.34	1.37
30	13	605	CHL	C1A-CHA	2.80	1.43	1.40
30	n	605	CHL	C1A-CHA	2.79	1.43	1.40
30	4	605	CHL	C2C-C3C	2.79	1.39	1.36
30	y	607	CHL	C1A-CHA	2.79	1.43	1.40
32	Y	616	LHG	O7-C7	2.79	1.42	1.34
32	a	411	LHG	P-O6	2.79	1.70	1.59
33	4	616	LUT	C22-C23	-2.79	1.49	1.52
32	A	411	LHG	C8-C7	2.78	1.58	1.50
31	R	602	CLA	C1D-ND	-2.78	1.34	1.37
32	D	412	LHG	O8-C23	2.78	1.41	1.33
30	N	607	CHL	C1A-CHA	2.78	1.43	1.40
32	d	413	LHG	O8-C23	2.78	1.41	1.33
31	r	602	CLA	C1D-ND	-2.78	1.34	1.37
31	c	510	CLA	C1D-ND	-2.78	1.34	1.37
30	S	607	CHL	C1A-CHA	2.78	1.43	1.40
32	A	413	LHG	C8-C7	2.78	1.58	1.50
32	14	615	LHG	C8-C7	2.78	1.58	1.50
32	R	618	LHG	P-O3	2.77	1.70	1.59
32	A	414	LHG	C8-C7	2.77	1.58	1.50
32	y	616	LHG	O7-C7	2.77	1.42	1.34
30	G	609	CHL	C1A-CHA	2.77	1.43	1.40
32	6	616	LHG	O8-C23	2.77	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	414	LHG	O8-C23	2.77	1.41	1.33
30	3	606	CHL	C1A-CHA	2.77	1.43	1.40
32	4	615	LHG	O8-C23	2.76	1.41	1.33
32	16	616	LHG	O8-C23	2.76	1.41	1.33
30	Y	605	CHL	C1A-CHA	2.76	1.43	1.40
32	D	408	LHG	C8-C7	2.76	1.58	1.50
32	s	621	LHG	O8-C23	2.76	1.41	1.33
32	r	621	LHG	O8-C23	2.76	1.41	1.33
32	a	413	LHG	C8-C7	2.76	1.58	1.50
32	R	621	LHG	O8-C23	2.76	1.41	1.33
32	S	621	LHG	O8-C23	2.76	1.41	1.33
30	13	601	CHL	C1A-CHA	2.76	1.43	1.40
32	3	617	LHG	O8-C23	2.76	1.41	1.33
30	13	609	CHL	MG-NB	2.75	2.11	2.05
32	3	616	LHG	O8-C23	2.75	1.41	1.33
32	G	615	LHG	P-O6	2.75	1.70	1.59
30	g	609	CHL	C1A-CHA	2.75	1.43	1.40
30	14	606	CHL	C1A-CHA	2.75	1.43	1.40
30	s	608	CHL	C1A-CHA	2.75	1.43	1.40
32	S	617	LHG	P-O6	2.75	1.70	1.59
31	C	508	CLA	C1D-ND	-2.75	1.34	1.37
30	4	608	CHL	C1A-CHA	2.75	1.43	1.40
32	a	414	LHG	C8-C7	2.75	1.58	1.50
30	n	607	CHL	C1A-CHA	2.75	1.43	1.40
32	r	619	LHG	C8-C7	2.74	1.58	1.50
32	G	615	LHG	O8-C23	2.74	1.41	1.33
31	c	511	CLA	C1D-ND	-2.74	1.34	1.37
32	c	521	LHG	O8-C23	2.74	1.41	1.33
32	L	102	LHG	O8-C23	2.74	1.41	1.33
32	L	102	LHG	P-O3	2.74	1.70	1.59
32	13	616	LHG	O8-C23	2.74	1.41	1.33
30	15	601	CHL	C1A-CHA	2.74	1.43	1.40
32	A	411	LHG	O8-C23	2.74	1.41	1.33
30	3	608	CHL	C1A-CHA	2.74	1.43	1.40
32	l	102	LHG	P-O3	2.74	1.70	1.59
32	S	621	LHG	C8-C7	2.73	1.58	1.50
33	n	618	LUT	C22-C23	-2.73	1.49	1.52
30	y	608	CHL	C1A-CHA	2.73	1.43	1.40
33	13	618	LUT	C22-C23	-2.73	1.49	1.52
32	D	409	LHG	P-O6	2.73	1.70	1.59
32	d	409	LHG	P-O6	2.73	1.70	1.59
30	14	609	CHL	C2C-C3C	2.73	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	618	LHG	O8-C23	2.73	1.41	1.33
32	4	615	LHG	C8-C7	2.73	1.58	1.50
32	s	621	LHG	C8-C7	2.73	1.58	1.50
30	5	608	CHL	C1A-CHA	2.73	1.43	1.40
32	a	411	LHG	C8-C7	2.72	1.58	1.50
30	s	606	CHL	C1A-CHA	2.72	1.43	1.40
31	C	511	CLA	C1D-ND	-2.72	1.34	1.37
32	Y	617	LHG	C8-C7	2.72	1.58	1.50
32	R	619	LHG	C8-C7	2.72	1.58	1.50
30	G	607	CHL	C1A-CHA	2.72	1.43	1.40
32	Y	618	LHG	O8-C23	2.72	1.41	1.33
31	C	509	CLA	C1D-ND	-2.72	1.34	1.37
34	6	621	NEX	C1-C6	-2.72	1.50	1.54
32	a	411	LHG	O8-C23	2.72	1.41	1.33
32	C	521	LHG	C8-C7	2.72	1.58	1.50
32	D	412	LHG	C6-C5	2.72	1.59	1.50
31	A	403	CLA	C1D-ND	-2.72	1.34	1.37
32	D	412	LHG	C8-C7	2.72	1.58	1.50
31	S	611	CLA	C1D-ND	-2.72	1.34	1.37
31	r	608	CLA	C1D-ND	-2.71	1.34	1.37
30	13	606	CHL	C1A-CHA	2.71	1.43	1.40
31	16	604	CLA	C1D-ND	-2.71	1.34	1.37
30	5	606	CHL	C1A-CHA	2.71	1.43	1.40
30	14	605	CHL	C1A-CHA	2.71	1.43	1.40
30	Y	608	CHL	C1A-CHA	2.71	1.43	1.40
32	l	102	LHG	O8-C23	2.71	1.41	1.33
32	s	617	LHG	C8-C7	2.71	1.58	1.50
32	G	615	LHG	C8-C7	2.71	1.58	1.50
30	n	609	CHL	C1A-CHA	2.71	1.43	1.40
32	d	413	LHG	C6-C5	2.71	1.59	1.50
30	N	605	CHL	C1A-CHA	2.71	1.43	1.40
32	N	616	LHG	P-O6	2.71	1.70	1.59
31	R	608	CLA	C1D-ND	-2.71	1.34	1.37
30	6	609	CHL	C1A-CHA	2.70	1.43	1.40
31	S	612	CLA	CHB-C1B	-2.70	1.33	1.39
32	6	617	LHG	O8-C23	2.70	1.41	1.33
30	N	609	CHL	C1A-CHA	2.70	1.43	1.40
32	S	617	LHG	C8-C7	2.70	1.58	1.50
32	11	615	LHG	C8-C7	2.69	1.58	1.50
32	a	401	LHG	C8-C7	2.69	1.58	1.50
30	16	606	CHL	C1A-CHA	2.69	1.43	1.40
30	g	607	CHL	C1A-CHA	2.69	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	608	CHL	C1A-CHA	2.69	1.43	1.40
30	11	605	CHL	C2C-C3C	2.69	1.39	1.36
32	N	616	LHG	O8-C23	2.69	1.41	1.33
31	4	610	CLA	MG-NB	2.69	2.11	2.05
32	A	415	LHG	C8-C7	2.69	1.58	1.50
30	12	607	CHL	C2C-C3C	2.69	1.39	1.36
32	R	618	LHG	C8-C7	2.69	1.58	1.50
30	3	609	CHL	C1A-CHA	2.69	1.43	1.40
30	2	608	CHL	C1A-CHA	2.69	1.43	1.40
30	14	601	CHL	C1A-CHA	2.68	1.43	1.40
30	5	607	CHL	C1A-CHA	2.68	1.43	1.40
32	g	615	LHG	P-O6	2.68	1.69	1.59
32	1	615	LHG	C8-C7	2.68	1.58	1.50
34	3	621	NEX	C1-C6	-2.68	1.50	1.54
32	6	616	LHG	C8-C7	2.68	1.58	1.50
31	G	603	CLA	C1D-ND	-2.68	1.34	1.37
32	d	409	LHG	O8-C23	2.68	1.41	1.33
31	n	613	CLA	C1D-ND	-2.68	1.34	1.37
30	1	601	CHL	C1A-CHA	2.68	1.43	1.40
32	S	617	LHG	O8-C23	2.68	1.41	1.33
32	a	414	LHG	O8-C23	2.67	1.41	1.33
34	S	620	NEX	C1-C6	-2.67	1.50	1.54
32	g	615	LHG	O8-C23	2.67	1.41	1.33
30	R	605	CHL	C1A-CHA	2.67	1.43	1.40
32	C	521	LHG	O8-C23	2.67	1.41	1.33
32	d	413	LHG	C8-C7	2.67	1.58	1.50
31	d	402	CLA	C1D-ND	-2.67	1.34	1.37
30	1	606	CHL	C2C-C3C	2.67	1.39	1.36
30	Y	601	CHL	C1A-CHA	2.67	1.43	1.40
31	S	604	CLA	C1D-ND	-2.67	1.34	1.37
30	13	609	CHL	C1A-CHA	2.67	1.43	1.40
30	N	608	CHL	C1A-CHA	2.67	1.43	1.40
30	6	605	CHL	C2-C3	2.67	1.39	1.33
32	y	617	LHG	C8-C7	2.67	1.58	1.50
32	c	521	LHG	C8-C7	2.67	1.58	1.50
31	d	404	CLA	C1D-ND	-2.66	1.34	1.37
32	R	618	LHG	P-O6	2.66	1.69	1.59
32	n	616	LHG	O8-C23	2.66	1.41	1.33
30	2	606	CHL	C1A-CHA	2.66	1.43	1.40
32	A	413	LHG	O8-C23	2.66	1.41	1.33
32	r	618	LHG	P-O6	2.66	1.69	1.59
30	13	601	CHL	C2C-C3C	2.66	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	502	CLA	C1D-ND	-2.66	1.34	1.37
32	3	616	LHG	C8-C7	2.66	1.58	1.50
30	16	601	CHL	C2C-C3C	2.66	1.38	1.36
31	A	406	CLA	C1D-ND	-2.66	1.34	1.37
33	N	618	LUT	C22-C23	-2.66	1.49	1.52
30	4	601	CHL	C1A-CHA	2.66	1.43	1.40
32	s	617	LHG	P-O6	2.66	1.69	1.59
30	15	606	CHL	C2C-C3C	2.66	1.38	1.36
32	a	413	LHG	O8-C23	2.65	1.41	1.33
31	Y	602	CLA	C1D-ND	-2.65	1.34	1.37
30	R	607	CHL	C1A-CHA	2.65	1.43	1.40
34	s	620	NEX	C1-C6	-2.65	1.50	1.54
32	Y	618	LHG	C8-C7	2.65	1.58	1.50
30	y	601	CHL	C1A-CHA	2.65	1.43	1.40
31	s	604	CLA	C1D-ND	-2.65	1.34	1.37
32	r	619	LHG	O8-C23	2.65	1.41	1.33
30	12	601	CHL	C1A-CHA	2.65	1.43	1.40
31	c	509	CLA	C1D-ND	-2.65	1.34	1.37
31	C	507	CLA	C1D-ND	-2.65	1.34	1.37
30	6	608	CHL	C1A-CHA	2.65	1.43	1.40
30	16	609	CHL	C1A-CHA	2.64	1.43	1.40
30	2	609	CHL	MG-NB	2.64	2.11	2.05
31	b	601	CLA	C1D-ND	-2.64	1.34	1.37
32	D	409	LHG	O8-C23	2.64	1.41	1.33
31	N	602	CLA	C1D-ND	-2.64	1.34	1.37
31	Y	603	CLA	C1D-ND	-2.64	1.34	1.37
31	y	611	CLA	C1D-ND	-2.64	1.34	1.37
32	L	102	LHG	P-O6	2.64	1.69	1.59
32	l	102	LHG	P-O6	2.64	1.69	1.59
31	4	612	CLA	MG-NB	2.64	2.11	2.05
31	C	502	CLA	C1D-ND	-2.64	1.34	1.37
30	1	605	CHL	C2C-C3C	2.64	1.38	1.36
32	R	619	LHG	O8-C23	2.64	1.41	1.33
32	R	618	LHG	O8-C23	2.64	1.41	1.33
31	b	613	CLA	C1D-ND	-2.64	1.34	1.37
33	Y	621	LUT	C22-C23	-2.63	1.49	1.52
31	y	615	CLA	C1D-ND	-2.63	1.34	1.37
31	1	604	CLA	C1D-ND	-2.63	1.34	1.37
31	d	405	CLA	C1D-ND	-2.63	1.34	1.37
31	2	604	CLA	C1D-ND	-2.63	1.34	1.37
31	r	601	CLA	C1D-ND	-2.63	1.34	1.37
30	2	607	CHL	C1A-CHA	2.63	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	603	CLA	C1D-ND	-2.63	1.34	1.37
31	B	613	CLA	C1D-ND	-2.63	1.34	1.37
31	s	602	CLA	C1D-ND	-2.63	1.34	1.37
31	b	602	CLA	C1D-ND	-2.62	1.34	1.37
31	r	612	CLA	C1D-ND	-2.62	1.34	1.37
31	c	512	CLA	C1D-ND	-2.62	1.34	1.37
31	Y	615	CLA	C1D-ND	-2.62	1.34	1.37
31	b	611	CLA	C1D-ND	-2.62	1.34	1.37
30	15	607	CHL	C2C-C3C	2.62	1.38	1.36
32	r	618	LHG	C8-C7	2.62	1.58	1.50
30	3	605	CHL	C2-C3	2.62	1.39	1.33
31	b	604	CLA	C1D-ND	-2.62	1.34	1.37
30	n	608	CHL	C1A-CHA	2.62	1.43	1.40
30	5	609	CHL	MG-NB	2.62	2.11	2.05
32	n	616	LHG	C8-C7	2.62	1.58	1.50
31	4	604	CLA	C1D-ND	-2.62	1.34	1.37
31	G	614	CLA	C1D-ND	-2.62	1.34	1.37
34	16	619	NEX	C1-C6	-2.62	1.50	1.54
30	2	609	CHL	C1A-CHA	2.62	1.43	1.40
31	a	404	CLA	C1D-ND	-2.62	1.34	1.37
32	D	409	LHG	C8-C7	2.61	1.58	1.50
31	6	604	CLA	C1D-ND	-2.61	1.34	1.37
31	11	610	CLA	CHC-C1C	2.61	1.43	1.38
31	D	404	CLA	C1D-ND	-2.61	1.34	1.37
31	C	513	CLA	C1D-ND	-2.61	1.34	1.37
31	D	405	CLA	C1D-ND	-2.61	1.34	1.37
31	a	407	CLA	C1D-ND	-2.61	1.34	1.37
31	c	508	CLA	C1D-ND	-2.61	1.34	1.37
30	3	601	CHL	C1A-CHA	2.61	1.43	1.40
30	14	608	CHL	MG-NB	2.61	2.11	2.05
30	2	609	CHL	C2-C3	2.61	1.39	1.33
31	B	601	CLA	C1D-ND	-2.61	1.34	1.37
31	B	607	CLA	C1D-ND	-2.61	1.34	1.37
31	S	602	CLA	C1D-ND	-2.61	1.34	1.37
32	r	618	LHG	O8-C23	2.61	1.41	1.33
31	B	611	CLA	C1D-ND	-2.61	1.34	1.37
30	16	601	CHL	C2-C3	2.61	1.39	1.33
31	s	610	CLA	C1D-ND	-2.61	1.34	1.37
31	R	601	CLA	C1D-ND	-2.61	1.34	1.37
30	12	608	CHL	C1A-CHA	2.61	1.43	1.40
31	g	610	CLA	C1D-ND	-2.61	1.34	1.37
32	Y	616	LHG	C8-C7	2.61	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	615	LHG	C8-C7	2.61	1.58	1.50
31	y	603	CLA	C1D-ND	-2.61	1.34	1.37
30	Y	609	CHL	C2C-C3C	2.60	1.38	1.36
31	B	609	CLA	C1D-ND	-2.60	1.34	1.37
30	r	607	CHL	C1A-CHA	2.60	1.43	1.40
30	g	609	CHL	C2C-C3C	2.60	1.38	1.36
31	5	604	CLA	C1D-ND	-2.60	1.34	1.37
31	S	610	CLA	C1D-ND	-2.60	1.34	1.37
31	c	506	CLA	C1D-ND	-2.60	1.34	1.37
30	12	608	CHL	C2C-C3C	2.60	1.38	1.36
30	16	608	CHL	C1A-CHA	2.60	1.43	1.40
31	C	506	CLA	C1D-ND	-2.60	1.34	1.37
30	16	605	CHL	C1A-CHA	2.60	1.43	1.40
33	y	622	LUT	C22-C23	-2.60	1.49	1.52
30	11	609	CHL	C2-C3	2.60	1.39	1.33
31	C	504	CLA	C1D-ND	-2.60	1.34	1.37
32	d	409	LHG	C8-C7	2.60	1.58	1.50
31	a	403	CLA	C1D-ND	-2.60	1.34	1.37
32	3	617	LHG	C6-C5	2.60	1.58	1.50
33	15	614	LUT	C22-C23	-2.60	1.49	1.52
30	3	606	CHL	C2C-C3C	2.60	1.38	1.36
31	6	615	CLA	C1D-ND	-2.60	1.34	1.37
31	y	613	CLA	C1D-ND	-2.60	1.34	1.37
30	5	601	CHL	C1A-CHA	2.60	1.43	1.40
31	b	608	CLA	C1D-ND	-2.60	1.34	1.37
30	y	606	CHL	C2-C3	2.59	1.39	1.33
30	16	609	CHL	C2C-C3C	2.59	1.38	1.36
30	1	609	CHL	C2-C3	2.59	1.39	1.33
30	N	606	CHL	C1A-CHA	2.59	1.42	1.40
30	15	608	CHL	C2-C3	2.59	1.39	1.33
30	G	609	CHL	C2C-C3C	2.59	1.38	1.36
34	2	616	NEX	C8-C9	-2.59	1.43	1.50
32	d	408	LHG	C8-C7	2.59	1.58	1.50
30	6	601	CHL	C1A-CHA	2.59	1.42	1.40
34	5	616	NEX	C8-C9	-2.59	1.43	1.50
31	B	614	CLA	C1D-ND	-2.59	1.34	1.37
31	N	613	CLA	C1D-ND	-2.59	1.34	1.37
32	s	617	LHG	O8-C23	2.59	1.40	1.33
31	b	614	CLA	C1D-ND	-2.59	1.34	1.37
32	D	408	LHG	P-O6	2.59	1.69	1.59
30	15	608	CHL	C1A-CHA	2.59	1.42	1.40
31	Y	611	CLA	C1D-ND	-2.59	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	616	LHG	O8-C23	2.59	1.40	1.33
31	R	611	CLA	C1D-ND	-2.59	1.34	1.37
30	6	606	CHL	C2-C3	2.59	1.39	1.33
31	N	603	CLA	C1D-ND	-2.59	1.34	1.37
30	11	608	CHL	C2C-C3C	2.59	1.38	1.36
30	r	605	CHL	C1A-CHA	2.58	1.42	1.40
31	c	507	CLA	C1D-ND	-2.58	1.34	1.37
30	13	601	CHL	C2-C3	2.58	1.39	1.33
30	13	607	CHL	C2-C3	2.58	1.39	1.33
30	14	609	CHL	C2-C3	2.58	1.39	1.33
31	Y	613	CLA	C1D-ND	-2.58	1.34	1.37
31	C	503	CLA	C1D-ND	-2.58	1.34	1.37
31	b	609	CLA	C1D-ND	-2.58	1.34	1.37
31	Y	610	CLA	CHC-C1C	2.58	1.43	1.38
31	13	604	CLA	C1D-ND	-2.58	1.34	1.37
31	y	602	CLA	C1D-ND	-2.58	1.34	1.37
30	Y	606	CHL	C2-C3	2.58	1.39	1.33
31	A	402	CLA	C1D-ND	-2.58	1.34	1.37
31	c	513	CLA	C1D-ND	-2.58	1.34	1.37
30	S	606	CHL	C1A-CHA	2.58	1.42	1.40
31	g	604	CLA	C1D-ND	-2.58	1.34	1.37
31	s	611	CLA	C1D-ND	-2.58	1.34	1.37
31	S	605	CLA	C1D-ND	-2.58	1.34	1.37
31	y	610	CLA	CHC-C1C	2.58	1.43	1.38
31	B	604	CLA	C1D-ND	-2.58	1.34	1.37
30	16	609	CHL	C2-C3	2.58	1.39	1.33
31	n	615	CLA	C1D-ND	-2.57	1.34	1.37
32	l	102	LHG	C8-C7	2.57	1.58	1.50
30	14	606	CHL	C2C-C3C	2.57	1.38	1.36
31	g	603	CLA	C1D-ND	-2.57	1.34	1.37
30	11	601	CHL	C1A-CHA	2.57	1.42	1.40
31	B	603	CLA	C1D-ND	-2.57	1.34	1.37
34	y	624	NEX	C1-C6	-2.57	1.50	1.54
32	3	616	LHG	C6-C5	2.57	1.58	1.50
31	14	610	CLA	C1D-ND	-2.57	1.34	1.37
31	B	602	CLA	C1D-ND	-2.57	1.34	1.37
31	n	602	CLA	C1D-ND	-2.57	1.34	1.37
31	A	404	CLA	C1D-ND	-2.57	1.34	1.37
31	R	603	CLA	C1D-ND	-2.57	1.34	1.37
30	Y	609	CHL	MG-NB	2.57	2.10	2.05
30	5	601	CHL	MG-NB	2.57	2.10	2.05
31	16	610	CLA	C1D-ND	-2.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r	609	CLA	C1D-ND	-2.57	1.34	1.37
34	n	619	NEX	C1-C6	-2.57	1.50	1.54
32	6	616	LHG	C6-C5	2.57	1.58	1.50
31	r	603	CLA	C1D-ND	-2.57	1.34	1.37
30	6	606	CHL	C2C-C3C	2.57	1.38	1.36
30	4	609	CHL	C2-C3	2.57	1.39	1.33
31	B	610	CLA	C1D-ND	-2.57	1.34	1.37
33	12	614	LUT	C22-C23	-2.57	1.49	1.52
31	3	604	CLA	C1D-ND	-2.57	1.34	1.37
31	s	615	CLA	C1D-ND	-2.57	1.34	1.37
32	L	102	LHG	C8-C7	2.57	1.58	1.50
30	3	609	CHL	C2-C3	2.56	1.39	1.33
31	1	611	CLA	C1D-ND	-2.56	1.34	1.37
30	n	606	CHL	C1A-CHA	2.56	1.42	1.40
31	N	610	CLA	CHC-C1C	2.56	1.43	1.38
30	5	609	CHL	C1A-CHA	2.56	1.42	1.40
30	6	609	CHL	MG-NB	2.56	2.10	2.05
30	g	605	CHL	MG-NB	2.56	2.10	2.05
31	3	615	CLA	C1D-ND	-2.56	1.34	1.37
32	D	408	LHG	O8-C23	2.56	1.40	1.33
31	14	610	CLA	CHC-C1C	2.56	1.43	1.38
31	3	602	CLA	C1D-ND	-2.56	1.34	1.37
31	b	607	CLA	C1D-ND	-2.56	1.34	1.37
31	c	504	CLA	C1D-ND	-2.56	1.34	1.37
31	B	608	CLA	C1D-ND	-2.56	1.34	1.37
31	C	514	CLA	C1D-ND	-2.56	1.34	1.37
30	N	609	CHL	MG-NB	2.56	2.10	2.05
30	16	609	CHL	MG-NB	2.56	2.10	2.05
31	s	610	CLA	CHC-C1C	2.56	1.43	1.38
30	1	607	CHL	MG-NB	2.56	2.10	2.05
31	1	604	CLA	CHC-C1C	2.56	1.43	1.38
30	4	609	CHL	MG-NB	2.56	2.10	2.05
30	14	605	CHL	MG-NB	2.56	2.10	2.05
30	s	606	CHL	MG-NB	2.56	2.10	2.05
31	g	610	CLA	CHC-C1C	2.56	1.43	1.38
31	y	614	CLA	C1D-ND	-2.56	1.34	1.37
32	N	616	LHG	C8-C7	2.56	1.58	1.50
32	d	409	LHG	P-O3	2.56	1.69	1.59
31	G	610	CLA	CHC-C1C	2.56	1.43	1.38
30	5	609	CHL	C2C-C3C	2.56	1.38	1.36
32	6	617	LHG	C8-C7	2.56	1.58	1.50
31	g	614	CLA	C1D-ND	-2.56	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	5	607	CHL	MG-NB	2.55	2.10	2.05
30	16	607	CHL	MG-NB	2.55	2.10	2.05
32	d	408	LHG	O8-C23	2.55	1.40	1.33
31	r	603	CLA	CHC-C1C	2.55	1.43	1.38
30	g	609	CHL	MG-NB	2.55	2.10	2.05
31	11	612	CLA	MG-NB	2.55	2.10	2.05
30	s	606	CHL	C2-C3	2.55	1.38	1.33
32	y	616	LHG	O8-C23	2.55	1.40	1.33
32	y	618	LHG	C8-C7	2.55	1.58	1.50
32	A	413	LHG	P-O6	2.55	1.69	1.59
31	S	615	CLA	C1D-ND	-2.55	1.34	1.37
31	r	613	CLA	C1D-ND	-2.55	1.34	1.37
32	Y	617	LHG	C6-C5	2.55	1.58	1.50
31	3	603	CLA	C1D-ND	-2.55	1.34	1.37
33	G	616	LUT	C22-C23	-2.55	1.49	1.52
31	6	603	CLA	C1D-ND	-2.55	1.34	1.37
30	r	605	CHL	C2-C3	2.55	1.38	1.33
31	G	602	CLA	CHC-C1C	2.55	1.43	1.38
31	B	615	CLA	C1D-ND	-2.55	1.34	1.37
31	S	609	CLA	C1D-ND	-2.55	1.34	1.37
32	Y	618	LHG	C6-C5	2.55	1.58	1.50
30	13	606	CHL	MG-NB	2.55	2.10	2.05
31	C	512	CLA	C1D-ND	-2.55	1.34	1.37
30	1	609	CHL	MG-NB	2.54	2.10	2.05
31	6	613	CLA	C1D-ND	-2.54	1.34	1.37
32	y	618	LHG	C6-C5	2.54	1.58	1.50
30	3	606	CHL	C2-C3	2.54	1.38	1.33
31	r	610	CLA	C1D-ND	-2.54	1.34	1.37
30	12	606	CHL	C2C-C3C	2.54	1.38	1.36
30	G	605	CHL	MG-NB	2.54	2.10	2.05
30	14	608	CHL	C2C-C3C	2.54	1.38	1.36
31	2	603	CLA	C1D-ND	-2.54	1.34	1.37
31	11	610	CLA	C1D-ND	-2.54	1.34	1.37
31	y	612	CLA	C1D-ND	-2.54	1.34	1.37
31	b	612	CLA	CHC-C1C	2.54	1.43	1.38
30	13	608	CHL	C1A-CHA	2.54	1.42	1.40
32	y	616	LHG	C8-C7	2.54	1.58	1.50
31	n	610	CLA	C1D-ND	-2.54	1.34	1.37
31	r	614	CLA	C1D-ND	-2.54	1.34	1.37
30	6	608	CHL	MG-NB	2.54	2.10	2.05
30	3	609	CHL	MG-NB	2.54	2.10	2.05
30	12	608	CHL	C2-C3	2.54	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	614	CLA	C1D-ND	-2.54	1.34	1.37
30	12	608	CHL	MG-NB	2.54	2.10	2.05
30	16	607	CHL	C2-C3	2.54	1.38	1.33
30	2	609	CHL	C2C-C3C	2.54	1.38	1.36
31	R	612	CLA	MG-NC	2.54	2.12	2.06
31	13	612	CLA	MG-NB	2.54	2.10	2.05
31	b	610	CLA	C1D-ND	-2.54	1.34	1.37
31	y	610	CLA	C1D-ND	-2.53	1.34	1.37
30	4	608	CHL	MG-NB	2.53	2.10	2.05
31	16	610	CLA	CHC-C1C	2.53	1.43	1.38
30	5	607	CHL	C2-C3	2.53	1.38	1.33
30	13	609	CHL	C2-C3	2.53	1.38	1.33
30	16	606	CHL	C2-C3	2.53	1.38	1.33
30	S	606	CHL	C2-C3	2.53	1.38	1.33
31	b	603	CLA	C1D-ND	-2.53	1.34	1.37
30	6	609	CHL	C2-C3	2.53	1.38	1.33
31	C	508	CLA	CHC-C1C	2.53	1.43	1.38
30	3	601	CHL	C2C-C3C	2.53	1.38	1.36
32	3	617	LHG	C8-C7	2.53	1.58	1.50
31	14	612	CLA	MG-NB	2.53	2.10	2.05
30	G	609	CHL	C2-C3	2.53	1.38	1.33
30	1	608	CHL	C2C-C3C	2.53	1.38	1.36
31	N	604	CLA	C1D-ND	-2.53	1.34	1.37
31	s	614	CLA	C1D-ND	-2.53	1.34	1.37
30	y	605	CHL	C2-C3	2.53	1.38	1.33
31	R	604	CLA	C1D-ND	-2.53	1.34	1.37
30	13	607	CHL	MG-NB	2.53	2.10	2.05
31	13	610	CLA	C1D-ND	-2.53	1.34	1.37
30	11	601	CHL	C2-C3	2.53	1.38	1.33
30	3	608	CHL	MG-NB	2.53	2.10	2.05
31	G	610	CLA	C1D-ND	-2.53	1.34	1.37
30	R	605	CHL	C2-C3	2.53	1.38	1.33
30	2	606	CHL	C2C-C3C	2.53	1.38	1.36
30	y	608	CHL	MG-NB	2.53	2.10	2.05
31	r	604	CLA	C1D-ND	-2.53	1.34	1.37
34	13	619	NEX	C1-C6	-2.53	1.50	1.54
32	D	409	LHG	P-O3	2.52	1.69	1.59
31	B	612	CLA	CHC-C1C	2.52	1.43	1.38
32	a	413	LHG	P-O6	2.52	1.69	1.59
31	R	613	CLA	C1D-ND	-2.52	1.34	1.37
30	5	606	CHL	MG-NB	2.52	2.10	2.05
31	R	602	CLA	CHC-C1C	2.52	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	16	602	CLA	C1D-ND	-2.52	1.34	1.37
31	6	602	CLA	C1D-ND	-2.52	1.34	1.37
31	R	614	CLA	C1D-ND	-2.52	1.34	1.37
31	c	505	CLA	C1D-ND	-2.52	1.34	1.37
30	13	605	CHL	C2-C3	2.52	1.38	1.33
30	2	605	CHL	MG-NB	2.52	2.10	2.05
34	N	619	NEX	C1-C6	-2.52	1.50	1.54
33	r	615	LUT	C22-C23	-2.52	1.49	1.52
30	11	606	CHL	MG-NB	2.52	2.10	2.05
30	15	608	CHL	MG-NB	2.52	2.10	2.05
31	3	611	CLA	C1D-ND	-2.52	1.34	1.37
30	S	606	CHL	MG-NB	2.52	2.10	2.05
30	N	601	CHL	C2-C3	2.52	1.38	1.33
30	N	606	CHL	C2-C3	2.52	1.38	1.33
30	5	608	CHL	MG-NB	2.52	2.10	2.05
31	g	613	CLA	C1D-ND	-2.52	1.34	1.37
31	n	604	CLA	C1D-ND	-2.52	1.34	1.37
31	b	611	CLA	CHC-C1C	2.52	1.43	1.38
30	4	607	CHL	MG-NB	2.52	2.10	2.05
30	y	609	CHL	MG-NB	2.52	2.10	2.05
30	2	607	CHL	MG-NB	2.51	2.10	2.05
30	g	608	CHL	C2C-C3C	2.51	1.38	1.36
30	5	609	CHL	C2-C3	2.51	1.38	1.33
31	4	610	CLA	MG-NC	2.51	2.12	2.06
31	13	611	CLA	C1D-ND	-2.51	1.34	1.37
31	16	611	CLA	C1D-ND	-2.51	1.34	1.37
32	d	408	LHG	P-O6	2.51	1.69	1.59
30	16	606	CHL	MG-NB	2.51	2.10	2.05
30	G	608	CHL	C2C-C3C	2.51	1.38	1.36
30	5	605	CHL	MG-NB	2.51	2.10	2.05
30	n	609	CHL	MG-NB	2.51	2.10	2.05
30	2	605	CHL	C2C-C3C	2.51	1.38	1.36
31	2	612	CLA	C1D-ND	-2.51	1.34	1.37
31	12	602	CLA	C1D-ND	-2.51	1.34	1.37
31	B	616	CLA	C1D-ND	-2.51	1.34	1.37
30	N	608	CHL	MG-NB	2.51	2.10	2.05
31	3	602	CLA	CHC-C1C	2.51	1.43	1.38
30	s	606	CHL	C2C-C3C	2.51	1.38	1.36
30	g	608	CHL	C2-C3	2.51	1.38	1.33
31	r	611	CLA	C1D-ND	-2.51	1.34	1.37
31	12	602	CLA	CHC-C1C	2.51	1.43	1.38
30	16	605	CHL	C2-C3	2.51	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	605	CHL	MG-NB	2.51	2.10	2.05
31	G	611	CLA	C1D-ND	-2.51	1.34	1.37
33	5	615	LUT	C22-C23	-2.51	1.49	1.52
32	a	401	LHG	C6-C5	2.51	1.58	1.50
31	6	615	CLA	CHC-C1C	2.51	1.43	1.38
32	y	617	LHG	C6-C5	2.51	1.58	1.50
31	Y	610	CLA	C1D-ND	-2.51	1.34	1.37
32	c	521	LHG	C6-C5	2.51	1.58	1.50
31	c	514	CLA	C1D-ND	-2.51	1.34	1.37
31	n	611	CLA	C1D-ND	-2.51	1.34	1.37
31	N	611	CLA	C1D-ND	-2.50	1.34	1.37
31	s	602	CLA	CHC-C1C	2.50	1.43	1.38
31	4	611	CLA	C1D-ND	-2.50	1.34	1.37
31	2	610	CLA	CHC-C1C	2.50	1.43	1.38
31	6	610	CLA	MG-NB	2.50	2.10	2.05
31	15	609	CLA	C1D-ND	-2.50	1.34	1.37
30	6	607	CHL	C2C-C3C	2.50	1.38	1.36
31	5	610	CLA	CHC-C1C	2.50	1.43	1.38
31	Y	615	CLA	CHC-C1C	2.50	1.43	1.38
30	Y	605	CHL	C2-C3	2.50	1.38	1.33
30	11	607	CHL	MG-NB	2.50	2.10	2.05
30	g	609	CHL	C2-C3	2.50	1.38	1.33
30	S	601	CHL	MG-NB	2.50	2.10	2.05
31	s	609	CLA	C1D-ND	-2.50	1.34	1.37
30	6	601	CHL	C2-C3	2.50	1.38	1.33
31	6	614	CLA	C1D-ND	-2.50	1.34	1.37
31	c	503	CLA	C1D-ND	-2.50	1.34	1.37
30	2	607	CHL	C2-C3	2.50	1.38	1.33
32	a	414	LHG	C6-C5	2.50	1.58	1.50
30	2	608	CHL	MG-NB	2.50	2.10	2.05
31	G	602	CLA	C1D-ND	-2.50	1.34	1.37
31	N	615	CLA	C1D-ND	-2.50	1.34	1.37
31	16	612	CLA	MG-NB	2.50	2.10	2.05
30	g	606	CHL	MG-NB	2.50	2.10	2.05
31	Y	612	CLA	CHB-C1B	-2.50	1.33	1.39
30	s	601	CHL	MG-NB	2.50	2.10	2.05
31	3	610	CLA	C1D-ND	-2.50	1.34	1.37
31	G	604	CLA	C1D-ND	-2.50	1.34	1.37
30	y	609	CHL	C2-C3	2.50	1.38	1.33
30	6	607	CHL	C2-C3	2.49	1.38	1.33
31	R	609	CLA	C1D-ND	-2.49	1.34	1.37
31	d	404	CLA	CHC-C1C	2.49	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	n	601	CHL	C2-C3	2.49	1.38	1.33
31	2	613	CLA	C1D-ND	-2.49	1.34	1.37
31	4	612	CLA	CHB-C1B	-2.49	1.33	1.39
31	5	602	CLA	C1D-ND	-2.49	1.34	1.37
30	2	606	CHL	MG-NB	2.49	2.10	2.05
30	r	605	CHL	MG-NB	2.49	2.10	2.05
30	N	609	CHL	C2-C3	2.49	1.38	1.33
30	g	606	CHL	C2C-C3C	2.49	1.38	1.36
31	13	602	CLA	C1D-ND	-2.49	1.34	1.37
31	Y	614	CLA	C1D-ND	-2.49	1.34	1.37
30	s	607	CHL	MG-NB	2.49	2.10	2.05
31	4	604	CLA	CHC-C1C	2.49	1.43	1.38
31	15	609	CLA	CHC-C1C	2.49	1.43	1.38
31	5	603	CLA	C1D-ND	-2.49	1.34	1.37
31	14	604	CLA	C1D-ND	-2.49	1.34	1.37
31	16	603	CLA	C1D-ND	-2.49	1.34	1.37
30	1	605	CHL	MG-NB	2.49	2.10	2.05
31	11	604	CLA	C1D-ND	-2.49	1.34	1.37
31	Y	612	CLA	C1D-ND	-2.49	1.34	1.37
31	B	611	CLA	CHC-C1C	2.49	1.43	1.38
31	R	609	CLA	CHC-C1C	2.49	1.43	1.38
30	11	609	CHL	MG-NB	2.49	2.10	2.05
30	14	606	CHL	MG-NB	2.49	2.10	2.05
30	3	607	CHL	C2-C3	2.49	1.38	1.33
31	13	610	CLA	CHC-C1C	2.49	1.43	1.38
31	15	613	CLA	CHC-C1C	2.49	1.43	1.38
31	R	608	CLA	CHC-C1C	2.49	1.43	1.38
31	11	611	CLA	C1D-ND	-2.49	1.34	1.37
31	R	610	CLA	C1D-ND	-2.49	1.34	1.37
31	b	606	CLA	C1D-ND	-2.49	1.34	1.37
30	4	605	CHL	MG-NB	2.49	2.10	2.05
31	1	602	CLA	C1D-ND	-2.49	1.34	1.37
31	6	611	CLA	C1D-ND	-2.49	1.34	1.37
31	C	505	CLA	C1D-ND	-2.49	1.34	1.37
30	n	608	CHL	MG-NB	2.49	2.10	2.05
30	G	601	CHL	MG-NB	2.48	2.10	2.05
30	4	608	CHL	C2C-C3C	2.48	1.38	1.36
32	14	615	LHG	C6-C5	2.48	1.58	1.50
31	14	614	CLA	C1D-ND	-2.48	1.34	1.37
30	5	605	CHL	C2C-C3C	2.48	1.38	1.36
31	n	602	CLA	CHC-C1C	2.48	1.43	1.38
31	1	610	CLA	MG-NB	2.48	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Y	607	CHL	C2-C3	2.48	1.38	1.33
30	R	605	CHL	MG-NB	2.48	2.10	2.05
30	n	606	CHL	C2-C3	2.48	1.38	1.33
30	N	607	CHL	MG-NB	2.48	2.10	2.05
30	S	607	CHL	MG-NB	2.48	2.10	2.05
31	b	615	CLA	C1D-ND	-2.48	1.34	1.37
30	14	609	CHL	MG-NB	2.48	2.10	2.05
32	16	616	LHG	C6-C5	2.48	1.58	1.50
31	2	602	CLA	C1D-ND	-2.48	1.34	1.37
31	Y	604	CLA	C1D-ND	-2.48	1.34	1.37
31	3	612	CLA	C1D-ND	-2.48	1.34	1.37
30	2	605	CHL	CBA-CGA	2.48	1.56	1.50
34	R	617	NEX	C1-C6	-2.48	1.50	1.54
31	B	605	CLA	C1D-ND	-2.48	1.34	1.37
30	4	609	CHL	C1A-CHA	2.48	1.42	1.40
30	6	607	CHL	MG-NB	2.48	2.10	2.05
30	13	608	CHL	MG-NB	2.48	2.10	2.05
30	G	606	CHL	MG-NB	2.48	2.10	2.05
31	2	604	CLA	CHC-C1C	2.48	1.43	1.38
31	Y	602	CLA	CHC-C1C	2.48	1.43	1.38
31	n	610	CLA	CHC-C1C	2.48	1.43	1.38
30	13	605	CHL	MG-NB	2.48	2.10	2.05
31	11	613	CLA	C1D-ND	-2.48	1.34	1.37
30	G	608	CHL	C2-C3	2.48	1.38	1.33
31	s	612	CLA	CHB-C1B	-2.47	1.33	1.39
31	3	614	CLA	C1D-ND	-2.47	1.34	1.37
30	R	606	CHL	C2-C3	2.47	1.38	1.33
30	14	601	CHL	MG-NB	2.47	2.10	2.05
32	13	616	LHG	C6-C5	2.47	1.58	1.50
31	G	613	CLA	C1D-ND	-2.47	1.34	1.37
31	g	602	CLA	C1D-ND	-2.47	1.34	1.37
30	1	609	CHL	C1A-CHA	2.47	1.42	1.40
31	12	611	CLA	C1D-ND	-2.47	1.34	1.37
31	g	602	CLA	CHC-C1C	2.47	1.43	1.38
31	r	609	CLA	CHC-C1C	2.47	1.43	1.38
30	3	605	CHL	MG-NB	2.47	2.10	2.05
31	r	608	CLA	CHC-C1C	2.47	1.43	1.38
31	6	612	CLA	C1D-ND	-2.47	1.34	1.37
31	3	615	CLA	CHC-C1C	2.47	1.43	1.38
31	n	615	CLA	CHC-C1C	2.47	1.43	1.38
31	y	602	CLA	CHC-C1C	2.47	1.43	1.38
30	13	601	CHL	MG-NB	2.47	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	610	CLA	C1D-ND	-2.47	1.34	1.37
30	n	606	CHL	C2C-C3C	2.47	1.38	1.36
31	12	611	CLA	MG-NB	2.47	2.10	2.05
31	b	605	CLA	C1D-ND	-2.47	1.34	1.37
30	16	608	CHL	MG-NB	2.47	2.10	2.05
30	Y	608	CHL	MG-NB	2.47	2.10	2.05
31	4	613	CLA	CHC-C1C	2.47	1.43	1.38
31	N	610	CLA	C1D-ND	-2.47	1.34	1.37
30	G	609	CHL	MG-NB	2.47	2.10	2.05
31	C	510	CLA	CHC-C1C	2.47	1.43	1.38
31	15	612	CLA	C1D-ND	-2.47	1.34	1.37
31	12	613	CLA	MG-NB	2.47	2.10	2.05
30	3	606	CHL	MG-NB	2.46	2.10	2.05
31	N	615	CLA	CHC-C1C	2.46	1.43	1.38
30	r	606	CHL	C2-C3	2.46	1.38	1.33
30	5	605	CHL	CBA-CGA	2.46	1.56	1.50
30	4	605	CHL	CBA-CGA	2.46	1.56	1.50
30	s	601	CHL	C2C-C3C	2.46	1.38	1.36
31	N	614	CLA	C1D-ND	-2.46	1.34	1.37
30	12	606	CHL	MG-NB	2.46	2.10	2.05
33	g	616	LUT	C22-C23	-2.46	1.49	1.52
32	A	415	LHG	C6-C5	2.46	1.58	1.50
30	n	609	CHL	C2-C3	2.46	1.38	1.33
31	5	604	CLA	CHC-C1C	2.46	1.43	1.38
31	14	602	CLA	CHC-C1C	2.46	1.43	1.38
31	5	610	CLA	C1D-ND	-2.46	1.34	1.37
30	N	606	CHL	C2C-C3C	2.46	1.38	1.36
30	3	601	CHL	C2-C3	2.46	1.38	1.33
31	12	604	CLA	C1D-ND	-2.46	1.34	1.37
30	6	601	CHL	MG-NB	2.46	2.10	2.05
31	1	612	CLA	MG-NB	2.46	2.10	2.05
31	4	602	CLA	C1D-ND	-2.46	1.34	1.37
31	4	613	CLA	C1D-ND	-2.46	1.34	1.37
30	y	607	CHL	C2-C3	2.46	1.38	1.33
30	6	601	CHL	C2C-C3C	2.46	1.38	1.36
30	6	606	CHL	MG-NB	2.46	2.10	2.05
31	b	616	CLA	C1D-ND	-2.46	1.34	1.37
30	g	601	CHL	MG-NB	2.46	2.10	2.05
31	6	610	CLA	C1D-ND	-2.46	1.34	1.37
31	c	510	CLA	CHC-C1C	2.46	1.43	1.38
30	14	607	CHL	MG-NB	2.46	2.10	2.05
31	15	611	CLA	MG-NB	2.46	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	n	607	CHL	MG-NB	2.46	2.10	2.05
32	16	616	LHG	C24-C23	2.45	1.57	1.50
32	1	615	LHG	C6-C5	2.45	1.58	1.50
30	Y	609	CHL	C2-C3	2.45	1.38	1.33
31	12	609	CLA	C1D-ND	-2.45	1.34	1.37
30	G	607	CHL	MG-NB	2.45	2.10	2.05
30	g	607	CHL	MG-NB	2.45	2.10	2.05
31	15	613	CLA	C1D-ND	-2.45	1.34	1.37
31	2	611	CLA	CHC-C1C	2.45	1.43	1.38
31	6	612	CLA	CHB-C1B	-2.45	1.33	1.39
31	2	611	CLA	C1D-ND	-2.45	1.34	1.37
31	g	611	CLA	C1D-ND	-2.45	1.34	1.37
32	A	411	LHG	C6-C5	2.45	1.58	1.50
30	14	601	CHL	C2-C3	2.45	1.38	1.33
30	6	605	CHL	MG-NB	2.45	2.10	2.05
31	1	610	CLA	C1D-ND	-2.45	1.34	1.37
31	6	602	CLA	CHC-C1C	2.45	1.43	1.38
30	3	607	CHL	C2C-C3C	2.45	1.38	1.36
32	r	621	LHG	C6-C5	2.45	1.58	1.50
31	N	612	CLA	C1D-ND	-2.45	1.34	1.37
32	a	413	LHG	C6-C5	2.45	1.58	1.50
30	16	605	CHL	MG-NB	2.45	2.10	2.05
31	15	602	CLA	CHC-C1C	2.45	1.43	1.38
30	1	608	CHL	MG-NB	2.45	2.10	2.05
31	13	612	CLA	CHB-C1B	-2.45	1.33	1.39
31	4	614	CLA	C1D-ND	-2.45	1.34	1.37
31	N	602	CLA	CHC-C1C	2.45	1.43	1.38
30	G	601	CHL	C2-C3	2.45	1.38	1.33
31	y	604	CLA	C1D-ND	-2.45	1.34	1.37
30	12	601	CHL	MG-NB	2.44	2.10	2.05
30	n	605	CHL	C2-C3	2.44	1.38	1.33
30	n	609	CHL	C2C-C3C	2.44	1.38	1.36
31	y	615	CLA	CHC-C1C	2.44	1.43	1.38
31	6	612	CLA	MG-NB	2.44	2.10	2.05
32	A	414	LHG	C6-C5	2.44	1.58	1.50
30	5	606	CHL	C2C-C3C	2.44	1.38	1.36
31	r	601	CLA	CHC-C1C	2.44	1.43	1.38
30	1	605	CHL	CBA-CGA	2.44	1.56	1.50
31	r	612	CLA	CHC-C1C	2.44	1.43	1.38
31	B	614	CLA	CHC-C1C	2.44	1.43	1.38
30	N	601	CHL	MG-NB	2.44	2.10	2.05
31	b	615	CLA	MG-NB	2.44	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	13	606	CHL	C2-C3	2.44	1.38	1.33
31	4	603	CLA	C1D-ND	-2.44	1.34	1.37
31	16	614	CLA	C1D-ND	-2.44	1.34	1.37
32	C	521	LHG	C6-C5	2.44	1.58	1.50
30	S	601	CHL	CBA-CGA	2.44	1.56	1.50
30	n	605	CHL	MG-NB	2.44	2.10	2.05
31	2	603	CLA	CHC-C1C	2.44	1.43	1.38
31	C	512	CLA	CHC-C1C	2.44	1.43	1.38
31	y	612	CLA	MG-NC	2.44	2.12	2.06
30	2	606	CHL	CBA-CGA	2.44	1.56	1.50
31	1	613	CLA	C1D-ND	-2.44	1.34	1.37
31	s	613	CLA	C1D-ND	-2.44	1.34	1.37
31	3	612	CLA	CHB-C1B	-2.44	1.34	1.39
31	11	604	CLA	CHC-C1C	2.44	1.43	1.38
31	r	604	CLA	CHC-C1C	2.44	1.43	1.38
31	y	612	CLA	CHB-C1B	-2.44	1.34	1.39
30	5	601	CHL	C2C-C3C	2.44	1.38	1.36
31	C	514	CLA	CHC-C1C	2.44	1.43	1.38
31	3	613	CLA	C1D-ND	-2.44	1.34	1.37
31	14	611	CLA	C1D-ND	-2.44	1.34	1.37
30	s	608	CHL	MG-NB	2.44	2.10	2.05
30	Y	605	CHL	MG-NB	2.44	2.10	2.05
31	16	602	CLA	CHC-C1C	2.44	1.43	1.38
31	S	613	CLA	C1D-ND	-2.44	1.34	1.37
31	B	615	CLA	CHB-C1B	-2.43	1.34	1.39
30	r	607	CHL	MG-NB	2.43	2.10	2.05
31	C	511	CLA	CHC-C1C	2.43	1.43	1.38
31	1	603	CLA	C1D-ND	-2.43	1.34	1.37
31	14	602	CLA	C1D-ND	-2.43	1.34	1.37
31	15	611	CLA	C1D-ND	-2.43	1.34	1.37
31	G	612	CLA	C1D-ND	-2.43	1.34	1.37
31	B	615	CLA	MG-NB	2.43	2.10	2.05
31	B	602	CLA	CHC-C1C	2.43	1.43	1.38
30	S	601	CHL	C2C-C3C	2.43	1.38	1.36
31	s	605	CLA	C1D-ND	-2.43	1.34	1.37
31	1	613	CLA	CHC-C1C	2.43	1.43	1.38
31	b	614	CLA	CHC-C1C	2.43	1.43	1.38
30	S	606	CHL	C2C-C3C	2.43	1.38	1.36
30	3	601	CHL	MG-NB	2.43	2.10	2.05
30	5	606	CHL	CBA-CGA	2.43	1.56	1.50
30	s	601	CHL	CBA-CGA	2.43	1.56	1.50
31	b	615	CLA	CHB-C1B	-2.43	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	601	CLA	CHC-C1C	2.43	1.43	1.38
30	3	607	CHL	MG-NB	2.43	2.10	2.05
31	Y	612	CLA	MG-NB	2.43	2.10	2.05
31	11	602	CLA	C1D-ND	-2.43	1.34	1.37
31	15	612	CLA	CHC-C1C	2.43	1.43	1.38
31	B	605	CLA	MG-NB	2.43	2.10	2.05
30	11	601	CHL	MG-NB	2.43	2.10	2.05
31	b	602	CLA	CHC-C1C	2.43	1.43	1.38
30	13	609	CHL	C2C-C3C	2.43	1.38	1.36
31	14	613	CLA	C1D-ND	-2.43	1.34	1.37
31	c	512	CLA	CHC-C1C	2.43	1.43	1.38
33	2	615	LUT	C22-C23	-2.43	1.49	1.52
31	13	603	CLA	C1D-ND	-2.43	1.34	1.37
30	16	601	CHL	MG-NB	2.43	2.10	2.05
30	12	605	CHL	CBA-CGA	2.43	1.56	1.50
31	2	613	CLA	CHC-C1C	2.43	1.43	1.38
32	11	615	LHG	C6-C5	2.43	1.58	1.50
31	s	612	CLA	C1D-ND	-2.43	1.34	1.37
30	15	601	CHL	MG-NB	2.43	2.10	2.05
30	G	608	CHL	MG-NB	2.43	2.10	2.05
30	y	601	CHL	MG-NB	2.42	2.10	2.05
31	B	606	CLA	C1D-ND	-2.42	1.34	1.37
31	n	612	CLA	C1D-ND	-2.42	1.34	1.37
31	b	608	CLA	CHC-C1C	2.42	1.43	1.38
31	5	613	CLA	C1D-ND	-2.42	1.34	1.37
32	Y	616	LHG	P-O6	2.42	1.68	1.59
30	16	606	CHL	C2C-C3C	2.42	1.38	1.36
31	14	613	CLA	CHC-C1C	2.42	1.43	1.38
31	d	402	CLA	CHC-C1C	2.42	1.43	1.38
31	3	604	CLA	CHC-C1C	2.42	1.43	1.38
31	11	602	CLA	CHC-C1C	2.42	1.43	1.38
31	C	509	CLA	CHC-C1C	2.42	1.43	1.38
31	a	404	CLA	CHC-C1C	2.42	1.43	1.38
31	4	612	CLA	MG-NC	2.42	2.12	2.06
31	A	402	CLA	CHC-C1C	2.42	1.43	1.38
31	S	610	CLA	CHC-C1C	2.42	1.43	1.38
31	c	509	CLA	CHC-C1C	2.42	1.43	1.38
30	N	607	CHL	C2-C3	2.42	1.38	1.33
31	11	614	CLA	C1D-ND	-2.42	1.34	1.37
31	g	612	CLA	C1D-ND	-2.42	1.34	1.37
30	N	606	CHL	MG-NB	2.42	2.10	2.05
31	g	613	CLA	CHC-C1C	2.42	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	615	LHG	C6-C5	2.42	1.58	1.50
31	B	603	CLA	CHB-C1B	-2.42	1.34	1.39
31	R	604	CLA	CHC-C1C	2.42	1.43	1.38
31	B	606	CLA	CHB-C1B	-2.42	1.34	1.39
32	a	411	LHG	C6-C5	2.42	1.58	1.50
30	G	606	CHL	C2C-C3C	2.42	1.38	1.36
30	N	605	CHL	C2-C3	2.42	1.38	1.33
31	5	611	CLA	C1D-ND	-2.42	1.34	1.37
30	11	607	CHL	CBA-CGA	2.42	1.56	1.50
30	Y	607	CHL	MG-NB	2.42	2.10	2.05
31	G	613	CLA	CHC-C1C	2.42	1.43	1.38
30	11	606	CHL	C2C-C3C	2.42	1.38	1.36
31	S	602	CLA	CHC-C1C	2.42	1.43	1.38
31	A	403	CLA	CHC-C1C	2.42	1.43	1.38
31	c	514	CLA	CHC-C1C	2.42	1.43	1.38
31	13	614	CLA	MG-NB	2.42	2.10	2.05
31	c	502	CLA	CHC-C1C	2.42	1.43	1.38
31	12	611	CLA	CHB-C1B	-2.41	1.34	1.39
31	y	612	CLA	MG-NB	2.41	2.10	2.05
30	15	605	CHL	CBA-CGA	2.41	1.56	1.50
31	b	606	CLA	CHB-C1B	-2.41	1.34	1.39
31	B	606	CLA	CHC-C1C	2.41	1.43	1.38
31	13	614	CLA	C1D-ND	-2.41	1.34	1.37
30	15	606	CHL	MG-NB	2.41	2.10	2.05
30	r	606	CHL	MG-NB	2.41	2.10	2.05
31	y	614	CLA	MG-NB	2.41	2.10	2.05
31	5	613	CLA	CHC-C1C	2.41	1.43	1.38
30	1	601	CHL	C2-C3	2.41	1.38	1.33
32	13	616	LHG	C24-C23	2.41	1.57	1.50
33	R	615	LUT	C22-C23	-2.41	1.49	1.52
31	11	611	CLA	CHC-C1C	2.41	1.43	1.38
30	11	607	CHL	C2C-C3C	2.41	1.38	1.36
32	a	401	LHG	C24-C23	2.41	1.57	1.50
32	y	616	LHG	P-O6	2.41	1.68	1.59
31	b	606	CLA	CHC-C1C	2.41	1.43	1.38
32	r	619	LHG	C24-C23	2.41	1.57	1.50
31	b	603	CLA	CHB-C1B	-2.41	1.34	1.39
31	4	602	CLA	CHC-C1C	2.41	1.43	1.38
31	13	602	CLA	CHC-C1C	2.41	1.43	1.38
32	D	412	LHG	C24-C23	2.41	1.57	1.50
32	Y	618	LHG	C24-C23	2.41	1.57	1.50
30	4	609	CHL	C2C-C3C	2.41	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	11	603	CLA	C1D-ND	-2.41	1.34	1.37
31	15	604	CLA	C1D-ND	-2.40	1.34	1.37
30	g	608	CHL	MG-NB	2.40	2.10	2.05
32	6	617	LHG	C6-C5	2.40	1.58	1.50
32	s	621	LHG	C6-C5	2.40	1.58	1.50
31	11	614	CLA	CHC-C1C	2.40	1.43	1.38
30	R	606	CHL	MG-NB	2.40	2.10	2.05
31	15	611	CLA	CHB-C1B	-2.40	1.34	1.39
30	15	608	CHL	C2C-C3C	2.40	1.38	1.36
31	S	605	CLA	CHC-C1C	2.40	1.43	1.38
31	11	613	CLA	CHC-C1C	2.40	1.43	1.38
31	s	611	CLA	CHC-C1C	2.40	1.43	1.38
31	12	613	CLA	C1D-ND	-2.40	1.34	1.37
30	1	609	CHL	C2C-C3C	2.40	1.38	1.36
31	14	614	CLA	CHC-C1C	2.40	1.43	1.38
30	S	608	CHL	MG-NB	2.40	2.10	2.05
30	n	606	CHL	MG-NB	2.40	2.10	2.05
31	12	612	CLA	C1D-ND	-2.40	1.34	1.37
32	A	413	LHG	C6-C5	2.40	1.58	1.50
30	g	601	CHL	C1A-CHA	2.40	1.42	1.40
31	s	605	CLA	CHC-C1C	2.40	1.43	1.38
31	y	613	CLA	CHC-C1C	2.40	1.43	1.38
31	A	406	CLA	CHC-C1C	2.40	1.43	1.38
32	S	621	LHG	C6-C5	2.40	1.58	1.50
31	C	502	CLA	CHC-C1C	2.40	1.43	1.38
31	r	610	CLA	CHC-C1C	2.40	1.43	1.38
31	S	613	CLA	CHC-C1C	2.40	1.43	1.38
32	A	415	LHG	C24-C23	2.40	1.57	1.50
31	15	603	CLA	C1D-ND	-2.40	1.34	1.37
31	r	602	CLA	CHC-C1C	2.40	1.43	1.38
31	R	611	CLA	CHC-C1C	2.40	1.43	1.38
30	y	607	CHL	MG-NB	2.40	2.10	2.05
30	13	606	CHL	C2C-C3C	2.40	1.38	1.36
31	C	512	CLA	CHB-C1B	-2.40	1.34	1.39
31	n	611	CLA	CHC-C1C	2.39	1.43	1.38
31	G	612	CLA	CHB-C1B	-2.39	1.34	1.39
31	Y	613	CLA	CHC-C1C	2.39	1.43	1.38
31	s	604	CLA	CHC-C1C	2.39	1.43	1.38
31	n	614	CLA	C1D-ND	-2.39	1.34	1.37
31	c	509	CLA	CHB-C1B	-2.39	1.34	1.39
31	12	603	CLA	C1D-ND	-2.39	1.34	1.37
30	12	607	CHL	MG-NB	2.39	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	r	617	NEX	C1-C6	-2.39	1.50	1.54
31	1	602	CLA	CHC-C1C	2.39	1.43	1.38
31	c	511	CLA	CHC-C1C	2.39	1.43	1.38
32	y	618	LHG	C24-C23	2.39	1.57	1.50
30	n	601	CHL	MG-NB	2.39	2.10	2.05
31	B	603	CLA	MG-NB	2.39	2.10	2.05
31	a	403	CLA	CHC-C1C	2.39	1.43	1.38
30	1	606	CHL	MG-NB	2.39	2.10	2.05
30	Y	601	CHL	MG-NB	2.39	2.10	2.05
31	Y	614	CLA	MG-NB	2.39	2.10	2.05
31	12	612	CLA	CHC-C1C	2.39	1.43	1.38
31	16	615	CLA	CHC-C1C	2.39	1.43	1.38
32	r	619	LHG	C6-C5	2.39	1.58	1.50
31	6	604	CLA	CHC-C1C	2.39	1.43	1.38
31	g	612	CLA	MG-NB	2.39	2.10	2.05
31	16	613	CLA	C1D-ND	-2.39	1.34	1.37
31	16	611	CLA	CHC-C1C	2.39	1.43	1.38
31	14	611	CLA	CHC-C1C	2.39	1.43	1.38
31	A	404	CLA	CHC-C1C	2.39	1.43	1.38
31	5	612	CLA	C1D-ND	-2.39	1.34	1.37
31	3	610	CLA	CHC-C1C	2.38	1.43	1.38
31	n	604	CLA	CHC-C1C	2.38	1.43	1.38
31	r	603	CLA	CHB-C1B	-2.38	1.34	1.39
31	S	609	CLA	CHC-C1C	2.38	1.43	1.38
30	g	601	CHL	C2-C3	2.38	1.38	1.33
30	15	607	CHL	MG-NB	2.38	2.10	2.05
32	r	621	LHG	C24-C23	2.38	1.57	1.50
31	15	602	CLA	C1D-ND	-2.38	1.34	1.37
31	4	610	CLA	CHC-C1C	2.38	1.43	1.38
31	12	609	CLA	CHC-C1C	2.38	1.43	1.38
31	g	614	CLA	CHC-C1C	2.38	1.43	1.38
30	14	607	CHL	C2C-C3C	2.38	1.38	1.36
31	s	603	CLA	C1D-ND	-2.38	1.34	1.37
31	C	504	CLA	CHC-C1C	2.38	1.43	1.38
31	5	603	CLA	CHC-C1C	2.38	1.43	1.38
31	Y	612	CLA	MG-NC	2.38	2.11	2.06
31	C	506	CLA	MG-NB	2.38	2.10	2.05
32	R	621	LHG	C6-C5	2.38	1.58	1.50
31	g	612	CLA	CHB-C1B	-2.38	1.34	1.39
31	G	612	CLA	MG-NB	2.38	2.10	2.05
31	11	603	CLA	MG-NB	2.38	2.10	2.05
30	14	605	CHL	C2C-C3C	2.38	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	521	LHG	C24-C23	2.38	1.57	1.50
31	11	612	CLA	MG-NC	2.38	2.11	2.06
31	3	614	CLA	CHC-C1C	2.38	1.43	1.38
32	D	408	LHG	C6-C5	2.38	1.58	1.50
32	d	413	LHG	C24-C23	2.38	1.57	1.50
31	14	612	CLA	CHB-C1B	-2.38	1.34	1.39
31	G	614	CLA	CHC-C1C	2.38	1.43	1.38
30	y	608	CHL	C2C-C3C	2.38	1.38	1.36
31	c	506	CLA	MG-NB	2.37	2.10	2.05
32	4	615	LHG	C6-C5	2.37	1.58	1.50
30	11	601	CHL	C2C-C3C	2.37	1.38	1.36
31	a	407	CLA	CHC-C1C	2.37	1.43	1.38
30	4	601	CHL	C2-C3	2.37	1.38	1.33
31	13	612	CLA	C1D-ND	-2.37	1.34	1.37
31	4	614	CLA	CHC-C1C	2.37	1.43	1.38
31	Y	603	CLA	CHC-C1C	2.37	1.43	1.38
31	g	604	CLA	CHB-C1B	-2.37	1.34	1.39
31	b	605	CLA	MG-NB	2.37	2.10	2.05
31	c	513	CLA	MG-NB	2.37	2.10	2.05
31	B	604	CLA	CHC-C1C	2.37	1.43	1.38
31	c	505	CLA	CHC-C1C	2.37	1.43	1.38
31	1	614	CLA	CHC-C1C	2.37	1.43	1.38
31	N	611	CLA	CHC-C1C	2.37	1.43	1.38
31	N	612	CLA	MG-NB	2.37	2.10	2.05
31	4	611	CLA	CHC-C1C	2.37	1.43	1.38
31	3	604	CLA	CHB-C1B	-2.37	1.34	1.39
31	16	612	CLA	CHB-C1B	-2.37	1.34	1.39
30	4	606	CHL	C2C-C3C	2.37	1.38	1.36
31	s	609	CLA	MG-NB	2.37	2.10	2.05
31	16	612	CLA	MG-NC	2.37	2.11	2.06
30	S	608	CHL	C2C-C3C	2.37	1.38	1.36
30	R	607	CHL	MG-NB	2.37	2.10	2.05
31	c	508	CLA	CHC-C1C	2.37	1.43	1.38
31	s	615	CLA	CHC-C1C	2.37	1.43	1.38
31	y	603	CLA	CHC-C1C	2.37	1.43	1.38
31	C	506	CLA	CHB-C1B	-2.37	1.34	1.39
30	1	601	CHL	MG-NB	2.37	2.10	2.05
31	15	612	CLA	MG-NB	2.37	2.10	2.05
31	12	604	CLA	CHC-C1C	2.36	1.43	1.38
31	S	604	CLA	CHC-C1C	2.36	1.43	1.38
32	d	409	LHG	C6-C5	2.36	1.58	1.50
31	2	612	CLA	CHC-C1C	2.36	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	505	CLA	CHB-C1B	-2.36	1.34	1.39
31	B	608	CLA	CHC-C1C	2.36	1.43	1.38
31	16	614	CLA	MG-NB	2.36	2.10	2.05
31	b	602	CLA	MG-NB	2.36	2.10	2.05
31	B	608	CLA	CHB-C1B	-2.36	1.34	1.39
33	N	617	LUT	C22-C23	-2.36	1.50	1.52
31	s	603	CLA	MG-NB	2.36	2.10	2.05
31	y	604	CLA	CHC-C1C	2.36	1.43	1.38
31	5	602	CLA	CHC-C1C	2.36	1.43	1.38
31	s	614	CLA	CHC-C1C	2.36	1.43	1.38
31	b	607	CLA	CHB-C1B	-2.36	1.34	1.39
31	n	604	CLA	CHB-C1B	-2.36	1.34	1.39
32	L	102	LHG	C6-C5	2.36	1.58	1.50
31	6	614	CLA	MG-NB	2.36	2.10	2.05
31	11	612	CLA	CHB-C1B	-2.36	1.34	1.39
31	C	505	CLA	CHC-C1C	2.36	1.43	1.38
31	13	612	CLA	MG-NC	2.36	2.11	2.06
31	14	603	CLA	MG-NB	2.36	2.10	2.05
31	2	612	CLA	CHB-C1B	-2.36	1.34	1.39
31	5	611	CLA	CHB-C1B	-2.36	1.34	1.39
31	N	604	CLA	CHC-C1C	2.36	1.43	1.38
31	C	508	CLA	C1B-NB	-2.36	1.34	1.37
31	B	607	CLA	CHB-C1B	-2.36	1.34	1.39
31	y	603	CLA	CHB-C1B	-2.36	1.34	1.39
31	c	504	CLA	CHC-C1C	2.35	1.43	1.38
30	G	601	CHL	C1A-CHA	2.35	1.42	1.40
31	2	602	CLA	CHC-C1C	2.35	1.43	1.38
33	1	617	LUT	C22-C23	-2.35	1.50	1.52
31	b	605	CLA	CHB-C1B	-2.35	1.34	1.39
31	14	603	CLA	CHC-C1C	2.35	1.43	1.38
31	6	610	CLA	CHC-C1C	2.35	1.43	1.38
31	a	403	CLA	CHB-C1B	-2.35	1.34	1.39
31	4	603	CLA	CHC-C1C	2.35	1.43	1.38
31	1	614	CLA	C1D-ND	-2.35	1.34	1.37
31	c	506	CLA	CHB-C1B	-2.35	1.34	1.39
31	b	605	CLA	CHC-C1C	2.35	1.43	1.38
31	G	604	CLA	CHB-C1B	-2.35	1.34	1.39
32	S	621	LHG	C4-C5	2.35	1.58	1.50
31	14	603	CLA	C1D-ND	-2.35	1.34	1.37
31	3	613	CLA	CHC-C1C	2.35	1.43	1.38
31	b	603	CLA	CHC-C1C	2.35	1.43	1.38
31	5	612	CLA	MG-NB	2.35	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	509	CLA	CHB-C1B	-2.35	1.34	1.39
31	1	611	CLA	CHC-C1C	2.35	1.43	1.38
32	y	617	LHG	C4-C5	2.35	1.58	1.50
31	B	605	CLA	CHB-C1B	-2.35	1.34	1.39
31	N	604	CLA	CHB-C1B	-2.35	1.34	1.39
30	s	608	CHL	C2C-C3C	2.35	1.38	1.36
31	n	614	CLA	MG-NB	2.35	2.10	2.05
31	11	612	CLA	C1D-ND	-2.35	1.34	1.37
30	4	607	CHL	C2C-C3C	2.35	1.38	1.36
31	15	604	CLA	CHC-C1C	2.35	1.43	1.38
31	c	512	CLA	CHB-C1B	-2.35	1.34	1.39
31	16	615	CLA	C1D-ND	-2.35	1.34	1.37
31	11	614	CLA	MG-NB	2.35	2.10	2.05
31	b	603	CLA	MG-NB	2.35	2.10	2.05
31	12	610	CLA	C1D-ND	-2.35	1.34	1.37
31	s	613	CLA	CHC-C1C	2.35	1.43	1.38
31	12	604	CLA	MG-NB	2.35	2.10	2.05
31	b	608	CLA	CHB-C1B	-2.34	1.34	1.39
31	14	612	CLA	C1D-ND	-2.34	1.34	1.37
31	c	508	CLA	CHB-C1B	-2.34	1.34	1.39
30	y	601	CHL	C2-C3	2.34	1.38	1.33
31	A	402	CLA	CHB-C1B	-2.34	1.34	1.39
31	B	604	CLA	CHB-C1B	-2.34	1.34	1.39
31	r	610	CLA	CHB-C1B	-2.34	1.34	1.39
31	N	613	CLA	CHC-C1C	2.34	1.43	1.38
32	A	415	LHG	C4-C5	2.34	1.58	1.50
32	D	409	LHG	C6-C5	2.34	1.58	1.50
31	11	603	CLA	CHC-C1C	2.34	1.43	1.38
31	15	611	CLA	CHC-C1C	2.34	1.43	1.38
31	s	609	CLA	CHC-C1C	2.34	1.43	1.38
31	1	610	CLA	MG-NC	2.34	2.11	2.06
31	14	604	CLA	CHC-C1C	2.34	1.43	1.38
31	S	615	CLA	CHC-C1C	2.34	1.43	1.38
32	d	408	LHG	C6-C5	2.34	1.58	1.50
31	13	604	CLA	CHB-C1B	-2.34	1.34	1.39
31	13	604	CLA	CHC-C1C	2.34	1.43	1.38
31	B	616	CLA	CHB-C1B	-2.34	1.34	1.39
30	11	608	CHL	MG-NB	2.34	2.10	2.05
31	16	604	CLA	CHC-C1C	2.34	1.43	1.38
30	15	601	CHL	C2C-C3C	2.34	1.38	1.36
34	g	618	NEX	C1-C6	-2.34	1.50	1.54
31	1	612	CLA	CHB-C1B	-2.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	612	CLA	MG-NB	2.34	2.10	2.05
32	R	619	LHG	C24-C23	2.34	1.57	1.50
31	12	613	CLA	CHC-C1C	2.34	1.43	1.38
30	n	607	CHL	C2-C3	2.34	1.38	1.33
30	s	607	CHL	C2C-C3C	2.34	1.38	1.36
31	B	603	CLA	CHC-C1C	2.34	1.43	1.38
31	15	613	CLA	MG-NB	2.34	2.10	2.05
31	d	405	CLA	CHC-C1C	2.34	1.43	1.38
31	15	604	CLA	MG-NB	2.34	2.10	2.05
31	Y	611	CLA	MG-NB	2.34	2.10	2.05
31	12	611	CLA	CHC-C1C	2.33	1.43	1.38
32	l	102	LHG	C6-C5	2.33	1.58	1.50
31	Y	604	CLA	CHC-C1C	2.33	1.43	1.38
32	g	615	LHG	C6-C5	2.33	1.58	1.50
32	s	621	LHG	C4-C5	2.33	1.58	1.50
30	g	607	CHL	C2C-C3C	2.33	1.38	1.36
31	15	602	CLA	MG-NB	2.33	2.10	2.05
31	R	613	CLA	CHC-C1C	2.33	1.43	1.38
30	12	601	CHL	C2C-C3C	2.33	1.38	1.36
31	s	614	CLA	MG-NB	2.33	2.10	2.05
30	Y	601	CHL	C2-C3	2.33	1.38	1.33
31	G	604	CLA	CHC-C1C	2.33	1.43	1.38
30	14	601	CHL	C2C-C3C	2.33	1.38	1.36
31	5	611	CLA	CHC-C1C	2.33	1.43	1.38
31	B	605	CLA	CHC-C1C	2.33	1.43	1.38
31	D	405	CLA	CHC-C1C	2.33	1.43	1.38
31	S	611	CLA	CHC-C1C	2.33	1.43	1.38
33	4	617	LUT	C22-C23	-2.33	1.50	1.52
31	4	614	CLA	MG-NB	2.33	2.10	2.05
31	g	604	CLA	CHC-C1C	2.33	1.43	1.38
31	d	404	CLA	CHB-C1B	-2.33	1.34	1.39
31	r	611	CLA	CHB-C1B	-2.33	1.34	1.39
31	c	505	CLA	CHB-C1B	-2.33	1.34	1.39
31	y	604	CLA	CHB-C1B	-2.33	1.34	1.39
31	S	603	CLA	C1D-ND	-2.33	1.34	1.37
31	12	610	CLA	MG-NB	2.33	2.10	2.05
31	14	611	CLA	MG-NB	2.33	2.10	2.05
31	1	612	CLA	C1D-ND	-2.33	1.34	1.37
31	16	612	CLA	C1D-ND	-2.33	1.34	1.37
31	2	613	CLA	MG-NB	2.33	2.10	2.05
31	s	612	CLA	MG-NC	2.33	2.11	2.06
31	6	614	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	616	LHG	C6-C5	2.33	1.58	1.50
31	b	616	CLA	CHB-C1B	-2.33	1.34	1.39
31	1	603	CLA	MG-NB	2.33	2.10	2.05
31	16	615	CLA	CHB-C1B	-2.33	1.34	1.39
30	4	601	CHL	MG-NB	2.32	2.10	2.05
31	S	614	CLA	CHC-C1C	2.32	1.43	1.38
31	6	610	CLA	CHB-C1B	-2.32	1.34	1.39
31	n	602	CLA	CHB-C1B	-2.32	1.34	1.39
31	N	603	CLA	CHC-C1C	2.32	1.43	1.38
32	S	617	LHG	C6-C5	2.32	1.58	1.50
31	B	613	CLA	CHC-C1C	2.32	1.43	1.38
31	b	613	CLA	CHC-C1C	2.32	1.43	1.38
31	16	604	CLA	CHB-C1B	-2.32	1.34	1.39
31	2	602	CLA	MG-NB	2.32	2.10	2.05
31	5	604	CLA	CHB-C1B	-2.32	1.34	1.39
31	S	611	CLA	CHB-C1B	-2.32	1.34	1.39
31	R	611	CLA	CHB-C1B	-2.32	1.34	1.39
31	11	611	CLA	MG-NB	2.32	2.10	2.05
31	N	612	CLA	CHC-C1C	2.32	1.43	1.38
31	N	603	CLA	CHB-C1B	-2.32	1.34	1.39
31	n	611	CLA	CHB-C1B	-2.32	1.34	1.39
32	14	615	LHG	C24-C23	2.32	1.57	1.50
31	N	612	CLA	CHB-C1B	-2.32	1.34	1.39
31	5	612	CLA	MG-NC	2.32	2.11	2.06
31	R	603	CLA	CHC-C1C	2.32	1.43	1.38
32	Y	617	LHG	C24-C23	2.32	1.57	1.50
31	3	611	CLA	CHB-C1B	-2.32	1.34	1.39
31	R	610	CLA	CHB-C1B	-2.32	1.34	1.39
31	r	608	CLA	CHB-C1B	-2.32	1.34	1.39
31	15	610	CLA	C1D-ND	-2.32	1.34	1.37
31	6	604	CLA	CHB-C1B	-2.32	1.34	1.39
31	R	610	CLA	CHC-C1C	2.32	1.43	1.38
31	4	603	CLA	MG-NB	2.32	2.10	2.05
30	S	607	CHL	C2C-C3C	2.32	1.38	1.36
31	R	604	CLA	CHB-C1B	-2.32	1.34	1.39
31	12	603	CLA	MG-NB	2.32	2.10	2.05
31	n	612	CLA	CHC-C1C	2.32	1.43	1.38
31	B	609	CLA	CHB-C1B	-2.32	1.34	1.39
31	b	601	CLA	CHB-C1B	-2.32	1.34	1.39
31	B	616	CLA	CHC-C1C	2.32	1.43	1.38
32	Y	617	LHG	C4-C5	2.32	1.58	1.50
31	15	604	CLA	CHB-C1B	-2.32	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	13	611	CLA	CHC-C1C	2.32	1.43	1.38
33	12	615	LUT	C22-C23	-2.32	1.50	1.52
31	12	604	CLA	CHB-C1B	-2.31	1.34	1.39
31	s	612	CLA	MG-NB	2.31	2.10	2.05
31	b	609	CLA	CHC-C1C	2.31	1.43	1.38
31	5	612	CLA	CHC-C1C	2.31	1.43	1.38
31	Y	614	CLA	CHB-C1B	-2.31	1.34	1.39
31	G	611	CLA	MG-NB	2.31	2.10	2.05
31	b	614	CLA	CHB-C1B	-2.31	1.34	1.39
31	13	603	CLA	CHC-C1C	2.31	1.43	1.38
31	g	603	CLA	CHC-C1C	2.31	1.43	1.38
32	R	621	LHG	C24-C23	2.31	1.57	1.50
31	1	613	CLA	CHB-C1B	-2.31	1.34	1.39
31	C	513	CLA	CHB-C1B	-2.31	1.34	1.39
31	15	603	CLA	CHC-C1C	2.31	1.43	1.38
32	1	615	LHG	C24-C23	2.31	1.57	1.50
31	R	603	CLA	CHB-C1B	-2.31	1.34	1.39
31	c	513	CLA	CHB-C1B	-2.31	1.34	1.39
31	c	509	CLA	MG-NB	2.31	2.10	2.05
31	G	611	CLA	CHC-C1C	2.31	1.43	1.38
32	A	411	LHG	C24-C23	2.31	1.57	1.50
31	n	612	CLA	MG-NB	2.31	2.10	2.05
31	R	602	CLA	CHB-C1B	-2.31	1.34	1.39
30	N	607	CHL	C2C-C3C	2.31	1.38	1.36
31	g	611	CLA	MG-NB	2.31	2.10	2.05
31	g	612	CLA	MG-NC	2.31	2.11	2.06
31	a	407	CLA	MG-NB	2.31	2.10	2.05
32	4	615	LHG	C24-C23	2.31	1.57	1.50
31	2	612	CLA	MG-NB	2.31	2.10	2.05
31	r	611	CLA	CHC-C1C	2.31	1.43	1.38
31	1	614	CLA	MG-NB	2.31	2.10	2.05
31	15	602	CLA	CHB-C1B	-2.31	1.34	1.39
31	14	612	CLA	CHC-C1C	2.31	1.43	1.38
31	S	609	CLA	CHB-C1B	-2.31	1.34	1.39
31	c	507	CLA	CHC-C1C	2.31	1.43	1.38
34	G	618	NEX	C1-C6	-2.31	1.50	1.54
31	R	612	CLA	CHC-C1C	2.31	1.43	1.38
31	G	603	CLA	CHB-C1B	-2.31	1.34	1.39
31	14	614	CLA	MG-NB	2.31	2.10	2.05
31	r	613	CLA	CHC-C1C	2.31	1.43	1.38
31	g	603	CLA	CHB-C1B	-2.31	1.34	1.39
31	r	602	CLA	CHB-C1B	-2.31	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	605	CHL	C2C-C3C	2.30	1.38	1.36
30	y	609	CHL	C2C-C3C	2.30	1.38	1.36
31	B	610	CLA	CHB-C1B	-2.30	1.34	1.39
31	b	610	CLA	CHB-C1B	-2.30	1.34	1.39
31	c	504	CLA	CHB-C1B	-2.30	1.34	1.39
32	A	413	LHG	C24-C23	2.30	1.57	1.50
31	s	603	CLA	CHB-C1B	-2.30	1.34	1.39
31	N	611	CLA	MG-NB	2.30	2.10	2.05
31	c	504	CLA	MG-NB	2.30	2.10	2.05
31	b	615	CLA	MG-NC	2.30	2.11	2.06
31	G	603	CLA	CHC-C1C	2.30	1.43	1.38
31	B	602	CLA	MG-NB	2.30	2.10	2.05
31	G	614	CLA	MG-NB	2.30	2.10	2.05
31	2	604	CLA	CHB-C1B	-2.30	1.34	1.39
31	6	613	CLA	CHC-C1C	2.30	1.43	1.38
31	16	612	CLA	CHC-C1C	2.30	1.43	1.38
31	16	613	CLA	MG-NB	2.30	2.10	2.05
31	B	601	CLA	CHB-C1B	-2.30	1.34	1.39
32	n	616	LHG	C6-C5	2.30	1.58	1.50
32	R	619	LHG	C6-C5	2.30	1.58	1.50
30	n	601	CHL	C2C-C3C	2.30	1.38	1.36
31	c	514	CLA	CHB-C1B	-2.30	1.34	1.39
31	3	614	CLA	MG-NB	2.30	2.10	2.05
31	B	606	CLA	MG-NB	2.30	2.10	2.05
31	5	612	CLA	CHB-C1B	-2.30	1.34	1.39
31	N	611	CLA	CHB-C1B	-2.30	1.34	1.39
32	y	616	LHG	C6-C5	2.30	1.58	1.50
31	13	613	CLA	C1D-ND	-2.30	1.34	1.37
31	6	614	CLA	CHB-C1B	-2.30	1.34	1.39
31	3	612	CLA	CHC-C1C	2.30	1.43	1.38
30	15	605	CHL	MG-NB	2.30	2.10	2.05
31	13	603	CLA	MG-NB	2.30	2.10	2.05
31	S	613	CLA	MG-NB	2.30	2.10	2.05
31	B	614	CLA	CHB-C1B	-2.30	1.34	1.39
31	s	615	CLA	CHB-C1B	-2.30	1.34	1.39
31	n	603	CLA	CHC-C1C	2.30	1.43	1.38
31	15	610	CLA	MG-NB	2.30	2.10	2.05
31	G	612	CLA	MG-NC	2.30	2.11	2.06
31	n	603	CLA	CHB-C1B	-2.30	1.34	1.39
31	14	612	CLA	MG-NC	2.30	2.11	2.06
31	16	603	CLA	MG-NB	2.30	2.10	2.05
31	B	609	CLA	MG-NB	2.30	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	606	CLA	MG-NB	2.30	2.10	2.05
31	13	615	CLA	C1D-ND	-2.30	1.34	1.37
31	R	608	CLA	CHB-C1B	-2.30	1.34	1.39
31	Y	602	CLA	CHB-C1B	-2.30	1.34	1.39
31	b	611	CLA	CHB-C1B	-2.30	1.34	1.39
31	y	604	CLA	MG-NB	2.30	2.10	2.05
31	12	610	CLA	CHB-C1B	-2.29	1.34	1.39
31	15	610	CLA	CHC-C1C	2.29	1.43	1.38
31	g	614	CLA	MG-NB	2.29	2.10	2.05
31	R	614	CLA	CHB-C1B	-2.29	1.34	1.39
31	2	611	CLA	MG-NB	2.29	2.10	2.05
31	6	612	CLA	MG-NC	2.29	2.11	2.06
30	2	608	CHL	C2C-C3C	2.29	1.38	1.36
32	a	413	LHG	C24-C23	2.29	1.57	1.50
31	n	612	CLA	MG-NC	2.29	2.11	2.06
31	3	603	CLA	CHC-C1C	2.29	1.43	1.38
31	b	604	CLA	CHC-C1C	2.29	1.43	1.38
31	C	513	CLA	MG-NB	2.29	2.10	2.05
31	s	615	CLA	MG-NB	2.29	2.10	2.05
32	R	619	LHG	C4-C5	2.29	1.58	1.50
31	6	611	CLA	CHB-C1B	-2.29	1.34	1.39
31	C	514	CLA	CHB-C1B	-2.29	1.34	1.39
30	12	605	CHL	MG-NB	2.29	2.10	2.05
31	R	610	CLA	MG-NB	2.29	2.10	2.05
31	y	611	CLA	MG-NB	2.29	2.10	2.05
31	N	614	CLA	CHC-C1C	2.29	1.43	1.38
31	1	602	CLA	CHB-C1B	-2.29	1.34	1.39
31	4	611	CLA	CHB-C1B	-2.29	1.34	1.39
31	5	602	CLA	CHB-C1B	-2.29	1.34	1.39
31	12	610	CLA	CHC-C1C	2.29	1.43	1.38
31	s	612	CLA	CHC-C1C	2.29	1.43	1.38
31	N	614	CLA	MG-NB	2.29	2.10	2.05
31	d	404	CLA	MG-NB	2.29	2.10	2.05
30	2	601	CHL	C2C-C3C	2.29	1.38	1.36
31	1	612	CLA	CHC-C1C	2.29	1.43	1.38
31	14	602	CLA	CHB-C1B	-2.29	1.34	1.39
31	1	612	CLA	MG-NC	2.29	2.11	2.06
31	4	602	CLA	CHB-C1B	-2.29	1.34	1.39
31	b	609	CLA	CHB-C1B	-2.29	1.34	1.39
31	y	611	CLA	CHC-C1C	2.29	1.43	1.38
31	r	614	CLA	CHB-C1B	-2.29	1.34	1.39
31	1	603	CLA	CHC-C1C	2.29	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	616	CLA	CHC-C1C	2.29	1.43	1.38
31	S	614	CLA	MG-NB	2.29	2.10	2.05
31	b	616	CLA	MG-NB	2.29	2.10	2.05
31	s	613	CLA	MG-NB	2.29	2.10	2.05
31	C	510	CLA	CHB-C1B	-2.29	1.34	1.39
31	D	404	CLA	MG-NB	2.29	2.10	2.05
31	n	612	CLA	CHB-C1B	-2.29	1.34	1.39
31	S	604	CLA	CHB-C1B	-2.29	1.34	1.39
30	4	606	CHL	MG-NB	2.29	2.10	2.05
31	N	612	CLA	MG-NC	2.28	2.11	2.06
31	12	603	CLA	CHC-C1C	2.28	1.43	1.38
31	G	613	CLA	CHB-C1B	-2.28	1.34	1.39
31	B	602	CLA	CHB-C1B	-2.28	1.34	1.39
31	Y	603	CLA	CHB-C1B	-2.28	1.34	1.39
31	r	604	CLA	CHB-C1B	-2.28	1.34	1.39
30	G	607	CHL	C2C-C3C	2.28	1.38	1.36
30	y	606	CHL	MG-NB	2.28	2.10	2.05
32	1	615	LHG	C4-C5	2.28	1.57	1.50
31	b	604	CLA	CHB-C1B	-2.28	1.34	1.39
31	r	613	CLA	CHB-C1B	-2.28	1.34	1.39
32	C	521	LHG	C24-C23	2.28	1.57	1.50
31	b	601	CLA	CHC-C1C	2.28	1.43	1.38
31	1	603	CLA	CHB-C1B	-2.28	1.34	1.39
31	S	603	CLA	CHB-C1B	-2.28	1.34	1.39
31	G	603	CLA	MG-NB	2.28	2.10	2.05
31	c	514	CLA	MG-NB	2.28	2.10	2.05
31	G	612	CLA	CHC-C1C	2.28	1.43	1.38
31	13	603	CLA	CHB-C1B	-2.28	1.34	1.39
31	g	613	CLA	CHB-C1B	-2.28	1.34	1.39
31	Y	604	CLA	CHB-C1B	-2.28	1.34	1.39
31	s	611	CLA	CHB-C1B	-2.28	1.34	1.39
32	y	617	LHG	C24-C23	2.28	1.57	1.50
30	Y	606	CHL	MG-NB	2.28	2.10	2.05
31	14	604	CLA	MG-NB	2.28	2.10	2.05
32	R	618	LHG	C6-C5	2.28	1.57	1.50
31	11	612	CLA	CHC-C1C	2.28	1.43	1.38
31	C	504	CLA	CHB-C1B	-2.28	1.34	1.39
31	s	609	CLA	CHB-C1B	-2.28	1.34	1.39
31	y	614	CLA	CHB-C1B	-2.28	1.34	1.39
31	a	403	CLA	MG-NB	2.28	2.10	2.05
31	13	615	CLA	CHC-C1C	2.28	1.43	1.38
31	C	509	CLA	MG-NB	2.28	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	609	CLA	CHC-C1C	2.27	1.43	1.38
31	y	614	CLA	CHC-C1C	2.27	1.43	1.38
31	13	602	CLA	MG-NB	2.27	2.10	2.05
31	16	602	CLA	MG-NB	2.27	2.10	2.05
31	4	603	CLA	CHB-C1B	-2.27	1.34	1.39
30	2	607	CHL	C2C-C3C	2.27	1.38	1.36
31	s	603	CLA	CHC-C1C	2.27	1.43	1.38
31	13	612	CLA	CHC-C1C	2.27	1.43	1.38
31	16	611	CLA	MG-NB	2.27	2.10	2.05
31	6	603	CLA	CHC-C1C	2.27	1.43	1.38
31	12	613	CLA	CHB-C1B	-2.27	1.34	1.39
31	14	611	CLA	CHB-C1B	-2.27	1.34	1.39
31	5	611	CLA	MG-NB	2.27	2.10	2.05
31	R	612	CLA	MG-NB	2.27	2.10	2.05
31	y	615	CLA	CHB-C1B	-2.27	1.34	1.39
31	3	610	CLA	MG-NB	2.27	2.10	2.05
30	5	608	CHL	C2C-C3C	2.27	1.38	1.36
32	11	615	LHG	C24-C23	2.27	1.57	1.50
31	S	615	CLA	CHB-C1B	-2.27	1.34	1.39
31	6	613	CLA	MG-NC	2.27	2.11	2.06
31	S	603	CLA	MG-NB	2.27	2.10	2.05
31	Y	615	CLA	CHB-C1B	-2.27	1.34	1.39
30	N	601	CHL	C2C-C3C	2.27	1.38	1.36
31	1	610	CLA	CHB-C1B	-2.27	1.34	1.39
31	s	613	CLA	CHB-C1B	-2.27	1.34	1.39
31	5	613	CLA	MG-NB	2.27	2.10	2.05
31	S	609	CLA	MG-NB	2.27	2.10	2.05
31	S	603	CLA	CHC-C1C	2.27	1.43	1.38
31	12	611	CLA	MG-NC	2.27	2.11	2.06
31	13	613	CLA	MG-NB	2.27	2.10	2.05
31	B	612	CLA	CHB-C1B	-2.27	1.34	1.39
30	1	601	CHL	C2C-C3C	2.27	1.38	1.36
31	12	612	CLA	MG-NB	2.27	2.10	2.05
31	g	603	CLA	MG-NB	2.27	2.10	2.05
31	3	602	CLA	CHB-C1B	-2.27	1.34	1.39
31	g	614	CLA	CHB-C1B	-2.27	1.34	1.39
31	13	614	CLA	CHC-C1C	2.27	1.43	1.38
31	3	612	CLA	MG-NC	2.27	2.11	2.06
32	3	616	LHG	C24-C23	2.27	1.57	1.50
31	D	405	CLA	MG-NB	2.26	2.10	2.05
31	G	610	CLA	MG-NB	2.26	2.10	2.05
33	1	616	LUT	C22-C23	-2.26	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	614	CLA	CHB-C1B	-2.26	1.34	1.39
31	C	513	CLA	MG-NC	2.26	2.11	2.06
31	c	513	CLA	MG-NC	2.26	2.11	2.06
31	n	611	CLA	MG-NB	2.26	2.10	2.05
31	R	613	CLA	CHB-C1B	-2.26	1.34	1.39
31	6	611	CLA	MG-NB	2.26	2.10	2.05
31	B	611	CLA	MG-NB	2.26	2.10	2.05
31	1	614	CLA	CHB-C1B	-2.26	1.34	1.39
31	B	615	CLA	MG-NC	2.26	2.11	2.06
31	4	612	CLA	C1D-ND	-2.26	1.34	1.37
31	2	602	CLA	CHB-C1B	-2.26	1.34	1.39
31	15	610	CLA	CHB-C1B	-2.26	1.34	1.39
31	14	604	CLA	CHB-C1B	-2.26	1.34	1.39
31	11	614	CLA	CHB-C1B	-2.26	1.34	1.39
31	Y	614	CLA	CHC-C1C	2.26	1.43	1.38
31	11	611	CLA	CHB-C1B	-2.26	1.34	1.39
31	y	611	CLA	CHB-C1B	-2.26	1.34	1.39
30	Y	605	CHL	C2C-C3C	2.26	1.38	1.36
31	s	614	CLA	CHB-C1B	-2.26	1.34	1.39
31	c	505	CLA	MG-NB	2.26	2.10	2.05
31	16	603	CLA	CHB-C1B	-2.26	1.34	1.39
31	2	612	CLA	MG-NC	2.26	2.11	2.06
30	Y	606	CHL	C2C-C3C	2.26	1.38	1.36
31	G	611	CLA	CHB-C1B	-2.26	1.34	1.39
32	D	412	LHG	C4-C5	2.26	1.57	1.50
31	n	615	CLA	MG-NB	2.26	2.10	2.05
31	4	611	CLA	MG-NB	2.26	2.10	2.05
31	3	603	CLA	CHB-C1B	-2.26	1.34	1.39
31	15	603	CLA	CHB-C1B	-2.26	1.34	1.39
31	5	602	CLA	MG-NB	2.26	2.10	2.05
31	g	610	CLA	MG-NB	2.26	2.10	2.05
31	g	612	CLA	CHC-C1C	2.26	1.43	1.38
31	B	611	CLA	CHB-C1B	-2.26	1.34	1.39
31	15	611	CLA	MG-NC	2.26	2.11	2.06
31	c	510	CLA	CHB-C1B	-2.26	1.34	1.39
31	b	611	CLA	MG-NB	2.26	2.10	2.05
31	g	611	CLA	CHB-C1B	-2.26	1.34	1.39
30	11	605	CHL	MG-NB	2.25	2.10	2.05
31	3	611	CLA	MG-NB	2.25	2.10	2.05
31	A	402	CLA	MG-NB	2.25	2.10	2.05
31	Y	604	CLA	MG-NB	2.25	2.10	2.05
31	13	611	CLA	MG-NC	2.25	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	613	CLA	MG-NB	2.25	2.10	2.05
31	1	611	CLA	CHB-C1B	-2.25	1.34	1.39
31	C	504	CLA	MG-NB	2.25	2.10	2.05
31	S	615	CLA	MG-NB	2.25	2.10	2.05
31	3	611	CLA	CHC-C1C	2.25	1.43	1.38
31	B	601	CLA	CHC-C1C	2.25	1.43	1.38
31	B	613	CLA	CHB-C1B	-2.25	1.34	1.39
31	C	502	CLA	CHB-C1B	-2.25	1.34	1.39
32	6	616	LHG	C24-C23	2.25	1.57	1.50
30	1	607	CHL	C2C-C3C	2.25	1.38	1.36
31	D	405	CLA	CHB-C1B	-2.25	1.34	1.39
32	a	411	LHG	C24-C23	2.25	1.57	1.50
31	n	614	CLA	CHC-C1C	2.25	1.43	1.38
31	N	611	CLA	MG-NC	2.25	2.11	2.06
31	6	612	CLA	CHC-C1C	2.25	1.43	1.38
31	S	614	CLA	CHB-C1B	-2.25	1.34	1.39
31	4	610	CLA	C1D-ND	-2.25	1.34	1.37
31	r	602	CLA	MG-NB	2.25	2.10	2.05
31	12	609	CLA	CHB-C1B	-2.25	1.34	1.39
31	15	609	CLA	CHB-C1B	-2.25	1.34	1.39
31	b	602	CLA	CHB-C1B	-2.25	1.34	1.39
31	s	604	CLA	CHB-C1B	-2.25	1.34	1.39
31	r	613	CLA	MG-NB	2.25	2.10	2.05
31	n	611	CLA	MG-NC	2.25	2.11	2.06
31	B	615	CLA	CHC-C1C	2.25	1.43	1.38
31	C	508	CLA	CHB-C1B	-2.25	1.34	1.39
31	15	603	CLA	MG-NB	2.25	2.10	2.05
31	b	609	CLA	MG-NB	2.25	2.10	2.05
31	b	612	CLA	CHB-C1B	-2.25	1.34	1.39
31	c	502	CLA	CHB-C1B	-2.25	1.34	1.39
31	c	507	CLA	CHB-C1B	-2.25	1.34	1.39
31	S	609	CLA	MG-NC	2.25	2.11	2.06
31	g	602	CLA	CHB-C1B	-2.25	1.34	1.39
31	B	607	CLA	CHC-C1C	2.25	1.43	1.38
31	n	604	CLA	MG-NB	2.25	2.10	2.05
31	11	602	CLA	CHB-C1B	-2.25	1.34	1.39
31	C	505	CLA	MG-NB	2.25	2.10	2.05
32	a	401	LHG	C4-C5	2.25	1.57	1.50
31	16	602	CLA	CHB-C1B	-2.25	1.34	1.39
31	r	610	CLA	MG-NB	2.25	2.10	2.05
31	S	611	CLA	MG-NB	2.24	2.10	2.05
31	C	507	CLA	CHB-C1B	-2.24	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	611	CLA	CHC-C1C	2.24	1.43	1.38
31	c	506	CLA	CHC-C1C	2.24	1.43	1.38
32	d	413	LHG	C4-C5	2.24	1.57	1.50
31	B	608	CLA	MG-NB	2.24	2.10	2.05
31	14	603	CLA	CHB-C1B	-2.24	1.34	1.39
31	y	602	CLA	CHB-C1B	-2.24	1.34	1.39
30	G	605	CHL	C2C-C3C	2.24	1.38	1.36
31	3	613	CLA	CHB-C1B	-2.24	1.34	1.39
31	13	611	CLA	MG-NB	2.24	2.10	2.05
31	G	602	CLA	MG-NB	2.24	2.10	2.05
30	2	601	CHL	MG-NB	2.24	2.10	2.05
31	13	602	CLA	CHB-C1B	-2.24	1.34	1.39
31	y	604	CLA	MG-NC	2.24	2.11	2.06
31	6	602	CLA	CHB-C1B	-2.24	1.34	1.39
32	3	617	LHG	C24-C23	2.24	1.57	1.50
31	14	614	CLA	CHB-C1B	-2.24	1.34	1.39
31	b	614	CLA	MG-NB	2.24	2.10	2.05
31	5	603	CLA	CHB-C1B	-2.24	1.34	1.39
31	G	602	CLA	CHB-C1B	-2.24	1.34	1.39
31	b	607	CLA	CHC-C1C	2.24	1.43	1.38
31	B	614	CLA	MG-NB	2.24	2.10	2.05
31	g	611	CLA	CHC-C1C	2.24	1.43	1.38
31	12	609	CLA	MG-NB	2.24	2.10	2.05
31	R	608	CLA	MG-NB	2.24	2.10	2.05
30	14	608	CHL	C2-C3	2.24	1.39	1.32
31	A	406	CLA	MG-NB	2.24	2.10	2.05
31	R	612	CLA	C1D-ND	-2.24	1.34	1.37
31	6	610	CLA	MG-NC	2.24	2.11	2.06
31	12	602	CLA	CHB-C1B	-2.24	1.34	1.39
31	R	602	CLA	MG-NB	2.24	2.10	2.05
31	c	513	CLA	CHC-C1C	2.23	1.43	1.38
31	13	614	CLA	CHB-C1B	-2.23	1.34	1.39
30	5	607	CHL	C2C-C3C	2.23	1.38	1.36
31	14	613	CLA	CHB-C1B	-2.23	1.34	1.39
31	Y	610	CLA	CHB-C1B	-2.23	1.34	1.39
30	Y	601	CHL	C2C-C3C	2.23	1.38	1.36
31	14	604	CLA	MG-NC	2.23	2.11	2.06
31	S	603	CLA	MG-NC	2.23	2.11	2.06
31	s	602	CLA	CHB-C1B	-2.23	1.34	1.39
31	b	615	CLA	CHC-C1C	2.23	1.43	1.38
31	Y	604	CLA	MG-NC	2.23	2.11	2.06
31	1	602	CLA	MG-NB	2.23	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	603	CLA	CHB-C1B	-2.23	1.34	1.39
31	C	503	CLA	CHB-C1B	-2.23	1.34	1.39
31	c	503	CLA	CHB-C1B	-2.23	1.34	1.39
31	B	604	CLA	MG-NB	2.23	2.10	2.05
32	a	414	LHG	C24-C23	2.23	1.57	1.50
31	R	603	CLA	MG-NB	2.23	2.10	2.05
31	s	611	CLA	MG-NB	2.23	2.10	2.05
31	14	611	CLA	MG-NC	2.23	2.11	2.06
31	16	603	CLA	CHC-C1C	2.23	1.43	1.38
31	r	601	CLA	CHB-C1B	-2.23	1.34	1.39
31	4	610	CLA	CHB-C1B	-2.23	1.34	1.39
31	s	604	CLA	MG-NB	2.23	2.10	2.05
31	d	405	CLA	CHB-C1B	-2.23	1.34	1.39
31	Y	611	CLA	CHB-C1B	-2.23	1.34	1.39
31	d	405	CLA	MG-NB	2.23	2.10	2.05
31	1	613	CLA	MG-NC	2.23	2.11	2.06
31	N	615	CLA	MG-NB	2.23	2.10	2.05
31	S	613	CLA	CHB-C1B	-2.23	1.34	1.39
31	15	609	CLA	MG-NB	2.23	2.10	2.05
31	D	404	CLA	CHB-C1B	-2.23	1.34	1.39
31	a	407	CLA	CHB-C1B	-2.23	1.34	1.39
32	N	616	LHG	C6-C5	2.23	1.57	1.50
32	S	617	LHG	C24-C23	2.23	1.57	1.50
30	y	605	CHL	MG-NB	2.23	2.10	2.05
31	A	406	CLA	CHB-C1B	-2.23	1.34	1.39
31	16	615	CLA	MG-NC	2.23	2.11	2.06
30	g	605	CHL	C2C-C3C	2.23	1.38	1.36
31	12	610	CLA	MG-NC	2.23	2.11	2.06
31	b	604	CLA	MG-NC	2.23	2.11	2.06
31	11	603	CLA	CHB-C1B	-2.22	1.34	1.39
31	C	507	CLA	CHC-C1C	2.22	1.42	1.38
31	14	613	CLA	MG-NB	2.22	2.10	2.05
31	C	513	CLA	CHC-C1C	2.22	1.42	1.38
31	S	612	CLA	CHC-C1C	2.22	1.42	1.38
31	r	608	CLA	MG-NB	2.22	2.10	2.05
31	16	614	CLA	CHC-C1C	2.22	1.42	1.38
32	r	619	LHG	C4-C5	2.22	1.57	1.50
31	4	613	CLA	CHB-C1B	-2.22	1.34	1.39
31	13	611	CLA	CHB-C1B	-2.22	1.34	1.39
31	2	603	CLA	CHB-C1B	-2.22	1.34	1.39
31	G	604	CLA	MG-NB	2.22	2.10	2.05
31	3	610	CLA	CHB-C1B	-2.22	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	15	613	CLA	CHB-C1B	-2.22	1.34	1.39
31	d	402	CLA	CHB-C1B	-2.22	1.34	1.39
31	y	610	CLA	CHB-C1B	-2.22	1.34	1.39
31	11	613	CLA	MG-NB	2.22	2.10	2.05
31	A	404	CLA	CHB-C1B	-2.22	1.34	1.39
31	B	604	CLA	MG-NC	2.22	2.11	2.06
31	r	611	CLA	MG-NC	2.22	2.11	2.06
31	r	614	CLA	CHC-C1C	2.22	1.42	1.38
30	11	608	CHL	C2-C3	2.22	1.39	1.32
31	g	614	CLA	MG-NC	2.22	2.11	2.06
31	s	603	CLA	MG-NC	2.22	2.11	2.06
31	16	611	CLA	CHB-C1B	-2.22	1.34	1.39
31	1	613	CLA	MG-NB	2.22	2.10	2.05
31	5	603	CLA	MG-NB	2.22	2.10	2.05
31	16	613	CLA	CHC-C1C	2.22	1.42	1.38
31	5	610	CLA	CHB-C1B	-2.22	1.34	1.39
31	r	611	CLA	MG-NB	2.22	2.10	2.05
31	11	611	CLA	MG-NC	2.22	2.11	2.06
31	R	612	CLA	CHB-C1B	-2.22	1.34	1.39
31	3	615	CLA	CHB-C1B	-2.22	1.34	1.39
31	16	613	CLA	CHB-C1B	-2.22	1.34	1.39
31	a	404	CLA	CHB-C1B	-2.22	1.34	1.39
31	n	613	CLA	MG-NB	2.22	2.10	2.05
31	S	612	CLA	C1D-ND	-2.22	1.34	1.37
31	N	610	CLA	CHB-C1B	-2.22	1.34	1.39
31	g	610	CLA	CHB-C1B	-2.22	1.34	1.39
31	12	602	CLA	MG-NB	2.22	2.10	2.05
31	s	602	CLA	MG-NC	2.22	2.11	2.06
31	11	604	CLA	MG-NB	2.22	2.10	2.05
31	g	602	CLA	MG-NB	2.22	2.10	2.05
31	2	613	CLA	CHB-C1B	-2.22	1.34	1.39
31	N	613	CLA	CHB-C1B	-2.22	1.34	1.39
31	s	609	CLA	MG-NC	2.22	2.11	2.06
30	n	607	CHL	C2C-C3C	2.22	1.38	1.36
31	B	616	CLA	MG-NB	2.21	2.10	2.05
31	b	613	CLA	C1B-NB	-2.21	1.35	1.37
31	B	605	CLA	MG-NC	2.21	2.11	2.06
31	13	613	CLA	CHB-C1B	-2.21	1.34	1.39
32	13	616	LHG	C4-C5	2.21	1.57	1.50
31	3	604	CLA	MG-NB	2.21	2.10	2.05
33	n	617	LUT	C22-C23	-2.21	1.50	1.52
31	3	613	CLA	MG-NC	2.21	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	613	CLA	MG-NC	2.21	2.11	2.06
32	R	618	LHG	C24-C23	2.21	1.57	1.50
31	6	611	CLA	MG-NC	2.21	2.11	2.06
31	3	614	CLA	CHB-C1B	-2.21	1.34	1.39
30	y	601	CHL	C2C-C3C	2.21	1.38	1.36
31	4	614	CLA	CHB-C1B	-2.21	1.34	1.39
31	16	614	CLA	CHB-C1B	-2.21	1.34	1.39
31	C	514	CLA	MG-NB	2.21	2.10	2.05
31	r	609	CLA	MG-NB	2.21	2.10	2.05
31	R	614	CLA	CHC-C1C	2.21	1.42	1.38
31	11	602	CLA	MG-NB	2.21	2.10	2.05
31	2	610	CLA	CHB-C1B	-2.21	1.34	1.39
31	6	613	CLA	CHB-C1B	-2.21	1.34	1.39
31	16	610	CLA	CHB-C1B	-2.21	1.34	1.39
31	2	604	CLA	MG-NB	2.21	2.10	2.05
31	4	602	CLA	MG-NB	2.21	2.10	2.05
31	r	609	CLA	CHB-C1B	-2.21	1.34	1.39
31	D	404	CLA	CHC-C1C	2.21	1.42	1.38
31	2	602	CLA	MG-NC	2.21	2.11	2.06
31	13	604	CLA	MG-NB	2.21	2.10	2.05
31	S	602	CLA	MG-NC	2.21	2.11	2.06
31	n	614	CLA	CHB-C1B	-2.21	1.34	1.39
31	Y	611	CLA	CHC-C1C	2.21	1.42	1.38
31	b	610	CLA	CHC-C1C	2.21	1.42	1.38
31	11	613	CLA	CHB-C1B	-2.21	1.34	1.39
31	16	611	CLA	MG-NC	2.20	2.11	2.06
31	2	603	CLA	MG-NB	2.20	2.10	2.05
31	13	615	CLA	CHB-C1B	-2.20	1.34	1.39
30	1	607	CHL	C2-C3	2.20	1.39	1.32
31	6	613	CLA	MG-NB	2.20	2.10	2.05
31	R	613	CLA	MG-NB	2.20	2.10	2.05
31	11	604	CLA	CHB-C1B	-2.20	1.34	1.39
31	S	610	CLA	CHB-C1B	-2.20	1.34	1.39
31	S	604	CLA	MG-NB	2.20	2.10	2.05
31	15	612	CLA	CHB-C1B	-2.20	1.34	1.39
31	c	511	CLA	CHB-C1B	-2.20	1.34	1.39
30	6	609	CHL	C2C-C3C	2.20	1.38	1.36
31	N	602	CLA	CHB-C1B	-2.20	1.34	1.39
31	16	613	CLA	MG-NC	2.20	2.11	2.06
31	B	610	CLA	CHC-C1C	2.20	1.42	1.38
31	13	610	CLA	CHB-C1B	-2.20	1.34	1.39
31	C	503	CLA	CHC-C1C	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	611	CLA	MG-NC	2.20	2.11	2.06
31	s	610	CLA	CHB-C1B	-2.20	1.34	1.39
31	11	604	CLA	MG-NC	2.20	2.11	2.06
31	1	611	CLA	MG-NC	2.20	2.11	2.06
31	g	611	CLA	MG-NC	2.20	2.11	2.06
31	g	604	CLA	MG-NB	2.20	2.10	2.05
30	4	607	CHL	C2-C3	2.20	1.39	1.32
31	A	403	CLA	CHB-C1B	-2.20	1.34	1.39
31	G	610	CLA	CHB-C1B	-2.20	1.34	1.39
31	15	613	CLA	MG-NC	2.20	2.11	2.06
31	R	613	CLA	MG-NC	2.20	2.11	2.06
31	C	511	CLA	CHB-C1B	-2.20	1.34	1.39
31	R	609	CLA	MG-NB	2.20	2.10	2.05
31	n	603	CLA	MG-NB	2.20	2.10	2.05
31	3	603	CLA	MG-NC	2.20	2.11	2.06
32	A	414	LHG	C24-C23	2.20	1.57	1.50
30	n	605	CHL	C2C-C3C	2.20	1.38	1.36
31	c	507	CLA	MG-NB	2.20	2.10	2.05
31	15	610	CLA	MG-NC	2.20	2.11	2.06
31	16	604	CLA	MG-NB	2.19	2.10	2.05
31	g	613	CLA	MG-NB	2.19	2.10	2.05
31	y	614	CLA	MG-NC	2.19	2.11	2.06
31	R	601	CLA	MG-NB	2.19	2.10	2.05
31	R	604	CLA	MG-NB	2.19	2.10	2.05
31	c	512	CLA	MG-NB	2.19	2.10	2.05
31	1	611	CLA	MG-NB	2.19	2.10	2.05
30	15	606	CHL	C2-C3	2.19	1.39	1.32
31	16	615	CLA	MG-NB	2.19	2.10	2.05
31	2	604	CLA	MG-NC	2.19	2.11	2.06
32	4	615	LHG	C4-C5	2.19	1.57	1.50
31	N	603	CLA	MG-NB	2.19	2.10	2.05
31	G	604	CLA	MG-NC	2.19	2.11	2.06
31	12	609	CLA	MG-NC	2.19	2.11	2.06
32	a	414	LHG	C4-C5	2.19	1.57	1.50
31	R	611	CLA	MG-NC	2.19	2.11	2.06
31	c	506	CLA	MG-NC	2.19	2.11	2.06
31	3	611	CLA	MG-NC	2.19	2.11	2.06
31	b	613	CLA	CHB-C1B	-2.19	1.34	1.39
31	S	602	CLA	CHB-C1B	-2.19	1.34	1.39
31	2	610	CLA	MG-NB	2.19	2.10	2.05
31	B	608	CLA	C1B-NB	-2.19	1.35	1.37
31	4	611	CLA	MG-NC	2.19	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	613	CLA	CHB-C1B	-2.19	1.34	1.39
31	13	610	CLA	MG-NB	2.19	2.10	2.05
30	y	606	CHL	C2C-C3C	2.19	1.38	1.36
31	N	610	CLA	MG-NB	2.19	2.10	2.05
31	s	613	CLA	MG-NC	2.19	2.11	2.06
31	Y	612	CLA	CHC-C1C	2.19	1.42	1.38
30	16	607	CHL	C2C-C3C	2.19	1.38	1.36
31	n	610	CLA	MG-NB	2.19	2.10	2.05
31	5	604	CLA	MG-NC	2.19	2.11	2.06
31	4	614	CLA	MG-NC	2.19	2.11	2.06
31	11	614	CLA	MG-NC	2.19	2.11	2.06
31	13	613	CLA	CHC-C1C	2.18	1.42	1.38
31	4	604	CLA	CHB-C1B	-2.18	1.34	1.39
31	n	610	CLA	CHB-C1B	-2.18	1.34	1.39
31	G	603	CLA	MG-NC	2.18	2.11	2.06
31	3	602	CLA	MG-NB	2.18	2.10	2.05
31	S	605	CLA	MG-NC	2.18	2.11	2.06
31	6	602	CLA	MG-NB	2.18	2.10	2.05
32	c	521	LHG	C4-C5	2.18	1.57	1.50
31	13	615	CLA	MG-NB	2.18	2.10	2.05
31	r	601	CLA	MG-NB	2.18	2.10	2.05
31	y	602	CLA	MG-NB	2.18	2.10	2.05
31	14	610	CLA	CHB-C1B	-2.18	1.34	1.39
31	14	602	CLA	MG-NB	2.18	2.10	2.05
31	c	503	CLA	CHC-C1C	2.18	1.42	1.38
31	6	614	CLA	MG-NC	2.18	2.11	2.06
31	G	614	CLA	MG-NC	2.18	2.11	2.06
32	A	411	LHG	C4-C5	2.18	1.57	1.50
31	12	603	CLA	CHB-C1B	-2.18	1.34	1.39
30	5	601	CHL	C2-C3	2.18	1.39	1.32
31	N	604	CLA	MG-NB	2.18	2.10	2.05
31	16	602	CLA	MG-NC	2.18	2.11	2.06
31	s	602	CLA	MG-NB	2.18	2.10	2.05
31	y	612	CLA	CHC-C1C	2.18	1.42	1.38
31	1	614	CLA	MG-NC	2.18	2.11	2.06
31	3	614	CLA	MG-NC	2.18	2.11	2.06
31	14	614	CLA	MG-NC	2.18	2.11	2.06
31	n	613	CLA	CHB-C1B	-2.18	1.34	1.39
31	n	604	CLA	MG-NC	2.18	2.11	2.06
31	3	603	CLA	MG-NB	2.18	2.10	2.05
31	r	604	CLA	MG-NB	2.18	2.10	2.05
31	12	613	CLA	MG-NC	2.18	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	14	602	CLA	MG-NC	2.17	2.11	2.06
31	G	611	CLA	MG-NC	2.17	2.11	2.06
31	4	612	CLA	CHC-C1C	2.17	1.42	1.38
31	B	607	CLA	MG-NB	2.17	2.10	2.05
31	r	602	CLA	C1B-NB	-2.17	1.35	1.37
31	a	407	CLA	MG-NC	2.17	2.11	2.06
31	Y	613	CLA	CHB-C1B	-2.17	1.34	1.39
31	1	604	CLA	CHB-C1B	-2.17	1.34	1.39
31	R	604	CLA	MG-NC	2.17	2.11	2.06
32	r	618	LHG	C6-C5	2.17	1.57	1.50
31	2	611	CLA	CHB-C1B	-2.17	1.34	1.39
31	4	613	CLA	MG-NC	2.17	2.11	2.06
31	5	602	CLA	MG-NC	2.17	2.11	2.06
31	5	604	CLA	MG-NB	2.17	2.10	2.05
32	C	521	LHG	C4-C5	2.17	1.57	1.50
31	11	602	CLA	MG-NC	2.17	2.11	2.06
31	13	603	CLA	MG-NC	2.17	2.11	2.06
31	13	615	CLA	MG-NC	2.17	2.11	2.06
31	b	603	CLA	MG-NC	2.17	2.11	2.06
31	13	602	CLA	MG-NC	2.17	2.11	2.06
31	16	614	CLA	MG-NC	2.17	2.11	2.06
31	n	602	CLA	MG-NB	2.17	2.10	2.05
31	3	604	CLA	MG-NC	2.17	2.11	2.06
31	Y	603	CLA	MG-NB	2.17	2.10	2.05
30	G	601	CHL	C2C-C3C	2.17	1.38	1.36
31	1	603	CLA	MG-NC	2.17	2.11	2.06
31	14	603	CLA	MG-NC	2.17	2.11	2.06
31	g	613	CLA	MG-NC	2.17	2.11	2.06
31	C	510	CLA	C1B-NB	-2.17	1.35	1.37
31	c	503	CLA	MG-NB	2.17	2.10	2.05
32	s	617	LHG	C6-C5	2.17	1.57	1.50
31	A	406	CLA	MG-NC	2.17	2.11	2.06
32	3	617	LHG	C4-C5	2.17	1.57	1.50
31	R	602	CLA	MG-NC	2.17	2.11	2.06
31	S	614	CLA	MG-NC	2.17	2.11	2.06
31	S	605	CLA	CHB-C1B	-2.16	1.34	1.39
30	13	605	CHL	C2C-C3C	2.16	1.38	1.36
31	2	603	CLA	MG-NC	2.16	2.11	2.06
31	15	604	CLA	MG-NC	2.16	2.11	2.06
31	G	613	CLA	MG-NC	2.16	2.11	2.06
31	13	613	CLA	MG-NC	2.16	2.11	2.06
31	c	509	CLA	MG-NC	2.16	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	15	602	CLA	MG-NC	2.16	2.11	2.06
31	b	612	CLA	C1B-NB	-2.16	1.35	1.37
31	n	615	CLA	CHB-C1B	-2.16	1.34	1.39
31	y	613	CLA	CHB-C1B	-2.16	1.34	1.39
31	B	611	CLA	MG-NC	2.16	2.11	2.06
31	r	602	CLA	MG-NC	2.16	2.11	2.06
31	B	603	CLA	MG-NC	2.16	2.11	2.06
30	4	601	CHL	C2C-C3C	2.16	1.38	1.36
31	6	603	CLA	MG-NC	2.16	2.11	2.06
31	11	603	CLA	MG-NC	2.16	2.11	2.06
31	C	506	CLA	MG-NC	2.16	2.11	2.06
31	y	610	CLA	MG-NB	2.16	2.10	2.05
31	16	603	CLA	MG-NC	2.16	2.11	2.06
30	N	609	CHL	C2C-C3C	2.16	1.38	1.36
31	S	611	CLA	MG-NC	2.16	2.11	2.06
31	R	609	CLA	CHB-C1B	-2.16	1.34	1.39
30	6	605	CHL	C2C-C3C	2.16	1.38	1.36
31	r	612	CLA	CHB-C1B	-2.16	1.34	1.39
31	R	611	CLA	MG-NB	2.16	2.10	2.05
31	b	604	CLA	MG-NB	2.16	2.10	2.05
31	b	605	CLA	MG-NC	2.16	2.11	2.06
30	3	609	CHL	C2C-C3C	2.16	1.38	1.36
31	g	604	CLA	MG-NC	2.16	2.11	2.06
31	R	601	CLA	CHB-C1B	-2.16	1.34	1.39
31	R	603	CLA	MG-NC	2.15	2.11	2.06
31	g	603	CLA	MG-NC	2.15	2.11	2.06
31	n	614	CLA	MG-NC	2.15	2.11	2.06
31	6	603	CLA	MG-NB	2.15	2.10	2.05
31	b	607	CLA	MG-NB	2.15	2.10	2.05
30	12	606	CHL	C2-C3	2.15	1.38	1.32
31	r	604	CLA	MG-NC	2.15	2.11	2.06
30	16	605	CHL	C2C-C3C	2.15	1.38	1.36
31	C	506	CLA	CHC-C1C	2.15	1.42	1.38
31	N	604	CLA	MG-NC	2.15	2.11	2.06
31	4	610	CLA	C3B-C4B	2.15	1.49	1.42
31	N	613	CLA	C1B-NB	-2.15	1.35	1.37
31	Y	602	CLA	MG-NB	2.15	2.10	2.05
31	C	509	CLA	MG-NC	2.15	2.11	2.06
33	16	617	LUT	C22-C23	-2.15	1.50	1.52
31	4	610	CLA	CMD-C2D	2.15	1.55	1.50
31	C	503	CLA	MG-NB	2.15	2.10	2.05
31	4	604	CLA	MG-NB	2.15	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	6	604	CLA	MG-NB	2.15	2.10	2.05
31	s	614	CLA	MG-NC	2.15	2.11	2.06
31	Y	613	CLA	MG-NB	2.15	2.10	2.05
30	Y	608	CHL	C2C-C3C	2.15	1.38	1.36
31	R	603	CLA	C1B-NB	-2.15	1.35	1.37
31	B	606	CLA	MG-NC	2.15	2.11	2.06
31	C	512	CLA	MG-NB	2.15	2.10	2.05
31	G	613	CLA	MG-NB	2.15	2.10	2.05
31	b	608	CLA	MG-NB	2.15	2.10	2.05
31	11	610	CLA	CHB-C1B	-2.15	1.34	1.39
31	6	615	CLA	CHB-C1B	-2.15	1.34	1.39
31	c	507	CLA	MG-NC	2.15	2.11	2.06
31	r	603	CLA	C1B-NB	-2.15	1.35	1.37
31	4	603	CLA	MG-NC	2.15	2.11	2.06
31	B	609	CLA	MG-NC	2.15	2.11	2.06
31	5	610	CLA	MG-NB	2.14	2.10	2.05
33	S	618	LUT	C22-C23	-2.14	1.50	1.52
32	16	616	LHG	C4-C5	2.14	1.57	1.50
31	c	504	CLA	MG-NC	2.14	2.11	2.06
31	s	605	CLA	MG-NC	2.14	2.11	2.06
31	2	611	CLA	MG-NC	2.14	2.11	2.06
31	12	603	CLA	MG-NC	2.14	2.11	2.06
31	y	613	CLA	MG-NC	2.14	2.11	2.06
31	B	613	CLA	MG-NC	2.14	2.11	2.06
30	13	607	CHL	C2C-C3C	2.14	1.38	1.36
31	1	602	CLA	MG-NC	2.14	2.11	2.06
31	r	613	CLA	MG-NC	2.14	2.11	2.06
31	s	615	CLA	MG-NC	2.14	2.11	2.06
32	A	414	LHG	C4-C5	2.14	1.57	1.50
31	y	613	CLA	MG-NB	2.14	2.10	2.05
31	N	614	CLA	CHB-C1B	-2.14	1.34	1.39
31	c	508	CLA	MG-NC	2.14	2.11	2.06
31	16	610	CLA	MG-NB	2.14	2.10	2.05
31	C	507	CLA	MG-NC	2.14	2.11	2.06
31	B	610	CLA	C1B-NB	-2.14	1.35	1.37
31	b	610	CLA	C1B-NB	-2.14	1.35	1.37
30	g	601	CHL	C2C-C3C	2.14	1.38	1.36
31	1	604	CLA	MG-NB	2.14	2.10	2.05
31	11	613	CLA	MG-NC	2.14	2.11	2.06
31	g	610	CLA	C3B-C4B	2.14	1.49	1.42
31	Y	610	CLA	MG-NB	2.14	2.10	2.05
31	b	606	CLA	MG-NC	2.14	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	602	CLA	MG-NB	2.14	2.10	2.05
31	Y	602	CLA	C3B-C4B	2.14	1.49	1.42
31	12	602	CLA	MG-NC	2.14	2.11	2.06
31	Y	611	CLA	MG-NC	2.14	2.11	2.06
31	y	611	CLA	MG-NC	2.14	2.11	2.06
31	B	613	CLA	C1B-NB	-2.14	1.35	1.37
31	s	605	CLA	CHB-C1B	-2.13	1.34	1.39
31	c	510	CLA	C1B-NB	-2.13	1.35	1.37
31	4	602	CLA	MG-NC	2.13	2.11	2.06
31	C	507	CLA	MG-NB	2.13	2.10	2.05
31	R	610	CLA	MG-NC	2.13	2.11	2.06
31	b	611	CLA	MG-NC	2.13	2.11	2.06
32	D	408	LHG	C24-C23	2.13	1.56	1.50
31	c	508	CLA	MG-NB	2.13	2.10	2.05
32	6	617	LHG	C4-C5	2.13	1.57	1.50
31	Y	615	CLA	C1B-NB	-2.13	1.35	1.37
31	C	502	CLA	C1B-NB	-2.13	1.35	1.37
31	B	610	CLA	MG-NB	2.13	2.10	2.05
30	r	607	CHL	C2-C3	2.13	1.38	1.32
31	s	605	CLA	MG-NB	2.13	2.10	2.05
31	S	612	CLA	C3B-C4B	2.13	1.48	1.42
31	3	613	CLA	MG-NB	2.13	2.10	2.05
31	15	609	CLA	MG-NC	2.13	2.11	2.06
31	Y	614	CLA	MG-NC	2.13	2.11	2.06
31	n	603	CLA	MG-NC	2.13	2.11	2.06
31	5	603	CLA	MG-NC	2.13	2.11	2.06
31	N	614	CLA	MG-NC	2.13	2.11	2.06
31	13	614	CLA	MG-NC	2.13	2.11	2.06
31	S	615	CLA	MG-NC	2.13	2.11	2.06
31	S	610	CLA	MG-NB	2.13	2.10	2.05
31	b	616	CLA	MG-NC	2.12	2.11	2.06
31	B	612	CLA	C1B-NB	-2.12	1.35	1.37
31	C	503	CLA	C1B-NB	-2.12	1.35	1.37
30	R	607	CHL	C2-C3	2.12	1.38	1.32
31	y	610	CLA	C3B-C4B	2.12	1.48	1.42
32	6	617	LHG	C24-C23	2.12	1.56	1.50
31	s	611	CLA	MG-NC	2.12	2.11	2.06
31	r	603	CLA	MG-NB	2.12	2.10	2.05
32	s	617	LHG	C24-C23	2.12	1.56	1.50
32	y	618	LHG	C4-C5	2.12	1.57	1.50
31	C	512	CLA	MG-NC	2.12	2.11	2.06
31	12	604	CLA	MG-NC	2.12	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r	610	CLA	MG-NC	2.12	2.11	2.06
31	14	610	CLA	MG-NB	2.12	2.10	2.05
31	11	610	CLA	C3B-C4B	2.12	1.48	1.42
31	6	604	CLA	MG-NC	2.12	2.11	2.06
31	16	602	CLA	CAA-C2A	2.12	1.57	1.54
31	R	614	CLA	MG-NB	2.12	2.10	2.05
31	y	602	CLA	C3B-C4B	2.12	1.48	1.42
32	Y	618	LHG	C4-C5	2.12	1.57	1.50
32	14	615	LHG	C4-C5	2.12	1.57	1.50
31	c	512	CLA	MG-NC	2.12	2.11	2.06
31	d	404	CLA	C3B-C4B	2.12	1.48	1.42
31	C	502	CLA	MG-NB	2.12	2.10	2.05
31	r	614	CLA	MG-NB	2.12	2.10	2.05
31	y	603	CLA	MG-NB	2.12	2.10	2.05
31	14	613	CLA	MG-NC	2.12	2.11	2.06
31	S	602	CLA	MG-NB	2.12	2.10	2.05
32	d	409	LHG	C24-C23	2.12	1.56	1.50
32	a	411	LHG	C4-C5	2.12	1.57	1.50
31	15	612	CLA	MG-NC	2.12	2.11	2.06
31	c	511	CLA	C1B-NB	-2.11	1.35	1.37
31	B	607	CLA	MG-NC	2.11	2.11	2.06
31	C	504	CLA	MG-NC	2.11	2.11	2.06
31	11	610	CLA	MG-NB	2.11	2.10	2.05
31	B	614	CLA	MG-NC	2.11	2.11	2.06
31	13	604	CLA	MG-NC	2.11	2.11	2.06
31	15	603	CLA	MG-NC	2.11	2.11	2.06
31	b	608	CLA	C1B-NB	-2.11	1.35	1.37
30	3	605	CHL	C2C-C3C	2.11	1.38	1.36
31	S	605	CLA	MG-NB	2.11	2.10	2.05
31	15	613	CLA	C3B-C4B	2.11	1.48	1.42
31	R	602	CLA	C3B-C4B	2.11	1.48	1.42
32	d	408	LHG	C24-C23	2.11	1.56	1.50
31	Y	603	CLA	C1B-NB	-2.11	1.35	1.37
32	L	102	LHG	C24-C23	2.11	1.56	1.50
31	N	610	CLA	C3B-C4B	2.11	1.48	1.42
30	Y	607	CHL	C2C-C3C	2.11	1.38	1.36
31	16	604	CLA	MG-NC	2.11	2.11	2.06
31	3	610	CLA	MG-NC	2.11	2.11	2.06
33	13	617	LUT	C22-C23	-2.11	1.50	1.52
31	n	602	CLA	MG-NC	2.11	2.11	2.06
31	N	615	CLA	CHB-C1B	-2.11	1.34	1.39
31	12	612	CLA	MG-NC	2.11	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	603	CLA	MG-NC	2.11	2.11	2.06
31	5	613	CLA	MG-NC	2.11	2.11	2.06
31	C	511	CLA	C1B-NB	-2.11	1.35	1.37
32	r	621	LHG	C4-C5	2.11	1.57	1.50
31	Y	610	CLA	C3B-C4B	2.10	1.48	1.42
31	B	608	CLA	MG-NC	2.10	2.11	2.06
31	D	404	CLA	MG-NC	2.10	2.11	2.06
31	r	602	CLA	C3B-C4B	2.10	1.48	1.42
32	r	618	LHG	C24-C23	2.10	1.56	1.50
31	B	601	CLA	MG-NB	2.10	2.10	2.05
31	b	613	CLA	MG-NB	2.10	2.10	2.05
31	14	610	CLA	C3B-C4B	2.10	1.48	1.42
32	l	102	LHG	C24-C23	2.10	1.56	1.50
31	1	610	CLA	CHC-C1C	2.10	1.42	1.38
31	b	616	CLA	C1B-NB	-2.10	1.35	1.37
31	15	612	CLA	CAA-C2A	2.10	1.57	1.54
31	b	608	CLA	MG-NC	2.10	2.11	2.06
31	c	503	CLA	C1B-NB	-2.10	1.35	1.37
31	A	402	CLA	C1B-NB	-2.10	1.35	1.37
31	12	612	CLA	CHB-C1B	-2.10	1.34	1.39
31	b	610	CLA	MG-NC	2.10	2.11	2.06
31	b	613	CLA	MG-NC	2.10	2.11	2.06
31	B	613	CLA	MG-NB	2.10	2.09	2.05
31	S	604	CLA	MG-NC	2.10	2.11	2.06
31	B	601	CLA	MG-NC	2.10	2.11	2.06
31	b	614	CLA	MG-NC	2.10	2.11	2.06
31	g	602	CLA	MG-NC	2.09	2.11	2.06
31	N	613	CLA	MG-NB	2.09	2.09	2.05
31	G	610	CLA	C3B-C4B	2.09	1.48	1.42
31	B	616	CLA	C1B-NB	-2.09	1.35	1.37
31	Y	613	CLA	MG-NC	2.09	2.11	2.06
31	B	610	CLA	MG-NC	2.09	2.11	2.06
31	b	612	CLA	MG-NC	2.09	2.11	2.06
30	y	607	CHL	C2C-C3C	2.09	1.38	1.36
31	R	611	CLA	C1B-NB	-2.09	1.35	1.37
31	b	604	CLA	C1B-NB	-2.09	1.35	1.37
32	11	615	LHG	C4-C5	2.09	1.57	1.50
31	B	616	CLA	MG-NC	2.09	2.11	2.06
31	R	601	CLA	MG-NC	2.09	2.11	2.06
31	N	611	CLA	CAA-C2A	2.09	1.57	1.54
31	C	505	CLA	MG-NC	2.09	2.11	2.06
31	c	503	CLA	MG-NC	2.09	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	615	CLA	C1B-NB	-2.09	1.35	1.37
31	y	603	CLA	MG-NC	2.09	2.11	2.06
31	N	615	CLA	MG-NC	2.09	2.11	2.06
31	c	510	CLA	MG-NC	2.09	2.11	2.06
31	b	601	CLA	MG-NB	2.08	2.09	2.05
31	15	613	CLA	CAA-C2A	2.08	1.57	1.54
31	G	602	CLA	C3B-C4B	2.08	1.48	1.42
31	r	612	CLA	MG-NB	2.08	2.09	2.05
30	n	608	CHL	C2C-C3C	2.08	1.38	1.36
31	b	601	CLA	MG-NC	2.08	2.11	2.06
32	G	615	LHG	C24-C23	2.08	1.56	1.50
31	s	604	CLA	MG-NC	2.08	2.11	2.06
31	y	615	CLA	MG-NC	2.08	2.11	2.06
31	r	611	CLA	C1B-NB	-2.08	1.35	1.37
31	c	502	CLA	C1B-NB	-2.08	1.35	1.37
31	y	603	CLA	C1B-NB	-2.08	1.35	1.37
31	N	614	CLA	CAA-C2A	2.08	1.57	1.54
31	D	405	CLA	MG-NC	2.08	2.11	2.06
31	y	602	CLA	MG-NC	2.08	2.11	2.06
31	15	602	CLA	C3B-C4B	2.08	1.48	1.42
31	s	610	CLA	MG-NB	2.08	2.09	2.05
31	a	403	CLA	C1B-NB	-2.08	1.35	1.37
31	c	512	CLA	C1B-NB	-2.08	1.35	1.37
31	C	513	CLA	C1B-NB	-2.08	1.35	1.37
31	c	513	CLA	C1B-NB	-2.08	1.35	1.37
31	R	609	CLA	MG-NC	2.08	2.11	2.06
31	b	609	CLA	MG-NC	2.08	2.11	2.06
31	n	610	CLA	MG-NC	2.08	2.11	2.06
31	5	602	CLA	C3B-C4B	2.08	1.48	1.42
31	S	612	CLA	CHD-C1D	2.08	1.42	1.38
31	r	609	CLA	MG-NC	2.08	2.11	2.06
31	A	402	CLA	MG-NC	2.08	2.11	2.06
31	4	604	CLA	C3B-C4B	2.07	1.48	1.42
31	n	610	CLA	C3B-C4B	2.07	1.48	1.42
31	r	614	CLA	MG-NC	2.07	2.11	2.06
31	b	609	CLA	C1B-NB	-2.07	1.35	1.37
31	1	604	CLA	C3B-C4B	2.07	1.48	1.42
31	R	614	CLA	MG-NC	2.07	2.11	2.06
31	c	511	CLA	MG-NC	2.07	2.11	2.06
31	13	610	CLA	C3B-C4B	2.07	1.48	1.42
30	R	605	CHL	C2C-C3C	2.07	1.38	1.36
31	Y	602	CLA	MG-NC	2.07	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	607	CLA	MG-NC	2.07	2.11	2.06
31	g	602	CLA	C3B-C4B	2.07	1.48	1.42
31	n	615	CLA	CAA-C2A	2.07	1.57	1.54
32	R	621	LHG	C4-C5	2.07	1.57	1.50
31	B	602	CLA	MG-NC	2.07	2.11	2.06
31	c	514	CLA	MG-NC	2.07	2.11	2.06
31	d	402	CLA	C1B-NB	-2.07	1.35	1.37
31	4	604	CLA	MG-NC	2.07	2.11	2.06
31	b	602	CLA	C3B-C4B	2.07	1.48	1.42
31	b	610	CLA	MG-NB	2.07	2.09	2.05
31	b	612	CLA	MG-NB	2.07	2.09	2.05
31	d	404	CLA	MG-NC	2.07	2.11	2.06
31	a	404	CLA	MG-NB	2.07	2.09	2.05
31	c	502	CLA	MG-NB	2.07	2.09	2.05
31	B	601	CLA	C1B-NB	-2.07	1.35	1.37
31	12	602	CLA	C3B-C4B	2.07	1.48	1.42
31	G	602	CLA	MG-NC	2.07	2.11	2.06
31	D	404	CLA	C1B-NB	-2.07	1.35	1.37
31	2	602	CLA	C3B-C4B	2.06	1.48	1.42
31	n	615	CLA	MG-NC	2.06	2.11	2.06
31	15	609	CLA	C3B-C4B	2.06	1.48	1.42
31	C	508	CLA	MG-NC	2.06	2.11	2.06
32	L	102	LHG	C4-C5	2.06	1.57	1.50
30	y	605	CHL	C2C-C3C	2.06	1.38	1.36
31	12	611	CLA	C3B-C4B	2.06	1.48	1.42
31	Y	615	CLA	MG-NC	2.06	2.11	2.06
31	A	404	CLA	MG-NB	2.06	2.09	2.05
31	N	610	CLA	MG-NC	2.06	2.11	2.06
31	N	603	CLA	C1B-NB	-2.06	1.35	1.37
31	C	504	CLA	C1B-NB	-2.06	1.35	1.37
31	1	611	CLA	CAA-C2A	2.06	1.57	1.54
31	1	602	CLA	C3B-C4B	2.06	1.48	1.42
31	13	602	CLA	C3B-C4B	2.06	1.48	1.42
31	b	602	CLA	MG-NC	2.06	2.11	2.06
31	6	602	CLA	MG-NC	2.06	2.11	2.06
31	r	609	CLA	C3B-C4B	2.05	1.48	1.42
31	N	613	CLA	MG-NC	2.05	2.11	2.06
31	r	612	CLA	MG-NC	2.05	2.11	2.06
31	5	610	CLA	MG-NC	2.05	2.11	2.06
31	15	611	CLA	C3B-C4B	2.05	1.48	1.42
31	6	602	CLA	C1B-NB	-2.05	1.35	1.37
31	s	602	CLA	C3B-C4B	2.05	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r	603	CLA	MG-NC	2.05	2.11	2.06
32	6	616	LHG	C4-C5	2.05	1.57	1.50
31	3	602	CLA	C3B-C4B	2.05	1.48	1.42
31	C	511	CLA	MG-NC	2.05	2.11	2.06
33	S	619	LUT	C22-C23	-2.05	1.50	1.52
31	c	504	CLA	C1B-NB	-2.05	1.35	1.37
31	A	404	CLA	MG-NC	2.05	2.11	2.06
31	2	604	CLA	CAA-C2A	2.05	1.57	1.54
31	n	602	CLA	C3B-C4B	2.05	1.48	1.42
31	C	502	CLA	MG-NC	2.05	2.11	2.06
31	c	502	CLA	MG-NC	2.05	2.11	2.06
31	n	614	CLA	CAA-C2A	2.05	1.57	1.54
31	2	604	CLA	C1B-NB	-2.05	1.35	1.37
30	5	605	CHL	O1D-CGD	2.05	1.26	1.21
31	3	602	CLA	MG-NC	2.05	2.11	2.06
31	A	403	CLA	C1B-NB	-2.05	1.35	1.37
31	3	615	CLA	MG-NC	2.05	2.11	2.06
31	B	612	CLA	MG-NC	2.05	2.11	2.06
31	r	601	CLA	MG-NC	2.05	2.11	2.06
31	C	509	CLA	C3B-C4B	2.05	1.48	1.42
32	3	616	LHG	C4-C5	2.05	1.57	1.50
30	16	608	CHL	C2C-C3C	2.05	1.38	1.36
31	y	615	CLA	MG-NB	2.05	2.09	2.05
31	4	614	CLA	C3B-C4B	2.05	1.48	1.42
31	C	514	CLA	MG-NC	2.05	2.11	2.06
30	2	605	CHL	O1D-CGD	2.05	1.26	1.21
31	c	505	CLA	MG-NC	2.04	2.11	2.06
31	C	507	CLA	C1B-NB	-2.04	1.35	1.37
30	r	605	CHL	C2C-C3C	2.04	1.38	1.36
33	5	614	LUT	C22-C23	-2.04	1.50	1.52
31	4	602	CLA	C3B-C4B	2.04	1.48	1.42
31	Y	615	CLA	MG-NB	2.04	2.09	2.05
31	16	602	CLA	C3B-C4B	2.04	1.48	1.42
30	3	608	CHL	C2C-C3C	2.04	1.38	1.36
30	2	601	CHL	O1D-CGD	2.04	1.26	1.21
31	11	611	CLA	C3B-C4B	2.04	1.48	1.42
31	14	612	CLA	C3B-C4B	2.04	1.48	1.42
31	C	510	CLA	MG-NC	2.04	2.11	2.06
31	3	615	CLA	MG-NB	2.04	2.09	2.05
31	C	505	CLA	C1B-NB	-2.04	1.35	1.37
31	A	403	CLA	C3D-C4D	-2.04	1.39	1.44
31	s	612	CLA	C1B-NB	-2.04	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	403	CLA	MG-NC	2.04	2.11	2.06
31	Y	610	CLA	MG-NC	2.04	2.11	2.06
31	5	610	CLA	C3B-C4B	2.04	1.48	1.42
31	2	610	CLA	MG-NC	2.04	2.11	2.06
32	n	616	LHG	C4-C5	2.04	1.57	1.50
31	n	602	CLA	C1B-NB	-2.04	1.35	1.37
31	N	615	CLA	CAA-C2A	2.04	1.57	1.54
31	Y	603	CLA	MG-NC	2.04	2.11	2.06
31	d	402	CLA	C3D-C4D	-2.04	1.39	1.44
31	C	511	CLA	MG-NB	2.04	2.09	2.05
31	5	613	CLA	C3B-C4B	2.04	1.48	1.42
31	d	405	CLA	MG-NC	2.04	2.11	2.06
31	2	611	CLA	CAA-C2A	2.04	1.57	1.54
31	2	613	CLA	MG-NC	2.04	2.11	2.06
31	2	610	CLA	C3B-C4B	2.04	1.48	1.42
31	C	503	CLA	MG-NC	2.04	2.11	2.06
31	r	610	CLA	C3B-C4B	2.04	1.48	1.42
31	A	404	CLA	C1B-NB	-2.04	1.35	1.37
31	y	612	CLA	C1B-NB	-2.04	1.35	1.37
31	12	613	CLA	C3B-C4B	2.04	1.48	1.42
31	R	609	CLA	C3B-C4B	2.04	1.48	1.42
30	14	607	CHL	O1D-CGD	2.03	1.26	1.21
31	2	611	CLA	C3B-C4B	2.03	1.48	1.42
32	D	409	LHG	C24-C23	2.03	1.56	1.50
31	a	403	CLA	C3B-C4B	2.03	1.48	1.42
31	3	604	CLA	C1B-NB	-2.03	1.35	1.37
31	n	603	CLA	C1B-NB	-2.03	1.35	1.37
31	16	610	CLA	C3B-C4B	2.03	1.48	1.42
31	r	603	CLA	C3B-C4B	2.03	1.48	1.42
31	b	607	CLA	C1B-NB	-2.03	1.35	1.37
31	S	610	CLA	MG-NC	2.03	2.11	2.06
31	2	612	CLA	C3B-C4B	2.03	1.48	1.42
30	Y	608	CHL	C3D-C2D	-2.03	1.36	1.39
31	c	509	CLA	C3B-C4B	2.03	1.48	1.42
31	12	612	CLA	CAA-C2A	2.03	1.57	1.54
31	3	613	CLA	C1B-NB	-2.03	1.35	1.37
31	N	602	CLA	C1B-NB	-2.03	1.35	1.37
33	11	616	LUT	C22-C23	-2.03	1.50	1.52
30	R	607	CHL	C3D-C2D	-2.03	1.36	1.39
31	4	604	CLA	CAA-C2A	2.03	1.57	1.54
31	14	614	CLA	C3B-C4B	2.03	1.48	1.42
32	l	102	LHG	C4-C5	2.03	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	615	CLA	C1B-NB	-2.03	1.35	1.37
31	R	611	CLA	C3B-C4B	2.03	1.48	1.42
32	S	617	LHG	C4-C5	2.03	1.57	1.50
30	4	606	CHL	O1D-CGD	2.03	1.26	1.21
31	13	604	CLA	C1B-NB	-2.03	1.35	1.37
31	5	604	CLA	C3B-C4B	2.03	1.48	1.42
31	3	602	CLA	C1B-NB	-2.03	1.35	1.37
30	5	601	CHL	O1D-CGD	2.03	1.26	1.21
31	3	604	CLA	CAA-C2A	2.03	1.57	1.54
31	b	601	CLA	C1B-NB	-2.03	1.35	1.37
31	14	602	CLA	C3B-C4B	2.03	1.48	1.42
31	A	402	CLA	C3B-C4B	2.03	1.48	1.42
31	2	604	CLA	C3B-C4B	2.03	1.48	1.42
32	s	621	LHG	C24-C23	2.03	1.56	1.50
31	b	615	CLA	C1B-NB	-2.03	1.35	1.37
31	g	610	CLA	MG-NC	2.03	2.11	2.06
31	B	602	CLA	C3B-C4B	2.02	1.48	1.42
31	C	510	CLA	MG-NB	2.02	2.09	2.05
30	11	608	CHL	O1D-CGD	2.02	1.26	1.21
31	2	613	CLA	C3B-C4B	2.02	1.48	1.42
31	N	602	CLA	C3B-C4B	2.02	1.48	1.42
31	A	403	CLA	MG-NB	2.02	2.09	2.05
31	a	404	CLA	MG-NC	2.02	2.11	2.06
31	c	508	CLA	C1B-NB	-2.02	1.35	1.37
31	1	614	CLA	C3B-C4B	2.02	1.48	1.42
30	2	606	CHL	O1D-CGD	2.02	1.26	1.21
32	S	621	LHG	C24-C23	2.02	1.56	1.50
31	3	615	CLA	C1B-NB	-2.02	1.35	1.37
30	N	601	CHL	C3D-C2D	-2.02	1.36	1.39
31	c	511	CLA	MG-NB	2.02	2.09	2.05
31	n	614	CLA	CMD-C2D	2.02	1.54	1.50
30	13	608	CHL	C2C-C3C	2.02	1.38	1.36
31	r	608	CLA	MG-NC	2.02	2.11	2.06
31	B	609	CLA	C1B-NB	-2.02	1.35	1.37
31	y	602	CLA	C1B-NB	-2.02	1.35	1.37
31	6	602	CLA	C3B-C4B	2.02	1.48	1.42
31	C	504	CLA	C3B-C4B	2.02	1.48	1.42
31	y	610	CLA	MG-NC	2.02	2.11	2.06
31	B	612	CLA	MG-NB	2.02	2.09	2.05
31	14	613	CLA	C3B-C4B	2.02	1.48	1.42
31	b	606	CLA	C3B-C4B	2.02	1.48	1.42
31	s	612	CLA	C3B-C4B	2.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	604	CLA	MG-NC	2.02	2.11	2.06
31	C	512	CLA	C1B-NB	-2.02	1.35	1.37
30	14	606	CHL	O1D-CGD	2.01	1.26	1.21
31	n	615	CLA	C3B-C4B	2.01	1.48	1.42
30	N	608	CHL	C2C-C3C	2.01	1.38	1.36
31	6	615	CLA	C1B-NB	-2.01	1.35	1.37
31	b	611	CLA	C3B-C4B	2.01	1.48	1.42
31	c	505	CLA	C1B-NB	-2.01	1.35	1.37
31	16	610	CLA	MG-NC	2.01	2.11	2.06
31	N	602	CLA	MG-NC	2.01	2.11	2.06
31	3	610	CLA	C3B-C4B	2.01	1.48	1.42
31	R	608	CLA	C3B-C4B	2.01	1.48	1.42
31	3	614	CLA	CAA-C2A	2.01	1.57	1.54
31	s	610	CLA	MG-NC	2.01	2.11	2.06
31	Y	610	CLA	C1B-NB	-2.01	1.35	1.37
31	n	611	CLA	CAA-C2A	2.01	1.57	1.54
31	s	610	CLA	C3B-C4B	2.01	1.48	1.42
31	s	611	CLA	C3B-C4B	2.01	1.48	1.42
31	16	611	CLA	C3B-C4B	2.01	1.48	1.42
32	d	409	LHG	C4-C5	2.01	1.57	1.50
31	6	604	CLA	C1B-NB	-2.01	1.35	1.37
31	11	602	CLA	C3B-C4B	2.01	1.48	1.42
31	3	615	CLA	C3B-C4B	2.01	1.48	1.42
31	2	602	CLA	C1B-NB	-2.01	1.35	1.37
31	r	612	CLA	C1B-NB	-2.01	1.35	1.37
31	12	604	CLA	C3B-C4B	2.01	1.48	1.42
31	B	614	CLA	C3B-C4B	2.01	1.48	1.42
30	1	606	CHL	O1D-CGD	2.01	1.26	1.21
30	s	607	CHL	O1D-CGD	2.01	1.26	1.21
31	S	602	CLA	C3B-C4B	2.01	1.48	1.42
31	6	615	CLA	C3B-C4B	2.01	1.48	1.42
31	6	604	CLA	CAA-C2A	2.01	1.57	1.54
31	c	507	CLA	C1B-NB	-2.01	1.35	1.37
31	s	611	CLA	C1B-NB	-2.01	1.35	1.37
31	11	614	CLA	C3B-C4B	2.01	1.48	1.42
31	d	402	CLA	MG-NB	2.01	2.09	2.05
31	R	608	CLA	MG-NC	2.01	2.11	2.06
30	2	608	CHL	O1D-CGD	2.00	1.26	1.21
31	16	604	CLA	C1B-NB	-2.00	1.35	1.37
31	R	614	CLA	C1B-NB	-2.00	1.35	1.37
31	B	611	CLA	C3B-C4B	2.00	1.48	1.42
31	S	609	CLA	C3B-C4B	2.00	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	11	604	CLA	CAA-C2A	2.00	1.57	1.54
30	1	605	CHL	O1D-CGD	2.00	1.26	1.21
30	5	606	CHL	O1D-CGD	2.00	1.26	1.21
32	N	616	LHG	C4-C5	2.00	1.57	1.50

All (4456) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	y	606	CHL	C1B-CHB-C4A	12.77	129.54	121.32
30	2	601	CHL	C1B-CHB-C4A	12.74	129.52	121.32
30	Y	606	CHL	C1B-CHB-C4A	12.66	129.47	121.32
30	4	605	CHL	C1B-CHB-C4A	12.61	129.43	121.32
30	y	605	CHL	C1B-CHB-C4A	12.58	129.41	121.32
30	n	601	CHL	C1B-CHB-C4A	12.53	129.39	121.32
30	6	605	CHL	C1B-CHB-C4A	12.52	129.38	121.32
30	G	606	CHL	C1B-CHB-C4A	12.48	129.35	121.32
30	N	601	CHL	C1B-CHB-C4A	12.48	129.35	121.32
30	N	606	CHL	C1B-CHB-C4A	12.48	129.35	121.32
30	g	606	CHL	C1B-CHB-C4A	12.45	129.33	121.32
30	S	601	CHL	C1B-CHB-C4A	12.44	129.32	121.32
30	n	606	CHL	C1B-CHB-C4A	12.43	129.32	121.32
30	1	605	CHL	C1B-CHB-C4A	12.42	129.31	121.32
30	1	606	CHL	C1B-CHB-C4A	12.39	129.29	121.32
30	4	606	CHL	C1B-CHB-C4A	12.39	129.29	121.32
30	3	605	CHL	C1B-CHB-C4A	12.38	129.29	121.32
30	s	601	CHL	C1B-CHB-C4A	12.35	129.27	121.32
30	16	601	CHL	C1B-CHB-C4A	12.35	129.27	121.32
30	13	601	CHL	C1B-CHB-C4A	12.34	129.26	121.32
30	2	606	CHL	C1B-CHB-C4A	12.33	129.26	121.32
30	s	606	CHL	C1B-CHB-C4A	12.33	129.25	121.32
30	R	607	CHL	C1B-CHB-C4A	12.30	129.24	121.32
30	12	608	CHL	C1B-CHB-C4A	12.29	129.23	121.32
30	r	607	CHL	C1B-CHB-C4A	12.29	129.23	121.32
30	y	607	CHL	C1B-CHB-C4A	12.29	129.23	121.32
30	11	606	CHL	C1B-CHB-C4A	12.28	129.22	121.32
30	5	606	CHL	C1B-CHB-C4A	12.27	129.22	121.32
30	r	605	CHL	C1B-CHB-C4A	12.26	129.21	121.32
30	R	605	CHL	C1B-CHB-C4A	12.26	129.21	121.32
30	6	601	CHL	C1B-CHB-C4A	12.23	129.19	121.32
30	Y	607	CHL	C1B-CHB-C4A	12.23	129.19	121.32
30	6	608	CHL	C1B-CHB-C4A	12.21	129.18	121.32
30	2	608	CHL	C1B-CHB-C4A	12.21	129.18	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	601	CHL	C1B-CHB-C4A	12.20	129.17	121.32
30	S	606	CHL	C1B-CHB-C4A	12.19	129.16	121.32
30	3	601	CHL	C1B-CHB-C4A	12.17	129.15	121.32
30	y	601	CHL	C1B-CHB-C4A	12.16	129.15	121.32
30	5	608	CHL	C1B-CHB-C4A	12.16	129.15	121.32
30	5	607	CHL	C1B-CHB-C4A	12.16	129.15	121.32
30	4	608	CHL	C1B-CHB-C4A	12.15	129.14	121.32
30	G	608	CHL	C1B-CHB-C4A	12.15	129.14	121.32
30	g	601	CHL	C1B-CHB-C4A	12.14	129.13	121.32
30	R	606	CHL	C1B-CHB-C4A	12.14	129.13	121.32
30	G	601	CHL	C1B-CHB-C4A	12.13	129.13	121.32
30	3	608	CHL	C1B-CHB-C4A	12.12	129.12	121.32
30	12	606	CHL	C1B-CHB-C4A	12.12	129.12	121.32
30	13	608	CHL	C1B-CHB-C4A	12.11	129.11	121.32
30	6	607	CHL	C1B-CHB-C4A	12.11	129.11	121.32
30	16	605	CHL	C1B-CHB-C4A	12.10	129.11	121.32
30	16	606	CHL	C1B-CHB-C4A	12.09	129.10	121.32
30	g	608	CHL	C1B-CHB-C4A	12.08	129.09	121.32
30	13	605	CHL	C1B-CHB-C4A	12.07	129.09	121.32
30	1	608	CHL	C1B-CHB-C4A	12.07	129.09	121.32
30	N	609	CHL	C1B-CHB-C4A	12.07	129.09	121.32
30	s	608	CHL	C1B-CHB-C4A	12.06	129.08	121.32
30	15	608	CHL	C1B-CHB-C4A	12.05	129.07	121.32
30	6	606	CHL	C1B-CHB-C4A	12.05	129.07	121.32
30	14	601	CHL	C1B-CHB-C4A	12.03	129.06	121.32
30	3	606	CHL	C1B-CHB-C4A	12.03	129.06	121.32
30	y	608	CHL	C1B-CHB-C4A	12.02	129.05	121.32
30	16	609	CHL	C1B-CHB-C4A	12.01	129.05	121.32
30	3	607	CHL	C1B-CHB-C4A	12.01	129.05	121.32
30	11	601	CHL	C1B-CHB-C4A	12.00	129.04	121.32
30	r	606	CHL	C1B-CHB-C4A	12.00	129.04	121.32
30	4	609	CHL	C1B-CHB-C4A	11.99	129.04	121.32
30	1	609	CHL	C1B-CHB-C4A	11.98	129.03	121.32
30	13	606	CHL	C1B-CHB-C4A	11.98	129.03	121.32
30	15	606	CHL	C1B-CHB-C4A	11.98	129.03	121.32
30	n	609	CHL	C1B-CHB-C4A	11.97	129.02	121.32
30	16	608	CHL	C1B-CHB-C4A	11.97	129.02	121.32
30	13	607	CHL	C1B-CHB-C4A	11.96	129.02	121.32
30	S	608	CHL	C1B-CHB-C4A	11.96	129.02	121.32
30	3	609	CHL	C1B-CHB-C4A	11.96	129.02	121.32
30	s	607	CHL	C1B-CHB-C4A	11.96	129.01	121.32
30	6	609	CHL	C1B-CHB-C4A	11.95	129.01	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	605	CHL	C1B-CHB-C4A	11.95	129.01	121.32
30	16	607	CHL	C1B-CHB-C4A	11.94	129.00	121.32
30	2	607	CHL	C1B-CHB-C4A	11.94	129.00	121.32
30	S	607	CHL	C1B-CHB-C4A	11.92	128.99	121.32
30	12	601	CHL	C1B-CHB-C4A	11.92	128.99	121.32
30	G	609	CHL	C1B-CHB-C4A	11.91	128.98	121.32
30	11	605	CHL	C1B-CHB-C4A	11.90	128.98	121.32
30	1	607	CHL	C1B-CHB-C4A	11.89	128.97	121.32
30	15	601	CHL	C1B-CHB-C4A	11.88	128.96	121.32
30	Y	608	CHL	C1B-CHB-C4A	11.87	128.96	121.32
30	n	607	CHL	C1B-CHB-C4A	11.87	128.96	121.32
30	g	609	CHL	C1B-CHB-C4A	11.87	128.96	121.32
30	11	607	CHL	C1B-CHB-C4A	11.87	128.96	121.32
30	N	605	CHL	C1B-CHB-C4A	11.87	128.96	121.32
30	5	601	CHL	C1B-CHB-C4A	11.86	128.95	121.32
30	g	605	CHL	C1B-CHB-C4A	11.85	128.94	121.32
30	14	607	CHL	C1B-CHB-C4A	11.84	128.94	121.32
30	2	605	CHL	C1B-CHB-C4A	11.83	128.94	121.32
30	5	605	CHL	C1B-CHB-C4A	11.82	128.92	121.32
30	N	607	CHL	C1B-CHB-C4A	11.81	128.92	121.32
30	Y	609	CHL	C1B-CHB-C4A	11.81	128.92	121.32
30	14	606	CHL	C1B-CHB-C4A	11.79	128.91	121.32
30	n	605	CHL	C1B-CHB-C4A	11.79	128.91	121.32
30	15	607	CHL	C1B-CHB-C4A	11.78	128.90	121.32
30	N	608	CHL	C1B-CHB-C4A	11.78	128.90	121.32
30	14	605	CHL	C1B-CHB-C4A	11.76	128.89	121.32
30	14	608	CHL	C1B-CHB-C4A	11.75	128.88	121.32
30	1	601	CHL	C1B-CHB-C4A	11.75	128.88	121.32
30	4	607	CHL	C1B-CHB-C4A	11.75	128.88	121.32
30	4	601	CHL	C1B-CHB-C4A	11.75	128.88	121.32
30	n	608	CHL	C1B-CHB-C4A	11.73	128.87	121.32
30	G	605	CHL	C1B-CHB-C4A	11.72	128.86	121.32
30	G	607	CHL	C1B-CHB-C4A	11.71	128.86	121.32
30	y	609	CHL	C1B-CHB-C4A	11.71	128.86	121.32
30	12	607	CHL	C1B-CHB-C4A	11.67	128.83	121.32
30	13	609	CHL	C1B-CHB-C4A	11.63	128.80	121.32
30	g	607	CHL	C1B-CHB-C4A	11.62	128.79	121.32
30	5	609	CHL	C1B-CHB-C4A	11.46	128.69	121.32
30	12	605	CHL	C1B-CHB-C4A	11.45	128.69	121.32
31	c	510	CLA	C4A-NA-C1A	11.40	111.88	106.68
31	C	510	CLA	C4A-NA-C1A	11.36	111.86	106.68
30	15	605	CHL	C1B-CHB-C4A	11.31	128.60	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	613	CLA	C4A-NA-C1A	11.31	111.84	106.68
31	b	613	CLA	C4A-NA-C1A	11.28	111.82	106.68
30	2	609	CHL	C1B-CHB-C4A	11.27	128.57	121.32
30	14	609	CHL	C1B-CHB-C4A	11.25	128.56	121.32
30	11	609	CHL	C1B-CHB-C4A	11.15	128.49	121.32
31	c	508	CLA	C4A-NA-C1A	11.14	111.76	106.68
31	B	612	CLA	C4A-NA-C1A	11.12	111.75	106.68
31	b	612	CLA	C4A-NA-C1A	10.87	111.64	106.68
31	2	603	CLA	C4A-NA-C1A	10.80	111.61	106.68
31	16	613	CLA	C4A-NA-C1A	10.77	111.59	106.68
31	n	603	CLA	C4A-NA-C1A	10.76	111.59	106.68
30	11	608	CHL	C1B-CHB-C4A	10.75	128.24	121.32
31	S	603	CLA	C4A-NA-C1A	10.71	111.57	106.68
31	c	511	CLA	C4A-NA-C1A	10.71	111.56	106.68
31	R	603	CLA	C4A-NA-C1A	10.70	111.56	106.68
31	6	603	CLA	C4A-NA-C1A	10.69	111.56	106.68
31	5	603	CLA	C4A-NA-C1A	10.68	111.55	106.68
31	C	511	CLA	C4A-NA-C1A	10.62	111.53	106.68
31	s	603	CLA	C4A-NA-C1A	10.60	111.52	106.68
31	13	613	CLA	C4A-NA-C1A	10.60	111.51	106.68
31	r	613	CLA	C4A-NA-C1A	10.59	111.51	106.68
31	C	503	CLA	C4A-NA-C1A	10.58	111.51	106.68
31	c	503	CLA	C4A-NA-C1A	10.58	111.51	106.68
31	15	603	CLA	C4A-NA-C1A	10.55	111.49	106.68
31	N	612	CLA	C4A-NA-C1A	10.55	111.49	106.68
31	R	613	CLA	C4A-NA-C1A	10.54	111.49	106.68
31	n	612	CLA	C4A-NA-C1A	10.54	111.49	106.68
31	g	603	CLA	C4A-NA-C1A	10.53	111.48	106.68
31	G	603	CLA	C4A-NA-C1A	10.51	111.48	106.68
31	13	603	CLA	C4A-NA-C1A	10.49	111.47	106.68
31	3	603	CLA	C4A-NA-C1A	10.45	111.45	106.68
31	B	615	CLA	C4A-NA-C1A	10.44	111.44	106.68
31	S	615	CLA	C4A-NA-C1A	10.43	111.44	106.68
31	B	616	CLA	C4A-NA-C1A	10.42	111.43	106.68
31	y	614	CLA	C4A-NA-C1A	10.40	111.42	106.68
31	N	613	CLA	C4A-NA-C1A	10.38	111.42	106.68
31	Y	603	CLA	C4A-NA-C1A	10.38	111.41	106.68
31	12	603	CLA	C4A-NA-C1A	10.37	111.41	106.68
31	1	603	CLA	C4A-NA-C1A	10.37	111.41	106.68
31	16	602	CLA	C4A-NA-C1A	10.36	111.41	106.68
31	1	614	CLA	C4A-NA-C1A	10.36	111.41	106.68
31	r	603	CLA	C4A-NA-C1A	10.35	111.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	612	CLA	C4A-NA-C1A	10.34	111.39	106.68
31	b	615	CLA	C4A-NA-C1A	10.33	111.39	106.68
31	b	605	CLA	C4A-NA-C1A	10.32	111.39	106.68
31	B	610	CLA	C4A-NA-C1A	10.30	111.38	106.68
31	c	504	CLA	C4A-NA-C1A	10.30	111.38	106.68
31	g	612	CLA	C4A-NA-C1A	10.30	111.38	106.68
31	s	615	CLA	C4A-NA-C1A	10.30	111.38	106.68
31	b	610	CLA	C4A-NA-C1A	10.29	111.37	106.68
31	4	603	CLA	C4A-NA-C1A	10.28	111.37	106.68
31	y	603	CLA	C4A-NA-C1A	10.27	111.36	106.68
31	Y	614	CLA	C4A-NA-C1A	10.27	111.36	106.68
31	C	504	CLA	C4A-NA-C1A	10.24	111.35	106.68
31	4	604	CLA	C4A-NA-C1A	10.24	111.35	106.68
31	D	404	CLA	C4A-NA-C1A	10.23	111.34	106.68
31	B	607	CLA	C4A-NA-C1A	10.22	111.34	106.68
31	N	615	CLA	C4A-NA-C1A	10.21	111.34	106.68
31	4	614	CLA	C4A-NA-C1A	10.18	111.32	106.68
31	c	512	CLA	C4A-NA-C1A	10.18	111.32	106.68
31	b	616	CLA	C4A-NA-C1A	10.17	111.32	106.68
31	r	611	CLA	C4A-NA-C1A	10.16	111.31	106.68
31	B	605	CLA	C4A-NA-C1A	10.16	111.31	106.68
31	3	612	CLA	C4A-NA-C1A	10.16	111.31	106.68
31	N	602	CLA	C4A-NA-C1A	10.15	111.31	106.68
31	N	603	CLA	C4A-NA-C1A	10.13	111.30	106.68
31	s	611	CLA	C4A-NA-C1A	10.13	111.30	106.68
31	b	607	CLA	C4A-NA-C1A	10.09	111.28	106.68
31	16	612	CLA	C4A-NA-C1A	10.09	111.28	106.68
31	n	615	CLA	C4A-NA-C1A	10.09	111.28	106.68
31	C	506	CLA	C4A-NA-C1A	10.08	111.28	106.68
31	6	612	CLA	C4A-NA-C1A	10.07	111.28	106.68
31	S	602	CLA	C4A-NA-C1A	10.05	111.27	106.68
31	15	610	CLA	C4A-NA-C1A	10.04	111.26	106.68
31	S	609	CLA	C4A-NA-C1A	10.04	111.26	106.68
31	C	512	CLA	C4A-NA-C1A	10.03	111.25	106.68
31	R	614	CLA	C4A-NA-C1A	10.03	111.25	106.68
31	c	506	CLA	C4A-NA-C1A	10.02	111.25	106.68
31	S	611	CLA	C4A-NA-C1A	10.00	111.24	106.68
31	14	614	CLA	C4A-NA-C1A	10.00	111.24	106.68
31	B	604	CLA	C4A-NA-C1A	9.99	111.24	106.68
31	c	513	CLA	C4A-NA-C1A	9.98	111.23	106.68
31	11	604	CLA	C4A-NA-C1A	9.97	111.23	106.68
31	b	604	CLA	C4A-NA-C1A	9.97	111.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	6	614	CLA	C4A-NA-C1A	9.97	111.23	106.68
31	3	615	CLA	C4A-NA-C1A	9.96	111.22	106.68
31	R	611	CLA	C4A-NA-C1A	9.96	111.22	106.68
31	13	612	CLA	C4A-NA-C1A	9.96	111.22	106.68
31	C	513	CLA	C4A-NA-C1A	9.95	111.22	106.68
31	6	615	CLA	C4A-NA-C1A	9.95	111.22	106.68
31	5	612	CLA	C4A-NA-C1A	9.94	111.21	106.68
31	12	610	CLA	C4A-NA-C1A	9.92	111.21	106.68
31	g	602	CLA	C4A-NA-C1A	9.92	111.20	106.68
31	r	610	CLA	C4A-NA-C1A	9.92	111.20	106.68
31	13	602	CLA	C4A-NA-C1A	9.91	111.20	106.68
31	a	403	CLA	C4A-NA-C1A	9.91	111.20	106.68
31	14	602	CLA	C4A-NA-C1A	9.90	111.20	106.68
31	A	402	CLA	C4A-NA-C1A	9.89	111.19	106.68
31	13	611	CLA	C4A-NA-C1A	9.89	111.19	106.68
31	Y	611	CLA	C4A-NA-C1A	9.89	111.19	106.68
31	3	613	CLA	C4A-NA-C1A	9.89	111.19	106.68
31	11	614	CLA	C4A-NA-C1A	9.88	111.19	106.68
31	n	602	CLA	C4A-NA-C1A	9.85	111.17	106.68
31	11	602	CLA	C4A-NA-C1A	9.85	111.17	106.68
31	15	609	CLA	C4A-NA-C1A	9.84	111.17	106.68
31	y	604	CLA	C4A-NA-C1A	9.83	111.16	106.68
31	2	612	CLA	C4A-NA-C1A	9.82	111.16	106.68
31	G	611	CLA	C4A-NA-C1A	9.81	111.16	106.68
31	4	611	CLA	C4A-NA-C1A	9.79	111.15	106.68
31	s	612	CLA	C4A-NA-C1A	9.79	111.14	106.68
31	G	604	CLA	C4A-NA-C1A	9.76	111.13	106.68
31	N	604	CLA	C4A-NA-C1A	9.76	111.13	106.68
31	N	611	CLA	C4A-NA-C1A	9.76	111.13	106.68
31	B	614	CLA	C4A-NA-C1A	9.76	111.13	106.68
31	6	613	CLA	C4A-NA-C1A	9.75	111.13	106.68
31	13	615	CLA	C4A-NA-C1A	9.75	111.13	106.68
31	y	611	CLA	C4A-NA-C1A	9.75	111.13	106.68
31	Y	604	CLA	C4A-NA-C1A	9.75	111.12	106.68
31	r	602	CLA	C4A-NA-C1A	9.74	111.12	106.68
31	11	610	CLA	C4A-NA-C1A	9.74	111.12	106.68
31	16	611	CLA	C4A-NA-C1A	9.73	111.12	106.68
31	n	611	CLA	C4A-NA-C1A	9.73	111.12	106.68
31	G	613	CLA	C4A-NA-C1A	9.72	111.11	106.68
31	g	604	CLA	C4A-NA-C1A	9.71	111.11	106.68
31	g	611	CLA	C4A-NA-C1A	9.70	111.11	106.68
31	s	602	CLA	C4A-NA-C1A	9.70	111.11	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	16	614	CLA	C4A-NA-C1A	9.70	111.10	106.68
31	14	610	CLA	C4A-NA-C1A	9.69	111.10	106.68
31	b	614	CLA	C4A-NA-C1A	9.69	111.10	106.68
31	n	604	CLA	C4A-NA-C1A	9.69	111.10	106.68
31	2	602	CLA	C4A-NA-C1A	9.69	111.10	106.68
31	B	611	CLA	C4A-NA-C1A	9.69	111.10	106.68
31	1	602	CLA	C4A-NA-C1A	9.68	111.09	106.68
31	14	611	CLA	C4A-NA-C1A	9.68	111.09	106.68
31	b	609	CLA	C4A-NA-C1A	9.68	111.09	106.68
31	B	601	CLA	C4A-NA-C1A	9.67	111.09	106.68
31	16	603	CLA	C4A-NA-C1A	9.67	111.09	106.68
31	Y	602	CLA	C4A-NA-C1A	9.66	111.09	106.68
31	4	602	CLA	C4A-NA-C1A	9.66	111.09	106.68
31	y	612	CLA	C4A-NA-C1A	9.66	111.09	106.68
31	B	603	CLA	C4A-NA-C1A	9.66	111.08	106.68
31	b	603	CLA	C4A-NA-C1A	9.66	111.08	106.68
31	Y	612	CLA	C4A-NA-C1A	9.65	111.08	106.68
31	g	613	CLA	C4A-NA-C1A	9.65	111.08	106.68
31	11	613	CLA	C4A-NA-C1A	9.63	111.07	106.68
31	b	601	CLA	C4A-NA-C1A	9.63	111.07	106.68
31	d	404	CLA	C4A-NA-C1A	9.61	111.06	106.68
31	G	610	CLA	C4A-NA-C1A	9.60	111.06	106.68
31	1	613	CLA	C4A-NA-C1A	9.60	111.06	106.68
31	13	614	CLA	C4A-NA-C1A	9.57	111.05	106.68
31	14	604	CLA	C4A-NA-C1A	9.57	111.05	106.68
31	A	406	CLA	C4A-NA-C1A	9.57	111.05	106.68
31	n	614	CLA	C4A-NA-C1A	9.57	111.04	106.68
31	16	610	CLA	C4A-NA-C1A	9.56	111.04	106.68
31	b	611	CLA	C4A-NA-C1A	9.54	111.03	106.68
31	R	602	CLA	C4A-NA-C1A	9.53	111.03	106.68
31	14	613	CLA	C4A-NA-C1A	9.53	111.03	106.68
31	11	611	CLA	C4A-NA-C1A	9.52	111.02	106.68
31	12	613	CLA	C4A-NA-C1A	9.52	111.02	106.68
31	y	610	CLA	C4A-NA-C1A	9.52	111.02	106.68
31	B	609	CLA	C4A-NA-C1A	9.52	111.02	106.68
31	r	609	CLA	C4A-NA-C1A	9.50	111.01	106.68
31	S	613	CLA	C4A-NA-C1A	9.49	111.01	106.68
31	C	507	CLA	C4A-NA-C1A	9.49	111.01	106.68
31	14	603	CLA	C4A-NA-C1A	9.48	111.00	106.68
31	C	505	CLA	C4A-NA-C1A	9.47	111.00	106.68
31	G	614	CLA	C4A-NA-C1A	9.47	111.00	106.68
31	a	407	CLA	C4A-NA-C1A	9.47	111.00	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	610	CLA	C4A-NA-C1A	9.46	111.00	106.68
31	14	612	CLA	C4A-NA-C1A	9.45	110.99	106.68
31	2	611	CLA	C4A-NA-C1A	9.43	110.98	106.68
31	g	610	CLA	C4A-NA-C1A	9.43	110.98	106.68
31	y	602	CLA	C4A-NA-C1A	9.42	110.98	106.68
31	c	505	CLA	C4A-NA-C1A	9.41	110.97	106.68
31	1	612	CLA	C4A-NA-C1A	9.39	110.96	106.68
31	g	614	CLA	C4A-NA-C1A	9.38	110.96	106.68
31	s	613	CLA	C4A-NA-C1A	9.36	110.95	106.68
31	n	610	CLA	C4A-NA-C1A	9.35	110.94	106.68
31	11	603	CLA	C4A-NA-C1A	9.35	110.94	106.68
31	y	615	CLA	C4A-NA-C1A	9.34	110.94	106.68
31	11	612	CLA	C4A-NA-C1A	9.34	110.94	106.68
31	3	614	CLA	C4A-NA-C1A	9.33	110.94	106.68
31	5	611	CLA	C4A-NA-C1A	9.33	110.94	106.68
31	N	610	CLA	C4A-NA-C1A	9.33	110.94	106.68
31	13	610	CLA	C4A-NA-C1A	9.32	110.93	106.68
31	c	509	CLA	C4A-NA-C1A	9.32	110.93	106.68
31	r	614	CLA	C4A-NA-C1A	9.30	110.92	106.68
31	C	509	CLA	C4A-NA-C1A	9.28	110.92	106.68
31	Y	615	CLA	C4A-NA-C1A	9.28	110.91	106.68
31	1	604	CLA	C4A-NA-C1A	9.28	110.91	106.68
31	S	610	CLA	C4A-NA-C1A	9.27	110.91	106.68
31	1	611	CLA	C4A-NA-C1A	9.26	110.91	106.68
31	12	609	CLA	C4A-NA-C1A	9.23	110.89	106.68
31	c	507	CLA	C4A-NA-C1A	9.21	110.88	106.68
31	B	602	CLA	C4A-NA-C1A	9.20	110.88	106.68
31	b	602	CLA	C4A-NA-C1A	9.19	110.87	106.68
31	2	604	CLA	C4A-NA-C1A	9.17	110.86	106.68
31	r	612	CLA	C4A-NA-C1A	9.16	110.86	106.68
31	C	502	CLA	C4A-NA-C1A	9.16	110.86	106.68
31	15	611	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	6	602	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	6	604	CLA	C4A-NA-C1A	9.13	110.84	106.68
31	12	611	CLA	C4A-NA-C1A	9.13	110.84	106.68
31	r	604	CLA	C4A-NA-C1A	9.12	110.84	106.68
31	s	610	CLA	C4A-NA-C1A	9.12	110.84	106.68
31	R	604	CLA	C4A-NA-C1A	9.11	110.83	106.68
31	2	610	CLA	C4A-NA-C1A	9.10	110.83	106.68
31	R	609	CLA	C4A-NA-C1A	9.10	110.83	106.68
31	12	602	CLA	C4A-NA-C1A	9.09	110.82	106.68
31	5	602	CLA	C4A-NA-C1A	9.08	110.82	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	502	CLA	C4A-NA-C1A	9.07	110.82	106.68
31	S	604	CLA	C4A-NA-C1A	9.07	110.82	106.68
31	3	602	CLA	C4A-NA-C1A	9.06	110.81	106.68
31	15	602	CLA	C4A-NA-C1A	9.03	110.80	106.68
31	3	604	CLA	C4A-NA-C1A	9.02	110.80	106.68
31	15	612	CLA	C4A-NA-C1A	9.02	110.79	106.68
31	S	605	CLA	C4A-NA-C1A	9.00	110.79	106.68
31	s	609	CLA	C4A-NA-C1A	9.00	110.79	106.68
31	3	610	CLA	C4A-NA-C1A	8.98	110.78	106.68
31	s	605	CLA	C4A-NA-C1A	8.97	110.77	106.68
31	12	612	CLA	C4A-NA-C1A	8.94	110.76	106.68
31	y	613	CLA	C4A-NA-C1A	8.93	110.75	106.68
31	s	604	CLA	C4A-NA-C1A	8.90	110.74	106.68
31	Y	613	CLA	C4A-NA-C1A	8.89	110.73	106.68
31	4	613	CLA	C4A-NA-C1A	8.86	110.72	106.68
31	5	604	CLA	C4A-NA-C1A	8.85	110.72	106.68
31	b	608	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	B	608	CLA	C4A-NA-C1A	8.75	110.67	106.68
31	R	610	CLA	C4A-NA-C1A	8.74	110.67	106.68
31	a	404	CLA	C4A-NA-C1A	8.70	110.65	106.68
31	13	604	CLA	C4A-NA-C1A	8.67	110.64	106.68
31	16	604	CLA	C4A-NA-C1A	8.63	110.62	106.68
31	3	611	CLA	C4A-NA-C1A	8.61	110.61	106.68
31	N	614	CLA	C4A-NA-C1A	8.60	110.60	106.68
31	4	612	CLA	C4A-NA-C1A	8.58	110.59	106.68
31	A	404	CLA	C4A-NA-C1A	8.56	110.58	106.68
31	s	614	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	S	614	CLA	C4A-NA-C1A	8.54	110.58	106.68
31	r	608	CLA	C4A-NA-C1A	8.52	110.57	106.68
31	R	608	CLA	C4A-NA-C1A	8.51	110.56	106.68
31	G	602	CLA	C4A-NA-C1A	8.50	110.56	106.68
31	r	601	CLA	C4A-NA-C1A	8.49	110.55	106.68
31	d	405	CLA	C4A-NA-C1A	8.46	110.54	106.68
31	15	613	CLA	C4A-NA-C1A	8.46	110.54	106.68
31	c	514	CLA	C4A-NA-C1A	8.45	110.53	106.68
31	5	610	CLA	C4A-NA-C1A	8.45	110.53	106.68
31	6	611	CLA	C4A-NA-C1A	8.44	110.53	106.68
31	A	403	CLA	C4A-NA-C1A	8.41	110.52	106.68
31	5	613	CLA	C4A-NA-C1A	8.39	110.51	106.68
31	R	601	CLA	C4A-NA-C1A	8.35	110.49	106.68
31	D	405	CLA	C4A-NA-C1A	8.35	110.49	106.68
31	15	604	CLA	C4A-NA-C1A	8.32	110.48	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	606	CLA	C4A-NA-C1A	8.32	110.47	106.68
31	C	514	CLA	C4A-NA-C1A	8.31	110.47	106.68
31	6	610	CLA	C4A-NA-C1A	8.28	110.45	106.68
31	16	615	CLA	C4A-NA-C1A	8.16	110.40	106.68
31	2	613	CLA	C4A-NA-C1A	8.13	110.39	106.68
31	B	606	CLA	C4A-NA-C1A	8.08	110.36	106.68
31	n	613	CLA	C4A-NA-C1A	8.06	110.36	106.68
31	d	402	CLA	C4A-NA-C1A	8.04	110.34	106.68
31	12	604	CLA	C4A-NA-C1A	8.02	110.34	106.68
31	1	610	CLA	C4A-NA-C1A	7.79	110.23	106.68
30	n	608	CHL	O2D-CGD-CBD	7.74	119.45	110.95
31	R	612	CLA	C4A-NA-C1A	7.73	110.21	106.68
30	s	607	CHL	O2D-CGD-CBD	7.71	119.42	110.95
30	13	607	CHL	O2D-CGD-CBD	7.62	119.32	110.95
30	S	607	CHL	O2D-CGD-CBD	7.58	119.28	110.95
31	S	612	CLA	C4A-NA-C1A	7.54	110.12	106.68
30	6	605	CHL	O2D-CGD-CBD	7.51	119.20	110.95
30	3	605	CHL	O2D-CGD-CBD	7.46	119.14	110.95
30	16	607	CHL	O2D-CGD-CBD	7.41	119.09	110.95
30	11	601	CHL	O2D-CGD-CBD	7.35	119.02	110.95
30	n	605	CHL	O2D-CGD-CBD	7.29	118.96	110.95
30	Y	601	CHL	O2D-CGD-CBD	7.27	118.93	110.95
30	G	605	CHL	O2D-CGD-CBD	7.22	118.88	110.95
30	y	601	CHL	O2D-CGD-CBD	7.21	118.87	110.95
30	y	609	CHL	O2D-CGD-CBD	7.20	118.86	110.95
30	Y	605	CHL	O2D-CGD-CBD	7.20	118.86	110.95
30	g	605	CHL	O2D-CGD-CBD	7.19	118.85	110.95
30	Y	609	CHL	O2D-CGD-CBD	7.11	118.76	110.95
30	y	605	CHL	O2D-CGD-CBD	7.07	118.72	110.95
30	n	601	CHL	O2D-CGD-CBD	7.06	118.70	110.95
30	G	607	CHL	O2D-CGD-CBD	7.05	118.70	110.95
30	13	606	CHL	O2D-CGD-CBD	7.03	118.67	110.95
30	y	608	CHL	O2D-CGD-CBD	7.02	118.66	110.95
30	g	607	CHL	O2D-CGD-CBD	7.02	118.66	110.95
30	N	601	CHL	O2D-CGD-CBD	7.01	118.65	110.95
30	N	605	CHL	O2D-CGD-CBD	7.01	118.65	110.95
30	6	607	CHL	O2D-CGD-CBD	7.01	118.65	110.95
30	13	609	CHL	O2D-CGD-CBD	7.00	118.64	110.95
30	14	601	CHL	O2D-CGD-CBD	6.99	118.62	110.95
30	Y	608	CHL	O2D-CGD-CBD	6.93	118.56	110.95
30	16	606	CHL	O2D-CGD-CBD	6.92	118.55	110.95
30	G	601	CHL	O2D-CGD-CBD	6.91	118.54	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	g	601	CHL	O2D-CGD-CBD	6.91	118.54	110.95
30	N	606	CHL	O2D-CGD-CBD	6.91	118.54	110.95
30	r	605	CHL	O2D-CGD-CBD	6.91	118.53	110.95
30	N	609	CHL	O2D-CGD-CBD	6.90	118.53	110.95
30	n	609	CHL	O2D-CGD-CBD	6.90	118.53	110.95
30	s	608	CHL	O2D-CGD-CBD	6.90	118.52	110.95
30	N	607	CHL	O2D-CGD-CBD	6.88	118.50	110.95
30	n	606	CHL	O2D-CGD-CBD	6.87	118.50	110.95
30	2	608	CHL	O2D-CGD-CBD	6.87	118.50	110.95
30	3	607	CHL	O2D-CGD-CBD	6.87	118.49	110.95
30	n	607	CHL	O2D-CGD-CBD	6.87	118.49	110.95
30	4	608	CHL	O2D-CGD-CBD	6.85	118.48	110.95
30	13	605	CHL	O2D-CGD-CBD	6.85	118.47	110.95
30	12	605	CHL	O2D-CGD-CBD	6.84	118.47	110.95
30	2	607	CHL	O2D-CGD-CBD	6.84	118.46	110.95
30	5	607	CHL	O2D-CGD-CBD	6.83	118.45	110.95
30	12	606	CHL	O2D-CGD-CBD	6.82	118.44	110.95
30	4	607	CHL	O2D-CGD-CBD	6.82	118.44	110.95
30	16	605	CHL	O2D-CGD-CBD	6.82	118.44	110.95
30	3	606	CHL	O2D-CGD-CBD	6.81	118.42	110.95
30	6	606	CHL	O2D-CGD-CBD	6.80	118.42	110.95
30	5	608	CHL	O2D-CGD-CBD	6.79	118.41	110.95
30	G	606	CHL	O2D-CGD-CBD	6.79	118.41	110.95
30	1	608	CHL	O2D-CGD-CBD	6.78	118.40	110.95
30	1	607	CHL	O2D-CGD-CBD	6.77	118.38	110.95
30	R	606	CHL	O2D-CGD-CBD	6.75	118.36	110.95
30	5	606	CHL	O2D-CGD-CBD	6.74	118.35	110.95
30	s	606	CHL	O2D-CGD-CBD	6.74	118.35	110.95
30	1	606	CHL	O2D-CGD-CBD	6.73	118.34	110.95
30	15	605	CHL	O2D-CGD-CBD	6.71	118.32	110.95
30	14	608	CHL	O2D-CGD-CBD	6.66	118.27	110.95
30	S	608	CHL	O2D-CGD-CBD	6.66	118.27	110.95
30	s	601	CHL	O2D-CGD-CBD	6.66	118.26	110.95
30	S	601	CHL	O2D-CGD-CBD	6.66	118.26	110.95
30	g	606	CHL	O2D-CGD-CBD	6.64	118.24	110.95
30	R	605	CHL	O2D-CGD-CBD	6.64	118.24	110.95
30	2	606	CHL	O2D-CGD-CBD	6.62	118.22	110.95
30	6	601	CHL	O2D-CGD-CBD	6.58	118.17	110.95
30	11	608	CHL	O2D-CGD-CBD	6.56	118.15	110.95
30	G	608	CHL	O2D-CGD-CBD	6.55	118.14	110.95
30	3	609	CHL	O2D-CGD-CBD	6.54	118.14	110.95
30	Y	607	CHL	O2D-CGD-CBD	6.53	118.12	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	14	605	CHL	O2D-CGD-CBD	6.52	118.11	110.95
30	r	606	CHL	O2D-CGD-CBD	6.51	118.10	110.95
30	y	607	CHL	O2D-CGD-CBD	6.49	118.08	110.95
30	6	608	CHL	O2D-CGD-CBD	6.49	118.08	110.95
30	3	601	CHL	O2D-CGD-CBD	6.48	118.07	110.95
30	g	608	CHL	O2D-CGD-CBD	6.48	118.07	110.95
30	S	606	CHL	O2D-CGD-CBD	6.47	118.05	110.95
30	N	608	CHL	O2D-CGD-CBD	6.45	118.03	110.95
30	6	609	CHL	O2D-CGD-CBD	6.45	118.03	110.95
30	y	606	CHL	O2D-CGD-CBD	6.43	118.02	110.95
30	5	609	CHL	O2D-CGD-CBD	6.39	117.97	110.95
30	3	608	CHL	O2D-CGD-CBD	6.39	117.96	110.95
30	12	607	CHL	O2D-CGD-CBD	6.37	117.95	110.95
30	11	609	CHL	O2D-CGD-CBD	6.37	117.95	110.95
30	15	606	CHL	O2D-CGD-CBD	6.36	117.94	110.95
30	16	609	CHL	O2D-CGD-CBD	6.35	117.92	110.95
30	4	605	CHL	O2D-CGD-CBD	6.34	117.91	110.95
30	g	609	CHL	O2D-CGD-CBD	6.33	117.91	110.95
30	15	607	CHL	O2D-CGD-CBD	6.32	117.90	110.95
30	11	605	CHL	O2D-CGD-CBD	6.32	117.89	110.95
30	13	607	CHL	C4D-CHA-CBD	-6.31	102.60	108.97
30	14	607	CHL	O2D-CGD-CBD	6.29	117.86	110.95
30	G	609	CHL	O2D-CGD-CBD	6.29	117.86	110.95
30	1	601	CHL	O2D-CGD-CBD	6.28	117.85	110.95
30	R	607	CHL	O2D-CGD-CBD	6.27	117.84	110.95
30	Y	606	CHL	O2D-CGD-CBD	6.26	117.82	110.95
30	r	607	CHL	O2D-CGD-CBD	6.24	117.80	110.95
30	1	605	CHL	O2D-CGD-CBD	6.23	117.80	110.95
30	15	601	CHL	O2D-CGD-CBD	6.23	117.80	110.95
30	12	601	CHL	O2D-CGD-CBD	6.23	117.79	110.95
30	16	601	CHL	O2D-CGD-CBD	6.20	117.76	110.95
30	2	609	CHL	O2D-CGD-CBD	6.20	117.76	110.95
30	4	606	CHL	O2D-CGD-CBD	6.15	117.71	110.95
30	14	609	CHL	O2D-CGD-CBD	6.13	117.68	110.95
30	13	608	CHL	O2D-CGD-CBD	6.11	117.66	110.95
30	4	601	CHL	O2D-CGD-CBD	6.11	117.66	110.95
30	5	601	CHL	O2D-CGD-CBD	6.08	117.63	110.95
30	16	608	CHL	O2D-CGD-CBD	6.03	117.58	110.95
30	13	601	CHL	O2D-CGD-CBD	6.03	117.57	110.95
31	C	508	CLA	C4A-NA-C1A	5.98	109.41	106.68
30	11	607	CHL	O2D-CGD-CBD	5.96	117.50	110.95
30	y	609	CHL	C4D-CHA-CBD	-5.93	102.99	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	605	CHL	O2D-CGD-CBD	5.90	117.43	110.95
30	4	609	CHL	O2D-CGD-CBD	5.85	117.37	110.95
30	Y	609	CHL	C4D-CHA-CBD	-5.83	103.09	108.97
30	2	605	CHL	O2D-CGD-CBD	5.82	117.34	110.95
30	11	606	CHL	O2D-CGD-CBD	5.78	117.30	110.95
30	15	608	CHL	O2D-CGD-CBD	5.78	117.30	110.95
30	12	608	CHL	O2D-CGD-CBD	5.74	117.26	110.95
30	1	609	CHL	O2D-CGD-CBD	5.73	117.25	110.95
30	s	607	CHL	C4D-CHA-CBD	-5.73	103.19	108.97
30	16	607	CHL	C4D-CHA-CBD	-5.72	103.21	108.97
30	4	607	CHL	C4D-CHA-CBD	-5.71	103.21	108.97
30	14	606	CHL	O2D-CGD-CBD	5.69	117.20	110.95
30	4	606	CHL	C4D-CHA-CBD	-5.66	103.26	108.97
30	2	601	CHL	O2D-CGD-CBD	5.60	117.10	110.95
30	S	607	CHL	C4D-CHA-CBD	-5.53	103.39	108.97
30	6	607	CHL	C4D-CHA-CBD	-5.53	103.39	108.97
30	3	607	CHL	C4D-CHA-CBD	-5.52	103.41	108.97
30	5	605	CHL	C4D-CHA-CBD	-5.10	103.83	108.97
30	n	608	CHL	C4D-CHA-CBD	-5.08	103.85	108.97
30	1	607	CHL	C4D-CHA-CBD	-5.07	103.86	108.97
30	n	609	CHL	C4D-CHA-CBD	-5.05	103.88	108.97
30	N	609	CHL	C4D-CHA-CBD	-5.03	103.90	108.97
30	N	601	CHL	C4D-CHA-CBD	-5.02	103.90	108.97
30	2	605	CHL	C4D-CHA-CBD	-5.02	103.91	108.97
30	11	608	CHL	C4D-CHA-CBD	-5.01	103.92	108.97
30	12	608	CHL	C4D-CHA-CBD	-4.92	104.01	108.97
30	2	601	CHL	C4D-CHA-CBD	-4.90	104.03	108.97
30	14	608	CHL	C4D-CHA-CBD	-4.90	104.03	108.97
30	2	601	CHL	C3D-C4D-CHA	4.87	115.95	108.54
30	S	601	CHL	C4D-CHA-CBD	-4.87	104.06	108.97
30	15	608	CHL	C4D-CHA-CBD	-4.82	104.11	108.97
30	y	605	CHL	C3D-C4D-CHA	4.81	115.85	108.54
30	11	605	CHL	C3D-C4D-CHA	4.80	115.83	108.54
31	b	606	CLA	O2D-CGD-CBD	4.78	119.58	111.23
30	s	601	CHL	C4D-CHA-CBD	-4.78	104.15	108.97
30	11	605	CHL	C4D-CHA-CBD	-4.77	104.16	108.97
31	B	606	CLA	O2D-CGD-CBD	4.76	119.55	111.23
30	y	605	CHL	C4D-CHA-CBD	-4.75	104.18	108.97
30	12	601	CHL	C4D-CHA-CBD	-4.73	104.20	108.97
31	R	610	CLA	O2D-CGD-CBD	4.73	119.50	111.23
30	3	605	CHL	C3D-C4D-CHA	4.72	115.71	108.54
31	r	610	CLA	O2D-CGD-CBD	4.71	119.47	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	601	CHL	C4D-CHA-CBD	-4.71	104.22	108.97
30	4	606	CHL	CBC-CAC-C3C	-4.71	106.13	112.87
30	1	606	CHL	C4D-CHA-CBD	-4.70	104.23	108.97
31	B	601	CLA	O2D-CGD-CBD	4.69	119.43	111.23
30	g	608	CHL	C4D-CHA-CBD	-4.68	104.25	108.97
30	6	605	CHL	C3D-C4D-CHA	4.68	115.65	108.54
30	G	606	CHL	C3D-C4D-CHA	4.67	115.64	108.54
30	Y	606	CHL	C4D-CHA-CBD	-4.67	104.26	108.97
31	B	612	CLA	O2D-CGD-CBD	4.67	119.39	111.23
30	11	601	CHL	C4D-CHA-CBD	-4.66	104.27	108.97
30	15	605	CHL	C3D-C4D-CHA	4.66	115.63	108.54
30	G	608	CHL	C4D-CHA-CBD	-4.65	104.28	108.97
30	15	607	CHL	C4D-CHA-CBD	-4.65	104.28	108.97
30	r	606	CHL	C3D-C4D-CHA	4.64	115.59	108.54
30	15	601	CHL	C4D-CHA-CBD	-4.63	104.30	108.97
30	G	607	CHL	C3D-C4D-CHA	4.63	115.58	108.54
30	12	605	CHL	C3D-C4D-CHA	4.63	115.58	108.54
30	S	608	CHL	C4D-CHA-CBD	-4.63	104.30	108.97
30	s	608	CHL	C4D-CHA-CBD	-4.63	104.30	108.97
30	Y	606	CHL	C3D-C4D-CHA	4.63	115.58	108.54
30	4	605	CHL	C3D-C4D-CHA	4.63	115.57	108.54
30	y	607	CHL	C3D-C4D-CHA	4.62	115.57	108.54
30	R	606	CHL	C3D-C4D-CHA	4.62	115.57	108.54
30	r	606	CHL	C4D-CHA-CBD	-4.62	104.31	108.97
30	11	608	CHL	C3D-C4D-CHA	4.62	115.56	108.54
31	b	601	CLA	O2D-CGD-CBD	4.62	119.30	111.23
30	12	607	CHL	C4D-CHA-CBD	-4.62	104.31	108.97
30	11	607	CHL	C4D-CHA-CBD	-4.61	104.31	108.97
31	b	612	CLA	O2D-CGD-CBD	4.61	119.30	111.23
30	y	606	CHL	C4D-CHA-CBD	-4.61	104.32	108.97
30	g	607	CHL	C3D-C4D-CHA	4.61	115.55	108.54
31	c	502	CLA	O2D-CGD-CBD	4.61	119.29	111.23
30	n	601	CHL	C4D-CHA-CBD	-4.61	104.32	108.97
30	g	608	CHL	C3D-C4D-CHA	4.61	115.54	108.54
30	Y	607	CHL	C3D-C4D-CHA	4.61	115.54	108.54
30	12	606	CHL	C4D-CHA-CBD	-4.61	104.32	108.97
30	1	605	CHL	C3D-C4D-CHA	4.60	115.53	108.54
30	G	608	CHL	C3D-C4D-CHA	4.60	115.53	108.54
30	g	606	CHL	C3D-C4D-CHA	4.60	115.53	108.54
30	1	606	CHL	C3D-C4D-CHA	4.60	115.53	108.54
31	c	506	CLA	O2D-CGD-CBD	4.59	119.26	111.23
30	3	605	CHL	C4D-CHA-CBD	-4.59	104.34	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	s	606	CHL	C3D-C4D-CHA	4.58	115.51	108.54
30	12	606	CHL	C3D-C4D-CHA	4.58	115.51	108.54
30	y	606	CHL	C3D-C4D-CHA	4.58	115.51	108.54
30	3	607	CHL	C3D-C4D-CHA	4.58	115.50	108.54
30	1	601	CHL	C4D-CHA-CBD	-4.58	104.35	108.97
30	11	607	CHL	C3D-C4D-CHA	4.57	115.49	108.54
31	4	610	CLA	C4A-NA-C1A	4.57	108.77	106.68
31	C	506	CLA	O2D-CGD-CBD	4.57	119.22	111.23
30	15	606	CHL	C3D-C4D-CHA	4.57	115.48	108.54
30	11	606	CHL	C3D-C4D-CHA	4.57	115.48	108.54
30	2	606	CHL	C4D-CHA-CBD	-4.56	104.37	108.97
30	6	607	CHL	C3D-C4D-CHA	4.56	115.48	108.54
30	y	608	CHL	C3D-C4D-CHA	4.56	115.47	108.54
30	15	608	CHL	C3D-C4D-CHA	4.56	115.46	108.54
30	S	606	CHL	C3D-C4D-CHA	4.55	115.46	108.54
30	Y	605	CHL	C3D-C4D-CHA	4.55	115.46	108.54
30	n	607	CHL	C3D-C4D-CHA	4.55	115.46	108.54
30	14	606	CHL	C3D-C4D-CHA	4.55	115.46	108.54
30	15	607	CHL	C3D-C4D-CHA	4.55	115.46	108.54
30	6	605	CHL	C4D-CHA-CBD	-4.55	104.38	108.97
30	3	606	CHL	C3D-C4D-CHA	4.55	115.46	108.54
30	Y	608	CHL	C3D-C4D-CHA	4.55	115.46	108.54
30	N	607	CHL	C3D-C4D-CHA	4.55	115.45	108.54
30	N	601	CHL	C3D-C4D-CHA	4.55	115.45	108.54
30	15	606	CHL	C4D-CHA-CBD	-4.54	104.39	108.97
30	12	608	CHL	C3D-C4D-CHA	4.54	115.44	108.54
30	R	607	CHL	C3D-C4D-CHA	4.54	115.44	108.54
30	6	601	CHL	C3D-C4D-CHA	4.54	115.43	108.54
30	N	608	CHL	C3D-C4D-CHA	4.53	115.43	108.54
30	n	605	CHL	C3D-C4D-CHA	4.53	115.42	108.54
30	6	606	CHL	C3D-C4D-CHA	4.53	115.42	108.54
30	Y	601	CHL	C3D-C4D-CHA	4.52	115.42	108.54
30	N	605	CHL	C3D-C4D-CHA	4.52	115.41	108.54
30	G	605	CHL	C3D-C4D-CHA	4.52	115.41	108.54
30	14	609	CHL	C4D-CHA-CBD	-4.51	104.42	108.97
30	13	607	CHL	C3D-C4D-CHA	4.51	115.40	108.54
30	11	609	CHL	C4D-CHA-CBD	-4.51	104.42	108.97
30	r	607	CHL	C3D-C4D-CHA	4.51	115.40	108.54
30	14	607	CHL	C4D-CHA-CBD	-4.51	104.42	108.97
30	16	608	CHL	C3D-C4D-CHA	4.51	115.40	108.54
30	5	607	CHL	C3D-C4D-CHA	4.51	115.39	108.54
30	13	608	CHL	C3D-C4D-CHA	4.51	115.39	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	609	CHL	C3D-C4D-CHA	4.51	115.39	108.54
30	3	601	CHL	C3D-C4D-CHA	4.51	115.39	108.54
30	g	609	CHL	C3D-C4D-CHA	4.51	115.39	108.54
30	R	606	CHL	C4D-CHA-CBD	-4.50	104.43	108.97
30	g	605	CHL	C3D-C4D-CHA	4.50	115.38	108.54
30	1	607	CHL	C3D-C4D-CHA	4.50	115.37	108.54
30	1	605	CHL	C4D-CHA-CBD	-4.49	104.44	108.97
30	G	609	CHL	C3D-C4D-CHA	4.49	115.37	108.54
30	Y	609	CHL	C3D-C4D-CHA	4.49	115.37	108.54
30	5	608	CHL	C3D-C4D-CHA	4.49	115.36	108.54
30	12	607	CHL	C3D-C4D-CHA	4.49	115.36	108.54
30	4	601	CHL	C4D-CHA-CBD	-4.49	104.44	108.97
30	4	605	CHL	C4D-CHA-CBD	-4.49	104.44	108.97
30	R	605	CHL	C3D-C4D-CHA	4.49	115.36	108.54
30	2	608	CHL	C3D-C4D-CHA	4.48	115.36	108.54
30	y	601	CHL	C3D-C4D-CHA	4.48	115.36	108.54
30	16	601	CHL	C3D-C4D-CHA	4.48	115.36	108.54
30	n	601	CHL	C3D-C4D-CHA	4.48	115.36	108.54
30	2	609	CHL	C4D-CHA-CBD	-4.48	104.45	108.97
30	5	609	CHL	C3D-C4D-CHA	4.48	115.35	108.54
30	16	605	CHL	C3D-C4D-CHA	4.48	115.35	108.54
30	y	609	CHL	C3D-C4D-CHA	4.48	115.34	108.54
30	14	609	CHL	C3D-C4D-CHA	4.47	115.34	108.54
30	G	606	CHL	C4D-CHA-CBD	-4.47	104.46	108.97
30	1	608	CHL	C4D-CHA-CBD	-4.47	104.46	108.97
30	16	607	CHL	C3D-C4D-CHA	4.47	115.33	108.54
30	n	608	CHL	C3D-C4D-CHA	4.47	115.33	108.54
30	G	607	CHL	C4D-CHA-CBD	-4.47	104.46	108.97
30	Y	608	CHL	C4D-CHA-CBD	-4.47	104.46	108.97
30	4	601	CHL	C3D-C4D-CHA	4.47	115.33	108.54
30	16	606	CHL	C3D-C4D-CHA	4.47	115.33	108.54
30	14	605	CHL	C3D-C4D-CHA	4.47	115.33	108.54
30	5	605	CHL	C3D-C4D-CHA	4.46	115.33	108.54
30	n	606	CHL	C4D-CHA-CBD	-4.46	104.47	108.97
30	3	608	CHL	C3D-C4D-CHA	4.46	115.32	108.54
30	4	608	CHL	C3D-C4D-CHA	4.46	115.32	108.54
30	13	606	CHL	C3D-C4D-CHA	4.46	115.32	108.54
30	r	605	CHL	C3D-C4D-CHA	4.46	115.32	108.54
30	y	608	CHL	C4D-CHA-CBD	-4.46	104.47	108.97
30	3	609	CHL	C3D-C4D-CHA	4.45	115.31	108.54
30	2	609	CHL	C3D-C4D-CHA	4.45	115.31	108.54
30	6	608	CHL	C3D-C4D-CHA	4.45	115.31	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	S	607	CHL	C3D-C4D-CHA	4.45	115.31	108.54
30	2	605	CHL	C3D-C4D-CHA	4.45	115.31	108.54
30	5	609	CHL	C4D-CHA-CBD	-4.45	104.48	108.97
30	1	608	CHL	C3D-C4D-CHA	4.45	115.30	108.54
31	c	512	CLA	O2D-CGD-CBD	4.45	119.01	111.23
30	S	608	CHL	C3D-C4D-CHA	4.45	115.30	108.54
30	3	609	CHL	C4D-CHA-CBD	-4.45	104.48	108.97
30	6	609	CHL	C3D-C4D-CHA	4.45	115.30	108.54
30	s	607	CHL	C3D-C4D-CHA	4.45	115.30	108.54
30	1	601	CHL	C3D-C4D-CHA	4.44	115.30	108.54
30	2	607	CHL	C3D-C4D-CHA	4.44	115.29	108.54
30	13	609	CHL	C3D-C4D-CHA	4.44	115.29	108.54
30	s	608	CHL	C3D-C4D-CHA	4.44	115.29	108.54
30	1	609	CHL	C3D-C4D-CHA	4.44	115.29	108.54
30	5	606	CHL	C3D-C4D-CHA	4.44	115.29	108.54
30	6	609	CHL	C4D-CHA-CBD	-4.44	104.49	108.97
30	14	607	CHL	C3D-C4D-CHA	4.44	115.28	108.54
31	C	502	CLA	O2D-CGD-CBD	4.44	118.98	111.23
30	N	609	CHL	C3D-C4D-CHA	4.43	115.28	108.54
30	n	609	CHL	C3D-C4D-CHA	4.43	115.27	108.54
30	13	601	CHL	C3D-C4D-CHA	4.43	115.27	108.54
30	G	601	CHL	C3D-C4D-CHA	4.43	115.27	108.54
30	g	609	CHL	C4D-CHA-CBD	-4.43	104.50	108.97
30	4	609	CHL	C3D-C4D-CHA	4.42	115.27	108.54
30	S	601	CHL	C3D-C4D-CHA	4.42	115.27	108.54
30	13	605	CHL	C3D-C4D-CHA	4.42	115.26	108.54
30	16	609	CHL	C3D-C4D-CHA	4.42	115.26	108.54
30	5	601	CHL	C3D-C4D-CHA	4.42	115.25	108.54
30	g	601	CHL	C3D-C4D-CHA	4.42	115.25	108.54
30	4	607	CHL	C3D-C4D-CHA	4.41	115.25	108.54
31	C	512	CLA	O2D-CGD-CBD	4.41	118.94	111.23
30	g	607	CHL	C4D-CHA-CBD	-4.41	104.52	108.97
30	n	606	CHL	C3D-C4D-CHA	4.40	115.23	108.54
31	S	611	CLA	O2D-CGD-CBD	4.40	118.93	111.23
30	s	601	CHL	C3D-C4D-CHA	4.40	115.22	108.54
30	15	605	CHL	C4D-CHA-CBD	-4.40	104.53	108.97
30	G	609	CHL	C4D-CHA-CBD	-4.39	104.54	108.97
31	a	407	CLA	O2D-CGD-CBD	4.38	118.89	111.23
30	11	601	CHL	C3D-C4D-CHA	4.38	115.19	108.54
30	g	606	CHL	C4D-CHA-CBD	-4.38	104.55	108.97
30	N	608	CHL	C4D-CHA-CBD	-4.37	104.56	108.97
30	12	601	CHL	C3D-C4D-CHA	4.37	115.18	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	612	CLA	O2D-CGD-CBD	4.37	118.86	111.23
30	N	606	CHL	C3D-C4D-CHA	4.36	115.17	108.54
30	4	606	CHL	C3D-C4D-CHA	4.36	115.17	108.54
30	4	608	CHL	C4D-CHA-CBD	-4.36	104.57	108.97
31	c	508	CLA	O2D-CGD-CBD	4.36	118.85	111.23
30	14	601	CHL	C3D-C4D-CHA	4.36	115.16	108.54
30	14	608	CHL	C3D-C4D-CHA	4.35	115.15	108.54
30	s	606	CHL	C4D-CHA-CBD	-4.35	104.58	108.97
30	y	607	CHL	C4D-CHA-CBD	-4.35	104.58	108.97
30	N	606	CHL	C4D-CHA-CBD	-4.35	104.59	108.97
31	A	406	CLA	O2D-CGD-CBD	4.34	118.81	111.23
30	2	606	CHL	C3D-C4D-CHA	4.33	115.13	108.54
30	15	601	CHL	C3D-C4D-CHA	4.33	115.12	108.54
31	4	604	CLA	O2D-CGD-CBD	4.33	118.80	111.23
30	Y	607	CHL	C4D-CHA-CBD	-4.33	104.60	108.97
30	G	605	CHL	C4D-CHA-CBD	-4.33	104.60	108.97
30	y	601	CHL	C4D-CHA-CBD	-4.33	104.60	108.97
30	11	606	CHL	C4D-CHA-CBD	-4.32	104.61	108.97
31	C	508	CLA	O2D-CGD-CBD	4.32	118.78	111.23
30	12	605	CHL	C4D-CHA-CBD	-4.32	104.62	108.97
30	Y	601	CHL	C4D-CHA-CBD	-4.32	104.62	108.97
31	S	614	CLA	O2D-CGD-CBD	4.31	118.77	111.23
30	5	607	CHL	C4D-CHA-CBD	-4.31	104.62	108.97
30	g	605	CHL	C4D-CHA-CBD	-4.30	104.63	108.97
30	13	605	CHL	C4D-CHA-CBD	-4.30	104.63	108.97
31	d	405	CLA	O2D-CGD-CBD	4.30	118.74	111.23
30	n	605	CHL	C4D-CHA-CBD	-4.30	104.64	108.97
31	6	610	CLA	O2D-CGD-CBD	4.29	118.74	111.23
30	2	608	CHL	C4D-CHA-CBD	-4.29	104.64	108.97
31	C	510	CLA	O2D-CGD-CBD	4.29	118.73	111.23
31	2	603	CLA	O2D-CGD-CBD	4.29	118.72	111.23
30	6	601	CHL	C4D-CHA-CBD	-4.29	104.65	108.97
30	R	607	CHL	C4D-CHA-CBD	-4.28	104.65	108.97
30	R	605	CHL	C4D-CHA-CBD	-4.28	104.65	108.97
30	5	608	CHL	C4D-CHA-CBD	-4.28	104.66	108.97
30	3	601	CHL	C4D-CHA-CBD	-4.27	104.66	108.97
30	2	607	CHL	C4D-CHA-CBD	-4.27	104.66	108.97
30	S	606	CHL	C4D-CHA-CBD	-4.27	104.67	108.97
30	r	605	CHL	C4D-CHA-CBD	-4.27	104.67	108.97
31	C	513	CLA	O2D-CGD-CBD	4.27	118.69	111.23
30	Y	605	CHL	C4D-CHA-CBD	-4.27	104.67	108.97
30	6	606	CHL	C4D-CHA-CBD	-4.26	104.67	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	603	CLA	O2D-CGD-CBD	4.26	118.68	111.23
30	3	606	CHL	C4D-CHA-CBD	-4.25	104.68	108.97
30	r	607	CHL	C4D-CHA-CBD	-4.25	104.68	108.97
30	4	609	CHL	C4D-CHA-CBD	-4.25	104.68	108.97
31	s	611	CLA	O2D-CGD-CBD	4.25	118.66	111.23
31	5	603	CLA	O2D-CGD-CBD	4.24	118.65	111.23
30	13	608	CHL	C4D-CHA-CBD	-4.24	104.69	108.97
31	r	613	CLA	O2D-CGD-CBD	4.24	118.65	111.23
30	1	609	CHL	C4D-CHA-CBD	-4.24	104.69	108.97
31	R	608	CLA	O2D-CGD-CBD	4.24	118.64	111.23
30	16	605	CHL	C4D-CHA-CBD	-4.24	104.69	108.97
31	r	608	CLA	O2D-CGD-CBD	4.24	118.64	111.23
31	N	615	CLA	O2D-CGD-CBD	4.24	118.64	111.23
30	16	608	CHL	C4D-CHA-CBD	-4.24	104.69	108.97
30	14	606	CHL	C4D-CHA-CBD	-4.24	104.70	108.97
31	1	603	CLA	O2D-CGD-CBD	4.23	118.63	111.23
31	1	612	CLA	O2D-CGD-CBD	4.23	118.63	111.23
31	D	405	CLA	O2D-CGD-CBD	4.23	118.63	111.23
30	16	601	CHL	C4D-CHA-CBD	-4.23	104.70	108.97
30	5	601	CHL	C4D-CHA-CBD	-4.22	104.71	108.97
31	1	604	CLA	O2D-CGD-CBD	4.22	118.61	111.23
31	A	402	CLA	O2D-CGD-CBD	4.22	118.61	111.23
31	b	608	CLA	O2D-CGD-CBD	4.22	118.61	111.23
31	S	605	CLA	O2D-CGD-CBD	4.22	118.60	111.23
30	5	606	CHL	C4D-CHA-CBD	-4.21	104.72	108.97
31	a	403	CLA	O2D-CGD-CBD	4.21	118.58	111.23
31	C	508	CLA	C3B-C4B-NB	-4.21	106.78	110.53
31	S	612	CLA	O2D-CGD-CBD	4.20	118.58	111.23
31	c	513	CLA	O2D-CGD-CBD	4.20	118.58	111.23
30	N	605	CHL	C4D-CHA-CBD	-4.20	104.74	108.97
31	b	615	CLA	O2D-CGD-CBD	4.19	118.56	111.23
30	G	601	CHL	C4D-CHA-CBD	-4.19	104.74	108.97
31	b	610	CLA	O2D-CGD-CBD	4.19	118.56	111.23
31	s	614	CLA	O2D-CGD-CBD	4.19	118.56	111.23
31	B	615	CLA	O2D-CGD-CBD	4.19	118.55	111.23
31	s	605	CLA	O2D-CGD-CBD	4.19	118.55	111.23
30	g	601	CHL	C4D-CHA-CBD	-4.19	104.75	108.97
31	n	613	CLA	O2D-CGD-CBD	4.19	118.55	111.23
31	D	404	CLA	O2D-CGD-CBD	4.19	118.55	111.23
30	14	605	CHL	C4D-CHA-CBD	-4.19	104.75	108.97
31	B	610	CLA	O2D-CGD-CBD	4.18	118.55	111.23
31	r	604	CLA	O2D-CGD-CBD	4.18	118.54	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	611	CLA	O2D-CGD-CBD	4.18	118.54	111.23
30	16	606	CHL	C4D-CHA-CBD	-4.18	104.75	108.97
31	b	605	CLA	O2D-CGD-CBD	4.18	118.54	111.23
31	g	611	CLA	O2D-CGD-CBD	4.18	118.54	111.23
31	Y	611	CLA	O2D-CGD-CBD	4.18	118.54	111.23
31	N	610	CLA	O2D-CGD-CBD	4.18	118.54	111.23
30	N	607	CHL	C4D-CHA-CBD	-4.18	104.75	108.97
30	6	608	CHL	C4D-CHA-CBD	-4.18	104.76	108.97
30	3	608	CHL	C4D-CHA-CBD	-4.18	104.76	108.97
31	c	510	CLA	O2D-CGD-CBD	4.18	118.53	111.23
31	R	604	CLA	O2D-CGD-CBD	4.17	118.53	111.23
30	r	605	CHL	OBD-CAD-CBD	-4.17	119.70	125.82
31	B	604	CLA	O2D-CGD-CBD	4.17	118.52	111.23
31	15	613	CLA	O2D-CGD-CBD	4.17	118.52	111.23
30	G	608	CHL	CAA-C2A-C3A	-4.17	101.73	113.00
31	N	603	CLA	O2D-CGD-CBD	4.17	118.52	111.23
31	3	610	CLA	O2D-CGD-CBD	4.17	118.52	111.23
31	13	610	CLA	O2D-CGD-CBD	4.16	118.51	111.23
31	n	603	CLA	O2D-CGD-CBD	4.16	118.51	111.23
30	R	605	CHL	OBD-CAD-CBD	-4.16	119.72	125.82
31	g	614	CLA	O2D-CGD-CBD	4.16	118.50	111.23
30	13	606	CHL	C4D-CHA-CBD	-4.14	104.79	108.97
31	n	615	CLA	O2D-CGD-CBD	4.14	118.47	111.23
31	G	611	CLA	O2D-CGD-CBD	4.14	118.46	111.23
31	S	610	CLA	O2D-CGD-CBD	4.13	118.45	111.23
31	g	603	CLA	O2D-CGD-CBD	4.13	118.45	111.23
31	d	404	CLA	O2D-CGD-CBD	4.13	118.44	111.23
30	g	608	CHL	CAA-C2A-C3A	-4.13	101.85	113.00
31	c	509	CLA	O2D-CGD-CBD	4.13	118.44	111.23
31	b	604	CLA	O2D-CGD-CBD	4.12	118.44	111.23
31	r	609	CLA	O2D-CGD-CBD	4.12	118.44	111.23
31	R	609	CLA	O2D-CGD-CBD	4.12	118.44	111.23
31	16	610	CLA	O2D-CGD-CBD	4.12	118.42	111.23
31	4	612	CLA	O2D-CGD-CBD	4.11	118.42	111.23
31	Y	613	CLA	O2D-CGD-CBD	4.11	118.42	111.23
30	11	608	CHL	CAA-C2A-C3A	-4.11	101.89	113.00
31	1	611	CLA	O2D-CGD-CBD	4.11	118.42	111.23
31	C	514	CLA	O2D-CGD-CBD	4.11	118.42	111.23
30	4	601	CHL	CBC-CAC-C3C	-4.11	106.99	112.87
31	4	603	CLA	O2D-CGD-CBD	4.11	118.41	111.23
31	G	614	CLA	O2D-CGD-CBD	4.11	118.41	111.23
31	12	603	CLA	O2D-CGD-CBD	4.10	118.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	608	CLA	O2D-CGD-CBD	4.10	118.40	111.23
31	N	602	CLA	O2D-CGD-CBD	4.10	118.40	111.23
31	B	616	CLA	O2D-CGD-CBD	4.10	118.40	111.23
31	C	509	CLA	O2D-CGD-CBD	4.10	118.40	111.23
31	B	605	CLA	O2D-CGD-CBD	4.10	118.40	111.23
30	13	601	CHL	C4D-CHA-CBD	-4.10	104.83	108.97
31	N	613	CLA	O2D-CGD-CBD	4.10	118.39	111.23
30	13	609	CHL	C4D-CHA-CBD	-4.10	104.84	108.97
31	12	612	CLA	O2D-CGD-CBD	4.09	118.38	111.23
31	16	612	CLA	O2D-CGD-CBD	4.09	118.38	111.23
31	N	611	CLA	O2D-CGD-CBD	4.09	118.38	111.23
30	n	607	CHL	C4D-CHA-CBD	-4.09	104.85	108.97
31	C	507	CLA	O2D-CGD-CBD	4.09	118.37	111.23
31	B	603	CLA	O2D-CGD-CBD	4.09	118.37	111.23
31	G	610	CLA	O2D-CGD-CBD	4.08	118.37	111.23
31	c	507	CLA	O2D-CGD-CBD	4.08	118.36	111.23
31	y	613	CLA	O2D-CGD-CBD	4.08	118.35	111.23
31	y	615	CLA	O2D-CGD-CBD	4.07	118.34	111.23
31	b	603	CLA	O2D-CGD-CBD	4.07	118.34	111.23
30	1	601	CHL	CBC-CAC-C3C	-4.07	107.05	112.87
31	g	610	CLA	O2D-CGD-CBD	4.06	118.33	111.23
31	16	613	CLA	O2D-CGD-CBD	4.06	118.33	111.23
31	Y	610	CLA	O2D-CGD-CBD	4.06	118.32	111.23
31	n	611	CLA	O2D-CGD-CBD	4.06	118.32	111.23
31	13	615	CLA	O2D-CGD-CBD	4.05	118.32	111.23
31	b	614	CLA	O2D-CGD-CBD	4.05	118.31	111.23
30	14	607	CHL	CAA-C2A-C3A	-4.05	102.06	113.00
31	13	612	CLA	O2D-CGD-CBD	4.05	118.30	111.23
31	b	616	CLA	O2D-CGD-CBD	4.04	118.30	111.23
31	B	614	CLA	O2D-CGD-CBD	4.04	118.29	111.23
31	16	603	CLA	O2D-CGD-CBD	4.03	118.27	111.23
30	R	606	CHL	CAA-C2A-C3A	-4.02	102.12	113.00
31	12	610	CLA	O2D-CGD-CBD	4.02	118.27	111.23
31	G	603	CLA	O2D-CGD-CBD	4.02	118.26	111.23
31	13	613	CLA	O2D-CGD-CBD	4.02	118.25	111.23
31	Y	604	CLA	O2D-CGD-CBD	4.02	118.25	111.23
31	b	607	CLA	O2D-CGD-CBD	4.01	118.25	111.23
31	15	610	CLA	O2D-CGD-CBD	4.01	118.24	111.23
31	3	611	CLA	O2D-CGD-CBD	4.01	118.24	111.23
31	3	614	CLA	O2D-CGD-CBD	4.01	118.24	111.23
31	s	610	CLA	O2D-CGD-CBD	4.01	118.24	111.23
31	y	610	CLA	O2D-CGD-CBD	4.01	118.24	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	1	610	CLA	O2D-CGD-CBD	4.01	118.24	111.23
30	16	609	CHL	C4D-CHA-CBD	-4.01	104.93	108.97
31	r	601	CLA	O2D-CGD-CBD	4.00	118.22	111.23
31	b	612	CLA	C3B-C4B-NB	-4.00	106.96	110.53
31	b	602	CLA	O2D-CGD-CBD	4.00	118.22	111.23
31	n	610	CLA	O2D-CGD-CBD	4.00	118.22	111.23
31	y	604	CLA	O2D-CGD-CBD	3.99	118.20	111.23
30	r	606	CHL	CAA-C2A-C3A	-3.98	102.23	113.00
31	12	611	CLA	O2D-CGD-CBD	3.98	118.19	111.23
31	3	613	CLA	O2D-CGD-CBD	3.98	118.19	111.23
31	15	611	CLA	O2D-CGD-CBD	3.98	118.19	111.23
31	B	602	CLA	O2D-CGD-CBD	3.98	118.19	111.23
31	S	604	CLA	O2D-CGD-CBD	3.98	118.18	111.23
31	6	614	CLA	O2D-CGD-CBD	3.98	118.18	111.23
31	15	612	CLA	O2D-CGD-CBD	3.97	118.17	111.23
48	d	403	BCT	O2-C-O1	3.97	129.82	119.68
31	b	609	CLA	O2D-CGD-CBD	3.96	118.16	111.23
31	c	514	CLA	O2D-CGD-CBD	3.96	118.16	111.23
31	4	602	CLA	O2D-CGD-CBD	3.96	118.16	111.23
31	6	604	CLA	O2D-CGD-CBD	3.96	118.15	111.23
31	Y	615	CLA	O2D-CGD-CBD	3.96	118.15	111.23
31	N	614	CLA	O2D-CGD-CBD	3.95	118.14	111.23
31	y	612	CLA	O2D-CGD-CBD	3.94	118.12	111.23
48	D	403	BCT	O2-C-O1	3.94	129.76	119.68
31	c	503	CLA	O2D-CGD-CBD	3.94	118.12	111.23
31	6	611	CLA	O2D-CGD-CBD	3.94	118.12	111.23
31	C	503	CLA	O2D-CGD-CBD	3.94	118.12	111.23
31	B	612	CLA	C3B-C4B-NB	-3.94	107.02	110.53
35	R	616	XAT	C7-C8-C9	3.94	131.64	125.53
31	14	610	CLA	O2D-CGD-CBD	3.93	118.11	111.23
31	B	609	CLA	O2D-CGD-CBD	3.93	118.10	111.23
31	B	607	CLA	O2D-CGD-CBD	3.93	118.10	111.23
31	11	610	CLA	O2D-CGD-CBD	3.93	118.10	111.23
31	6	603	CLA	O2D-CGD-CBD	3.92	118.09	111.23
31	r	603	CLA	C3B-C4B-NB	-3.92	107.03	110.53
31	11	603	CLA	O2D-CGD-CBD	3.92	118.08	111.23
31	R	612	CLA	O2D-CGD-CBD	3.92	118.08	111.23
31	11	611	CLA	O2D-CGD-CBD	3.92	118.08	111.23
35	r	616	XAT	C7-C8-C9	3.92	131.61	125.53
31	y	610	CLA	C3B-C4B-NB	-3.92	107.03	110.53
31	C	505	CLA	O2D-CGD-CBD	3.91	118.07	111.23
31	c	505	CLA	O2D-CGD-CBD	3.91	118.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	612	CLA	O2D-CGD-CBD	3.90	118.06	111.23
31	n	614	CLA	O2D-CGD-CBD	3.90	118.05	111.23
31	Y	610	CLA	C3B-C4B-NB	-3.90	107.05	110.53
31	R	613	CLA	O2D-CGD-CBD	3.90	118.05	111.23
31	R	602	CLA	C3B-C4B-NB	-3.89	107.05	110.53
30	3	607	CHL	CAA-C2A-C3A	-3.89	102.49	113.00
31	11	614	CLA	O2D-CGD-CBD	3.89	118.02	111.23
30	14	608	CHL	CAA-C2A-C3A	-3.88	102.51	113.00
31	c	511	CLA	O2D-CGD-CBD	3.88	118.01	111.23
31	C	510	CLA	C3B-C4B-NB	-3.88	107.07	110.53
31	14	603	CLA	O2D-CGD-CBD	3.87	118.00	111.23
31	c	510	CLA	C3B-C4B-NB	-3.87	107.08	110.53
31	G	602	CLA	O2D-CGD-CBD	3.87	117.99	111.23
31	n	602	CLA	O2D-CGD-CBD	3.85	117.96	111.23
31	3	604	CLA	O2D-CGD-CBD	3.85	117.95	111.23
31	g	610	CLA	C3B-C4B-NB	-3.84	107.10	110.53
31	C	511	CLA	O2D-CGD-CBD	3.84	117.94	111.23
31	R	611	CLA	O2D-CGD-CBD	3.84	117.94	111.23
31	Y	614	CLA	O2D-CGD-CBD	3.83	117.93	111.23
30	13	605	CHL	CMA-C3A-C4A	-3.83	106.36	114.61
31	r	609	CLA	C3B-C4B-NB	-3.83	107.11	110.53
38	a	406	PHO	C4D-CHA-CBD	3.82	110.29	108.45
31	6	615	CLA	C3B-C4B-NB	-3.82	107.12	110.53
31	6	613	CLA	O2D-CGD-CBD	3.82	117.91	111.23
31	14	614	CLA	O2D-CGD-CBD	3.82	117.91	111.23
30	g	601	CHL	CMA-C3A-C4A	-3.82	106.39	114.61
31	s	609	CLA	O2D-CGD-CBD	3.82	117.90	111.23
31	14	611	CLA	O2D-CGD-CBD	3.81	117.90	111.23
30	6	607	CHL	CAA-C2A-C3A	-3.81	102.69	113.00
31	6	612	CLA	O2D-CGD-CBD	3.81	117.89	111.23
31	4	611	CLA	O2D-CGD-CBD	3.81	117.89	111.23
31	R	601	CLA	O2D-CGD-CBD	3.81	117.89	111.23
31	1	613	CLA	O2D-CGD-CBD	3.81	117.89	111.23
31	S	602	CLA	O2D-CGD-CBD	3.81	117.89	111.23
31	y	614	CLA	O2D-CGD-CBD	3.81	117.89	111.23
31	13	611	CLA	O2D-CGD-CBD	3.81	117.89	111.23
31	5	611	CLA	O2D-CGD-CBD	3.80	117.88	111.23
31	r	611	CLA	O2D-CGD-CBD	3.80	117.88	111.23
31	13	602	CLA	O2D-CGD-CBD	3.79	117.86	111.23
31	13	603	CLA	O2D-CGD-CBD	3.79	117.86	111.23
31	3	612	CLA	O2D-CGD-CBD	3.79	117.86	111.23
31	s	613	CLA	O2D-CGD-CBD	3.79	117.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	610	CLA	C3B-C4B-NB	-3.79	107.15	110.53
31	r	602	CLA	O2D-CGD-CBD	3.78	117.84	111.23
31	2	612	CLA	O2D-CGD-CBD	3.78	117.84	111.23
31	15	603	CLA	O2D-CGD-CBD	3.78	117.84	111.23
31	16	614	CLA	O2D-CGD-CBD	3.78	117.84	111.23
31	5	612	CLA	O2D-CGD-CBD	3.78	117.84	111.23
31	s	604	CLA	O2D-CGD-CBD	3.78	117.83	111.23
31	s	615	CLA	O2D-CGD-CBD	3.78	117.83	111.23
30	Y	608	CHL	OBD-CAD-CBD	-3.78	120.28	125.82
31	13	614	CLA	O2D-CGD-CBD	3.78	117.83	111.23
31	d	402	CLA	C3B-C4B-NB	-3.78	107.16	110.53
31	N	610	CLA	C3B-C4B-NB	-3.78	107.16	110.53
31	R	602	CLA	O2D-CGD-CBD	3.77	117.83	111.23
30	2	601	CHL	CBC-CAC-C3C	-3.77	107.47	112.87
31	R	609	CLA	C3B-C4B-NB	-3.77	107.16	110.53
31	6	615	CLA	O2D-CGD-CBD	3.77	117.82	111.23
31	g	613	CLA	O2D-CGD-CBD	3.77	117.82	111.23
31	13	610	CLA	C3B-C4B-NB	-3.76	107.17	110.53
30	5	601	CHL	CBC-CAC-C3C	-3.76	107.49	112.87
30	n	601	CHL	CMA-C3A-C4A	-3.76	106.51	114.61
31	12	613	CLA	O2D-CGD-CBD	3.76	117.80	111.23
31	G	613	CLA	O2D-CGD-CBD	3.76	117.80	111.23
31	y	602	CLA	O2D-CGD-CBD	3.76	117.80	111.23
31	15	604	CLA	O2D-CGD-CBD	3.76	117.80	111.23
31	g	602	CLA	O2D-CGD-CBD	3.76	117.80	111.23
31	14	610	CLA	C3B-C4B-NB	-3.75	107.18	110.53
31	N	604	CLA	O2D-CGD-CBD	3.75	117.79	111.23
31	11	610	CLA	C3B-C4B-NB	-3.75	107.19	110.53
31	Y	615	CLA	C3B-C4B-NB	-3.75	107.19	110.53
31	r	603	CLA	O2D-CGD-CBD	3.75	117.78	111.23
31	y	602	CLA	C3B-C4B-NB	-3.74	107.19	110.53
31	5	604	CLA	O2D-CGD-CBD	3.74	117.78	111.23
30	R	606	CHL	CBC-CAC-C3C	-3.74	107.51	112.87
30	s	607	CHL	CBC-CAC-C3C	-3.74	107.51	112.87
31	n	604	CLA	O2D-CGD-CBD	3.74	117.77	111.23
31	c	502	CLA	C3B-C4B-NB	-3.74	107.19	110.53
30	G	601	CHL	CMA-C3A-C4A	-3.73	106.56	114.61
31	A	403	CLA	C3B-C4B-NB	-3.73	107.20	110.53
31	1	602	CLA	O2D-CGD-CBD	3.73	117.75	111.23
31	2	610	CLA	O2D-CGD-CBD	3.73	117.75	111.23
31	16	610	CLA	C3B-C4B-NB	-3.73	107.20	110.53
31	4	610	CLA	O2D-CGD-CBD	3.73	117.75	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	609	CHL	CMA-C3A-C4A	-3.73	106.58	114.61
31	Y	602	CLA	C3B-C4B-NB	-3.73	107.20	110.53
31	b	611	CLA	O2D-CGD-CBD	3.73	117.74	111.23
31	b	602	CLA	C3B-C4B-NB	-3.72	107.21	110.53
31	S	613	CLA	O2D-CGD-CBD	3.72	117.74	111.23
31	n	612	CLA	O2D-CGD-CBD	3.72	117.74	111.23
30	N	608	CHL	CBC-CAC-C3C	-3.72	107.54	112.87
30	13	607	CHL	CMA-C3A-C4A	-3.72	106.59	114.61
38	D	402	PHO	C4D-CHA-CBD	3.72	110.24	108.45
30	4	605	CHL	CMA-C3A-C4A	-3.72	106.60	114.61
31	G	602	CLA	C3B-C4B-NB	-3.72	107.21	110.53
30	3	609	CHL	CBC-CAC-C3C	-3.72	107.55	112.87
30	n	605	CHL	CAA-C2A-C3A	-3.72	102.96	113.00
31	6	602	CLA	O2D-CGD-CBD	3.72	117.73	111.23
31	r	614	CLA	O2D-CGD-CBD	3.72	117.72	111.23
30	Y	605	CHL	CMA-C3A-C4A	-3.71	106.61	114.61
31	2	604	CLA	O2D-CGD-CBD	3.71	117.72	111.23
31	11	604	CLA	O2D-CGD-CBD	3.71	117.72	111.23
31	S	615	CLA	O2D-CGD-CBD	3.71	117.72	111.23
30	y	608	CHL	OBD-CAD-CBD	-3.71	120.38	125.82
31	s	602	CLA	O2D-CGD-CBD	3.71	117.72	111.23
31	C	502	CLA	C3B-C4B-NB	-3.71	107.22	110.53
31	S	609	CLA	O2D-CGD-CBD	3.71	117.71	111.23
31	4	614	CLA	O2D-CGD-CBD	3.71	117.71	111.23
31	s	602	CLA	C3B-C4B-NB	-3.71	107.22	110.53
31	g	612	CLA	O2D-CGD-CBD	3.70	117.71	111.23
30	y	601	CHL	CBC-CAC-C3C	-3.70	107.57	112.87
31	2	610	CLA	C3B-C4B-NB	-3.70	107.22	110.53
31	y	603	CLA	O2D-CGD-CBD	3.70	117.70	111.23
30	14	601	CHL	CMA-C3A-C4A	-3.70	106.64	114.61
31	g	602	CLA	C3B-C4B-NB	-3.70	107.23	110.53
31	3	615	CLA	O2D-CGD-CBD	3.70	117.70	111.23
30	S	607	CHL	CBC-CAC-C3C	-3.70	107.58	112.87
31	B	611	CLA	O2D-CGD-CBD	3.69	117.69	111.23
31	13	604	CLA	O2D-CGD-CBD	3.69	117.69	111.23
30	16	605	CHL	CMA-C3A-C4A	-3.69	106.66	114.61
31	n	602	CLA	O2A-CGA-CBA	3.69	123.09	111.83
31	Y	602	CLA	O2D-CGD-CBD	3.69	117.68	111.23
31	14	604	CLA	O2D-CGD-CBD	3.69	117.68	111.23
31	3	615	CLA	C3B-C4B-NB	-3.69	107.24	110.53
31	G	612	CLA	O2D-CGD-CBD	3.68	117.67	111.23
31	3	602	CLA	O2D-CGD-CBD	3.68	117.66	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	601	CHL	CBC-CAC-C3C	-3.68	107.60	112.87
31	s	610	CLA	C3B-C4B-NB	-3.68	107.25	110.53
38	A	405	PHO	C4D-CHA-CBD	3.68	110.22	108.45
31	r	609	CLA	O2A-CGA-CBA	3.68	123.05	111.83
30	14	606	CHL	CMA-C3A-C4A	-3.68	106.69	114.61
30	g	606	CHL	CBC-CAC-C3C	-3.67	107.61	112.87
30	2	609	CHL	CMA-C3A-C4A	-3.67	106.70	114.61
31	5	610	CLA	C3B-C4B-NB	-3.67	107.25	110.53
31	Y	603	CLA	O2D-CGD-CBD	3.67	117.64	111.23
30	1	605	CHL	CMA-C3A-C4A	-3.67	106.71	114.61
30	n	609	CHL	CAA-C2A-C3A	-3.67	103.09	113.00
31	1	614	CLA	O2D-CGD-CBD	3.67	117.64	111.23
30	N	608	CHL	CMA-C3A-C4A	-3.66	106.72	114.61
31	16	611	CLA	O2D-CGD-CBD	3.66	117.63	111.23
30	13	609	CHL	CMA-C3A-C4A	-3.66	106.72	114.61
31	s	612	CLA	O2D-CGD-CBD	3.66	117.62	111.23
30	Y	606	CHL	CAA-C2A-C3A	-3.66	103.12	113.00
31	12	604	CLA	O2D-CGD-CBD	3.65	117.62	111.23
31	A	406	CLA	C3B-C4B-NB	-3.65	107.27	110.53
31	d	404	CLA	C3B-C4B-NB	-3.65	107.27	110.53
30	16	609	CHL	CMA-C3A-C4A	-3.65	106.75	114.61
30	N	609	CHL	CMA-C3A-C4A	-3.65	106.75	114.61
30	4	606	CHL	CMA-C3A-C4A	-3.65	106.76	114.61
31	N	612	CLA	O2D-CGD-CBD	3.64	117.60	111.23
31	r	612	CLA	C3B-C4B-NB	-3.64	107.28	110.53
31	c	511	CLA	C3B-C4B-NB	-3.64	107.28	110.53
31	1	604	CLA	C3B-C4B-NB	-3.64	107.28	110.53
31	y	615	CLA	C3B-C4B-NB	-3.64	107.28	110.53
31	15	609	CLA	C3B-C4B-NB	-3.64	107.28	110.53
31	b	611	CLA	C3B-C4B-NB	-3.64	107.28	110.53
30	G	606	CHL	CBC-CAC-C3C	-3.64	107.67	112.87
31	s	611	CLA	O2A-CGA-CBA	3.64	122.92	111.83
31	B	602	CLA	C3B-C4B-NB	-3.64	107.28	110.53
30	N	609	CHL	CAA-C2A-C3A	-3.63	103.18	113.00
30	n	608	CHL	CBC-CAC-C3C	-3.63	107.67	112.87
31	14	612	CLA	O2D-CGD-CBD	3.63	117.58	111.23
30	16	607	CHL	CAA-C2A-C3A	-3.63	103.18	113.00
38	a	405	PHO	C4D-CHA-CBD	3.63	110.20	108.45
30	S	601	CHL	CBC-CAC-C3C	-3.63	107.67	112.87
30	s	601	CHL	CBC-CAC-C3C	-3.63	107.68	112.87
30	n	608	CHL	CMA-C3A-C4A	-3.63	106.80	114.61
30	2	605	CHL	CMA-C3A-C4A	-3.63	106.80	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n	602	CLA	C3B-C4B-NB	-3.62	107.30	110.53
30	16	607	CHL	C1-C2-C3	3.62	132.13	126.20
31	3	602	CLA	C3B-C4B-NB	-3.62	107.30	110.53
30	6	609	CHL	CAA-C2A-C3A	-3.62	103.22	113.00
31	12	609	CLA	O2D-CGD-CBD	3.62	117.55	111.23
31	N	615	CLA	C3B-C4B-NB	-3.62	107.30	110.53
30	16	606	CHL	CBC-CAC-C3C	-3.62	107.70	112.87
30	y	605	CHL	CMA-C3A-C4A	-3.62	106.82	114.61
31	16	602	CLA	O2D-CGD-CBD	3.61	117.55	111.23
30	16	607	CHL	CMA-C3A-C4A	-3.61	106.83	114.61
30	6	609	CHL	CMA-C3A-C4A	-3.61	106.83	114.61
31	b	608	CLA	C3B-C4B-NB	-3.61	107.31	110.53
30	1	601	CHL	CMA-C3A-C4A	-3.61	106.83	114.61
30	13	606	CHL	CBC-CAC-C3C	-3.61	107.70	112.87
31	n	615	CLA	C3B-C4B-NB	-3.61	107.31	110.53
30	3	609	CHL	CMA-C3A-C4A	-3.61	106.83	114.61
30	13	609	CHL	CAA-C2A-C3A	-3.61	103.25	113.00
30	5	605	CHL	CMA-C3A-C4A	-3.61	106.84	114.61
31	C	509	CLA	C3B-C4B-NB	-3.61	107.31	110.53
30	11	607	CHL	CAA-C2A-C3A	-3.60	103.26	113.00
30	13	606	CHL	CAA-C2A-C3A	-3.60	103.27	113.00
31	C	504	CLA	O2D-CGD-CBD	3.60	117.52	111.23
30	y	609	CHL	C1-C2-C3	3.60	132.09	126.20
30	6	609	CHL	CBC-CAC-C3C	-3.60	107.72	112.87
31	c	504	CLA	O2D-CGD-CBD	3.60	117.52	111.23
32	A	413	LHG	O7-C7-C8	3.60	119.26	111.48
30	3	609	CHL	CAA-C2A-C3A	-3.59	103.29	113.00
30	6	608	CHL	CMA-C3A-C4A	-3.59	106.87	114.61
30	G	607	CHL	CMA-C3A-C4A	-3.59	106.87	114.61
31	C	511	CLA	C3B-C4B-NB	-3.59	107.32	110.53
31	5	613	CLA	O2D-CGD-CBD	3.59	117.51	111.23
31	16	602	CLA	O2A-CGA-CBA	3.59	122.79	111.83
31	a	403	CLA	C3B-C4B-NB	-3.59	107.32	110.53
31	c	508	CLA	C3B-C4B-NB	-3.59	107.32	110.53
30	Y	609	CHL	CMA-C3A-C4A	-3.59	106.87	114.61
30	3	605	CHL	CAA-C2A-C3A	-3.59	103.30	113.00
30	y	608	CHL	CMA-C3A-C4A	-3.59	106.88	114.61
30	G	607	CHL	CAA-C2A-C3A	-3.59	103.30	113.00
30	y	606	CHL	CAA-C2A-C3A	-3.59	103.30	113.00
31	c	512	CLA	C3B-C4B-NB	-3.59	107.33	110.53
31	2	604	CLA	C3B-C4B-NB	-3.59	107.33	110.53
31	R	601	CLA	C3B-C4B-NB	-3.59	107.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	601	CLA	C3B-C4B-NB	-3.59	107.33	110.53
31	c	509	CLA	C3B-C4B-NB	-3.58	107.33	110.53
31	6	602	CLA	C3B-C4B-NB	-3.58	107.33	110.53
30	g	607	CHL	CAA-C2A-C3A	-3.58	103.33	113.00
31	14	602	CLA	O2D-CGD-CBD	3.58	117.49	111.23
31	C	512	CLA	C3B-C4B-NB	-3.58	107.34	110.53
30	y	607	CHL	CAA-C2A-C3A	-3.58	103.33	113.00
31	11	602	CLA	O2D-CGD-CBD	3.58	117.48	111.23
32	s	621	LHG	O7-C7-C8	3.58	119.22	111.48
30	1	606	CHL	CBC-CAC-C3C	-3.57	107.75	112.87
30	14	609	CHL	CMA-C3A-C4A	-3.57	106.91	114.61
31	Y	613	CLA	C3B-C4B-NB	-3.57	107.34	110.53
31	r	610	CLA	C3B-C4B-NB	-3.57	107.34	110.53
30	Y	606	CHL	OBD-CAD-CBD	-3.57	120.58	125.82
31	s	605	CLA	C3B-C4B-NB	-3.57	107.34	110.53
30	Y	609	CHL	C1-C2-C3	3.57	132.05	126.20
30	S	601	CHL	CMA-C3A-C4A	-3.57	106.92	114.61
30	Y	608	CHL	CMA-C3A-C4A	-3.57	106.92	114.61
30	Y	607	CHL	CAA-C2A-C3A	-3.57	103.35	113.00
32	a	413	LHG	O7-C7-C8	3.57	119.20	111.48
31	4	613	CLA	O2D-CGD-CBD	3.57	117.47	111.23
30	n	609	CHL	C1-C2-C3	3.57	132.04	126.20
31	4	604	CLA	C3B-C4B-NB	-3.57	107.35	110.53
30	s	601	CHL	CMA-C3A-C4A	-3.57	106.93	114.61
31	2	611	CLA	O2D-CGD-CBD	3.57	117.47	111.23
30	g	607	CHL	CMA-C3A-C4A	-3.56	106.93	114.61
30	r	607	CHL	CMA-C3A-C4A	-3.56	106.93	114.61
30	11	606	CHL	CMA-C3A-C4A	-3.56	106.94	114.61
31	A	402	CLA	C3B-C4B-NB	-3.56	107.35	110.53
30	N	609	CHL	C1-C2-C3	3.56	132.02	126.20
31	S	603	CLA	O2D-CGD-CBD	3.56	117.44	111.23
30	1	607	CHL	CMA-C3A-C4A	-3.55	106.95	114.61
30	12	606	CHL	CBC-CAC-C3C	-3.55	107.78	112.87
31	R	603	CLA	O2D-CGD-CBD	3.55	117.44	111.23
31	R	614	CLA	O2D-CGD-CBD	3.55	117.44	111.23
31	B	611	CLA	C3B-C4B-NB	-3.55	107.36	110.53
31	11	612	CLA	O2D-CGD-CBD	3.55	117.44	111.23
30	y	609	CHL	CMA-C3A-C4A	-3.55	106.96	114.61
30	3	608	CHL	CBC-CAC-C3C	-3.55	107.79	112.87
30	n	606	CHL	CBC-CAC-C3C	-3.55	107.79	112.87
30	5	605	CHL	CBC-CAC-C3C	-3.55	107.79	112.87
30	n	607	CHL	CMA-C3A-C4A	-3.55	106.96	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	609	CHL	CAA-C2A-C3A	-3.55	103.41	113.00
30	r	605	CHL	CMA-C3A-C4A	-3.55	106.97	114.61
31	G	610	CLA	O2A-CGA-CBA	3.55	122.65	111.83
30	6	601	CHL	C1-C2-C3	3.55	132.01	126.20
31	y	613	CLA	C3B-C4B-NB	-3.55	107.36	110.53
30	5	606	CHL	CMA-C3A-C4A	-3.54	106.97	114.61
31	16	615	CLA	C3B-C4B-NB	-3.54	107.37	110.53
31	B	609	CLA	O2A-CGA-CBA	3.54	122.64	111.83
32	S	621	LHG	O7-C7-C8	3.54	119.14	111.48
30	2	605	CHL	CBC-CAC-C3C	-3.54	107.80	112.87
30	2	607	CHL	CMA-C3A-C4A	-3.54	106.98	114.61
31	4	613	CLA	C3B-C4B-NB	-3.54	107.37	110.53
31	a	404	CLA	C3B-C4B-NB	-3.54	107.37	110.53
30	11	601	CHL	CMA-C3A-C4A	-3.54	106.98	114.61
30	16	609	CHL	CBC-CAC-C3C	-3.54	107.81	112.87
30	g	601	CHL	CBC-CAC-C3C	-3.54	107.81	112.87
31	5	602	CLA	O2D-CGD-CBD	3.54	117.42	111.23
30	N	608	CHL	OBD-CAD-CBD	-3.54	120.63	125.82
30	y	606	CHL	OBD-CAD-CBD	-3.54	120.63	125.82
30	N	605	CHL	CAA-C2A-C3A	-3.54	103.44	113.00
30	g	605	CHL	CAA-C2A-C3A	-3.54	103.44	113.00
31	15	609	CLA	O2D-CGD-CBD	3.54	117.41	111.23
30	y	609	CHL	CAA-C2A-C3A	-3.54	103.44	113.00
30	y	607	CHL	CMA-C3A-C4A	-3.54	106.99	114.61
30	N	601	CHL	CBC-CAC-C3C	-3.54	107.81	112.87
30	4	601	CHL	CMA-C3A-C4A	-3.54	106.99	114.61
30	5	609	CHL	CAA-C2A-C3A	-3.53	103.45	113.00
30	15	606	CHL	CBC-CAC-C3C	-3.53	107.81	112.87
31	14	602	CLA	C3B-C4B-NB	-3.53	107.38	110.53
31	a	407	CLA	C3B-C4B-NB	-3.53	107.38	110.53
31	g	610	CLA	O2A-CGA-CBA	3.53	122.60	111.83
30	s	607	CHL	CMA-C3A-C4A	-3.53	107.01	114.61
30	3	608	CHL	CMA-C3A-C4A	-3.53	107.01	114.61
30	16	608	CHL	CMA-C3A-C4A	-3.53	107.01	114.61
31	A	404	CLA	C3B-C4B-NB	-3.53	107.38	110.53
30	N	607	CHL	CMA-C3A-C4A	-3.53	107.01	114.61
30	s	608	CHL	CMA-C3A-C4A	-3.52	107.02	114.61
30	Y	601	CHL	CMA-C3A-C4A	-3.52	107.02	114.61
30	y	601	CHL	CMA-C3A-C4A	-3.52	107.02	114.61
31	b	613	CLA	O2D-CGD-CBD	3.52	117.39	111.23
30	13	609	CHL	CBC-CAC-C3C	-3.52	107.83	112.87
31	3	604	CLA	C3B-C4B-NB	-3.52	107.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	13	606	CHL	OBD-CAD-CBD	-3.52	120.66	125.82
31	s	614	CLA	O2A-CGA-CBA	3.52	122.57	111.83
30	3	606	CHL	CBC-CAC-C3C	-3.52	107.83	112.87
30	R	607	CHL	CMA-C3A-C4A	-3.52	107.03	114.61
30	g	605	CHL	CMA-C3A-C4A	-3.52	107.03	114.61
30	S	607	CHL	CMA-C3A-C4A	-3.52	107.03	114.61
30	Y	607	CHL	CMA-C3A-C4A	-3.52	107.03	114.61
30	3	606	CHL	CMA-C3A-C4A	-3.51	107.04	114.61
31	b	606	CLA	C3B-C4B-NB	-3.51	107.39	110.53
30	6	606	CHL	CMA-C3A-C4A	-3.51	107.04	114.61
30	13	608	CHL	CMA-C3A-C4A	-3.51	107.04	114.61
31	16	604	CLA	O2D-CGD-CBD	3.51	117.37	111.23
31	B	606	CLA	C3B-C4B-NB	-3.51	107.39	110.53
31	d	402	CLA	O2D-CGD-CBD	3.51	117.37	111.23
31	S	602	CLA	C3B-C4B-NB	-3.51	107.40	110.53
30	16	606	CHL	OBD-CAD-CBD	-3.51	120.67	125.82
30	1	607	CHL	CAA-C2A-C3A	-3.51	103.52	113.00
30	4	607	CHL	CAA-C2A-C3A	-3.51	103.52	113.00
31	n	613	CLA	O2A-CGA-CBA	3.51	122.53	111.83
31	c	507	CLA	C3B-C4B-NB	-3.51	107.40	110.53
30	5	607	CHL	CMA-C3A-C4A	-3.51	107.06	114.61
31	b	609	CLA	O2A-CGA-CBA	3.51	122.52	111.83
30	S	601	CHL	CAA-C2A-C3A	-3.51	103.53	113.00
31	14	613	CLA	O2D-CGD-CBD	3.51	117.36	111.23
31	6	604	CLA	C3B-C4B-NB	-3.50	107.40	110.53
30	G	605	CHL	CMA-C3A-C4A	-3.50	107.06	114.61
31	S	605	CLA	C3B-C4B-NB	-3.50	107.40	110.53
30	1	606	CHL	CAA-C2A-C3A	-3.50	103.54	113.00
30	N	606	CHL	CMA-C3A-C4A	-3.50	107.07	114.61
30	14	608	CHL	OBD-CAD-CBD	-3.50	120.69	125.82
31	5	604	CLA	C3B-C4B-NB	-3.50	107.41	110.53
31	y	603	CLA	C3B-C4B-NB	-3.50	107.41	110.53
30	G	605	CHL	CAA-C2A-C3A	-3.50	103.55	113.00
30	16	606	CHL	CMA-C3A-C4A	-3.50	107.08	114.61
31	c	514	CLA	C3B-C4B-NB	-3.50	107.41	110.53
30	5	601	CHL	CMA-C3A-C4A	-3.50	107.08	114.61
30	3	601	CHL	CMA-C3A-C4A	-3.50	107.08	114.61
31	B	613	CLA	O2D-CGD-CBD	3.50	117.34	111.23
30	6	608	CHL	CBC-CAC-C3C	-3.49	107.87	112.87
31	s	603	CLA	O2D-CGD-CBD	3.49	117.34	111.23
30	14	605	CHL	CBC-CAC-C3C	-3.49	107.87	112.87
31	2	603	CLA	C3B-C4B-NB	-3.49	107.41	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	611	CLA	C3B-C4B-NB	-3.49	107.41	110.53
30	15	606	CHL	CMA-C3A-C4A	-3.49	107.09	114.61
30	13	605	CHL	CBC-CAC-C3C	-3.49	107.88	112.87
31	B	608	CLA	C3B-C4B-NB	-3.49	107.42	110.53
30	6	607	CHL	CMA-C3A-C4A	-3.49	107.10	114.61
30	6	606	CHL	CBC-CAC-C3C	-3.48	107.89	112.87
31	c	508	CLA	O2A-CGA-CBA	3.48	122.45	111.83
31	12	602	CLA	C3B-C4B-NB	-3.48	107.42	110.53
30	4	607	CHL	CMA-C3A-C4A	-3.48	107.11	114.61
30	6	605	CHL	CMA-C3A-C4A	-3.48	107.11	114.61
30	R	605	CHL	CBC-CAC-C3C	-3.48	107.89	112.87
30	n	605	CHL	CMA-C3A-C4A	-3.48	107.11	114.61
31	s	611	CLA	C3B-C4B-NB	-3.48	107.42	110.53
30	s	601	CHL	CAA-C2A-C3A	-3.48	103.60	113.00
32	Y	616	LHG	O7-C7-C8	3.48	119.00	111.48
30	14	605	CHL	CMA-C3A-C4A	-3.48	107.12	114.61
32	Y	617	LHG	O7-C7-C8	3.48	119.00	111.48
31	C	508	CLA	O2A-CGA-CBA	3.48	122.43	111.83
31	13	604	CLA	O2A-CGA-CBA	3.47	122.43	111.83
30	6	601	CHL	CMA-C3A-C4A	-3.47	107.13	114.61
31	R	608	CLA	O2A-CGA-CBA	3.47	122.42	111.83
31	2	602	CLA	O2D-CGD-CBD	3.47	117.30	111.23
31	B	614	CLA	C3B-C4B-NB	-3.47	107.43	110.53
32	r	621	LHG	O7-C7-C8	3.47	118.98	111.48
31	16	610	CLA	O2A-CGA-CBA	3.47	122.40	111.83
30	3	607	CHL	CMA-C3A-C4A	-3.47	107.14	114.61
30	11	609	CHL	CMA-C3A-C4A	-3.47	107.14	114.61
30	g	606	CHL	CMA-C3A-C4A	-3.47	107.14	114.61
31	13	604	CLA	C3B-C4B-NB	-3.47	107.44	110.53
31	r	602	CLA	C3B-C4B-NB	-3.47	107.44	110.53
31	11	602	CLA	C3B-C4B-NB	-3.46	107.44	110.53
31	n	610	CLA	C3B-C4B-NB	-3.46	107.44	110.53
30	N	606	CHL	CBC-CAC-C3C	-3.46	107.91	112.87
30	14	607	CHL	CMA-C3A-C4A	-3.46	107.15	114.61
30	R	605	CHL	CMA-C3A-C4A	-3.46	107.15	114.61
30	n	606	CHL	CMA-C3A-C4A	-3.46	107.15	114.61
30	2	606	CHL	CMA-C3A-C4A	-3.46	107.16	114.61
31	R	610	CLA	C3B-C4B-NB	-3.46	107.44	110.53
30	G	606	CHL	CMA-C3A-C4A	-3.46	107.16	114.61
31	b	614	CLA	C3B-C4B-NB	-3.46	107.44	110.53
31	b	604	CLA	C3B-C4B-NB	-3.45	107.45	110.53
30	13	606	CHL	CMA-C3A-C4A	-3.45	107.17	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	r	606	CHL	CBC-CAC-C3C	-3.45	107.93	112.87
31	G	604	CLA	O2D-CGD-CBD	3.45	117.27	111.23
30	r	605	CHL	CBC-CAC-C3C	-3.45	107.93	112.87
30	6	608	CHL	OBD-CAD-CBD	-3.45	120.76	125.82
30	12	608	CHL	CMA-C3A-C4A	-3.45	107.18	114.61
31	11	604	CLA	C3B-C4B-NB	-3.45	107.45	110.53
30	13	607	CHL	CAA-C2A-C3A	-3.45	103.69	113.00
32	S	617	LHG	O7-C7-C8	3.45	118.94	111.48
31	N	611	CLA	C3B-C4B-NB	-3.45	107.45	110.53
31	2	613	CLA	O2D-CGD-CBD	3.45	117.25	111.23
31	16	604	CLA	C3B-C4B-NB	-3.44	107.45	110.53
31	D	405	CLA	C3B-C4B-NB	-3.44	107.45	110.53
31	b	601	CLA	C3B-C4B-NB	-3.44	107.46	110.53
30	N	607	CHL	CAA-C2A-C3A	-3.44	103.69	113.00
30	S	608	CHL	CMA-C3A-C4A	-3.44	107.20	114.61
30	5	609	CHL	CMA-C3A-C4A	-3.44	107.20	114.61
30	11	609	CHL	CAA-C2A-C3A	-3.44	103.70	113.00
30	G	609	CHL	CMA-C3A-C4A	-3.44	107.20	114.61
30	2	609	CHL	C1-C2-C3	3.44	131.83	126.20
30	14	607	CHL	CBC-CAC-C3C	-3.44	107.95	112.87
31	r	601	CLA	O2A-CGA-CBA	3.44	122.31	111.83
31	13	602	CLA	C3B-C4B-NB	-3.44	107.46	110.53
31	15	613	CLA	C3B-C4B-NB	-3.44	107.46	110.53
31	13	610	CLA	O2A-CGA-CBA	3.44	122.31	111.83
30	N	605	CHL	CMA-C3A-C4A	-3.43	107.21	114.61
31	c	505	CLA	C3B-C4B-NB	-3.43	107.46	110.53
30	2	608	CHL	CBC-CAC-C3C	-3.43	107.96	112.87
31	s	609	CLA	O2A-CGA-CBA	3.43	122.31	111.83
31	11	613	CLA	C3B-C4B-NB	-3.43	107.47	110.53
31	G	614	CLA	O2A-CGA-CBA	3.43	122.30	111.83
30	16	606	CHL	CAA-C2A-C3A	-3.43	103.73	113.00
31	1	613	CLA	C3B-C4B-NB	-3.43	107.47	110.53
31	15	602	CLA	C3B-C4B-NB	-3.43	107.47	110.53
30	N	601	CHL	CAA-C2A-C3A	-3.43	103.73	113.00
31	12	609	CLA	C3B-C4B-NB	-3.43	107.47	110.53
31	14	613	CLA	C3B-C4B-NB	-3.43	107.47	110.53
31	C	514	CLA	C3B-C4B-NB	-3.43	107.47	110.53
31	y	613	CLA	O2A-CGA-CBA	3.43	122.29	111.83
31	12	612	CLA	C3B-C4B-NB	-3.43	107.47	110.53
31	g	604	CLA	C3B-C4B-NB	-3.43	107.47	110.53
30	16	601	CHL	CAA-C2A-C3A	-3.42	103.74	113.00
31	S	614	CLA	C3B-C4B-NB	-3.42	107.47	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	6	605	CHL	CAA-C2A-C3A	-3.42	103.75	113.00
30	1	605	CHL	CBC-CAC-C3C	-3.42	107.97	112.87
32	A	415	LHG	O7-C7-C8	3.42	118.89	111.48
30	11	605	CHL	CMA-C3A-C4A	-3.42	107.24	114.61
30	n	601	CHL	CBC-CAC-C3C	-3.42	107.98	112.87
30	13	608	CHL	CBC-CAC-C3C	-3.42	107.98	112.87
31	4	602	CLA	C3B-C4B-NB	-3.42	107.48	110.53
31	11	613	CLA	O2D-CGD-CBD	3.42	117.20	111.23
32	y	616	LHG	O7-C7-C8	3.42	118.87	111.48
31	2	611	CLA	C3B-C4B-NB	-3.42	107.48	110.53
31	Y	603	CLA	C3B-C4B-NB	-3.41	107.48	110.53
30	15	607	CHL	CMA-C3A-C4A	-3.41	107.25	114.61
31	g	604	CLA	O2D-CGD-CBD	3.41	117.20	111.23
30	g	609	CHL	CMA-C3A-C4A	-3.41	107.26	114.61
31	B	601	CLA	C3B-C4B-NB	-3.41	107.49	110.53
30	3	605	CHL	CMA-C3A-C4A	-3.41	107.26	114.61
30	S	606	CHL	CMA-C3A-C4A	-3.41	107.27	114.61
31	G	613	CLA	C3B-C4B-NB	-3.41	107.49	110.53
32	A	411	LHG	O7-C7-C8	3.41	118.85	111.48
30	14	609	CHL	CAA-C2A-C3A	-3.41	103.79	113.00
30	s	606	CHL	CBC-CAC-C3C	-3.41	108.00	112.87
31	r	608	CLA	O2A-CGA-CBA	3.41	122.22	111.83
31	1	602	CLA	C3B-C4B-NB	-3.40	107.49	110.53
31	g	613	CLA	C3B-C4B-NB	-3.40	107.49	110.53
30	12	607	CHL	CMA-C3A-C4A	-3.40	107.28	114.61
30	16	608	CHL	CBC-CAC-C3C	-3.40	108.00	112.87
31	R	604	CLA	C3B-C4B-NB	-3.40	107.49	110.53
30	1	601	CHL	CAA-C2A-C3A	-3.40	103.81	113.00
30	16	605	CHL	CBC-CAC-C3C	-3.40	108.00	112.87
30	15	601	CHL	CMA-C3A-C4A	-3.40	107.29	114.61
30	2	601	CHL	CMA-C3A-C4A	-3.40	107.29	114.61
30	2	608	CHL	CMA-C3A-C4A	-3.40	107.29	114.61
31	C	514	CLA	O2A-CGA-CBA	3.40	122.19	111.83
31	g	614	CLA	O2A-CGA-CBA	3.40	122.19	111.83
31	S	610	CLA	C3B-C4B-NB	-3.40	107.50	110.53
31	b	604	CLA	O2A-CGA-CBA	3.40	122.19	111.83
30	12	605	CHL	CAA-C2A-C3A	-3.39	103.83	113.00
31	16	602	CLA	C3B-C4B-NB	-3.39	107.50	110.53
30	G	609	CHL	CAA-C2A-C3A	-3.39	103.83	113.00
30	12	607	CHL	CBC-CAC-C3C	-3.39	108.02	112.87
31	S	609	CLA	C3B-C4B-NB	-3.39	107.50	110.53
30	R	605	CHL	CAA-C2A-C3A	-3.39	103.83	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	601	CHL	CMA-C3A-C4A	-3.39	107.30	114.61
30	12	606	CHL	CMA-C3A-C4A	-3.39	107.30	114.61
30	15	608	CHL	CAA-C2A-C3A	-3.39	103.83	113.00
31	C	507	CLA	C3B-C4B-NB	-3.39	107.50	110.53
31	d	405	CLA	C3B-C4B-NB	-3.39	107.50	110.53
31	r	604	CLA	C3B-C4B-NB	-3.39	107.50	110.53
30	15	605	CHL	CMA-C3A-C4A	-3.39	107.31	114.61
30	5	607	CHL	CAA-C2A-C3A	-3.39	103.84	113.00
30	15	608	CHL	CMA-C3A-C4A	-3.39	107.31	114.61
31	C	505	CLA	C3B-C4B-NB	-3.39	107.51	110.53
30	g	605	CHL	CBC-CAC-C3C	-3.39	108.03	112.87
30	14	606	CHL	O1D-CGD-CBD	-3.38	119.59	124.72
31	S	614	CLA	O2A-CGA-CBA	3.38	122.15	111.83
30	11	607	CHL	CMA-C3A-C4A	-3.38	107.32	114.61
31	B	604	CLA	C3B-C4B-NB	-3.38	107.51	110.53
32	R	619	LHG	O7-C7-C8	3.38	118.79	111.48
32	r	618	LHG	O7-C7-C8	3.38	118.79	111.48
30	15	606	CHL	CAA-C2A-C3A	-3.38	103.86	113.00
30	15	605	CHL	CAA-C2A-C3A	-3.38	103.87	113.00
30	11	608	CHL	CMA-C3A-C4A	-3.38	107.33	114.61
30	s	606	CHL	CMA-C3A-C4A	-3.38	107.33	114.61
30	G	606	CHL	CAA-C2A-C3A	-3.38	103.87	113.00
30	12	605	CHL	CMA-C3A-C4A	-3.38	107.33	114.61
30	Y	607	CHL	CBC-CAC-C3C	-3.38	108.04	112.87
31	n	613	CLA	C3B-C4B-NB	-3.38	107.52	110.53
31	r	614	CLA	C3B-C4B-NB	-3.38	107.52	110.53
31	6	610	CLA	C3B-C4B-NB	-3.38	107.52	110.53
31	D	405	CLA	O2A-CGA-CBA	3.38	122.13	111.83
30	5	608	CHL	CMA-C3A-C4A	-3.37	107.34	114.61
30	12	606	CHL	CAA-C2A-C3A	-3.37	103.89	113.00
31	s	614	CLA	C3B-C4B-NB	-3.37	107.52	110.53
31	B	603	CLA	O2A-CGA-CBA	3.37	122.11	111.83
30	14	605	CHL	CAA-C2A-C3A	-3.37	103.89	113.00
30	11	606	CHL	CBC-CAC-C3C	-3.37	108.05	112.87
31	B	604	CLA	O2A-CGA-CBA	3.37	122.11	111.83
31	6	610	CLA	O2A-CGA-CBA	3.37	122.11	111.83
31	S	611	CLA	C3B-C4B-NB	-3.37	107.52	110.53
31	Y	613	CLA	O2A-CGA-CBA	3.37	122.10	111.83
31	b	609	CLA	C3B-C4B-NB	-3.37	107.52	110.53
31	n	611	CLA	C3B-C4B-NB	-3.37	107.52	110.53
32	6	616	LHG	O7-C7-C8	3.37	118.77	111.48
30	14	609	CHL	OBD-CAD-CBD	-3.37	120.88	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	505	CLA	O2A-CGA-CBA	3.37	122.10	111.83
31	N	604	CLA	C3B-C4B-NB	-3.37	107.53	110.53
31	b	603	CLA	O2A-CGA-CBA	3.36	122.09	111.83
30	11	605	CHL	CBC-CAC-C3C	-3.36	108.06	112.87
30	G	605	CHL	CBC-CAC-C3C	-3.36	108.06	112.87
30	G	601	CHL	CBC-CAC-C3C	-3.36	108.06	112.87
30	16	609	CHL	C1-C2-C3	3.36	131.71	126.20
31	S	613	CLA	C3B-C4B-NB	-3.36	107.53	110.53
31	d	405	CLA	O2A-CGA-CBA	3.36	122.09	111.83
31	B	612	CLA	O2A-CGA-CBA	3.36	122.08	111.83
30	13	601	CHL	CBC-CAC-C3C	-3.36	108.06	112.87
30	14	608	CHL	CMA-C3A-C4A	-3.36	107.37	114.61
30	5	608	CHL	CBC-CAC-C3C	-3.36	108.06	112.87
31	16	611	CLA	C3B-C4B-NB	-3.36	107.53	110.53
30	4	608	CHL	CMA-C3A-C4A	-3.36	107.38	114.61
31	B	610	CLA	C3B-C4B-NB	-3.36	107.53	110.53
30	11	601	CHL	CAA-C2A-C3A	-3.36	103.93	113.00
30	1	609	CHL	CMA-C3A-C4A	-3.36	107.38	114.61
32	3	616	LHG	O7-C7-C8	3.36	118.74	111.48
31	2	613	CLA	C3B-C4B-NB	-3.35	107.54	110.53
31	B	613	CLA	O2A-CGA-CBA	3.35	122.06	111.83
30	y	607	CHL	CBC-CAC-C3C	-3.35	108.07	112.87
31	4	611	CLA	O2A-CGA-CBA	3.35	122.06	111.83
31	R	608	CLA	C3B-C4B-NB	-3.35	107.54	110.53
30	6	609	CHL	C1-C2-C3	3.35	131.69	126.20
31	3	610	CLA	O2A-CGA-CBA	3.35	122.05	111.83
30	y	605	CHL	O1D-CGD-CBD	-3.35	119.64	124.72
30	15	607	CHL	CBC-CAC-C3C	-3.35	108.08	112.87
31	b	613	CLA	O2A-CGA-CBA	3.35	122.05	111.83
30	1	608	CHL	CMA-C3A-C4A	-3.35	107.39	114.61
31	B	607	CLA	O2A-CGA-CBA	3.35	122.05	111.83
31	y	604	CLA	C3B-C4B-NB	-3.35	107.54	110.53
30	14	601	CHL	CBC-CAC-C3C	-3.35	108.08	112.87
30	5	601	CHL	CAA-C2A-C3A	-3.35	103.96	113.00
30	11	601	CHL	CBC-CAC-C3C	-3.35	108.08	112.87
31	b	612	CLA	O2A-CGA-CBA	3.34	122.03	111.83
31	C	504	CLA	C3B-C4B-NB	-3.34	107.54	110.53
30	g	601	CHL	OBD-CAD-CBD	-3.34	120.92	125.82
30	13	608	CHL	O1D-CGD-CBD	-3.34	119.65	124.72
30	3	606	CHL	CAA-C2A-C3A	-3.34	103.96	113.00
30	11	601	CHL	OBD-CAD-CBD	-3.34	120.92	125.82
31	15	602	CLA	O2D-CGD-CBD	3.34	117.07	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	609	CHL	CMA-C3A-C4A	-3.34	107.41	114.61
31	b	610	CLA	C3B-C4B-NB	-3.34	107.55	110.53
30	1	606	CHL	CMA-C3A-C4A	-3.34	107.42	114.61
30	15	608	CHL	CHA-C1A-C2A	-3.34	125.47	133.31
30	y	605	CHL	CAA-C2A-C3A	-3.34	103.98	113.00
30	5	609	CHL	CBC-CAC-C3C	-3.34	108.09	112.87
31	G	603	CLA	C3B-C4B-NB	-3.34	107.55	110.53
30	N	601	CHL	CMA-C3A-C4A	-3.33	107.43	114.61
32	L	102	LHG	O7-C7-C8	3.33	118.69	111.48
30	3	605	CHL	CBC-CAC-C3C	-3.33	108.10	112.87
31	c	505	CLA	O2A-CGA-CBA	3.33	122.00	111.83
31	5	603	CLA	C3B-C4B-NB	-3.33	107.56	110.53
30	1	607	CHL	CBC-CAC-C3C	-3.33	108.10	112.87
31	c	504	CLA	C3B-C4B-NB	-3.33	107.56	110.53
31	c	503	CLA	O2A-CGA-CBA	3.33	121.99	111.83
31	16	615	CLA	O2D-CGD-CBD	3.33	117.05	111.23
31	C	503	CLA	O2A-CGA-CBA	3.33	121.99	111.83
30	3	608	CHL	OBD-CAD-CBD	-3.33	120.94	125.82
31	B	607	CLA	C3B-C4B-NB	-3.33	107.56	110.53
31	N	602	CLA	C3B-C4B-NB	-3.33	107.56	110.53
31	r	611	CLA	C3B-C4B-NB	-3.33	107.56	110.53
31	n	604	CLA	C3B-C4B-NB	-3.33	107.56	110.53
30	14	606	CHL	CBC-CAC-C3C	-3.33	108.11	112.87
30	6	606	CHL	CAA-C2A-C3A	-3.33	104.01	113.00
31	11	611	CLA	C3B-C4B-NB	-3.33	107.56	110.53
31	3	610	CLA	C3B-C4B-NB	-3.32	107.56	110.53
31	R	614	CLA	C3B-C4B-NB	-3.32	107.56	110.53
31	13	611	CLA	O2A-CGA-CBA	3.32	121.97	111.83
31	N	604	CLA	O2A-CGA-CBA	3.32	121.97	111.83
32	r	619	LHG	O7-C7-C8	3.32	118.66	111.48
31	5	613	CLA	C3B-C4B-NB	-3.32	107.57	110.53
32	a	414	LHG	O7-C7-C8	3.32	118.66	111.48
31	1	611	CLA	C3B-C4B-NB	-3.32	107.57	110.53
31	r	608	CLA	C3B-C4B-NB	-3.32	107.57	110.53
30	n	607	CHL	CAA-C2A-C3A	-3.32	104.03	113.00
32	R	621	LHG	O7-C7-C8	3.32	118.66	111.48
31	3	614	CLA	C3B-C4B-NB	-3.32	107.57	110.53
32	l	102	LHG	O7-C7-C8	3.32	118.66	111.48
31	b	613	CLA	C3B-C4B-NB	-3.32	107.57	110.53
31	c	507	CLA	O2A-CGA-CBA	3.32	121.94	111.83
30	16	608	CHL	O1D-CGD-CBD	-3.31	119.70	124.72
30	14	601	CHL	CAA-C2A-C3A	-3.31	104.05	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	R	618	LHG	O7-C7-C8	3.31	118.65	111.48
31	R	604	CLA	O2A-CGA-CBA	3.31	121.94	111.83
31	R	612	CLA	C3B-C4B-NB	-3.31	107.57	110.53
31	n	610	CLA	O2A-CGA-CBA	3.31	121.93	111.83
31	N	610	CLA	O2A-CGA-CBA	3.31	121.93	111.83
30	2	607	CHL	CAA-C2A-C3A	-3.31	104.05	113.00
31	B	610	CLA	O2A-CGA-CBA	3.31	121.93	111.83
31	Y	604	CLA	C3B-C4B-NB	-3.31	107.58	110.53
32	n	616	LHG	O7-C7-C8	3.31	118.64	111.48
31	3	611	CLA	C3B-C4B-NB	-3.31	107.58	110.53
31	s	604	CLA	C3B-C4B-NB	-3.31	107.58	110.53
31	s	613	CLA	C3B-C4B-NB	-3.31	107.58	110.53
30	5	607	CHL	OBD-CAD-CBD	-3.30	120.97	125.82
31	r	610	CLA	O2A-CGA-CBA	3.30	121.91	111.83
30	Y	605	CHL	CAA-C2A-C3A	-3.30	104.07	113.00
31	11	614	CLA	C3B-C4B-NB	-3.30	107.58	110.53
31	B	613	CLA	C3B-C4B-NB	-3.30	107.58	110.53
32	16	616	LHG	O7-C7-C8	3.30	118.62	111.48
30	r	607	CHL	CBC-CAC-C3C	-3.30	108.14	112.87
31	r	603	CLA	O2A-CGA-CBA	3.30	121.90	111.83
30	2	601	CHL	OBD-CAD-CBD	-3.30	120.98	125.82
31	S	615	CLA	C3B-C4B-NB	-3.30	107.58	110.53
31	B	605	CLA	O2A-CGA-CBA	3.30	121.90	111.83
30	1	609	CHL	O1D-CGD-CBD	-3.30	119.72	124.72
30	6	605	CHL	C1-C2-C3	3.30	131.60	126.20
31	n	604	CLA	O2A-CGA-CBA	3.30	121.89	111.83
31	4	614	CLA	C3B-C4B-NB	-3.30	107.58	110.53
31	1	604	CLA	O2A-CGA-CBA	3.30	121.89	111.83
31	15	602	CLA	O2A-CGA-CBA	3.30	121.89	111.83
30	6	605	CHL	CBC-CAC-C3C	-3.30	108.15	112.87
30	16	601	CHL	CBC-CAC-C3C	-3.30	108.15	112.87
30	2	609	CHL	CBC-CAC-C3C	-3.30	108.15	112.87
30	S	606	CHL	CBC-CAC-C3C	-3.30	108.15	112.87
30	6	605	CHL	O2A-CGA-CBA	3.30	121.89	111.83
30	2	606	CHL	CBC-CAC-C3C	-3.30	108.15	112.87
30	Y	608	CHL	CAA-C2A-C3A	-3.30	104.09	113.00
31	6	603	CLA	C3B-C4B-NB	-3.30	107.59	110.53
32	y	617	LHG	O7-C7-C8	3.30	118.61	111.48
30	4	607	CHL	CBC-CAC-C3C	-3.30	108.16	112.87
31	N	615	CLA	O2A-CGA-CBA	3.30	121.88	111.83
31	B	609	CLA	C3B-C4B-NB	-3.29	107.59	110.53
31	S	604	CLA	C3B-C4B-NB	-3.29	107.59	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	601	CHL	CBC-CAC-C3C	-3.29	108.16	112.87
31	16	611	CLA	O2A-CGA-CBA	3.29	121.87	111.83
31	3	603	CLA	C3B-C4B-NB	-3.29	107.59	110.53
31	C	503	CLA	C3B-C4B-NB	-3.29	107.59	110.53
31	N	603	CLA	C3B-C4B-NB	-3.29	107.59	110.53
31	3	614	CLA	O2A-CGA-CBA	3.29	121.87	111.83
31	2	612	CLA	C3B-C4B-NB	-3.29	107.59	110.53
31	r	604	CLA	O2A-CGA-CBA	3.29	121.87	111.83
30	n	609	CHL	CBC-CAC-C3C	-3.29	108.17	112.87
31	n	603	CLA	C3B-C4B-NB	-3.29	107.59	110.53
31	R	609	CLA	O2A-CGA-CBA	3.29	121.86	111.83
31	5	602	CLA	C3B-C4B-NB	-3.29	107.60	110.53
31	s	613	CLA	O2A-CGA-CBA	3.29	121.86	111.83
31	b	610	CLA	O2A-CGA-CBA	3.29	121.85	111.83
31	G	604	CLA	O2A-CGA-CBA	3.29	121.85	111.83
31	3	613	CLA	C3B-C4B-NB	-3.28	107.60	110.53
30	12	601	CHL	CBC-CAC-C3C	-3.28	108.17	112.87
32	13	616	LHG	O7-C7-C8	3.28	118.58	111.48
30	r	606	CHL	CMA-C3A-C4A	-3.28	107.54	114.61
30	r	605	CHL	C1-C2-C3	3.28	131.57	126.20
31	s	610	CLA	O2A-CGA-CBA	3.28	121.84	111.83
30	g	609	CHL	CAA-C2A-C3A	-3.28	104.14	113.00
31	g	603	CLA	C3B-C4B-NB	-3.28	107.60	110.53
31	R	603	CLA	O2A-CGA-CBA	3.28	121.83	111.83
30	S	606	CHL	CAA-C2A-C3A	-3.28	104.14	113.00
30	11	606	CHL	CAA-C2A-C3A	-3.28	104.14	113.00
31	4	604	CLA	O2A-CGA-CBA	3.28	121.83	111.83
31	G	604	CLA	C3B-C4B-NB	-3.28	107.60	110.53
31	s	615	CLA	C3B-C4B-NB	-3.28	107.60	110.53
31	b	607	CLA	C3B-C4B-NB	-3.28	107.61	110.53
30	13	609	CHL	C1-C2-C3	3.28	131.56	126.20
30	g	608	CHL	CMA-C3A-C4A	-3.27	107.56	114.61
30	y	606	CHL	CMA-C3A-C4A	-3.27	107.56	114.61
30	y	608	CHL	CAA-C2A-C3A	-3.27	104.15	113.00
31	g	602	CLA	O2A-CGA-CBA	3.27	121.82	111.83
31	14	614	CLA	C3B-C4B-NB	-3.27	107.61	110.53
31	c	503	CLA	C3B-C4B-NB	-3.27	107.61	110.53
32	A	414	LHG	O7-C7-C8	3.27	118.56	111.48
30	13	601	CHL	CMA-C3A-C4A	-3.27	107.56	114.61
31	4	613	CLA	O2A-CGA-CBA	3.27	121.81	111.83
31	16	613	CLA	O2A-CGA-CBA	3.27	121.81	111.83
31	S	613	CLA	O2A-CGA-CBA	3.27	121.81	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	507	CLA	O2A-CGA-CBA	3.27	121.80	111.83
30	1	606	CHL	OBD-CAD-CBD	-3.27	121.03	125.82
30	Y	606	CHL	CMA-C3A-C4A	-3.27	107.57	114.61
30	6	607	CHL	CBC-CAC-C3C	-3.27	108.20	112.87
31	11	613	CLA	O2A-CGA-CBA	3.27	121.79	111.83
32	d	413	LHG	O7-C7-C8	3.27	118.55	111.48
31	4	610	CLA	O2A-CGA-CBA	3.26	121.79	111.83
32	a	411	LHG	O7-C7-C8	3.26	118.54	111.48
30	1	609	CHL	OBD-CAD-CBD	-3.26	121.03	125.82
31	14	604	CLA	C3B-C4B-NB	-3.26	107.62	110.53
31	12	602	CLA	O2A-CGA-CBA	3.26	121.78	111.83
31	G	614	CLA	C3B-C4B-NB	-3.26	107.62	110.53
30	4	609	CHL	OBD-CAD-CBD	-3.26	121.04	125.82
31	6	611	CLA	C3B-C4B-NB	-3.26	107.62	110.53
32	N	616	LHG	O7-C7-C8	3.26	118.53	111.48
30	Y	609	CHL	CBC-CAC-C3C	-3.26	108.21	112.87
32	Y	618	LHG	O7-C7-C8	3.26	118.53	111.48
31	R	603	CLA	C3B-C4B-NB	-3.26	107.62	110.53
31	Y	603	CLA	O2A-CGA-CBA	3.25	121.76	111.83
30	4	609	CHL	O1D-CGD-CBD	-3.25	119.79	124.72
31	14	611	CLA	C3B-C4B-NB	-3.25	107.62	110.53
31	15	612	CLA	C3B-C4B-NB	-3.25	107.62	110.53
31	Y	615	CLA	O2A-CGA-CBA	3.25	121.76	111.83
30	R	607	CHL	CBC-CAC-C3C	-3.25	108.21	112.87
32	a	401	LHG	O7-C7-C8	3.25	118.52	111.48
30	s	606	CHL	CAA-C2A-C3A	-3.25	104.21	113.00
30	5	608	CHL	CAA-C2A-C3A	-3.25	104.21	113.00
30	13	601	CHL	CAA-C2A-C3A	-3.25	104.21	113.00
31	1	602	CLA	O2A-CGA-CBA	3.25	121.75	111.83
31	4	611	CLA	C3B-C4B-NB	-3.25	107.63	110.53
31	G	611	CLA	C3B-C4B-NB	-3.25	107.63	110.53
31	A	404	CLA	O2D-CGD-CBD	3.25	116.91	111.23
31	a	404	CLA	O2D-CGD-CBD	3.25	116.91	111.23
30	4	605	CHL	CBC-CAC-C3C	-3.25	108.22	112.87
30	Y	605	CHL	C1-C2-C3	3.25	131.52	126.20
31	b	603	CLA	C3B-C4B-NB	-3.25	107.63	110.53
30	16	601	CHL	CMA-C3A-C4A	-3.25	107.62	114.61
31	y	615	CLA	O2A-CGA-CBA	3.25	121.73	111.83
31	Y	604	CLA	O2A-CGA-CBA	3.24	121.73	111.83
31	5	611	CLA	C3B-C4B-NB	-3.24	107.63	110.53
31	B	606	CLA	O2A-CGA-CBA	3.24	121.72	111.83
30	1	608	CHL	OBD-CAD-CBD	-3.24	121.07	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	605	CHL	CAA-C2A-C3A	-3.24	104.24	113.00
30	G	608	CHL	CMA-C3A-C4A	-3.24	107.63	114.61
32	C	521	LHG	O7-C7-C8	3.24	118.49	111.48
30	G	607	CHL	OBD-CAD-CBD	-3.24	121.07	125.82
31	4	602	CLA	O2A-CGA-CBA	3.24	121.71	111.83
31	y	604	CLA	O2A-CGA-CBA	3.24	121.71	111.83
30	3	607	CHL	CBC-CAC-C3C	-3.24	108.23	112.87
30	y	601	CHL	CAA-C2A-C3A	-3.24	104.25	113.00
31	14	613	CLA	O2A-CGA-CBA	3.24	121.71	111.83
31	N	602	CLA	O2A-CGA-CBA	3.24	121.71	111.83
30	12	608	CHL	CHA-C1A-C2A	-3.24	125.70	133.31
30	15	607	CHL	CAA-C2A-C3A	-3.24	104.25	113.00
31	16	604	CLA	O2A-CGA-CBA	3.24	121.70	111.83
30	g	607	CHL	OBD-CAD-CBD	-3.24	121.08	125.82
31	b	607	CLA	O2A-CGA-CBA	3.23	121.70	111.83
31	g	611	CLA	C3B-C4B-NB	-3.23	107.64	110.53
30	2	601	CHL	CAA-C2A-C3A	-3.23	104.26	113.00
31	12	604	CLA	C3B-C4B-NB	-3.23	107.65	110.53
30	g	607	CHL	CBC-CAC-C3C	-3.23	108.25	112.87
30	S	608	CHL	CAA-C2A-C3A	-3.23	104.28	113.00
30	5	606	CHL	CBC-CAC-C3C	-3.23	108.25	112.87
31	11	611	CLA	O2A-CGA-CBA	3.23	121.67	111.83
30	G	607	CHL	CBC-CAC-C3C	-3.23	108.25	112.87
31	N	603	CLA	O2A-CGA-CBA	3.23	121.67	111.83
30	6	601	CHL	OBD-CAD-CBD	-3.23	121.09	125.82
30	14	609	CHL	C1-C2-C3	3.22	131.48	126.20
31	13	611	CLA	C3B-C4B-NB	-3.22	107.65	110.53
32	D	412	LHG	O7-C7-C8	3.22	118.45	111.48
30	11	609	CHL	OBD-CAD-CBD	-3.22	121.10	125.82
30	n	605	CHL	CBC-CAC-C3C	-3.22	108.26	112.87
31	15	603	CLA	C3B-C4B-NB	-3.22	107.66	110.53
30	r	606	CHL	O1D-CGD-CBD	-3.22	119.84	124.72
31	C	510	CLA	O2A-CGA-CBA	3.22	121.64	111.83
30	11	606	CHL	O1D-CGD-CBD	-3.22	119.84	124.72
30	2	608	CHL	CAA-C2A-C3A	-3.22	104.31	113.00
31	A	406	CLA	O2A-CGA-CBA	3.22	121.64	111.83
30	R	606	CHL	CMA-C3A-C4A	-3.22	107.68	114.61
30	12	608	CHL	CBC-CAC-C3C	-3.22	108.27	112.87
30	2	607	CHL	OBD-CAD-CBD	-3.21	121.11	125.82
31	12	602	CLA	O2D-CGD-CBD	3.21	116.85	111.23
30	11	606	CHL	CHA-C1A-C2A	-3.21	125.76	133.31
31	15	604	CLA	C3B-C4B-NB	-3.21	107.66	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	y	618	LHG	O7-C7-C8	3.21	118.43	111.48
31	c	504	CLA	O2A-CGA-CBA	3.21	121.63	111.83
31	D	404	CLA	C3B-C4B-NB	-3.21	107.66	110.53
31	2	602	CLA	C3B-C4B-NB	-3.21	107.67	110.53
31	b	605	CLA	C3B-C4B-NB	-3.21	107.67	110.53
30	2	607	CHL	C1-C2-C3	3.21	131.45	126.20
31	g	613	CLA	O2A-CGA-CBA	3.21	121.61	111.83
31	g	614	CLA	C3B-C4B-NB	-3.21	107.67	110.53
31	R	614	CLA	O2A-CGA-CBA	3.21	121.61	111.83
31	2	610	CLA	O2A-CGA-CBA	3.21	121.61	111.83
31	13	615	CLA	C3B-C4B-NB	-3.20	107.67	110.53
30	1	609	CHL	CBC-CAC-C3C	-3.20	108.29	112.87
31	s	604	CLA	O2A-CGA-CBA	3.20	121.60	111.83
31	1	614	CLA	C3B-C4B-NB	-3.20	107.67	110.53
31	5	612	CLA	C3B-C4B-NB	-3.20	107.67	110.53
31	s	602	CLA	O2A-CGA-CBA	3.20	121.60	111.83
30	y	605	CHL	CBC-CAC-C3C	-3.20	108.29	112.87
31	12	612	CLA	O2A-CGA-CBA	3.20	121.59	111.83
30	3	601	CHL	OBD-CAD-CBD	-3.20	121.13	125.82
31	A	403	CLA	O2D-CGD-CBD	3.20	116.82	111.23
31	13	613	CLA	O2A-CGA-CBA	3.20	121.59	111.83
31	5	610	CLA	O2A-CGA-CBA	3.20	121.59	111.83
31	14	603	CLA	C3B-C4B-NB	-3.19	107.68	110.53
31	11	614	CLA	O2A-CGA-CBA	3.19	121.58	111.83
31	14	611	CLA	O2A-CGA-CBA	3.19	121.58	111.83
31	2	613	CLA	O2A-CGA-CBA	3.19	121.57	111.83
31	C	504	CLA	O2A-CGA-CBA	3.19	121.57	111.83
32	11	615	LHG	O7-C7-C8	3.19	118.39	111.48
31	B	603	CLA	C3B-C4B-NB	-3.19	107.68	110.53
30	4	609	CHL	CBC-CAC-C3C	-3.19	108.31	112.87
31	b	605	CLA	O2A-CGA-CBA	3.19	121.56	111.83
30	3	608	CHL	O1D-CGD-CBD	-3.19	119.89	124.72
30	r	605	CHL	CAA-C2A-C3A	-3.19	104.38	113.00
31	S	615	CLA	O2A-CGA-CBA	3.19	121.56	111.83
31	14	614	CLA	O2A-CGA-CBA	3.19	121.55	111.83
31	y	603	CLA	O2A-CGA-CBA	3.19	121.55	111.83
30	Y	601	CHL	OBD-CAD-CBD	-3.19	121.15	125.82
31	6	613	CLA	O2A-CGA-CBA	3.19	121.55	111.83
31	s	612	CLA	C3B-C4B-NB	-3.19	107.69	110.53
30	5	606	CHL	CAA-C2A-C3A	-3.19	104.39	113.00
30	13	606	CHL	C1-C2-C3	3.18	131.41	126.20
30	g	609	CHL	CBC-CAC-C3C	-3.18	108.31	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	15	604	CLA	O2A-CGA-CBA	3.18	121.54	111.83
30	Y	608	CHL	CBC-CAC-C3C	-3.18	108.32	112.87
31	Y	614	CLA	C3B-C4B-NB	-3.18	107.69	110.53
30	Y	601	CHL	CAA-C2A-C3A	-3.18	104.41	113.00
30	n	606	CHL	CAA-C2A-C3A	-3.18	104.41	113.00
31	Y	611	CLA	C3B-C4B-NB	-3.18	107.69	110.53
32	c	521	LHG	O7-C7-C8	3.18	118.35	111.48
31	12	611	CLA	C3B-C4B-NB	-3.18	107.69	110.53
31	4	603	CLA	C3B-C4B-NB	-3.18	107.69	110.53
31	13	603	CLA	C3B-C4B-NB	-3.18	107.69	110.53
30	y	609	CHL	CBC-CAC-C3C	-3.18	108.33	112.87
31	c	514	CLA	O2A-CGA-CBA	3.18	121.52	111.83
30	13	607	CHL	C1-C2-C3	3.18	131.40	126.20
30	1	607	CHL	OBD-CAD-CBD	-3.17	121.17	125.82
31	G	613	CLA	O2A-CGA-CBA	3.17	121.51	111.83
30	6	608	CHL	O1D-CGD-CBD	-3.17	119.91	124.72
30	11	609	CHL	C1-C2-C3	3.17	131.39	126.20
31	6	603	CLA	O2A-CGA-CBA	3.17	121.50	111.83
31	11	610	CLA	O2A-CGA-CBA	3.17	121.50	111.83
31	16	603	CLA	O2A-CGA-CBA	3.17	121.50	111.83
31	s	609	CLA	C3B-C4B-NB	-3.17	107.70	110.53
31	C	506	CLA	O2A-CGA-CBA	3.17	121.49	111.83
31	3	603	CLA	O2A-CGA-CBA	3.16	121.48	111.83
30	3	609	CHL	C1-C2-C3	3.16	131.38	126.20
30	S	606	CHL	C1-C2-C3	3.16	131.38	126.20
30	s	608	CHL	CAA-C2A-C3A	-3.16	104.45	113.00
31	S	602	CLA	O2A-CGA-CBA	3.16	121.48	111.83
31	b	601	CLA	O2A-CGA-CBA	3.16	121.47	111.83
30	y	605	CHL	C1-C2-C3	3.16	131.38	126.20
31	6	614	CLA	C3B-C4B-NB	-3.16	107.71	110.53
30	4	608	CHL	CAA-C2A-C3A	-3.16	104.46	113.00
32	6	617	LHG	O7-C7-C8	3.16	118.32	111.48
31	r	613	CLA	C3B-C4B-NB	-3.16	107.71	110.53
31	a	407	CLA	O2A-CGA-CBA	3.16	121.47	111.83
30	R	607	CHL	OBD-CAD-CBD	-3.16	121.19	125.82
30	5	601	CHL	OBD-CAD-CBD	-3.16	121.19	125.82
30	6	601	CHL	CAA-C2A-C3A	-3.16	104.47	113.00
31	r	613	CLA	O2A-CGA-CBA	3.16	121.46	111.83
31	R	612	CLA	O2A-CGA-CBA	3.16	121.46	111.83
30	11	607	CHL	CBC-CAC-C3C	-3.15	108.36	112.87
30	G	609	CHL	CBC-CAC-C3C	-3.15	108.36	112.87
31	S	610	CLA	O2A-CGA-CBA	3.15	121.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	608	CHL	CAA-C2A-C3A	-3.15	104.48	113.00
30	2	606	CHL	CAA-C2A-C3A	-3.15	104.48	113.00
32	1	615	LHG	O7-C7-C8	3.15	118.30	111.48
30	g	608	CHL	OBD-CAD-CBD	-3.15	121.20	125.82
30	Y	606	CHL	C1-C2-C3	3.15	131.36	126.20
30	g	607	CHL	O2A-CGA-CBA	3.15	121.44	111.83
30	5	607	CHL	C1-C2-C3	3.15	131.36	126.20
30	R	605	CHL	C1-C2-C3	3.15	131.35	126.20
30	R	606	CHL	O1D-CGD-CBD	-3.15	119.95	124.72
31	15	611	CLA	C3B-C4B-NB	-3.15	107.72	110.53
31	R	613	CLA	C3B-C4B-NB	-3.15	107.72	110.53
31	r	612	CLA	O2A-CGA-CBA	3.15	121.43	111.83
31	C	506	CLA	C3B-C4B-NB	-3.15	107.72	110.53
32	G	615	LHG	O7-C7-C8	3.14	118.28	111.48
30	s	606	CHL	C1-C2-C3	3.14	131.35	126.20
30	12	607	CHL	CAA-C2A-C3A	-3.14	104.50	113.00
31	11	603	CLA	C3B-C4B-NB	-3.14	107.72	110.53
31	n	611	CLA	O2A-CGA-CBA	3.14	121.42	111.83
30	G	607	CHL	O2A-CGA-CBA	3.14	121.41	111.83
31	r	614	CLA	O2A-CGA-CBA	3.14	121.41	111.83
31	N	613	CLA	C3B-C4B-NB	-3.14	107.73	110.53
31	G	611	CLA	O2A-CGA-CBA	3.14	121.41	111.83
30	R	607	CHL	C1-C2-C3	3.14	131.84	126.76
31	y	602	CLA	O2A-CGA-CBA	3.14	121.41	111.83
31	N	614	CLA	C3B-C4B-NB	-3.14	107.73	110.53
30	Y	607	CHL	C1-C2-C3	3.14	131.33	126.20
30	g	609	CHL	C1-C2-C3	3.14	131.33	126.20
30	14	606	CHL	CHA-C1A-C2A	-3.14	125.94	133.31
31	b	614	CLA	O2A-CGA-CBA	3.13	121.39	111.83
30	R	605	CHL	O2A-CGA-CBA	3.13	121.39	111.83
30	16	609	CHL	O1D-CGD-CBD	-3.13	119.97	124.72
32	14	615	LHG	O7-C7-C8	3.13	118.26	111.48
31	B	614	CLA	C1-C2-C3	3.13	131.33	126.20
32	d	408	LHG	O7-C7-C8	3.13	118.25	111.48
31	c	510	CLA	O2A-CGA-CBA	3.13	121.38	111.83
30	g	608	CHL	CBC-CAC-C3C	-3.13	108.39	112.87
31	3	613	CLA	O2A-CGA-CBA	3.13	121.38	111.83
31	12	609	CLA	O2A-CGA-CBA	3.13	121.37	111.83
30	g	606	CHL	O2A-CGA-CBA	3.13	121.37	111.83
30	N	601	CHL	CHA-C1A-C2A	-3.13	125.96	133.31
30	3	607	CHL	O1D-CGD-CBD	-3.13	119.98	124.72
30	G	601	CHL	OBD-CAD-CBD	-3.13	121.24	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	610	CLA	O2A-CGA-CBA	3.12	121.36	111.83
30	G	608	CHL	OBD-CAD-CBD	-3.12	121.24	125.82
30	y	601	CHL	OBD-CAD-CBD	-3.12	121.24	125.82
31	Y	602	CLA	O2A-CGA-CBA	3.12	121.36	111.83
31	y	614	CLA	C3B-C4B-NB	-3.12	107.74	110.53
31	Y	614	CLA	O2A-CGA-CBA	3.12	121.35	111.83
31	R	613	CLA	O2A-CGA-CBA	3.12	121.35	111.83
30	13	601	CHL	O1D-CGD-CBD	-3.12	119.99	124.72
31	Y	610	CLA	O2A-CGA-CBA	3.12	121.35	111.83
30	13	605	CHL	CHA-C1A-C2A	-3.12	125.98	133.31
31	16	603	CLA	C3B-C4B-NB	-3.12	107.75	110.53
30	4	607	CHL	CHA-C1A-C2A	-3.12	125.98	133.31
30	y	608	CHL	CBC-CAC-C3C	-3.12	108.41	112.87
31	1	603	CLA	C3B-C4B-NB	-3.12	107.75	110.53
30	Y	605	CHL	CBC-CAC-C3C	-3.12	108.41	112.87
31	14	610	CLA	O2A-CGA-CBA	3.12	121.34	111.83
31	b	614	CLA	C1-C2-C3	3.12	131.30	126.20
30	G	601	CHL	C1-C2-C3	3.12	131.30	126.20
31	6	613	CLA	C3B-C4B-NB	-3.12	107.75	110.53
30	1	605	CHL	O1D-CGD-CBD	-3.11	120.00	124.72
31	g	603	CLA	O2A-CGA-CBA	3.11	121.33	111.83
31	2	603	CLA	O2A-CGA-CBA	3.11	121.33	111.83
31	5	603	CLA	O2A-CGA-CBA	3.11	121.33	111.83
31	5	613	CLA	O2A-CGA-CBA	3.11	121.33	111.83
31	B	601	CLA	O2A-CGA-CBA	3.11	121.32	111.83
30	N	606	CHL	CAA-C2A-C3A	-3.11	104.59	113.00
30	12	601	CHL	OBD-CAD-CBD	-3.11	121.26	125.82
32	3	617	LHG	O7-C7-C8	3.11	118.21	111.48
30	n	605	CHL	C1-C2-C3	3.11	131.29	126.20
31	12	603	CLA	C3B-C4B-NB	-3.11	107.76	110.53
32	D	408	LHG	O7-C7-C8	3.11	118.20	111.48
30	16	601	CHL	O2A-CGA-CBA	3.11	121.31	111.83
31	c	506	CLA	O2A-CGA-CBA	3.11	121.31	111.83
30	14	607	CHL	O1D-CGD-CBD	-3.11	120.01	124.72
30	r	607	CHL	OBD-CAD-CBD	-3.11	121.27	125.82
30	13	607	CHL	CBC-CAC-C3C	-3.11	108.43	112.87
30	4	607	CHL	C1-C2-C3	3.11	131.79	126.76
31	C	502	CLA	O2A-CGA-CBA	3.10	121.30	111.83
31	12	613	CLA	C3B-C4B-NB	-3.10	107.76	110.53
31	y	611	CLA	C3B-C4B-NB	-3.10	107.76	110.53
31	A	404	CLA	O2A-CGA-CBA	3.10	121.29	111.83
30	6	607	CHL	OBD-CAD-CBD	-3.10	121.27	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	512	CLA	O2A-CGA-CBA	3.10	121.28	111.83
30	N	609	CHL	CBC-CAC-C3C	-3.10	108.44	112.87
30	3	606	CHL	O2A-CGA-CBA	3.10	121.28	111.83
31	a	404	CLA	O2A-CGA-CBA	3.10	121.28	111.83
31	G	603	CLA	O2A-CGA-CBA	3.10	121.28	111.83
31	b	616	CLA	O2A-CGA-CBA	3.10	121.28	111.83
31	g	604	CLA	O2A-CGA-CBA	3.10	121.27	111.83
30	5	608	CHL	O2A-CGA-CBA	3.09	121.27	111.83
31	c	506	CLA	C3B-C4B-NB	-3.09	107.77	110.53
31	6	610	CLA	C1-C2-C3	3.09	131.26	126.20
30	4	601	CHL	OBD-CAD-CBD	-3.09	121.28	125.82
30	y	607	CHL	C1-C2-C3	3.09	131.26	126.20
30	6	606	CHL	C1-C2-C3	3.09	131.26	126.20
30	2	609	CHL	O2A-CGA-CBA	3.09	121.25	111.83
31	5	610	CLA	O2D-CGD-CBD	3.09	116.63	111.23
31	c	513	CLA	C3B-C4B-NB	-3.09	107.77	110.53
30	3	605	CHL	O2A-CGA-CBA	3.09	121.25	111.83
31	1	610	CLA	C3B-C4B-NB	-3.09	107.78	110.53
31	c	512	CLA	O2A-CGA-CBA	3.08	121.24	111.83
31	15	603	CLA	O2A-CGA-CBA	3.08	121.24	111.83
30	1	609	CHL	C1-C2-C3	3.08	131.25	126.20
30	2	609	CHL	O1D-CGD-CBD	-3.08	120.05	124.72
30	12	608	CHL	C1-C2-C3	3.08	131.25	126.20
30	12	608	CHL	O1D-CGD-CBD	-3.08	120.05	124.72
35	6	620	XAT	O4-C5-C4	-3.08	110.60	113.49
31	3	611	CLA	O2A-CGA-CBA	3.08	121.23	111.83
30	3	607	CHL	OBD-CAD-CBD	-3.08	121.31	125.82
30	G	609	CHL	O1D-CGD-CBD	-3.08	120.05	124.72
31	Y	611	CLA	O2A-CGA-CBA	3.08	121.22	111.83
31	S	614	CLA	C1-C2-C3	3.08	131.24	126.20
31	R	611	CLA	O2A-CGA-CBA	3.08	121.21	111.83
30	12	601	CHL	CAA-C2A-C3A	-3.08	104.69	113.00
31	12	604	CLA	O2A-CGA-CBA	3.08	121.21	111.83
31	G	602	CLA	O2A-CGA-CBA	3.08	121.21	111.83
30	15	608	CHL	O2A-CGA-CBA	3.08	121.21	111.83
31	B	605	CLA	C3B-C4B-NB	-3.07	107.78	110.53
30	13	601	CHL	O2A-CGA-CBA	3.07	121.21	111.83
31	B	615	CLA	O2A-CGA-CBA	3.07	121.21	111.83
31	n	603	CLA	O2A-CGA-CBA	3.07	121.21	111.83
30	15	601	CHL	OBD-CAD-CBD	-3.07	121.31	125.82
30	n	601	CHL	CAA-C2A-C3A	-3.07	104.70	113.00
31	b	616	CLA	C3B-C4B-NB	-3.07	107.79	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	614	CLA	O2A-CGA-CBA	3.07	121.20	111.83
30	G	608	CHL	CBC-CAC-C3C	-3.07	108.48	112.87
31	12	610	CLA	C3B-C4B-NB	-3.07	107.79	110.53
30	n	607	CHL	C1-C2-C3	3.07	131.23	126.20
30	4	601	CHL	CAA-C2A-C3A	-3.07	104.71	113.00
30	y	609	CHL	O2A-CGA-CBA	3.07	121.18	111.83
31	r	611	CLA	O2A-CGA-CBA	3.06	121.18	111.83
31	y	614	CLA	O2A-CGA-CBA	3.06	121.18	111.83
30	13	605	CHL	C1-C2-C3	3.06	131.22	126.20
30	4	608	CHL	CBC-CAC-C3C	-3.06	108.49	112.87
30	16	607	CHL	CBC-CAC-C3C	-3.06	108.49	112.87
30	15	608	CHL	O1D-CGD-CBD	-3.06	120.08	124.72
30	14	606	CHL	CAA-C2A-C3A	-3.06	104.72	113.00
32	s	617	LHG	O7-C7-C8	3.06	118.10	111.48
31	s	615	CLA	O2A-CGA-CBA	3.06	121.17	111.83
30	15	608	CHL	CBC-CAC-C3C	-3.06	108.49	112.87
31	c	502	CLA	O2A-CGA-CBA	3.06	121.17	111.83
30	Y	609	CHL	O2A-CGA-CBA	3.06	121.17	111.83
31	6	604	CLA	O2A-CGA-CBA	3.06	121.16	111.83
31	3	612	CLA	C3B-C4B-NB	-3.06	107.80	110.53
30	3	606	CHL	C1-C2-C3	3.06	131.21	126.20
31	3	612	CLA	O2A-CGA-CBA	3.06	121.16	111.83
31	y	611	CLA	O2A-CGA-CBA	3.06	121.16	111.83
30	4	605	CHL	CAA-C2A-C3A	-3.06	104.73	113.00
30	4	609	CHL	C1-C2-C3	3.06	131.21	126.20
30	n	609	CHL	OBD-CAD-CBD	-3.06	121.34	125.82
30	15	601	CHL	CAA-C2A-C3A	-3.06	104.74	113.00
32	4	615	LHG	O7-C7-C8	3.06	118.09	111.48
30	g	605	CHL	OBD-CAD-CBD	-3.06	121.34	125.82
31	3	604	CLA	O2A-CGA-CBA	3.06	121.15	111.83
30	2	606	CHL	O1D-CGD-CBD	-3.06	120.09	124.72
31	s	614	CLA	C1-C2-C3	3.05	131.20	126.20
31	b	608	CLA	O2A-CGA-CBA	3.05	121.15	111.83
31	15	610	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	B	616	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	6	611	CLA	O2A-CGA-CBA	3.05	121.14	111.83
30	G	605	CHL	O2A-CGA-CBA	3.05	121.14	111.83
31	2	604	CLA	O2A-CGA-CBA	3.05	121.14	111.83
31	12	603	CLA	O2A-CGA-CBA	3.05	121.14	111.83
30	N	609	CHL	OBD-CAD-CBD	-3.05	121.35	125.82
30	12	608	CHL	O2A-CGA-CBA	3.05	121.14	111.83
31	S	603	CLA	C3B-C4B-NB	-3.05	107.81	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	611	CLA	O2A-CGA-CBA	3.05	121.13	111.83
31	r	602	CLA	O2A-CGA-CBA	3.05	121.13	111.83
31	3	602	CLA	O2A-CGA-CBA	3.05	121.13	111.83
30	2	607	CHL	CBC-CAC-C3C	-3.05	108.51	112.87
31	y	612	CLA	C3B-C4B-NB	-3.05	107.81	110.53
30	2	608	CHL	OBD-CAD-CBD	-3.04	121.36	125.82
30	4	608	CHL	OBD-CAD-CBD	-3.04	121.36	125.82
31	15	612	CLA	O2A-CGA-CBA	3.04	121.12	111.83
31	b	602	CLA	O2A-CGA-CBA	3.04	121.11	111.83
31	13	614	CLA	C3B-C4B-NB	-3.04	107.81	110.53
31	S	604	CLA	O2A-CGA-CBA	3.04	121.11	111.83
31	C	513	CLA	C3B-C4B-NB	-3.04	107.82	110.53
31	1	611	CLA	O2A-CGA-CBA	3.04	121.10	111.83
30	Y	605	CHL	OMC-CMC-C2C	-3.04	119.84	125.12
30	16	607	CHL	O2A-CGA-CBA	3.04	121.10	111.83
31	b	615	CLA	O2A-CGA-CBA	3.04	121.09	111.83
30	11	608	CHL	OBD-CAD-CBD	-3.04	121.37	125.82
30	14	607	CHL	O2A-CGA-CBA	3.04	121.09	111.83
31	B	608	CLA	O2A-CGA-CBA	3.04	121.09	111.83
30	G	605	CHL	OBD-CAD-CBD	-3.04	121.37	125.82
30	13	605	CHL	O2A-CGA-CBA	3.03	121.09	111.83
31	n	614	CLA	C3B-C4B-NB	-3.03	107.82	110.53
30	G	601	CHL	CAA-C2A-C3A	-3.03	104.80	113.00
30	g	609	CHL	O2A-CGA-CBA	3.03	121.08	111.83
32	d	409	LHG	O7-C7-C8	3.03	118.04	111.48
31	g	611	CLA	O2A-CGA-CBA	3.03	121.08	111.83
31	n	615	CLA	O2A-CGA-CBA	3.03	121.08	111.83
30	15	606	CHL	O1D-CGD-CBD	-3.03	120.12	124.72
30	15	608	CHL	C1-C2-C3	3.03	131.16	126.20
31	N	613	CLA	O2A-CGA-CBA	3.03	121.08	111.83
30	16	609	CHL	OBD-CAD-CBD	-3.03	121.38	125.82
30	2	605	CHL	CAA-C2A-C3A	-3.03	104.81	113.00
30	N	608	CHL	O1D-CGD-CBD	-3.03	120.13	124.72
30	2	606	CHL	OBD-CAD-CBD	-3.03	121.38	125.82
30	3	609	CHL	OBD-CAD-CBD	-3.03	121.38	125.82
31	Y	612	CLA	C3B-C4B-NB	-3.03	107.83	110.53
30	y	606	CHL	C1-C2-C3	3.03	131.16	126.20
31	n	612	CLA	C3B-C4B-NB	-3.03	107.83	110.53
30	g	608	CHL	C1-C2-C3	3.02	131.15	126.20
31	6	615	CLA	O2A-CGA-CBA	3.02	121.05	111.83
30	g	609	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
31	B	602	CLA	C1-C2-C3	3.02	131.15	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	609	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
31	1	603	CLA	O2A-CGA-CBA	3.02	121.05	111.83
30	5	609	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
30	6	607	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
30	6	605	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
30	16	605	CHL	O1D-CGD-CBD	-3.02	120.14	124.72
30	5	608	CHL	OBD-CAD-CBD	-3.02	121.39	125.82
30	13	608	CHL	OBD-CAD-CBD	-3.02	121.39	125.82
30	16	608	CHL	CAA-C2A-C3A	-3.02	104.84	113.00
30	13	608	CHL	CAA-C2A-C3A	-3.02	104.85	113.00
32	D	409	LHG	O7-C7-C8	3.02	118.01	111.48
31	16	614	CLA	C3B-C4B-NB	-3.01	107.84	110.53
30	11	606	CHL	C1A-CHA-C4D	3.01	124.01	118.98
30	n	601	CHL	C1-C2-C3	3.01	131.13	126.20
30	r	607	CHL	C1-C2-C3	3.01	131.64	126.76
31	B	602	CLA	O2A-CGA-CBA	3.01	121.02	111.83
31	S	609	CLA	O2A-CGA-CBA	3.01	121.02	111.83
30	16	608	CHL	OBD-CAD-CBD	-3.01	121.41	125.82
30	4	605	CHL	O1D-CGD-CBD	-3.01	120.16	124.72
30	3	601	CHL	CAA-C2A-C3A	-3.01	104.87	113.00
30	S	608	CHL	O2A-CGA-CBA	3.01	121.01	111.83
31	R	602	CLA	O2A-CGA-CBA	3.01	121.01	111.83
30	16	605	CHL	C1-C2-C3	3.01	131.12	126.20
31	s	603	CLA	C3B-C4B-NB	-3.01	107.85	110.53
30	11	605	CHL	O1D-CGD-CBD	-3.01	120.17	124.72
31	g	612	CLA	C3B-C4B-NB	-3.01	107.85	110.53
30	Y	605	CHL	O1D-CGD-CBD	-3.00	120.17	124.72
30	2	608	CHL	O2A-CGA-CBA	3.00	120.99	111.83
31	S	605	CLA	O2A-CGA-CBA	3.00	120.99	111.83
31	12	609	CLA	C1-C2-C3	3.00	131.12	126.20
30	11	607	CHL	O1D-CGD-CBD	-3.00	120.17	124.72
30	N	607	CHL	O2A-CGA-CBA	3.00	120.99	111.83
31	13	603	CLA	O2A-CGA-CBA	3.00	120.98	111.83
30	R	607	CHL	CHA-C1A-C2A	-3.00	126.26	133.31
30	N	605	CHL	CBC-CAC-C3C	-3.00	108.58	112.87
31	N	612	CLA	C3B-C4B-NB	-3.00	107.85	110.53
31	C	506	CLA	C1-C2-C3	3.00	131.11	126.20
31	G	612	CLA	C3B-C4B-NB	-3.00	107.86	110.53
30	5	607	CHL	CBC-CAC-C3C	-3.00	108.58	112.87
30	y	606	CHL	O2A-CGA-CBA	3.00	120.97	111.83
30	13	601	CHL	C1-C2-C3	2.99	131.10	126.20
31	B	615	CLA	C3B-C4B-NB	-2.99	107.86	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	1	605	CHL	CAA-C2A-C3A	-2.99	104.91	113.00
30	N	606	CHL	O2A-CGA-CBA	2.99	120.96	111.83
31	s	605	CLA	O2A-CGA-CBA	2.99	120.96	111.83
30	6	608	CHL	O2A-CGA-CBA	2.99	120.96	111.83
30	15	606	CHL	OBD-CAD-CBD	-2.99	121.43	125.82
30	N	609	CHL	O2A-CGA-CBA	2.99	120.95	111.83
30	R	606	CHL	OBD-CAD-CBD	-2.99	121.44	125.82
30	11	609	CHL	CBC-CAC-C3C	-2.99	108.59	112.87
31	6	602	CLA	O2A-CGA-CBA	2.99	120.94	111.83
31	c	509	CLA	O2A-CGA-CBA	2.99	120.94	111.83
30	12	606	CHL	OBD-CAD-CBD	-2.99	121.44	125.82
30	g	605	CHL	O2A-CGA-CBA	2.99	120.94	111.83
31	R	601	CLA	O2A-CGA-CBA	2.99	120.94	111.83
30	2	601	CHL	O1D-CGD-CBD	-2.99	120.20	124.72
31	A	403	CLA	O1D-CGD-CBD	-2.98	118.63	124.52
30	G	608	CHL	C1-C2-C3	2.98	131.09	126.20
30	16	601	CHL	O1D-CGD-CBD	-2.98	120.20	124.72
30	4	605	CHL	OBD-CAD-CBD	-2.98	121.45	125.82
31	r	603	CLA	C1-C2-C3	2.98	131.08	126.20
30	6	609	CHL	OBD-CAD-CBD	-2.98	121.45	125.82
30	r	606	CHL	C1A-CHA-C4D	2.98	123.95	118.98
30	1	601	CHL	OBD-CAD-CBD	-2.98	121.46	125.82
30	4	607	CHL	OBD-CAD-CBD	-2.98	121.46	125.82
30	Y	606	CHL	O2A-CGA-CBA	2.97	120.90	111.83
30	G	606	CHL	C1A-CHA-C4D	2.97	123.94	118.98
31	R	603	CLA	C1-C2-C3	2.97	131.07	126.20
38	a	406	PHO	C2D-C1D-ND	-2.97	107.28	109.43
30	3	609	CHL	O2A-CGA-CBA	2.97	120.89	111.83
31	11	602	CLA	O2A-CGA-CBA	2.97	120.88	111.83
30	16	606	CHL	C1-C2-C3	2.97	131.06	126.20
30	r	605	CHL	O2A-CGA-CBA	2.97	120.88	111.83
30	4	601	CHL	C1A-CHA-C4D	2.97	123.93	118.98
30	3	605	CHL	C1A-CHA-C4D	2.97	123.93	118.98
31	b	602	CLA	C1-C2-C3	2.97	131.06	126.20
30	g	606	CHL	OBD-CAD-CBD	-2.96	121.47	125.82
30	13	608	CHL	O2A-CGA-CBA	2.96	120.87	111.83
30	5	605	CHL	CAA-C2A-C3A	-2.96	104.99	113.00
31	y	612	CLA	O2A-CGA-CBA	2.96	120.86	111.83
30	14	606	CHL	C1A-CHA-C4D	2.96	123.92	118.98
31	c	513	CLA	O2A-CGA-CBA	2.96	120.86	111.83
30	n	607	CHL	O2A-CGA-CBA	2.96	120.86	111.83
30	1	607	CHL	O2A-CGA-CBA	2.96	120.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	14	604	CLA	O2A-CGA-CBA	2.96	120.85	111.83
31	C	509	CLA	O2A-CGA-CBA	2.96	120.85	111.83
30	G	606	CHL	OBD-CAD-CBD	-2.96	121.48	125.82
30	r	606	CHL	OBD-CAD-CBD	-2.96	121.48	125.82
30	4	606	CHL	CAA-C2A-C3A	-2.96	105.01	113.00
30	13	607	CHL	O2A-CGA-CBA	2.96	120.85	111.83
30	n	609	CHL	O2A-CGA-CBA	2.96	120.85	111.83
31	c	514	CLA	O1D-CGD-CBD	-2.96	118.69	124.52
31	b	606	CLA	O2A-CGA-CBA	2.96	120.85	111.83
31	N	602	CLA	C1-C2-C3	2.96	131.04	126.20
30	15	601	CHL	O2A-CGA-CBA	2.96	120.85	111.83
30	G	609	CHL	C1-C2-C3	2.95	131.03	126.20
30	s	606	CHL	O2A-CGA-CBA	2.95	120.83	111.83
30	16	608	CHL	O2A-CGA-CBA	2.95	120.83	111.83
30	y	607	CHL	O1D-CGD-CBD	-2.95	120.25	124.72
30	6	605	CHL	C1A-CHA-C4D	2.95	123.90	118.98
30	R	606	CHL	C1A-CHA-C4D	2.95	123.90	118.98
30	14	609	CHL	CBC-CAC-C3C	-2.95	108.65	112.87
30	14	605	CHL	O1D-CGD-CBD	-2.95	120.25	124.72
31	Y	612	CLA	O2A-CGA-CBA	2.95	120.82	111.83
31	b	609	CLA	C1-C2-C3	2.95	131.02	126.20
30	R	606	CHL	OMC-CMC-C2C	-2.94	120.01	125.12
32	g	615	LHG	O7-C7-C8	2.94	117.85	111.48
30	r	607	CHL	CAA-C2A-C3A	-2.94	105.05	113.00
30	12	601	CHL	O2A-CGA-CBA	2.94	120.81	111.83
31	6	614	CLA	O2A-CGA-CBA	2.94	120.81	111.83
30	16	605	CHL	O2A-CGA-CBA	2.94	120.81	111.83
30	3	605	CHL	C1-C2-C3	2.94	131.01	126.20
31	14	602	CLA	O2A-CGA-CBA	2.94	120.80	111.83
31	6	612	CLA	C3B-C4B-NB	-2.94	107.91	110.53
30	16	609	CHL	O2A-CGA-CBA	2.94	120.79	111.83
31	c	509	CLA	O1D-CGD-CBD	-2.94	118.72	124.52
31	11	603	CLA	O2A-CGA-CBA	2.94	120.79	111.83
31	13	613	CLA	C3B-C4B-NB	-2.94	107.91	110.53
30	y	601	CHL	O2A-CGA-CBA	2.94	120.79	111.83
31	16	613	CLA	C3B-C4B-NB	-2.94	107.91	110.53
31	C	513	CLA	O2A-CGA-CBA	2.94	120.79	111.83
30	R	606	CHL	C1-C2-C3	2.94	131.01	126.20
30	n	605	CHL	O1D-CGD-CBD	-2.93	120.27	124.72
30	r	607	CHL	O1D-CGD-CBD	-2.93	120.27	124.72
30	S	606	CHL	O2A-CGA-CBA	2.93	120.78	111.83
30	1	607	CHL	C1-C2-C3	2.93	131.51	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	610	CLA	C1-C2-C3	2.93	131.00	126.20
38	D	402	PHO	C2D-C1D-ND	-2.93	107.31	109.43
30	3	607	CHL	C1-C2-C3	2.93	131.00	126.20
30	3	608	CHL	O2A-CGA-CBA	2.93	120.77	111.83
30	G	601	CHL	O2A-CGA-CBA	2.93	120.77	111.83
30	s	608	CHL	C1A-CHA-C4D	2.93	123.87	118.98
30	14	608	CHL	C1A-CHA-C4D	2.93	123.87	118.98
30	r	607	CHL	CHA-C1A-C2A	-2.93	126.43	133.31
30	2	607	CHL	O2A-CGA-CBA	2.93	120.77	111.83
31	R	602	CLA	C1-C2-C3	2.93	130.99	126.20
30	12	601	CHL	O1D-CGD-CBD	-2.92	120.29	124.72
30	R	607	CHL	CAA-C2A-C3A	-2.92	105.10	113.00
31	4	603	CLA	O2A-CGA-CBA	2.92	120.75	111.83
30	1	601	CHL	C1A-CHA-C4D	2.92	123.86	118.98
30	6	607	CHL	C1-C2-C3	2.92	130.99	126.20
30	3	605	CHL	O1D-CGD-CBD	-2.92	120.29	124.72
30	3	601	CHL	C1-C2-C3	2.92	130.98	126.20
31	C	509	CLA	O1D-CGD-CBD	-2.92	118.76	124.52
30	n	601	CHL	O2A-CGA-CBA	2.92	120.74	111.83
30	14	607	CHL	OBD-CAD-CBD	-2.92	121.54	125.82
31	15	609	CLA	O2A-CGA-CBA	2.92	120.73	111.83
30	s	608	CHL	CBC-CAC-C3C	-2.92	108.69	112.87
30	11	607	CHL	C1A-CHA-C4D	2.92	123.85	118.98
30	n	606	CHL	O2A-CGA-CBA	2.92	120.73	111.83
38	a	405	PHO	C2D-C1D-ND	-2.92	107.32	109.43
30	13	605	CHL	O1D-CGD-CBD	-2.92	120.30	124.72
31	R	613	CLA	C1-C2-C3	2.92	130.97	126.20
30	12	606	CHL	O2A-CGA-CBA	2.91	120.72	111.83
30	6	608	CHL	CAA-C2A-C3A	-2.91	105.13	113.00
30	R	607	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
30	6	601	CHL	O2A-CGA-CBA	2.91	120.72	111.83
30	15	601	CHL	O1D-CGD-CBD	-2.91	120.31	124.72
30	11	605	CHL	O2A-CGA-CBA	2.91	120.71	111.83
30	1	609	CHL	O2A-CGA-CBA	2.91	120.71	111.83
30	1	605	CHL	OBD-CAD-CBD	-2.91	121.55	125.82
30	11	607	CHL	OBD-CAD-CBD	-2.91	121.56	125.82
30	R	607	CHL	O2A-CGA-CBA	2.91	120.69	111.83
30	6	601	CHL	CBC-CAC-C3C	-2.91	108.71	112.87
31	15	603	CLA	C1-C2-C3	2.91	130.96	126.20
30	11	601	CHL	C1A-CHA-C4D	2.90	123.83	118.98
31	1	613	CLA	O2A-CGA-CBA	2.90	120.69	111.83
30	4	609	CHL	CAA-C2A-C3A	-2.90	105.16	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	607	CHL	O1D-CGD-CBD	-2.90	120.32	124.72
31	G	610	CLA	C1-C2-C3	2.90	130.95	126.20
31	15	609	CLA	O1D-CGD-CBD	-2.90	118.80	124.52
31	14	612	CLA	C3B-C4B-NB	-2.90	107.94	110.53
30	g	601	CHL	C1-C2-C3	2.90	130.95	126.20
30	Y	601	CHL	O2A-CGA-CBA	2.90	120.67	111.83
35	3	620	XAT	O4-C5-C4	-2.90	110.78	113.49
30	5	607	CHL	O2A-CGA-CBA	2.90	120.67	111.83
30	3	601	CHL	O2A-CGA-CBA	2.90	120.66	111.83
30	S	606	CHL	O1D-CGD-CBD	-2.89	120.33	124.72
30	N	605	CHL	O2A-CGA-CBA	2.89	120.66	111.83
30	s	606	CHL	OBD-CAD-CBD	-2.89	121.58	125.82
31	13	602	CLA	O2A-CGA-CBA	2.89	120.66	111.83
30	r	606	CHL	OMC-CMC-C2C	-2.89	120.10	125.12
30	2	609	CHL	CHA-C1A-C2A	-2.89	126.52	133.31
30	14	601	CHL	C1-C2-C3	2.89	130.93	126.20
31	6	604	CLA	C1-C2-C3	2.89	130.93	126.20
31	c	504	CLA	C1-C2-C3	2.89	130.93	126.20
30	Y	605	CHL	O2A-CGA-CBA	2.89	120.64	111.83
30	6	605	CHL	CHA-C1A-C2A	-2.89	126.53	133.31
31	1	612	CLA	C3B-C4B-NB	-2.89	107.95	110.53
30	13	606	CHL	C1A-CHA-C4D	2.89	123.80	118.98
30	1	609	CHL	CAA-C2A-C3A	-2.88	105.21	113.00
30	16	606	CHL	C1A-CHA-C4D	2.88	123.79	118.98
30	N	607	CHL	C1A-CHA-C4D	2.88	123.79	118.98
30	S	608	CHL	C1A-CHA-C4D	2.88	123.79	118.98
30	3	601	CHL	CBC-CAC-C3C	-2.88	108.75	112.87
30	16	601	CHL	OBD-CAD-CBD	-2.88	121.59	125.82
30	15	606	CHL	O2A-CGA-CBA	2.88	120.62	111.83
30	s	601	CHL	OBD-CAD-CBD	-2.88	121.60	125.82
30	s	607	CHL	O1D-CGD-CBD	-2.88	120.35	124.72
31	B	611	CLA	O2A-CGA-CBA	2.88	120.62	111.83
30	g	606	CHL	CAA-C2A-C3A	-2.88	105.21	113.00
31	C	504	CLA	C1-C2-C3	2.88	130.92	126.20
30	y	605	CHL	CHA-C1A-C2A	-2.88	126.55	133.31
30	16	601	CHL	C1A-CHA-C4D	2.88	123.78	118.98
30	5	609	CHL	O2A-CGA-CBA	2.88	120.60	111.83
31	A	404	CLA	C1-C2-C3	2.88	130.91	126.20
38	A	405	PHO	C2D-C1D-ND	-2.88	107.35	109.43
31	B	616	CLA	O2A-CGA-CBA	2.87	120.60	111.83
31	b	611	CLA	O2A-CGA-CBA	2.87	120.60	111.83
30	3	601	CHL	C1A-CHA-C4D	2.87	123.78	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	608	CHL	CBC-CAC-C3C	-2.87	108.76	112.87
31	5	602	CLA	O2A-CGA-CBA	2.87	120.59	111.83
30	S	608	CHL	CBC-CAC-C3C	-2.87	108.76	112.87
31	c	511	CLA	O2A-CGA-CBA	2.87	120.59	111.83
30	3	605	CHL	CHA-C1A-C2A	-2.87	126.57	133.31
30	13	601	CHL	C1A-CHA-C4D	2.87	123.77	118.98
30	16	607	CHL	O1D-CGD-CBD	-2.87	120.37	124.72
30	16	609	CHL	CAA-C2A-C3A	-2.87	105.25	113.00
31	a	404	CLA	C1-C2-C3	2.87	130.89	126.20
30	4	607	CHL	O2A-CGA-CBA	2.87	120.57	111.83
31	Y	610	CLA	C1-C2-C3	2.86	130.89	126.20
31	3	604	CLA	C1-C2-C3	2.86	130.89	126.20
30	13	607	CHL	OBD-CAD-CBD	-2.86	121.62	125.82
30	y	607	CHL	O2A-CGA-CBA	2.86	120.56	111.83
30	6	609	CHL	O1D-CGD-CBD	-2.86	120.39	124.72
30	6	601	CHL	C1A-CHA-C4D	2.86	123.75	118.98
30	Y	607	CHL	O2A-CGA-CBA	2.86	120.55	111.83
30	s	608	CHL	O2A-CGA-CBA	2.86	120.55	111.83
30	5	601	CHL	O1D-CGD-CBD	-2.86	120.39	124.72
31	13	612	CLA	C3B-C4B-NB	-2.85	107.98	110.53
30	11	608	CHL	C1C-CHC-C4B	2.85	126.28	116.07
31	S	611	CLA	C1-C2-C3	2.85	130.87	126.20
31	4	610	CLA	C2D-C1D-ND	2.85	112.95	110.13
30	1	601	CHL	C1-C2-C3	2.85	130.87	126.20
30	14	605	CHL	O2A-CGA-CBA	2.85	120.52	111.83
30	G	608	CHL	O2A-CGA-CBA	2.85	120.52	111.83
30	g	606	CHL	C1A-CHA-C4D	2.85	123.73	118.98
31	C	511	CLA	O2A-CGA-CBA	2.85	120.51	111.83
31	c	509	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
30	s	608	CHL	O2A-CGA-O1A	-2.84	116.51	123.63
31	2	602	CLA	O2A-CGA-CBA	2.84	120.51	111.83
30	2	607	CHL	C1A-CHA-C4D	2.84	123.73	118.98
31	6	612	CLA	O2A-CGA-CBA	2.84	120.50	111.83
30	5	605	CHL	C1C-CHC-C4B	2.84	126.23	116.07
30	r	607	CHL	O2A-CGA-CBA	2.84	120.50	111.83
31	1	610	CLA	O2A-CGA-CBA	2.84	120.50	111.83
30	n	606	CHL	C1A-CHA-C4D	2.84	123.72	118.98
31	y	610	CLA	C1-C2-C3	2.84	130.85	126.20
30	15	608	CHL	OBD-CAD-CBD	-2.84	121.66	125.82
31	d	405	CLA	C1-C2-C3	2.84	130.85	126.20
30	S	606	CHL	OBD-CAD-CBD	-2.84	121.66	125.82
30	5	601	CHL	O2A-CGA-CBA	2.84	120.49	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	608	CHL	CAA-C2A-C3A	-2.84	105.33	113.00
30	15	601	CHL	OMC-CMC-C2C	-2.84	120.19	125.12
31	c	514	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
31	b	615	CLA	C3B-C4B-NB	-2.84	108.00	110.53
30	14	601	CHL	C1A-CHA-C4D	2.83	123.71	118.98
30	4	606	CHL	C1A-CHA-C4D	2.83	123.71	118.98
30	5	606	CHL	C1A-CHA-C4D	2.83	123.71	118.98
31	d	402	CLA	O1D-CGD-CBD	-2.83	118.93	124.52
31	B	609	CLA	C1-C2-C3	2.83	130.84	126.20
30	11	609	CHL	C1A-CHA-C4D	2.83	123.71	118.98
30	15	607	CHL	C1A-CHA-C4D	2.83	123.70	118.98
31	C	509	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
30	14	601	CHL	OBD-CAD-CBD	-2.83	121.67	125.82
30	n	606	CHL	C1-C2-C3	2.83	130.83	126.20
30	n	607	CHL	C1A-CHA-C4D	2.83	123.70	118.98
30	6	606	CHL	O2A-CGA-CBA	2.83	120.46	111.83
30	3	609	CHL	O1D-CGD-CBD	-2.83	120.43	124.72
31	r	613	CLA	C1-C2-C3	2.83	130.83	126.20
31	S	611	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
30	5	607	CHL	C1A-CHA-C4D	2.83	123.70	118.98
30	3	608	CHL	CAA-C2A-C3A	-2.83	105.36	113.00
30	4	601	CHL	O1D-CGD-CBD	-2.82	120.44	124.72
30	5	609	CHL	C1-C2-C3	2.82	130.82	126.20
30	G	606	CHL	CHA-C1A-C2A	-2.82	126.67	133.31
31	D	405	CLA	C1-C2-C3	2.82	130.82	126.20
30	y	605	CHL	O2A-CGA-CBA	2.82	120.44	111.83
30	1	608	CHL	CBC-CAC-C3C	-2.82	108.83	112.87
30	1	601	CHL	O1D-CGD-CBD	-2.82	120.44	124.72
31	14	603	CLA	O2A-CGA-CBA	2.82	120.44	111.83
30	N	608	CHL	CAA-C2A-C3A	-2.82	105.37	113.00
31	A	402	CLA	O2A-CGA-CBA	2.82	120.44	111.83
30	12	608	CHL	CAA-C2A-C3A	-2.82	105.38	113.00
30	12	601	CHL	OMC-CMC-C2C	-2.82	120.22	125.12
30	y	605	CHL	OMC-CMC-C2C	-2.82	120.22	125.12
31	a	403	CLA	O2A-CGA-CBA	2.82	120.44	111.83
30	4	607	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
31	D	404	CLA	O2A-CGA-CBA	2.82	120.43	111.83
30	1	608	CHL	C1A-CHA-C4D	2.82	123.68	118.98
30	N	606	CHL	C1A-CHA-C4D	2.82	123.68	118.98
30	g	601	CHL	C1A-CHA-C4D	2.82	123.68	118.98
30	14	607	CHL	C1C-CHC-C4B	2.82	126.14	116.07
31	3	611	CLA	C1-C2-C3	2.82	130.81	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	601	CHL	C1C-CHC-C4B	2.81	126.14	116.07
30	y	601	CHL	C1C-CHC-C4B	2.81	126.14	116.07
30	G	601	CHL	C1A-CHA-C4D	2.81	123.68	118.98
30	2	601	CHL	C1A-CHA-C4D	2.81	123.67	118.98
30	2	605	CHL	C1C-CHC-C4B	2.81	126.13	116.07
30	n	609	CHL	O1D-CGD-CBD	-2.81	120.46	124.72
30	16	605	CHL	C1A-CHA-C4D	2.81	123.67	118.98
31	N	611	CLA	C1-C2-C3	2.81	130.80	126.20
31	5	604	CLA	O2A-CGA-CBA	2.81	120.40	111.83
30	16	601	CHL	C1-C2-C3	2.81	130.80	126.20
30	S	601	CHL	OBD-CAD-CBD	-2.81	121.70	125.82
30	y	601	CHL	C1A-CHA-C4D	2.81	123.67	118.98
30	11	609	CHL	C1C-CHC-C4B	2.81	126.11	116.07
31	11	612	CLA	C3B-C4B-NB	-2.81	108.03	110.53
31	d	404	CLA	O2A-CGA-CBA	2.81	120.39	111.83
30	y	605	CHL	O2D-CGD-O1D	-2.81	118.39	123.85
30	2	606	CHL	CHA-C1A-C2A	-2.80	126.72	133.31
31	3	613	CLA	C1-C2-C3	2.80	130.79	126.20
30	16	609	CHL	CHA-C1A-C2A	-2.80	126.72	133.31
30	N	609	CHL	O1D-CGD-CBD	-2.80	120.47	124.72
30	3	601	CHL	C1C-CHC-C4B	2.80	126.10	116.07
30	16	609	CHL	C1A-CHA-C4D	2.80	123.66	118.98
30	12	607	CHL	O2A-CGA-CBA	2.80	120.38	111.83
30	4	608	CHL	O2A-CGA-CBA	2.80	120.38	111.83
30	6	601	CHL	C1C-CHC-C4B	2.80	126.09	116.07
31	A	402	CLA	C1-C2-C3	2.80	130.79	126.20
30	14	609	CHL	C1A-CHA-C4D	2.80	123.66	118.98
30	n	605	CHL	O2A-CGA-CBA	2.80	120.37	111.83
30	1	605	CHL	C4C-CHD-C1D	2.80	126.08	116.07
30	2	606	CHL	C1A-CHA-C4D	2.80	123.65	118.98
31	S	609	CLA	C1-C2-C3	2.80	130.78	126.20
30	6	601	CHL	O1D-CGD-CBD	-2.80	120.48	124.72
30	3	605	CHL	C1C-CHC-C4B	2.80	126.08	116.07
30	12	607	CHL	C1A-CHA-C4D	2.80	123.65	118.98
30	15	605	CHL	CBC-CAC-C3C	-2.80	108.87	112.87
30	r	605	CHL	C1A-CHA-C4D	2.80	123.65	118.98
30	3	607	CHL	O2A-CGA-CBA	2.80	120.36	111.83
30	11	608	CHL	O1D-CGD-CBD	-2.80	120.48	124.72
30	Y	606	CHL	C1A-CHA-C4D	2.79	123.64	118.98
30	12	605	CHL	C1A-CHA-C4D	2.79	123.64	118.98
30	3	606	CHL	C1A-CHA-C4D	2.79	123.64	118.98
30	3	601	CHL	O1D-CGD-CBD	-2.79	120.49	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	609	CHL	OBD-CAD-CBD	-2.79	121.72	125.82
30	11	601	CHL	O2A-CGA-CBA	2.79	120.35	111.83
30	N	605	CHL	C1C-CHC-C4B	2.79	126.06	116.07
30	s	608	CHL	OBD-CAD-CBD	-2.79	121.73	125.82
30	4	605	CHL	C4C-CHD-C1D	2.79	126.06	116.07
31	R	610	CLA	O2A-CGA-CBA	2.79	120.35	111.83
30	Y	605	CHL	C1C-CHC-C4B	2.79	126.06	116.07
30	R	605	CHL	C1A-CHA-C4D	2.79	123.64	118.98
30	11	605	CHL	C1C-CHC-C4B	2.79	126.05	116.07
30	n	605	CHL	C1C-CHC-C4B	2.79	126.05	116.07
30	g	608	CHL	O2A-CGA-CBA	2.79	120.34	111.83
30	6	605	CHL	C1C-CHC-C4B	2.79	126.05	116.07
30	N	607	CHL	C1C-CHC-C4B	2.79	126.05	116.07
30	n	608	CHL	O2A-CGA-CBA	2.79	120.34	111.83
30	Y	609	CHL	O1D-CGD-CBD	-2.79	120.50	124.72
31	a	403	CLA	C1-C2-C3	2.79	130.76	126.20
31	c	505	CLA	C1-C2-C3	2.79	130.76	126.20
31	6	613	CLA	C1-C2-C3	2.79	130.76	126.20
31	16	612	CLA	C3B-C4B-NB	-2.79	108.04	110.53
30	G	605	CHL	C1C-CHC-C4B	2.79	126.04	116.07
30	y	605	CHL	C1C-CHC-C4B	2.79	126.04	116.07
30	11	601	CHL	C1C-CHC-C4B	2.79	126.04	116.07
30	g	606	CHL	O1D-CGD-CBD	-2.79	120.50	124.72
30	11	607	CHL	C1C-CHC-C4B	2.79	126.03	116.07
31	N	611	CLA	O2A-CGA-CBA	2.79	120.33	111.83
30	r	605	CHL	OMC-CMC-C2C	-2.78	120.29	125.12
31	4	610	CLA	C3B-C4B-NB	-2.78	108.05	110.53
30	1	608	CHL	O2A-CGA-CBA	2.78	120.32	111.83
30	Y	601	CHL	C1A-CHA-C4D	2.78	123.63	118.98
30	Y	605	CHL	C1A-CHA-C4D	2.78	123.63	118.98
30	11	601	CHL	C1-C2-C3	2.78	130.76	126.20
30	y	606	CHL	C1A-CHA-C4D	2.78	123.62	118.98
30	14	601	CHL	C1C-CHC-C4B	2.78	126.02	116.07
30	g	605	CHL	C1C-CHC-C4B	2.78	126.02	116.07
30	13	601	CHL	OBD-CAD-CBD	-2.78	121.74	125.82
30	R	607	CHL	C1A-CHA-C4D	2.78	123.62	118.98
30	12	605	CHL	C1C-CHC-C4B	2.78	126.01	116.07
30	n	607	CHL	C1C-CHC-C4B	2.78	126.01	116.07
30	y	607	CHL	OBD-CAD-CBD	-2.78	121.75	125.82
31	12	602	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
30	14	609	CHL	C1C-CHC-C4B	2.78	126.00	116.07
30	y	609	CHL	C1C-CHC-C4B	2.78	126.00	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	15	605	CHL	C1C-CHC-C4B	2.78	126.00	116.07
30	N	601	CHL	O2A-CGA-CBA	2.78	120.30	111.83
31	1	613	CLA	C1-C2-C3	2.78	130.74	126.20
31	R	608	CLA	C1-C2-C3	2.78	130.74	126.20
31	n	603	CLA	C1-C2-C3	2.77	130.74	126.20
30	N	608	CHL	O2A-CGA-CBA	2.77	120.29	111.83
31	B	603	CLA	O1D-CGD-CBD	-2.77	119.05	124.52
30	6	607	CHL	O2A-CGA-CBA	2.77	120.28	111.83
30	5	601	CHL	C1A-CHA-C4D	2.77	123.60	118.98
31	b	603	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
30	15	605	CHL	C1A-CHA-C4D	2.77	123.60	118.98
30	5	606	CHL	C1C-CHC-C4B	2.77	125.97	116.07
30	R	605	CHL	OMC-CMC-C2C	-2.77	120.32	125.12
30	5	607	CHL	C1C-CHC-C4B	2.76	125.96	116.07
30	5	609	CHL	CHA-C1A-C2A	-2.76	126.81	133.31
30	13	607	CHL	O1D-CGD-CBD	-2.76	120.53	124.72
30	5	601	CHL	C1-C2-C3	2.76	131.24	126.76
30	2	601	CHL	C1C-CHC-C4B	2.76	125.96	116.07
30	Y	607	CHL	OBD-CAD-CBD	-2.76	121.77	125.82
31	A	403	CLA	O2A-CGA-CBA	2.76	120.26	111.83
30	r	606	CHL	C1-C2-C3	2.76	130.72	126.20
30	15	607	CHL	O2A-CGA-CBA	2.76	120.25	111.83
30	N	605	CHL	OBD-CAD-CBD	-2.76	121.78	125.82
30	4	608	CHL	C1A-CHA-C4D	2.76	123.58	118.98
30	Y	608	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
31	d	402	CLA	O2A-CGA-CBA	2.76	120.24	111.83
30	4	601	CHL	O2A-CGA-CBA	2.76	120.24	111.83
30	r	606	CHL	C1C-CHC-C4B	2.76	125.93	116.07
30	y	606	CHL	CBC-CAC-C3C	-2.76	108.93	112.87
30	N	607	CHL	O1D-CGD-CBD	-2.75	120.55	124.72
30	16	605	CHL	CHA-C1A-C2A	-2.75	126.84	133.31
30	15	601	CHL	C1C-CHC-C4B	2.75	125.92	116.07
30	11	609	CHL	O1D-CGD-CBD	-2.75	120.55	124.72
31	C	508	CLA	C1-C2-C3	2.75	130.71	126.20
30	1	601	CHL	C1C-CHC-C4B	2.75	125.92	116.07
30	g	607	CHL	C1C-CHC-C4B	2.75	125.92	116.07
30	G	607	CHL	C1C-CHC-C4B	2.75	125.91	116.07
30	N	607	CHL	OBD-CAD-CBD	-2.75	121.79	125.82
30	y	607	CHL	C4C-CHD-C1D	2.75	125.91	116.07
30	13	605	CHL	C1A-CHA-C4D	2.75	123.57	118.98
30	12	601	CHL	C1C-CHC-C4B	2.75	125.91	116.07
30	4	601	CHL	C1C-CHC-C4B	2.75	125.91	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	605	CHL	C4C-CHD-C1D	2.75	125.91	116.07
30	n	606	CHL	OBD-CAD-CBD	-2.75	121.79	125.82
30	13	601	CHL	C1C-CHC-C4B	2.75	125.90	116.07
30	6	606	CHL	C1A-CHA-C4D	2.75	123.56	118.98
30	13	605	CHL	C1C-CHC-C4B	2.75	125.89	116.07
30	12	607	CHL	OBD-CAD-CBD	-2.75	121.79	125.82
30	1	606	CHL	C4C-CHD-C1D	2.75	125.89	116.07
30	16	608	CHL	C4C-CHD-C1D	2.75	125.89	116.07
30	S	606	CHL	C1A-CHA-C4D	2.74	123.56	118.98
31	A	403	CLA	C1-C2-C3	2.74	130.69	126.20
30	N	605	CHL	C4C-CHD-C1D	2.74	125.88	116.07
31	d	402	CLA	C1-C2-C3	2.74	130.69	126.20
30	N	606	CHL	C1C-CHC-C4B	2.74	125.88	116.07
30	13	608	CHL	C4C-CHD-C1D	2.74	125.88	116.07
30	16	605	CHL	CAA-C2A-C3A	-2.74	105.59	113.00
30	6	606	CHL	C1C-CHC-C4B	2.74	125.88	116.07
30	Y	607	CHL	C4C-CHD-C1D	2.74	125.88	116.07
44	B	623	STE	O1-C1-C2	-2.74	114.40	123.09
30	13	605	CHL	OMC-CMC-C2C	-2.74	120.36	125.12
30	n	606	CHL	C1C-CHC-C4B	2.74	125.87	116.07
30	g	601	CHL	CAA-C2A-C3A	-2.74	105.59	113.00
31	3	610	CLA	C1-C2-C3	2.74	130.69	126.20
30	15	608	CHL	C1C-CHC-C4B	2.74	125.87	116.07
30	6	607	CHL	C1C-CHC-C4B	2.74	125.87	116.07
30	S	601	CHL	C1A-CHA-C4D	2.74	123.55	118.98
30	3	606	CHL	C1C-CHC-C4B	2.74	125.86	116.07
30	2	608	CHL	C1C-CHC-C4B	2.74	125.86	116.07
30	5	606	CHL	OBD-CAD-CBD	-2.74	121.81	125.82
30	r	607	CHL	C1A-CHA-C4D	2.74	123.55	118.98
30	5	608	CHL	C1C-CHC-C4B	2.74	125.86	116.07
30	16	605	CHL	C1C-CHC-C4B	2.74	125.86	116.07
30	14	605	CHL	C1C-CHC-C4B	2.73	125.85	116.07
30	N	601	CHL	C4C-CHD-C1D	2.73	125.85	116.07
31	B	603	CLA	C1-C2-C3	2.73	130.67	126.20
30	12	608	CHL	OBD-CAD-CBD	-2.73	121.82	125.82
30	16	601	CHL	C1C-CHC-C4B	2.73	125.84	116.07
30	y	608	CHL	O1D-CGD-CBD	-2.73	120.58	124.72
30	16	606	CHL	C1C-CHC-C4B	2.73	125.84	116.07
30	G	601	CHL	C1C-CHC-C4B	2.73	125.84	116.07
30	12	608	CHL	C4C-CHD-C1D	2.73	125.83	116.07
30	14	605	CHL	OBD-CAD-CBD	-2.73	121.82	125.82
30	r	607	CHL	C1C-CHC-C4B	2.73	125.83	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	601	CHL	C4C-CHD-C1D	2.73	125.83	116.07
30	12	601	CHL	C1A-CHA-C4D	2.73	123.53	118.98
30	16	605	CHL	OMC-CMC-C2C	-2.73	120.38	125.12
30	g	608	CHL	O1D-CGD-CBD	-2.73	120.59	124.72
30	N	607	CHL	C1-C2-C3	2.73	130.66	126.20
30	13	606	CHL	C1C-CHC-C4B	2.73	125.83	116.07
30	N	606	CHL	C1-C2-C3	2.73	130.66	126.20
30	3	609	CHL	C4C-CHD-C1D	2.73	125.82	116.07
31	15	611	CLA	CHD-C1D-ND	-2.73	120.97	124.80
30	Y	606	CHL	CBC-CAC-C3C	-2.73	108.97	112.87
31	r	614	CLA	C1-C2-C3	2.73	130.66	126.20
30	4	609	CHL	O2A-CGA-CBA	2.72	120.14	111.83
30	15	608	CHL	C4C-CHD-C1D	2.72	125.82	116.07
30	R	607	CHL	C1C-CHC-C4B	2.72	125.81	116.07
30	G	606	CHL	O1D-CGD-CBD	-2.72	120.59	124.72
30	6	609	CHL	C4C-CHD-C1D	2.72	125.81	116.07
30	15	606	CHL	C1C-CHC-C4B	2.72	125.81	116.07
30	S	608	CHL	OBD-CAD-CBD	-2.72	121.83	125.82
30	1	609	CHL	C1A-CHA-C4D	2.72	123.53	118.98
30	n	608	CHL	C1C-CHC-C4B	2.72	125.81	116.07
30	14	607	CHL	C1A-CHA-C4D	2.72	123.52	118.98
30	2	606	CHL	C1C-CHC-C4B	2.72	125.81	116.07
30	12	607	CHL	C1C-CHC-C4B	2.72	125.81	116.07
30	g	606	CHL	C4C-CHD-C1D	2.72	125.81	116.07
30	13	609	CHL	O1D-CGD-CBD	-2.72	120.59	124.72
30	y	609	CHL	C4C-CHD-C1D	2.72	125.80	116.07
30	14	608	CHL	O2A-CGA-CBA	2.72	120.13	111.83
30	3	607	CHL	C1C-CHC-C4B	2.72	125.80	116.07
30	y	605	CHL	OBD-CAD-CBD	-2.72	121.83	125.82
31	r	608	CLA	C1-C2-C3	2.72	130.65	126.20
30	n	607	CHL	OBD-CAD-CBD	-2.72	121.84	125.82
30	12	606	CHL	O1D-CGD-CBD	-2.72	120.60	124.72
30	N	608	CHL	C1C-CHC-C4B	2.72	125.79	116.07
30	14	608	CHL	CBC-CAC-C3C	-2.72	108.98	112.87
30	G	608	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
31	A	404	CLA	O1D-CGD-CBD	-2.71	119.17	124.52
30	2	608	CHL	C4C-CHD-C1D	2.71	125.78	116.07
30	16	605	CHL	C4C-CHD-C1D	2.71	125.78	116.07
30	4	609	CHL	C1A-CHA-C4D	2.71	123.51	118.98
30	15	607	CHL	C1C-CHC-C4B	2.71	125.77	116.07
30	n	607	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
30	S	608	CHL	C1C-CHC-C4B	2.71	125.77	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	s	601	CHL	C1A-CHA-C4D	2.71	123.50	118.98
30	2	609	CHL	OBD-CAD-CBD	-2.71	121.85	125.82
30	N	606	CHL	OBD-CAD-CBD	-2.71	121.85	125.82
30	14	606	CHL	C1C-CHC-C4B	2.71	125.77	116.07
30	14	609	CHL	O2A-CGA-CBA	2.71	120.10	111.83
30	3	601	CHL	C4C-CHD-C1D	2.71	125.77	116.07
30	s	608	CHL	C1C-CHC-C4B	2.71	125.77	116.07
30	16	607	CHL	C4C-CHD-C1D	2.71	125.77	116.07
30	13	606	CHL	O2A-CGA-CBA	2.71	120.10	111.83
30	y	605	CHL	C1A-CHA-C4D	2.71	123.50	118.98
31	12	611	CLA	CHD-C1D-ND	-2.71	120.99	124.80
44	b	622	STE	O1-C1-C2	-2.71	114.50	123.09
30	6	609	CHL	O2A-CGA-CBA	2.71	120.09	111.83
30	g	601	CHL	C1C-CHC-C4B	2.71	125.76	116.07
30	S	608	CHL	OMC-CMC-C2C	-2.71	120.42	125.12
31	11	610	CLA	CHD-C1D-ND	-2.71	120.99	124.80
30	Y	609	CHL	C1C-CHC-C4B	2.71	125.75	116.07
30	13	605	CHL	OBD-CAD-CBD	-2.71	121.85	125.82
30	G	609	CHL	C1A-CHA-C4D	2.71	123.50	118.98
30	G	606	CHL	C4C-CHD-C1D	2.71	125.75	116.07
30	R	606	CHL	C1C-CHC-C4B	2.71	125.75	116.07
30	6	601	CHL	C4C-CHD-C1D	2.71	125.75	116.07
30	N	609	CHL	C4C-CHD-C1D	2.71	125.75	116.07
31	4	612	CLA	C3B-C4B-NB	-2.70	108.12	110.53
30	n	605	CHL	C4C-CHD-C1D	2.70	125.74	116.07
30	13	606	CHL	CHA-C1A-C2A	-2.70	126.96	133.31
30	2	601	CHL	C4C-CHD-C1D	2.70	125.74	116.07
30	2	607	CHL	C1C-CHC-C4B	2.70	125.74	116.07
30	16	606	CHL	O2A-CGA-CBA	2.70	120.08	111.83
30	s	606	CHL	C1A-CHA-C4D	2.70	123.49	118.98
30	12	607	CHL	O1D-CGD-CBD	-2.70	120.62	124.72
30	3	605	CHL	C4C-CHD-C1D	2.70	125.74	116.07
30	13	607	CHL	C4C-CHD-C1D	2.70	125.74	116.07
30	16	607	CHL	C1C-CHC-C4B	2.70	125.74	116.07
31	r	602	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
30	4	607	CHL	C1C-CHC-C4B	2.70	125.73	116.07
30	4	601	CHL	C1-C2-C3	2.70	130.62	126.20
31	b	603	CLA	C1-C2-C3	2.70	130.62	126.20
30	5	608	CHL	C4C-CHD-C1D	2.70	125.73	116.07
30	g	609	CHL	C1A-CHA-C4D	2.70	123.48	118.98
30	y	609	CHL	O1D-CGD-CBD	-2.70	120.63	124.72
30	6	609	CHL	C1C-CHC-C4B	2.70	125.72	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	607	CHL	C1C-CHC-C4B	2.70	125.72	116.07
31	n	611	CLA	C1-C2-C3	2.70	130.62	126.20
31	c	508	CLA	C1-C2-C3	2.70	130.62	126.20
30	3	609	CHL	C1C-CHC-C4B	2.70	125.72	116.07
30	13	609	CHL	C1A-CHA-C4D	2.70	123.48	118.98
30	y	607	CHL	C1C-CHC-C4B	2.70	125.72	116.07
30	n	608	CHL	C4C-CHD-C1D	2.70	125.72	116.07
30	12	606	CHL	C1A-CHA-C4D	2.70	123.48	118.98
30	13	605	CHL	C4C-CHD-C1D	2.70	125.71	116.07
30	y	606	CHL	C1C-CHC-C4B	2.69	125.71	116.07
31	11	602	CLA	C1-C2-C3	2.69	130.61	126.20
30	y	607	CHL	C1A-CHA-C4D	2.69	123.48	118.98
30	S	606	CHL	C4C-CHD-C1D	2.69	125.70	116.07
30	N	609	CHL	C1C-CHC-C4B	2.69	125.70	116.07
30	s	606	CHL	C4C-CHD-C1D	2.69	125.70	116.07
30	Y	609	CHL	C4C-CHD-C1D	2.69	125.70	116.07
30	5	609	CHL	C1A-CHA-C4D	2.69	123.47	118.98
30	6	605	CHL	C4C-CHD-C1D	2.69	125.69	116.07
30	n	609	CHL	C4C-CHD-C1D	2.69	125.69	116.07
31	14	610	CLA	C1-C2-C3	2.69	130.60	126.20
31	N	603	CLA	C1-C2-C3	2.69	130.60	126.20
30	r	605	CHL	C4C-CHD-C1D	2.69	125.68	116.07
30	3	605	CHL	OBD-CAD-CBD	-2.69	121.88	125.82
30	g	608	CHL	C1A-CHA-C4D	2.69	123.47	118.98
30	Y	606	CHL	C1C-CHC-C4B	2.69	125.68	116.07
30	15	601	CHL	C1A-CHA-C4D	2.69	123.46	118.98
30	4	609	CHL	C4C-CHD-C1D	2.69	125.68	116.07
30	N	605	CHL	C1A-CHA-C4D	2.69	123.46	118.98
30	5	601	CHL	C1C-CHC-C4B	2.69	125.68	116.07
30	6	607	CHL	C1A-CHA-C4D	2.69	123.46	118.98
30	11	608	CHL	C1A-CHA-C4D	2.69	123.46	118.98
30	4	608	CHL	C1C-CHC-C4B	2.68	125.67	116.07
30	y	605	CHL	C4C-CHD-C1D	2.68	125.67	116.07
30	1	609	CHL	C4C-CHD-C1D	2.68	125.67	116.07
30	2	609	CHL	C1C-CHC-C4B	2.68	125.67	116.07
30	g	605	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
30	4	608	CHL	C4C-CHD-C1D	2.68	125.66	116.07
31	a	404	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
30	N	608	CHL	C4C-CHD-C1D	2.68	125.66	116.07
30	2	609	CHL	CAA-C2A-C3A	-2.68	105.76	113.00
30	13	608	CHL	C1C-CHC-C4B	2.68	125.66	116.07
30	13	607	CHL	C1C-CHC-C4B	2.68	125.66	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	14	608	CHL	C1C-CHC-C4B	2.68	125.65	116.07
30	5	606	CHL	C4C-CHD-C1D	2.68	125.65	116.07
30	3	607	CHL	C1A-CHA-C4D	2.68	123.45	118.98
31	14	602	CLA	C1-C2-C3	2.68	130.59	126.20
30	11	605	CHL	OBD-CAD-CBD	-2.68	121.89	125.82
31	12	604	CLA	C1-C2-C3	2.68	130.58	126.20
30	R	605	CHL	C4C-CHD-C1D	2.68	125.65	116.07
30	G	608	CHL	C4C-CHD-C1D	2.68	125.65	116.07
30	y	606	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
30	14	608	CHL	C1-C2-C3	2.68	131.09	126.76
30	13	606	CHL	C4C-CHD-C1D	2.68	125.64	116.07
30	R	605	CHL	O1D-CGD-CBD	-2.68	120.67	124.72
30	S	601	CHL	C1C-CHC-C4B	2.68	125.64	116.07
30	S	606	CHL	C1C-CHC-C4B	2.68	125.64	116.07
30	Y	608	CHL	C1C-CHC-C4B	2.68	125.64	116.07
30	1	607	CHL	C1C-CHC-C4B	2.67	125.64	116.07
30	15	606	CHL	C1A-CHA-C4D	2.67	123.44	118.98
31	14	610	CLA	CHD-C1D-ND	-2.67	121.04	124.80
30	r	607	CHL	C4C-CHD-C1D	2.67	125.64	116.07
31	15	604	CLA	C1-C2-C3	2.67	130.58	126.20
31	16	604	CLA	C1-C2-C3	2.67	130.58	126.20
31	c	507	CLA	C1-C2-C3	2.67	130.58	126.20
30	5	609	CHL	C1C-CHC-C4B	2.67	125.64	116.07
30	12	606	CHL	C1C-CHC-C4B	2.67	125.64	116.07
30	y	608	CHL	C1A-CHA-C4D	2.67	123.44	118.98
30	g	609	CHL	C1C-CHC-C4B	2.67	125.63	116.07
30	G	605	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
30	Y	601	CHL	CHA-C1A-C2A	-2.67	127.03	133.31
30	Y	607	CHL	C1A-CHA-C4D	2.67	123.44	118.98
30	S	607	CHL	O1D-CGD-CBD	-2.67	120.67	124.72
30	13	601	CHL	C4C-CHD-C1D	2.67	125.63	116.07
30	s	601	CHL	C1C-CHC-C4B	2.67	125.63	116.07
30	n	606	CHL	C4C-CHD-C1D	2.67	125.62	116.07
31	6	611	CLA	C1-C2-C3	2.67	130.57	126.20
30	11	606	CHL	C1C-CHC-C4B	2.67	125.62	116.07
30	11	609	CHL	O2A-CGA-CBA	2.67	119.97	111.83
30	16	608	CHL	C1C-CHC-C4B	2.67	125.61	116.07
31	C	509	CLA	C1-C2-C3	2.67	130.57	126.20
31	Y	603	CLA	C1-C2-C3	2.67	130.57	126.20
30	2	606	CHL	C4C-CHD-C1D	2.67	125.61	116.07
30	4	609	CHL	C1C-CHC-C4B	2.67	125.61	116.07
30	1	608	CHL	C4C-CHD-C1D	2.67	125.61	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	G	609	CHL	O2A-CGA-CBA	2.67	119.97	111.83
30	3	608	CHL	C1A-CHA-C4D	2.67	123.43	118.98
30	1	609	CHL	C1C-CHC-C4B	2.67	125.61	116.07
30	16	606	CHL	C4C-CHD-C1D	2.67	125.61	116.07
30	12	608	CHL	C1A-CHA-C4D	2.67	123.43	118.98
30	Y	606	CHL	O1D-CGD-CBD	-2.67	120.68	124.72
30	6	608	CHL	C4C-CHD-C1D	2.67	125.61	116.07
31	R	602	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
30	G	609	CHL	C1C-CHC-C4B	2.66	125.60	116.07
30	R	607	CHL	C4C-CHD-C1D	2.66	125.60	116.07
30	y	601	CHL	C4C-CHD-C1D	2.66	125.60	116.07
31	2	602	CLA	C1-C2-C3	2.66	130.56	126.20
30	N	606	CHL	C4C-CHD-C1D	2.66	125.60	116.07
31	R	612	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
30	g	608	CHL	C4C-CHD-C1D	2.66	125.59	116.07
30	16	601	CHL	C4C-CHD-C1D	2.66	125.59	116.07
30	s	606	CHL	C1C-CHC-C4B	2.66	125.59	116.07
31	5	602	CLA	C1-C2-C3	2.66	130.56	126.20
30	Y	605	CHL	OBD-CAD-CBD	-2.66	121.92	125.82
30	15	607	CHL	O1D-CGD-CBD	-2.66	120.69	124.72
30	5	605	CHL	CHA-C1A-C2A	-2.66	127.06	133.31
30	n	601	CHL	C1C-CHC-C4B	2.66	125.58	116.07
30	3	608	CHL	C4C-CHD-C1D	2.66	125.58	116.07
30	g	607	CHL	C4C-CHD-C1D	2.66	125.58	116.07
30	g	601	CHL	O2A-CGA-CBA	2.66	119.94	111.83
30	Y	608	CHL	C1A-CHA-C4D	2.66	123.42	118.98
30	R	605	CHL	C1C-CHC-C4B	2.66	125.58	116.07
31	c	509	CLA	C1-C2-C3	2.66	130.55	126.20
30	Y	606	CHL	C4C-CHD-C1D	2.66	125.58	116.07
30	12	608	CHL	C1C-CHC-C4B	2.66	125.58	116.07
30	g	609	CHL	C4C-CHD-C1D	2.66	125.58	116.07
31	1	610	CLA	CHD-C1D-ND	-2.66	121.06	124.80
30	N	605	CHL	C1-C2-C3	2.66	130.55	126.20
31	13	611	CLA	C1-C2-C3	2.66	130.55	126.20
31	r	602	CLA	C1-C2-C3	2.66	130.55	126.20
30	g	609	CHL	OBD-CAD-CBD	-2.66	121.93	125.82
30	G	609	CHL	C4C-CHD-C1D	2.66	125.57	116.07
30	N	601	CHL	C1C-CHC-C4B	2.66	125.57	116.07
30	6	608	CHL	C1A-CHA-C4D	2.66	123.41	118.98
30	Y	601	CHL	C4C-CHD-C1D	2.65	125.57	116.07
30	1	607	CHL	C4C-CHD-C1D	2.65	125.57	116.07
30	g	601	CHL	C4C-CHD-C1D	2.65	125.57	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	n	609	CHL	C1C-CHC-C4B	2.65	125.57	116.07
30	3	601	CHL	CHA-C1A-C2A	-2.65	127.07	133.31
30	5	605	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
31	12	612	CLA	C1-C2-C3	2.65	131.06	126.76
31	b	605	CLA	C12-C11-C10	-2.65	101.39	113.28
31	g	610	CLA	C1-C2-C3	2.65	130.54	126.20
30	S	607	CHL	C1C-CHC-C4B	2.65	125.56	116.07
30	G	605	CHL	C4C-CHD-C1D	2.65	125.56	116.07
30	G	607	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
30	g	606	CHL	C1C-CHC-C4B	2.65	125.56	116.07
30	5	606	CHL	CHA-C1A-C2A	-2.65	127.08	133.31
31	B	605	CLA	C12-C11-C10	-2.65	101.40	113.28
30	y	608	CHL	C4C-CHD-C1D	2.65	125.56	116.07
30	G	607	CHL	C4C-CHD-C1D	2.65	125.56	116.07
30	g	605	CHL	C4C-CHD-C1D	2.65	125.56	116.07
31	s	612	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
30	6	606	CHL	O1D-CGD-CBD	-2.65	120.70	124.72
30	S	601	CHL	C4C-CHD-C1D	2.65	125.55	116.07
30	y	606	CHL	C4C-CHD-C1D	2.65	125.55	116.07
31	r	610	CLA	C1-C2-C3	2.65	130.53	126.20
30	16	609	CHL	C4C-CHD-C1D	2.65	125.54	116.07
30	14	608	CHL	OMC-CMC-C2C	-2.65	120.52	125.12
30	G	606	CHL	C1C-CHC-C4B	2.65	125.54	116.07
30	G	608	CHL	C1A-CHA-C4D	2.65	123.40	118.98
30	S	608	CHL	O1D-CGD-CBD	-2.65	120.71	124.72
30	5	608	CHL	C1A-CHA-C4D	2.65	123.40	118.98
30	s	607	CHL	C1C-CHC-C4B	2.64	125.53	116.07
30	13	609	CHL	O2A-CGA-CBA	2.64	119.90	111.83
30	g	607	CHL	O1D-CGD-CBD	-2.64	120.71	124.72
31	B	603	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
30	S	607	CHL	C4C-CHD-C1D	2.64	125.52	116.07
31	6	615	CLA	C1-C2-C3	2.64	131.04	126.76
30	G	601	CHL	CHA-C1A-C2A	-2.64	127.10	133.31
30	2	608	CHL	C1A-CHA-C4D	2.64	123.39	118.98
30	6	606	CHL	C4C-CHD-C1D	2.64	125.52	116.07
30	2	605	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
30	3	606	CHL	C4C-CHD-C1D	2.64	125.52	116.07
30	12	605	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
30	s	608	CHL	OMC-CMC-C2C	-2.64	120.54	125.12
30	13	608	CHL	C1A-CHA-C4D	2.64	123.38	118.98
30	g	601	CHL	CHA-C1A-C2A	-2.64	127.11	133.31
30	4	601	CHL	C4C-CHD-C1D	2.64	125.51	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	606	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
30	y	601	CHL	CHA-C1A-C2A	-2.64	127.11	133.31
30	4	609	CHL	CHA-C1A-C2A	-2.64	127.11	133.31
30	n	608	CHL	O2D-CGD-O1D	-2.64	118.72	123.85
30	Y	608	CHL	C4C-CHD-C1D	2.64	125.50	116.07
30	G	601	CHL	C4C-CHD-C1D	2.64	125.50	116.07
30	6	608	CHL	C1C-CHC-C4B	2.64	125.50	116.07
30	s	608	CHL	C4C-CHD-C1D	2.64	125.50	116.07
30	5	601	CHL	C4C-CHD-C1D	2.63	125.50	116.07
30	s	601	CHL	C4C-CHD-C1D	2.63	125.50	116.07
30	1	605	CHL	C1A-CHA-C4D	2.63	123.38	118.98
30	6	607	CHL	C4C-CHD-C1D	2.63	125.50	116.07
31	n	602	CLA	C1-C2-C3	2.63	130.51	126.20
31	c	513	CLA	C1-C2-C3	2.63	130.51	126.20
31	2	603	CLA	C1-C2-C3	2.63	130.51	126.20
30	2	609	CHL	C1A-CHA-C4D	2.63	123.38	118.98
30	4	606	CHL	C1C-CHC-C4B	2.63	125.49	116.07
31	n	604	CLA	C1-C2-C3	2.63	130.51	126.20
30	S	608	CHL	C4C-CHD-C1D	2.63	125.48	116.07
30	n	607	CHL	CBC-CAC-C3C	-2.63	109.11	112.87
30	S	607	CHL	OBD-CAD-CBD	-2.63	121.96	125.82
31	R	614	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
30	16	608	CHL	C1A-CHA-C4D	2.63	123.37	118.98
30	N	607	CHL	CBC-CAC-C3C	-2.63	109.11	112.87
30	3	606	CHL	CHA-C1A-C2A	-2.63	127.13	133.31
30	3	608	CHL	C1C-CHC-C4B	2.63	125.48	116.07
30	13	609	CHL	CHA-C1A-C2A	-2.63	127.13	133.31
30	r	605	CHL	C1C-CHC-C4B	2.63	125.47	116.07
30	y	601	CHL	C1-C2-C3	2.63	130.50	126.20
30	2	605	CHL	CHA-C1A-C2A	-2.63	127.14	133.31
30	6	605	CHL	OBD-CAD-CBD	-2.63	121.97	125.82
30	14	606	CHL	OBD-CAD-CBD	-2.63	121.97	125.82
30	r	606	CHL	C4C-CHD-C1D	2.63	125.46	116.07
30	R	606	CHL	C4C-CHD-C1D	2.63	125.46	116.07
31	N	604	CLA	C1-C2-C3	2.63	130.50	126.20
30	Y	605	CHL	C4C-CHD-C1D	2.62	125.46	116.07
30	11	601	CHL	C4C-CHD-C1D	2.62	125.46	116.07
30	s	607	CHL	C4C-CHD-C1D	2.62	125.46	116.07
30	N	607	CHL	C4C-CHD-C1D	2.62	125.45	116.07
30	16	605	CHL	OBD-CAD-CBD	-2.62	121.97	125.82
31	C	513	CLA	C1-C2-C3	2.62	130.49	126.20
30	15	605	CHL	O1D-CGD-CBD	-2.62	120.75	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	16	609	CHL	C1C-CHC-C4B	2.62	125.45	116.07
30	n	607	CHL	C4C-CHD-C1D	2.62	125.45	116.07
31	b	612	CLA	C12-C11-C10	-2.62	101.53	113.28
31	C	510	CLA	C1-C2-C3	2.62	130.49	126.20
30	16	606	CHL	CHA-C1A-C2A	-2.62	127.15	133.31
31	B	612	CLA	C1-C2-C3	2.62	130.49	126.20
30	14	601	CHL	O2A-CGA-CBA	2.62	119.82	111.83
30	5	606	CHL	O1D-CGD-CBD	-2.62	120.75	124.72
31	b	603	CLA	C12-C11-C10	-2.62	101.55	113.28
30	G	609	CHL	OBD-CAD-CBD	-2.62	121.98	125.82
31	11	613	CLA	C1-C2-C3	2.62	130.49	126.20
31	Y	604	CLA	C1-C2-C3	2.62	130.49	126.20
30	1	608	CHL	C1C-CHC-C4B	2.62	125.44	116.07
30	6	609	CHL	CHA-C1A-C2A	-2.62	127.16	133.31
31	15	602	CLA	O1D-CGD-CBD	-2.62	119.36	124.52
30	s	606	CHL	O1D-CGD-CBD	-2.62	120.76	124.72
31	g	604	CLA	O1D-CGD-CBD	-2.61	119.36	124.52
30	13	609	CHL	OBD-CAD-CBD	-2.61	121.99	125.82
30	n	605	CHL	C1A-CHA-C4D	2.61	123.34	118.98
31	16	615	CLA	O1D-CGD-CBD	-2.61	119.36	124.52
31	s	603	CLA	O1D-CGD-CBD	-2.61	119.36	124.52
30	3	606	CHL	O1D-CGD-CBD	-2.61	120.76	124.72
31	N	612	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
30	G	601	CHL	O1D-CGD-CBD	-2.61	120.76	124.72
30	1	601	CHL	C4C-CHD-C1D	2.61	125.41	116.07
31	b	603	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
30	y	608	CHL	C1C-CHC-C4B	2.61	125.41	116.07
31	B	612	CLA	C12-C11-C10	-2.61	101.58	113.28
31	5	603	CLA	C1-C2-C3	2.61	130.47	126.20
30	15	607	CHL	OBD-CAD-CBD	-2.61	122.00	125.82
30	r	607	CHL	O2A-CGA-O1A	-2.61	117.10	123.63
30	n	601	CHL	OBD-CAD-CBD	-2.61	122.00	125.82
30	3	607	CHL	C4C-CHD-C1D	2.61	125.39	116.07
30	11	605	CHL	C1A-CHA-C4D	2.61	123.33	118.98
30	n	608	CHL	CHA-C1A-C2A	-2.60	127.19	133.31
30	g	606	CHL	CHA-C1A-C2A	-2.60	127.19	133.31
30	15	607	CHL	C4C-CHD-C1D	2.60	125.39	116.07
30	15	606	CHL	C1-C2-C3	2.60	130.98	126.76
30	4	607	CHL	C4C-CHD-C1D	2.60	125.38	116.07
30	1	606	CHL	C1C-CHC-C4B	2.60	125.38	116.07
30	14	605	CHL	C4C-CHD-C1D	2.60	125.38	116.07
30	4	605	CHL	C1A-CHA-C4D	2.60	123.32	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	603	CLA	C12-C11-C10	-2.60	101.63	113.28
31	g	613	CLA	C1-C2-C3	2.60	130.46	126.20
30	1	609	CHL	CHA-C1A-C2A	-2.60	127.20	133.31
30	14	601	CHL	C4C-CHD-C1D	2.60	125.37	116.07
31	14	611	CLA	C1-C2-C3	2.60	130.46	126.20
30	S	607	CHL	C1A-CHA-C4D	2.60	123.32	118.98
30	5	607	CHL	C4C-CHD-C1D	2.60	125.36	116.07
30	n	607	CHL	CHA-C1A-C2A	-2.60	127.21	133.31
31	6	614	CLA	C1-C2-C3	2.60	130.96	126.76
30	2	601	CHL	CHA-C1A-C2A	-2.60	127.21	133.31
31	b	616	CLA	O1D-CGD-CBD	-2.59	119.40	124.52
31	c	510	CLA	C1-C2-C3	2.59	130.44	126.20
30	6	607	CHL	OMC-CMC-C2C	-2.59	120.62	125.12
31	B	616	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
30	Y	608	CHL	OMC-CMC-C2C	-2.59	120.62	125.12
31	R	603	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
30	12	607	CHL	C4C-CHD-C1D	2.59	125.34	116.07
30	13	606	CHL	O1D-CGD-CBD	-2.59	120.80	124.72
30	3	609	CHL	CHA-C1A-C2A	-2.59	127.23	133.31
31	c	506	CLA	C1-C2-C3	2.59	130.44	126.20
31	y	603	CLA	C1-C2-C3	2.59	130.44	126.20
31	y	604	CLA	C1-C2-C3	2.59	130.44	126.20
30	1	601	CHL	O2A-CGA-CBA	2.59	119.72	111.83
31	1	604	CLA	CHD-C1D-ND	-2.59	121.16	124.80
30	6	605	CHL	OMC-CMC-C2C	-2.59	120.63	125.12
30	n	605	CHL	OMC-CMC-C2C	-2.59	120.63	125.12
31	6	615	CLA	O1D-CGD-CBD	-2.59	119.42	124.52
30	3	607	CHL	OMC-CMC-C2C	-2.59	120.63	125.12
30	4	608	CHL	O1D-CGD-CBD	-2.58	120.80	124.72
30	4	606	CHL	C4C-CHD-C1D	2.58	125.32	116.07
30	g	608	CHL	C1C-CHC-C4B	2.58	125.30	116.07
30	11	606	CHL	C4C-CHD-C1D	2.58	125.29	116.07
30	n	605	CHL	OBD-CAD-CBD	-2.58	122.04	125.82
31	15	613	CLA	CHD-C1D-ND	-2.58	121.17	124.80
30	15	605	CHL	OBD-CAD-CBD	-2.58	122.04	125.82
31	b	612	CLA	C1-C2-C3	2.58	130.42	126.20
30	2	607	CHL	C4C-CHD-C1D	2.58	125.29	116.07
30	3	605	CHL	OMC-CMC-C2C	-2.58	120.65	125.12
30	14	605	CHL	C1A-CHA-C4D	2.58	123.28	118.98
31	6	602	CLA	C1-C2-C3	2.57	130.41	126.20
31	s	611	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
31	y	615	CLA	C1-C2-C3	2.57	130.41	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	611	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
31	c	504	CLA	C12-C11-C10	-2.57	101.76	113.28
31	g	603	CLA	C1-C2-C3	2.57	130.41	126.20
31	Y	603	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
30	2	601	CHL	C3C-C4C-NC	-2.57	108.37	114.65
30	2	609	CHL	C4C-CHD-C1D	2.57	125.26	116.07
30	14	607	CHL	C4C-CHD-C1D	2.57	125.26	116.07
30	15	608	CHL	C1A-CHA-C4D	2.57	123.27	118.98
30	R	606	CHL	O2A-CGA-CBA	2.57	119.67	111.83
31	6	603	CLA	C1-C2-C3	2.57	130.40	126.20
31	G	613	CLA	C1-C2-C3	2.57	130.40	126.20
30	Y	605	CHL	O2D-CGD-O1D	-2.57	118.85	123.85
30	6	606	CHL	OBD-CAD-CBD	-2.56	122.06	125.82
30	14	605	CHL	OMC-CMC-C2C	-2.56	120.67	125.12
30	1	607	CHL	C1A-CHA-C4D	2.56	123.26	118.98
30	G	608	CHL	C1C-CHC-C4B	2.56	125.24	116.07
30	11	608	CHL	C3C-C4C-NC	-2.56	108.39	114.65
30	12	606	CHL	C1-C2-C3	2.56	130.91	126.76
30	g	601	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
30	6	601	CHL	CHA-C1A-C2A	-2.56	127.30	133.31
31	2	604	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
31	s	604	CLA	C12-C11-C10	-2.56	101.82	113.28
30	14	608	CHL	C4C-CHD-C1D	2.56	125.22	116.07
30	6	606	CHL	CHA-C1A-C2A	-2.56	127.30	133.31
30	5	608	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
30	15	601	CHL	CHA-C1A-C2A	-2.56	127.30	133.31
30	r	605	CHL	O1D-CGD-CBD	-2.56	120.85	124.72
30	r	606	CHL	O2A-CGA-CBA	2.56	119.63	111.83
30	5	609	CHL	C4C-CHD-C1D	2.56	125.21	116.07
30	1	607	CHL	O1D-CGD-CBD	-2.56	120.85	124.72
30	15	606	CHL	CHA-C1A-C2A	-2.55	127.31	133.31
30	N	608	CHL	C1A-CHA-C4D	2.55	123.24	118.98
31	5	604	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
30	14	601	CHL	OMC-CMC-C2C	-2.55	120.69	125.12
31	C	505	CLA	C1-C2-C3	2.55	130.38	126.20
30	N	607	CHL	CHA-C1A-C2A	-2.55	127.31	133.31
30	12	605	CHL	OBD-CAD-CBD	-2.55	122.08	125.82
31	16	613	CLA	C1-C2-C3	2.55	130.89	126.76
31	2	611	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
30	2	607	CHL	CHA-C1A-C2A	-2.55	127.32	133.31
30	1	606	CHL	C3C-C4C-NC	-2.55	108.42	114.65
31	G	603	CLA	C1-C2-C3	2.55	130.37	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	604	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
30	N	606	CHL	CHA-C1A-C2A	-2.55	127.32	133.31
30	4	605	CHL	C1C-CHC-C4B	2.55	125.18	116.07
31	r	608	CLA	C12-C11-C10	-2.55	101.86	113.28
31	3	602	CLA	C1-C2-C3	2.55	130.37	126.20
31	s	610	CLA	O1D-CGD-CBD	-2.55	119.50	124.52
30	1	605	CHL	C1C-CHC-C4B	2.55	125.17	116.07
30	13	609	CHL	C1C-CHC-C4B	2.54	125.17	116.07
31	5	610	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
31	S	603	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
30	2	605	CHL	C4C-CHD-C1D	2.54	125.16	116.07
30	s	608	CHL	O1D-CGD-CBD	-2.54	120.87	124.72
30	g	609	CHL	CHA-C1A-C2A	-2.54	127.34	133.31
31	1	604	CLA	C1-C2-C3	2.54	130.87	126.76
31	n	613	CLA	CED-O2D-CGD	2.54	121.68	115.92
31	3	603	CLA	C1-C2-C3	2.54	130.36	126.20
30	Y	608	CHL	CHA-C1A-C2A	-2.54	127.34	133.31
30	N	605	CHL	OMC-CMC-C2C	-2.54	120.71	125.12
31	b	604	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
30	3	608	CHL	CHA-C1A-C2A	-2.54	127.35	133.31
30	3	606	CHL	OBD-CAD-CBD	-2.54	122.10	125.82
31	R	613	CLA	C12-C11-C10	-2.54	101.90	113.28
30	6	608	CHL	CHA-C1A-C2A	-2.54	127.35	133.31
31	n	612	CLA	O1D-CGD-CBD	-2.54	119.52	124.52
30	5	605	CHL	OMC-CMC-C2C	-2.54	120.72	125.12
31	1	612	CLA	O2A-CGA-CBA	2.54	121.72	112.14
31	C	504	CLA	C12-C11-C10	-2.54	101.92	113.28
31	4	604	CLA	CHD-C1D-ND	-2.53	121.23	124.80
30	4	606	CHL	CHA-C1A-C2A	-2.53	127.36	133.31
30	4	606	CHL	O1D-CGD-CBD	-2.53	120.88	124.72
30	14	606	CHL	C4C-CHD-C1D	2.53	125.13	116.07
31	b	608	CLA	C1-C2-C3	2.53	130.35	126.20
31	3	614	CLA	C1-C2-C3	2.53	130.86	126.76
31	B	607	CLA	C1-C2-C3	2.53	130.35	126.20
30	y	608	CHL	CHA-C1A-C2A	-2.53	127.36	133.31
31	15	613	CLA	O2A-CGA-CBA	2.53	122.00	114.00
30	G	609	CHL	CHA-C1A-C2A	-2.53	127.36	133.31
30	n	609	CHL	CHA-C1A-C2A	-2.53	127.36	133.31
31	6	611	CLA	C12-C11-C10	-2.53	101.94	113.28
31	y	611	CLA	C1-C2-C3	2.53	130.34	126.20
30	16	608	CHL	CHA-C1A-C2A	-2.53	127.37	133.31
31	S	612	CLA	O2A-CGA-CBA	2.53	121.99	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	602	CLA	C12-C11-C10	-2.53	101.94	113.28
31	11	610	CLA	C1-C2-C3	2.53	130.34	126.20
30	16	608	CHL	C3C-C4C-NC	-2.53	108.47	114.65
30	11	606	CHL	OBD-CAD-CBD	-2.53	122.11	125.82
30	n	606	CHL	O2A-CGA-O1A	-2.53	117.31	123.63
30	5	605	CHL	C1A-CHA-C4D	2.53	123.20	118.98
30	11	601	CHL	OMC-CMC-C2C	-2.53	120.73	125.12
30	13	608	CHL	C3C-C4C-NC	-2.53	108.48	114.65
31	Y	611	CLA	C1-C2-C3	2.53	130.34	126.20
31	r	602	CLA	C12-C11-C10	-2.53	101.96	113.28
30	13	608	CHL	CHA-C1A-C2A	-2.52	127.38	133.31
31	3	615	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
31	14	613	CLA	C1-C2-C3	2.52	130.33	126.20
30	4	601	CHL	C3C-C4C-NC	-2.52	108.48	114.65
31	c	512	CLA	C1-C2-C3	2.52	130.33	126.20
31	y	603	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
30	2	608	CHL	CHA-C1A-C2A	-2.52	127.39	133.31
31	R	608	CLA	C12-C11-C10	-2.52	101.98	113.28
31	g	612	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
30	12	601	CHL	CHA-C1A-C2A	-2.52	127.39	133.31
31	D	404	CLA	C12-C11-C10	-2.52	101.98	113.28
31	1	602	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
30	N	601	CHL	C1-C2-C3	2.52	130.33	126.20
30	11	607	CHL	C4C-CHD-C1D	2.52	125.08	116.07
31	1	602	CLA	C12-C11-C10	-2.52	101.99	113.28
31	Y	602	CLA	C12-C11-C10	-2.52	101.99	113.28
30	2	605	CHL	OMC-CMC-C2C	-2.52	120.75	125.12
31	g	611	CLA	C12-C11-C10	-2.52	101.99	113.28
30	6	609	CHL	C1A-CHA-C4D	2.52	123.19	118.98
31	13	610	CLA	C1-C2-C3	2.52	130.32	126.20
30	2	605	CHL	OBD-CAD-CBD	-2.52	122.13	125.82
30	13	601	CHL	CHA-C1A-C2A	-2.52	127.39	133.31
30	15	606	CHL	C4C-CHD-C1D	2.52	125.08	116.07
31	13	603	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
31	Y	615	CLA	C1-C2-C3	2.52	130.32	126.20
30	15	608	CHL	C3C-C4C-NC	-2.52	108.50	114.65
30	1	608	CHL	O1D-CGD-CBD	-2.52	120.91	124.72
30	N	608	CHL	CHA-C1A-C2A	-2.52	127.40	133.31
30	N	609	CHL	C1A-CHA-C4D	2.52	123.18	118.98
31	B	608	CLA	C1-C2-C3	2.52	130.32	126.20
31	b	607	CLA	C1-C2-C3	2.52	130.32	126.20
30	y	601	CHL	C3C-C4C-NC	-2.51	108.50	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	15	602	CLA	C1-C2-C3	2.51	130.31	126.20
30	11	605	CHL	C3C-C4C-NC	-2.51	108.51	114.65
30	G	605	CHL	C1A-CHA-C4D	2.51	123.17	118.98
30	5	607	CHL	CHA-C1A-C2A	-2.51	127.41	133.31
30	N	608	CHL	OMC-CMC-C2C	-2.51	120.76	125.12
30	12	608	CHL	C3C-C4C-NC	-2.51	108.51	114.65
30	n	609	CHL	C1A-CHA-C4D	2.51	123.17	118.98
30	G	605	CHL	OMC-CMC-C2C	-2.51	120.76	125.12
30	5	605	CHL	C4C-CHD-C1D	2.51	125.05	116.07
30	N	609	CHL	CHA-C1A-C2A	-2.51	127.41	133.31
30	S	607	CHL	CHA-C1A-C2A	-2.51	127.41	133.31
30	1	601	CHL	O2A-CGA-O1A	-2.51	117.35	123.63
31	13	604	CLA	C1-C2-C3	2.51	130.31	126.20
31	11	602	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
31	A	403	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
30	Y	601	CHL	C3C-C4C-NC	-2.51	108.52	114.65
30	2	608	CHL	O1D-CGD-CBD	-2.51	120.92	124.72
30	n	608	CHL	OMC-CMC-C2C	-2.51	120.77	125.12
30	1	601	CHL	C3C-C4C-NC	-2.51	108.53	114.65
30	12	606	CHL	C4C-CHD-C1D	2.51	125.03	116.07
30	s	606	CHL	CHA-C1A-C2A	-2.51	127.42	133.31
30	y	608	CHL	OMC-CMC-C2C	-2.50	120.77	125.12
30	13	605	CHL	CAA-C2A-C3A	-2.50	106.23	113.00
31	G	612	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
30	g	605	CHL	C1A-CHA-C4D	2.50	123.16	118.98
30	y	609	CHL	CHA-C1A-C2A	-2.50	127.43	133.31
30	11	601	CHL	O2A-CGA-O1A	-2.50	117.37	123.63
30	16	605	CHL	C3C-C4C-NC	-2.50	108.54	114.65
31	3	615	CLA	CHD-C1D-ND	-2.50	121.28	124.80
30	12	601	CHL	C4C-CHD-C1D	2.50	125.01	116.07
31	R	614	CLA	C1-C2-C3	2.50	130.29	126.20
30	n	601	CHL	C3C-C4C-NC	-2.50	108.54	114.65
31	b	615	CLA	C1-C2-C3	2.50	130.29	126.20
31	s	610	CLA	CHD-C1D-ND	-2.50	121.29	124.80
30	1	605	CHL	C3C-C4C-NC	-2.50	108.54	114.65
30	16	607	CHL	CHA-C1A-C2A	-2.50	127.44	133.31
31	14	602	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
30	3	609	CHL	C3C-C4C-NC	-2.50	108.55	114.65
30	5	605	CHL	C3C-C4C-NC	-2.50	108.55	114.65
30	N	605	CHL	C3C-C4C-NC	-2.50	108.55	114.65
30	15	607	CHL	C3C-C4C-NC	-2.49	108.55	114.65
31	d	404	CLA	C12-C11-C10	-2.49	102.10	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	N	601	CHL	C3C-C4C-NC	-2.49	108.55	114.65
31	c	511	CLA	C12-C11-C10	-2.49	102.10	113.28
30	3	609	CHL	C1A-CHA-C4D	2.49	123.14	118.98
30	n	608	CHL	C3C-C4C-NC	-2.49	108.56	114.65
30	3	601	CHL	C3C-C4C-NC	-2.49	108.56	114.65
30	y	606	CHL	OMC-CMC-C2C	-2.49	120.79	125.12
30	15	601	CHL	C4C-CHD-C1D	2.49	124.99	116.07
31	C	511	CLA	C12-C11-C10	-2.49	102.11	113.28
31	r	609	CLA	C12-C11-C10	-2.49	102.11	113.28
31	c	508	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
31	c	511	CLA	C1-C2-C3	2.49	130.28	126.20
30	n	601	CHL	C1A-CHA-C4D	2.49	123.14	118.98
31	B	604	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
30	y	607	CHL	C3C-C4C-NC	-2.49	108.56	114.65
30	14	609	CHL	C3C-C4C-NC	-2.49	108.56	114.65
31	13	603	CLA	C12-C11-C10	-2.49	102.12	113.28
31	4	611	CLA	C1-C2-C3	2.49	130.79	126.76
31	16	611	CLA	C1-C2-C3	2.49	130.28	126.20
31	4	610	CLA	C1-C2-C3	2.49	130.28	126.20
31	S	614	CLA	C12-C11-C10	-2.49	102.12	113.28
31	B	615	CLA	C1-C2-C3	2.49	130.28	126.20
30	14	609	CHL	C4C-CHD-C1D	2.49	124.97	116.07
30	11	609	CHL	C3C-C4C-NC	-2.49	108.57	114.65
30	12	607	CHL	C3C-C4C-NC	-2.49	108.57	114.65
30	g	605	CHL	OMC-CMC-C2C	-2.49	120.80	125.12
31	3	612	CLA	C1-C2-C3	2.49	130.27	126.20
31	N	610	CLA	C1-C2-C3	2.49	130.27	126.20
30	11	609	CHL	OMC-CMC-C2C	-2.49	120.80	125.12
31	s	611	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
30	5	601	CHL	CHA-C1A-C2A	-2.49	127.47	133.31
30	n	606	CHL	CHA-C1A-C2A	-2.48	127.47	133.31
30	R	605	CHL	C3C-C4C-NC	-2.48	108.58	114.65
30	12	605	CHL	CBC-CAC-C3C	-2.48	109.32	112.87
30	11	607	CHL	CHA-C1A-C2A	-2.48	127.47	133.31
30	14	601	CHL	C3C-C4C-NC	-2.48	108.58	114.65
31	G	602	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
31	r	614	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
30	14	607	CHL	C3C-C4C-NC	-2.48	108.58	114.65
30	G	605	CHL	C3C-C4C-NC	-2.48	108.58	114.65
31	C	511	CLA	C1-C2-C3	2.48	130.26	126.20
30	5	608	CHL	CHA-C1A-C2A	-2.48	127.48	133.31
30	12	606	CHL	CHA-C1A-C2A	-2.48	127.48	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	y	606	CHL	CHA-C1A-C2A	-2.48	127.48	133.31
31	b	611	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
30	n	608	CHL	O1D-CGD-CBD	-2.48	120.96	124.72
30	16	608	CHL	OMC-CMC-C2C	-2.48	120.81	125.12
30	2	605	CHL	C1A-CHA-C4D	2.48	123.12	118.98
30	5	608	CHL	C3C-C4C-NC	-2.48	108.59	114.65
31	B	604	CLA	C1-C2-C3	2.48	130.26	126.20
30	N	608	CHL	C3C-C4C-NC	-2.48	108.59	114.65
31	B	604	CLA	C12-C11-C10	-2.48	102.17	113.28
31	b	604	CLA	C12-C11-C10	-2.48	102.17	113.28
31	2	610	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
30	15	605	CHL	C3C-C4C-NC	-2.48	108.59	114.65
31	6	615	CLA	CHD-C1D-ND	-2.48	121.31	124.80
31	G	611	CLA	C12-C11-C10	-2.48	102.18	113.28
30	6	601	CHL	C3C-C4C-NC	-2.48	108.60	114.65
30	16	601	CHL	C3C-C4C-NC	-2.48	108.60	114.65
30	1	607	CHL	CHA-C1A-C2A	-2.48	127.49	133.31
30	1	609	CHL	O2D-CGD-O1D	-2.48	119.03	123.85
30	2	608	CHL	C3C-C4C-NC	-2.48	108.60	114.65
30	13	601	CHL	C3C-C4C-NC	-2.48	108.60	114.65
30	R	606	CHL	C3C-C4C-NC	-2.47	108.60	114.65
30	S	601	CHL	C3C-C4C-NC	-2.47	108.60	114.65
30	6	608	CHL	OMC-CMC-C2C	-2.47	120.83	125.12
30	13	605	CHL	C3C-C4C-NC	-2.47	108.61	114.65
30	Y	609	CHL	O2D-CGD-O1D	-2.47	119.03	123.85
31	R	614	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
30	n	609	CHL	C3C-C4C-NC	-2.47	108.61	114.65
31	3	611	CLA	C12-C11-C10	-2.47	102.20	113.28
31	B	602	CLA	C12-C11-C10	-2.47	102.20	113.28
30	4	608	CHL	C3C-C4C-NC	-2.47	108.61	114.65
30	N	609	CHL	C3C-C4C-NC	-2.47	108.61	114.65
31	N	602	CLA	C12-C11-C10	-2.47	102.20	113.28
30	11	608	CHL	C1-O2A-CGA	2.47	122.63	116.65
30	N	609	CHL	OMC-CMC-C2C	-2.47	120.83	125.12
30	13	608	CHL	OMC-CMC-C2C	-2.47	120.83	125.12
30	s	608	CHL	CHA-C1A-C2A	-2.47	127.51	133.31
30	R	607	CHL	C3C-C4C-NC	-2.47	108.61	114.65
31	A	404	CLA	C12-C11-C10	-2.47	102.21	113.28
30	n	601	CHL	O1D-CGD-CBD	-2.47	120.98	124.72
31	S	611	CLA	C12-C11-C10	-2.47	102.21	113.28
30	11	601	CHL	C3C-C4C-NC	-2.47	108.61	114.65
30	Y	607	CHL	C3C-C4C-NC	-2.47	108.61	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	2	607	CHL	O1D-CGD-CBD	-2.47	120.98	124.72
30	N	606	CHL	O1D-CGD-CBD	-2.47	120.98	124.72
30	s	607	CHL	CHA-C1A-C2A	-2.47	127.51	133.31
31	S	612	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
30	6	605	CHL	O2D-CGD-O1D	-2.47	119.05	123.85
31	14	604	CLA	C1-C2-C3	2.47	130.24	126.20
30	r	606	CHL	C3C-C4C-NC	-2.47	108.62	114.65
31	D	405	CLA	C12-C11-C10	-2.47	102.23	113.28
30	g	601	CHL	C3C-C4C-NC	-2.47	108.62	114.65
31	12	602	CLA	C12-C11-C10	-2.47	102.23	113.28
44	B	623	STE	O2-C1-C2	2.47	121.79	114.00
30	N	601	CHL	OBD-CAD-CBD	-2.46	122.21	125.82
30	n	601	CHL	CHA-C1A-C2A	-2.46	127.52	133.31
30	14	601	CHL	O1D-CGD-CBD	-2.46	120.99	124.72
31	G	610	CLA	O1D-CGD-CBD	-2.46	119.66	124.52
31	c	502	CLA	C12-C11-C10	-2.46	102.24	113.28
30	4	601	CHL	OMC-CMC-C2C	-2.46	120.84	125.12
30	12	605	CHL	C4C-CHD-C1D	2.46	124.88	116.07
30	S	606	CHL	CHA-C1A-C2A	-2.46	127.52	133.31
31	d	405	CLA	C12-C11-C10	-2.46	102.24	113.28
31	b	615	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
31	b	602	CLA	C12-C11-C10	-2.46	102.24	113.28
31	B	611	CLA	O1D-CGD-CBD	-2.46	119.66	124.52
30	2	605	CHL	C3C-C4C-NC	-2.46	108.63	114.65
31	r	613	CLA	C12-C11-C10	-2.46	102.24	113.28
31	N	615	CLA	CHD-C1D-ND	-2.46	121.34	124.80
30	4	606	CHL	C3C-C4C-NC	-2.46	108.64	114.65
30	g	605	CHL	C3C-C4C-NC	-2.46	108.64	114.65
31	C	510	CLA	C12-C11-C10	-2.46	102.25	113.28
30	6	609	CHL	C3C-C4C-NC	-2.46	108.64	114.65
30	16	609	CHL	C3C-C4C-NC	-2.46	108.64	114.65
30	n	605	CHL	C3C-C4C-NC	-2.46	108.64	114.65
31	1	614	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
30	1	601	CHL	OMC-CMC-C2C	-2.46	120.85	125.12
30	14	601	CHL	O2A-CGA-O1A	-2.46	117.48	123.63
30	n	606	CHL	O1D-CGD-CBD	-2.46	121.00	124.72
30	s	601	CHL	C3C-C4C-NC	-2.46	108.65	114.65
30	4	605	CHL	C3C-C4C-NC	-2.46	108.65	114.65
30	G	607	CHL	C3C-C4C-NC	-2.46	108.65	114.65
31	N	604	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
31	16	610	CLA	C1-C2-C3	2.45	130.22	126.20
31	5	610	CLA	CHD-C1D-ND	-2.45	121.35	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	r	607	CHL	C3C-C4C-NC	-2.45	108.65	114.65
30	11	607	CHL	OMC-CMC-C2C	-2.45	120.86	125.12
31	4	614	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
31	d	405	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
30	1	609	CHL	C3C-C4C-NC	-2.45	108.66	114.65
31	a	404	CLA	C12-C11-C10	-2.45	102.29	113.28
31	c	510	CLA	C12-C11-C10	-2.45	102.29	113.28
30	S	608	CHL	C3C-C4C-NC	-2.45	108.66	114.65
30	5	605	CHL	OBD-CAD-CBD	-2.45	122.22	125.82
30	3	608	CHL	O2A-CGA-O1A	-2.45	117.49	123.63
31	C	502	CLA	C12-C11-C10	-2.45	102.29	113.28
30	r	605	CHL	C3C-C4C-NC	-2.45	108.66	114.65
31	r	612	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
30	G	601	CHL	C3C-C4C-NC	-2.45	108.66	114.65
30	y	605	CHL	C3C-C4C-NC	-2.45	108.66	114.65
31	13	602	CLA	C1-C2-C3	2.45	130.21	126.20
31	y	613	CLA	C12-C11-C10	-2.45	102.30	113.28
30	1	608	CHL	C3C-C4C-NC	-2.45	108.67	114.65
30	N	601	CHL	OMC-CMC-C2C	-2.45	120.87	125.12
30	4	609	CHL	C3C-C4C-NC	-2.45	108.67	114.65
30	n	607	CHL	O2A-CGA-O1A	-2.45	117.51	123.63
31	g	613	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
31	15	609	CLA	C1-C2-C3	2.45	130.21	126.20
31	n	614	CLA	O2A-CGA-CBA	2.45	121.73	114.00
30	16	607	CHL	O2D-CGD-O1D	-2.45	119.09	123.85
30	n	606	CHL	C3C-C4C-NC	-2.45	108.67	114.65
30	Y	606	CHL	CHA-C1A-C2A	-2.45	127.56	133.31
30	Y	609	CHL	CHA-C1A-C2A	-2.45	127.56	133.31
31	C	508	CLA	C12-C11-C10	-2.45	102.32	113.28
30	4	608	CHL	CHA-C1A-C2A	-2.45	127.56	133.31
31	b	610	CLA	C1-C2-C3	2.44	130.20	126.20
31	6	602	CLA	C12-C11-C10	-2.44	102.32	113.28
30	n	601	CHL	OMC-CMC-C2C	-2.44	120.88	125.12
31	2	611	CLA	O2A-CGA-CBA	2.44	121.37	112.14
31	4	610	CLA	C4D-CHA-C1A	2.44	124.16	121.24
30	Y	609	CHL	C3C-C4C-NC	-2.44	108.68	114.65
30	g	607	CHL	C3C-C4C-NC	-2.44	108.68	114.65
30	y	601	CHL	O1D-CGD-CBD	-2.44	121.02	124.72
31	s	609	CLA	C1-C2-C3	2.44	130.20	126.20
30	4	607	CHL	C1A-CHA-C4D	2.44	123.05	118.98
31	13	613	CLA	C1-C2-C3	2.44	130.71	126.76
31	n	604	CLA	O1D-CGD-CBD	-2.44	119.70	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	405	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
31	B	610	CLA	C1-C2-C3	2.44	130.19	126.20
30	13	606	CHL	C3C-C4C-NC	-2.44	108.69	114.65
30	s	608	CHL	C3C-C4C-NC	-2.44	108.69	114.65
31	b	616	CLA	C12-C11-C10	-2.44	102.35	113.28
31	c	506	CLA	C12-C11-C10	-2.44	102.35	113.28
31	R	603	CLA	C12-C11-C10	-2.44	102.35	113.28
31	c	508	CLA	C12-C11-C10	-2.44	102.35	113.28
30	3	607	CHL	C3C-C4C-NC	-2.44	108.69	114.65
30	11	601	CHL	O1D-CGD-CBD	-2.44	121.03	124.72
30	S	607	CHL	C3C-C4C-NC	-2.44	108.69	114.65
31	4	602	CLA	C1-C2-C3	2.44	130.19	126.20
31	C	507	CLA	C1-C2-C3	2.44	130.19	126.20
31	C	506	CLA	C12-C11-C10	-2.44	102.36	113.28
30	3	607	CHL	O2D-CGD-O1D	-2.44	119.11	123.85
30	16	607	CHL	C3C-C4C-NC	-2.44	108.70	114.65
31	c	505	CLA	O1D-CGD-CBD	-2.44	119.71	124.52
30	5	607	CHL	O1D-CGD-CBD	-2.44	121.03	124.72
30	N	605	CHL	O2D-CGD-O1D	-2.44	119.11	123.85
31	16	603	CLA	C12-C11-C10	-2.44	102.37	113.28
30	g	606	CHL	C3C-C4C-NC	-2.43	108.70	114.65
30	16	606	CHL	O2A-CGA-O1A	-2.43	117.54	123.63
31	N	613	CLA	C1-C2-C3	2.43	130.19	126.20
30	3	608	CHL	OMC-CMC-C2C	-2.43	120.89	125.12
30	G	609	CHL	C3C-C4C-NC	-2.43	108.70	114.65
30	g	609	CHL	C3C-C4C-NC	-2.43	108.70	114.65
30	N	601	CHL	O1D-CGD-CBD	-2.43	121.03	124.72
31	14	602	CLA	C12-C11-C10	-2.43	102.38	113.28
44	b	622	STE	O2-C1-C2	2.43	121.69	114.00
30	16	606	CHL	C3C-C4C-NC	-2.43	108.71	114.65
30	11	609	CHL	C4C-CHD-C1D	2.43	124.77	116.07
30	2	607	CHL	C3C-C4C-NC	-2.43	108.71	114.65
31	C	512	CLA	C1-C2-C3	2.43	130.18	126.20
30	13	609	CHL	C4C-CHD-C1D	2.43	124.77	116.07
31	C	505	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
30	2	601	CHL	O2A-CGA-CBA	2.43	121.32	112.14
31	C	514	CLA	C12-C11-C10	-2.43	102.38	113.28
30	Y	607	CHL	CHA-C1A-C2A	-2.43	127.60	133.31
31	6	612	CLA	C1-C2-C3	2.43	130.18	126.20
30	4	607	CHL	C3C-C4C-NC	-2.43	108.71	114.65
30	11	608	CHL	O2A-CGA-O1A	-2.43	117.55	123.63
30	s	601	CHL	OMC-CMC-C2C	-2.43	120.90	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	507	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
30	N	606	CHL	C3C-C4C-NC	-2.43	108.71	114.65
31	B	613	CLA	C1-C2-C3	2.43	130.18	126.20
31	y	602	CLA	C1-C2-C3	2.43	130.18	126.20
30	6	608	CHL	C3C-C4C-NC	-2.43	108.72	114.65
30	16	607	CHL	C1A-CHA-C4D	2.43	123.03	118.98
31	16	614	CLA	O2A-CGA-CBA	2.43	121.67	114.00
31	G	613	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
31	B	615	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
30	4	609	CHL	O2D-CGD-O1D	-2.43	119.12	123.85
31	2	602	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
30	y	609	CHL	C3C-C4C-NC	-2.43	108.72	114.65
30	4	601	CHL	CHA-C1A-C2A	-2.43	127.61	133.31
31	y	602	CLA	C12-C11-C10	-2.43	102.41	113.28
30	1	607	CHL	C3C-C4C-NC	-2.43	108.72	114.65
31	g	610	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
31	S	610	CLA	C12-C11-C10	-2.43	102.41	113.28
31	c	503	CLA	C12-C11-C10	-2.43	102.41	113.28
30	5	601	CHL	C3C-C4C-NC	-2.42	108.72	114.65
31	c	507	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
30	Y	605	CHL	C3C-C4C-NC	-2.42	108.73	114.65
31	b	615	CLA	C12-C11-C10	-2.42	102.42	113.28
30	S	608	CHL	CHA-C1A-C2A	-2.42	127.62	133.31
30	6	608	CHL	O2A-CGA-O1A	-2.42	117.57	123.63
31	15	612	CLA	C1-C2-C3	2.42	130.68	126.76
30	5	607	CHL	C3C-C4C-NC	-2.42	108.73	114.65
30	1	606	CHL	CHA-C1A-C2A	-2.42	127.62	133.31
31	N	611	CLA	C12-C11-C10	-2.42	102.42	113.28
30	6	607	CHL	C3C-C4C-NC	-2.42	108.73	114.65
32	l	102	LHG	O8-C23-C24	2.42	119.22	111.83
30	G	606	CHL	C3C-C4C-NC	-2.42	108.73	114.65
31	s	602	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
30	16	601	CHL	CHA-C1A-C2A	-2.42	127.62	133.31
30	3	608	CHL	C3C-C4C-NC	-2.42	108.73	114.65
30	12	605	CHL	C3C-C4C-NC	-2.42	108.73	114.65
32	L	102	LHG	O8-C23-C24	2.42	119.21	111.83
31	12	609	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
30	3	601	CHL	O2D-CGD-O1D	-2.42	119.14	123.85
30	1	608	CHL	OMC-CMC-C2C	-2.42	120.92	125.12
31	11	602	CLA	C12-C11-C10	-2.42	102.44	113.28
31	14	610	CLA	C12-C11-C10	-2.42	102.44	113.28
30	4	608	CHL	OMC-CMC-C2C	-2.42	120.92	125.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	R	606	CHL	CHA-C1A-C2A	-2.42	127.63	133.31
31	s	602	CLA	C12-C11-C10	-2.42	102.45	113.28
31	16	611	CLA	C12-C11-C10	-2.42	102.45	113.28
31	12	602	CLA	C1-C2-C3	2.42	130.16	126.20
31	2	610	CLA	CHD-C1D-ND	-2.42	121.40	124.80
30	14	608	CHL	C3C-C4C-NC	-2.42	108.75	114.65
30	G	608	CHL	C3C-C4C-NC	-2.42	108.75	114.65
31	Y	613	CLA	C12-C11-C10	-2.41	102.46	113.28
31	15	602	CLA	C12-C11-C10	-2.41	102.46	113.28
31	3	602	CLA	C12-C11-C10	-2.41	102.46	113.28
31	14	613	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
30	y	609	CHL	O2D-CGD-O1D	-2.41	119.15	123.85
31	R	604	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
31	r	603	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
30	Y	605	CHL	CHA-C1A-C2A	-2.41	127.64	133.31
30	n	608	CHL	C1A-CHA-C4D	2.41	123.01	118.98
31	R	614	CLA	C4-C3-C5	-2.41	111.04	115.23
30	y	609	CHL	OBD-CAD-CBD	-2.41	122.28	125.82
30	1	609	CHL	OMC-CMC-C2C	-2.41	120.93	125.12
30	14	606	CHL	C3C-C4C-NC	-2.41	108.76	114.65
30	15	606	CHL	C3C-C4C-NC	-2.41	108.76	114.65
30	11	608	CHL	C1-C2-C3	2.41	130.66	126.76
30	r	605	CHL	CHA-C1A-C2A	-2.41	127.65	133.31
31	5	611	CLA	O2A-CGA-CBA	2.41	121.25	112.14
30	6	606	CHL	C3C-C4C-NC	-2.41	108.76	114.65
30	15	601	CHL	C3C-C4C-NC	-2.41	108.76	114.65
30	Y	607	CHL	OMC-CMC-C2C	-2.41	120.94	125.12
30	3	605	CHL	C3C-C4C-NC	-2.41	108.76	114.65
30	3	605	CHL	O2D-CGD-O1D	-2.41	119.16	123.85
31	s	613	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
30	13	607	CHL	C3C-C4C-NC	-2.41	108.76	114.65
31	R	613	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
31	13	614	CLA	O2A-CGA-CBA	2.41	121.61	114.00
31	B	616	CLA	C12-C11-C10	-2.41	102.49	113.28
30	14	605	CHL	C3C-C4C-NC	-2.41	108.77	114.65
30	1	607	CHL	O2A-CGA-O1A	-2.41	117.61	123.63
30	12	601	CHL	C3C-C4C-NC	-2.41	108.77	114.65
30	y	607	CHL	OMC-CMC-C2C	-2.41	120.94	125.12
30	y	607	CHL	CHA-C1A-C2A	-2.41	127.66	133.31
30	2	606	CHL	C3C-C4C-NC	-2.41	108.77	114.65
30	g	608	CHL	C3C-C4C-NC	-2.41	108.77	114.65
30	16	607	CHL	OBD-CAD-CBD	-2.40	122.30	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	615	CLA	C12-C11-C10	-2.40	102.50	113.28
31	d	404	CLA	C1-C2-C3	2.40	130.13	126.20
31	y	611	CLA	C12-C11-C10	-2.40	102.51	113.28
30	6	605	CHL	C3C-C4C-NC	-2.40	108.78	114.65
31	D	404	CLA	C1-C2-C3	2.40	130.13	126.20
31	3	610	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
31	r	604	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
30	11	607	CHL	C3C-C4C-NC	-2.40	108.78	114.65
30	12	606	CHL	C3C-C4C-NC	-2.40	108.78	114.65
31	n	615	CLA	CHD-C1D-ND	-2.40	121.42	124.80
30	3	606	CHL	C3C-C4C-NC	-2.40	108.78	114.65
31	Y	610	CLA	CHD-C1D-ND	-2.40	121.43	124.80
30	5	606	CHL	C3C-C4C-NC	-2.40	108.79	114.65
30	14	608	CHL	C1-O2A-CGA	2.40	122.46	116.65
31	B	609	CLA	C12-C11-C10	-2.40	102.53	113.28
30	r	606	CHL	CHA-C1A-C2A	-2.40	127.68	133.31
30	S	601	CHL	O1D-CGD-CBD	-2.40	121.09	124.72
30	N	601	CHL	C1A-CHA-C4D	2.40	122.98	118.98
31	5	602	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
30	1	606	CHL	C1A-CHA-C4D	2.39	122.98	118.98
30	1	605	CHL	CHA-C1A-C2A	-2.39	127.68	133.31
31	B	614	CLA	C12-C11-C10	-2.39	102.55	113.28
31	n	612	CLA	O2A-CGA-CBA	2.39	121.56	114.00
30	6	607	CHL	CHA-C1A-C2A	-2.39	127.69	133.31
31	b	616	CLA	C1-C2-C3	2.39	130.12	126.20
31	S	613	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
30	1	608	CHL	CHA-C1A-C2A	-2.39	127.69	133.31
31	Y	615	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
30	11	606	CHL	C3C-C4C-NC	-2.39	108.80	114.65
31	N	603	CLA	C12-C11-C10	-2.39	102.56	113.28
31	4	611	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
31	c	509	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
31	b	614	CLA	C12-C11-C10	-2.39	102.56	113.28
31	G	603	CLA	C4-C3-C5	-2.39	111.08	115.23
31	1	610	CLA	C1-C2-C3	2.39	130.11	126.20
31	R	610	CLA	C1-C2-C3	2.39	130.11	126.20
31	b	606	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
31	A	403	CLA	CHD-C1D-ND	-2.39	121.44	124.80
30	13	606	CHL	OMC-CMC-C2C	-2.39	120.97	125.12
31	2	602	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
31	14	611	CLA	C12-C11-C10	-2.39	102.57	113.28
31	12	602	CLA	O2D-CGD-O1D	-2.39	119.20	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	614	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
31	16	610	CLA	CHD-C1D-ND	-2.39	121.44	124.80
30	4	609	CHL	OMC-CMC-C2C	-2.39	120.97	125.12
30	11	608	CHL	OMC-CMC-C2C	-2.39	120.97	125.12
30	1	601	CHL	CHA-C1A-C2A	-2.39	127.70	133.31
31	C	509	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
31	11	603	CLA	C1-C2-C3	2.39	130.11	126.20
31	S	610	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
31	16	602	CLA	C1-C2-C3	2.39	130.11	126.20
30	r	607	CHL	O2D-CGD-O1D	-2.39	119.20	123.85
31	b	609	CLA	C12-C11-C10	-2.39	102.59	113.28
30	6	601	CHL	OMC-CMC-C2C	-2.38	120.98	125.12
30	n	607	CHL	C3C-C4C-NC	-2.38	108.82	114.65
31	2	603	CLA	CHD-C1D-ND	-2.38	121.45	124.80
30	16	608	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
30	11	609	CHL	O2A-CGA-O1A	-2.38	117.66	123.63
30	N	607	CHL	C3C-C4C-NC	-2.38	108.83	114.65
31	13	615	CLA	CHD-C1D-ND	-2.38	121.45	124.80
31	n	603	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
30	S	606	CHL	C3C-C4C-NC	-2.38	108.83	114.65
30	1	606	CHL	O1D-CGD-CBD	-2.38	121.11	124.72
31	16	604	CLA	O1D-CGD-CBD	-2.38	119.82	124.52
32	A	414	LHG	O8-C23-C24	2.38	119.09	111.83
30	R	607	CHL	O2D-CGD-O1D	-2.38	119.21	123.85
31	3	615	CLA	O2A-CGA-CBA	2.38	121.13	112.14
31	3	612	CLA	C12-C11-C10	-2.38	102.61	113.28
30	n	605	CHL	O2D-CGD-O1D	-2.38	119.22	123.85
31	15	604	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
31	c	514	CLA	C12-C11-C10	-2.38	102.62	113.28
31	d	402	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
30	1	606	CHL	OMC-CMC-C2C	-2.38	120.99	125.12
31	12	613	CLA	O2A-CGA-CBA	2.38	121.51	114.00
30	S	601	CHL	OMC-CMC-C2C	-2.38	120.99	125.12
30	13	608	CHL	O2D-CGD-O1D	-2.38	119.22	123.85
30	16	606	CHL	OMC-CMC-C2C	-2.38	120.99	125.12
31	12	603	CLA	C1-C2-C3	2.38	130.09	126.20
30	Y	601	CHL	O1D-CGD-CBD	-2.38	121.12	124.72
31	11	613	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
31	d	402	CLA	CHD-C1D-ND	-2.38	121.46	124.80
31	Y	611	CLA	C12-C11-C10	-2.38	102.63	113.28
30	R	605	CHL	CHA-C1A-C2A	-2.38	127.73	133.31
31	13	602	CLA	O2A-CGA-O1A	-2.38	117.69	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	614	CLA	O2A-CGA-CBA	2.37	121.11	112.14
31	n	611	CLA	C12-C11-C10	-2.37	102.64	113.28
30	2	609	CHL	C3C-C4C-NC	-2.37	108.85	114.65
30	s	606	CHL	C3C-C4C-NC	-2.37	108.85	114.65
30	Y	609	CHL	OBD-CAD-CBD	-2.37	122.34	125.82
30	14	607	CHL	OMC-CMC-C2C	-2.37	121.00	125.12
31	Y	602	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
30	14	609	CHL	OMC-CMC-C2C	-2.37	121.00	125.12
31	S	604	CLA	C12-C11-C10	-2.37	102.65	113.28
31	6	612	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
30	3	607	CHL	CHA-C1A-C2A	-2.37	127.74	133.31
31	c	512	CLA	C12-C11-C10	-2.37	102.66	113.28
31	13	603	CLA	C1-C2-C3	2.37	130.08	126.20
31	B	616	CLA	C1-C2-C3	2.37	130.08	126.20
30	Y	606	CHL	OMC-CMC-C2C	-2.37	121.01	125.12
31	C	512	CLA	C12-C11-C10	-2.37	102.66	113.28
30	y	608	CHL	C3C-C4C-NC	-2.37	108.86	114.65
30	15	605	CHL	C4C-CHD-C1D	2.37	124.54	116.07
30	5	609	CHL	C3C-C4C-NC	-2.37	108.86	114.65
31	4	612	CLA	O2A-CGA-CBA	2.37	121.09	112.14
31	y	610	CLA	CHD-C1D-ND	-2.37	121.47	124.80
30	4	606	CHL	OBD-CAD-CBD	-2.37	122.35	125.82
31	5	612	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
31	g	602	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
31	y	615	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
31	5	612	CLA	O2A-CGA-CBA	2.37	121.08	112.14
31	S	602	CLA	C1-C2-C3	2.36	130.07	126.20
30	s	607	CHL	C3C-C4C-NC	-2.36	108.87	114.65
31	15	610	CLA	O2A-CGA-CBA	2.36	121.47	114.00
30	1	607	CHL	OMC-CMC-C2C	-2.36	121.02	125.12
31	5	602	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
31	3	612	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
31	B	602	CLA	CHD-C1D-ND	-2.36	121.48	124.80
31	g	603	CLA	C4-C3-C5	-2.36	111.13	115.23
31	1	614	CLA	O2A-CGA-CBA	2.36	121.06	112.14
31	13	611	CLA	C12-C11-C10	-2.36	102.70	113.28
31	G	610	CLA	C12-C11-C10	-2.36	102.70	113.28
30	R	607	CHL	O2A-CGA-O1A	-2.36	117.72	123.63
31	b	613	CLA	C1-C2-C3	2.36	130.06	126.20
31	15	603	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
31	4	602	CLA	C12-C11-C10	-2.36	102.71	113.28
31	s	610	CLA	C12-C11-C10	-2.36	102.71	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	3	601	CHL	OMC-CMC-C2C	-2.36	121.03	125.12
31	b	614	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
31	Y	603	CLA	C12-C11-C10	-2.36	102.71	113.28
30	14	609	CHL	CHA-C1A-C2A	-2.36	127.77	133.31
31	13	602	CLA	C12-C11-C10	-2.36	102.72	113.28
31	2	612	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
30	14	608	CHL	CHA-C1A-C2A	-2.36	127.77	133.31
30	Y	606	CHL	C3C-C4C-NC	-2.36	108.89	114.65
31	4	613	CLA	C1-C2-C3	2.36	130.06	126.20
30	y	606	CHL	C3C-C4C-NC	-2.36	108.89	114.65
31	1	602	CLA	C1-C2-C3	2.36	130.06	126.20
30	12	605	CHL	O2A-CGA-CBA	2.36	121.44	114.00
31	5	603	CLA	CHD-C1D-ND	-2.36	121.49	124.80
32	3	617	LHG	O8-C23-C24	2.36	119.02	111.83
31	N	612	CLA	O2A-CGA-CBA	2.35	121.44	114.00
30	14	609	CHL	O2A-CGA-O1A	-2.35	117.74	123.63
31	11	604	CLA	O2A-CGA-CBA	2.35	121.03	112.14
31	Y	612	CLA	C12-C11-C10	-2.35	102.73	113.28
31	y	610	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
31	3	604	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
31	B	605	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
31	13	610	CLA	CHD-C1D-ND	-2.35	121.49	124.80
31	a	403	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
30	N	605	CHL	O1D-CGD-CBD	-2.35	121.16	124.72
30	s	601	CHL	O1D-CGD-CBD	-2.35	121.16	124.72
30	13	607	CHL	CHA-C1A-C2A	-2.35	127.78	133.31
30	6	607	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
30	1	601	CHL	O2D-CGD-O1D	-2.35	119.27	123.85
30	S	607	CHL	OMC-CMC-C2C	-2.35	121.04	125.12
31	15	609	CLA	CHD-C1D-ND	-2.35	121.50	124.80
30	11	606	CHL	OMC-CMC-C2C	-2.35	121.04	125.12
30	5	601	CHL	O2A-CGA-O1A	-2.35	117.75	123.63
31	6	604	CLA	C12-C11-C10	-2.35	102.75	113.28
30	s	607	CHL	C1A-CHA-C4D	2.35	122.90	118.98
31	s	604	CLA	C1-C2-C3	2.35	130.04	126.20
31	2	611	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	Y	604	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
30	R	606	CHL	O2D-CGD-O1D	-2.35	119.28	123.85
31	B	604	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
31	b	604	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
31	B	609	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
30	Y	608	CHL	C3C-C4C-NC	-2.35	108.92	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	12	610	CLA	O2A-CGA-CBA	2.34	121.41	114.00
31	n	610	CLA	C12-C11-C10	-2.34	102.77	113.28
31	y	603	CLA	C12-C11-C10	-2.34	102.77	113.28
30	N	606	CHL	OMC-CMC-C2C	-2.34	121.05	125.12
30	N	608	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
30	r	606	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
30	n	609	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
31	r	612	CLA	C1-C2-C3	2.34	130.55	126.76
31	A	402	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
31	c	503	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
30	11	608	CHL	O2A-CGA-CBA	2.34	118.97	111.83
31	13	612	CLA	O2A-CGA-CBA	2.34	121.40	114.00
31	6	610	CLA	C12-C11-C10	-2.34	102.79	113.28
30	6	601	CHL	O2D-CGD-O1D	-2.34	119.29	123.85
30	n	606	CHL	OMC-CMC-C2C	-2.34	121.06	125.12
31	3	604	CLA	C12-C11-C10	-2.34	102.80	113.28
31	g	610	CLA	C12-C11-C10	-2.34	102.80	113.28
31	G	602	CLA	C12-C11-C10	-2.34	102.80	113.28
31	16	612	CLA	O2A-CGA-CBA	2.34	121.39	114.00
30	4	601	CHL	O2D-CGD-O1D	-2.34	119.30	123.85
30	15	605	CHL	O2A-CGA-CBA	2.34	121.39	114.00
31	n	603	CLA	C12-C11-C10	-2.34	102.81	113.28
31	g	602	CLA	C12-C11-C10	-2.34	102.81	113.28
31	1	604	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
30	4	605	CHL	CHA-C1A-C2A	-2.33	127.82	133.31
31	C	507	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
32	Y	616	LHG	O8-C23-C24	2.33	118.95	111.83
30	N	609	CHL	O2D-CGD-O1D	-2.33	119.31	123.85
31	b	602	CLA	CHD-C1D-ND	-2.33	121.52	124.80
31	N	612	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	s	611	CLA	C4-C3-C5	-2.33	111.18	115.23
31	G	610	CLA	CHD-C1D-ND	-2.33	121.52	124.80
31	A	404	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	Y	610	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
31	b	616	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	r	610	CLA	C12-C11-C10	-2.33	102.84	113.28
30	s	607	CHL	OMC-CMC-C2C	-2.33	121.08	125.12
30	Y	609	CHL	C1A-CHA-C4D	2.33	122.87	118.98
31	b	609	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
31	r	612	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
31	G	613	CLA	C12-C11-C10	-2.33	102.84	113.28
31	16	615	CLA	O2A-CGA-CBA	2.33	121.35	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	11	601	CHL	CHA-C1A-C2A	-2.33	127.84	133.31
32	r	621	LHG	O8-C23-C24	2.33	118.93	111.83
31	y	602	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
32	y	618	LHG	O8-C23-C24	2.32	118.92	111.83
31	a	404	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
31	14	603	CLA	C1-C2-C3	2.32	130.00	126.20
31	6	603	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
31	g	610	CLA	CHD-C1D-ND	-2.32	121.53	124.80
31	c	507	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
31	s	614	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
31	6	610	CLA	CHD-C1D-ND	-2.32	121.53	124.80
30	1	608	CHL	O2A-CGA-O1A	-2.32	117.82	123.63
31	b	607	CLA	C12-C11-C10	-2.32	102.87	113.28
31	N	610	CLA	C12-C11-C10	-2.32	102.88	113.28
31	R	610	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
31	C	503	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
31	y	612	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
30	14	608	CHL	O1D-CGD-CBD	-2.32	121.21	124.72
31	13	604	CLA	CHD-C1D-ND	-2.32	121.54	124.80
30	N	607	CHL	O2A-CGA-O1A	-2.32	117.83	123.63
31	b	601	CLA	O1D-CGD-CBD	-2.32	119.95	124.52
30	12	607	CHL	CHA-C1A-C2A	-2.32	127.86	133.31
30	11	608	CHL	C4C-CHD-C1D	2.32	124.36	116.07
31	11	610	CLA	C4-C3-C5	-2.32	111.21	115.23
30	s	607	CHL	O2D-CGD-O1D	-2.32	119.34	123.85
32	d	409	LHG	O8-C23-C24	2.32	118.90	111.83
30	g	608	CHL	CHA-C1A-C2A	-2.32	127.87	133.31
32	y	616	LHG	O8-C23-C24	2.32	118.90	111.83
30	4	608	CHL	O2A-CGA-O1A	-2.32	117.84	123.63
31	16	614	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
31	C	509	CLA	C12-C11-C10	-2.31	102.91	113.28
31	R	601	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
30	Y	601	CHL	C1-C2-C3	2.31	129.99	126.20
32	R	619	LHG	O8-C23-C24	2.31	118.89	111.83
31	5	613	CLA	C1-C2-C3	2.31	130.51	126.76
30	6	609	CHL	O2A-CGA-O1A	-2.31	117.84	123.63
31	13	603	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
30	r	607	CHL	OMC-CMC-C2C	-2.31	121.11	125.12
30	y	609	CHL	OMC-CMC-C2C	-2.31	121.11	125.12
31	A	406	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
32	d	413	LHG	O8-C23-C24	2.31	118.88	111.83
30	s	601	CHL	CHA-C1A-C2A	-2.31	127.88	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	604	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
32	D	409	LHG	O8-C23-C24	2.31	118.87	111.83
30	N	606	CHL	O2A-CGA-O1A	-2.31	117.86	123.63
31	16	604	CLA	CHD-C1D-ND	-2.31	121.56	124.80
31	5	613	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
30	11	609	CHL	CHA-C1A-C2A	-2.31	127.89	133.31
30	n	608	CHL	OBD-CAD-CBD	-2.31	122.44	125.82
31	N	614	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
31	Y	611	CLA	O1D-CGD-CBD	-2.30	119.97	124.52
31	B	601	CLA	O1D-CGD-CBD	-2.30	119.97	124.52
31	b	606	CLA	C1-C2-C3	2.30	129.97	126.20
32	R	618	LHG	O8-C23-C24	2.30	118.86	111.83
31	c	509	CLA	C12-C11-C10	-2.30	102.95	113.28
31	N	603	CLA	O1D-CGD-CBD	-2.30	119.97	124.52
31	13	614	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
31	a	407	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
31	2	612	CLA	CHD-C1D-ND	-2.30	121.56	124.80
30	14	606	CHL	O2A-CGA-CBA	2.30	120.83	112.14
31	Y	602	CLA	C1-C2-C3	2.30	129.97	126.20
31	16	611	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
30	g	601	CHL	OMC-CMC-C2C	-2.30	121.12	125.12
32	D	412	LHG	O8-C23-C24	2.30	118.85	111.83
30	11	607	CHL	O2A-CGA-CBA	2.30	121.27	114.00
31	B	607	CLA	C12-C11-C10	-2.30	102.97	113.28
30	R	607	CHL	OMC-CMC-C2C	-2.30	121.13	125.12
30	15	607	CHL	CHA-C1A-C2A	-2.30	127.91	133.31
30	5	601	CHL	OMC-CMC-C2C	-2.30	121.13	125.12
30	G	608	CHL	O2A-CGA-O1A	-2.30	117.88	123.63
31	15	609	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
30	1	605	CHL	O2A-CGA-CBA	2.30	121.26	114.00
31	s	612	CLA	O2A-CGA-CBA	2.30	121.26	114.00
31	y	612	CLA	C12-C11-C10	-2.30	102.98	113.28
31	n	610	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
30	6	606	CHL	O2A-CGA-O1A	-2.30	117.88	123.63
31	11	611	CLA	C1-C2-C3	2.30	130.48	126.76
31	4	610	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	2	613	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
31	G	602	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
32	G	615	LHG	O8-C23-C24	2.30	118.83	111.83
30	5	609	CHL	O2A-CGA-O1A	-2.29	117.89	123.63
30	G	608	CHL	CHA-C1A-C2A	-2.29	127.92	133.31
31	C	503	CLA	C12-C11-C10	-2.29	103.00	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	508	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
31	S	602	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
31	g	611	CLA	C1-C2-C3	2.29	129.95	126.20
30	G	606	CHL	O2A-CGA-CBA	2.29	120.80	112.14
31	2	612	CLA	O2A-CGA-CBA	2.29	120.80	112.14
31	n	613	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
32	a	414	LHG	O8-C23-C24	2.29	118.82	111.83
31	13	615	CLA	O2A-CGA-CBA	2.29	121.24	114.00
31	13	610	CLA	C12-C11-C10	-2.29	103.01	113.28
30	15	607	CHL	O2A-CGA-O1A	-2.29	117.90	123.63
31	16	615	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
31	b	608	CLA	C12-C11-C10	-2.29	103.03	113.28
31	16	602	CLA	C12-C11-C10	-2.29	103.03	113.28
31	13	604	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
31	B	608	CLA	C12-C11-C10	-2.28	103.04	113.28
30	y	609	CHL	C1A-CHA-C4D	2.28	122.79	118.98
31	16	610	CLA	C12-C11-C10	-2.28	103.04	113.28
31	R	602	CLA	C12-C11-C10	-2.28	103.04	113.28
31	Y	612	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
30	S	601	CHL	CHA-C1A-C2A	-2.28	127.95	133.31
31	4	610	CLA	C12-C11-C10	-2.28	103.05	113.28
30	4	605	CHL	O2A-CGA-CBA	2.28	121.21	114.00
31	B	606	CLA	CHD-C1D-ND	-2.28	121.59	124.80
30	12	608	CHL	OMC-CMC-C2C	-2.28	121.16	125.12
31	S	610	CLA	C1-C2-C3	2.28	129.93	126.20
31	3	610	CLA	C12-C11-C10	-2.28	103.06	113.28
30	13	609	CHL	C3C-C4C-NC	-2.28	109.08	114.65
31	S	611	CLA	C4-C3-C5	-2.28	111.27	115.23
30	2	608	CHL	OMC-CMC-C2C	-2.28	121.17	125.12
31	c	508	CLA	CHD-C1D-ND	-2.28	121.60	124.80
31	11	610	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
31	B	601	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
30	14	601	CHL	CHA-C1A-C2A	-2.28	127.96	133.31
31	C	508	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
31	y	611	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
31	a	407	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
31	16	602	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
31	R	610	CLA	C12-C11-C10	-2.28	103.08	113.28
31	c	511	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
31	n	614	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
31	n	602	CLA	C12-C11-C10	-2.27	103.09	113.28
30	11	606	CHL	O2A-CGA-CBA	2.27	120.73	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	612	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
31	s	611	CLA	C1-C2-C3	2.27	129.92	126.20
31	1	613	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
30	12	605	CHL	CHA-C1A-C2A	-2.27	127.97	133.31
31	B	616	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
31	d	402	CLA	CMD-C2D-C1D	2.27	128.73	124.73
31	Y	614	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
31	N	604	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
30	G	601	CHL	OMC-CMC-C2C	-2.27	121.17	125.12
32	Y	618	LHG	O8-C23-C24	2.27	118.76	111.83
30	13	605	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
31	Y	615	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	B	608	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
31	S	611	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
32	6	617	LHG	O8-C23-C24	2.27	118.76	111.83
30	16	605	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
31	S	610	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	A	403	CLA	C12-C11-C10	-2.27	103.11	113.28
32	a	413	LHG	O8-C23-C24	2.27	118.75	111.83
31	C	504	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
31	b	601	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
31	2	604	CLA	C1-C2-C3	2.27	130.43	126.76
32	14	615	LHG	O8-C23-C24	2.27	118.75	111.83
31	g	602	CLA	C1-C2-C3	2.27	129.91	126.20
31	12	611	CLA	O2A-CGA-CBA	2.27	121.16	114.00
31	15	611	CLA	O2A-CGA-CBA	2.27	121.16	114.00
30	R	606	CHL	O2A-CGA-O1A	-2.27	117.96	123.63
31	b	608	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
31	3	602	CLA	CHD-C1D-ND	-2.27	121.61	124.80
30	11	605	CHL	O2A-CGA-O1A	-2.27	117.96	123.63
30	n	608	CHL	O2A-CGA-O1A	-2.26	117.97	123.63
31	c	511	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
31	c	504	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	4	613	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
31	13	614	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	6	611	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
31	12	604	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
32	R	621	LHG	O8-C23-C24	2.26	118.73	111.83
31	n	602	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
32	11	615	LHG	O8-C23-C24	2.26	118.72	111.83
30	13	609	CHL	O2A-CGA-O1A	-2.26	117.98	123.63
31	R	612	CLA	O1D-CGD-CBD	-2.26	120.07	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	606	CLA	CHD-C1D-ND	-2.26	121.63	124.80
31	d	402	CLA	C12-C11-C10	-2.25	103.17	113.28
30	14	606	CHL	O2D-CGD-O1D	-2.25	119.46	123.85
31	R	613	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
30	5	606	CHL	OMC-CMC-C2C	-2.25	121.21	125.12
31	4	602	CLA	O1D-CGD-CBD	-2.25	120.07	124.52
31	1	611	CLA	C1-C2-C3	2.25	130.41	126.76
30	13	609	CHL	OMC-CMC-C2C	-2.25	121.21	125.12
31	s	614	CLA	C12-C11-C10	-2.25	103.19	113.28
30	3	608	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
31	12	613	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
30	15	605	CHL	CHA-C1A-C2A	-2.25	128.02	133.31
31	N	614	CLA	O2A-CGA-CBA	2.25	121.11	114.00
32	A	413	LHG	O8-C23-C24	2.25	118.69	111.83
31	B	613	CLA	C12-C11-C10	-2.25	103.20	113.28
31	n	610	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
31	2	610	CLA	C1-C2-C3	2.25	130.40	126.76
31	n	615	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
31	G	611	CLA	C1-C2-C3	2.25	129.88	126.20
30	g	608	CHL	O2A-CGA-O1A	-2.25	118.01	123.63
31	15	609	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
31	n	604	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
31	b	613	CLA	C12-C11-C10	-2.25	103.21	113.28
30	14	605	CHL	CHA-C1A-C2A	-2.25	128.03	133.31
31	s	614	CLA	CHD-C1D-ND	-2.25	121.64	124.80
31	r	602	CLA	O2D-CGD-O1D	-2.25	119.48	123.85
30	n	601	CHL	O2A-CGA-O1A	-2.25	118.01	123.63
30	2	601	CHL	OMC-CMC-C2C	-2.25	121.22	125.12
31	11	604	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
31	C	511	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
31	14	604	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
31	b	611	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
31	A	406	CLA	C4-C3-C5	-2.24	111.33	115.23
31	c	513	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
31	a	407	CLA	C4-C3-C5	-2.24	111.33	115.23
30	3	606	CHL	OMC-CMC-C2C	-2.24	121.23	125.12
30	s	607	CHL	OBD-CAD-CBD	-2.24	122.53	125.82
31	c	504	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
30	Y	601	CHL	O2A-CGA-O1A	-2.24	118.02	123.63
30	5	608	CHL	OMC-CMC-C2C	-2.24	121.23	125.12
30	Y	601	CHL	OMC-CMC-C2C	-2.24	121.23	125.12
32	r	618	LHG	O8-C23-C24	2.24	118.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	404	CLA	CHD-C1D-ND	-2.24	121.65	124.80
30	13	607	CHL	C1A-CHA-C4D	2.24	122.72	118.98
31	B	606	CLA	C12-C11-C10	-2.24	103.24	113.28
31	r	608	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
31	B	601	CLA	C1-C2-C3	2.24	129.87	126.20
31	11	604	CLA	CHD-C1D-ND	-2.24	121.65	124.80
32	D	408	LHG	O8-C23-C24	2.24	118.66	111.83
30	N	608	CHL	O2A-CGA-O1A	-2.24	118.03	123.63
30	6	607	CHL	O2A-CGA-O1A	-2.24	118.03	123.63
30	12	607	CHL	O2A-CGA-O1A	-2.24	118.03	123.63
31	A	403	CLA	CMD-C2D-C1D	2.24	128.67	124.73
31	N	610	CLA	CHD-C1D-ND	-2.24	121.66	124.80
30	2	609	CHL	O2A-CGA-O1A	-2.24	118.03	123.63
30	5	609	CHL	O2D-CGD-O1D	-2.24	119.50	123.85
31	b	606	CLA	C12-C11-C10	-2.24	103.26	113.28
30	y	601	CHL	OMC-CMC-C2C	-2.24	121.24	125.12
31	d	405	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
31	r	614	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
30	4	606	CHL	OMC-CMC-C2C	-2.23	121.24	125.12
31	a	403	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	n	613	CLA	C4-C3-C5	-2.23	111.35	115.23
30	4	606	CHL	O2A-CGA-CBA	2.23	120.58	112.14
31	C	513	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
31	S	614	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	n	610	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	B	611	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
30	6	606	CHL	OMC-CMC-C2C	-2.23	121.24	125.12
31	14	614	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
31	S	609	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
30	13	607	CHL	OMC-CMC-C2C	-2.23	121.25	125.12
30	2	609	CHL	O2D-CGD-O1D	-2.23	119.50	123.85
31	C	511	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
32	1	615	LHG	O8-C23-C24	2.23	118.64	111.83
31	B	608	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
32	d	408	LHG	O8-C23-C24	2.23	118.64	111.83
31	4	604	CLA	C1-C2-C3	2.23	130.37	126.76
31	n	612	CLA	O2D-CGD-O1D	-2.23	119.51	123.85
31	6	612	CLA	CHD-C1D-ND	-2.23	121.67	124.80
32	A	415	LHG	O8-C23-C24	2.23	118.63	111.83
31	12	612	CLA	CHD-C1D-ND	-2.23	121.67	124.80
30	S	607	CHL	O2D-CGD-O1D	-2.23	119.51	123.85
31	y	612	CLA	O2A-CGA-O1A	-2.23	118.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	3	610	CLA	CHD-C1D-ND	-2.23	121.67	124.80
31	b	611	CLA	C12-C11-C10	-2.23	103.30	113.28
32	n	616	LHG	O8-C23-C24	2.23	118.62	111.83
30	4	607	CHL	OMC-CMC-C2C	-2.23	121.25	125.12
31	3	612	CLA	CHD-C1D-ND	-2.23	121.67	124.80
38	a	405	PHO	C2B-C1B-NB	-2.22	107.82	109.43
30	16	605	CHL	O2A-CGA-O1A	-2.22	118.06	123.63
32	r	619	LHG	O8-C23-C24	2.22	118.61	111.83
31	C	504	CLA	CHD-C1D-ND	-2.22	121.67	124.80
30	3	605	CHL	O2A-CGA-O1A	-2.22	118.07	123.63
31	6	602	CLA	CHD-C1D-ND	-2.22	121.68	124.80
31	3	614	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
31	B	616	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
32	a	401	LHG	O8-C23-C24	2.22	118.60	111.83
30	16	607	CHL	OMC-CMC-C2C	-2.22	121.27	125.12
30	g	607	CHL	OMC-CMC-C2C	-2.22	121.27	125.12
31	R	609	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
31	13	611	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
31	B	611	CLA	C12-C11-C10	-2.22	103.34	113.28
31	r	612	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
30	6	608	CHL	O2D-CGD-O1D	-2.22	119.54	123.85
30	5	606	CHL	CMB-C2B-C3B	2.21	129.11	124.68
31	D	405	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
31	y	614	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
30	2	605	CHL	O2A-CGA-CBA	2.21	121.00	114.00
32	N	616	LHG	O8-C23-C24	2.21	118.59	111.83
31	1	610	CLA	C4-C3-C5	-2.21	111.39	115.23
31	14	603	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
30	3	607	CHL	O2A-CGA-O1A	-2.21	118.09	123.63
31	15	602	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
31	16	603	CLA	C1-C2-C3	2.21	129.82	126.20
30	G	605	CHL	CHA-C1A-C2A	-2.21	128.11	133.31
30	2	606	CHL	OMC-CMC-C2C	-2.21	121.28	125.12
30	5	605	CHL	O2A-CGA-CBA	2.21	120.99	114.00
31	5	610	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
31	b	608	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
31	A	402	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	4	602	CLA	C4-C3-C5	-2.21	111.39	115.23
30	11	605	CHL	OMC-CMC-C2C	-2.21	121.28	125.12
30	N	605	CHL	CHA-C1A-C2A	-2.21	128.12	133.31
30	2	606	CHL	O2A-CGA-CBA	2.21	120.98	114.00
31	y	603	CLA	CHD-C1D-ND	-2.21	121.69	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	612	CLA	CHD-C1D-ND	-2.21	121.70	124.80
30	y	606	CHL	O2A-CGA-O1A	-2.21	118.11	123.63
31	A	406	CLA	O2D-CGD-O1D	-2.21	119.56	123.85
31	14	614	CLA	CHD-C1D-ND	-2.21	121.70	124.80
30	s	606	CHL	OMC-CMC-C2C	-2.20	121.29	125.12
32	Y	617	LHG	O8-C23-C24	2.20	118.56	111.83
30	g	601	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
31	y	603	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
31	N	615	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
31	13	611	CLA	C4-C3-C5	-2.20	111.40	115.23
32	a	411	LHG	O8-C23-C24	2.20	118.55	111.83
30	G	601	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
30	15	607	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
30	N	601	CHL	O2A-CGA-O1A	-2.20	118.12	123.63
32	6	616	LHG	O8-C23-C24	2.20	118.55	111.83
30	S	601	CHL	O2A-CGA-CBA	2.20	120.95	114.00
31	g	613	CLA	C12-C11-C10	-2.20	103.42	113.28
31	a	403	CLA	C12-C11-C10	-2.20	103.42	113.28
30	12	607	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
30	15	606	CHL	O2D-CGD-O1D	-2.20	119.57	123.85
30	G	607	CHL	OMC-CMC-C2C	-2.20	121.30	125.12
31	B	602	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
30	r	606	CHL	O2A-CGA-O1A	-2.20	118.13	123.63
30	s	601	CHL	O2A-CGA-CBA	2.20	120.94	114.00
32	3	616	LHG	O8-C23-C24	2.20	118.53	111.83
31	s	612	CLA	CHD-C1D-ND	-2.20	121.71	124.80
31	y	612	CLA	C1-C2-C3	2.19	129.79	126.20
31	1	610	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
30	G	609	CHL	O2D-CGD-O1D	-2.19	119.58	123.85
31	Y	603	CLA	CHD-C1D-ND	-2.19	121.72	124.80
30	1	605	CHL	OMC-CMC-C2C	-2.19	121.31	125.12
31	c	507	CLA	C12-C11-C10	-2.19	103.45	113.28
31	C	512	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
31	b	606	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
31	y	615	CLA	CHD-C1D-ND	-2.19	121.72	124.80
32	A	411	LHG	O8-C23-C24	2.19	118.52	111.83
31	Y	612	CLA	C1-C2-C3	2.19	129.79	126.20
31	C	503	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
31	15	603	CLA	C4-C3-C5	-2.19	111.42	115.23
30	g	601	CHL	O2A-CGA-O1A	-2.19	118.15	123.63
31	r	613	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	B	615	CLA	O2D-CGD-O1D	-2.19	119.58	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	612	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
31	11	614	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
31	C	505	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
31	R	603	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
30	n	607	CHL	OMC-CMC-C2C	-2.19	121.32	125.12
31	C	508	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	y	611	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
30	R	605	CHL	O2D-CGD-O1D	-2.19	119.59	123.85
31	c	503	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
30	Y	607	CHL	O2D-CGD-O1D	-2.19	119.59	123.85
31	y	612	CLA	C4-C3-C5	-2.19	111.43	115.23
30	11	607	CHL	O2D-CGD-O1D	-2.19	119.59	123.85
31	b	615	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
31	c	505	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
31	1	613	CLA	O1D-CGD-CBD	-2.19	120.21	124.52
48	d	403	BCT	O3-C-O1	-2.18	114.09	119.68
30	5	607	CHL	O2A-CGA-O1A	-2.18	118.16	123.63
31	6	613	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
31	c	512	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
31	Y	603	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
31	c	503	CLA	C1-C2-C3	2.18	129.78	126.20
31	6	614	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
32	S	621	LHG	O8-C23-C24	2.18	118.49	111.83
31	s	609	CLA	CHD-C1D-ND	-2.18	121.73	124.80
30	13	606	CHL	O2A-CGA-O1A	-2.18	118.17	123.63
31	15	610	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
31	S	614	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
30	Y	606	CHL	O2A-CGA-O1A	-2.18	118.17	123.63
31	S	604	CLA	C1-C2-C3	2.18	129.77	126.20
32	y	617	LHG	O8-C23-C24	2.18	118.48	111.83
31	r	608	CLA	CHD-C1D-ND	-2.18	121.74	124.80
31	5	602	CLA	CHD-C1D-ND	-2.18	121.74	124.80
31	A	404	CLA	CHD-C1D-ND	-2.18	121.74	124.80
31	b	609	CLA	CHD-C1D-ND	-2.18	121.74	124.80
32	4	615	LHG	O8-C23-C24	2.18	118.47	111.83
38	A	405	PHO	C2B-C1B-NB	-2.18	107.86	109.43
30	13	607	CHL	O2D-CGD-O1D	-2.18	119.61	123.85
31	b	605	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
31	B	609	CLA	CHD-C1D-ND	-2.18	121.74	124.80
30	13	601	CHL	OMC-CMC-C2C	-2.18	121.34	125.12
30	S	606	CHL	OMC-CMC-C2C	-2.18	121.34	125.12
30	1	605	CHL	O2D-CGD-O1D	-2.18	119.61	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	12	601	CHL	O2A-CGA-O1A	-2.18	118.19	123.63
31	r	603	CLA	C12-C11-C10	-2.18	103.53	113.28
31	3	602	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
32	s	621	LHG	O8-C23-C24	2.17	118.47	111.83
31	16	604	CLA	CHB-C1B-NB	2.17	127.31	124.05
31	A	402	CLA	C12-C11-C10	-2.17	103.54	113.28
32	g	615	LHG	O8-C23-C24	2.17	118.46	111.83
31	14	604	CLA	CHD-C1D-ND	-2.17	121.74	124.80
31	R	608	CLA	CHD-C1D-ND	-2.17	121.74	124.80
31	g	604	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
30	15	601	CHL	O2A-CGA-O1A	-2.17	118.19	123.63
31	1	603	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
31	S	609	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	16	615	CLA	CHB-C1B-NB	2.17	127.31	124.05
30	12	608	CHL	O2D-CGD-O1D	-2.17	119.62	123.85
31	16	610	CLA	C2A-C1A-CHA	2.17	127.64	123.87
30	2	606	CHL	O2D-CGD-O1D	-2.17	119.62	123.85
31	1	610	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
30	g	605	CHL	CHA-C1A-C2A	-2.17	128.21	133.31
31	12	612	CLA	C2A-C1A-CHA	2.17	127.63	123.87
30	15	608	CHL	O2D-CGD-O1D	-2.17	119.62	123.85
31	C	507	CLA	C12-C11-C10	-2.17	103.55	113.28
31	14	612	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
31	11	614	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	13	604	CLA	CHB-C1B-NB	2.17	127.30	124.05
30	2	607	CHL	O2A-CGA-O1A	-2.17	118.20	123.63
31	r	604	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
31	b	616	CLA	CHD-C1D-ND	-2.17	121.75	124.80
30	g	609	CHL	O2D-CGD-O1D	-2.17	119.63	123.85
31	16	603	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
30	y	609	CHL	O2A-CGA-O1A	-2.17	118.21	123.63
31	6	615	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
31	Y	604	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
31	12	610	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
31	s	605	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
30	14	609	CHL	C1-O2A-CGA	2.16	121.89	116.65
31	12	602	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	c	507	CLA	CHD-C1D-ND	-2.16	121.76	124.80
30	G	606	CHL	OMC-CMC-C2C	-2.16	121.36	125.12
31	b	601	CLA	C1-C2-C3	2.16	129.74	126.20
31	Y	611	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
31	D	404	CLA	CHD-C1D-ND	-2.16	121.76	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	613	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	r	603	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	11	612	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	a	404	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	6	604	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
31	S	612	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
31	c	504	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
31	11	602	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
38	a	406	PHO	C2B-C1B-NB	-2.16	107.87	109.43
31	s	611	CLA	C12-C11-C10	-2.16	103.60	113.28
30	s	606	CHL	O2A-CGA-O1A	-2.16	118.23	123.63
31	6	602	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
31	4	603	CLA	C1-C2-C3	2.16	129.73	126.20
30	Y	609	CHL	O2A-CGA-O1A	-2.16	118.23	123.63
30	14	607	CHL	O2D-CGD-O1D	-2.16	119.65	123.85
30	15	608	CHL	OMC-CMC-C2C	-2.16	121.37	125.12
30	G	608	CHL	OMC-CMC-C2C	-2.16	121.37	125.12
31	B	616	CLA	CHD-C1D-ND	-2.16	121.77	124.80
31	b	610	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
30	n	609	CHL	O2A-CGA-O1A	-2.16	118.23	123.63
31	R	602	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
48	D	403	BCT	O3-C-O1	-2.16	114.16	119.68
30	4	609	CHL	O2A-CGA-O1A	-2.16	118.23	123.63
31	3	611	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
31	C	504	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
31	b	602	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
31	g	604	CLA	CHD-C1D-ND	-2.16	121.77	124.80
32	C	521	LHG	O8-C23-C24	2.15	118.41	111.83
31	R	609	CLA	CHD-C1D-ND	-2.15	121.77	124.80
30	16	609	CHL	O2D-CGD-O1D	-2.15	119.66	123.85
31	13	610	CLA	C2A-C1A-CHA	2.15	127.61	123.87
30	g	606	CHL	OMC-CMC-C2C	-2.15	121.38	125.12
31	16	615	CLA	CHD-C1D-ND	-2.15	121.77	124.80
31	1	612	CLA	CHD-C1D-ND	-2.15	121.77	124.80
31	5	611	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
32	c	521	LHG	O8-C23-C24	2.15	118.40	111.83
31	y	613	CLA	C2A-C1A-CHA	2.15	127.60	123.87
30	11	608	CHL	CHA-C1A-C2A	-2.15	128.26	133.31
31	15	612	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	R	604	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
31	4	603	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
31	y	604	CLA	CHD-C1D-ND	-2.15	121.78	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	11	603	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
31	r	604	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	14	602	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
31	s	605	CLA	C1-C2-C3	2.15	130.24	126.76
31	s	609	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
31	d	405	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	r	614	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	s	602	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
31	C	503	CLA	C1-C2-C3	2.15	129.71	126.20
31	B	606	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
31	B	610	CLA	C12-C11-C10	-2.14	103.67	113.28
31	B	610	CLA	O2D-CGD-O1D	-2.14	119.67	123.85
31	b	602	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
31	B	603	CLA	CHD-C1D-ND	-2.14	121.79	124.80
30	13	607	CHL	O2A-CGA-O1A	-2.14	118.27	123.63
30	14	605	CHL	O2A-CGA-O1A	-2.14	118.27	123.63
30	N	607	CHL	OMC-CMC-C2C	-2.14	121.40	125.12
31	G	612	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
31	R	602	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
31	r	609	CLA	CHD-C1D-ND	-2.14	121.79	124.80
30	2	608	CHL	O2A-CGA-O1A	-2.14	118.27	123.63
31	b	610	CLA	C12-C11-C10	-2.14	103.68	113.28
31	n	613	CLA	C1-C2-C3	2.14	129.71	126.20
31	B	614	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
30	13	605	CHL	O2A-CGA-O1A	-2.14	118.27	123.63
31	g	612	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
31	12	612	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
31	2	613	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	d	404	CLA	CMD-C2D-C1D	2.14	128.50	124.73
31	Y	612	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
31	B	602	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
31	y	604	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
31	4	603	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	4	603	CLA	C4-C3-C5	-2.14	111.52	115.23
31	14	610	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
31	4	603	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
31	13	602	CLA	C4-C3-C5	-2.14	111.52	115.23
31	D	405	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	R	614	CLA	CHD-C1D-ND	-2.14	121.79	124.80
30	n	605	CHL	CHA-C1A-C2A	-2.14	128.29	133.31
31	12	603	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
31	b	614	CLA	O2D-CGD-O1D	-2.14	119.69	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	404	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
30	r	605	CHL	O2A-CGA-O1A	-2.14	118.28	123.63
31	B	607	CLA	CHD-C1D-ND	-2.14	121.80	124.80
31	S	613	CLA	CHD-C1D-ND	-2.14	121.80	124.80
31	R	612	CLA	C1-C2-C3	2.13	130.22	126.76
30	5	606	CHL	O2A-CGA-CBA	2.13	120.74	114.00
31	n	615	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
30	G	607	CHL	C1A-CHA-C4D	2.13	122.54	118.98
31	s	603	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
31	Y	610	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
31	g	602	CLA	CHD-C1D-ND	-2.13	121.80	124.80
31	s	613	CLA	CHD-C1D-ND	-2.13	121.80	124.80
31	3	611	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
31	Y	612	CLA	C4-C3-C5	-2.13	111.53	115.23
31	11	602	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
31	3	615	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
31	14	611	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
38	A	405	PHO	CMD-C2D-C3D	2.13	128.94	124.68
31	6	615	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
30	y	601	CHL	O2D-CGD-O1D	-2.13	119.70	123.85
30	15	605	CHL	OMC-CMC-C2C	-2.13	121.42	125.12
31	3	604	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	5	613	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	y	602	CLA	CHD-C1D-ND	-2.13	121.81	124.80
32	S	617	LHG	O8-C23-C24	2.13	118.32	111.83
31	R	609	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
30	y	601	CHL	O2A-CGA-O1A	-2.12	118.31	123.63
31	3	611	CLA	C4-C3-C5	-2.12	111.54	115.23
31	5	604	CLA	CHD-C1D-ND	-2.12	121.81	124.80
31	6	603	CLA	CHD-C1D-ND	-2.12	121.81	124.80
31	14	611	CLA	CHD-C1D-ND	-2.12	121.81	124.80
31	d	402	CLA	C3C-C4C-NC	-2.12	107.71	110.43
30	n	607	CHL	O2D-CGD-O1D	-2.12	119.72	123.85
31	B	610	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
30	15	606	CHL	O2A-CGA-O1A	-2.12	118.32	123.63
30	y	607	CHL	O2D-CGD-O1D	-2.12	119.72	123.85
31	14	610	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
30	g	605	CHL	O2A-CGA-O1A	-2.12	118.32	123.63
31	6	610	CLA	CMD-C2D-C1D	2.12	128.46	124.73
31	16	602	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	N	603	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	11	612	CLA	O1D-CGD-CBD	-2.12	120.34	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	2	604	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
31	S	602	CLA	C4-C3-C5	-2.12	111.55	115.23
31	C	507	CLA	CHD-C1D-ND	-2.12	121.82	124.80
38	a	405	PHO	CMD-C2D-C3D	2.12	128.92	124.68
31	y	612	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
31	c	511	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
31	c	512	CLA	C4-C3-C5	-2.12	111.55	115.23
31	6	602	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
31	2	611	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
31	c	505	CLA	CHD-C1D-ND	-2.12	121.82	124.80
30	16	601	CHL	OMC-CMC-C2C	-2.12	121.44	125.12
31	3	613	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
31	13	610	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
32	13	616	LHG	O8-C23-C24	2.12	118.29	111.83
31	G	604	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
31	11	611	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	15	612	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
30	R	605	CHL	O2A-CGA-O1A	-2.12	118.34	123.63
30	2	601	CHL	O2D-CGD-O1D	-2.12	119.73	123.85
31	b	603	CLA	CHD-C1D-ND	-2.11	121.83	124.80
30	Y	601	CHL	O2D-CGD-O1D	-2.11	119.73	123.85
31	r	613	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
31	11	602	CLA	CHD-C1D-ND	-2.11	121.83	124.80
30	13	601	CHL	O2D-CGD-O1D	-2.11	119.73	123.85
31	C	511	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
31	C	514	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
31	C	514	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
30	g	609	CHL	O2A-CGA-O1A	-2.11	118.34	123.63
38	a	406	PHO	CMD-C2D-C3D	2.11	128.90	124.68
31	C	512	CLA	C4-C3-C5	-2.11	111.56	115.23
35	r	616	XAT	O24-C25-C24	-2.11	111.51	113.49
31	14	613	CLA	CHD-C1D-ND	-2.11	121.83	124.80
38	D	402	PHO	C2B-C1B-NB	-2.11	107.90	109.43
31	3	602	CLA	CMD-C2D-C1D	2.11	128.45	124.73
31	2	604	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
31	c	504	CLA	CED-O2D-CGD	2.11	120.70	115.92
31	y	610	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
31	A	403	CLA	C3C-C4C-NC	-2.11	107.73	110.43
31	6	610	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	15	613	CLA	CMD-C2D-C1D	2.11	128.44	124.73
30	n	601	CHL	C4-C3-C5	-2.11	113.64	116.13
31	14	603	CLA	CHD-C1D-ND	-2.11	121.83	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	15	603	CLA	CHD-C1D-ND	-2.11	121.83	124.80
30	12	606	CHL	O2A-CGA-O1A	-2.11	118.35	123.63
31	c	506	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	C	506	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	R	604	CLA	CHD-C1D-ND	-2.11	121.84	124.80
31	Y	602	CLA	CHD-C1D-ND	-2.11	121.84	124.80
32	s	617	LHG	O8-C23-C24	2.11	118.26	111.83
31	R	601	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
31	G	602	CLA	CHD-C1D-ND	-2.11	121.84	124.80
31	y	602	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
30	y	605	CHL	O2A-CGA-O1A	-2.11	118.36	123.63
31	B	615	CLA	CHD-C1D-ND	-2.11	121.84	124.80
30	S	606	CHL	O2A-CGA-O1A	-2.10	118.36	123.63
31	Y	604	CLA	CHD-C1D-ND	-2.10	121.84	124.80
31	12	604	CLA	CHD-C1D-ND	-2.10	121.84	124.80
31	3	602	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
31	B	606	CLA	C4-C3-C5	-2.10	111.58	115.23
31	y	610	CLA	C12-C11-C10	-2.10	103.86	113.28
31	B	614	CLA	CHD-C1D-ND	-2.10	121.84	124.80
30	11	606	CHL	O2D-CGD-O1D	-2.10	119.76	123.85
31	16	602	CLA	C4-C3-C5	-2.10	111.58	115.23
31	5	603	CLA	CMD-C2D-C1D	2.10	128.43	124.73
30	4	601	CHL	O2A-CGA-O1A	-2.10	118.37	123.63
31	1	602	CLA	C4-C3-C5	-2.10	111.58	115.23
30	G	605	CHL	O2A-CGA-O1A	-2.10	118.37	123.63
31	S	602	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
31	r	609	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
31	6	602	CLA	CMD-C2D-C1D	2.10	128.43	124.73
31	R	610	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
31	N	611	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
31	4	614	CLA	CHD-C1D-ND	-2.10	121.85	124.80
38	D	402	PHO	CMD-C2D-C3D	2.10	128.88	124.68
31	r	601	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
31	6	604	CLA	CHD-C1D-ND	-2.10	121.85	124.80
30	1	606	CHL	O2A-CGA-CBA	2.10	120.07	112.14
31	B	606	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
31	R	608	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
31	4	602	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	s	605	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	s	611	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	a	404	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
31	Y	602	CLA	O2D-CGD-O1D	-2.10	119.77	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	604	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	1	602	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
31	6	604	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
31	14	612	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	N	614	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	C	504	CLA	CED-O2D-CGD	2.10	120.67	115.92
31	b	608	CLA	O1D-CGD-CBD	-2.10	120.39	124.52
31	R	601	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
31	g	604	CLA	C1-C2-C3	2.09	130.15	126.76
30	N	609	CHL	O2A-CGA-O1A	-2.09	118.39	123.63
31	12	609	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	D	404	CLA	CMD-C2D-C1D	2.09	128.41	124.73
30	g	607	CHL	C1A-CHA-C4D	2.09	122.47	118.98
31	Y	613	CLA	C4-C3-C5	-2.09	111.59	115.23
31	5	610	CLA	CED-O2D-CGD	2.09	120.66	115.92
31	A	404	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
31	2	602	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	b	607	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	Y	610	CLA	C12-C11-C10	-2.09	103.90	113.28
31	c	502	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
31	A	402	CLA	CMD-C2D-C1D	2.09	128.41	124.73
31	b	615	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
31	b	613	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
31	16	610	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
31	5	604	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
31	15	602	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	C	505	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	S	604	CLA	CHD-C1D-ND	-2.09	121.86	124.80
32	16	616	LHG	O8-C23-C24	2.09	118.21	111.83
31	15	603	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
31	r	601	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
30	14	609	CHL	O2D-CGD-O1D	-2.09	119.78	123.85
30	1	609	CHL	O2A-CGA-O1A	-2.09	118.41	123.63
31	s	613	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
31	b	614	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	1	611	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
31	y	603	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
31	G	603	CLA	O1D-CGD-CBD	-2.09	120.41	124.52
31	6	611	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
31	1	614	CLA	CHD-C1D-ND	-2.08	121.87	124.80
31	14	602	CLA	CHD-C1D-ND	-2.08	121.87	124.80
31	N	604	CLA	CHD-C1D-ND	-2.08	121.87	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	611	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
31	6	604	CLA	CMD-C2D-C1D	2.08	128.40	124.73
31	n	615	CLA	C2A-C1A-CHA	2.08	127.48	123.87
31	G	602	CLA	C1-C2-C3	2.08	129.61	126.20
31	13	602	CLA	CHD-C1D-ND	-2.08	121.87	124.80
31	n	604	CLA	CHD-C1D-ND	-2.08	121.87	124.80
31	16	604	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
30	r	605	CHL	O2D-CGD-O1D	-2.08	119.80	123.85
31	D	404	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
30	11	605	CHL	O2D-CGD-O1D	-2.08	119.80	123.85
31	C	510	CLA	CHD-C1D-ND	-2.08	121.88	124.80
31	3	610	CLA	CMD-C2D-C1D	2.08	128.39	124.73
30	N	607	CHL	O2D-CGD-O1D	-2.08	119.80	123.85
30	14	608	CHL	O2A-CGA-O1A	-2.08	118.43	123.63
31	g	603	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
30	15	608	CHL	O2A-CGA-O1A	-2.08	118.43	123.63
31	B	608	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
31	S	609	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
31	6	614	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
30	4	605	CHL	O2D-CGD-O1D	-2.08	119.81	123.85
31	r	602	CLA	CHD-C1D-ND	-2.08	121.88	124.80
30	5	609	CHL	OMC-CMC-C2C	-2.08	121.52	125.12
31	Y	613	CLA	C2A-C1A-CHA	2.07	127.47	123.87
31	14	603	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
31	15	612	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
30	G	607	CHL	CHA-C1A-C2A	-2.07	128.44	133.31
31	3	604	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
31	16	614	CLA	CHD-C1D-ND	-2.07	121.88	124.80
31	2	602	CLA	C4-C3-C5	-2.07	111.63	115.23
31	11	603	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	1	612	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
31	1	614	CLA	CMD-C2D-C1D	2.07	128.38	124.73
31	a	403	CLA	CMD-C2D-C1D	2.07	128.38	124.73
31	4	611	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
31	b	615	CLA	CHD-C1D-ND	-2.07	121.89	124.80
30	16	608	CHL	O2A-CGA-O1A	-2.07	118.45	123.63
31	3	604	CLA	CMD-C2D-C1D	2.07	128.38	124.73
31	Y	602	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
31	15	609	CLA	CMD-C2D-C1D	2.07	128.38	124.73
31	5	604	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
30	2	606	CHL	CMB-C2B-C3B	2.07	128.82	124.68
31	15	610	CLA	CED-O2D-CGD	2.07	120.61	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	11	608	CHL	O2D-CGD-O1D	-2.07	119.82	123.85
30	S	606	CHL	O2D-CGD-O1D	-2.07	119.82	123.85
31	B	610	CLA	C4-C3-C5	-2.07	111.64	115.23
31	b	610	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	5	610	CLA	C1-C2-C3	2.07	130.11	126.76
31	b	610	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
31	n	611	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	n	602	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	Y	615	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
30	n	605	CHL	O2A-CGA-O1A	-2.07	118.46	123.63
31	16	611	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
30	13	608	CHL	O2A-CGA-O1A	-2.07	118.46	123.63
31	A	403	CLA	C4-C3-C5	-2.07	111.64	115.23
30	16	609	CHL	O2A-CGA-O1A	-2.07	118.46	123.63
30	G	609	CHL	O2A-CGA-O1A	-2.07	118.46	123.63
31	S	605	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
31	Y	614	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
31	1	611	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	3	614	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	4	610	CLA	C4-C3-C5	-2.06	111.64	115.23
31	C	502	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
31	B	611	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	s	615	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	c	510	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
31	s	615	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
31	2	610	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
31	b	610	CLA	C4-C3-C5	-2.06	111.65	115.23
31	15	604	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	c	513	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	14	602	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
31	B	613	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
31	4	602	CLA	CMD-C2D-C1D	2.06	128.36	124.73
31	4	614	CLA	CMD-C2D-C1D	2.06	128.36	124.73
31	G	602	CLA	CMD-C2D-C1D	2.06	128.36	124.73
31	y	614	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
31	R	602	CLA	CHD-C1D-ND	-2.06	121.90	124.80
30	3	609	CHL	O2D-CGD-O1D	-2.06	119.84	123.85
30	6	609	CHL	O2D-CGD-O1D	-2.06	119.84	123.85
30	g	607	CHL	CHA-C1A-C2A	-2.06	128.47	133.31
31	11	610	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
30	12	605	CHL	OMC-CMC-C2C	-2.06	121.55	125.12
31	S	610	CLA	O2A-CGA-O1A	-2.06	118.48	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	402	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
31	1	603	CLA	CHD-C1D-ND	-2.06	121.91	124.80
31	13	615	CLA	CMD-C2D-C1D	2.06	128.35	124.73
31	B	610	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
31	G	610	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
31	R	603	CLA	CHD-C1D-ND	-2.06	121.91	124.80
31	g	602	CLA	CMD-C2D-C1D	2.06	128.35	124.73
31	S	613	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
31	Y	615	CLA	CMD-C2D-C1D	2.06	128.35	124.73
31	r	604	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
31	5	610	CLA	CMD-C2D-C1D	2.06	128.35	124.73
31	R	601	CLA	CHD-C1D-ND	-2.06	121.91	124.80
31	12	611	CLA	CMD-C2D-C1D	2.06	128.35	124.73
31	S	615	CLA	CHD-C1D-ND	-2.05	121.91	124.80
31	c	514	CLA	C1-C2-C3	2.05	129.56	126.20
31	B	613	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	r	610	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
31	B	615	CLA	C4-C3-C5	-2.05	111.67	115.23
31	y	614	CLA	CMD-C2D-C1D	2.05	128.34	124.73
31	C	513	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
31	G	611	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	y	613	CLA	C4-C3-C5	-2.05	111.67	115.23
31	R	604	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
31	4	613	CLA	CED-O2D-CGD	2.05	120.57	115.92
31	1	604	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
31	n	614	CLA	CHD-C1D-ND	-2.05	121.92	124.80
34	y	624	NEX	C27-C28-C29	-2.05	122.35	125.53
31	d	402	CLA	C4-C3-C5	-2.05	111.67	115.23
31	6	612	CLA	CMD-C2D-C1D	2.05	128.34	124.73
31	B	607	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
30	4	609	CHL	C1-O2A-CGA	2.05	121.61	116.65
31	b	615	CLA	C4-C3-C5	-2.05	111.67	115.23
31	c	502	CLA	CHD-C1D-ND	-2.05	121.92	124.80
31	B	604	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
31	1	604	CLA	C2A-C1A-CHA	2.05	127.42	123.87
31	R	610	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
30	3	609	CHL	OMC-CMC-C2C	-2.05	121.56	125.12
31	B	612	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
31	3	612	CLA	C4-C3-C5	-2.05	111.67	115.23
31	r	610	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
30	4	605	CHL	OMC-CMC-C2C	-2.05	121.57	125.12
31	R	608	CLA	CMB-C2B-C1B	-2.05	122.30	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	613	CLA	CMD-C2D-C1D	2.05	128.33	124.73
31	r	609	CLA	C4-C3-C5	-2.05	111.68	115.23
31	C	502	CLA	CHD-C1D-ND	-2.05	121.92	124.80
31	b	613	CLA	O1D-CGD-CBD	-2.04	120.48	124.52
31	g	611	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
31	1	602	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	g	603	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	g	611	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	N	602	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	b	611	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	r	601	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	n	610	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
31	N	615	CLA	CMD-C2D-C1D	2.04	128.32	124.73
31	S	614	CLA	CMD-C2D-C1D	2.04	128.32	124.73
31	13	613	CLA	CED-O2D-CGD	2.04	120.55	115.92
31	r	608	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
30	G	601	CHL	O2A-CGA-O1A	-2.04	118.52	123.63
31	6	611	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	C	514	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	n	602	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
31	15	611	CLA	CMD-C2D-C1D	2.04	128.32	124.73
31	3	604	CLA	CHB-C1B-NB	2.04	127.11	124.05
31	s	602	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	s	614	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
30	G	607	CHL	O2A-CGA-O1A	-2.04	118.53	123.63
30	2	609	CHL	OMC-CMC-C2C	-2.04	121.58	125.12
31	d	405	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
31	B	615	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
31	d	404	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
31	n	603	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	r	611	CLA	CHD-C1D-ND	-2.04	121.93	124.80
30	6	609	CHL	OMC-CMC-C2C	-2.04	121.58	125.12
31	S	605	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
31	1	602	CLA	CMD-C2D-C1D	2.04	128.32	124.73
31	6	610	CLA	C5-C3-C2	2.04	125.74	121.17
31	3	612	CLA	CMD-C2D-C1D	2.04	128.32	124.73
31	g	610	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
30	Y	606	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
31	S	603	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
31	2	604	CLA	CHD-C1D-ND	-2.04	121.94	124.80
31	C	513	CLA	CHD-C1D-ND	-2.04	121.94	124.80
31	N	602	CLA	CMD-C2D-C1D	2.04	128.31	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	613	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
30	G	609	CHL	OMC-CMC-C2C	-2.04	121.58	125.12
30	14	601	CHL	O2D-CGD-O1D	-2.04	119.88	123.85
31	16	610	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
31	C	508	CLA	C4D-CHA-C1A	2.04	123.67	121.24
30	15	601	CHL	O2D-CGD-O1D	-2.04	119.89	123.85
30	15	607	CHL	O2D-CGD-O1D	-2.04	119.89	123.85
31	N	604	CLA	CHB-C1B-NB	2.04	127.10	124.05
30	G	609	CHL	C1-O2A-CGA	2.03	121.57	116.65
31	b	611	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
31	16	612	CLA	CED-O2D-CGD	2.03	120.53	115.92
31	16	603	CLA	C2A-C1A-CHA	2.03	127.40	123.87
30	g	608	CHL	OMC-CMC-C2C	-2.03	121.59	125.12
30	11	609	CHL	C1-O2A-CGA	2.03	121.57	116.65
30	12	608	CHL	O2A-CGA-O1A	-2.03	118.54	123.63
31	4	614	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
31	c	502	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
30	s	601	CHL	O2A-CGA-O1A	-2.03	118.11	123.33
31	S	605	CLA	CHD-C1D-ND	-2.03	121.94	124.80
31	r	603	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
31	R	613	CLA	CMD-C2D-C1D	2.03	128.30	124.73
30	g	606	CHL	O2D-CGD-O1D	-2.03	119.90	123.85
31	4	604	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
31	r	611	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
31	N	615	CLA	C2A-C1A-CHA	2.03	127.39	123.87
31	6	612	CLA	C4-C3-C5	-2.03	111.71	115.23
31	b	614	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
31	g	604	CLA	CHB-C1B-NB	2.03	127.09	124.05
31	16	611	CLA	CHD-C1D-ND	-2.03	121.95	124.80
31	16	614	CLA	CED-O2D-CGD	2.03	120.51	115.92
31	1	614	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
31	14	604	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
31	B	614	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
31	C	508	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
31	4	612	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
31	13	604	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
31	4	612	CLA	CMD-C2D-C1D	2.03	128.29	124.73
31	12	610	CLA	CED-O2D-CGD	2.03	120.51	115.92
31	A	403	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
31	3	603	CLA	CHD-C1D-ND	-2.02	121.95	124.80
30	16	607	CHL	O2A-CGA-O1A	-2.02	118.56	123.63
31	S	602	CLA	CHD-C1D-ND	-2.02	121.95	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	604	CLA	CHB-C1B-NB	2.02	127.08	124.05
31	S	604	CLA	CMD-C2D-C1D	2.02	128.29	124.73
30	3	609	CHL	O2A-CGA-O1A	-2.02	118.57	123.63
31	S	610	CLA	CMD-C2D-C1D	2.02	128.29	124.73
31	Y	611	CLA	CHD-C1D-ND	-2.02	121.96	124.80
31	13	614	CLA	CED-O2D-CGD	2.02	120.50	115.92
31	6	612	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
31	n	615	CLA	CMD-C2D-C1D	2.02	128.29	124.73
31	2	603	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
31	4	612	CLA	CHD-C1D-ND	-2.02	121.96	124.80
31	s	614	CLA	CMD-C2D-C1D	2.02	128.29	124.73
31	c	513	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
31	5	611	CLA	CHD-C1D-ND	-2.02	121.96	124.80
31	12	603	CLA	CHD-C1D-ND	-2.02	121.96	124.80
31	13	602	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
31	6	613	CLA	CED-O2D-CGD	2.02	120.50	115.92
31	15	613	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
31	D	404	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
31	b	607	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
31	B	604	CLA	CMD-C2D-C1D	2.02	128.28	124.73
31	b	614	CLA	C4-C3-C5	-2.02	111.72	115.23
31	n	604	CLA	CHB-C1B-NB	2.02	127.08	124.05
31	D	405	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
31	2	613	CLA	CMD-C2D-C1D	2.02	128.28	124.73
31	b	604	CLA	CMD-C2D-C1D	2.02	128.28	124.73
31	n	611	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
30	11	601	CHL	O2D-CGD-O1D	-2.02	119.92	123.85
30	3	606	CHL	O2A-CGA-O1A	-2.02	118.59	123.63
31	n	610	CLA	C1-C2-C3	2.02	129.50	126.20
31	y	615	CLA	CMD-C2D-C1D	2.02	128.28	124.73
31	C	509	CLA	CHD-C1D-ND	-2.01	121.97	124.80
31	12	604	CLA	CMD-C2D-C1D	2.01	128.28	124.73
31	16	615	CLA	CMD-C2D-C1D	2.01	128.28	124.73
31	c	504	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
31	g	614	CLA	CHD-C1D-ND	-2.01	121.97	124.80
31	y	611	CLA	CHD-C1D-ND	-2.01	121.97	124.80
35	R	616	XAT	O24-C25-C24	-2.01	111.60	113.49
31	b	612	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
31	a	407	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
31	6	610	CLA	CHB-C1B-NB	2.01	127.07	124.05
30	4	607	CHL	O2A-CGA-O1A	-2.01	118.59	123.63
31	G	611	CLA	CHD-C1D-ND	-2.01	121.97	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	12	613	CLA	CHD-C1D-ND	-2.01	121.97	124.80
31	12	609	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
31	C	504	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
31	C	510	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
31	B	606	CLA	C1-C2-C3	2.01	129.49	126.20
31	S	615	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
31	G	613	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
31	11	612	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
31	s	604	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
31	13	612	CLA	CED-O2D-CGD	2.01	120.47	115.92
31	N	613	CLA	CED-O2D-CGD	2.01	120.47	115.92
31	A	404	CLA	C3C-C4C-NC	-2.01	107.86	110.43
30	16	601	CHL	O2D-CGD-O1D	-2.01	119.94	123.85
31	12	602	CLA	CMD-C2D-C1D	2.01	128.27	124.73
31	16	613	CLA	CED-O2D-CGD	2.01	120.47	115.92
31	N	614	CLA	CBA-CAA-C2A	2.01	119.77	113.79
31	1	604	CLA	CMD-C2D-C1D	2.01	128.26	124.73
31	N	610	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
31	11	613	CLA	CHD-C1D-ND	-2.01	121.98	124.80
30	g	609	CHL	OMC-CMC-C2C	-2.01	121.64	125.12
31	r	602	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
31	N	602	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
31	11	613	CLA	CED-O2D-CGD	2.01	120.47	115.92
31	1	603	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
31	N	613	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
31	y	613	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
31	B	610	CLA	CHD-C1D-ND	-2.01	121.98	124.80
31	C	508	CLA	CHB-C4A-NA	2.01	127.29	124.40
31	11	603	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
31	14	613	CLA	CED-O2D-CGD	2.01	120.46	115.92
31	13	610	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
31	13	611	CLA	CHD-C1D-ND	-2.00	121.98	124.80
31	c	510	CLA	CHD-C1D-ND	-2.00	121.98	124.80
31	c	509	CLA	CHD-C1D-ND	-2.00	121.98	124.80
30	4	607	CHL	O2D-CGD-O1D	-2.00	119.95	123.85
31	13	611	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
30	S	601	CHL	O2A-CGA-O1A	-2.00	118.18	123.33
31	2	603	CLA	CMD-C2D-C1D	2.00	128.26	124.73
31	S	613	CLA	CMD-C2D-C1D	2.00	128.26	124.73
31	1	611	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
31	15	612	CLA	C2A-C1A-CHA	2.00	127.34	123.87
30	2	606	CHL	O2A-CGA-O1A	-2.00	118.18	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	11	602	CLA	CMD-C2D-C1D	2.00	128.25	124.73
31	Y	614	CLA	CMD-C2D-C1D	2.00	128.25	124.73
31	1	613	CLA	CED-O2D-CGD	2.00	120.46	115.92
31	13	614	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
31	C	513	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
31	11	612	CLA	CED-O2D-CGD	2.00	120.46	115.92
31	B	605	CLA	CHD-C1D-ND	-2.00	121.98	124.80
31	14	603	CLA	CMD-C2D-C1D	2.00	128.25	124.73
31	15	611	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
31	G	603	CLA	CHD-C1D-ND	-2.00	121.99	124.80
31	b	606	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
31	14	613	CLA	O2D-CGD-O1D	-2.00	119.95	123.85

All (621) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	1	601	CHL	ND
30	1	601	CHL	NC
30	1	601	CHL	NA
30	1	605	CHL	ND
30	1	605	CHL	NC
30	1	605	CHL	NA
30	1	606	CHL	ND
30	1	606	CHL	NC
30	1	606	CHL	NA
30	1	607	CHL	ND
30	1	607	CHL	NC
30	1	607	CHL	NA
30	1	608	CHL	ND
30	1	608	CHL	NC
30	1	608	CHL	NA
30	1	609	CHL	ND
30	1	609	CHL	NC
30	1	609	CHL	NA
30	2	601	CHL	ND
30	2	601	CHL	NC
30	2	605	CHL	ND
30	2	605	CHL	NC
30	2	605	CHL	NA
30	2	606	CHL	ND
30	2	606	CHL	NC
30	2	606	CHL	NA

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Mol	Chain	Res	Type	Atom
30	2	608	CHL	ND
30	2	608	CHL	NC
30	2	608	CHL	NA
30	2	609	CHL	ND
30	2	609	CHL	NC
30	2	609	CHL	NA
30	2	607	CHL	ND
30	2	607	CHL	NC
30	2	607	CHL	NA
30	3	601	CHL	ND
30	3	601	CHL	NC
30	3	601	CHL	NA
30	3	605	CHL	ND
30	3	605	CHL	NC
30	3	605	CHL	NA
30	3	606	CHL	ND
30	3	606	CHL	NC
30	3	606	CHL	NA
30	3	607	CHL	ND
30	3	607	CHL	NC
30	3	607	CHL	NA
30	3	608	CHL	ND
30	3	608	CHL	NC
30	3	608	CHL	NA
30	3	609	CHL	ND
30	3	609	CHL	NC
30	3	609	CHL	NA
30	4	601	CHL	ND
30	4	601	CHL	NC
30	4	601	CHL	NA
30	4	605	CHL	ND
30	4	605	CHL	NC
30	4	605	CHL	NA
30	4	606	CHL	ND
30	4	606	CHL	NC
30	4	607	CHL	ND
30	4	607	CHL	NC
30	4	607	CHL	NA
30	4	608	CHL	ND
30	4	608	CHL	NC
30	4	608	CHL	NA
30	4	609	CHL	ND

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Mol	Chain	Res	Type	Atom
30	4	609	CHL	NC
30	4	609	CHL	NA
30	5	601	CHL	ND
30	5	601	CHL	NC
30	5	601	CHL	NA
30	5	605	CHL	ND
30	5	605	CHL	NC
30	5	605	CHL	NA
30	5	606	CHL	ND
30	5	606	CHL	NC
30	5	606	CHL	NA
30	5	608	CHL	ND
30	5	608	CHL	NC
30	5	608	CHL	NA
30	5	609	CHL	ND
30	5	609	CHL	NC
30	5	609	CHL	NA
30	5	607	CHL	ND
30	5	607	CHL	NC
30	5	607	CHL	NA
30	6	601	CHL	ND
30	6	601	CHL	NC
30	6	601	CHL	NA
30	6	605	CHL	ND
30	6	605	CHL	NC
30	6	605	CHL	NA
30	6	606	CHL	ND
30	6	606	CHL	NC
30	6	606	CHL	NA
30	6	607	CHL	ND
30	6	607	CHL	NC
30	6	607	CHL	NA
30	6	608	CHL	ND
30	6	608	CHL	NC
30	6	608	CHL	NA
30	6	609	CHL	ND
30	6	609	CHL	NC
30	6	609	CHL	NA
30	11	601	CHL	ND
30	11	601	CHL	NC
30	11	601	CHL	NA
30	11	605	CHL	ND

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Mol	Chain	Res	Type	Atom
30	11	605	CHL	NC
30	11	606	CHL	ND
30	11	606	CHL	NC
30	11	606	CHL	NA
30	11	607	CHL	ND
30	11	607	CHL	NC
30	11	607	CHL	NA
30	11	608	CHL	ND
30	11	608	CHL	NC
30	11	608	CHL	NA
30	11	609	CHL	ND
30	11	609	CHL	NC
30	11	609	CHL	NA
30	12	601	CHL	ND
30	12	601	CHL	NC
30	12	601	CHL	NA
30	12	605	CHL	ND
30	12	605	CHL	NC
30	12	605	CHL	NA
30	12	606	CHL	ND
30	12	606	CHL	NC
30	12	606	CHL	NA
30	12	607	CHL	ND
30	12	607	CHL	NC
30	12	607	CHL	NA
30	12	608	CHL	ND
30	12	608	CHL	NC
30	12	608	CHL	NA
30	13	601	CHL	ND
30	13	601	CHL	NC
30	13	601	CHL	NA
30	13	605	CHL	ND
30	13	605	CHL	NC
30	13	605	CHL	NA
30	13	606	CHL	ND
30	13	606	CHL	NC
30	13	606	CHL	NA
30	13	607	CHL	ND
30	13	607	CHL	NC
30	13	607	CHL	NA
30	13	608	CHL	ND
30	13	608	CHL	NC

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Mol	Chain	Res	Type	Atom
30	13	608	CHL	NA
30	13	609	CHL	ND
30	13	609	CHL	NC
30	13	609	CHL	NA
30	14	601	CHL	ND
30	14	601	CHL	NC
30	14	601	CHL	NA
30	14	605	CHL	ND
30	14	605	CHL	NC
30	14	605	CHL	NA
30	14	606	CHL	ND
30	14	606	CHL	NC
30	14	606	CHL	NA
30	14	607	CHL	ND
30	14	607	CHL	NC
30	14	607	CHL	NA
30	14	608	CHL	ND
30	14	608	CHL	NC
30	14	608	CHL	NA
30	14	609	CHL	ND
30	14	609	CHL	NC
30	14	609	CHL	NA
30	15	601	CHL	ND
30	15	601	CHL	NC
30	15	601	CHL	NA
30	15	605	CHL	ND
30	15	605	CHL	NC
30	15	605	CHL	NA
30	15	606	CHL	ND
30	15	606	CHL	NC
30	15	606	CHL	NA
30	15	607	CHL	ND
30	15	607	CHL	NC
30	15	607	CHL	NA
30	15	608	CHL	ND
30	15	608	CHL	NC
30	15	608	CHL	NA
30	16	601	CHL	ND
30	16	601	CHL	NC
30	16	601	CHL	NA
30	16	605	CHL	ND
30	16	605	CHL	NC

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Mol	Chain	Res	Type	Atom
30	16	605	CHL	NA
30	16	606	CHL	ND
30	16	606	CHL	NC
30	16	606	CHL	NA
30	16	607	CHL	ND
30	16	607	CHL	NC
30	16	607	CHL	NA
30	16	608	CHL	ND
30	16	608	CHL	NC
30	16	608	CHL	NA
30	16	609	CHL	ND
30	16	609	CHL	NC
30	16	609	CHL	NA
30	G	601	CHL	ND
30	G	601	CHL	NC
30	G	601	CHL	NA
30	G	605	CHL	ND
30	G	605	CHL	NC
30	G	605	CHL	NA
30	G	606	CHL	ND
30	G	606	CHL	NC
30	G	606	CHL	NA
30	G	608	CHL	ND
30	G	608	CHL	NC
30	G	608	CHL	NA
30	G	609	CHL	ND
30	G	609	CHL	NC
30	G	609	CHL	NA
30	G	607	CHL	ND
30	G	607	CHL	NC
30	G	607	CHL	NA
30	N	601	CHL	ND
30	N	601	CHL	NC
30	N	601	CHL	NA
30	N	605	CHL	ND
30	N	605	CHL	NC
30	N	605	CHL	NA
30	N	606	CHL	ND
30	N	606	CHL	NC
30	N	606	CHL	NA
30	N	608	CHL	ND
30	N	608	CHL	NC

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Mol	Chain	Res	Type	Atom
30	N	608	CHL	NA
30	N	609	CHL	ND
30	N	609	CHL	NC
30	N	609	CHL	NA
30	N	607	CHL	ND
30	N	607	CHL	NC
30	N	607	CHL	NA
30	R	605	CHL	ND
30	R	605	CHL	NC
30	R	605	CHL	NA
30	R	606	CHL	ND
30	R	606	CHL	NC
30	R	606	CHL	NA
30	R	607	CHL	ND
30	R	607	CHL	NC
30	R	607	CHL	NA
30	S	601	CHL	ND
30	S	601	CHL	NC
30	S	601	CHL	NA
30	S	606	CHL	ND
30	S	606	CHL	NC
30	S	606	CHL	NA
30	S	607	CHL	ND
30	S	607	CHL	NC
30	S	607	CHL	NA
30	S	608	CHL	ND
30	S	608	CHL	NC
30	S	608	CHL	NA
30	Y	607	CHL	ND
30	Y	607	CHL	NC
30	Y	607	CHL	NA
30	Y	601	CHL	ND
30	Y	601	CHL	NC
30	Y	601	CHL	NA
30	Y	605	CHL	ND
30	Y	605	CHL	NC
30	Y	605	CHL	NA
30	Y	606	CHL	ND
30	Y	606	CHL	NC
30	Y	606	CHL	NA
30	Y	608	CHL	ND
30	Y	608	CHL	NC

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Mol	Chain	Res	Type	Atom
30	Y	608	CHL	NA
30	Y	609	CHL	ND
30	Y	609	CHL	NC
30	Y	609	CHL	NA
30	g	601	CHL	ND
30	g	601	CHL	NC
30	g	601	CHL	NA
30	g	605	CHL	ND
30	g	605	CHL	NC
30	g	605	CHL	NA
30	g	606	CHL	ND
30	g	606	CHL	NC
30	g	606	CHL	NA
30	g	608	CHL	ND
30	g	608	CHL	NC
30	g	608	CHL	NA
30	g	609	CHL	ND
30	g	609	CHL	NC
30	g	609	CHL	NA
30	g	607	CHL	ND
30	g	607	CHL	NC
30	g	607	CHL	NA
30	n	601	CHL	ND
30	n	601	CHL	NC
30	n	601	CHL	NA
30	n	605	CHL	ND
30	n	605	CHL	NC
30	n	605	CHL	NA
30	n	606	CHL	ND
30	n	606	CHL	NC
30	n	606	CHL	NA
30	n	608	CHL	ND
30	n	608	CHL	NC
30	n	608	CHL	NA
30	n	609	CHL	ND
30	n	609	CHL	NC
30	n	609	CHL	NA
30	n	607	CHL	ND
30	n	607	CHL	NC
30	n	607	CHL	NA
30	r	605	CHL	ND
30	r	605	CHL	NC

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Mol	Chain	Res	Type	Atom
30	r	605	CHL	NA
30	r	606	CHL	ND
30	r	606	CHL	NC
30	r	606	CHL	NA
30	r	607	CHL	ND
30	r	607	CHL	NC
30	r	607	CHL	NA
30	s	601	CHL	ND
30	s	601	CHL	NC
30	s	601	CHL	NA
30	s	606	CHL	ND
30	s	606	CHL	NC
30	s	606	CHL	NA
30	s	607	CHL	ND
30	s	607	CHL	NC
30	s	607	CHL	NA
30	s	608	CHL	ND
30	s	608	CHL	NC
30	s	608	CHL	NA
30	y	607	CHL	ND
30	y	607	CHL	NC
30	y	607	CHL	NA
30	y	601	CHL	ND
30	y	601	CHL	NC
30	y	601	CHL	NA
30	y	605	CHL	ND
30	y	605	CHL	NA
30	y	605	CHL	NC
30	y	606	CHL	ND
30	y	606	CHL	NA
30	y	606	CHL	NC
30	y	608	CHL	ND
30	y	608	CHL	NC
30	y	608	CHL	NA
30	y	609	CHL	ND
30	y	609	CHL	NC
30	y	609	CHL	NA
31	1	602	CLA	ND
31	1	603	CLA	ND
31	1	604	CLA	ND
31	1	610	CLA	ND
31	1	611	CLA	ND

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Mol	Chain	Res	Type	Atom
31	1	612	CLA	ND
31	1	613	CLA	ND
31	1	614	CLA	ND
31	2	602	CLA	ND
31	2	603	CLA	ND
31	2	604	CLA	ND
31	2	610	CLA	ND
31	2	611	CLA	ND
31	2	612	CLA	ND
31	2	613	CLA	ND
31	3	602	CLA	ND
31	3	603	CLA	ND
31	3	604	CLA	ND
31	3	610	CLA	ND
31	3	611	CLA	ND
31	3	612	CLA	ND
31	3	613	CLA	ND
31	3	614	CLA	ND
31	3	615	CLA	ND
31	4	602	CLA	ND
31	4	603	CLA	ND
31	4	604	CLA	ND
31	4	610	CLA	ND
31	4	611	CLA	ND
31	4	612	CLA	ND
31	4	613	CLA	ND
31	4	614	CLA	ND
31	5	602	CLA	ND
31	5	603	CLA	ND
31	5	604	CLA	ND
31	5	610	CLA	ND
31	5	611	CLA	ND
31	5	612	CLA	ND
31	5	613	CLA	ND
31	6	602	CLA	ND
31	6	603	CLA	ND
31	6	604	CLA	ND
31	6	610	CLA	ND
31	6	611	CLA	ND
31	6	612	CLA	ND
31	6	613	CLA	ND
31	6	614	CLA	ND

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Mol	Chain	Res	Type	Atom
31	6	615	CLA	ND
31	11	602	CLA	ND
31	11	603	CLA	ND
31	11	604	CLA	ND
31	11	610	CLA	ND
31	11	611	CLA	ND
31	11	612	CLA	ND
31	11	613	CLA	ND
31	11	614	CLA	ND
31	12	602	CLA	ND
31	12	603	CLA	ND
31	12	604	CLA	ND
31	12	609	CLA	ND
31	12	610	CLA	ND
31	12	611	CLA	ND
31	12	612	CLA	ND
31	12	613	CLA	ND
31	13	602	CLA	ND
31	13	603	CLA	ND
31	13	604	CLA	ND
31	13	610	CLA	ND
31	13	611	CLA	ND
31	13	612	CLA	ND
31	13	613	CLA	ND
31	13	614	CLA	ND
31	13	615	CLA	ND
31	14	602	CLA	ND
31	14	603	CLA	ND
31	14	604	CLA	ND
31	14	610	CLA	ND
31	14	611	CLA	ND
31	14	612	CLA	ND
31	14	613	CLA	ND
31	14	614	CLA	ND
31	15	602	CLA	ND
31	15	603	CLA	ND
31	15	604	CLA	ND
31	15	609	CLA	ND
31	15	610	CLA	ND
31	15	611	CLA	ND
31	15	612	CLA	ND
31	15	613	CLA	ND

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Mol	Chain	Res	Type	Atom
31	16	602	CLA	ND
31	16	603	CLA	ND
31	16	604	CLA	ND
31	16	610	CLA	ND
31	16	611	CLA	ND
31	16	612	CLA	ND
31	16	613	CLA	ND
31	16	614	CLA	ND
31	16	615	CLA	ND
31	A	402	CLA	ND
31	A	403	CLA	ND
31	A	404	CLA	ND
31	A	406	CLA	ND
31	B	601	CLA	ND
31	B	602	CLA	ND
31	B	603	CLA	ND
31	B	604	CLA	ND
31	B	605	CLA	ND
31	B	606	CLA	ND
31	B	607	CLA	ND
31	B	608	CLA	ND
31	B	609	CLA	ND
31	B	610	CLA	ND
31	B	611	CLA	ND
31	B	612	CLA	ND
31	B	613	CLA	ND
31	B	614	CLA	ND
31	B	615	CLA	ND
31	B	616	CLA	ND
31	C	502	CLA	ND
31	C	503	CLA	ND
31	C	504	CLA	ND
31	C	505	CLA	ND
31	C	506	CLA	ND
31	C	507	CLA	ND
31	C	508	CLA	ND
31	C	509	CLA	ND
31	C	510	CLA	ND
31	C	511	CLA	ND
31	C	512	CLA	ND
31	C	513	CLA	ND
31	C	514	CLA	ND

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Mol	Chain	Res	Type	Atom
31	D	404	CLA	ND
31	D	405	CLA	ND
31	G	602	CLA	ND
31	G	603	CLA	ND
31	G	604	CLA	ND
31	G	610	CLA	ND
31	G	611	CLA	ND
31	G	612	CLA	ND
31	G	613	CLA	ND
31	G	614	CLA	ND
31	N	602	CLA	ND
31	N	603	CLA	ND
31	N	604	CLA	ND
31	N	610	CLA	ND
31	N	611	CLA	ND
31	N	612	CLA	ND
31	N	613	CLA	ND
31	N	614	CLA	ND
31	N	615	CLA	ND
31	R	601	CLA	ND
31	R	602	CLA	ND
31	R	603	CLA	ND
31	R	604	CLA	ND
31	R	608	CLA	ND
31	R	609	CLA	ND
31	R	610	CLA	ND
31	R	611	CLA	ND
31	R	612	CLA	ND
31	R	613	CLA	ND
31	R	614	CLA	ND
31	S	602	CLA	ND
31	S	603	CLA	ND
31	S	604	CLA	ND
31	S	605	CLA	ND
31	S	609	CLA	ND
31	S	610	CLA	ND
31	S	611	CLA	ND
31	S	612	CLA	ND
31	S	613	CLA	ND
31	S	614	CLA	ND
31	S	615	CLA	ND
31	Y	615	CLA	ND

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Mol	Chain	Res	Type	Atom
31	Y	602	CLA	ND
31	Y	603	CLA	ND
31	Y	604	CLA	ND
31	Y	610	CLA	ND
31	Y	611	CLA	ND
31	Y	612	CLA	ND
31	Y	613	CLA	ND
31	Y	614	CLA	ND
31	a	403	CLA	ND
31	a	404	CLA	ND
31	a	407	CLA	ND
31	b	601	CLA	ND
31	b	602	CLA	ND
31	b	603	CLA	ND
31	b	604	CLA	ND
31	b	605	CLA	ND
31	b	606	CLA	ND
31	b	607	CLA	ND
31	b	608	CLA	ND
31	b	609	CLA	ND
31	b	610	CLA	ND
31	b	611	CLA	ND
31	b	612	CLA	ND
31	b	613	CLA	ND
31	b	614	CLA	ND
31	b	615	CLA	ND
31	b	616	CLA	ND
31	c	502	CLA	ND
31	c	503	CLA	ND
31	c	504	CLA	ND
31	c	505	CLA	ND
31	c	506	CLA	ND
31	c	507	CLA	ND
31	c	508	CLA	ND
31	c	509	CLA	ND
31	c	510	CLA	ND
31	c	511	CLA	ND
31	c	512	CLA	ND
31	c	513	CLA	ND
31	c	514	CLA	ND
31	d	402	CLA	ND
31	d	404	CLA	ND

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Mol	Chain	Res	Type	Atom
31	d	405	CLA	ND
31	g	602	CLA	ND
31	g	603	CLA	ND
31	g	604	CLA	ND
31	g	610	CLA	ND
31	g	611	CLA	ND
31	g	612	CLA	ND
31	g	613	CLA	ND
31	g	614	CLA	ND
31	n	602	CLA	ND
31	n	603	CLA	ND
31	n	604	CLA	ND
31	n	610	CLA	ND
31	n	611	CLA	ND
31	n	612	CLA	ND
31	n	613	CLA	ND
31	n	614	CLA	ND
31	n	615	CLA	ND
31	r	601	CLA	ND
31	r	602	CLA	ND
31	r	603	CLA	ND
31	r	604	CLA	ND
31	r	608	CLA	ND
31	r	609	CLA	ND
31	r	610	CLA	ND
31	r	611	CLA	ND
31	r	612	CLA	ND
31	r	613	CLA	ND
31	r	614	CLA	ND
31	s	602	CLA	ND
31	s	603	CLA	ND
31	s	604	CLA	ND
31	s	605	CLA	ND
31	s	609	CLA	ND
31	s	610	CLA	ND
31	s	611	CLA	ND
31	s	612	CLA	ND
31	s	613	CLA	ND
31	s	614	CLA	ND
31	s	615	CLA	ND
31	y	602	CLA	ND
31	y	603	CLA	ND

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Mol	Chain	Res	Type	Atom
31	y	604	CLA	ND
31	y	610	CLA	ND
31	y	611	CLA	ND
31	y	612	CLA	ND
31	y	613	CLA	ND
31	y	614	CLA	ND
31	y	615	CLA	ND

All (5794) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	1	601	CHL	C1C-C2C-CMC-OMC
30	1	601	CHL	C3C-C2C-CMC-OMC
30	1	606	CHL	C1C-C2C-CMC-OMC
30	1	606	CHL	C3C-C2C-CMC-OMC
30	1	608	CHL	O1A-CGA-O2A-C1
30	1	608	CHL	C1C-C2C-CMC-OMC
30	1	608	CHL	C3C-C2C-CMC-OMC
30	1	609	CHL	C3A-C2A-CAA-CBA
30	1	609	CHL	C1C-C2C-CMC-OMC
30	1	609	CHL	C3C-C2C-CMC-OMC
30	1	609	CHL	C1-C2-C3-C5
30	1	609	CHL	C4-C3-C5-C6
30	2	605	CHL	C3A-C2A-CAA-CBA
30	2	605	CHL	C1C-C2C-CMC-OMC
30	2	605	CHL	C3C-C2C-CMC-OMC
30	2	605	CHL	CAD-CBD-CGD-O2D
30	2	606	CHL	C1A-C2A-CAA-CBA
30	2	606	CHL	C3A-C2A-CAA-CBA
30	2	608	CHL	CBA-CGA-O2A-C1
30	2	608	CHL	O1A-CGA-O2A-C1
30	2	609	CHL	C3A-C2A-CAA-CBA
30	2	609	CHL	C1-C2-C3-C5
30	2	609	CHL	C4-C3-C5-C6
30	3	601	CHL	C4C-C3C-CAC-CBC
30	3	605	CHL	C1A-C2A-CAA-CBA
30	3	605	CHL	C1C-C2C-CMC-OMC
30	3	605	CHL	C3C-C2C-CMC-OMC
30	3	605	CHL	CAD-CBD-CGD-O1D
30	3	605	CHL	CAD-CBD-CGD-O2D
30	3	607	CHL	C1A-C2A-CAA-CBA
30	3	607	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
30	3	607	CHL	C1-C2-C3-C5
30	3	608	CHL	C3A-C2A-CAA-CBA
30	3	608	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	C3A-C2A-CAA-CBA
30	4	601	CHL	C1C-C2C-CMC-OMC
30	4	601	CHL	C3C-C2C-CMC-OMC
30	4	606	CHL	C1C-C2C-CMC-OMC
30	4	606	CHL	C3C-C2C-CMC-OMC
30	4	607	CHL	C1-C2-C3-C4
30	4	607	CHL	C1-C2-C3-C5
30	4	608	CHL	O1A-CGA-O2A-C1
30	4	608	CHL	C1C-C2C-CMC-OMC
30	4	608	CHL	C3C-C2C-CMC-OMC
30	4	609	CHL	C3A-C2A-CAA-CBA
30	4	609	CHL	C1C-C2C-CMC-OMC
30	4	609	CHL	C3C-C2C-CMC-OMC
30	5	601	CHL	C1C-C2C-CMC-OMC
30	5	601	CHL	C3C-C2C-CMC-OMC
30	5	605	CHL	C3A-C2A-CAA-CBA
30	5	605	CHL	C1C-C2C-CMC-OMC
30	5	605	CHL	C3C-C2C-CMC-OMC
30	5	605	CHL	CAD-CBD-CGD-O2D
30	5	606	CHL	C1A-C2A-CAA-CBA
30	5	606	CHL	C3C-C2C-CMC-OMC
30	5	608	CHL	CBA-CGA-O2A-C1
30	6	601	CHL	C4C-C3C-CAC-CBC
30	6	605	CHL	C1A-C2A-CAA-CBA
30	6	605	CHL	C1C-C2C-CMC-OMC
30	6	605	CHL	C3C-C2C-CMC-OMC
30	6	605	CHL	CAD-CBD-CGD-O1D
30	6	605	CHL	CAD-CBD-CGD-O2D
30	6	606	CHL	C3A-C2A-CAA-CBA
30	6	606	CHL	C2-C3-C5-C6
30	6	607	CHL	C1A-C2A-CAA-CBA
30	6	607	CHL	C1C-C2C-CMC-OMC
30	6	607	CHL	C1-C2-C3-C4
30	6	607	CHL	C1-C2-C3-C5
30	6	608	CHL	C3A-C2A-CAA-CBA
30	11	601	CHL	O1A-CGA-O2A-C1
30	11	601	CHL	C1C-C2C-CMC-OMC
30	11	601	CHL	C3C-C2C-CMC-OMC
30	11	605	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	11	605	CHL	C3A-C2A-CAA-CBA
30	11	605	CHL	CBD-CGD-O2D-CED
30	11	606	CHL	C1C-C2C-CMC-OMC
30	11	606	CHL	C3C-C2C-CMC-OMC
30	11	607	CHL	C1A-C2A-CAA-CBA
30	11	607	CHL	C1C-C2C-CMC-OMC
30	11	607	CHL	C3C-C2C-CMC-OMC
30	11	607	CHL	CBD-CGD-O2D-CED
30	11	607	CHL	O1D-CGD-O2D-CED
30	11	608	CHL	C2-C1-O2A-CGA
30	11	608	CHL	C1-C2-C3-C5
30	11	609	CHL	C1A-C2A-CAA-CBA
30	11	609	CHL	C1C-C2C-CMC-OMC
30	11	609	CHL	C4C-C3C-CAC-CBC
30	12	601	CHL	CBA-CGA-O2A-C1
30	12	601	CHL	C1C-C2C-CMC-OMC
30	12	601	CHL	C3C-C2C-CMC-OMC
30	12	607	CHL	C3A-C2A-CAA-CBA
30	12	607	CHL	C1C-C2C-CMC-OMC
30	12	607	CHL	C3C-C2C-CMC-OMC
30	12	608	CHL	C1A-C2A-CAA-CBA
30	12	608	CHL	C3A-C2A-CAA-CBA
30	12	608	CHL	C1C-C2C-CMC-OMC
30	12	608	CHL	C3C-C2C-CMC-OMC
30	13	601	CHL	C3C-C2C-CMC-OMC
30	13	601	CHL	C4C-C3C-CAC-CBC
30	13	601	CHL	C1-C2-C3-C5
30	13	605	CHL	C3A-C2A-CAA-CBA
30	13	605	CHL	C1C-C2C-CMC-OMC
30	13	605	CHL	C3C-C2C-CMC-OMC
30	13	605	CHL	C1-C2-C3-C5
30	13	606	CHL	C1A-C2A-CAA-CBA
30	13	606	CHL	C1C-C2C-CMC-OMC
30	13	606	CHL	C3C-C2C-CMC-OMC
30	13	606	CHL	C1-C2-C3-C5
30	13	607	CHL	C1-C2-C3-C5
30	13	608	CHL	C3A-C2A-CAA-CBA
30	13	608	CHL	CBD-CGD-O2D-CED
30	13	609	CHL	C1A-C2A-CAA-CBA
30	13	609	CHL	C1-C2-C3-C4
30	13	609	CHL	C1-C2-C3-C5
30	14	601	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	14	601	CHL	C1C-C2C-CMC-OMC
30	14	601	CHL	C3C-C2C-CMC-OMC
30	14	601	CHL	C14-C13-C15-C16
30	14	605	CHL	C1A-C2A-CAA-CBA
30	14	605	CHL	C3A-C2A-CAA-CBA
30	14	605	CHL	C1C-C2C-CMC-OMC
30	14	605	CHL	CBD-CGD-O2D-CED
30	14	608	CHL	C2-C1-O2A-CGA
30	14	608	CHL	C1C-C2C-CMC-OMC
30	14	608	CHL	C3C-C2C-CMC-OMC
30	14	608	CHL	C4C-C3C-CAC-CBC
30	14	608	CHL	CBD-CGD-O2D-CED
30	14	609	CHL	C1A-C2A-CAA-CBA
30	14	609	CHL	C1C-C2C-CMC-OMC
30	14	609	CHL	C4C-C3C-CAC-CBC
30	15	601	CHL	CBA-CGA-O2A-C1
30	15	601	CHL	C1C-C2C-CMC-OMC
30	15	601	CHL	C3C-C2C-CMC-OMC
30	15	607	CHL	C3A-C2A-CAA-CBA
30	15	607	CHL	C1C-C2C-CMC-OMC
30	15	607	CHL	C3C-C2C-CMC-OMC
30	16	601	CHL	C3C-C2C-CMC-OMC
30	16	601	CHL	C4C-C3C-CAC-CBC
30	16	605	CHL	C3A-C2A-CAA-CBA
30	16	605	CHL	C1C-C2C-CMC-OMC
30	16	605	CHL	C3C-C2C-CMC-OMC
30	16	606	CHL	C1A-C2A-CAA-CBA
30	16	606	CHL	C1C-C2C-CMC-OMC
30	16	606	CHL	C3C-C2C-CMC-OMC
30	16	606	CHL	C1-C2-C3-C5
30	16	607	CHL	O2A-C1-C2-C3
30	16	607	CHL	C1-C2-C3-C4
30	16	607	CHL	C1-C2-C3-C5
30	16	608	CHL	C3A-C2A-CAA-CBA
30	16	608	CHL	CBD-CGD-O2D-CED
30	16	609	CHL	C3A-C2A-CAA-CBA
30	16	609	CHL	C1C-C2C-CMC-OMC
30	16	609	CHL	C3C-C2C-CMC-OMC
30	G	605	CHL	C1A-C2A-CAA-CBA
30	G	608	CHL	C3C-C2C-CMC-OMC
30	G	607	CHL	C1A-C2A-CAA-CBA
30	N	605	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
30	N	605	CHL	C3C-C2C-CMC-OMC
30	N	605	CHL	CAD-CBD-CGD-O1D
30	N	605	CHL	CAD-CBD-CGD-O2D
30	N	606	CHL	C3A-C2A-CAA-CBA
30	N	606	CHL	C1C-C2C-CMC-OMC
30	N	606	CHL	C3C-C2C-CMC-OMC
30	N	608	CHL	C3A-C2A-CAA-CBA
30	N	609	CHL	C1C-C2C-CMC-OMC
30	N	609	CHL	C3C-C2C-CMC-OMC
30	N	609	CHL	C4C-C3C-CAC-CBC
30	N	609	CHL	CAD-CBD-CGD-O2D
30	N	609	CHL	C1-C2-C3-C4
30	R	605	CHL	C1C-C2C-CMC-OMC
30	R	606	CHL	C1A-C2A-CAA-CBA
30	R	607	CHL	CBD-CGD-O2D-CED
30	S	601	CHL	C1C-C2C-CMC-OMC
30	S	601	CHL	C3C-C2C-CMC-OMC
30	S	606	CHL	C1A-C2A-CAA-CBA
30	S	607	CHL	C1A-C2A-CAA-CBA
30	S	607	CHL	C3A-C2A-CAA-CBA
30	S	607	CHL	C1C-C2C-CMC-OMC
30	S	607	CHL	C3C-C2C-CMC-OMC
30	S	608	CHL	C1C-C2C-CMC-OMC
30	S	608	CHL	C3C-C2C-CMC-OMC
30	Y	607	CHL	C1A-C2A-CAA-CBA
30	Y	607	CHL	C1C-C2C-CMC-OMC
30	Y	607	CHL	C3C-C2C-CMC-OMC
30	Y	601	CHL	C2-C3-C5-C6
30	Y	601	CHL	C4-C3-C5-C6
30	Y	605	CHL	C1C-C2C-CMC-OMC
30	Y	605	CHL	C3C-C2C-CMC-OMC
30	Y	605	CHL	C1-C2-C3-C4
30	Y	605	CHL	C1-C2-C3-C5
30	Y	606	CHL	C1C-C2C-CMC-OMC
30	Y	608	CHL	C1A-C2A-CAA-CBA
30	Y	608	CHL	CBD-CGD-O2D-CED
30	Y	609	CHL	C1C-C2C-CMC-OMC
30	Y	609	CHL	C3C-C2C-CMC-OMC
30	Y	609	CHL	C1-C2-C3-C4
30	Y	609	CHL	C1-C2-C3-C5
30	g	605	CHL	C1A-C2A-CAA-CBA
30	g	606	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	g	607	CHL	C1A-C2A-CAA-CBA
30	n	601	CHL	C2-C3-C5-C6
30	n	601	CHL	C4-C3-C5-C6
30	n	605	CHL	C1A-C2A-CAA-CBA
30	n	605	CHL	CBA-CGA-O2A-C1
30	n	605	CHL	O1A-CGA-O2A-C1
30	n	605	CHL	C1C-C2C-CMC-OMC
30	n	605	CHL	C3C-C2C-CMC-OMC
30	n	606	CHL	C3A-C2A-CAA-CBA
30	n	606	CHL	C1C-C2C-CMC-OMC
30	n	606	CHL	C3C-C2C-CMC-OMC
30	n	608	CHL	C3A-C2A-CAA-CBA
30	n	608	CHL	CAD-CBD-CGD-O2D
30	n	609	CHL	CAD-CBD-CGD-O2D
30	r	605	CHL	C1C-C2C-CMC-OMC
30	r	606	CHL	C1A-C2A-CAA-CBA
30	r	606	CHL	CBD-CGD-O2D-CED
30	r	606	CHL	C11-C10-C8-C9
30	r	607	CHL	CBD-CGD-O2D-CED
30	s	601	CHL	C1C-C2C-CMC-OMC
30	s	606	CHL	C1A-C2A-CAA-CBA
30	s	607	CHL	C1A-C2A-CAA-CBA
30	s	607	CHL	C3A-C2A-CAA-CBA
30	s	607	CHL	C3C-C2C-CMC-OMC
30	s	608	CHL	C1C-C2C-CMC-OMC
30	s	608	CHL	C3C-C2C-CMC-OMC
30	y	607	CHL	C1A-C2A-CAA-CBA
30	y	607	CHL	C1C-C2C-CMC-OMC
30	y	607	CHL	C3C-C2C-CMC-OMC
30	y	605	CHL	C1C-C2C-CMC-OMC
30	y	605	CHL	C3C-C2C-CMC-OMC
30	y	605	CHL	C1-C2-C3-C4
30	y	606	CHL	C1C-C2C-CMC-OMC
30	y	606	CHL	C4-C3-C5-C6
30	y	608	CHL	C1A-C2A-CAA-CBA
30	y	608	CHL	C1C-C2C-CMC-OMC
30	y	608	CHL	CBD-CGD-O2D-CED
30	y	609	CHL	C1-C2-C3-C4
30	y	609	CHL	C1-C2-C3-C5
31	1	602	CLA	C2B-C3B-CAB-CBB
31	1	602	CLA	C4B-C3B-CAB-CBB
31	1	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	1	604	CLA	C4B-C3B-CAB-CBB
31	1	604	CLA	CAD-CBD-CGD-O1D
31	1	604	CLA	CAD-CBD-CGD-O2D
31	1	604	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	C1-C2-C3-C5
31	1	610	CLA	C1A-C2A-CAA-CBA
31	1	610	CLA	C3A-C2A-CAA-CBA
31	1	612	CLA	C1A-C2A-CAA-CBA
31	1	612	CLA	C3A-C2A-CAA-CBA
31	1	612	CLA	CBD-CGD-O2D-CED
31	1	613	CLA	C1-C2-C3-C4
31	1	614	CLA	C1A-C2A-CAA-CBA
31	1	614	CLA	C3A-C2A-CAA-CBA
31	2	602	CLA	C3A-C2A-CAA-CBA
31	2	602	CLA	C2B-C3B-CAB-CBB
31	2	602	CLA	C4B-C3B-CAB-CBB
31	2	602	CLA	CHA-CBD-CGD-O1D
31	2	602	CLA	CHA-CBD-CGD-O2D
31	2	603	CLA	CBD-CGD-O2D-CED
31	2	604	CLA	C1A-C2A-CAA-CBA
31	2	610	CLA	C1A-C2A-CAA-CBA
31	2	610	CLA	C3A-C2A-CAA-CBA
31	2	610	CLA	C2B-C3B-CAB-CBB
31	2	610	CLA	C4B-C3B-CAB-CBB
31	2	611	CLA	C1A-C2A-CAA-CBA
31	2	611	CLA	CBA-CGA-O2A-C1
31	2	611	CLA	C2B-C3B-CAB-CBB
31	2	611	CLA	C4B-C3B-CAB-CBB
31	2	612	CLA	CHA-CBD-CGD-O1D
31	2	612	CLA	CHA-CBD-CGD-O2D
31	2	613	CLA	CBD-CGD-O2D-CED
31	3	602	CLA	C3A-C2A-CAA-CBA
31	3	602	CLA	CHA-CBD-CGD-O1D
31	3	602	CLA	CHA-CBD-CGD-O2D
31	3	604	CLA	CHA-CBD-CGD-O1D
31	3	604	CLA	CHA-CBD-CGD-O2D
31	3	604	CLA	C1-C2-C3-C5
31	3	610	CLA	C3A-C2A-CAA-CBA
31	3	610	CLA	C2B-C3B-CAB-CBB
31	3	610	CLA	C4B-C3B-CAB-CBB
31	3	610	CLA	C1-C2-C3-C4
31	3	610	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
31	3	610	CLA	C4-C3-C5-C6
31	3	611	CLA	C1A-C2A-CAA-CBA
31	3	612	CLA	CHA-CBD-CGD-O1D
31	3	612	CLA	C1-C2-C3-C5
31	3	614	CLA	CHA-CBD-CGD-O2D
31	3	615	CLA	CAD-CBD-CGD-O1D
31	4	602	CLA	CHA-CBD-CGD-O2D
31	4	603	CLA	C1-C2-C3-C5
31	4	604	CLA	C2B-C3B-CAB-CBB
31	4	604	CLA	C4B-C3B-CAB-CBB
31	4	604	CLA	CAD-CBD-CGD-O1D
31	4	604	CLA	CAD-CBD-CGD-O2D
31	4	610	CLA	C1A-C2A-CAA-CBA
31	4	610	CLA	C3A-C2A-CAA-CBA
31	4	610	CLA	C1-C2-C3-C5
31	4	612	CLA	CBD-CGD-O2D-CED
31	4	614	CLA	C1A-C2A-CAA-CBA
31	4	614	CLA	C3A-C2A-CAA-CBA
31	5	602	CLA	C3A-C2A-CAA-CBA
31	5	602	CLA	C2B-C3B-CAB-CBB
31	5	602	CLA	C4B-C3B-CAB-CBB
31	5	602	CLA	CHA-CBD-CGD-O2D
31	5	602	CLA	C2-C3-C5-C6
31	5	603	CLA	CBD-CGD-O2D-CED
31	5	610	CLA	C3A-C2A-CAA-CBA
31	5	610	CLA	C2B-C3B-CAB-CBB
31	5	610	CLA	C4B-C3B-CAB-CBB
31	5	610	CLA	C1-C2-C3-C5
31	5	611	CLA	CBD-CGD-O2D-CED
31	5	612	CLA	CHA-CBD-CGD-O1D
31	5	612	CLA	CHA-CBD-CGD-O2D
31	5	613	CLA	CBD-CGD-O2D-CED
31	6	602	CLA	C3A-C2A-CAA-CBA
31	6	602	CLA	CHA-CBD-CGD-O1D
31	6	602	CLA	CHA-CBD-CGD-O2D
31	6	604	CLA	CHA-CBD-CGD-O1D
31	6	604	CLA	CHA-CBD-CGD-O2D
31	6	604	CLA	C1-C2-C3-C5
31	6	610	CLA	C3A-C2A-CAA-CBA
31	6	610	CLA	C1-C2-C3-C4
31	6	610	CLA	C1-C2-C3-C5
31	6	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	6	611	CLA	C14-C13-C15-C16
31	6	612	CLA	CHA-CBD-CGD-O1D
31	6	612	CLA	C1-C2-C3-C5
31	6	614	CLA	C1A-C2A-CAA-CBA
31	6	614	CLA	C3A-C2A-CAA-CBA
31	6	614	CLA	CHA-CBD-CGD-O2D
31	6	615	CLA	CAD-CBD-CGD-O1D
31	11	602	CLA	C1A-C2A-CAA-CBA
31	11	602	CLA	C3A-C2A-CAA-CBA
31	11	602	CLA	CBD-CGD-O2D-CED
31	11	603	CLA	CBA-CGA-O2A-C1
31	11	604	CLA	C1A-C2A-CAA-CBA
31	11	604	CLA	CBA-CGA-O2A-C1
31	11	610	CLA	C1A-C2A-CAA-CBA
31	11	610	CLA	C2B-C3B-CAB-CBB
31	11	610	CLA	C4B-C3B-CAB-CBB
31	11	612	CLA	C2A-CAA-CBA-CGA
31	11	612	CLA	C2B-C3B-CAB-CBB
31	11	612	CLA	C4B-C3B-CAB-CBB
31	12	602	CLA	CBD-CGD-O2D-CED
31	12	603	CLA	CBD-CGD-O2D-CED
31	12	603	CLA	C1-C2-C3-C5
31	12	604	CLA	C2B-C3B-CAB-CBB
31	12	604	CLA	C4B-C3B-CAB-CBB
31	12	604	CLA	CHA-CBD-CGD-O2D
31	12	609	CLA	C3A-C2A-CAA-CBA
31	12	609	CLA	C2B-C3B-CAB-CBB
31	12	609	CLA	C4B-C3B-CAB-CBB
31	12	609	CLA	CBD-CGD-O2D-CED
31	12	610	CLA	CBD-CGD-O2D-CED
31	12	611	CLA	CBD-CGD-O2D-CED
31	12	612	CLA	CBD-CGD-O2D-CED
31	12	612	CLA	O1D-CGD-O2D-CED
31	12	612	CLA	O2A-C1-C2-C3
31	12	612	CLA	C1-C2-C3-C4
31	12	612	CLA	C1-C2-C3-C5
31	12	613	CLA	C1A-C2A-CAA-CBA
31	12	613	CLA	C2B-C3B-CAB-CBB
31	12	613	CLA	C4B-C3B-CAB-CBB
31	13	602	CLA	C2B-C3B-CAB-CBB
31	13	602	CLA	C4B-C3B-CAB-CBB
31	13	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	13	602	CLA	CHA-CBD-CGD-O2D
31	13	602	CLA	C1-C2-C3-C4
31	13	602	CLA	C1-C2-C3-C5
31	13	604	CLA	C1A-C2A-CAA-CBA
31	13	610	CLA	C1A-C2A-CAA-CBA
31	13	610	CLA	C4B-C3B-CAB-CBB
31	13	614	CLA	C1A-C2A-CAA-CBA
31	13	614	CLA	CBD-CGD-O2D-CED
31	13	615	CLA	CBD-CGD-O2D-CED
31	14	602	CLA	C1A-C2A-CAA-CBA
31	14	602	CLA	C3A-C2A-CAA-CBA
31	14	602	CLA	CBD-CGD-O2D-CED
31	14	603	CLA	CAD-CBD-CGD-O1D
31	14	604	CLA	C1A-C2A-CAA-CBA
31	14	604	CLA	C3A-C2A-CAA-CBA
31	14	604	CLA	CBA-CGA-O2A-C1
31	14	604	CLA	CBD-CGD-O2D-CED
31	14	604	CLA	C1-C2-C3-C4
31	14	604	CLA	C1-C2-C3-C5
31	14	610	CLA	C1A-C2A-CAA-CBA
31	14	610	CLA	C2B-C3B-CAB-CBB
31	14	610	CLA	C4B-C3B-CAB-CBB
31	14	611	CLA	CBD-CGD-O2D-CED
31	14	611	CLA	C1-C2-C3-C5
31	14	612	CLA	C1A-C2A-CAA-CBA
31	14	612	CLA	C3A-C2A-CAA-CBA
31	14	612	CLA	C2A-CAA-CBA-CGA
31	14	612	CLA	CBD-CGD-O2D-CED
31	14	614	CLA	CAD-CBD-CGD-O1D
31	15	602	CLA	C1A-C2A-CAA-CBA
31	15	602	CLA	C4B-C3B-CAB-CBB
31	15	602	CLA	CBD-CGD-O2D-CED
31	15	603	CLA	C1-C2-C3-C5
31	15	604	CLA	C2B-C3B-CAB-CBB
31	15	604	CLA	C4B-C3B-CAB-CBB
31	15	609	CLA	C1A-C2A-CAA-CBA
31	15	609	CLA	C3A-C2A-CAA-CBA
31	15	609	CLA	C2B-C3B-CAB-CBB
31	15	609	CLA	C4B-C3B-CAB-CBB
31	15	609	CLA	C4-C3-C5-C6
31	15	610	CLA	CBD-CGD-O2D-CED
31	15	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	15	612	CLA	C1A-C2A-CAA-CBA
31	15	612	CLA	CBD-CGD-O2D-CED
31	15	612	CLA	C1-C2-C3-C4
31	15	612	CLA	C1-C2-C3-C5
31	15	613	CLA	C1A-C2A-CAA-CBA
31	15	613	CLA	C3A-C2A-CAA-CBA
31	15	613	CLA	C2B-C3B-CAB-CBB
31	15	613	CLA	C4B-C3B-CAB-CBB
31	16	602	CLA	C2B-C3B-CAB-CBB
31	16	602	CLA	C4B-C3B-CAB-CBB
31	16	602	CLA	CHA-CBD-CGD-O2D
31	16	602	CLA	CBD-CGD-O2D-CED
31	16	602	CLA	C2-C3-C5-C6
31	16	603	CLA	C1-C2-C3-C5
31	16	610	CLA	C1A-C2A-CAA-CBA
31	16	610	CLA	C2B-C3B-CAB-CBB
31	16	610	CLA	C4B-C3B-CAB-CBB
31	16	613	CLA	C1-C2-C3-C5
31	16	614	CLA	C1A-C2A-CAA-CBA
31	16	614	CLA	CBD-CGD-O2D-CED
31	16	615	CLA	C2B-C3B-CAB-CBB
31	16	615	CLA	C4B-C3B-CAB-CBB
31	A	403	CLA	C1A-C2A-CAA-CBA
31	A	403	CLA	C3A-C2A-CAA-CBA
31	A	404	CLA	C1A-C2A-CAA-CBA
31	A	404	CLA	C3A-C2A-CAA-CBA
31	A	406	CLA	C2B-C3B-CAB-CBB
31	A	406	CLA	C4B-C3B-CAB-CBB
31	B	601	CLA	C1A-C2A-CAA-CBA
31	B	601	CLA	CAD-CBD-CGD-O1D
31	B	603	CLA	C2B-C3B-CAB-CBB
31	B	603	CLA	C4B-C3B-CAB-CBB
31	B	603	CLA	CAD-CBD-CGD-O1D
31	B	603	CLA	CAD-CBD-CGD-O2D
31	B	605	CLA	CBD-CGD-O2D-CED
31	B	605	CLA	C4-C3-C5-C6
31	B	607	CLA	C1A-C2A-CAA-CBA
31	B	607	CLA	C3A-C2A-CAA-CBA
31	B	608	CLA	C1A-C2A-CAA-CBA
31	B	608	CLA	C1-C2-C3-C5
31	B	608	CLA	C11-C10-C8-C9
31	B	609	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	B	610	CLA	C1-C2-C3-C5
31	B	612	CLA	C1A-C2A-CAA-CBA
31	B	612	CLA	C3A-C2A-CAA-CBA
31	B	613	CLA	C2B-C3B-CAB-CBB
31	B	613	CLA	C4B-C3B-CAB-CBB
31	B	613	CLA	C11-C10-C8-C7
31	B	614	CLA	C2B-C3B-CAB-CBB
31	B	614	CLA	C4B-C3B-CAB-CBB
31	B	614	CLA	CAD-CBD-CGD-O1D
31	B	614	CLA	CAD-CBD-CGD-O2D
31	B	615	CLA	C1-C2-C3-C5
31	B	615	CLA	C11-C10-C8-C9
31	B	616	CLA	C4B-C3B-CAB-CBB
31	B	616	CLA	CHA-CBD-CGD-O1D
31	B	616	CLA	CHA-CBD-CGD-O2D
31	C	502	CLA	CAD-CBD-CGD-O1D
31	C	502	CLA	CAD-CBD-CGD-O2D
31	C	507	CLA	C1A-C2A-CAA-CBA
31	C	507	CLA	C3A-C2A-CAA-CBA
31	C	507	CLA	C2B-C3B-CAB-CBB
31	C	507	CLA	C4B-C3B-CAB-CBB
31	C	508	CLA	CHA-CBD-CGD-O1D
31	C	508	CLA	CHA-CBD-CGD-O2D
31	C	508	CLA	C1-C2-C3-C5
31	C	508	CLA	C11-C10-C8-C9
31	C	509	CLA	CHA-CBD-CGD-O2D
31	C	511	CLA	C2B-C3B-CAB-CBB
31	C	511	CLA	C4B-C3B-CAB-CBB
31	C	512	CLA	O1A-CGA-O2A-C1
31	C	512	CLA	C2B-C3B-CAB-CBB
31	C	512	CLA	C4B-C3B-CAB-CBB
31	C	512	CLA	C1-C2-C3-C5
31	C	513	CLA	C2B-C3B-CAB-CBB
31	C	513	CLA	C4B-C3B-CAB-CBB
31	C	514	CLA	C1A-C2A-CAA-CBA
31	C	514	CLA	C1-C2-C3-C5
31	D	404	CLA	C2B-C3B-CAB-CBB
31	D	404	CLA	C4B-C3B-CAB-CBB
31	D	405	CLA	C1-C2-C3-C5
31	G	602	CLA	CHA-CBD-CGD-O2D
31	G	603	CLA	CAD-CBD-CGD-O2D
31	G	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	G	604	CLA	C3A-C2A-CAA-CBA
31	G	604	CLA	C2B-C3B-CAB-CBB
31	G	604	CLA	C4B-C3B-CAB-CBB
31	G	604	CLA	C1-C2-C3-C5
31	G	611	CLA	C4-C3-C5-C6
31	G	612	CLA	CHA-CBD-CGD-O1D
31	G	614	CLA	C3A-C2A-CAA-CBA
31	N	602	CLA	C2B-C3B-CAB-CBB
31	N	602	CLA	C4B-C3B-CAB-CBB
31	N	602	CLA	CHA-CBD-CGD-O1D
31	N	602	CLA	CHA-CBD-CGD-O2D
31	N	603	CLA	C1-C2-C3-C5
31	N	604	CLA	C4B-C3B-CAB-CBB
31	N	604	CLA	C1-C2-C3-C4
31	N	604	CLA	C1-C2-C3-C5
31	N	604	CLA	C4-C3-C5-C6
31	N	610	CLA	C4-C3-C5-C6
31	N	611	CLA	C1A-C2A-CAA-CBA
31	N	612	CLA	CHA-CBD-CGD-O1D
31	N	612	CLA	CBD-CGD-O2D-CED
31	N	614	CLA	CBD-CGD-O2D-CED
31	R	601	CLA	C1A-C2A-CAA-CBA
31	R	601	CLA	C3A-C2A-CAA-CBA
31	R	603	CLA	C2B-C3B-CAB-CBB
31	R	603	CLA	C4B-C3B-CAB-CBB
31	R	604	CLA	C2B-C3B-CAB-CBB
31	R	604	CLA	C4B-C3B-CAB-CBB
31	R	609	CLA	C3A-C2A-CAA-CBA
31	R	610	CLA	CHA-CBD-CGD-O1D
31	R	610	CLA	CHA-CBD-CGD-O2D
31	R	614	CLA	C1-C2-C3-C4
31	R	614	CLA	C1-C2-C3-C5
31	S	602	CLA	C2B-C3B-CAB-CBB
31	S	602	CLA	C4B-C3B-CAB-CBB
31	S	603	CLA	C1A-C2A-CAA-CBA
31	S	603	CLA	C2B-C3B-CAB-CBB
31	S	603	CLA	C4B-C3B-CAB-CBB
31	S	603	CLA	CHA-CBD-CGD-O1D
31	S	603	CLA	CBD-CGD-O2D-CED
31	S	604	CLA	C1A-C2A-CAA-CBA
31	S	604	CLA	C4B-C3B-CAB-CBB
31	S	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	S	604	CLA	CHA-CBD-CGD-O2D
31	S	604	CLA	C11-C10-C8-C7
31	S	605	CLA	C1A-C2A-CAA-CBA
31	S	605	CLA	C3A-C2A-CAA-CBA
31	S	610	CLA	C1A-C2A-CAA-CBA
31	S	610	CLA	C3A-C2A-CAA-CBA
31	S	610	CLA	C2B-C3B-CAB-CBB
31	S	610	CLA	C4B-C3B-CAB-CBB
31	S	612	CLA	CHA-CBD-CGD-O1D
31	S	613	CLA	CBA-CGA-O2A-C1
31	S	613	CLA	O1A-CGA-O2A-C1
31	S	614	CLA	C1-C2-C3-C5
31	S	615	CLA	CBA-CGA-O2A-C1
31	S	615	CLA	CBD-CGD-O2D-CED
31	S	615	CLA	O1D-CGD-O2D-CED
31	Y	615	CLA	C1A-C2A-CAA-CBA
31	Y	602	CLA	CHA-CBD-CGD-O2D
31	Y	603	CLA	C1-C2-C3-C4
31	Y	603	CLA	C1-C2-C3-C5
31	Y	612	CLA	C2B-C3B-CAB-CBB
31	Y	612	CLA	C4B-C3B-CAB-CBB
31	a	404	CLA	C1A-C2A-CAA-CBA
31	a	404	CLA	C3A-C2A-CAA-CBA
31	a	407	CLA	C2B-C3B-CAB-CBB
31	a	407	CLA	C4B-C3B-CAB-CBB
31	b	601	CLA	C1A-C2A-CAA-CBA
31	b	601	CLA	CAD-CBD-CGD-O1D
31	b	603	CLA	C2B-C3B-CAB-CBB
31	b	603	CLA	C4B-C3B-CAB-CBB
31	b	603	CLA	CAD-CBD-CGD-O1D
31	b	603	CLA	CAD-CBD-CGD-O2D
31	b	605	CLA	CBD-CGD-O2D-CED
31	b	605	CLA	C4-C3-C5-C6
31	b	606	CLA	C1-C2-C3-C4
31	b	607	CLA	C1A-C2A-CAA-CBA
31	b	607	CLA	C3A-C2A-CAA-CBA
31	b	608	CLA	C1A-C2A-CAA-CBA
31	b	609	CLA	CAD-CBD-CGD-O1D
31	b	610	CLA	C1-C2-C3-C5
31	b	612	CLA	C1A-C2A-CAA-CBA
31	b	612	CLA	C3A-C2A-CAA-CBA
31	b	612	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
31	b	613	CLA	C2B-C3B-CAB-CBB
31	b	613	CLA	C4B-C3B-CAB-CBB
31	b	614	CLA	C2B-C3B-CAB-CBB
31	b	614	CLA	C4B-C3B-CAB-CBB
31	b	614	CLA	CAD-CBD-CGD-O1D
31	b	614	CLA	CAD-CBD-CGD-O2D
31	b	615	CLA	C1-C2-C3-C5
31	b	615	CLA	C11-C10-C8-C9
31	b	616	CLA	C4B-C3B-CAB-CBB
31	b	616	CLA	CHA-CBD-CGD-O1D
31	b	616	CLA	CHA-CBD-CGD-O2D
31	c	502	CLA	CAD-CBD-CGD-O1D
31	c	502	CLA	CAD-CBD-CGD-O2D
31	c	502	CLA	C11-C12-C13-C14
31	c	505	CLA	C1-C2-C3-C5
31	c	507	CLA	C1A-C2A-CAA-CBA
31	c	507	CLA	C3A-C2A-CAA-CBA
31	c	507	CLA	C2B-C3B-CAB-CBB
31	c	507	CLA	C4B-C3B-CAB-CBB
31	c	508	CLA	CHA-CBD-CGD-O1D
31	c	508	CLA	CHA-CBD-CGD-O2D
31	c	508	CLA	C1-C2-C3-C5
31	c	508	CLA	C11-C10-C8-C9
31	c	509	CLA	CHA-CBD-CGD-O2D
31	c	511	CLA	C2B-C3B-CAB-CBB
31	c	511	CLA	C4B-C3B-CAB-CBB
31	c	512	CLA	C2B-C3B-CAB-CBB
31	c	512	CLA	C4B-C3B-CAB-CBB
31	c	513	CLA	C2B-C3B-CAB-CBB
31	c	513	CLA	C4B-C3B-CAB-CBB
31	c	514	CLA	C1A-C2A-CAA-CBA
31	c	514	CLA	C1-C2-C3-C5
31	d	402	CLA	C1A-C2A-CAA-CBA
31	d	402	CLA	C3A-C2A-CAA-CBA
31	d	405	CLA	C1-C2-C3-C5
31	g	602	CLA	CHA-CBD-CGD-O2D
31	g	602	CLA	C4-C3-C5-C6
31	g	603	CLA	CAD-CBD-CGD-O2D
31	g	603	CLA	C1-C2-C3-C5
31	g	604	CLA	C1A-C2A-CAA-CBA
31	g	604	CLA	C2B-C3B-CAB-CBB
31	g	604	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	g	610	CLA	C1-C2-C3-C5
31	g	611	CLA	C4-C3-C5-C6
31	g	612	CLA	CHA-CBD-CGD-O1D
31	g	614	CLA	C3A-C2A-CAA-CBA
31	n	602	CLA	CHA-CBD-CGD-O2D
31	n	602	CLA	C1-C2-C3-C5
31	n	603	CLA	C1-C2-C3-C5
31	n	604	CLA	C4B-C3B-CAB-CBB
31	n	604	CLA	C1-C2-C3-C4
31	n	604	CLA	C1-C2-C3-C5
31	n	604	CLA	C4-C3-C5-C6
31	n	610	CLA	C1A-C2A-CAA-CBA
31	n	610	CLA	C2-C3-C5-C6
31	n	611	CLA	CBA-CGA-O2A-C1
31	n	611	CLA	O1A-CGA-O2A-C1
31	n	612	CLA	CHA-CBD-CGD-O1D
31	n	612	CLA	CHA-CBD-CGD-O2D
31	n	613	CLA	C1A-C2A-CAA-CBA
31	n	614	CLA	C1A-C2A-CAA-CBA
31	n	614	CLA	C3A-C2A-CAA-CBA
31	n	614	CLA	CHA-CBD-CGD-O1D
31	n	614	CLA	CBD-CGD-O2D-CED
31	r	603	CLA	C4-C3-C5-C6
31	r	604	CLA	C2B-C3B-CAB-CBB
31	r	604	CLA	C4B-C3B-CAB-CBB
31	r	609	CLA	C1A-C2A-CAA-CBA
31	r	609	CLA	C3A-C2A-CAA-CBA
31	r	609	CLA	C1-C2-C3-C4
31	r	609	CLA	C1-C2-C3-C5
31	r	610	CLA	CHA-CBD-CGD-O1D
31	r	610	CLA	CHA-CBD-CGD-O2D
31	r	611	CLA	C2B-C3B-CAB-CBB
31	r	611	CLA	C4B-C3B-CAB-CBB
31	r	612	CLA	C3A-C2A-CAA-CBA
31	r	612	CLA	CAD-CBD-CGD-O1D
31	r	614	CLA	C1-C2-C3-C5
31	r	614	CLA	C4-C3-C5-C6
31	s	603	CLA	C2B-C3B-CAB-CBB
31	s	603	CLA	C4B-C3B-CAB-CBB
31	s	603	CLA	CHA-CBD-CGD-O1D
31	s	604	CLA	C3A-C2A-CAA-CBA
31	s	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	s	604	CLA	C4B-C3B-CAB-CBB
31	s	604	CLA	CHA-CBD-CGD-O1D
31	s	604	CLA	CHA-CBD-CGD-O2D
31	s	605	CLA	C1A-C2A-CAA-CBA
31	s	605	CLA	C3A-C2A-CAA-CBA
31	s	610	CLA	C3A-C2A-CAA-CBA
31	s	610	CLA	C1-C2-C3-C5
31	s	611	CLA	CBA-CGA-O2A-C1
31	s	611	CLA	O1A-CGA-O2A-C1
31	s	611	CLA	C1-C2-C3-C5
31	s	612	CLA	CHA-CBD-CGD-O1D
31	s	613	CLA	CBA-CGA-O2A-C1
31	s	613	CLA	O1A-CGA-O2A-C1
31	s	613	CLA	CBD-CGD-O2D-CED
31	s	614	CLA	C1-C2-C3-C5
31	s	615	CLA	C1A-C2A-CAA-CBA
31	s	615	CLA	CBD-CGD-O2D-CED
31	s	615	CLA	O1D-CGD-O2D-CED
31	y	602	CLA	CHA-CBD-CGD-O2D
31	y	603	CLA	C4-C3-C5-C6
31	y	612	CLA	C2B-C3B-CAB-CBB
31	y	612	CLA	C4B-C3B-CAB-CBB
31	y	615	CLA	C1A-C2A-CAA-CBA
31	y	615	CLA	C2B-C3B-CAB-CBB
31	y	615	CLA	C4B-C3B-CAB-CBB
31	y	615	CLA	CAD-CBD-CGD-O1D
32	1	615	LHG	C4-O6-P-O3
32	1	615	LHG	C4-O6-P-O4
32	3	616	LHG	O1-C1-C2-C3
32	3	616	LHG	C4-O6-P-O3
32	3	616	LHG	C4-O6-P-O5
32	3	617	LHG	O2-C2-C3-O3
32	3	617	LHG	C3-O3-P-O4
32	3	617	LHG	C3-O3-P-O5
32	3	617	LHG	C3-O3-P-O6
32	3	617	LHG	C4-O6-P-O4
32	3	617	LHG	C8-C7-O7-C5
32	4	615	LHG	O1-C1-C2-C3
32	4	615	LHG	C4-O6-P-O3
32	4	615	LHG	C4-O6-P-O4
32	4	615	LHG	C4-O6-P-O5
32	6	616	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
32	6	616	LHG	C4-O6-P-O4
32	6	616	LHG	C4-O6-P-O5
32	6	617	LHG	C4-O6-P-O4
32	6	617	LHG	O7-C5-C6-O8
32	6	617	LHG	C8-C7-O7-C5
32	11	615	LHG	C3-O3-P-O4
32	11	615	LHG	C3-O3-P-O5
32	11	615	LHG	C3-O3-P-O6
32	13	616	LHG	C3-O3-P-O4
32	13	616	LHG	C3-O3-P-O6
32	13	616	LHG	C4-O6-P-O3
32	13	616	LHG	C4-O6-P-O4
32	13	616	LHG	C4-O6-P-O5
32	13	616	LHG	C8-C7-O7-C5
32	14	615	LHG	C4-O6-P-O5
32	16	616	LHG	C1-C2-C3-O3
32	16	616	LHG	C4-O6-P-O3
32	16	616	LHG	C4-O6-P-O4
32	16	616	LHG	C4-O6-P-O5
32	16	616	LHG	O9-C7-O7-C5
32	16	616	LHG	C8-C7-O7-C5
32	A	411	LHG	C3-O3-P-O4
32	A	411	LHG	C3-O3-P-O6
32	A	411	LHG	O9-C7-O7-C5
32	A	411	LHG	C8-C7-O7-C5
32	A	413	LHG	C3-O3-P-O6
32	A	414	LHG	O1-C1-C2-C3
32	A	414	LHG	C4-O6-P-O5
32	A	414	LHG	O9-C7-O7-C5
32	A	414	LHG	C8-C7-O7-C5
32	A	415	LHG	O2-C2-C3-O3
32	A	415	LHG	C3-O3-P-O4
32	A	415	LHG	C3-O3-P-O6
32	A	415	LHG	C4-O6-P-O4
32	A	415	LHG	C4-O6-P-O5
32	C	521	LHG	C3-O3-P-O5
32	C	521	LHG	C3-O3-P-O6
32	D	409	LHG	O1-C1-C2-C3
32	D	412	LHG	O1-C1-C2-C3
32	D	412	LHG	C3-O3-P-O5
32	D	412	LHG	C3-O3-P-O6
32	G	615	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	G	615	LHG	C4-O6-P-O3
32	G	615	LHG	C4-O6-P-O4
32	G	615	LHG	O9-C7-O7-C5
32	L	102	LHG	C4-O6-P-O3
32	L	102	LHG	C4-O6-P-O5
32	N	616	LHG	O1-C1-C2-C3
32	N	616	LHG	C1-C2-C3-O3
32	N	616	LHG	C3-O3-P-O4
32	N	616	LHG	C3-O3-P-O6
32	N	616	LHG	C4-O6-P-O3
32	N	616	LHG	C4-O6-P-O4
32	R	621	LHG	C4-O6-P-O3
32	R	621	LHG	C4-O6-P-O5
32	R	618	LHG	C3-O3-P-O4
32	R	618	LHG	C3-O3-P-O6
32	R	618	LHG	C4-O6-P-O3
32	R	618	LHG	C4-O6-P-O4
32	R	618	LHG	C4-O6-P-O5
32	R	619	LHG	O6-C4-C5-O7
32	R	619	LHG	O9-C7-O7-C5
32	R	619	LHG	C8-C7-O7-C5
32	S	621	LHG	C1-C2-C3-O3
32	S	621	LHG	O2-C2-C3-O3
32	S	621	LHG	C4-O6-P-O3
32	S	621	LHG	C4-O6-P-O4
32	S	621	LHG	C4-O6-P-O5
32	S	617	LHG	C1-C2-C3-O3
32	Y	618	LHG	O1-C1-C2-O2
32	Y	618	LHG	O1-C1-C2-C3
32	Y	618	LHG	C1-C2-C3-O3
32	Y	618	LHG	C4-O6-P-O3
32	Y	618	LHG	C4-O6-P-O4
32	Y	618	LHG	O9-C7-O7-C5
32	Y	616	LHG	C4-O6-P-O3
32	Y	616	LHG	C4-O6-P-O5
32	Y	616	LHG	O7-C5-C6-O8
32	Y	617	LHG	O2-C2-C3-O3
32	Y	617	LHG	C3-O3-P-O5
32	Y	617	LHG	C4-O6-P-O3
32	Y	617	LHG	C4-O6-P-O4
32	Y	617	LHG	C4-O6-P-O5
32	a	401	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
32	a	411	LHG	O1-C1-C2-O2
32	a	411	LHG	O1-C1-C2-C3
32	a	411	LHG	C3-O3-P-O4
32	a	411	LHG	C3-O3-P-O6
32	a	411	LHG	O9-C7-O7-C5
32	a	411	LHG	C8-C7-O7-C5
32	a	413	LHG	C3-O3-P-O4
32	a	413	LHG	C3-O3-P-O5
32	a	413	LHG	C3-O3-P-O6
32	a	414	LHG	O1-C1-C2-C3
32	a	414	LHG	C4-O6-P-O5
32	a	414	LHG	O9-C7-O7-C5
32	c	521	LHG	C3-O3-P-O5
32	c	521	LHG	C3-O3-P-O6
32	d	413	LHG	O1-C1-C2-C3
32	d	413	LHG	C3-O3-P-O5
32	d	413	LHG	C3-O3-P-O6
32	g	615	LHG	O1-C1-C2-C3
32	g	615	LHG	C1-C2-C3-O3
32	g	615	LHG	C4-O6-P-O3
32	g	615	LHG	C4-O6-P-O4
32	l	102	LHG	C4-O6-P-O3
32	l	102	LHG	C4-O6-P-O5
32	n	616	LHG	O1-C1-C2-C3
32	n	616	LHG	C3-O3-P-O4
32	n	616	LHG	C4-O6-P-O3
32	n	616	LHG	C4-O6-P-O4
32	n	616	LHG	C4-O6-P-O5
32	n	616	LHG	C8-C7-O7-C5
32	r	621	LHG	C4-O6-P-O5
32	r	618	LHG	C4-O6-P-O3
32	r	618	LHG	C4-O6-P-O4
32	r	618	LHG	C4-O6-P-O5
32	r	619	LHG	O1-C1-C2-O2
32	r	619	LHG	O1-C1-C2-C3
32	r	619	LHG	C4-O6-P-O3
32	r	619	LHG	C4-O6-P-O4
32	r	619	LHG	C4-O6-P-O5
32	r	619	LHG	C8-C7-O7-C5
32	s	621	LHG	C1-C2-C3-O3
32	s	621	LHG	O2-C2-C3-O3
32	s	621	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
32	s	621	LHG	C4-O6-P-O4
32	s	621	LHG	C4-O6-P-O5
32	s	617	LHG	C3-O3-P-O4
32	s	617	LHG	C3-O3-P-O5
32	s	617	LHG	C3-O3-P-O6
32	y	618	LHG	O1-C1-C2-O2
32	y	618	LHG	O1-C1-C2-C3
32	y	618	LHG	C1-C2-C3-O3
32	y	618	LHG	C4-O6-P-O3
32	y	618	LHG	C4-O6-P-O4
32	y	618	LHG	O9-C7-O7-C5
32	y	616	LHG	C1-C2-C3-O3
32	y	616	LHG	C4-O6-P-O3
32	y	616	LHG	C4-O6-P-O4
32	y	616	LHG	C4-O6-P-O5
32	y	616	LHG	O7-C5-C6-O8
32	y	617	LHG	C1-C2-C3-O3
32	y	617	LHG	O2-C2-C3-O3
32	y	617	LHG	C3-O3-P-O5
32	y	617	LHG	C4-O6-P-O3
32	y	617	LHG	C4-O6-P-O4
32	y	617	LHG	C4-O6-P-O5
34	R	617	NEX	C7-C8-C9-C10
34	r	617	NEX	C7-C8-C9-C10
36	8	201	3PH	O22-C21-O21-C2
36	8	201	3PH	C22-C21-O21-C2
36	8	201	3PH	O32-C31-O31-C3
36	8	201	3PH	C32-C31-O31-C3
36	B	620	3PH	O22-C21-O21-C2
36	B	620	3PH	C22-C21-O21-C2
36	T	101	3PH	O21-C2-C3-O31
36	T	101	3PH	O22-C21-O21-C2
36	T	101	3PH	C22-C21-O21-C2
36	T	101	3PH	O32-C31-O31-C3
36	T	101	3PH	C32-C31-O31-C3
38	D	402	PHO	C3A-C2A-CAA-CBA
38	D	402	PHO	C1-C2-C3-C5
39	D	406	BCR	C23-C24-C25-C26
39	J	101	BCR	C1-C6-C7-C8
39	J	101	BCR	C5-C6-C7-C8
39	J	101	BCR	C23-C24-C25-C26
39	J	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
39	d	406	BCR	C23-C24-C25-C26
39	j	101	BCR	C1-C6-C7-C8
39	j	101	BCR	C5-C6-C7-C8
39	j	101	BCR	C23-C24-C25-C26
39	j	101	BCR	C23-C24-C25-C30
40	A	408	SQD	O5-C5-C6-S
40	D	413	SQD	O10-C23-O48-C46
40	D	413	SQD	C24-C23-O48-C46
40	D	413	SQD	C5-C6-S-O7
40	D	413	SQD	C5-C6-S-O8
40	D	413	SQD	C5-C6-S-O9
40	L	101	SQD	C5-C6-S-O7
40	L	101	SQD	C5-C6-S-O8
40	L	101	SQD	C5-C6-S-O9
40	a	409	SQD	O5-C5-C6-S
40	d	412	SQD	O47-C45-C46-O48
40	l	101	SQD	C5-C6-S-O7
40	l	101	SQD	C5-C6-S-O8
40	l	101	SQD	C5-C6-S-O9
41	J	102	LMG	O6-C1-O1-C7
41	S	616	LMG	O6-C1-O1-C7
41	j	102	LMG	O6-C1-O1-C7
41	s	616	LMG	O6-C1-O1-C7
43	Y	620	LNL	C9-C10-C11-C12
43	a	412	LNL	C13-C14-C15-C16
43	x	201	LNL	C12-C13-C14-C15
46	C	517	DGD	C2A-C1A-O1G-C1G
46	C	517	DGD	O1A-C1A-O1G-C1G
46	C	517	DGD	O6E-C1E-O5D-C6D
46	W	501	DGD	C2D-C1D-O3G-C3G
46	c	517	DGD	C2A-C1A-O1G-C1G
46	c	517	DGD	O1A-C1A-O1G-C1G
46	c	517	DGD	O6E-C1E-O5D-C6D
49	F	101	HEM	C2B-C3B-CAB-CBB
49	f	101	HEM	C2B-C3B-CAB-CBB
30	2	601	CHL	O1D-CGD-O2D-CED
30	4	606	CHL	O1D-CGD-O2D-CED
30	4	608	CHL	O1D-CGD-O2D-CED
30	15	605	CHL	O1D-CGD-O2D-CED
31	4	612	CLA	O1D-CGD-O2D-CED
31	5	611	CLA	O1D-CGD-O2D-CED
31	13	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	13	615	CLA	O1D-CGD-O2D-CED
31	16	612	CLA	O1D-CGD-O2D-CED
30	1	608	CHL	O1D-CGD-O2D-CED
30	12	605	CHL	O1D-CGD-O2D-CED
30	14	608	CHL	O1D-CGD-O2D-CED
31	11	612	CLA	O1D-CGD-O2D-CED
31	12	611	CLA	O1D-CGD-O2D-CED
31	13	614	CLA	O1D-CGD-O2D-CED
31	14	612	CLA	O1D-CGD-O2D-CED
31	15	611	CLA	O1D-CGD-O2D-CED
31	15	612	CLA	O1D-CGD-O2D-CED
31	16	614	CLA	O1D-CGD-O2D-CED
30	1	605	CHL	CBD-CGD-O2D-CED
30	1	608	CHL	CBD-CGD-O2D-CED
30	2	601	CHL	CBD-CGD-O2D-CED
30	2	605	CHL	CBD-CGD-O2D-CED
30	2	608	CHL	CBD-CGD-O2D-CED
30	3	608	CHL	CBD-CGD-O2D-CED
30	4	605	CHL	CBD-CGD-O2D-CED
30	4	606	CHL	CBD-CGD-O2D-CED
30	4	608	CHL	CBD-CGD-O2D-CED
30	5	601	CHL	CBD-CGD-O2D-CED
30	5	605	CHL	CBD-CGD-O2D-CED
30	5	608	CHL	CBD-CGD-O2D-CED
30	6	608	CHL	CBD-CGD-O2D-CED
30	11	608	CHL	CBD-CGD-O2D-CED
30	12	605	CHL	CBD-CGD-O2D-CED
30	12	607	CHL	CBD-CGD-O2D-CED
30	15	605	CHL	CBD-CGD-O2D-CED
30	15	607	CHL	CBD-CGD-O2D-CED
30	G	605	CHL	CBD-CGD-O2D-CED
30	N	608	CHL	CBD-CGD-O2D-CED
30	R	606	CHL	CBD-CGD-O2D-CED
30	g	605	CHL	CBD-CGD-O2D-CED
31	1	602	CLA	CBD-CGD-O2D-CED
31	1	613	CLA	CBD-CGD-O2D-CED
31	3	610	CLA	CBD-CGD-O2D-CED
31	3	614	CLA	CBD-CGD-O2D-CED
31	5	602	CLA	CBD-CGD-O2D-CED
31	6	614	CLA	CBD-CGD-O2D-CED
31	11	604	CLA	CBD-CGD-O2D-CED
31	11	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	11	612	CLA	CBD-CGD-O2D-CED
31	13	612	CLA	CBD-CGD-O2D-CED
31	15	604	CLA	CBD-CGD-O2D-CED
31	16	612	CLA	CBD-CGD-O2D-CED
31	16	613	CLA	CBD-CGD-O2D-CED
31	16	615	CLA	CBD-CGD-O2D-CED
31	A	402	CLA	CBD-CGD-O2D-CED
31	C	504	CLA	CBD-CGD-O2D-CED
31	G	603	CLA	CBD-CGD-O2D-CED
31	N	610	CLA	CBD-CGD-O2D-CED
31	N	613	CLA	CBD-CGD-O2D-CED
31	N	615	CLA	CBD-CGD-O2D-CED
31	R	614	CLA	CBD-CGD-O2D-CED
31	S	613	CLA	CBD-CGD-O2D-CED
31	a	403	CLA	CBD-CGD-O2D-CED
31	c	504	CLA	CBD-CGD-O2D-CED
31	g	603	CLA	CBD-CGD-O2D-CED
31	n	610	CLA	CBD-CGD-O2D-CED
31	n	615	CLA	CBD-CGD-O2D-CED
31	r	614	CLA	CBD-CGD-O2D-CED
31	s	603	CLA	CBD-CGD-O2D-CED
31	y	614	CLA	CBD-CGD-O2D-CED
30	1	601	CHL	O1A-CGA-O2A-C1
30	3	609	CHL	O1A-CGA-O2A-C1
30	5	608	CHL	O1A-CGA-O2A-C1
30	12	601	CHL	O1A-CGA-O2A-C1
30	15	601	CHL	O1A-CGA-O2A-C1
30	N	605	CHL	O1A-CGA-O2A-C1
31	1	613	CLA	O1A-CGA-O2A-C1
31	11	602	CLA	O1A-CGA-O2A-C1
31	11	614	CLA	O1A-CGA-O2A-C1
31	14	602	CLA	O1A-CGA-O2A-C1
31	14	604	CLA	O1A-CGA-O2A-C1
31	14	614	CLA	O1A-CGA-O2A-C1
31	C	511	CLA	O1A-CGA-O2A-C1
31	S	605	CLA	O1A-CGA-O2A-C1
31	S	611	CLA	O1A-CGA-O2A-C1
31	S	615	CLA	O1A-CGA-O2A-C1
31	c	511	CLA	O1A-CGA-O2A-C1
32	R	618	LHG	O10-C23-O8-C6
31	2	611	CLA	O1A-CGA-O2A-C1
31	5	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	11	604	CLA	O1A-CGA-O2A-C1
30	12	607	CHL	O1D-CGD-O2D-CED
30	15	607	CHL	O1D-CGD-O2D-CED
31	5	613	CLA	O1D-CGD-O2D-CED
30	1	606	CHL	CBA-CGA-O2A-C1
31	3	615	CLA	CBA-CGA-O2A-C1
31	4	612	CLA	CBA-CGA-O2A-C1
31	5	611	CLA	CBA-CGA-O2A-C1
30	Y	608	CHL	O1D-CGD-O2D-CED
31	1	604	CLA	O1D-CGD-O2D-CED
31	1	612	CLA	O1D-CGD-O2D-CED
31	2	613	CLA	O1D-CGD-O2D-CED
31	12	610	CLA	O1D-CGD-O2D-CED
31	15	610	CLA	O1D-CGD-O2D-CED
30	1	601	CHL	CBA-CGA-O2A-C1
30	1	608	CHL	CBA-CGA-O2A-C1
30	3	607	CHL	CBA-CGA-O2A-C1
30	3	609	CHL	CBA-CGA-O2A-C1
30	4	608	CHL	CBA-CGA-O2A-C1
30	11	601	CHL	CBA-CGA-O2A-C1
30	13	607	CHL	CBA-CGA-O2A-C1
30	14	601	CHL	CBA-CGA-O2A-C1
30	15	606	CHL	CBA-CGA-O2A-C1
30	g	605	CHL	CBA-CGA-O2A-C1
31	14	603	CLA	CBA-CGA-O2A-C1
31	r	614	CLA	CBA-CGA-O2A-C1
31	s	615	CLA	CBA-CGA-O2A-C1
31	5	610	CLA	CBD-CGD-O2D-CED
31	12	604	CLA	CBD-CGD-O2D-CED
31	B	609	CLA	CBD-CGD-O2D-CED
30	6	601	CHL	O1A-CGA-O2A-C1
30	11	605	CHL	O1A-CGA-O2A-C1
30	12	606	CHL	O1A-CGA-O2A-C1
30	13	607	CHL	O1A-CGA-O2A-C1
30	14	607	CHL	O1A-CGA-O2A-C1
30	15	606	CHL	O1A-CGA-O2A-C1
30	G	601	CHL	O1A-CGA-O2A-C1
30	G	605	CHL	O1A-CGA-O2A-C1
30	g	605	CHL	O1A-CGA-O2A-C1
31	1	610	CLA	O1A-CGA-O2A-C1
31	2	610	CLA	O1A-CGA-O2A-C1
31	11	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	11	613	CLA	O1A-CGA-O2A-C1
31	12	612	CLA	O1A-CGA-O2A-C1
31	14	603	CLA	O1A-CGA-O2A-C1
31	14	613	CLA	O1A-CGA-O2A-C1
31	15	612	CLA	O1A-CGA-O2A-C1
31	B	604	CLA	O1A-CGA-O2A-C1
31	B	613	CLA	O1A-CGA-O2A-C1
31	R	611	CLA	O1A-CGA-O2A-C1
31	b	613	CLA	O1A-CGA-O2A-C1
31	r	611	CLA	O1A-CGA-O2A-C1
31	r	614	CLA	O1A-CGA-O2A-C1
31	s	605	CLA	O1A-CGA-O2A-C1
31	s	615	CLA	O1A-CGA-O2A-C1
32	3	617	LHG	O10-C23-O8-C6
32	6	617	LHG	O10-C23-O8-C6
32	13	616	LHG	O10-C23-O8-C6
32	16	616	LHG	O10-C23-O8-C6
32	A	414	LHG	O10-C23-O8-C6
32	r	621	LHG	O10-C23-O8-C6
32	r	618	LHG	O10-C23-O8-C6
31	1	614	CLA	O1A-CGA-O2A-C1
30	2	605	CHL	O1D-CGD-O2D-CED
30	5	601	CHL	O1D-CGD-O2D-CED
30	y	608	CHL	O1D-CGD-O2D-CED
31	5	610	CLA	O1D-CGD-O2D-CED
31	12	603	CLA	O1D-CGD-O2D-CED
31	16	615	CLA	O1D-CGD-O2D-CED
31	N	615	CLA	O1D-CGD-O2D-CED
31	n	610	CLA	O1D-CGD-O2D-CED
31	n	615	CLA	O1D-CGD-O2D-CED
30	5	605	CHL	O1D-CGD-O2D-CED
30	6	608	CHL	O1D-CGD-O2D-CED
31	1	613	CLA	O1D-CGD-O2D-CED
31	2	603	CLA	O1D-CGD-O2D-CED
31	3	610	CLA	O1D-CGD-O2D-CED
31	4	613	CLA	O1D-CGD-O2D-CED
31	5	603	CLA	O1D-CGD-O2D-CED
31	12	604	CLA	O1D-CGD-O2D-CED
31	G	603	CLA	O1D-CGD-O2D-CED
31	g	603	CLA	O1D-CGD-O2D-CED
31	G	602	CLA	C15-C16-C17-C18
31	g	602	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	n	613	CLA	CBD-CGD-O2D-CED
30	3	605	CHL	O1A-CGA-O2A-C1
32	3	617	LHG	O9-C7-O7-C5
32	6	617	LHG	O9-C7-O7-C5
32	13	616	LHG	O9-C7-O7-C5
32	N	616	LHG	O9-C7-O7-C5
32	n	616	LHG	O9-C7-O7-C5
32	r	621	LHG	O9-C7-O7-C5
32	r	619	LHG	O9-C7-O7-C5
30	4	606	CHL	CBA-CGA-O2A-C1
31	2	612	CLA	CBA-CGA-O2A-C1
31	5	612	CLA	CBA-CGA-O2A-C1
30	1	606	CHL	O1A-CGA-O2A-C1
30	4	606	CHL	O1A-CGA-O2A-C1
30	3	606	CHL	C3-C5-C6-C7
30	3	607	CHL	C3-C5-C6-C7
30	3	609	CHL	C3-C5-C6-C7
30	11	609	CHL	C3-C5-C6-C7
30	14	609	CHL	C3-C5-C6-C7
30	16	606	CHL	C3-C5-C6-C7
30	G	601	CHL	C3-C5-C6-C7
30	G	609	CHL	C3-C5-C6-C7
30	R	606	CHL	C3-C5-C6-C7
30	Y	609	CHL	C3-C5-C6-C7
30	g	601	CHL	C3-C5-C6-C7
30	g	609	CHL	C3-C5-C6-C7
30	r	606	CHL	C3-C5-C6-C7
30	y	609	CHL	C3-C5-C6-C7
31	3	602	CLA	C3-C5-C6-C7
31	6	602	CLA	C3-C5-C6-C7
31	11	613	CLA	C3-C5-C6-C7
31	12	603	CLA	C3-C5-C6-C7
31	14	613	CLA	C3-C5-C6-C7
31	B	601	CLA	C3-C5-C6-C7
31	B	608	CLA	C3-C5-C6-C7
31	G	610	CLA	C3-C5-C6-C7
31	R	603	CLA	C3-C5-C6-C7
31	S	602	CLA	C3-C5-C6-C7
31	S	614	CLA	C3-C5-C6-C7
31	Y	603	CLA	C3-C5-C6-C7
31	a	407	CLA	C3-C5-C6-C7
31	b	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	n	602	CLA	C3-C5-C6-C7
31	s	609	CLA	C3-C5-C6-C7
31	s	614	CLA	C3-C5-C6-C7
31	y	603	CLA	C3-C5-C6-C7
30	3	605	CHL	CBA-CGA-O2A-C1
30	6	607	CHL	CBA-CGA-O2A-C1
30	12	606	CHL	CBA-CGA-O2A-C1
30	G	601	CHL	CBA-CGA-O2A-C1
30	G	605	CHL	CBA-CGA-O2A-C1
31	1	610	CLA	CBA-CGA-O2A-C1
31	1	613	CLA	CBA-CGA-O2A-C1
31	5	602	CLA	CBA-CGA-O2A-C1
31	11	602	CLA	CBA-CGA-O2A-C1
31	11	613	CLA	CBA-CGA-O2A-C1
31	11	614	CLA	CBA-CGA-O2A-C1
31	12	612	CLA	CBA-CGA-O2A-C1
31	14	602	CLA	CBA-CGA-O2A-C1
31	14	613	CLA	CBA-CGA-O2A-C1
31	14	614	CLA	CBA-CGA-O2A-C1
31	15	612	CLA	CBA-CGA-O2A-C1
31	B	606	CLA	CBA-CGA-O2A-C1
31	C	512	CLA	CBA-CGA-O2A-C1
31	S	605	CLA	CBA-CGA-O2A-C1
31	S	611	CLA	CBA-CGA-O2A-C1
31	Y	603	CLA	CBA-CGA-O2A-C1
31	c	508	CLA	CBA-CGA-O2A-C1
31	s	605	CLA	CBA-CGA-O2A-C1
32	6	617	LHG	C24-C23-O8-C6
32	13	616	LHG	C24-C23-O8-C6
32	16	616	LHG	C24-C23-O8-C6
32	A	414	LHG	C24-C23-O8-C6
32	R	618	LHG	C24-C23-O8-C6
32	r	618	LHG	C24-C23-O8-C6
30	1	609	CHL	CBD-CGD-O2D-CED
30	4	609	CHL	CBD-CGD-O2D-CED
30	13	601	CHL	CBD-CGD-O2D-CED
30	S	601	CHL	CBD-CGD-O2D-CED
30	s	601	CHL	CBD-CGD-O2D-CED
31	2	602	CLA	CBD-CGD-O2D-CED
31	2	604	CLA	CBD-CGD-O2D-CED
31	2	611	CLA	CBD-CGD-O2D-CED
31	3	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	4	611	CLA	CBD-CGD-O2D-CED
31	4	613	CLA	CBD-CGD-O2D-CED
31	5	604	CLA	CBD-CGD-O2D-CED
31	6	610	CLA	CBD-CGD-O2D-CED
31	13	602	CLA	CBD-CGD-O2D-CED
31	13	613	CLA	CBD-CGD-O2D-CED
31	B	610	CLA	CBD-CGD-O2D-CED
31	C	509	CLA	CBD-CGD-O2D-CED
31	S	612	CLA	CBD-CGD-O2D-CED
31	Y	614	CLA	CBD-CGD-O2D-CED
31	b	609	CLA	CBD-CGD-O2D-CED
31	b	610	CLA	CBD-CGD-O2D-CED
31	c	509	CLA	CBD-CGD-O2D-CED
31	g	614	CLA	CBD-CGD-O2D-CED
31	n	602	CLA	CBD-CGD-O2D-CED
31	s	602	CLA	CBD-CGD-O2D-CED
31	s	612	CLA	CBD-CGD-O2D-CED
32	G	615	LHG	C8-C7-O7-C5
32	N	616	LHG	C8-C7-O7-C5
32	Y	618	LHG	C8-C7-O7-C5
32	a	414	LHG	C8-C7-O7-C5
32	r	621	LHG	C8-C7-O7-C5
32	y	618	LHG	C8-C7-O7-C5
30	1	605	CHL	O1D-CGD-O2D-CED
30	4	605	CHL	O1D-CGD-O2D-CED
30	g	605	CHL	O1D-CGD-O2D-CED
31	c	504	CLA	O1D-CGD-O2D-CED
31	2	612	CLA	O1A-CGA-O2A-C1
31	4	614	CLA	O1A-CGA-O2A-C1
30	G	605	CHL	O1D-CGD-O2D-CED
31	C	504	CLA	O1D-CGD-O2D-CED
30	3	605	CHL	C4-C3-C5-C6
30	3	606	CHL	C4-C3-C5-C6
30	11	609	CHL	C4-C3-C5-C6
30	r	605	CHL	C4-C3-C5-C6
30	y	601	CHL	C4-C3-C5-C6
31	5	602	CLA	C4-C3-C5-C6
31	6	610	CLA	C4-C3-C5-C6
31	11	602	CLA	C4-C3-C5-C6
31	12	609	CLA	C4-C3-C5-C6
31	13	602	CLA	C4-C3-C5-C6
31	13	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	14	602	CLA	C4-C3-C5-C6
31	16	610	CLA	C4-C3-C5-C6
31	B	603	CLA	C4-C3-C5-C6
31	B	613	CLA	C4-C3-C5-C6
31	B	614	CLA	C4-C3-C5-C6
31	C	505	CLA	C4-C3-C5-C6
31	C	508	CLA	C4-C3-C5-C6
31	G	602	CLA	C4-C3-C5-C6
31	N	603	CLA	C4-C3-C5-C6
31	R	603	CLA	C4-C3-C5-C6
31	R	609	CLA	C4-C3-C5-C6
31	S	610	CLA	C4-C3-C5-C6
31	Y	602	CLA	C4-C3-C5-C6
31	b	603	CLA	C4-C3-C5-C6
31	b	613	CLA	C4-C3-C5-C6
31	c	508	CLA	C4-C3-C5-C6
31	n	602	CLA	C4-C3-C5-C6
31	n	610	CLA	C4-C3-C5-C6
31	r	609	CLA	C4-C3-C5-C6
31	s	609	CLA	C4-C3-C5-C6
31	s	610	CLA	C4-C3-C5-C6
31	y	602	CLA	C4-C3-C5-C6
42	A	410	PL9	C45-C44-C46-C47
42	D	407	PL9	C20-C19-C21-C22
42	d	407	PL9	C20-C19-C21-C22
30	1	609	CHL	C2-C3-C5-C6
30	3	606	CHL	C2-C3-C5-C6
30	4	609	CHL	C2-C3-C5-C6
30	14	609	CHL	C2-C3-C5-C6
30	16	609	CHL	C2-C3-C5-C6
30	N	601	CHL	C2-C3-C5-C6
30	N	609	CHL	C2-C3-C5-C6
30	R	605	CHL	C2-C3-C5-C6
30	Y	606	CHL	C2-C3-C5-C6
30	n	609	CHL	C2-C3-C5-C6
30	n	607	CHL	C2-C3-C5-C6
30	r	605	CHL	C2-C3-C5-C6
31	2	602	CLA	C2-C3-C5-C6
31	3	604	CLA	C2-C3-C5-C6
31	6	604	CLA	C2-C3-C5-C6
31	6	610	CLA	C2-C3-C5-C6
31	12	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	15	602	CLA	C2-C3-C5-C6
31	A	404	CLA	C2-C3-C5-C6
31	B	603	CLA	C2-C3-C5-C6
31	C	505	CLA	C2-C3-C5-C6
31	C	508	CLA	C2-C3-C5-C6
31	G	602	CLA	C2-C3-C5-C6
31	G	611	CLA	C2-C3-C5-C6
31	N	603	CLA	C2-C3-C5-C6
31	R	603	CLA	C2-C3-C5-C6
31	a	404	CLA	C2-C3-C5-C6
31	b	603	CLA	C2-C3-C5-C6
31	b	614	CLA	C2-C3-C5-C6
31	c	508	CLA	C2-C3-C5-C6
31	d	405	CLA	C2-C3-C5-C6
31	g	611	CLA	C2-C3-C5-C6
31	r	603	CLA	C2-C3-C5-C6
42	D	407	PL9	C18-C19-C21-C22
42	d	407	PL9	C18-C19-C21-C22
31	1	614	CLA	CBA-CGA-O2A-C1
31	4	614	CLA	CBA-CGA-O2A-C1
30	S	608	CHL	CBD-CGD-O2D-CED
31	4	602	CLA	CBD-CGD-O2D-CED
31	G	614	CLA	CBD-CGD-O2D-CED
31	N	613	CLA	O1D-CGD-O2D-CED
30	2	606	CHL	C2A-CAA-CBA-CGA
30	5	606	CHL	C2A-CAA-CBA-CGA
30	6	601	CHL	C2A-CAA-CBA-CGA
30	11	607	CHL	C2A-CAA-CBA-CGA
30	13	606	CHL	C2A-CAA-CBA-CGA
30	15	605	CHL	C2A-CAA-CBA-CGA
30	16	606	CHL	C2A-CAA-CBA-CGA
30	G	608	CHL	C2A-CAA-CBA-CGA
30	N	606	CHL	C2A-CAA-CBA-CGA
30	n	606	CHL	C2A-CAA-CBA-CGA
30	n	608	CHL	C2A-CAA-CBA-CGA
31	1	612	CLA	C2A-CAA-CBA-CGA
31	5	612	CLA	C2A-CAA-CBA-CGA
31	C	507	CLA	C2A-CAA-CBA-CGA
31	S	605	CLA	C2A-CAA-CBA-CGA
31	s	605	CLA	C2A-CAA-CBA-CGA
31	c	508	CLA	O1A-CGA-O2A-C1
30	6	606	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	Y	605	CHL	C3-C5-C6-C7
30	s	606	CHL	C3-C5-C6-C7
31	2	603	CLA	C3-C5-C6-C7
31	3	604	CLA	C3-C5-C6-C7
31	3	613	CLA	C3-C5-C6-C7
31	6	604	CLA	C3-C5-C6-C7
31	g	610	CLA	C3-C5-C6-C7
30	3	608	CHL	CBA-CGA-O2A-C1
30	6	609	CHL	CBA-CGA-O2A-C1
30	11	605	CHL	CBA-CGA-O2A-C1
30	14	607	CHL	CBA-CGA-O2A-C1
30	N	605	CHL	CBA-CGA-O2A-C1
30	S	606	CHL	CBA-CGA-O2A-C1
30	g	601	CHL	CBA-CGA-O2A-C1
30	s	606	CHL	CBA-CGA-O2A-C1
31	2	604	CLA	CBA-CGA-O2A-C1
31	2	610	CLA	CBA-CGA-O2A-C1
31	6	614	CLA	CBA-CGA-O2A-C1
31	12	609	CLA	CBA-CGA-O2A-C1
31	13	602	CLA	CBA-CGA-O2A-C1
31	B	604	CLA	CBA-CGA-O2A-C1
31	B	613	CLA	CBA-CGA-O2A-C1
31	C	508	CLA	CBA-CGA-O2A-C1
31	C	511	CLA	CBA-CGA-O2A-C1
31	N	611	CLA	CBA-CGA-O2A-C1
31	R	611	CLA	CBA-CGA-O2A-C1
31	R	614	CLA	CBA-CGA-O2A-C1
31	b	612	CLA	CBA-CGA-O2A-C1
31	b	613	CLA	CBA-CGA-O2A-C1
31	c	511	CLA	CBA-CGA-O2A-C1
31	c	513	CLA	CBA-CGA-O2A-C1
31	n	615	CLA	CBA-CGA-O2A-C1
31	r	611	CLA	CBA-CGA-O2A-C1
32	3	617	LHG	C24-C23-O8-C6
32	r	621	LHG	C24-C23-O8-C6
31	5	612	CLA	O1A-CGA-O2A-C1
46	C	517	DGD	C4D-C5D-C6D-O5D
46	c	517	DGD	C4D-C5D-C6D-O5D
30	4	607	CHL	O1A-CGA-O2A-C1
30	6	607	CHL	O1A-CGA-O2A-C1
30	G	607	CHL	O1A-CGA-O2A-C1
30	g	601	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	g	607	CHL	O1A-CGA-O2A-C1
31	5	602	CLA	O1A-CGA-O2A-C1
31	12	609	CLA	O1A-CGA-O2A-C1
31	B	606	CLA	O1A-CGA-O2A-C1
31	C	508	CLA	O1A-CGA-O2A-C1
31	N	615	CLA	O1A-CGA-O2A-C1
31	R	609	CLA	O1A-CGA-O2A-C1
31	R	614	CLA	O1A-CGA-O2A-C1
32	G	615	LHG	O10-C23-O8-C6
31	N	614	CLA	O1D-CGD-O2D-CED
31	S	613	CLA	O1D-CGD-O2D-CED
31	5	602	CLA	C3-C5-C6-C7
31	6	613	CLA	C3-C5-C6-C7
31	15	602	CLA	C3-C5-C6-C7
31	A	406	CLA	C3-C5-C6-C7
31	R	613	CLA	C3-C5-C6-C7
31	S	609	CLA	C3-C5-C6-C7
30	15	606	CHL	CBD-CGD-O2D-CED
30	s	608	CHL	CBD-CGD-O2D-CED
31	4	604	CLA	CBD-CGD-O2D-CED
31	6	613	CLA	CBD-CGD-O2D-CED
31	R	611	CLA	CBD-CGD-O2D-CED
31	Y	613	CLA	CBD-CGD-O2D-CED
31	n	612	CLA	CBD-CGD-O2D-CED
32	6	617	LHG	O2-C2-C3-O3
32	N	616	LHG	O2-C2-C3-O3
32	Y	618	LHG	O2-C2-C3-O3
32	y	618	LHG	O2-C2-C3-O3
30	S	601	CHL	O1D-CGD-O2D-CED
30	s	601	CHL	O1D-CGD-O2D-CED
31	A	402	CLA	O1D-CGD-O2D-CED
31	N	610	CLA	O1D-CGD-O2D-CED
31	a	403	CLA	O1D-CGD-O2D-CED
31	b	605	CLA	O1D-CGD-O2D-CED
31	n	613	CLA	O1D-CGD-O2D-CED
31	s	613	CLA	O1D-CGD-O2D-CED
30	5	607	CHL	CBA-CGA-O2A-C1
30	6	601	CHL	CBA-CGA-O2A-C1
30	6	608	CHL	CBA-CGA-O2A-C1
30	G	607	CHL	CBA-CGA-O2A-C1
30	N	609	CHL	CBA-CGA-O2A-C1
30	S	608	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	g	607	CHL	CBA-CGA-O2A-C1
30	n	609	CHL	CBA-CGA-O2A-C1
31	15	609	CLA	CBA-CGA-O2A-C1
31	C	513	CLA	CBA-CGA-O2A-C1
32	G	615	LHG	C24-C23-O8-C6
30	3	607	CHL	O1A-CGA-O2A-C1
31	3	603	CLA	O1A-CGA-O2A-C1
31	6	603	CLA	O1A-CGA-O2A-C1
46	W	501	DGD	C4D-C5D-C6D-O5D
31	Y	604	CLA	CBD-CGD-O2D-CED
31	r	611	CLA	CBD-CGD-O2D-CED
30	S	606	CHL	O1A-CGA-O2A-C1
30	S	608	CHL	O1D-CGD-O2D-CED
31	B	605	CLA	O1D-CGD-O2D-CED
31	1	602	CLA	C3-C5-C6-C7
31	G	613	CLA	C3-C5-C6-C7
31	r	603	CLA	C3-C5-C6-C7
31	3	615	CLA	CBD-CGD-O2D-CED
31	11	614	CLA	CBD-CGD-O2D-CED
31	B	603	CLA	CBD-CGD-O2D-CED
31	R	609	CLA	CBD-CGD-O2D-CED
31	S	602	CLA	CBD-CGD-O2D-CED
31	b	603	CLA	CBD-CGD-O2D-CED
31	y	604	CLA	CBD-CGD-O2D-CED
46	W	501	DGD	O6D-C5D-C6D-O5D
31	14	611	CLA	O1D-CGD-O2D-CED
30	4	607	CHL	CBA-CGA-O2A-C1
31	2	602	CLA	CBA-CGA-O2A-C1
31	N	615	CLA	CBA-CGA-O2A-C1
31	y	603	CLA	CBA-CGA-O2A-C1
30	14	609	CHL	C4-C3-C5-C6
30	N	601	CHL	C4-C3-C5-C6
30	N	607	CHL	C4-C3-C5-C6
30	R	606	CHL	C4-C3-C5-C6
30	n	607	CHL	C4-C3-C5-C6
30	r	606	CHL	C4-C3-C5-C6
31	3	604	CLA	C4-C3-C5-C6
31	6	604	CLA	C4-C3-C5-C6
31	15	602	CLA	C4-C3-C5-C6
31	D	405	CLA	C4-C3-C5-C6
31	d	405	CLA	C4-C3-C5-C6
30	3	605	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	11	602	CLA	C2-C3-C5-C6
31	12	609	CLA	C2-C3-C5-C6
31	14	602	CLA	C2-C3-C5-C6
31	B	606	CLA	C2-C3-C5-C6
31	B	614	CLA	C2-C3-C5-C6
31	D	405	CLA	C2-C3-C5-C6
31	n	602	CLA	C2-C3-C5-C6
30	2	607	CHL	O1A-CGA-O2A-C1
30	3	608	CHL	O1A-CGA-O2A-C1
30	14	605	CHL	O1A-CGA-O2A-C1
30	14	608	CHL	O1A-CGA-O2A-C1
30	R	605	CHL	O1A-CGA-O2A-C1
31	5	603	CLA	O1A-CGA-O2A-C1
31	13	603	CLA	O1A-CGA-O2A-C1
31	16	603	CLA	O1A-CGA-O2A-C1
31	16	610	CLA	O1A-CGA-O2A-C1
31	B	614	CLA	O1A-CGA-O2A-C1
31	N	611	CLA	O1A-CGA-O2A-C1
31	S	610	CLA	O1A-CGA-O2A-C1
31	n	610	CLA	O1A-CGA-O2A-C1
30	14	605	CHL	O1D-CGD-O2D-CED
42	A	410	PL9	C14-C16-C17-C18
42	a	410	PL9	C14-C16-C17-C18
31	r	609	CLA	CBD-CGD-O2D-CED
30	2	608	CHL	O1D-CGD-O2D-CED
30	14	608	CHL	C2A-CAA-CBA-CGA
30	N	601	CHL	C2A-CAA-CBA-CGA
30	g	608	CHL	C2A-CAA-CBA-CGA
30	3	601	CHL	O1A-CGA-O2A-C1
30	4	601	CHL	O1A-CGA-O2A-C1
30	6	608	CHL	O1A-CGA-O2A-C1
30	r	606	CHL	O1A-CGA-O2A-C1
30	s	606	CHL	O1A-CGA-O2A-C1
31	13	610	CLA	O1A-CGA-O2A-C1
31	b	614	CLA	O1A-CGA-O2A-C1
41	A	409	LMG	O6-C1-O1-C7
41	K	102	LMG	O6-C1-O1-C7
41	v	101	LMG	O6-C1-O1-C7
41	w	501	LMG	O6-C1-O1-C7
46	W	501	DGD	O6D-C1D-O3G-C3G
31	6	603	CLA	O1D-CGD-O2D-CED
31	16	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	13	603	CLA	CBA-CGA-O2A-C1
31	B	614	CLA	CBA-CGA-O2A-C1
30	5	607	CHL	CBD-CGD-O2D-CED
30	N	601	CHL	CBD-CGD-O2D-CED
31	6	615	CLA	CBD-CGD-O2D-CED
31	14	614	CLA	CBD-CGD-O2D-CED
31	C	505	CLA	CBD-CGD-O2D-CED
31	c	505	CLA	CBD-CGD-O2D-CED
31	c	514	CLA	CBD-CGD-O2D-CED
32	13	616	LHG	C23-C24-C25-C26
32	16	616	LHG	C23-C24-C25-C26
30	11	609	CHL	O1A-CGA-O2A-C1
46	w	502	DGD	O6D-C5D-C6D-O5D
30	Y	606	CHL	O1D-CGD-O2D-CED
31	6	610	CLA	O1D-CGD-O2D-CED
31	12	613	CLA	O1D-CGD-O2D-CED
31	15	602	CLA	O1D-CGD-O2D-CED
31	Y	613	CLA	O1D-CGD-O2D-CED
32	14	615	LHG	C13-C14-C15-C16
30	2	609	CHL	CBD-CGD-O2D-CED
30	2	607	CHL	CBD-CGD-O2D-CED
30	n	601	CHL	CBD-CGD-O2D-CED
30	n	605	CHL	CBD-CGD-O2D-CED
31	15	613	CLA	CBD-CGD-O2D-CED
31	C	503	CLA	CBD-CGD-O2D-CED
31	c	503	CLA	CBD-CGD-O2D-CED
31	s	604	CLA	CBD-CGD-O2D-CED
34	y	624	NEX	C33-C34-C35-C15
31	2	602	CLA	O1A-CGA-O2A-C1
31	2	603	CLA	O1A-CGA-O2A-C1
31	15	609	CLA	O1A-CGA-O2A-C1
31	Y	603	CLA	O1A-CGA-O2A-C1
31	n	604	CLA	O1A-CGA-O2A-C1
32	14	615	LHG	C1-C2-C3-O3
32	A	415	LHG	C1-C2-C3-O3
32	D	412	LHG	C1-C2-C3-O3
32	G	615	LHG	C1-C2-C3-O3
32	Y	617	LHG	C1-C2-C3-O3
32	d	413	LHG	C1-C2-C3-O3
32	n	616	LHG	C1-C2-C3-O3
32	s	617	LHG	C1-C2-C3-O3
30	2	607	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	3	601	CHL	CBA-CGA-O2A-C1
30	14	605	CHL	CBA-CGA-O2A-C1
30	14	608	CHL	CBA-CGA-O2A-C1
30	N	601	CHL	CBA-CGA-O2A-C1
30	R	605	CHL	CBA-CGA-O2A-C1
30	Y	609	CHL	CBA-CGA-O2A-C1
30	y	609	CHL	CBA-CGA-O2A-C1
31	1	611	CLA	CBA-CGA-O2A-C1
31	2	603	CLA	CBA-CGA-O2A-C1
31	3	603	CLA	CBA-CGA-O2A-C1
31	5	603	CLA	CBA-CGA-O2A-C1
31	6	603	CLA	CBA-CGA-O2A-C1
31	13	610	CLA	CBA-CGA-O2A-C1
31	16	603	CLA	CBA-CGA-O2A-C1
31	16	610	CLA	CBA-CGA-O2A-C1
31	A	404	CLA	CBA-CGA-O2A-C1
31	B	612	CLA	CBA-CGA-O2A-C1
31	B	616	CLA	CBA-CGA-O2A-C1
31	C	507	CLA	CBA-CGA-O2A-C1
31	N	604	CLA	CBA-CGA-O2A-C1
31	R	609	CLA	CBA-CGA-O2A-C1
31	S	610	CLA	CBA-CGA-O2A-C1
31	a	404	CLA	CBA-CGA-O2A-C1
31	c	507	CLA	CBA-CGA-O2A-C1
31	n	604	CLA	CBA-CGA-O2A-C1
32	14	615	LHG	C24-C23-O8-C6
32	11	615	LHG	C28-C29-C30-C31
30	Y	606	CHL	CBD-CGD-O2D-CED
32	14	615	LHG	C11-C12-C13-C14
30	R	607	CHL	O1D-CGD-O2D-CED
30	r	607	CHL	O1D-CGD-O2D-CED
31	3	603	CLA	O1D-CGD-O2D-CED
31	14	604	CLA	O1D-CGD-O2D-CED
31	G	614	CLA	O1D-CGD-O2D-CED
31	s	604	CLA	O1D-CGD-O2D-CED
31	14	611	CLA	C4-C3-C5-C6
31	A	404	CLA	C4-C3-C5-C6
31	a	404	CLA	C4-C3-C5-C6
30	2	609	CHL	C2-C3-C5-C6
30	N	607	CHL	C2-C3-C5-C6
30	y	601	CHL	C2-C3-C5-C6
30	y	606	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	3	610	CLA	C2-C3-C5-C6
31	12	602	CLA	C2-C3-C5-C6
31	13	602	CLA	C2-C3-C5-C6
31	14	611	CLA	C2-C3-C5-C6
31	G	603	CLA	C2-C3-C5-C6
31	R	602	CLA	C2-C3-C5-C6
31	n	603	CLA	C2-C3-C5-C6
31	s	609	CLA	C2-C3-C5-C6
31	y	603	CLA	C2-C3-C5-C6
42	A	410	PL9	C43-C44-C46-C47
30	2	609	CHL	C3-C5-C6-C7
30	g	608	CHL	CBD-CGD-O2D-CED
31	6	603	CLA	CBD-CGD-O2D-CED
30	2	609	CHL	C6-C7-C8-C9
30	2	609	CHL	C11-C12-C13-C14
30	3	601	CHL	C11-C10-C8-C9
30	3	605	CHL	C11-C10-C8-C9
30	3	607	CHL	C6-C7-C8-C9
30	3	609	CHL	C11-C10-C8-C9
30	4	609	CHL	C11-C10-C8-C9
30	4	609	CHL	C14-C13-C15-C16
30	5	609	CHL	C11-C12-C13-C14
30	6	601	CHL	C6-C7-C8-C9
30	6	605	CHL	C11-C10-C8-C9
30	6	607	CHL	C11-C12-C13-C14
30	11	601	CHL	C11-C10-C8-C9
30	13	609	CHL	C6-C7-C8-C9
30	G	609	CHL	C11-C10-C8-C9
30	G	609	CHL	C14-C13-C15-C16
30	N	606	CHL	C6-C7-C8-C9
30	R	606	CHL	C11-C10-C8-C9
30	R	606	CHL	C14-C13-C15-C16
30	S	606	CHL	C11-C10-C8-C9
30	S	606	CHL	C14-C13-C15-C16
30	Y	607	CHL	C14-C13-C15-C16
30	Y	601	CHL	C14-C13-C15-C16
30	Y	606	CHL	C14-C13-C15-C16
30	Y	609	CHL	C6-C7-C8-C9
30	Y	609	CHL	C11-C10-C8-C9
30	Y	609	CHL	C11-C12-C13-C14
30	g	609	CHL	C14-C13-C15-C16
30	n	605	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	n	609	CHL	C6-C7-C8-C9
30	r	606	CHL	C11-C12-C13-C14
30	r	606	CHL	C14-C13-C15-C16
30	s	606	CHL	C6-C7-C8-C9
30	s	606	CHL	C14-C13-C15-C16
30	y	607	CHL	C14-C13-C15-C16
30	y	601	CHL	C14-C13-C15-C16
30	y	606	CHL	C11-C10-C8-C9
30	y	609	CHL	C6-C7-C8-C9
30	y	609	CHL	C11-C10-C8-C9
30	y	609	CHL	C11-C12-C13-C14
31	3	610	CLA	C11-C10-C8-C9
31	4	602	CLA	C6-C7-C8-C9
31	6	610	CLA	C11-C10-C8-C9
31	13	603	CLA	C6-C7-C8-C9
31	14	610	CLA	C14-C13-C15-C16
31	16	603	CLA	C6-C7-C8-C9
31	A	403	CLA	C14-C13-C15-C16
31	A	404	CLA	C11-C10-C8-C9
31	B	602	CLA	C14-C13-C15-C16
31	B	605	CLA	C11-C10-C8-C9
31	B	608	CLA	C11-C12-C13-C14
31	B	610	CLA	C11-C12-C13-C14
31	B	612	CLA	C11-C10-C8-C9
31	B	614	CLA	C14-C13-C15-C16
31	B	616	CLA	C11-C10-C8-C9
31	C	508	CLA	C11-C12-C13-C14
31	D	404	CLA	C11-C10-C8-C9
31	D	405	CLA	C11-C10-C8-C9
31	G	602	CLA	C11-C10-C8-C9
31	G	602	CLA	C11-C12-C13-C14
31	G	613	CLA	C11-C12-C13-C14
31	N	602	CLA	C11-C10-C8-C9
31	N	602	CLA	C14-C13-C15-C16
31	R	602	CLA	C11-C12-C13-C14
31	S	602	CLA	C11-C10-C8-C9
31	S	604	CLA	C11-C12-C13-C14
31	S	611	CLA	C6-C7-C8-C9
31	S	611	CLA	C11-C12-C13-C14
31	Y	612	CLA	C11-C10-C8-C9
31	a	404	CLA	C11-C10-C8-C9
31	b	602	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	b	604	CLA	C11-C10-C8-C9
31	b	605	CLA	C11-C10-C8-C9
31	b	608	CLA	C11-C10-C8-C9
31	b	610	CLA	C11-C12-C13-C14
31	b	612	CLA	C11-C10-C8-C9
31	b	616	CLA	C11-C10-C8-C9
31	c	508	CLA	C11-C12-C13-C14
31	d	402	CLA	C14-C13-C15-C16
31	d	404	CLA	C11-C10-C8-C9
31	d	405	CLA	C11-C10-C8-C9
31	g	602	CLA	C11-C10-C8-C9
31	g	602	CLA	C11-C12-C13-C14
31	g	611	CLA	C11-C10-C8-C9
31	r	609	CLA	C11-C10-C8-C9
31	r	613	CLA	C14-C13-C15-C16
31	s	602	CLA	C11-C10-C8-C9
31	s	604	CLA	C11-C10-C8-C9
31	s	611	CLA	C11-C12-C13-C14
31	s	614	CLA	C11-C12-C13-C14
31	y	612	CLA	C11-C10-C8-C9
46	w	502	DGD	C4D-C5D-C6D-O5D
31	n	603	CLA	O1D-CGD-O2D-CED
41	A	409	LMG	C2-C1-O1-C7
41	J	102	LMG	C2-C1-O1-C7
41	K	102	LMG	C2-C1-O1-C7
41	j	102	LMG	C2-C1-O1-C7
41	v	101	LMG	C2-C1-O1-C7
41	w	501	LMG	C2-C1-O1-C7
32	14	615	LHG	O2-C2-C3-O3
32	16	616	LHG	O2-C2-C3-O3
32	S	617	LHG	O2-C2-C3-O3
32	a	401	LHG	O2-C2-C3-O3
32	s	617	LHG	O2-C2-C3-O3
30	6	609	CHL	O1A-CGA-O2A-C1
30	R	606	CHL	O1A-CGA-O2A-C1
31	2	604	CLA	O1A-CGA-O2A-C1
31	3	602	CLA	O1A-CGA-O2A-C1
31	5	604	CLA	O1A-CGA-O2A-C1
31	6	602	CLA	O1A-CGA-O2A-C1
31	N	604	CLA	O1A-CGA-O2A-C1
31	b	612	CLA	O1A-CGA-O2A-C1
31	b	616	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	N	604	CLA	CBD-CGD-O2D-CED
30	g	608	CHL	O1D-CGD-O2D-CED
30	s	608	CHL	O1D-CGD-O2D-CED
31	11	602	CLA	O1D-CGD-O2D-CED
31	N	603	CLA	O1D-CGD-O2D-CED
33	12	614	LUT	C11-C12-C13-C20
33	15	614	LUT	C11-C12-C13-C20
39	J	101	BCR	C37-C22-C23-C24
39	j	101	BCR	C37-C22-C23-C24
33	12	614	LUT	C11-C12-C13-C14
33	15	614	LUT	C11-C12-C13-C14
30	5	601	CHL	C2A-CAA-CBA-CGA
31	c	507	CLA	C2A-CAA-CBA-CGA
31	6	614	CLA	O1D-CGD-O2D-CED
32	Y	617	LHG	C26-C27-C28-C29
30	11	608	CHL	O1A-CGA-O2A-C1
30	14	609	CHL	O1A-CGA-O2A-C1
31	13	602	CLA	O1A-CGA-O2A-C1
31	A	402	CLA	O1A-CGA-O2A-C1
31	B	612	CLA	O1A-CGA-O2A-C1
31	R	602	CLA	O1A-CGA-O2A-C1
31	a	403	CLA	O1A-CGA-O2A-C1
31	c	507	CLA	O1A-CGA-O2A-C1
31	n	603	CLA	O1A-CGA-O2A-C1
30	13	605	CHL	CBD-CGD-O2D-CED
31	y	613	CLA	CBD-CGD-O2D-CED
40	D	411	SQD	O47-C45-C46-O48
31	b	614	CLA	CBA-CGA-O2A-C1
31	g	611	CLA	CBA-CGA-O2A-C1
31	n	610	CLA	CBA-CGA-O2A-C1
32	s	617	LHG	C24-C23-O8-C6
30	13	607	CHL	C5-C6-C7-C8
30	Y	607	CHL	C15-C16-C17-C18
30	y	607	CHL	C15-C16-C17-C18
30	y	601	CHL	C8-C10-C11-C12
31	B	606	CLA	C5-C6-C7-C8
31	C	507	CLA	C15-C16-C17-C18
41	B	622	LMG	C28-C29-C30-C31
32	y	616	LHG	C13-C14-C15-C16
30	r	606	CHL	O1D-CGD-O2D-CED
31	3	612	CLA	O1D-CGD-O2D-CED
31	6	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	11	611	CLA	O1D-CGD-O2D-CED
31	S	603	CLA	O1D-CGD-O2D-CED
31	g	614	CLA	O1D-CGD-O2D-CED
31	n	614	CLA	O1D-CGD-O2D-CED
30	2	606	CHL	CBD-CGD-O2D-CED
32	n	616	LHG	C28-C29-C30-C31
31	Y	602	CLA	C2C-C3C-CAC-CBC
30	2	609	CHL	C5-C6-C7-C8
30	R	606	CHL	C8-C10-C11-C12
31	3	604	CLA	C13-C15-C16-C17
31	4	610	CLA	C15-C16-C17-C18
31	B	614	CLA	C10-C11-C12-C13
31	C	507	CLA	C10-C11-C12-C13
31	S	614	CLA	C15-C16-C17-C18
31	Y	613	CLA	C10-C11-C12-C13
31	c	514	CLA	C15-C16-C17-C18
31	s	602	CLA	C15-C16-C17-C18
32	N	616	LHG	O1-C1-C2-O2
32	n	616	LHG	O1-C1-C2-O2
30	16	607	CHL	C3-C5-C6-C7
30	11	605	CHL	O1D-CGD-O2D-CED
31	14	613	CLA	O1D-CGD-O2D-CED
31	N	613	CLA	O1A-CGA-O2A-C1
31	c	502	CLA	O1A-CGA-O2A-C1
31	16	610	CLA	C5-C6-C7-C8
31	B	610	CLA	C15-C16-C17-C18
31	Y	603	CLA	C5-C6-C7-C8
31	c	504	CLA	C15-C16-C17-C18
31	y	613	CLA	C10-C11-C12-C13
31	y	602	CLA	C2C-C3C-CAC-CBC
30	4	601	CHL	C11-C10-C8-C7
30	13	606	CHL	C11-C10-C8-C7
30	16	606	CHL	C11-C10-C8-C7
30	16	607	CHL	C11-C10-C8-C7
30	N	609	CHL	C11-C10-C8-C7
30	N	607	CHL	C12-C13-C15-C16
30	n	609	CHL	C11-C10-C8-C7
30	n	607	CHL	C12-C13-C15-C16
30	s	606	CHL	C11-C10-C8-C7
31	6	611	CLA	C11-C10-C8-C7
31	14	610	CLA	C11-C12-C13-C15
31	A	402	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	B	611	CLA	C11-C10-C8-C7
31	C	509	CLA	C11-C10-C8-C7
31	S	610	CLA	C11-C10-C8-C7
31	S	611	CLA	C11-C10-C8-C7
31	a	403	CLA	C11-C10-C8-C7
31	b	611	CLA	C11-C10-C8-C7
31	b	613	CLA	C11-C10-C8-C7
31	c	509	CLA	C11-C10-C8-C7
31	r	613	CLA	C11-C12-C13-C15
31	s	610	CLA	C11-C10-C8-C7
31	s	611	CLA	C11-C10-C8-C7
31	s	614	CLA	C11-C10-C8-C7
30	4	601	CHL	CBA-CGA-O2A-C1
32	a	414	LHG	C24-C23-O8-C6
42	a	410	PL9	C25-C24-C26-C27
31	6	604	CLA	C13-C15-C16-C17
31	13	610	CLA	C5-C6-C7-C8
31	G	610	CLA	C15-C16-C17-C18
31	S	611	CLA	C5-C6-C7-C8
31	3	613	CLA	O1D-CGD-O2D-CED
31	16	602	CLA	O1D-CGD-O2D-CED
34	y	624	NEX	C13-C14-C15-C35
30	5	608	CHL	O1D-CGD-O2D-CED
30	y	606	CHL	O1D-CGD-O2D-CED
31	4	610	CLA	C3-C5-C6-C7
31	R	610	CLA	C3-C5-C6-C7
31	b	613	CLA	C5-C6-C7-C8
31	b	613	CLA	C8-C10-C11-C12
31	d	404	CLA	C15-C16-C17-C18
31	s	611	CLA	C15-C16-C17-C18
31	s	614	CLA	C10-C11-C12-C13
32	3	617	LHG	C17-C18-C19-C20
32	n	616	LHG	C7-C8-C9-C10
32	y	618	LHG	C7-C8-C9-C10
30	N	609	CHL	O1A-CGA-O2A-C1
30	S	608	CHL	O1A-CGA-O2A-C1
31	C	502	CLA	O1A-CGA-O2A-C1
31	C	507	CLA	O1A-CGA-O2A-C1
31	Y	611	CLA	O1A-CGA-O2A-C1
31	b	606	CLA	O1A-CGA-O2A-C1
31	n	615	CLA	O1A-CGA-O2A-C1
31	y	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	12	613	CLA	CBD-CGD-O2D-CED
31	B	604	CLA	CBD-CGD-O2D-CED
31	b	604	CLA	CBD-CGD-O2D-CED
30	11	608	CHL	O1D-CGD-O2D-CED
31	y	613	CLA	O1D-CGD-O2D-CED
30	2	609	CHL	C10-C11-C12-C13
30	3	609	CHL	C15-C16-C17-C18
30	4	609	CHL	C8-C10-C11-C12
30	13	609	CHL	C10-C11-C12-C13
30	14	609	CHL	C5-C6-C7-C8
30	16	606	CHL	C10-C11-C12-C13
30	S	606	CHL	C8-C10-C11-C12
30	Y	606	CHL	C8-C10-C11-C12
30	Y	606	CHL	C15-C16-C17-C18
31	6	602	CLA	C10-C11-C12-C13
31	6	610	CLA	C10-C11-C12-C13
31	6	612	CLA	C5-C6-C7-C8
31	12	603	CLA	C5-C6-C7-C8
31	14	610	CLA	C8-C10-C11-C12
31	16	611	CLA	C8-C10-C11-C12
31	B	602	CLA	C10-C11-C12-C13
31	C	508	CLA	C13-C15-C16-C17
31	C	514	CLA	C10-C11-C12-C13
31	Y	602	CLA	C8-C10-C11-C12
31	Y	602	CLA	C10-C11-C12-C13
31	Y	611	CLA	C15-C16-C17-C18
31	b	602	CLA	C10-C11-C12-C13
31	b	610	CLA	C15-C16-C17-C18
31	c	507	CLA	C10-C11-C12-C13
31	c	508	CLA	C13-C15-C16-C17
31	c	512	CLA	C15-C16-C17-C18
31	c	514	CLA	C10-C11-C12-C13
31	g	611	CLA	C15-C16-C17-C18
31	n	610	CLA	C5-C6-C7-C8
31	y	611	CLA	C15-C16-C17-C18
30	2	601	CHL	C2A-CAA-CBA-CGA
30	2	609	CHL	C2A-CAA-CBA-CGA
30	3	601	CHL	C2A-CAA-CBA-CGA
30	4	609	CHL	C2A-CAA-CBA-CGA
30	11	606	CHL	C2A-CAA-CBA-CGA
30	12	605	CHL	C2A-CAA-CBA-CGA
30	13	608	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	16	608	CHL	C2A-CAA-CBA-CGA
30	G	607	CHL	C2A-CAA-CBA-CGA
30	N	608	CHL	C2A-CAA-CBA-CGA
30	g	607	CHL	C2A-CAA-CBA-CGA
31	1	611	CLA	C2A-CAA-CBA-CGA
31	1	613	CLA	C2A-CAA-CBA-CGA
31	1	614	CLA	C2A-CAA-CBA-CGA
31	4	613	CLA	C2A-CAA-CBA-CGA
31	4	614	CLA	C2A-CAA-CBA-CGA
31	6	614	CLA	C2A-CAA-CBA-CGA
31	11	613	CLA	C2A-CAA-CBA-CGA
31	11	614	CLA	C2A-CAA-CBA-CGA
31	14	613	CLA	C2A-CAA-CBA-CGA
31	14	614	CLA	C2A-CAA-CBA-CGA
31	A	402	CLA	C2A-CAA-CBA-CGA
31	B	606	CLA	C2A-CAA-CBA-CGA
31	B	613	CLA	C2A-CAA-CBA-CGA
31	C	514	CLA	C2A-CAA-CBA-CGA
31	N	615	CLA	C2A-CAA-CBA-CGA
31	S	613	CLA	C2A-CAA-CBA-CGA
31	a	403	CLA	C2A-CAA-CBA-CGA
31	b	606	CLA	C2A-CAA-CBA-CGA
31	b	613	CLA	C2A-CAA-CBA-CGA
31	c	514	CLA	C2A-CAA-CBA-CGA
31	n	613	CLA	C2A-CAA-CBA-CGA
31	n	615	CLA	C2A-CAA-CBA-CGA
31	s	613	CLA	C2A-CAA-CBA-CGA
31	y	604	CLA	C2A-CAA-CBA-CGA
30	G	608	CHL	O1D-CGD-O2D-CED
30	1	609	CHL	C5-C6-C7-C8
30	5	609	CHL	C10-C11-C12-C13
30	6	601	CHL	C8-C10-C11-C12
30	13	601	CHL	C5-C6-C7-C8
30	14	601	CHL	C13-C15-C16-C17
30	14	601	CHL	C15-C16-C17-C18
30	N	605	CHL	C10-C11-C12-C13
30	Y	601	CHL	C8-C10-C11-C12
30	Y	606	CHL	C10-C11-C12-C13
30	r	606	CHL	C8-C10-C11-C12
30	y	609	CHL	C15-C16-C17-C18
31	1	613	CLA	C5-C6-C7-C8
31	13	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	14	613	CLA	C5-C6-C7-C8
31	A	404	CLA	C15-C16-C17-C18
31	B	610	CLA	C13-C15-C16-C17
31	B	613	CLA	C5-C6-C7-C8
31	B	613	CLA	C8-C10-C11-C12
31	C	506	CLA	C15-C16-C17-C18
31	C	507	CLA	C5-C6-C7-C8
31	C	508	CLA	C10-C11-C12-C13
31	R	610	CLA	C5-C6-C7-C8
31	R	610	CLA	C10-C11-C12-C13
31	Y	603	CLA	C10-C11-C12-C13
31	Y	610	CLA	C5-C6-C7-C8
31	a	404	CLA	C15-C16-C17-C18
31	b	610	CLA	C13-C15-C16-C17
31	b	612	CLA	C15-C16-C17-C18
31	b	614	CLA	C10-C11-C12-C13
31	c	507	CLA	C15-C16-C17-C18
31	g	611	CLA	C5-C6-C7-C8
31	g	613	CLA	C10-C11-C12-C13
31	r	609	CLA	C5-C6-C7-C8
31	s	604	CLA	C15-C16-C17-C18
31	s	611	CLA	C13-C15-C16-C17
31	y	610	CLA	C5-C6-C7-C8
32	11	615	LHG	C7-C8-C9-C10
32	N	616	LHG	C23-C24-C25-C26
36	B	620	3PH	C31-C32-C33-C34
30	n	608	CHL	O1A-CGA-O2A-C1
31	3	610	CLA	O1A-CGA-O2A-C1
31	15	602	CLA	O1A-CGA-O2A-C1
31	c	512	CLA	O1A-CGA-O2A-C1
31	c	513	CLA	O1A-CGA-O2A-C1
32	14	615	LHG	O10-C23-O8-C6
30	2	607	CHL	C3-C5-C6-C7
30	5	607	CHL	C3-C5-C6-C7
30	14	601	CHL	C3-C5-C6-C7
31	14	603	CLA	C3-C5-C6-C7
31	D	405	CLA	C3-C5-C6-C7
31	C	512	CLA	CBD-CGD-O2D-CED
40	D	411	SQD	O5-C1-O6-C44
40	d	412	SQD	O5-C1-O6-C44
46	C	517	DGD	O6D-C1D-O3G-C3G
46	c	517	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
31	14	602	CLA	O1D-CGD-O2D-CED
30	4	601	CHL	C10-C11-C12-C13
30	6	609	CHL	C5-C6-C7-C8
30	15	608	CHL	C8-C10-C11-C12
30	G	609	CHL	C5-C6-C7-C8
30	N	609	CHL	C15-C16-C17-C18
30	N	607	CHL	C8-C10-C11-C12
30	S	606	CHL	C15-C16-C17-C18
30	n	607	CHL	C8-C10-C11-C12
31	1	602	CLA	C10-C11-C12-C13
31	3	602	CLA	C10-C11-C12-C13
31	3	610	CLA	C10-C11-C12-C13
31	3	611	CLA	C10-C11-C12-C13
31	4	602	CLA	C5-C6-C7-C8
31	6	611	CLA	C10-C11-C12-C13
31	11	613	CLA	C5-C6-C7-C8
31	13	611	CLA	C5-C6-C7-C8
31	13	611	CLA	C10-C11-C12-C13
31	14	610	CLA	C15-C16-C17-C18
31	15	609	CLA	C5-C6-C7-C8
31	B	603	CLA	C5-C6-C7-C8
31	B	608	CLA	C10-C11-C12-C13
31	B	611	CLA	C13-C15-C16-C17
31	B	612	CLA	C15-C16-C17-C18
31	B	614	CLA	C8-C10-C11-C12
31	C	506	CLA	C10-C11-C12-C13
31	C	511	CLA	C15-C16-C17-C18
31	C	512	CLA	C15-C16-C17-C18
31	D	404	CLA	C15-C16-C17-C18
31	D	405	CLA	C15-C16-C17-C18
31	G	602	CLA	C5-C6-C7-C8
31	G	611	CLA	C15-C16-C17-C18
31	N	613	CLA	C5-C6-C7-C8
31	R	602	CLA	C10-C11-C12-C13
31	R	603	CLA	C10-C11-C12-C13
31	R	608	CLA	C13-C15-C16-C17
31	S	604	CLA	C15-C16-C17-C18
31	S	610	CLA	C15-C16-C17-C18
31	b	603	CLA	C5-C6-C7-C8
31	b	607	CLA	C15-C16-C17-C18
31	b	608	CLA	C10-C11-C12-C13
31	b	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	b	614	CLA	C8-C10-C11-C12
31	c	507	CLA	C5-C6-C7-C8
31	c	508	CLA	C10-C11-C12-C13
31	s	602	CLA	C10-C11-C12-C13
31	y	612	CLA	C8-C10-C11-C12
46	C	517	DGD	O6D-C5D-C6D-O5D
46	c	517	DGD	O6D-C5D-C6D-O5D
32	A	414	LHG	O2-C2-C3-O3
32	G	615	LHG	O2-C2-C3-O3
32	a	414	LHG	O2-C2-C3-O3
32	g	615	LHG	O2-C2-C3-O3
32	r	621	LHG	O2-C2-C3-O3
32	y	616	LHG	O2-C2-C3-O3
30	12	607	CHL	CBA-CGA-O2A-C1
30	15	607	CHL	CBA-CGA-O2A-C1
30	r	606	CHL	CBA-CGA-O2A-C1
31	12	603	CLA	CBA-CGA-O2A-C1
31	15	602	CLA	CBA-CGA-O2A-C1
31	a	407	CLA	CBA-CGA-O2A-C1
30	16	601	CHL	O1A-CGA-O2A-C1
30	N	608	CHL	O1A-CGA-O2A-C1
31	6	614	CLA	O1A-CGA-O2A-C1
31	14	610	CLA	O1A-CGA-O2A-C1
31	Y	612	CLA	O1A-CGA-O2A-C1
31	y	612	CLA	O1A-CGA-O2A-C1
32	d	408	LHG	C7-C8-C9-C10
32	s	617	LHG	C23-C24-C25-C26
30	Y	609	CHL	C15-C16-C17-C18
31	14	602	CLA	C8-C10-C11-C12
31	14	611	CLA	C5-C6-C7-C8
31	16	611	CLA	C13-C15-C16-C17
31	N	611	CLA	C10-C11-C12-C13
31	Y	610	CLA	C10-C11-C12-C13
31	Y	612	CLA	C8-C10-C11-C12
31	c	511	CLA	C15-C16-C17-C18
31	n	602	CLA	C13-C15-C16-C17
31	r	608	CLA	C15-C16-C17-C18
31	s	610	CLA	C15-C16-C17-C18
31	C	513	CLA	C3-C5-C6-C7
31	11	613	CLA	O1D-CGD-O2D-CED
31	13	613	CLA	O1D-CGD-O2D-CED
31	15	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	G	601	CHL	C5-C6-C7-C8
31	3	612	CLA	C5-C6-C7-C8
31	14	610	CLA	C10-C11-C12-C13
31	B	604	CLA	C15-C16-C17-C18
31	b	606	CLA	C5-C6-C7-C8
31	c	506	CLA	C15-C16-C17-C18
31	d	404	CLA	C8-C10-C11-C12
31	d	405	CLA	C15-C16-C17-C18
31	r	609	CLA	C10-C11-C12-C13
31	n	603	CLA	CBD-CGD-O2D-CED
30	n	609	CHL	O1A-CGA-O2A-C1
30	13	608	CHL	O1D-CGD-O2D-CED
30	16	608	CHL	O1D-CGD-O2D-CED
31	4	604	CLA	O1D-CGD-O2D-CED
31	12	609	CLA	O1D-CGD-O2D-CED
31	G	613	CLA	O1D-CGD-O2D-CED
31	g	613	CLA	O1D-CGD-O2D-CED
32	L	102	LHG	C12-C13-C14-C15
30	3	609	CHL	C5-C6-C7-C8
30	n	609	CHL	C15-C16-C17-C18
31	14	611	CLA	C10-C11-C12-C13
31	16	603	CLA	C8-C10-C11-C12
31	B	605	CLA	C10-C11-C12-C13
31	C	503	CLA	C15-C16-C17-C18
31	C	512	CLA	C10-C11-C12-C13
31	R	609	CLA	C5-C6-C7-C8
31	Y	613	CLA	C15-C16-C17-C18
31	c	503	CLA	C13-C15-C16-C17
31	n	602	CLA	C5-C6-C7-C8
31	s	610	CLA	C10-C11-C12-C13
30	16	601	CHL	CBA-CGA-O2A-C1
31	1	603	CLA	CBA-CGA-O2A-C1
31	b	616	CLA	CBA-CGA-O2A-C1
30	16	605	CHL	CBD-CGD-O2D-CED
30	G	608	CHL	CBD-CGD-O2D-CED
31	N	603	CLA	CBD-CGD-O2D-CED
32	c	521	LHG	C8-C7-O7-C5
32	s	621	LHG	C27-C28-C29-C30
30	5	607	CHL	O1A-CGA-O2A-C1
31	C	513	CLA	O1A-CGA-O2A-C1
31	R	610	CLA	O1A-CGA-O2A-C1
32	s	617	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
31	r	601	CLA	O1D-CGD-O2D-CED
32	3	617	LHG	C7-C8-C9-C10
31	13	602	CLA	C13-C15-C16-C17
31	13	603	CLA	C10-C11-C12-C13
31	c	506	CLA	C10-C11-C12-C13
31	s	602	CLA	C3-C5-C6-C7
31	6	604	CLA	CBD-CGD-O2D-CED
32	S	621	LHG	C27-C28-C29-C30
32	l	102	LHG	C12-C13-C14-C15
30	6	601	CHL	C5-C6-C7-C8
31	A	402	CLA	C13-C15-C16-C17
31	a	403	CLA	C13-C15-C16-C17
31	b	615	CLA	C8-C10-C11-C12
32	a	414	LHG	O10-C23-O8-C6
32	A	413	LHG	C31-C32-C33-C34
32	c	521	LHG	O9-C7-O7-C5
32	6	617	LHG	C1-C2-C3-O3
32	A	414	LHG	C1-C2-C3-O3
32	a	414	LHG	C1-C2-C3-O3
30	6	606	CHL	C2A-CAA-CBA-CGA
31	3	614	CLA	C2A-CAA-CBA-CGA
31	5	611	CLA	C2A-CAA-CBA-CGA
30	11	609	CHL	CBA-CGA-O2A-C1
30	n	601	CHL	CBA-CGA-O2A-C1
31	3	602	CLA	CBA-CGA-O2A-C1
31	A	403	CLA	CBA-CGA-O2A-C1
31	G	611	CLA	CBA-CGA-O2A-C1
31	b	604	CLA	CBA-CGA-O2A-C1
31	c	512	CLA	CBA-CGA-O2A-C1
31	n	603	CLA	CBA-CGA-O2A-C1
32	Y	618	LHG	C33-C34-C35-C36
30	3	607	CHL	C10-C11-C12-C13
30	4	609	CHL	C15-C16-C17-C18
30	5	609	CHL	C15-C16-C17-C18
30	6	601	CHL	C10-C11-C12-C13
30	6	607	CHL	C5-C6-C7-C8
30	16	601	CHL	C5-C6-C7-C8
30	Y	607	CHL	C5-C6-C7-C8
30	y	606	CHL	C15-C16-C17-C18
31	3	604	CLA	C10-C11-C12-C13
31	3	610	CLA	C5-C6-C7-C8
31	3	611	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	6	604	CLA	C15-C16-C17-C18
31	12	602	CLA	C5-C6-C7-C8
31	14	610	CLA	C13-C15-C16-C17
31	16	611	CLA	C10-C11-C12-C13
31	B	602	CLA	C15-C16-C17-C18
31	B	604	CLA	C5-C6-C7-C8
31	B	613	CLA	C10-C11-C12-C13
31	B	615	CLA	C8-C10-C11-C12
31	b	602	CLA	C15-C16-C17-C18
31	b	613	CLA	C10-C11-C12-C13
31	c	505	CLA	C5-C6-C7-C8
31	c	509	CLA	C10-C11-C12-C13
31	d	405	CLA	C10-C11-C12-C13
31	y	610	CLA	C10-C11-C12-C13
31	4	614	CLA	CBD-CGD-O2D-CED
31	c	512	CLA	CBD-CGD-O2D-CED
31	g	610	CLA	CBD-CGD-O2D-CED
31	r	603	CLA	O1D-CGD-O2D-CED
30	4	609	CHL	C10-C11-C12-C13
30	N	606	CHL	C5-C6-C7-C8
31	3	604	CLA	C15-C16-C17-C18
31	3	612	CLA	C10-C11-C12-C13
31	3	613	CLA	C5-C6-C7-C8
31	6	610	CLA	C5-C6-C7-C8
31	16	603	CLA	C5-C6-C7-C8
31	A	402	CLA	C15-C16-C17-C18
31	C	509	CLA	C10-C11-C12-C13
31	N	602	CLA	C13-C15-C16-C17
31	N	603	CLA	C8-C10-C11-C12
31	N	603	CLA	C10-C11-C12-C13
31	N	610	CLA	C5-C6-C7-C8
31	b	605	CLA	C5-C6-C7-C8
31	b	605	CLA	C10-C11-C12-C13
31	c	509	CLA	C8-C10-C11-C12
32	1	615	LHG	C26-C27-C28-C29
41	D	414	LMG	C15-C16-C17-C18
41	d	415	LMG	C15-C16-C17-C18
31	4	612	CLA	O1A-CGA-O2A-C1
30	R	606	CHL	O1D-CGD-O2D-CED
31	3	614	CLA	O1D-CGD-O2D-CED
30	6	607	CHL	C10-C11-C12-C13
30	6	609	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	13	606	CHL	C8-C10-C11-C12
30	N	607	CHL	C5-C6-C7-C8
30	s	606	CHL	C15-C16-C17-C18
30	y	607	CHL	C5-C6-C7-C8
31	2	603	CLA	C5-C6-C7-C8
31	11	610	CLA	C5-C6-C7-C8
31	A	404	CLA	C8-C10-C11-C12
31	B	609	CLA	C5-C6-C7-C8
31	B	610	CLA	C10-C11-C12-C13
31	S	610	CLA	C10-C11-C12-C13
31	b	609	CLA	C5-C6-C7-C8
31	b	610	CLA	C10-C11-C12-C13
31	b	612	CLA	C10-C11-C12-C13
31	b	612	CLA	C13-C15-C16-C17
31	n	602	CLA	C8-C10-C11-C12
30	Y	605	CHL	CBA-CGA-O2A-C1
31	B	609	CLA	CBA-CGA-O2A-C1
31	d	402	CLA	CBA-CGA-O2A-C1
32	G	615	LHG	C7-C8-C9-C10
30	4	609	CHL	C4-C3-C5-C6
42	a	410	PL9	C30-C29-C31-C32
31	g	603	CLA	C2-C3-C5-C6
31	12	602	CLA	O1D-CGD-O2D-CED
31	R	603	CLA	O1D-CGD-O2D-CED
31	6	613	CLA	C5-C6-C7-C8
31	B	605	CLA	C5-C6-C7-C8
31	C	509	CLA	C8-C10-C11-C12
31	S	611	CLA	C15-C16-C17-C18
31	a	403	CLA	C15-C16-C17-C18
30	14	608	CHL	C1-C2-C3-C5
30	R	607	CHL	C1-C2-C3-C4
31	2	610	CLA	C1-C2-C3-C4
31	3	614	CLA	C1-C2-C3-C5
31	4	604	CLA	C1-C2-C3-C5
31	4	611	CLA	C1-C2-C3-C5
31	5	610	CLA	C1-C2-C3-C4
31	5	613	CLA	C1-C2-C3-C5
31	6	614	CLA	C1-C2-C3-C5
31	6	615	CLA	C1-C2-C3-C5
31	11	611	CLA	C1-C2-C3-C5
31	G	604	CLA	C1-C2-C3-C4
31	g	604	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
30	16	605	CHL	C3-C5-C6-C7
32	C	521	LHG	C8-C7-O7-C5
32	R	621	LHG	C8-C7-O7-C5
31	N	603	CLA	C6-C7-C8-C9
31	15	603	CLA	O1D-CGD-O2D-CED
32	C	521	LHG	O9-C7-O7-C5
32	R	621	LHG	O9-C7-O7-C5
40	D	411	SQD	C2-C1-O6-C44
40	d	412	SQD	C2-C1-O6-C44
41	b	621	LMG	C2-C1-O1-C7
46	C	517	DGD	C2D-C1D-O3G-C3G
46	C	517	DGD	C2E-C1E-O5D-C6D
46	c	517	DGD	C2D-C1D-O3G-C3G
46	c	517	DGD	C2E-C1E-O5D-C6D
31	d	404	CLA	C13-C15-C16-C17
31	y	615	CLA	O1D-CGD-O2D-CED
32	D	412	LHG	O2-C2-C3-O3
32	d	413	LHG	O2-C2-C3-O3
32	n	616	LHG	O2-C2-C3-O3
30	r	605	CHL	CBA-CGA-O2A-C1
31	6	602	CLA	CBA-CGA-O2A-C1
31	b	609	CLA	CBA-CGA-O2A-C1
31	N	602	CLA	C16-C17-C18-C20
31	c	502	CLA	C16-C17-C18-C20
31	c	514	CLA	C16-C17-C18-C19
31	g	602	CLA	C16-C17-C18-C20
32	a	413	LHG	C31-C32-C33-C34
31	c	509	CLA	C2C-C3C-CAC-CBC
31	c	512	CLA	C10-C11-C12-C13
31	c	506	CLA	O1A-CGA-O2A-C1
32	11	615	LHG	C13-C14-C15-C16
32	c	521	LHG	C25-C26-C27-C28
30	4	609	CHL	C13-C15-C16-C17
31	3	612	CLA	C15-C16-C17-C18
31	B	612	CLA	C13-C15-C16-C17
31	G	611	CLA	C5-C6-C7-C8
32	D	412	LHG	C5-C4-O6-P
32	d	413	LHG	C5-C4-O6-P
31	C	509	CLA	C2C-C3C-CAC-CBC
39	J	101	BCR	C21-C22-C23-C24
39	j	101	BCR	C21-C22-C23-C24
31	6	615	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	11	610	CLA	O1A-CGA-O2A-C1
31	g	604	CLA	O1A-CGA-O2A-C1
31	y	603	CLA	O1A-CGA-O2A-C1
30	11	608	CHL	C2A-CAA-CBA-CGA
30	14	601	CHL	C2A-CAA-CBA-CGA
30	15	606	CHL	C2A-CAA-CBA-CGA
30	S	606	CHL	C2A-CAA-CBA-CGA
30	r	605	CHL	C2A-CAA-CBA-CGA
30	s	606	CHL	C2A-CAA-CBA-CGA
31	2	613	CLA	C2A-CAA-CBA-CGA
31	3	604	CLA	C2A-CAA-CBA-CGA
31	3	610	CLA	C2A-CAA-CBA-CGA
31	3	613	CLA	C2A-CAA-CBA-CGA
31	4	604	CLA	C2A-CAA-CBA-CGA
31	5	604	CLA	C2A-CAA-CBA-CGA
31	6	604	CLA	C2A-CAA-CBA-CGA
31	C	513	CLA	C2A-CAA-CBA-CGA
31	G	613	CLA	C2A-CAA-CBA-CGA
31	Y	604	CLA	C2A-CAA-CBA-CGA
31	r	614	CLA	C2A-CAA-CBA-CGA
30	2	609	CHL	C8-C10-C11-C12
30	16	606	CHL	C8-C10-C11-C12
30	g	601	CHL	C5-C6-C7-C8
31	14	610	CLA	C5-C6-C7-C8
31	A	406	CLA	C5-C6-C7-C8
31	B	612	CLA	C10-C11-C12-C13
32	1	615	LHG	O1-C1-C2-C3
32	6	616	LHG	O1-C1-C2-C3
32	A	411	LHG	O1-C1-C2-C3
32	L	102	LHG	O1-C1-C2-C3
32	S	621	LHG	O1-C1-C2-C3
32	S	617	LHG	O1-C1-C2-C3
32	d	409	LHG	O1-C1-C2-C3
32	l	102	LHG	O1-C1-C2-C3
32	r	618	LHG	O1-C1-C2-C3
32	s	621	LHG	O1-C1-C2-C3
32	s	617	LHG	O1-C1-C2-C3
36	b	623	3PH	C31-C32-C33-C34
30	6	601	CHL	O2A-C1-C2-C3
31	A	403	CLA	O2A-C1-C2-C3
31	d	402	CLA	O2A-C1-C2-C3
38	D	402	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	Y	605	CHL	C6-C7-C8-C9
31	13	603	CLA	C11-C12-C13-C14
31	14	603	CLA	C6-C7-C8-C10
31	B	607	CLA	C16-C17-C18-C20
31	G	602	CLA	C16-C17-C18-C19
31	G	602	CLA	C16-C17-C18-C20
31	a	403	CLA	C16-C17-C18-C19
32	R	621	LHG	C17-C18-C19-C20
31	B	611	CLA	O1D-CGD-O2D-CED
31	6	612	CLA	O1A-CGA-O2A-C1
31	r	602	CLA	O1A-CGA-O2A-C1
30	13	601	CHL	C3-C5-C6-C7
31	G	611	CLA	C3-C5-C6-C7
31	Y	615	CLA	C3-C5-C6-C7
31	G	613	CLA	C15-C16-C17-C18
31	y	612	CLA	C15-C16-C17-C18
40	d	414	SQD	O5-C1-O6-C44
41	b	621	LMG	O6-C1-O1-C7
30	n	608	CHL	CBD-CGD-O2D-CED
32	y	617	LHG	C8-C7-O7-C5
32	r	621	LHG	C17-C18-C19-C20
30	11	601	CHL	C10-C11-C12-C13
31	y	603	CLA	C10-C11-C12-C13
31	B	615	CLA	C2-C3-C5-C6
31	N	613	CLA	C2-C3-C5-C6
31	R	609	CLA	C2-C3-C5-C6
31	b	615	CLA	C2-C3-C5-C6
30	11	609	CHL	O1D-CGD-O2D-CED
32	c	521	LHG	C30-C31-C32-C33
31	2	612	CLA	O1D-CGD-O2D-CED
31	b	611	CLA	O1D-CGD-O2D-CED
31	3	610	CLA	CBA-CGA-O2A-C1
31	A	406	CLA	CBA-CGA-O2A-C1
31	C	502	CLA	CBA-CGA-O2A-C1
31	N	613	CLA	CBA-CGA-O2A-C1
31	c	502	CLA	CBA-CGA-O2A-C1
30	13	609	CHL	C5-C6-C7-C8
31	15	602	CLA	C8-C10-C11-C12
31	N	603	CLA	C5-C6-C7-C8
30	14	607	CHL	CBD-CGD-O2D-CED
32	D	408	LHG	C7-C8-C9-C10
31	15	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	R	601	CLA	O1D-CGD-O2D-CED
31	N	613	CLA	C2C-C3C-CAC-CBC
31	11	610	CLA	C6-C7-C8-C10
31	14	604	CLA	C6-C7-C8-C9
31	14	610	CLA	C16-C17-C18-C20
31	s	604	CLA	C16-C17-C18-C20
32	13	616	LHG	C32-C33-C34-C35
30	13	601	CHL	O1A-CGA-O2A-C1
31	1	611	CLA	O1A-CGA-O2A-C1
31	B	609	CLA	O1A-CGA-O2A-C1
31	b	609	CLA	O1A-CGA-O2A-C1
31	3	612	CLA	C13-C15-C16-C17
31	16	602	CLA	C13-C15-C16-C17
31	B	603	CLA	C10-C11-C12-C13
31	B	607	CLA	C10-C11-C12-C13
31	y	611	CLA	C10-C11-C12-C13
30	1	607	CHL	O1D-CGD-O2D-CED
32	Y	617	LHG	C29-C30-C31-C32
32	3	617	LHG	C25-C26-C27-C28
32	S	617	LHG	C24-C25-C26-C27
32	Y	618	LHG	C34-C35-C36-C37
32	Y	617	LHG	C11-C10-C9-C8
32	c	521	LHG	C33-C34-C35-C36
32	y	617	LHG	C32-C33-C34-C35
31	11	604	CLA	O1D-CGD-O2D-CED
31	Y	612	CLA	O1D-CGD-O2D-CED
32	1	615	LHG	C7-C8-C9-C10
30	6	609	CHL	C13-C15-C16-C17
31	Y	602	CLA	C13-C15-C16-C17
32	3	617	LHG	C27-C28-C29-C30
32	A	414	LHG	C28-C29-C30-C31
32	Y	617	LHG	C9-C10-C11-C12
41	d	410	LMG	C11-C12-C13-C14
31	3	604	CLA	O1A-CGA-O2A-C1
31	14	611	CLA	O1A-CGA-O2A-C1
32	4	615	LHG	C24-C25-C26-C27
32	a	413	LHG	C27-C28-C29-C30
32	y	617	LHG	C26-C27-C28-C29
46	c	519	DGD	C2B-C3B-C4B-C5B
32	y	617	LHG	O9-C7-O7-C5
32	1	615	LHG	O1-C1-C2-O2
32	4	615	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
32	6	616	LHG	O1-C1-C2-O2
32	A	411	LHG	O1-C1-C2-O2
32	A	414	LHG	O1-C1-C2-O2
32	D	412	LHG	O1-C1-C2-O2
32	G	615	LHG	O1-C1-C2-O2
32	a	414	LHG	O1-C1-C2-O2
32	d	413	LHG	O1-C1-C2-O2
32	g	615	LHG	O1-C1-C2-O2
32	1	615	LHG	C11-C12-C13-C14
32	6	617	LHG	C12-C13-C14-C15
32	d	408	LHG	C13-C14-C15-C16
30	3	608	CHL	O1D-CGD-O2D-CED
30	16	609	CHL	O1D-CGD-O2D-CED
31	N	612	CLA	O1D-CGD-O2D-CED
30	2	609	CHL	C15-C16-C17-C18
31	6	611	CLA	C15-C16-C17-C18
31	5	604	CLA	C4B-C3B-CAB-CBB
31	12	602	CLA	C4B-C3B-CAB-CBB
31	R	608	CLA	C4B-C3B-CAB-CBB
31	n	610	CLA	C4B-C3B-CAB-CBB
31	r	602	CLA	C4B-C3B-CAB-CBB
31	r	608	CLA	C4B-C3B-CAB-CBB
32	3	617	LHG	C12-C13-C14-C15
30	1	609	CHL	C6-C7-C8-C9
31	4	610	CLA	C16-C17-C18-C20
31	11	610	CLA	C6-C7-C8-C9
31	A	402	CLA	C16-C17-C18-C19
31	A	402	CLA	C16-C17-C18-C20
31	G	610	CLA	C16-C17-C18-C19
31	G	610	CLA	C16-C17-C18-C20
31	S	614	CLA	C16-C17-C18-C20
31	Y	613	CLA	C16-C17-C18-C20
31	a	403	CLA	C16-C17-C18-C20
31	g	610	CLA	C16-C17-C18-C20
31	s	604	CLA	C16-C17-C18-C19
31	y	612	CLA	O1D-CGD-O2D-CED
30	Y	609	CHL	O1A-CGA-O2A-C1
31	6	604	CLA	O1A-CGA-O2A-C1
31	y	615	CLA	O1A-CGA-O2A-C1
30	3	608	CHL	C2A-CAA-CBA-CGA
30	13	607	CHL	C2A-CAA-CBA-CGA
31	2	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	5	613	CLA	C2A-CAA-CBA-CGA
31	6	615	CLA	C2A-CAA-CBA-CGA
31	A	403	CLA	C2A-CAA-CBA-CGA
31	C	502	CLA	C2A-CAA-CBA-CGA
31	c	513	CLA	C2A-CAA-CBA-CGA
31	g	604	CLA	C2A-CAA-CBA-CGA
31	g	613	CLA	C2A-CAA-CBA-CGA
31	s	615	CLA	C2A-CAA-CBA-CGA
30	G	609	CHL	C8-C10-C11-C12
30	R	606	CHL	C15-C16-C17-C18
31	13	610	CLA	C15-C16-C17-C18
31	13	611	CLA	C15-C16-C17-C18
31	16	610	CLA	C15-C16-C17-C18
31	D	405	CLA	C10-C11-C12-C13
31	S	602	CLA	C15-C16-C17-C18
31	b	605	CLA	C15-C16-C17-C18
31	n	603	CLA	C10-C11-C12-C13
31	r	609	CLA	C15-C16-C17-C18
31	r	610	CLA	C10-C11-C12-C13
31	s	604	CLA	C8-C10-C11-C12
32	16	616	LHG	C33-C34-C35-C36
30	3	605	CHL	C6-C7-C8-C10
30	15	608	CHL	C11-C10-C8-C7
31	3	611	CLA	C11-C10-C8-C7
31	13	611	CLA	C11-C12-C13-C15
31	R	610	CLA	C11-C10-C8-C7
31	Y	610	CLA	C6-C7-C8-C10
31	b	613	CLA	C11-C12-C13-C15
31	y	610	CLA	C6-C7-C8-C10
38	a	406	PHO	C12-C13-C15-C16
41	D	410	LMG	C12-C13-C14-C15
46	C	519	DGD	C2B-C3B-C4B-C5B
32	c	521	LHG	C23-C24-C25-C26
36	T	101	3PH	C21-C22-C23-C24
31	5	604	CLA	CBA-CGA-O2A-C1
30	3	607	CHL	C15-C16-C17-C18
30	r	606	CHL	C15-C16-C17-C18
31	B	603	CLA	C15-C16-C17-C18
31	n	604	CLA	C5-C6-C7-C8
32	A	413	LHG	C27-C28-C29-C30
32	D	409	LHG	C25-C26-C27-C28
32	N	616	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	y	617	LHG	C10-C11-C12-C13
41	c	520	LMG	C39-C40-C41-C42
31	5	613	CLA	O1A-CGA-O2A-C1
30	n	607	CHL	C3-C5-C6-C7
30	y	605	CHL	C3-C5-C6-C7
31	c	513	CLA	C3-C5-C6-C7
31	d	405	CLA	C3-C5-C6-C7
30	3	605	CHL	C3A-C2A-CAA-CBA
30	3	606	CHL	C3A-C2A-CAA-CBA
30	3	607	CHL	C3A-C2A-CAA-CBA
30	5	606	CHL	C3A-C2A-CAA-CBA
30	6	605	CHL	C3A-C2A-CAA-CBA
30	6	607	CHL	C3A-C2A-CAA-CBA
30	11	607	CHL	C3A-C2A-CAA-CBA
30	13	606	CHL	C3A-C2A-CAA-CBA
30	14	607	CHL	C3A-C2A-CAA-CBA
30	15	605	CHL	C3A-C2A-CAA-CBA
30	16	601	CHL	C3A-C2A-CAA-CBA
30	16	606	CHL	C3A-C2A-CAA-CBA
30	G	605	CHL	C3A-C2A-CAA-CBA
30	G	607	CHL	C3A-C2A-CAA-CBA
30	R	606	CHL	C3A-C2A-CAA-CBA
30	S	606	CHL	C3A-C2A-CAA-CBA
30	Y	607	CHL	C3A-C2A-CAA-CBA
30	Y	601	CHL	C3A-C2A-CAA-CBA
30	g	605	CHL	C3A-C2A-CAA-CBA
30	g	607	CHL	C3A-C2A-CAA-CBA
30	n	605	CHL	C3A-C2A-CAA-CBA
30	r	606	CHL	C3A-C2A-CAA-CBA
30	s	606	CHL	C3A-C2A-CAA-CBA
30	y	607	CHL	C3A-C2A-CAA-CBA
30	y	601	CHL	C3A-C2A-CAA-CBA
31	1	611	CLA	C3A-C2A-CAA-CBA
31	2	604	CLA	C3A-C2A-CAA-CBA
31	3	604	CLA	C3A-C2A-CAA-CBA
31	3	611	CLA	C3A-C2A-CAA-CBA
31	3	614	CLA	C3A-C2A-CAA-CBA
31	4	612	CLA	C3A-C2A-CAA-CBA
31	6	604	CLA	C3A-C2A-CAA-CBA
31	6	611	CLA	C3A-C2A-CAA-CBA
31	11	604	CLA	C3A-C2A-CAA-CBA
31	11	610	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	11	612	CLA	C3A-C2A-CAA-CBA
31	12	604	CLA	C3A-C2A-CAA-CBA
31	12	612	CLA	C3A-C2A-CAA-CBA
31	12	613	CLA	C3A-C2A-CAA-CBA
31	13	604	CLA	C3A-C2A-CAA-CBA
31	13	610	CLA	C3A-C2A-CAA-CBA
31	13	614	CLA	C3A-C2A-CAA-CBA
31	14	610	CLA	C3A-C2A-CAA-CBA
31	15	612	CLA	C3A-C2A-CAA-CBA
31	16	604	CLA	C3A-C2A-CAA-CBA
31	16	610	CLA	C3A-C2A-CAA-CBA
31	16	614	CLA	C3A-C2A-CAA-CBA
31	B	601	CLA	C3A-C2A-CAA-CBA
31	B	608	CLA	C3A-C2A-CAA-CBA
31	N	611	CLA	C3A-C2A-CAA-CBA
31	N	612	CLA	C3A-C2A-CAA-CBA
31	R	610	CLA	C3A-C2A-CAA-CBA
31	R	612	CLA	C3A-C2A-CAA-CBA
31	S	604	CLA	C3A-C2A-CAA-CBA
31	b	601	CLA	C3A-C2A-CAA-CBA
31	b	608	CLA	C3A-C2A-CAA-CBA
31	n	610	CLA	C3A-C2A-CAA-CBA
31	n	612	CLA	C3A-C2A-CAA-CBA
31	r	614	CLA	C3A-C2A-CAA-CBA
31	s	615	CLA	C3A-C2A-CAA-CBA
31	Y	615	CLA	O1D-CGD-O2D-CED
41	c	520	LMG	C35-C36-C37-C38
30	15	608	CHL	C5-C6-C7-C8
30	G	601	CHL	C15-C16-C17-C18
30	g	609	CHL	C5-C6-C7-C8
30	n	605	CHL	C10-C11-C12-C13
31	2	602	CLA	C5-C6-C7-C8
31	15	602	CLA	C10-C11-C12-C13
31	16	602	CLA	C15-C16-C17-C18
31	B	605	CLA	C15-C16-C17-C18
31	B	614	CLA	C13-C15-C16-C17
31	D	404	CLA	C10-C11-C12-C13
31	N	604	CLA	C5-C6-C7-C8
31	S	604	CLA	C8-C10-C11-C12
31	S	609	CLA	C5-C6-C7-C8
31	Y	611	CLA	C10-C11-C12-C13
31	Y	612	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	Y	612	CLA	C15-C16-C17-C18
31	b	603	CLA	C10-C11-C12-C13
31	b	603	CLA	C15-C16-C17-C18
31	y	613	CLA	C15-C16-C17-C18
31	13	603	CLA	O1D-CGD-O2D-CED
41	c	520	LMG	C41-C42-C43-C44
30	Y	605	CHL	C6-C7-C8-C10
31	14	604	CLA	C6-C7-C8-C10
31	N	602	CLA	C16-C17-C18-C19
31	S	602	CLA	C16-C17-C18-C20
31	g	602	CLA	C16-C17-C18-C19
31	g	610	CLA	C16-C17-C18-C19
31	y	613	CLA	C16-C17-C18-C20
31	11	611	CLA	O1A-CGA-O2A-C1
31	C	506	CLA	O1A-CGA-O2A-C1
31	c	514	CLA	O1A-CGA-O2A-C1
32	13	616	LHG	C9-C10-C11-C12
32	A	413	LHG	C28-C29-C30-C31
32	d	413	LHG	C9-C10-C11-C12
32	Y	618	LHG	C24-C25-C26-C27
32	s	617	LHG	C31-C32-C33-C34
32	y	618	LHG	C25-C26-C27-C28
41	b	621	LMG	C12-C13-C14-C15
30	R	606	CHL	CBA-CGA-O2A-C1
31	4	613	CLA	CBA-CGA-O2A-C1
31	R	602	CLA	CBA-CGA-O2A-C1
31	Y	614	CLA	CBA-CGA-O2A-C1
31	c	506	CLA	CBA-CGA-O2A-C1
32	a	411	LHG	C27-C28-C29-C30
32	n	616	LHG	C11-C12-C13-C14
44	B	623	STE	C3-C4-C5-C6
44	b	622	STE	C2-C3-C4-C5
32	4	615	LHG	C7-C8-C9-C10
44	b	622	STE	C1-C2-C3-C4
30	6	605	CHL	C10-C11-C12-C13
30	g	601	CHL	C15-C16-C17-C18
31	a	404	CLA	C8-C10-C11-C12
32	6	617	LHG	C15-C16-C17-C18
32	C	521	LHG	C31-C32-C33-C34
32	D	412	LHG	C9-C10-C11-C12
32	l	102	LHG	C10-C11-C12-C13
32	y	618	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
41	C	520	LMG	C39-C40-C41-C42
30	y	609	CHL	O1A-CGA-O2A-C1
31	S	609	CLA	O1A-CGA-O2A-C1
31	r	601	CLA	O1A-CGA-O2A-C1
30	11	606	CHL	O1A-CGA-O2A-C1
32	L	102	LHG	C10-C11-C12-C13
32	R	619	LHG	C28-C29-C30-C31
41	C	520	LMG	C35-C36-C37-C38
41	C	520	LMG	C41-C42-C43-C44
31	5	612	CLA	O1D-CGD-O2D-CED
31	16	604	CLA	O1D-CGD-O2D-CED
32	r	618	LHG	C9-C10-C11-C12
41	d	411	LMG	C34-C35-C36-C37
30	16	606	CHL	C5-C6-C7-C8
32	3	617	LHG	C11-C10-C9-C8
32	A	413	LHG	C26-C27-C28-C29
32	Y	617	LHG	C10-C11-C12-C13
32	r	618	LHG	C24-C25-C26-C27
31	B	614	CLA	C16-C17-C18-C20
31	n	611	CLA	C11-C12-C13-C14
32	a	414	LHG	C23-C24-C25-C26
30	N	601	CHL	O1A-CGA-O2A-C1
31	5	604	CLA	C2B-C3B-CAB-CBB
31	12	602	CLA	C2B-C3B-CAB-CBB
31	13	610	CLA	C2B-C3B-CAB-CBB
31	15	602	CLA	C2B-C3B-CAB-CBB
31	B	616	CLA	C2B-C3B-CAB-CBB
31	N	604	CLA	C2B-C3B-CAB-CBB
31	S	604	CLA	C2B-C3B-CAB-CBB
31	b	616	CLA	C2B-C3B-CAB-CBB
31	n	604	CLA	C2B-C3B-CAB-CBB
31	n	610	CLA	C2B-C3B-CAB-CBB
31	r	602	CLA	C2B-C3B-CAB-CBB
39	B	617	BCR	C1-C6-C7-C8
39	D	406	BCR	C23-C24-C25-C30
39	b	617	BCR	C1-C6-C7-C8
39	d	406	BCR	C23-C24-C25-C30
31	1	614	CLA	CBD-CGD-O2D-CED
31	3	613	CLA	CBD-CGD-O2D-CED
31	G	610	CLA	CBD-CGD-O2D-CED
31	n	604	CLA	CBD-CGD-O2D-CED
32	d	408	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
30	g	609	CHL	CBA-CGA-O2A-C1
31	y	611	CLA	CBA-CGA-O2A-C1
32	y	618	LHG	C24-C23-O8-C6
32	y	617	LHG	C5-C4-O6-P
32	A	411	LHG	C11-C10-C9-C8
31	n	602	CLA	C2C-C3C-CAC-CBC
31	13	602	CLA	O1D-CGD-O2D-CED
30	1	609	CHL	C2A-CAA-CBA-CGA
30	6	608	CHL	C2A-CAA-CBA-CGA
30	12	606	CHL	C2A-CAA-CBA-CGA
30	r	607	CHL	C2A-CAA-CBA-CGA
31	6	613	CLA	C2A-CAA-CBA-CGA
31	12	610	CLA	C2A-CAA-CBA-CGA
31	15	610	CLA	C2A-CAA-CBA-CGA
31	B	602	CLA	C2A-CAA-CBA-CGA
31	b	602	CLA	C2A-CAA-CBA-CGA
31	c	502	CLA	C2A-CAA-CBA-CGA
31	y	612	CLA	C5-C6-C7-C8
32	4	615	LHG	C11-C12-C13-C14
32	14	615	LHG	C25-C26-C27-C28
30	11	606	CHL	CBD-CGD-O2D-CED
31	r	602	CLA	C2C-C3C-CAC-CBC
31	s	609	CLA	C2C-C3C-CAC-CBC
31	15	603	CLA	C4-C3-C5-C6
42	A	410	PL9	C25-C24-C26-C27
42	A	410	PL9	C30-C29-C31-C32
42	D	407	PL9	C12-C11-C9-C10
31	B	609	CLA	C15-C16-C17-C18
31	R	608	CLA	C8-C10-C11-C12
31	13	610	CLA	C2-C3-C5-C6
31	15	609	CLA	C2-C3-C5-C6
31	s	610	CLA	C2-C3-C5-C6
42	a	410	PL9	C23-C24-C26-C27
42	a	410	PL9	C28-C29-C31-C32
31	13	603	CLA	C11-C12-C13-C15
31	c	502	CLA	C16-C17-C18-C19
30	1	607	CHL	CBA-CGA-O2A-C1
30	6	606	CHL	CBA-CGA-O2A-C1
30	13	609	CHL	CBA-CGA-O2A-C1
30	14	609	CHL	CBA-CGA-O2A-C1
31	3	613	CLA	CBA-CGA-O2A-C1
31	6	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	C	506	CLA	CBA-CGA-O2A-C1
31	Y	611	CLA	CBA-CGA-O2A-C1
30	2	609	CHL	O1A-CGA-O2A-C1
30	N	609	CHL	C6-C7-C8-C9
30	N	607	CHL	C11-C10-C8-C9
30	R	606	CHL	C11-C12-C13-C14
31	C	507	CLA	C11-C12-C13-C14
31	R	608	CLA	C14-C13-C15-C16
32	11	615	LHG	C10-C11-C12-C13
32	G	615	LHG	C16-C17-C18-C19
32	S	617	LHG	C11-C10-C9-C8
32	Y	616	LHG	C24-C25-C26-C27
32	y	618	LHG	C34-C35-C36-C37
31	s	604	CLA	C10-C11-C12-C13
32	a	413	LHG	C28-C29-C30-C31
32	a	414	LHG	C11-C10-C9-C8
41	J	102	LMG	C22-C23-C24-C25
41	j	102	LMG	C22-C23-C24-C25
32	11	615	LHG	C27-C28-C29-C30
32	y	616	LHG	C24-C25-C26-C27
41	B	621	LMG	C2-C1-O1-C7
41	B	622	LMG	C2-C1-O1-C7
31	B	611	CLA	C15-C16-C17-C18
31	b	611	CLA	C15-C16-C17-C18
31	d	402	CLA	C15-C16-C17-C18
32	13	616	LHG	C11-C10-C9-C8
32	16	616	LHG	C11-C10-C9-C8
43	H	101	LNL	C15-C16-C17-C18
43	R	620	LNL	C15-C16-C17-C18
43	Y	619	LNL	C15-C16-C17-C18
43	c	523	LNL	C15-C16-C17-C18
43	y	619	LNL	C15-C16-C17-C18
32	3	617	LHG	C31-C32-C33-C34
46	c	519	DGD	C7B-C8B-C9B-CAB
31	6	604	CLA	C10-C11-C12-C13
31	B	614	CLA	C15-C16-C17-C18
31	C	504	CLA	C10-C11-C12-C13
31	b	609	CLA	C15-C16-C17-C18
30	n	608	CHL	CBA-CGA-O2A-C1
31	13	613	CLA	CBA-CGA-O2A-C1
31	y	612	CLA	CBA-CGA-O2A-C1
31	c	514	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
32	14	615	LHG	C8-C7-O7-C5
32	D	408	LHG	C8-C7-O7-C5
31	B	616	CLA	O1A-CGA-O2A-C1
31	G	613	CLA	O1A-CGA-O2A-C1
32	l	102	LHG	C23-C24-C25-C26
40	L	101	SQD	C7-C8-C9-C10
44	B	623	STE	C15-C16-C17-C18
31	14	603	CLA	C5-C6-C7-C8
32	A	411	LHG	C12-C13-C14-C15
32	A	411	LHG	C17-C18-C19-C20
43	H	101	LNL	C2-C3-C4-C5
31	Y	602	CLA	C4C-C3C-CAC-CBC
41	K	102	LMG	C32-C33-C34-C35
43	h	101	LNL	C2-C3-C4-C5
30	Y	601	CHL	C10-C11-C12-C13
30	Y	601	CHL	C15-C16-C17-C18
31	4	603	CLA	C5-C6-C7-C8
31	A	402	CLA	C10-C11-C12-C13
31	a	403	CLA	C10-C11-C12-C13
31	b	608	CLA	C15-C16-C17-C18
32	G	615	LHG	C24-C25-C26-C27
32	S	617	LHG	C32-C33-C34-C35
41	s	616	LMG	C13-C14-C15-C16
31	g	611	CLA	C3-C5-C6-C7
40	L	101	SQD	C45-C44-O6-C1
40	l	101	SQD	C45-C44-O6-C1
32	11	615	LHG	C14-C15-C16-C17
30	s	608	CHL	C2A-CAA-CBA-CGA
31	c	512	CLA	C2A-CAA-CBA-CGA
31	6	604	CLA	C16-C17-C18-C19
31	6	604	CLA	C16-C17-C18-C20
31	11	602	CLA	C11-C12-C13-C14
31	11	603	CLA	C6-C7-C8-C9
31	14	610	CLA	C16-C17-C18-C19
31	B	614	CLA	C16-C17-C18-C19
31	C	507	CLA	C16-C17-C18-C19
31	b	614	CLA	C16-C17-C18-C19
31	b	614	CLA	C16-C17-C18-C20
32	C	521	LHG	C29-C30-C31-C32
32	n	616	LHG	C15-C16-C17-C18
30	1	601	CHL	C4-C3-C5-C6
30	6	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	g	601	CHL	C4-C3-C5-C6
42	d	407	PL9	C12-C11-C9-C10
31	C	509	CLA	O1A-CGA-O2A-C1
49	F	101	HEM	C2C-C3C-CAC-CBC
49	f	101	HEM	C2C-C3C-CAC-CBC
31	b	610	CLA	C5-C6-C7-C8
31	g	613	CLA	C15-C16-C17-C18
32	a	414	LHG	C31-C32-C33-C34
46	C	517	DGD	C6A-C7A-C8A-C9A
46	c	517	DGD	C6A-C7A-C8A-C9A
31	y	603	CLA	O1D-CGD-O2D-CED
31	R	612	CLA	CBD-CGD-O2D-CED
32	Y	618	LHG	C17-C18-C19-C20
31	Y	615	CLA	O1A-CGA-O2A-C1
31	c	509	CLA	O1A-CGA-O2A-C1
31	R	603	CLA	C13-C15-C16-C17
31	Y	611	CLA	C5-C6-C7-C8
31	b	604	CLA	C10-C11-C12-C13
32	y	617	LHG	C29-C30-C31-C32
32	L	102	LHG	C23-C24-C25-C26
32	a	411	LHG	C23-C24-C25-C26
32	A	414	LHG	O6-C4-C5-O7
32	S	621	LHG	O6-C4-C5-O7
32	s	621	LHG	O6-C4-C5-O7
31	Y	603	CLA	O1D-CGD-O2D-CED
30	3	605	CHL	C15-C16-C17-C18
31	A	403	CLA	C15-C16-C17-C18
31	C	504	CLA	C8-C10-C11-C12
31	y	602	CLA	C10-C11-C12-C13
31	y	611	CLA	C5-C6-C7-C8
49	F	101	HEM	C4B-C3B-CAB-CBB
49	f	101	HEM	C4B-C3B-CAB-CBB
31	4	610	CLA	C16-C17-C18-C19
31	11	603	CLA	C6-C7-C8-C10
31	C	514	CLA	O1A-CGA-O2A-C1
31	G	611	CLA	O1A-CGA-O2A-C1
31	g	613	CLA	O1A-CGA-O2A-C1
32	a	411	LHG	C25-C26-C27-C28
32	a	413	LHG	C12-C13-C14-C15
32	y	618	LHG	C30-C31-C32-C33
36	B	624	3PH	C31-C32-C33-C34
31	b	614	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	N	601	CHL	O1D-CGD-O2D-CED
32	s	621	LHG	C9-C10-C11-C12
41	C	520	LMG	O6-C5-C6-O5
41	c	520	LMG	O6-C5-C6-O5
46	C	517	DGD	O6E-C5E-C6E-O5E
46	c	517	DGD	O6E-C5E-C6E-O5E
30	11	601	CHL	C3-C5-C6-C7
30	16	601	CHL	C3-C5-C6-C7
31	C	507	CLA	C3-C5-C6-C7
30	1	607	CHL	CBD-CGD-O2D-CED
32	n	616	LHG	O7-C5-C6-O8
36	B	624	3PH	O21-C2-C3-O31
41	b	621	LMG	O7-C8-C9-O8
46	C	518	DGD	O1G-C1G-C2G-O2G
46	c	518	DGD	O1G-C1G-C2G-O2G
31	y	602	CLA	C4C-C3C-CAC-CBC
31	a	403	CLA	CBA-CGA-O2A-C1
32	14	615	LHG	C18-C19-C20-C21
46	C	519	DGD	C7B-C8B-C9B-CAB
31	s	602	CLA	C5-C6-C7-C8
32	A	413	LHG	C12-C13-C14-C15
31	3	615	CLA	O1A-CGA-O2A-C1
31	B	607	CLA	C16-C17-C18-C19
31	B	610	CLA	C5-C6-C7-C8
31	C	502	CLA	C10-C11-C12-C13
31	b	614	CLA	C13-C15-C16-C17
32	S	621	LHG	C25-C26-C27-C28
32	d	408	LHG	C14-C15-C16-C17
32	s	621	LHG	C33-C34-C35-C36
31	Y	615	CLA	C4-C3-C5-C6
31	Y	604	CLA	C4-C3-C5-C6
31	12	609	CLA	C3-C5-C6-C7
30	5	609	CHL	C2-C3-C5-C6
31	14	613	CLA	C2-C3-C5-C6
31	y	604	CLA	C2-C3-C5-C6
42	A	410	PL9	C28-C29-C31-C32
32	14	615	LHG	O9-C7-O7-C5
32	D	408	LHG	O9-C7-O7-C5
32	3	617	LHG	C1-C2-C3-O3
32	r	621	LHG	C1-C2-C3-O3
31	B	607	CLA	C5-C6-C7-C8
31	G	611	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	D	408	LHG	O2-C2-C3-O3
32	Y	616	LHG	O2-C2-C3-O3
32	g	615	LHG	C24-C25-C26-C27
30	12	601	CHL	C2A-CAA-CBA-CGA
30	15	601	CHL	C2A-CAA-CBA-CGA
30	R	607	CHL	C2A-CAA-CBA-CGA
31	2	604	CLA	C2A-CAA-CBA-CGA
31	5	602	CLA	C2A-CAA-CBA-CGA
31	6	610	CLA	C2A-CAA-CBA-CGA
31	12	609	CLA	C2A-CAA-CBA-CGA
31	N	613	CLA	C2A-CAA-CBA-CGA
31	Y	613	CLA	C2A-CAA-CBA-CGA
31	d	402	CLA	C2A-CAA-CBA-CGA
30	5	606	CHL	CBD-CGD-O2D-CED
30	S	606	CHL	CBD-CGD-O2D-CED
30	N	608	CHL	CBA-CGA-O2A-C1
31	A	402	CLA	CBA-CGA-O2A-C1
31	y	615	CLA	CBA-CGA-O2A-C1
32	r	619	LHG	C10-C11-C12-C13
30	s	606	CHL	C10-C11-C12-C13
30	11	606	CHL	CBA-CGA-O2A-C1
36	8	201	3PH	C22-C23-C24-C25
46	C	517	DGD	C8A-C9A-CAA-CBA
41	K	102	LMG	O6-C5-C6-O5
41	v	101	LMG	O6-C5-C6-O5
32	3	616	LHG	O1-C1-C2-O2
32	L	102	LHG	O1-C1-C2-O2
32	S	621	LHG	O1-C1-C2-O2
32	l	102	LHG	O1-C1-C2-O2
30	R	607	CHL	O1A-CGA-O2A-C1
31	S	614	CLA	O1A-CGA-O2A-C1
31	b	604	CLA	O1A-CGA-O2A-C1
31	s	614	CLA	O1A-CGA-O2A-C1
32	y	618	LHG	O10-C23-O8-C6
30	13	605	CHL	C3-C5-C6-C7
31	c	507	CLA	C3-C5-C6-C7
46	c	517	DGD	C8A-C9A-CAA-CBA
31	1	611	CLA	C1A-C2A-CAA-CBA
31	2	602	CLA	C1A-C2A-CAA-CBA
31	3	602	CLA	C1A-C2A-CAA-CBA
31	3	604	CLA	C1A-C2A-CAA-CBA
31	3	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	3	614	CLA	C1A-C2A-CAA-CBA
31	4	612	CLA	C1A-C2A-CAA-CBA
31	5	602	CLA	C1A-C2A-CAA-CBA
31	5	610	CLA	C1A-C2A-CAA-CBA
31	5	613	CLA	C1A-C2A-CAA-CBA
31	6	602	CLA	C1A-C2A-CAA-CBA
31	6	604	CLA	C1A-C2A-CAA-CBA
31	6	610	CLA	C1A-C2A-CAA-CBA
31	6	615	CLA	C1A-C2A-CAA-CBA
31	11	612	CLA	C1A-C2A-CAA-CBA
31	12	602	CLA	C1A-C2A-CAA-CBA
31	12	609	CLA	C1A-C2A-CAA-CBA
31	12	612	CLA	C1A-C2A-CAA-CBA
31	13	611	CLA	C1A-C2A-CAA-CBA
31	16	602	CLA	C1A-C2A-CAA-CBA
31	16	604	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C1A-C2A-CAA-CBA
31	B	611	CLA	C1A-C2A-CAA-CBA
31	G	610	CLA	C1A-C2A-CAA-CBA
31	G	614	CLA	C1A-C2A-CAA-CBA
31	N	612	CLA	C1A-C2A-CAA-CBA
31	R	609	CLA	C1A-C2A-CAA-CBA
31	R	612	CLA	C1A-C2A-CAA-CBA
31	R	613	CLA	C1A-C2A-CAA-CBA
31	S	615	CLA	C1A-C2A-CAA-CBA
31	a	407	CLA	C1A-C2A-CAA-CBA
31	c	512	CLA	C1A-C2A-CAA-CBA
31	g	610	CLA	C1A-C2A-CAA-CBA
31	g	611	CLA	C1A-C2A-CAA-CBA
31	g	614	CLA	C1A-C2A-CAA-CBA
31	n	602	CLA	C1A-C2A-CAA-CBA
31	n	611	CLA	C1A-C2A-CAA-CBA
31	n	612	CLA	C1A-C2A-CAA-CBA
31	r	612	CLA	C1A-C2A-CAA-CBA
31	r	613	CLA	C1A-C2A-CAA-CBA
31	r	614	CLA	C1A-C2A-CAA-CBA
31	s	604	CLA	C1A-C2A-CAA-CBA
31	s	610	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	C13-C15-C16-C17
31	c	511	CLA	C10-C11-C12-C13
32	6	617	LHG	C32-C33-C34-C35
32	A	414	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
31	S	604	CLA	C10-C11-C12-C13
31	b	601	CLA	C5-C6-C7-C8
32	A	414	LHG	O6-C4-C5-C6
32	R	619	LHG	O6-C4-C5-C6
32	S	621	LHG	O6-C4-C5-C6
32	Y	617	LHG	O6-C4-C5-C6
32	r	618	LHG	O6-C4-C5-C6
32	s	621	LHG	O6-C4-C5-C6
41	D	414	LMG	O6-C5-C6-O5
41	d	415	LMG	O6-C5-C6-O5
32	d	408	LHG	O9-C7-O7-C5
32	Y	617	LHG	C23-C24-C25-C26
30	3	607	CHL	C11-C10-C8-C7
30	4	609	CHL	C11-C10-C8-C7
30	4	609	CHL	C11-C12-C13-C15
30	6	601	CHL	C6-C7-C8-C10
30	6	601	CHL	C11-C10-C8-C7
30	6	605	CHL	C11-C10-C8-C7
30	14	601	CHL	C11-C10-C8-C7
30	N	606	CHL	C6-C7-C8-C10
30	R	606	CHL	C12-C13-C15-C16
30	r	606	CHL	C12-C13-C15-C16
30	s	606	CHL	C11-C12-C13-C15
30	s	606	CHL	C12-C13-C15-C16
31	14	610	CLA	C12-C13-C15-C16
31	16	611	CLA	C11-C10-C8-C7
31	A	404	CLA	C11-C10-C8-C7
31	B	602	CLA	C12-C13-C15-C16
31	B	605	CLA	C11-C10-C8-C7
31	B	613	CLA	C11-C12-C13-C15
31	B	613	CLA	C12-C13-C15-C16
31	C	508	CLA	C11-C10-C8-C7
31	C	510	CLA	C11-C10-C8-C7
31	D	404	CLA	C11-C10-C8-C7
31	G	602	CLA	C6-C7-C8-C10
31	G	602	CLA	C11-C10-C8-C7
31	N	602	CLA	C6-C7-C8-C10
31	N	602	CLA	C11-C10-C8-C7
31	R	610	CLA	C6-C7-C8-C10
31	Y	602	CLA	C6-C7-C8-C10
31	b	602	CLA	C12-C13-C15-C16
31	b	604	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	b	605	CLA	C11-C10-C8-C7
31	b	613	CLA	C12-C13-C15-C16
31	c	510	CLA	C11-C10-C8-C7
31	d	404	CLA	C11-C10-C8-C7
31	g	602	CLA	C11-C10-C8-C7
31	n	611	CLA	C6-C7-C8-C10
31	r	609	CLA	C12-C13-C15-C16
31	s	614	CLA	C6-C7-C8-C10
31	y	612	CLA	C11-C12-C13-C15
36	8	201	3PH	C36-C37-C38-C39
31	3	604	CLA	C16-C17-C18-C19
31	C	511	CLA	C16-C17-C18-C20
31	C	511	CLA	C10-C11-C12-C13
32	y	616	LHG	C28-C29-C30-C31
31	S	603	CLA	C3A-C2A-CAA-CBA
30	n	609	CHL	C13-C15-C16-C17
30	y	601	CHL	C15-C16-C17-C18
31	R	603	CLA	C15-C16-C17-C18
31	b	602	CLA	C13-C15-C16-C17
31	n	602	CLA	C10-C11-C12-C13
41	D	410	LMG	C10-C11-C12-C13
31	y	604	CLA	C4-C3-C5-C6
31	y	611	CLA	C4-C3-C5-C6
38	A	405	PHO	C4-C3-C5-C6
38	a	405	PHO	C4-C3-C5-C6
30	12	608	CHL	C2-C3-C5-C6
30	g	601	CHL	C2-C3-C5-C6
31	3	612	CLA	C2-C3-C5-C6
31	6	611	CLA	C2-C3-C5-C6
31	6	612	CLA	C2-C3-C5-C6
31	11	613	CLA	C2-C3-C5-C6
31	Y	615	CLA	C2-C3-C5-C6
31	Y	611	CLA	C2-C3-C5-C6
38	A	405	PHO	C2-C3-C5-C6
38	a	405	PHO	C2-C3-C5-C6
31	r	610	CLA	O1A-CGA-O2A-C1
41	b	621	LMG	O6-C5-C6-O5
32	Y	618	LHG	C32-C33-C34-C35
31	12	602	CLA	C10-C11-C12-C13
31	B	608	CLA	C15-C16-C17-C18
31	s	611	CLA	C10-C11-C12-C13
31	1	611	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
31	5	604	CLA	C1-C2-C3-C5
31	R	612	CLA	C1-C2-C3-C5
30	4	608	CHL	C2A-CAA-CBA-CGA
30	5	607	CHL	C2A-CAA-CBA-CGA
30	16	601	CHL	C2A-CAA-CBA-CGA
30	Y	601	CHL	C2A-CAA-CBA-CGA
31	13	613	CLA	C2A-CAA-CBA-CGA
31	N	611	CLA	C2A-CAA-CBA-CGA
31	y	613	CLA	C2A-CAA-CBA-CGA
30	3	607	CHL	C11-C10-C8-C9
30	14	601	CHL	C11-C10-C8-C9
30	N	607	CHL	C14-C13-C15-C16
30	n	606	CHL	C6-C7-C8-C9
31	B	610	CLA	C11-C10-C8-C9
31	B	613	CLA	C14-C13-C15-C16
31	C	504	CLA	C11-C10-C8-C9
31	G	602	CLA	C6-C7-C8-C9
31	R	609	CLA	C14-C13-C15-C16
31	R	610	CLA	C11-C10-C8-C9
31	S	610	CLA	C11-C12-C13-C14
31	b	606	CLA	C11-C10-C8-C9
31	b	610	CLA	C11-C10-C8-C9
31	b	613	CLA	C14-C13-C15-C16
31	g	613	CLA	C6-C7-C8-C9
31	n	611	CLA	C6-C7-C8-C9
31	r	609	CLA	C14-C13-C15-C16
31	r	613	CLA	C11-C12-C13-C14
31	s	610	CLA	C11-C12-C13-C14
31	s	614	CLA	C6-C7-C8-C9
31	y	602	CLA	C6-C7-C8-C9
36	T	101	3PH	C24-C25-C26-C27
30	11	609	CHL	C6-C7-C8-C10
32	D	412	LHG	C11-C12-C13-C14
32	a	413	LHG	C26-C27-C28-C29
30	5	607	CHL	O1D-CGD-O2D-CED
31	y	614	CLA	O1D-CGD-O2D-CED
30	11	608	CHL	CBA-CGA-O2A-C1
30	13	601	CHL	CBA-CGA-O2A-C1
30	N	607	CHL	CBA-CGA-O2A-C1
30	y	605	CHL	CBA-CGA-O2A-C1
31	Y	612	CLA	CBA-CGA-O2A-C1
31	g	604	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	R	621	LHG	C24-C23-O8-C6
32	g	615	LHG	C24-C23-O8-C6
32	11	615	LHG	C24-C25-C26-C27
41	d	411	LMG	C12-C13-C14-C15
31	4	603	CLA	O1D-CGD-O2D-CED
32	R	618	LHG	C9-C10-C11-C12
31	S	602	CLA	C10-C11-C12-C13
41	B	622	LMG	O6-C5-C6-O5
32	C	521	LHG	C4-C5-C6-O8
32	c	521	LHG	C4-C5-C6-O8
40	D	411	SQD	C44-C45-C46-O48
40	d	412	SQD	C44-C45-C46-O48
41	S	616	LMG	O1-C7-C8-C9
46	C	518	DGD	O1G-C1G-C2G-C3G
46	c	518	DGD	O1G-C1G-C2G-C3G
32	N	616	LHG	C24-C25-C26-C27
31	g	610	CLA	C10-C11-C12-C13
32	d	409	LHG	C27-C28-C29-C30
30	N	608	CHL	O1D-CGD-O2D-CED
30	5	609	CHL	CBA-CGA-O2A-C1
30	n	606	CHL	CBA-CGA-O2A-C1
30	s	608	CHL	CBA-CGA-O2A-C1
31	C	509	CLA	C11-C12-C13-C14
31	C	511	CLA	C16-C17-C18-C19
31	c	509	CLA	C11-C12-C13-C14
31	Y	615	CLA	C5-C6-C7-C8
32	a	414	LHG	C28-C29-C30-C31
32	y	617	LHG	C13-C14-C15-C16
41	D	410	LMG	O6-C5-C6-O5
30	15	608	CHL	O1D-CGD-O2D-CED
30	1	608	CHL	CHA-CBD-CGD-O2D
30	N	605	CHL	CHA-CBD-CGD-O2D
30	N	608	CHL	CHA-CBD-CGD-O2D
30	R	605	CHL	CHA-CBD-CGD-O2D
30	R	607	CHL	CHA-CBD-CGD-O2D
30	r	607	CHL	CHA-CBD-CGD-O2D
30	s	607	CHL	CHA-CBD-CGD-O1D
30	s	607	CHL	CHA-CBD-CGD-O2D
38	a	406	PHO	CHA-CBD-CGD-O1D
38	a	406	PHO	CHA-CBD-CGD-O2D
31	B	609	CLA	C10-C11-C12-C13
31	C	508	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	b	609	CLA	C10-C11-C12-C13
31	d	404	CLA	C10-C11-C12-C13
31	N	613	CLA	C3-C5-C6-C7
41	c	522	LMG	C28-C29-C30-C31
31	5	610	CLA	O1A-CGA-O2A-C1
31	A	404	CLA	O1A-CGA-O2A-C1
31	a	404	CLA	O1A-CGA-O2A-C1
32	G	615	LHG	C28-C29-C30-C31
31	R	608	CLA	C4-C3-C5-C6
31	Y	611	CLA	C4-C3-C5-C6
31	b	601	CLA	C4-C3-C5-C6
42	a	410	PL9	C45-C44-C46-C47
30	13	601	CHL	C2-C3-C5-C6
30	15	608	CHL	C2-C3-C5-C6
31	C	507	CLA	C2-C3-C5-C6
31	Y	604	CLA	C2-C3-C5-C6
31	y	611	CLA	C2-C3-C5-C6
30	3	609	CHL	C8-C10-C11-C12
30	s	606	CHL	C13-C15-C16-C17
31	B	611	CLA	C8-C10-C11-C12
31	R	609	CLA	C15-C16-C17-C18
31	b	611	CLA	C8-C10-C11-C12
31	r	603	CLA	C10-C11-C12-C13
32	n	616	LHG	C24-C25-C26-C27
32	S	621	LHG	C16-C17-C18-C19
41	d	410	LMG	O6-C5-C6-O5
31	g	611	CLA	O1A-CGA-O2A-C1
31	13	610	CLA	C8-C10-C11-C12
30	14	606	CHL	C2A-CAA-CBA-CGA
30	n	607	CHL	C2A-CAA-CBA-CGA
31	4	612	CLA	C2A-CAA-CBA-CGA
31	13	615	CLA	C2A-CAA-CBA-CGA
30	14	606	CHL	CBA-CGA-O2A-C1
31	c	510	CLA	C8-C10-C11-C12
31	11	611	CLA	CBA-CGA-O2A-C1
31	14	610	CLA	CBA-CGA-O2A-C1
31	14	611	CLA	CBA-CGA-O2A-C1
31	16	613	CLA	CBA-CGA-O2A-C1
31	Y	615	CLA	CBA-CGA-O2A-C1
31	12	609	CLA	O2A-C1-C2-C3
31	15	612	CLA	O2A-C1-C2-C3
31	r	614	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	G	615	LHG	C6-C5-O7-C7
32	16	616	LHG	C29-C30-C31-C32
31	16	610	CLA	C8-C10-C11-C12
31	B	615	CLA	C15-C16-C17-C18
31	N	602	CLA	C15-C16-C17-C18
31	S	610	CLA	C5-C6-C7-C8
31	s	610	CLA	C5-C6-C7-C8
32	C	521	LHG	C34-C35-C36-C37
32	g	615	LHG	C28-C29-C30-C31
32	y	618	LHG	C26-C27-C28-C29
40	A	408	SQD	C27-C28-C29-C30
40	a	409	SQD	C27-C28-C29-C30
30	1	607	CHL	C3C-C2C-CMC-OMC
30	2	606	CHL	C3C-C2C-CMC-OMC
30	3	607	CHL	C3C-C2C-CMC-OMC
30	6	607	CHL	C3C-C2C-CMC-OMC
30	11	608	CHL	C3C-C2C-CMC-OMC
30	11	609	CHL	C3C-C2C-CMC-OMC
30	14	605	CHL	C3C-C2C-CMC-OMC
30	14	607	CHL	C3C-C2C-CMC-OMC
30	14	609	CHL	C3C-C2C-CMC-OMC
30	G	605	CHL	C3C-C2C-CMC-OMC
30	G	606	CHL	C3C-C2C-CMC-OMC
30	N	601	CHL	C3C-C2C-CMC-OMC
30	R	605	CHL	C3C-C2C-CMC-OMC
30	S	606	CHL	C3C-C2C-CMC-OMC
30	Y	606	CHL	C3C-C2C-CMC-OMC
30	g	605	CHL	C3C-C2C-CMC-OMC
30	r	605	CHL	C3C-C2C-CMC-OMC
30	s	601	CHL	C3C-C2C-CMC-OMC
30	s	606	CHL	C3C-C2C-CMC-OMC
30	y	606	CHL	C3C-C2C-CMC-OMC
30	y	608	CHL	C3C-C2C-CMC-OMC
32	6	616	LHG	C9-C10-C11-C12
32	n	616	LHG	C23-C24-C25-C26
30	4	609	CHL	C3-C5-C6-C7
30	S	606	CHL	C13-C15-C16-C17
31	C	510	CLA	C8-C10-C11-C12
41	c	522	LMG	C22-C23-C24-C25
31	g	612	CLA	C2A-CAA-CBA-CGA
32	3	616	LHG	C9-C10-C11-C12
32	14	615	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	13	616	LHG	C1-C2-C3-O3
32	D	408	LHG	C1-C2-C3-O3
32	Y	616	LHG	C1-C2-C3-O3
32	Y	618	LHG	O6-C4-C5-O7
32	11	615	LHG	C11-C10-C9-C8
31	B	609	CLA	O1D-CGD-O2D-CED
31	5	613	CLA	CBA-CGA-O2A-C1
31	c	514	CLA	CBA-CGA-O2A-C1
30	y	606	CHL	CBD-CGD-O2D-CED
32	y	618	LHG	C12-C13-C14-C15
32	R	618	LHG	C24-C25-C26-C27
32	y	618	LHG	C16-C17-C18-C19
32	y	617	LHG	C9-C10-C11-C12
44	B	623	STE	C7-C8-C9-C10
30	15	608	CHL	C4-C3-C5-C6
31	16	610	CLA	C2-C3-C5-C6
31	B	611	CLA	C2-C3-C5-C6
31	b	601	CLA	C2-C3-C5-C6
31	b	611	CLA	C2-C3-C5-C6
38	D	402	PHO	C2-C3-C5-C6
32	s	617	LHG	C35-C36-C37-C38
32	g	615	LHG	C14-C15-C16-C17
32	n	616	LHG	C16-C17-C18-C19
31	3	604	CLA	C16-C17-C18-C20
32	y	617	LHG	C24-C25-C26-C27
41	D	410	LMG	C11-C12-C13-C14
32	13	616	LHG	C29-C30-C31-C32
32	n	616	LHG	C13-C14-C15-C16
41	C	522	LMG	C22-C23-C24-C25
32	3	617	LHG	O7-C5-C6-O8
32	R	618	LHG	O7-C5-C6-O8
32	Y	618	LHG	O7-C5-C6-O8
32	r	618	LHG	O7-C5-C6-O8
36	B	620	3PH	O21-C2-C3-O31
46	w	502	DGD	O1G-C1G-C2G-O2G
32	13	616	LHG	O2-C2-C3-O3
32	d	408	LHG	O2-C2-C3-O3
31	b	607	CLA	CBA-CGA-O2A-C1
31	r	602	CLA	CBA-CGA-O2A-C1
31	G	612	CLA	C2A-CAA-CBA-CGA
31	13	604	CLA	CAA-CBA-CGA-O2A
32	11	615	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
41	c	520	LMG	C12-C13-C14-C15
44	b	622	STE	C10-C11-C12-C13
32	N	616	LHG	C19-C20-C21-C22
46	C	519	DGD	O6D-C5D-C6D-O5D
46	c	519	DGD	O6D-C5D-C6D-O5D
30	n	606	CHL	C5-C6-C7-C8
41	d	415	LMG	C32-C33-C34-C35
30	15	608	CHL	O1A-CGA-O2A-C1
32	6	617	LHG	C7-C8-C9-C10
31	c	508	CLA	C15-C16-C17-C18
41	D	414	LMG	C32-C33-C34-C35
30	n	607	CHL	CBA-CGA-O2A-C1
31	6	615	CLA	CBA-CGA-O2A-C1
31	11	610	CLA	CBA-CGA-O2A-C1
31	16	602	CLA	CBA-CGA-O2A-C1
31	b	606	CLA	CBA-CGA-O2A-C1
31	g	613	CLA	CBA-CGA-O2A-C1
31	r	601	CLA	CBA-CGA-O2A-C1
32	Y	618	LHG	C24-C23-O8-C6
32	c	521	LHG	C35-C36-C37-C38
31	R	610	CLA	CAA-CBA-CGA-O2A
32	3	617	LHG	C10-C11-C12-C13
30	1	605	CHL	C1C-C2C-CMC-OMC
30	1	607	CHL	C1C-C2C-CMC-OMC
30	2	606	CHL	C1C-C2C-CMC-OMC
30	5	606	CHL	C1C-C2C-CMC-OMC
30	13	601	CHL	C1C-C2C-CMC-OMC
30	13	609	CHL	C1C-C2C-CMC-OMC
30	14	607	CHL	C1C-C2C-CMC-OMC
30	16	601	CHL	C1C-C2C-CMC-OMC
30	G	605	CHL	C1C-C2C-CMC-OMC
30	G	606	CHL	C1C-C2C-CMC-OMC
30	G	608	CHL	C1C-C2C-CMC-OMC
30	G	609	CHL	C1C-C2C-CMC-OMC
30	S	606	CHL	C1C-C2C-CMC-OMC
30	g	605	CHL	C1C-C2C-CMC-OMC
30	g	606	CHL	C1C-C2C-CMC-OMC
30	s	606	CHL	C1C-C2C-CMC-OMC
30	s	607	CHL	C1C-C2C-CMC-OMC
30	14	609	CHL	C2C-C3C-CAC-CBC
32	D	408	LHG	C13-C14-C15-C16
36	B	620	3PH	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
31	c	512	CLA	O1D-CGD-O2D-CED
32	d	409	LHG	C23-C24-C25-C26
32	r	618	LHG	C26-C27-C28-C29
41	C	520	LMG	C12-C13-C14-C15
30	g	609	CHL	C8-C10-C11-C12
31	C	507	CLA	C13-C15-C16-C17
31	b	615	CLA	C15-C16-C17-C18
31	r	608	CLA	C8-C10-C11-C12
33	15	614	LUT	C9-C10-C11-C12
31	R	610	CLA	C4-C3-C5-C6
31	R	613	CLA	C4-C3-C5-C6
31	c	507	CLA	C4-C3-C5-C6
31	r	610	CLA	C4-C3-C5-C6
38	a	406	PHO	C4-C3-C5-C6
42	D	407	PL9	C15-C14-C16-C17
42	d	407	PL9	C15-C14-C16-C17
32	Y	618	LHG	C35-C36-C37-C38
44	b	622	STE	C15-C16-C17-C18
31	s	611	CLA	C2-C3-C5-C6
32	14	615	LHG	C9-C10-C11-C12
32	Y	617	LHG	C13-C14-C15-C16
32	d	408	LHG	C30-C31-C32-C33
30	16	607	CHL	CBA-CGA-O2A-C1
31	G	613	CLA	CBA-CGA-O2A-C1
31	r	610	CLA	CBA-CGA-O2A-C1
31	4	613	CLA	C5-C6-C7-C8
32	Y	617	LHG	C7-C8-C9-C10
32	S	617	LHG	C33-C34-C35-C36
32	Y	618	LHG	C25-C26-C27-C28
32	a	401	LHG	C14-C15-C16-C17
32	S	621	LHG	C33-C34-C35-C36
32	y	616	LHG	C12-C13-C14-C15
32	D	409	LHG	O1-C1-C2-O2
32	s	621	LHG	O1-C1-C2-O2
32	s	617	LHG	O1-C1-C2-O2
30	4	609	CHL	C6-C7-C8-C9
30	13	606	CHL	C11-C10-C8-C9
30	16	609	CHL	C11-C10-C8-C9
30	G	601	CHL	C11-C12-C13-C14
30	N	605	CHL	C11-C10-C8-C9
30	N	609	CHL	C11-C10-C8-C9
30	g	609	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	n	609	CHL	C11-C10-C8-C9
30	s	606	CHL	C11-C10-C8-C9
30	s	606	CHL	C11-C12-C13-C14
31	4	610	CLA	C11-C10-C8-C9
31	14	602	CLA	C11-C10-C8-C9
31	14	610	CLA	C11-C12-C13-C14
31	A	402	CLA	C11-C10-C8-C9
31	B	606	CLA	C11-C10-C8-C9
31	B	616	CLA	C6-C7-C8-C9
31	C	502	CLA	C11-C10-C8-C9
31	C	510	CLA	C11-C10-C8-C9
31	G	602	CLA	C14-C13-C15-C16
31	N	602	CLA	C6-C7-C8-C9
31	R	602	CLA	C11-C10-C8-C9
31	R	608	CLA	C11-C12-C13-C14
31	Y	615	CLA	C6-C7-C8-C9
31	Y	602	CLA	C6-C7-C8-C9
31	a	403	CLA	C11-C10-C8-C9
31	b	616	CLA	C6-C7-C8-C9
31	c	510	CLA	C11-C10-C8-C9
31	g	602	CLA	C6-C7-C8-C9
31	s	610	CLA	C11-C10-C8-C9
32	a	414	LHG	C32-C33-C34-C35
46	w	502	DGD	C4B-C5B-C6B-C7B
31	6	603	CLA	C5-C6-C7-C8
31	16	611	CLA	C15-C16-C17-C18
31	S	602	CLA	C5-C6-C7-C8
31	a	407	CLA	C5-C6-C7-C8
32	Y	618	LHG	C5-C4-O6-P
32	Y	617	LHG	C5-C4-O6-P
32	d	413	LHG	C2-C3-O3-P
31	16	613	CLA	O1A-CGA-O2A-C1
31	11	614	CLA	C4B-C3B-CAB-CBB
31	B	611	CLA	C4B-C3B-CAB-CBB
31	R	602	CLA	C4B-C3B-CAB-CBB
31	Y	604	CLA	C4B-C3B-CAB-CBB
31	b	611	CLA	C4B-C3B-CAB-CBB
31	y	604	CLA	C4B-C3B-CAB-CBB
32	S	617	LHG	C25-C26-C27-C28
32	s	617	LHG	C25-C26-C27-C28
41	C	522	LMG	C28-C29-C30-C31
31	c	509	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	d	404	CLA	C16-C17-C18-C20
30	2	608	CHL	C2A-CAA-CBA-CGA
30	S	608	CHL	C2A-CAA-CBA-CGA
46	C	518	DGD	C2E-C1E-O5D-C6D
46	c	518	DGD	C2E-C1E-O5D-C6D
30	r	605	CHL	C5-C6-C7-C8
31	13	603	CLA	C8-C10-C11-C12
32	L	102	LHG	C29-C30-C31-C32
31	N	604	CLA	C3-C5-C6-C7
32	d	408	LHG	C23-C24-C25-C26
32	C	521	LHG	O6-C4-C5-C6
32	R	621	LHG	O6-C4-C5-C6
32	c	521	LHG	O6-C4-C5-C6
32	y	617	LHG	O6-C4-C5-C6
36	B	620	3PH	O11-C1-C2-C3
44	B	623	STE	C14-C15-C16-C17
30	n	601	CHL	O1D-CGD-O2D-CED
31	R	602	CLA	C2C-C3C-CAC-CBC
41	C	520	LMG	C32-C33-C34-C35
41	H	102	LMG	C12-C13-C14-C15
30	3	601	CHL	C11-C10-C8-C7
30	3	607	CHL	C11-C12-C13-C15
30	13	609	CHL	C6-C7-C8-C10
30	14	601	CHL	C12-C13-C15-C16
30	N	605	CHL	C11-C10-C8-C7
30	R	606	CHL	C11-C10-C8-C7
30	Y	601	CHL	C12-C13-C15-C16
30	r	606	CHL	C11-C10-C8-C7
31	4	610	CLA	C11-C10-C8-C7
31	6	610	CLA	C11-C10-C8-C7
31	6	611	CLA	C12-C13-C15-C16
31	14	602	CLA	C11-C10-C8-C7
31	16	603	CLA	C6-C7-C8-C10
31	B	606	CLA	C11-C10-C8-C7
31	B	608	CLA	C11-C10-C8-C7
31	B	610	CLA	C11-C10-C8-C7
31	B	612	CLA	C11-C10-C8-C7
31	B	612	CLA	C11-C12-C13-C15
31	B	615	CLA	C11-C10-C8-C7
31	B	616	CLA	C6-C7-C8-C10
31	R	602	CLA	C11-C10-C8-C7
31	S	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
31	a	404	CLA	C11-C10-C8-C7
31	b	606	CLA	C11-C10-C8-C7
31	b	610	CLA	C11-C10-C8-C7
31	b	612	CLA	C11-C10-C8-C7
31	b	615	CLA	C11-C10-C8-C7
31	c	502	CLA	C11-C12-C13-C15
31	c	508	CLA	C11-C10-C8-C7
31	c	508	CLA	C11-C12-C13-C15
31	g	602	CLA	C6-C7-C8-C10
31	g	611	CLA	C11-C10-C8-C7
31	g	611	CLA	C12-C13-C15-C16
31	r	613	CLA	C12-C13-C15-C16
31	s	610	CLA	C11-C12-C13-C15
31	y	602	CLA	C6-C7-C8-C10
31	y	612	CLA	C11-C10-C8-C7
38	A	405	PHO	C11-C10-C8-C7
38	a	405	PHO	C11-C10-C8-C7
30	y	609	CHL	C5-C6-C7-C8
31	R	613	CLA	C10-C11-C12-C13
32	R	618	LHG	C11-C12-C13-C14
30	n	609	CHL	C5-C6-C7-C8
30	R	606	CHL	C16-C17-C18-C20
32	s	621	LHG	C25-C26-C27-C28
41	w	501	LMG	C40-C41-C42-C43
31	5	602	CLA	O1D-CGD-O2D-CED
30	1	605	CHL	C3A-C2A-CAA-CBA
30	1	608	CHL	C3A-C2A-CAA-CBA
30	4	605	CHL	C3A-C2A-CAA-CBA
30	12	605	CHL	C3A-C2A-CAA-CBA
30	14	606	CHL	C3A-C2A-CAA-CBA
30	14	608	CHL	C3A-C2A-CAA-CBA
30	16	605	CHL	C4-C3-C5-C6
30	G	601	CHL	C4-C3-C5-C6
30	G	609	CHL	C4-C3-C5-C6
30	R	607	CHL	C3A-C2A-CAA-CBA
30	n	601	CHL	C3A-C2A-CAA-CBA
30	r	607	CHL	C3A-C2A-CAA-CBA
31	6	615	CLA	C3A-C2A-CAA-CBA
31	11	614	CLA	C3A-C2A-CAA-CBA
31	13	611	CLA	C3A-C2A-CAA-CBA
31	16	611	CLA	C3A-C2A-CAA-CBA
31	B	605	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	C	510	CLA	C3A-C2A-CAA-CBA
31	S	615	CLA	C3A-C2A-CAA-CBA
31	c	510	CLA	C3A-C2A-CAA-CBA
31	c	512	CLA	C3A-C2A-CAA-CBA
31	g	604	CLA	C3A-C2A-CAA-CBA
31	Y	610	CLA	C13-C15-C16-C17
31	g	610	CLA	C5-C6-C7-C8
31	n	613	CLA	C2-C3-C5-C6
31	b	609	CLA	O1D-CGD-O2D-CED
31	Y	612	CLA	C2C-C3C-CAC-CBC
31	16	602	CLA	O1A-CGA-O2A-C1
31	G	603	CLA	O1A-CGA-O2A-C1
31	a	407	CLA	O1A-CGA-O2A-C1
32	R	621	LHG	O10-C23-O8-C6
31	3	603	CLA	C5-C6-C7-C8
31	B	606	CLA	C10-C11-C12-C13
31	C	510	CLA	C10-C11-C12-C13
31	C	514	CLA	CBA-CGA-O2A-C1
31	s	614	CLA	CBA-CGA-O2A-C1
44	b	622	STE	C7-C8-C9-C10
33	12	614	LUT	C9-C10-C11-C12
31	n	604	CLA	C3-C5-C6-C7
31	c	505	CLA	C6-C7-C8-C10
31	N	613	CLA	C4C-C3C-CAC-CBC
30	G	608	CHL	C4-C3-C5-C6
30	g	608	CHL	C4-C3-C5-C6
30	4	609	CHL	O1A-CGA-O2A-C1
31	3	612	CLA	O1A-CGA-O2A-C1
32	g	615	LHG	O10-C23-O8-C6
31	C	508	CLA	O1D-CGD-O2D-CED
30	Y	609	CHL	C5-C6-C7-C8
31	15	602	CLA	C5-C6-C7-C8
31	B	609	CLA	C13-C15-C16-C17
32	14	615	LHG	C29-C30-C31-C32
32	D	408	LHG	C30-C31-C32-C33
32	14	615	LHG	C23-C24-C25-C26
46	W	501	DGD	C4B-C5B-C6B-C7B
31	b	609	CLA	C13-C15-C16-C17
32	3	617	LHG	C4-C5-C6-O8
32	A	414	LHG	C4-C5-C6-O8
32	D	412	LHG	C4-C5-C6-O8
32	Y	618	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
32	d	413	LHG	C4-C5-C6-O8
36	T	101	3PH	C1-C2-C3-O31
40	l	101	SQD	O6-C44-C45-C46
41	B	621	LMG	O1-C7-C8-C9
41	b	620	LMG	O1-C7-C8-C9
41	b	621	LMG	C7-C8-C9-O8
41	s	616	LMG	O1-C7-C8-C9
46	c	517	DGD	C1G-C2G-C3G-O3G
46	w	502	DGD	O1G-C1G-C2G-C3G
32	a	413	LHG	C32-C33-C34-C35
31	n	602	CLA	C4C-C3C-CAC-CBC
32	D	408	LHG	C26-C27-C28-C29
31	C	509	CLA	C11-C12-C13-C15
31	c	509	CLA	C11-C12-C13-C15
31	c	511	CLA	C16-C17-C18-C20
30	6	605	CHL	C15-C16-C17-C18
31	b	606	CLA	C10-C11-C12-C13
31	c	510	CLA	C10-C11-C12-C13
32	A	413	LHG	C24-C25-C26-C27
32	14	615	LHG	C27-C28-C29-C30
32	R	619	LHG	C11-C12-C13-C14
30	11	609	CHL	C2C-C3C-CAC-CBC
30	3	607	CHL	C1-C2-C3-C4
30	4	601	CHL	C1A-C2A-CAA-CBA
30	6	606	CHL	C1A-C2A-CAA-CBA
30	14	609	CHL	C1-C2-C3-C4
30	16	601	CHL	C1A-C2A-CAA-CBA
30	N	606	CHL	C1A-C2A-CAA-CBA
30	N	609	CHL	C1A-C2A-CAA-CBA
30	R	605	CHL	C1-C2-C3-C4
30	Y	609	CHL	C1A-C2A-CAA-CBA
30	n	601	CHL	C1A-C2A-CAA-CBA
30	n	601	CHL	C1-C2-C3-C4
30	n	606	CHL	C1A-C2A-CAA-CBA
30	n	609	CHL	C1A-C2A-CAA-CBA
30	y	609	CHL	C1A-C2A-CAA-CBA
31	1	610	CLA	C1-C2-C3-C4
31	2	602	CLA	C1-C2-C3-C4
31	11	613	CLA	C1-C2-C3-C4
31	12	603	CLA	C1-C2-C3-C4
31	12	609	CLA	C1-C2-C3-C4
31	13	611	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
31	14	613	CLA	C1-C2-C3-C4
31	16	602	CLA	C1-C2-C3-C4
31	B	604	CLA	C1-C2-C3-C4
31	y	603	CLA	C1-C2-C3-C4
38	D	402	PHO	C1A-C2A-CAA-CBA
31	B	601	CLA	C5-C6-C7-C8
32	N	616	LHG	C32-C33-C34-C35
30	14	601	CHL	C4-C3-C5-C6
30	16	601	CHL	C4-C3-C5-C6
31	6	611	CLA	C4-C3-C5-C6
31	C	507	CLA	C4-C3-C5-C6
31	r	608	CLA	C4-C3-C5-C6
38	D	402	PHO	C4-C3-C5-C6
30	2	607	CHL	O1D-CGD-O2D-CED
31	y	612	CLA	C2C-C3C-CAC-CBC
32	g	615	LHG	C31-C32-C33-C34
36	7	201	3PH	C2A-C2B-C2C-C2D
36	T	101	3PH	C35-C36-C37-C38
41	c	520	LMG	C32-C33-C34-C35
30	1	601	CHL	C2-C3-C5-C6
38	a	406	PHO	C2-C3-C5-C6
42	D	407	PL9	C13-C14-C16-C17
31	3	611	CLA	O1A-CGA-O2A-C1
32	d	409	LHG	C29-C30-C31-C32
41	B	622	LMG	C14-C15-C16-C17
31	C	509	CLA	C5-C6-C7-C8
30	y	607	CHL	O1D-CGD-O2D-CED
32	Y	617	LHG	C24-C25-C26-C27
31	r	614	CLA	O1D-CGD-O2D-CED
31	c	505	CLA	C6-C7-C8-C9
31	c	507	CLA	C16-C17-C18-C19
31	c	511	CLA	C16-C17-C18-C19
31	d	405	CLA	C16-C17-C18-C19
31	d	405	CLA	C16-C17-C18-C20
31	n	611	CLA	C11-C12-C13-C15
32	c	521	LHG	O6-C4-C5-O7
32	y	618	LHG	O6-C4-C5-O7
32	y	617	LHG	O6-C4-C5-O7
32	l	102	LHG	C9-C10-C11-C12
31	11	614	CLA	C2B-C3B-CAB-CBB
31	Y	604	CLA	C2B-C3B-CAB-CBB
31	y	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
33	s	618	LUT	C1-C6-C7-C8
39	B	617	BCR	C5-C6-C7-C8
39	C	515	BCR	C1-C6-C7-C8
39	c	515	BCR	C1-C6-C7-C8
32	6	617	LHG	C17-C18-C19-C20
32	S	617	LHG	C8-C7-O7-C5
32	D	412	LHG	C2-C3-O3-P
32	a	413	LHG	C25-C26-C27-C28
31	n	611	CLA	C10-C11-C12-C13
31	b	607	CLA	CBD-CGD-O2D-CED
31	c	508	CLA	O1D-CGD-O2D-CED
32	14	615	LHG	C30-C31-C32-C33
32	N	616	LHG	C29-C30-C31-C32
32	d	408	LHG	C12-C13-C14-C15
32	A	413	LHG	C32-C33-C34-C35
31	S	602	CLA	C16-C17-C18-C19
31	S	614	CLA	C16-C17-C18-C19
30	3	605	CHL	C2A-CAA-CBA-CGA
31	15	612	CLA	C2A-CAA-CBA-CGA
31	C	512	CLA	O1D-CGD-O2D-CED
31	b	607	CLA	C5-C6-C7-C8
32	C	521	LHG	O7-C5-C6-O8
32	D	412	LHG	O7-C5-C6-O8
36	b	623	3PH	O21-C2-C3-O31
40	d	412	SQD	O6-C44-C45-O47
41	B	621	LMG	O1-C7-C8-O7
41	D	414	LMG	O7-C8-C9-O8
41	K	102	LMG	O1-C7-C8-O7
41	b	620	LMG	O1-C7-C8-O7
41	d	415	LMG	O7-C8-C9-O8
41	v	101	LMG	O1-C7-C8-O7
46	C	517	DGD	O2G-C2G-C3G-O3G
46	C	519	DGD	O1G-C1G-C2G-O2G
46	c	517	DGD	O2G-C2G-C3G-O3G
46	c	519	DGD	O1G-C1G-C2G-O2G
42	D	407	PL9	C4-C3-C7-C8
42	d	407	PL9	C4-C3-C7-C8
43	C	523	LNL	C12-C13-C14-C15
43	H	101	LNL	C10-C11-C12-C13
43	I	101	LNL	C9-C10-C11-C12
43	R	620	LNL	C9-C10-C11-C12
43	R	620	LNL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
43	R	620	LNL	C13-C14-C15-C16
43	W	502	LNL	C9-C10-C11-C12
43	W	502	LNL	C10-C11-C12-C13
43	W	502	LNL	C12-C13-C14-C15
43	W	503	LNL	C12-C13-C14-C15
43	X	201	LNL	C10-C11-C12-C13
43	X	201	LNL	C12-C13-C14-C15
43	X	201	LNL	C13-C14-C15-C16
43	Y	620	LNL	C10-C11-C12-C13
43	a	412	LNL	C12-C13-C14-C15
43	c	523	LNL	C12-C13-C14-C15
43	h	101	LNL	C10-C11-C12-C13
43	i	101	LNL	C9-C10-C11-C12
43	r	620	LNL	C12-C13-C14-C15
43	w	503	LNL	C9-C10-C11-C12
43	w	503	LNL	C10-C11-C12-C13
43	w	503	LNL	C12-C13-C14-C15
43	x	201	LNL	C10-C11-C12-C13
43	y	619	LNL	C9-C10-C11-C12
43	y	619	LNL	C13-C14-C15-C16
43	y	620	LNL	C12-C13-C14-C15
43	y	620	LNL	C13-C14-C15-C16
43	y	621	LNL	C12-C13-C14-C15
32	6	617	LHG	C24-C25-C26-C27
31	B	611	CLA	C10-C11-C12-C13
31	R	613	CLA	C8-C10-C11-C12
32	N	616	LHG	C9-C10-C11-C12
32	Y	616	LHG	C28-C29-C30-C31
31	y	615	CLA	C11-C10-C8-C7
32	D	412	LHG	C13-C14-C15-C16
30	16	607	CHL	C5-C6-C7-C8
31	C	512	CLA	C8-C10-C11-C12
30	16	601	CHL	C2-C3-C5-C6
30	16	605	CHL	C2-C3-C5-C6
30	N	605	CHL	C2-C3-C5-C6
42	d	407	PL9	C13-C14-C16-C17
30	3	601	CHL	C1-C2-C3-C5
30	4	609	CHL	C1-C2-C3-C5
30	6	606	CHL	C1-C2-C3-C5
30	6	609	CHL	C1-C2-C3-C5
30	11	609	CHL	C1-C2-C3-C5
30	12	608	CHL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
30	16	601	CHL	C1-C2-C3-C5
30	G	608	CHL	C1-C2-C3-C5
30	N	601	CHL	C1-C2-C3-C5
30	N	607	CHL	C1-C2-C3-C5
30	S	606	CHL	C1-C2-C3-C5
30	Y	607	CHL	C1-C2-C3-C5
30	g	608	CHL	C1-C2-C3-C5
30	g	609	CHL	C1-C2-C3-C5
30	n	605	CHL	C1-C2-C3-C5
30	n	606	CHL	C1-C2-C3-C5
30	n	607	CHL	C1-C2-C3-C5
30	s	606	CHL	C1-C2-C3-C5
30	y	607	CHL	C1-C2-C3-C5
31	1	613	CLA	C1-C2-C3-C5
31	4	602	CLA	C1-C2-C3-C5
31	11	602	CLA	C1-C2-C3-C5
31	11	610	CLA	C1-C2-C3-C5
31	12	604	CLA	C1-C2-C3-C5
31	13	603	CLA	C1-C2-C3-C5
31	A	403	CLA	C1-C2-C3-C5
31	A	406	CLA	C1-C2-C3-C5
31	B	603	CLA	C1-C2-C3-C5
31	B	606	CLA	C1-C2-C3-C5
31	B	613	CLA	C1-C2-C3-C5
31	C	503	CLA	C1-C2-C3-C5
31	C	504	CLA	C1-C2-C3-C5
31	R	603	CLA	C1-C2-C3-C5
31	R	609	CLA	C1-C2-C3-C5
31	R	613	CLA	C1-C2-C3-C5
31	S	602	CLA	C1-C2-C3-C5
31	S	604	CLA	C1-C2-C3-C5
31	S	610	CLA	C1-C2-C3-C5
31	Y	602	CLA	C1-C2-C3-C5
31	Y	613	CLA	C1-C2-C3-C5
31	a	407	CLA	C1-C2-C3-C5
31	b	603	CLA	C1-C2-C3-C5
31	b	607	CLA	C1-C2-C3-C5
31	b	608	CLA	C1-C2-C3-C5
31	b	613	CLA	C1-C2-C3-C5
31	c	503	CLA	C1-C2-C3-C5
31	c	504	CLA	C1-C2-C3-C5
31	c	506	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
31	c	512	CLA	C1-C2-C3-C5
31	d	402	CLA	C1-C2-C3-C5
31	n	611	CLA	C1-C2-C3-C5
31	r	603	CLA	C1-C2-C3-C5
31	s	602	CLA	C1-C2-C3-C5
31	s	609	CLA	C1-C2-C3-C5
31	y	602	CLA	C1-C2-C3-C5
31	y	613	CLA	C1-C2-C3-C5
31	b	601	CLA	C6-C7-C8-C9
32	A	413	LHG	C25-C26-C27-C28
32	a	413	LHG	C9-C10-C11-C12
32	d	408	LHG	C26-C27-C28-C29
32	g	615	LHG	C7-C8-C9-C10
30	11	608	CHL	C1-C2-C3-C4
31	16	613	CLA	C1-C2-C3-C4
31	S	605	CLA	C1-C2-C3-C5
31	n	602	CLA	O1A-CGA-O2A-C1
30	16	609	CHL	C3-C5-C6-C7
30	1	601	CHL	C11-C10-C8-C9
30	6	601	CHL	C11-C10-C8-C9
30	n	607	CHL	C14-C13-C15-C16
31	13	602	CLA	C6-C7-C8-C9
31	b	608	CLA	C11-C12-C13-C14
31	b	609	CLA	C6-C7-C8-C9
31	c	508	CLA	C14-C13-C15-C16
31	g	602	CLA	C14-C13-C15-C16
38	A	405	PHO	C11-C10-C8-C9
38	a	405	PHO	C11-C10-C8-C9
30	g	607	CHL	O1D-CGD-O2D-CED
44	b	622	STE	C5-C6-C7-C8
30	1	606	CHL	CAA-CBA-CGA-O2A
32	4	615	LHG	C12-C13-C14-C15
32	A	414	LHG	C32-C33-C34-C35
32	a	411	LHG	C11-C12-C13-C14
32	l	102	LHG	C29-C30-C31-C32
43	x	201	LNL	C4-C5-C6-C7
32	A	414	LHG	C9-C10-C11-C12
32	y	616	LHG	C18-C19-C20-C21
40	L	101	SQD	C30-C31-C32-C33
30	1	609	CHL	C6-C7-C8-C10
30	R	606	CHL	C16-C17-C18-C19
31	14	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	C	507	CLA	C16-C17-C18-C20
31	Y	613	CLA	C16-C17-C18-C19
31	c	507	CLA	C16-C17-C18-C20
31	y	613	CLA	C16-C17-C18-C19
31	b	610	CLA	O1D-CGD-O2D-CED
30	13	607	CHL	C10-C11-C12-C13
30	R	606	CHL	C10-C11-C12-C13
32	13	616	LHG	C33-C34-C35-C36
32	G	615	LHG	C31-C32-C33-C34
43	C	523	LNL	C15-C16-C17-C18
43	W	503	LNL	C15-C16-C17-C18
43	a	412	LNL	C15-C16-C17-C18
43	h	101	LNL	C15-C16-C17-C18
43	y	621	LNL	C15-C16-C17-C18
32	r	619	LHG	C26-C27-C28-C29
31	c	504	CLA	C8-C10-C11-C12
32	S	617	LHG	O1-C1-C2-O2
32	d	409	LHG	O1-C1-C2-O2
32	r	618	LHG	O1-C1-C2-O2
30	1	609	CHL	C3-C5-C6-C7
31	C	514	CLA	C3-C5-C6-C7
31	6	612	CLA	CBA-CGA-O2A-C1
32	A	411	LHG	C24-C23-O8-C6
32	Y	617	LHG	C24-C23-O8-C6
32	A	415	LHG	C14-C15-C16-C17
31	s	604	CLA	CAA-CBA-CGA-O2A
31	13	604	CLA	C2-C3-C5-C6
31	c	507	CLA	C2-C3-C5-C6
30	11	609	CHL	C6-C7-C8-C9
31	a	404	CLA	C5-C6-C7-C8
30	16	608	CHL	O1A-CGA-O2A-C1
30	12	608	CHL	O1D-CGD-O2D-CED
31	A	404	CLA	C5-C6-C7-C8
32	S	621	LHG	C9-C10-C11-C12
41	B	621	LMG	C13-C14-C15-C16
31	s	609	CLA	C4C-C3C-CAC-CBC
36	B	620	3PH	C21-C22-C23-C24
30	N	606	CHL	C10-C11-C12-C13
30	y	605	CHL	C5-C6-C7-C8
31	C	510	CLA	C5-C6-C7-C8
40	d	412	SQD	C9-C10-C11-C12
32	A	411	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	R	618	LHG	O6-C4-C5-C6
32	g	615	LHG	O6-C4-C5-C6
32	s	617	LHG	O6-C4-C5-C6
32	y	618	LHG	O6-C4-C5-C6
30	13	609	CHL	C11-C12-C13-C15
31	d	404	CLA	C16-C17-C18-C19
31	13	613	CLA	O1A-CGA-O2A-C1
31	12	602	CLA	C8-C10-C11-C12
31	15	603	CLA	C5-C6-C7-C8
31	c	510	CLA	C5-C6-C7-C8
31	d	404	CLA	C5-C6-C7-C8
32	s	617	LHG	C30-C31-C32-C33
30	3	601	CHL	C6-C7-C8-C10
30	G	609	CHL	C6-C7-C8-C10
30	Y	609	CHL	C11-C10-C8-C7
31	6	604	CLA	C6-C7-C8-C10
31	13	602	CLA	C6-C7-C8-C10
31	A	403	CLA	C12-C13-C15-C16
31	C	502	CLA	C11-C10-C8-C7
31	C	508	CLA	C12-C13-C15-C16
31	G	611	CLA	C12-C13-C15-C16
31	Y	612	CLA	C11-C12-C13-C15
31	b	608	CLA	C11-C10-C8-C7
31	b	612	CLA	C11-C12-C13-C15
31	b	616	CLA	C6-C7-C8-C10
31	c	508	CLA	C12-C13-C15-C16
31	r	603	CLA	C11-C10-C8-C7
32	D	409	LHG	C28-C29-C30-C31
31	c	504	CLA	C10-C11-C12-C13
31	r	610	CLA	C5-C6-C7-C8
39	D	406	BCR	C7-C8-C9-C10
39	d	406	BCR	C7-C8-C9-C10
31	Y	610	CLA	CBA-CGA-O2A-C1
32	y	617	LHG	C24-C23-O8-C6
30	12	607	CHL	O1A-CGA-O2A-C1
31	2	613	CLA	O1A-CGA-O2A-C1
31	12	603	CLA	O1A-CGA-O2A-C1
40	A	408	SQD	C5-C6-S-O8
40	a	409	SQD	C5-C6-S-O8
46	C	518	DGD	C5D-C6D-O5D-C1E
46	c	518	DGD	C5D-C6D-O5D-C1E
31	4	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	c	512	CLA	C8-C10-C11-C12
30	13	601	CHL	C2A-CAA-CBA-CGA
31	B	601	CLA	C2A-CAA-CBA-CGA
31	B	616	CLA	C2A-CAA-CBA-CGA
31	N	604	CLA	C2A-CAA-CBA-CGA
31	R	612	CLA	C2A-CAA-CBA-CGA
31	n	604	CLA	C2A-CAA-CBA-CGA
31	s	610	CLA	C2A-CAA-CBA-CGA
32	3	616	LHG	C27-C28-C29-C30
32	Y	617	LHG	C25-C26-C27-C28
41	J	102	LMG	C11-C12-C13-C14
31	11	602	CLA	C11-C12-C13-C15
31	A	403	CLA	C16-C17-C18-C20
31	D	405	CLA	C16-C17-C18-C19
31	12	603	CLA	C4-C3-C5-C6
31	b	614	CLA	C4-C3-C5-C6
30	N	601	CHL	CAA-CBA-CGA-O2A
30	13	608	CHL	O1A-CGA-O2A-C1
30	Y	606	CHL	O1A-CGA-O2A-C1
31	A	406	CLA	O1A-CGA-O2A-C1
31	g	603	CLA	O1A-CGA-O2A-C1
31	S	610	CLA	C2-C3-C5-C6
32	Y	616	LHG	O1-C1-C2-C3
31	g	613	CLA	C3-C5-C6-C7
31	y	615	CLA	C3-C5-C6-C7
31	5	610	CLA	CBA-CGA-O2A-C1
41	j	102	LMG	C11-C12-C13-C14
30	N	609	CHL	C13-C15-C16-C17
31	B	608	CLA	C5-C6-C7-C8
31	3	604	CLA	O2A-C1-C2-C3
31	6	604	CLA	O2A-C1-C2-C3
31	S	614	CLA	O2A-C1-C2-C3
31	Y	615	CLA	O2A-C1-C2-C3
31	s	614	CLA	O2A-C1-C2-C3
32	Y	618	LHG	O10-C23-O8-C6
32	r	621	LHG	C10-C11-C12-C13
30	Y	607	CHL	O1D-CGD-O2D-CED
31	b	615	CLA	C16-C17-C18-C19
31	d	402	CLA	C16-C17-C18-C20
44	b	622	STE	C14-C15-C16-C17
30	15	607	CHL	O1A-CGA-O2A-C1
30	y	606	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	13	604	CLA	O1A-CGA-O2A-C1
31	y	614	CLA	CBA-CGA-O2A-C1
41	A	409	LMG	C28-C29-C30-C31
32	A	411	LHG	O6-C4-C5-O7
32	C	521	LHG	O6-C4-C5-O7
32	a	411	LHG	O6-C4-C5-O7
36	B	620	3PH	O11-C1-C2-O21
46	C	518	DGD	O6E-C1E-O5D-C6D
46	c	518	DGD	O6E-C1E-O5D-C6D
30	N	607	CHL	O1D-CGD-O2D-CED
31	n	602	CLA	O1D-CGD-O2D-CED
32	6	617	LHG	C4-C5-C6-O8
32	Y	616	LHG	C4-C5-C6-O8
32	y	616	LHG	C4-C5-C6-O8
36	B	620	3PH	C1-C2-C3-O31
36	B	624	3PH	C1-C2-C3-O31
40	L	101	SQD	O6-C44-C45-C46
41	C	520	LMG	O1-C7-C8-C9
41	D	414	LMG	C7-C8-C9-O8
41	K	102	LMG	O1-C7-C8-C9
41	d	410	LMG	O1-C7-C8-C9
41	d	415	LMG	C7-C8-C9-O8
41	v	101	LMG	O1-C7-C8-C9
41	w	501	LMG	O1-C7-C8-C9
46	C	517	DGD	C1G-C2G-C3G-O3G
46	C	519	DGD	O1G-C1G-C2G-C3G
46	c	519	DGD	O1G-C1G-C2G-C3G
32	3	616	LHG	C7-C8-C9-C10
31	R	614	CLA	C5-C6-C7-C8
31	r	602	CLA	C10-C11-C12-C13
31	B	615	CLA	C16-C17-C18-C19
31	b	601	CLA	C6-C7-C8-C10
31	b	604	CLA	C16-C17-C18-C20
31	b	611	CLA	C16-C17-C18-C20
32	A	413	LHG	C9-C10-C11-C12
31	B	610	CLA	O1D-CGD-O2D-CED
30	13	607	CHL	C3-C5-C6-C7
30	N	609	CHL	C5-C6-C7-C8
31	c	502	CLA	C8-C10-C11-C12
31	r	613	CLA	C13-C15-C16-C17
30	12	608	CHL	C4-C3-C5-C6
30	4	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	11	609	CHL	C2-C3-C5-C6
31	B	613	CLA	C2-C3-C5-C6
31	b	613	CLA	C2-C3-C5-C6
42	D	407	PL9	C12-C11-C9-C8
32	y	618	LHG	C10-C11-C12-C13
31	b	604	CLA	C5-C6-C7-C8
31	c	503	CLA	C15-C16-C17-C18
31	5	603	CLA	C3-C5-C6-C7
32	A	414	LHG	O7-C5-C6-O8
32	c	521	LHG	O7-C5-C6-O8
32	d	413	LHG	O7-C5-C6-O8
40	L	101	SQD	O6-C44-C45-O47
40	l	101	SQD	O6-C44-C45-O47
41	S	616	LMG	O1-C7-C8-O7
41	d	410	LMG	O1-C7-C8-O7
41	s	616	LMG	O1-C7-C8-O7
41	w	501	LMG	O1-C7-C8-O7
30	3	607	CHL	C11-C12-C13-C14
30	6	609	CHL	C14-C13-C15-C16
30	16	607	CHL	C11-C10-C8-C9
30	Y	607	CHL	C11-C10-C8-C9
30	g	601	CHL	C11-C12-C13-C14
30	n	607	CHL	C11-C10-C8-C9
31	16	611	CLA	C11-C10-C8-C9
31	B	609	CLA	C6-C7-C8-C9
31	C	514	CLA	C6-C7-C8-C9
31	C	514	CLA	C11-C12-C13-C14
31	G	611	CLA	C14-C13-C15-C16
31	G	613	CLA	C6-C7-C8-C9
31	S	604	CLA	C11-C10-C8-C9
31	b	614	CLA	C14-C13-C15-C16
31	c	504	CLA	C11-C10-C8-C9
31	c	507	CLA	C11-C12-C13-C14
31	c	507	CLA	C14-C13-C15-C16
31	n	602	CLA	C14-C13-C15-C16
31	s	610	CLA	C6-C7-C8-C9
31	3	604	CLA	CBA-CGA-O2A-C1
41	D	414	LMG	C17-C18-C19-C20
41	d	415	LMG	C17-C18-C19-C20
30	Y	605	CHL	O1A-CGA-O2A-C1
32	14	615	LHG	C26-C27-C28-C29
31	R	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	b	611	CLA	C10-C11-C12-C13
30	Y	605	CHL	CBD-CGD-O2D-CED
31	D	404	CLA	C5-C6-C7-C8
32	A	411	LHG	O10-C23-O8-C6
32	Y	617	LHG	O10-C23-O8-C6
30	13	606	CHL	C3-C5-C6-C7
40	D	411	SQD	C9-C10-C11-C12
41	D	414	LMG	C34-C35-C36-C37
31	y	610	CLA	CBA-CGA-O2A-C1
31	B	601	CLA	C6-C7-C8-C9
31	B	606	CLA	C16-C17-C18-C19
31	B	610	CLA	C16-C17-C18-C20
31	B	611	CLA	C16-C17-C18-C20
31	b	610	CLA	C16-C17-C18-C20
31	d	402	CLA	C16-C17-C18-C19
31	c	511	CLA	C13-C15-C16-C17
31	s	614	CLA	C13-C15-C16-C17
30	S	606	CHL	C10-C11-C12-C13
30	n	609	CHL	C4-C3-C5-C6
31	3	611	CLA	C4-C3-C5-C6
31	r	602	CLA	C4-C3-C5-C6
30	3	601	CHL	C3-C5-C6-C7
32	r	618	LHG	C23-C24-C25-C26
30	G	609	CHL	C2-C3-C5-C6
41	v	101	LMG	C32-C33-C34-C35
32	d	408	LHG	C1-C2-C3-O3
32	d	409	LHG	O2-C2-C3-O3
30	5	608	CHL	C2A-CAA-CBA-CGA
31	n	611	CLA	C2A-CAA-CBA-CGA
30	13	601	CHL	C6-C7-C8-C10
31	s	609	CLA	C6-C7-C8-C9
32	6	616	LHG	C27-C28-C29-C30
32	a	413	LHG	C24-C25-C26-C27
41	d	415	LMG	C34-C35-C36-C37
31	4	613	CLA	O1A-CGA-O2A-C1
31	13	611	CLA	O1A-CGA-O2A-C1
30	G	609	CHL	C15-C16-C17-C18
31	c	506	CLA	C3-C5-C6-C7
30	1	606	CHL	C4C-C3C-CAC-CBC
30	1	608	CHL	C4C-C3C-CAC-CBC
30	1	609	CHL	C4C-C3C-CAC-CBC
30	2	609	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
30	2	607	CHL	C4C-C3C-CAC-CBC
30	3	609	CHL	C4C-C3C-CAC-CBC
30	4	608	CHL	C4C-C3C-CAC-CBC
30	4	609	CHL	C4C-C3C-CAC-CBC
30	5	609	CHL	C4C-C3C-CAC-CBC
30	5	607	CHL	C4C-C3C-CAC-CBC
30	6	609	CHL	C4C-C3C-CAC-CBC
30	12	608	CHL	C4C-C3C-CAC-CBC
30	15	608	CHL	C4C-C3C-CAC-CBC
30	G	608	CHL	C4C-C3C-CAC-CBC
30	G	609	CHL	C4C-C3C-CAC-CBC
30	N	605	CHL	C4C-C3C-CAC-CBC
30	N	607	CHL	C4C-C3C-CAC-CBC
30	S	608	CHL	C4C-C3C-CAC-CBC
30	g	609	CHL	C4C-C3C-CAC-CBC
30	n	609	CHL	C4C-C3C-CAC-CBC
30	s	608	CHL	C4C-C3C-CAC-CBC
30	y	609	CHL	C4C-C3C-CAC-CBC
31	y	615	CLA	C11-C10-C8-C9
32	s	617	LHG	C11-C12-C13-C14
40	D	413	SQD	C25-C26-C27-C28
31	A	406	CLA	O1D-CGD-O2D-CED
31	B	615	CLA	C16-C17-C18-C20
31	b	615	CLA	C16-C17-C18-C20
32	S	617	LHG	O9-C7-O7-C5
31	a	407	CLA	O1D-CGD-O2D-CED
31	13	602	CLA	C3-C5-C6-C7
31	13	611	CLA	C3-C5-C6-C7
32	R	621	LHG	C10-C11-C12-C13
32	r	619	LHG	C31-C32-C33-C34
31	y	614	CLA	O2A-C1-C2-C3
31	2	604	CLA	C4B-C3B-CAB-CBB
31	11	614	CLA	C1A-C2A-CAA-CBA
31	13	604	CLA	C4B-C3B-CAB-CBB
31	16	604	CLA	C4B-C3B-CAB-CBB
31	A	404	CLA	C4B-C3B-CAB-CBB
31	C	510	CLA	C4B-C3B-CAB-CBB
31	N	614	CLA	C1A-C2A-CAA-CBA
31	R	610	CLA	C1A-C2A-CAA-CBA
31	Y	610	CLA	C4B-C3B-CAB-CBB
31	a	404	CLA	C4B-C3B-CAB-CBB
31	b	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	c	510	CLA	C4B-C3B-CAB-CBB
31	y	610	CLA	C4B-C3B-CAB-CBB
31	1	602	CLA	O1D-CGD-O2D-CED
31	6	604	CLA	CBA-CGA-O2A-C1
43	C	524	LNL	C4-C5-C6-C7
30	r	605	CHL	O1A-CGA-O2A-C1
32	R	621	LHG	O7-C7-C8-C9
43	c	524	LNL	C4-C5-C6-C7
41	b	620	LMG	C13-C14-C15-C16
30	5	609	CHL	C16-C17-C18-C20
31	A	403	CLA	C16-C17-C18-C19
31	G	603	CLA	C6-C7-C8-C9
31	g	603	CLA	C6-C7-C8-C9
32	L	102	LHG	C9-C10-C11-C12
40	d	414	SQD	C25-C26-C27-C28
30	1	608	CHL	C2A-CAA-CBA-CGA
30	6	605	CHL	C2A-CAA-CBA-CGA
30	15	607	CHL	C2A-CAA-CBA-CGA
30	N	607	CHL	C2A-CAA-CBA-CGA
31	12	602	CLA	C2A-CAA-CBA-CGA
32	y	618	LHG	C29-C30-C31-C32
31	13	602	CLA	C15-C16-C17-C18
31	r	603	CLA	C15-C16-C17-C18
32	S	617	LHG	O6-C4-C5-C6
32	Y	618	LHG	O6-C4-C5-C6
32	a	411	LHG	O6-C4-C5-C6
32	11	615	LHG	C32-C33-C34-C35
32	Y	617	LHG	C32-C33-C34-C35
30	G	608	CHL	C2-C3-C5-C6
30	g	608	CHL	C2-C3-C5-C6
40	A	408	SQD	C5-C6-S-O7
40	a	409	SQD	C5-C6-S-O7
32	A	411	LHG	C9-C10-C11-C12
32	N	616	LHG	C10-C11-C12-C13
30	16	607	CHL	C6-C7-C8-C10
30	S	606	CHL	C12-C13-C15-C16
30	Y	606	CHL	C12-C13-C15-C16
30	n	606	CHL	C11-C10-C8-C7
30	y	601	CHL	C12-C13-C15-C16
30	y	609	CHL	C11-C10-C8-C7
31	1	602	CLA	C11-C10-C8-C7
31	3	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	13	603	CLA	C6-C7-C8-C10
31	14	610	CLA	C11-C10-C8-C7
31	B	610	CLA	C11-C12-C13-C15
31	C	508	CLA	C11-C12-C13-C15
31	D	404	CLA	C6-C7-C8-C10
31	R	609	CLA	C12-C13-C15-C16
31	b	607	CLA	C6-C7-C8-C10
31	b	610	CLA	C11-C12-C13-C15
31	c	512	CLA	C11-C12-C13-C15
31	n	603	CLA	C11-C10-C8-C7
31	r	609	CLA	C11-C10-C8-C7
30	N	606	CHL	C11-C12-C13-C14
31	4	602	CLA	C11-C12-C13-C15
31	b	606	CLA	C16-C17-C18-C20
31	r	609	CLA	C16-C17-C18-C20
31	y	602	CLA	C11-C12-C13-C14
32	6	617	LHG	C28-C29-C30-C31
32	r	621	LHG	C9-C10-C11-C12
32	D	409	LHG	O2-C2-C3-O3
32	y	617	LHG	O10-C23-O8-C6
41	K	102	LMG	C30-C31-C32-C33
32	6	617	LHG	C5-C4-O6-P
32	13	616	LHG	C5-C4-O6-P
32	r	619	LHG	C5-C4-O6-P
32	y	617	LHG	C2-C3-O3-P
32	l	102	LHG	C11-C10-C9-C8
30	N	605	CHL	C3A-C2A-CAA-CBA
30	N	605	CHL	C4-C3-C5-C6
30	y	606	CHL	C3A-C2A-CAA-CBA
31	4	611	CLA	C3A-C2A-CAA-CBA
31	13	604	CLA	C4-C3-C5-C6
31	14	613	CLA	C4-C3-C5-C6
31	N	614	CLA	C3A-C2A-CAA-CBA
31	R	604	CLA	C3A-C2A-CAA-CBA
31	r	604	CLA	C3A-C2A-CAA-CBA
30	13	607	CHL	C11-C12-C13-C15
31	B	601	CLA	C6-C7-C8-C10
31	N	611	CLA	C11-C12-C13-C15
32	N	616	LHG	C16-C17-C18-C19
32	c	521	LHG	C31-C32-C33-C34
30	6	609	CHL	CBD-CGD-O2D-CED
31	3	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	L	102	LHG	O6-C4-C5-O7
32	R	621	LHG	O6-C4-C5-O7
32	R	618	LHG	O6-C4-C5-O7
32	S	617	LHG	O6-C4-C5-O7
32	Y	617	LHG	O6-C4-C5-O7
32	g	615	LHG	O6-C4-C5-O7
32	r	618	LHG	O6-C4-C5-O7
31	C	512	CLA	C2A-CAA-CBA-CGA
31	R	611	CLA	C2A-CAA-CBA-CGA
31	r	611	CLA	C2A-CAA-CBA-CGA
30	16	606	CHL	C11-C10-C8-C9
31	14	610	CLA	C11-C10-C8-C9
31	C	508	CLA	C14-C13-C15-C16
31	b	607	CLA	C14-C13-C15-C16
31	b	612	CLA	C11-C12-C13-C14
31	g	611	CLA	C14-C13-C15-C16
31	n	603	CLA	C11-C10-C8-C9
31	r	603	CLA	C11-C10-C8-C9
31	6	611	CLA	CAA-CBA-CGA-O2A
30	g	609	CHL	C15-C16-C17-C18
31	R	610	CLA	C11-C12-C13-C14
30	G	607	CHL	O1D-CGD-O2D-CED
30	1	608	CHL	C1-C2-C3-C4
30	4	608	CHL	C1-C2-C3-C4
30	5	608	CHL	C1-C2-C3-C4
30	6	608	CHL	C1-C2-C3-C4
30	12	601	CHL	C1-C2-C3-C4
30	15	601	CHL	C1-C2-C3-C4
30	N	608	CHL	C1-C2-C3-C4
30	g	606	CHL	C1-C2-C3-C4
30	n	608	CHL	C1-C2-C3-C4
31	11	614	CLA	C1-C2-C3-C4
31	14	614	CLA	C1-C2-C3-C4
31	R	611	CLA	C1-C2-C3-C4
31	S	613	CLA	C1-C2-C3-C4
31	r	611	CLA	C1-C2-C3-C4
31	s	613	CLA	C1-C2-C3-C4
31	b	616	CLA	O1D-CGD-O2D-CED
31	s	603	CLA	O1D-CGD-O2D-CED
32	11	615	LHG	C16-C17-C18-C19
32	r	619	LHG	C14-C15-C16-C17
32	r	621	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
41	C	520	LMG	O1-C7-C8-O7
41	S	616	LMG	O7-C8-C9-O8
41	c	520	LMG	O1-C7-C8-O7
32	3	617	LHG	C15-C16-C17-C18
32	C	521	LHG	C9-C10-C11-C12
40	d	412	SQD	C26-C27-C28-C29
30	r	606	CHL	C10-C11-C12-C13
31	G	613	CLA	C13-C15-C16-C17
41	J	102	LMG	C10-C11-C12-C13
31	5	602	CLA	C6-C7-C8-C9
31	s	609	CLA	C6-C7-C8-C10
32	N	616	LHG	C33-C34-C35-C36
32	n	616	LHG	C4-C5-C6-O8
40	d	412	SQD	O6-C44-C45-C46
40	d	414	SQD	O6-C44-C45-C46
41	A	409	LMG	O1-C7-C8-C9
41	c	520	LMG	O1-C7-C8-C9
32	S	617	LHG	C31-C32-C33-C34
31	y	615	CLA	C5-C6-C7-C8
42	a	410	PL9	C43-C44-C46-C47
42	d	407	PL9	C12-C11-C9-C8
32	1	615	LHG	C15-C16-C17-C18
32	16	616	LHG	C26-C27-C28-C29
30	4	607	CHL	CAD-CBD-CGD-O2D
30	11	601	CHL	CAD-CBD-CGD-O2D
30	14	601	CHL	CAD-CBD-CGD-O2D
30	16	607	CHL	CAD-CBD-CGD-O2D
31	3	603	CLA	CAD-CBD-CGD-O2D
31	14	603	CLA	CAD-CBD-CGD-O2D
31	14	614	CLA	CAD-CBD-CGD-O2D
31	B	601	CLA	CAD-CBD-CGD-O2D
31	B	606	CLA	CAD-CBD-CGD-O2D
31	B	609	CLA	CAD-CBD-CGD-O2D
31	B	612	CLA	CAD-CBD-CGD-O2D
31	C	506	CLA	CAD-CBD-CGD-O2D
31	C	513	CLA	CAD-CBD-CGD-O2D
31	N	603	CLA	CAD-CBD-CGD-O2D
31	Y	612	CLA	CAD-CBD-CGD-O2D
31	b	601	CLA	CAD-CBD-CGD-O2D
31	b	606	CLA	CAD-CBD-CGD-O2D
31	b	607	CLA	CAD-CBD-CGD-O2D
31	b	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	b	612	CLA	CAD-CBD-CGD-O2D
31	c	513	CLA	CAD-CBD-CGD-O2D
31	n	603	CLA	CAD-CBD-CGD-O2D
31	r	612	CLA	CAD-CBD-CGD-O2D
31	y	612	CLA	CAD-CBD-CGD-O2D
31	y	615	CLA	CAD-CBD-CGD-O2D
32	Y	618	LHG	C30-C31-C32-C33
30	2	609	CHL	CBA-CGA-O2A-C1
31	R	610	CLA	CBA-CGA-O2A-C1
30	5	609	CHL	C16-C17-C18-C19
31	6	610	CLA	C11-C12-C13-C14
31	12	602	CLA	C11-C12-C13-C15
31	g	603	CLA	C6-C7-C8-C10
40	D	411	SQD	C26-C27-C28-C29
31	B	614	CLA	C3-C5-C6-C7
31	g	603	CLA	C3-C5-C6-C7
31	B	614	CLA	C2A-CAA-CBA-CGA
31	C	506	CLA	C2A-CAA-CBA-CGA
31	b	612	CLA	C2A-CAA-CBA-CGA
36	T	101	3PH	C26-C27-C28-C29
30	n	601	CHL	O1A-CGA-O2A-C1
32	S	621	LHG	C18-C19-C20-C21
32	n	616	LHG	C11-C10-C9-C8
32	6	616	LHG	C12-C13-C14-C15
30	16	601	CHL	C2C-C3C-CAC-CBC
31	12	604	CLA	CAA-CBA-CGA-O2A
32	a	411	LHG	C16-C17-C18-C19
41	B	622	LMG	C16-C17-C18-C19
30	1	608	CHL	CHA-CBD-CGD-O1D
30	1	609	CHL	CHA-CBD-CGD-O1D
30	2	605	CHL	CAD-CBD-CGD-O1D
30	2	609	CHL	CHA-CBD-CGD-O2D
30	3	605	CHL	CHA-CBD-CGD-O2D
30	3	609	CHL	CHA-CBD-CGD-O2D
30	4	609	CHL	CHA-CBD-CGD-O1D
30	5	605	CHL	CAD-CBD-CGD-O1D
30	5	609	CHL	CHA-CBD-CGD-O2D
30	6	605	CHL	CHA-CBD-CGD-O2D
30	6	608	CHL	CHA-CBD-CGD-O2D
30	6	609	CHL	CHA-CBD-CGD-O2D
30	11	601	CHL	CAD-CBD-CGD-O1D
30	11	607	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	11	608	CHL	CHA-CBD-CGD-O2D
30	13	608	CHL	CHA-CBD-CGD-O2D
30	14	601	CHL	CAD-CBD-CGD-O1D
30	14	606	CHL	CHA-CBD-CGD-O1D
30	14	607	CHL	CHA-CBD-CGD-O2D
30	16	601	CHL	CHA-CBD-CGD-O1D
30	16	608	CHL	CHA-CBD-CGD-O2D
30	16	609	CHL	CHA-CBD-CGD-O1D
30	G	601	CHL	CAD-CBD-CGD-O1D
30	G	606	CHL	CHA-CBD-CGD-O2D
30	G	609	CHL	CHA-CBD-CGD-O2D
30	N	601	CHL	CHA-CBD-CGD-O1D
30	N	601	CHL	CHA-CBD-CGD-O2D
30	N	609	CHL	CAD-CBD-CGD-O1D
30	S	606	CHL	CHA-CBD-CGD-O2D
30	g	601	CHL	CAD-CBD-CGD-O1D
30	g	606	CHL	CHA-CBD-CGD-O2D
30	g	609	CHL	CHA-CBD-CGD-O2D
30	n	608	CHL	CAD-CBD-CGD-O1D
30	n	609	CHL	CAD-CBD-CGD-O1D
30	r	605	CHL	CHA-CBD-CGD-O2D
31	1	602	CLA	CHA-CBD-CGD-O2D
31	2	604	CLA	CAD-CBD-CGD-O1D
31	3	603	CLA	CAD-CBD-CGD-O1D
31	3	614	CLA	CHA-CBD-CGD-O1D
31	4	602	CLA	CHA-CBD-CGD-O1D
31	5	602	CLA	CHA-CBD-CGD-O1D
31	5	604	CLA	CAD-CBD-CGD-O1D
31	6	614	CLA	CHA-CBD-CGD-O1D
31	11	603	CLA	CAD-CBD-CGD-O1D
31	11	604	CLA	CAD-CBD-CGD-O1D
31	11	614	CLA	CAD-CBD-CGD-O1D
31	13	604	CLA	CAD-CBD-CGD-O1D
31	14	602	CLA	CHA-CBD-CGD-O2D
31	14	604	CLA	CAD-CBD-CGD-O1D
31	15	603	CLA	CHA-CBD-CGD-O1D
31	16	602	CLA	CHA-CBD-CGD-O1D
31	16	603	CLA	CAD-CBD-CGD-O1D
31	16	604	CLA	CAD-CBD-CGD-O1D
31	B	604	CLA	CHA-CBD-CGD-O1D
31	B	605	CLA	CAD-CBD-CGD-O1D
31	B	606	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	B	607	CLA	CAD-CBD-CGD-O1D
31	B	612	CLA	CAD-CBD-CGD-O1D
31	C	503	CLA	CAD-CBD-CGD-O1D
31	C	504	CLA	CAD-CBD-CGD-O1D
31	C	505	CLA	CAD-CBD-CGD-O1D
31	C	507	CLA	CAD-CBD-CGD-O1D
31	C	509	CLA	CHA-CBD-CGD-O1D
31	C	513	CLA	CAD-CBD-CGD-O1D
31	G	602	CLA	CHA-CBD-CGD-O1D
31	G	603	CLA	CAD-CBD-CGD-O1D
31	N	604	CLA	CAD-CBD-CGD-O1D
31	N	612	CLA	CHA-CBD-CGD-O2D
31	N	614	CLA	CHA-CBD-CGD-O1D
31	R	609	CLA	CHA-CBD-CGD-O1D
31	R	612	CLA	CAD-CBD-CGD-O1D
31	R	614	CLA	CHA-CBD-CGD-O2D
31	S	603	CLA	CHA-CBD-CGD-O2D
31	S	611	CLA	CAD-CBD-CGD-O1D
31	S	612	CLA	CHA-CBD-CGD-O2D
31	Y	615	CLA	CAD-CBD-CGD-O1D
31	Y	602	CLA	CHA-CBD-CGD-O1D
31	Y	603	CLA	CHA-CBD-CGD-O1D
31	Y	604	CLA	CAD-CBD-CGD-O1D
31	b	604	CLA	CHA-CBD-CGD-O1D
31	b	605	CLA	CAD-CBD-CGD-O1D
31	b	606	CLA	CAD-CBD-CGD-O1D
31	b	607	CLA	CAD-CBD-CGD-O1D
31	b	612	CLA	CAD-CBD-CGD-O1D
31	c	503	CLA	CAD-CBD-CGD-O1D
31	c	504	CLA	CAD-CBD-CGD-O1D
31	c	505	CLA	CAD-CBD-CGD-O1D
31	c	506	CLA	CAD-CBD-CGD-O1D
31	c	507	CLA	CAD-CBD-CGD-O1D
31	c	509	CLA	CHA-CBD-CGD-O1D
31	c	513	CLA	CAD-CBD-CGD-O1D
31	c	514	CLA	CHA-CBD-CGD-O1D
31	g	602	CLA	CHA-CBD-CGD-O1D
31	g	603	CLA	CAD-CBD-CGD-O1D
31	g	604	CLA	CAD-CBD-CGD-O1D
31	n	604	CLA	CAD-CBD-CGD-O1D
31	n	614	CLA	CHA-CBD-CGD-O2D
31	r	609	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	s	612	CLA	CHA-CBD-CGD-O2D
31	y	602	CLA	CHA-CBD-CGD-O1D
31	y	603	CLA	CHA-CBD-CGD-O1D
31	y	604	CLA	CAD-CBD-CGD-O1D
32	1	615	LHG	C4-O6-P-O5
32	3	616	LHG	C4-O6-P-O4
32	3	617	LHG	C4-O6-P-O3
32	3	617	LHG	C4-O6-P-O5
32	6	617	LHG	C3-O3-P-O5
32	6	617	LHG	C4-O6-P-O3
32	6	617	LHG	C4-O6-P-O5
32	14	615	LHG	C3-O3-P-O5
32	14	615	LHG	C4-O6-P-O3
32	A	413	LHG	C3-O3-P-O5
32	A	415	LHG	C3-O3-P-O5
32	A	415	LHG	C4-O6-P-O3
32	C	521	LHG	C4-O6-P-O5
32	D	412	LHG	C3-O3-P-O4
32	D	412	LHG	C4-O6-P-O5
32	G	615	LHG	C3-O3-P-O5
32	L	102	LHG	C3-O3-P-O5
32	L	102	LHG	C4-O6-P-O4
32	R	621	LHG	C3-O3-P-O5
32	R	619	LHG	C3-O3-P-O5
32	S	621	LHG	C3-O3-P-O5
32	Y	616	LHG	C4-O6-P-O4
32	a	401	LHG	C4-O6-P-O3
32	a	401	LHG	C4-O6-P-O5
32	d	413	LHG	C3-O3-P-O4
32	d	413	LHG	C4-O6-P-O5
32	g	615	LHG	C3-O3-P-O5
32	l	102	LHG	C3-O3-P-O5
32	l	102	LHG	C4-O6-P-O4
32	r	621	LHG	C3-O3-P-O5
32	r	621	LHG	C4-O6-P-O3
32	r	619	LHG	C3-O3-P-O5
32	s	621	LHG	C3-O3-P-O5
32	y	616	LHG	C3-O3-P-O4
38	D	402	PHO	CHA-CBD-CGD-O1D
38	D	402	PHO	CHA-CBD-CGD-O2D
32	n	616	LHG	C18-C19-C20-C21
41	j	102	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	G	615	LHG	C15-C16-C17-C18
31	12	602	CLA	C4-C3-C5-C6
31	s	602	CLA	C4-C3-C5-C6
31	13	604	CLA	C2B-C3B-CAB-CBB
31	16	604	CLA	C2B-C3B-CAB-CBB
31	B	611	CLA	C2B-C3B-CAB-CBB
31	C	510	CLA	C2B-C3B-CAB-CBB
31	R	602	CLA	C2B-C3B-CAB-CBB
31	R	608	CLA	C2B-C3B-CAB-CBB
31	b	611	CLA	C2B-C3B-CAB-CBB
31	c	510	CLA	C2B-C3B-CAB-CBB
31	r	608	CLA	C2B-C3B-CAB-CBB
39	C	516	BCR	C1-C6-C7-C8
39	b	617	BCR	C5-C6-C7-C8
41	D	414	LMG	O7-C10-C11-C12
41	d	415	LMG	O7-C10-C11-C12
31	R	608	CLA	C2-C3-C5-C6
42	A	410	PL9	C23-C24-C26-C27
32	D	409	LHG	C29-C30-C31-C32
44	B	623	STE	C10-C11-C12-C13
30	4	609	CHL	C5-C6-C7-C8
30	6	609	CHL	C10-C11-C12-C13
32	4	615	LHG	C5-C4-O6-P
32	C	521	LHG	C2-C3-O3-P
32	C	521	LHG	C5-C4-O6-P
32	S	621	LHG	C5-C4-O6-P
32	Y	617	LHG	C2-C3-O3-P
32	c	521	LHG	C2-C3-O3-P
32	c	521	LHG	C5-C4-O6-P
32	n	616	LHG	C5-C4-O6-P
32	r	621	LHG	C5-C4-O6-P
32	s	621	LHG	C5-C4-O6-P
32	y	616	LHG	C5-C4-O6-P
31	b	608	CLA	C5-C6-C7-C8
31	n	603	CLA	C5-C6-C7-C8
31	4	602	CLA	C11-C12-C13-C14
31	C	514	CLA	C16-C17-C18-C20
31	G	603	CLA	C6-C7-C8-C10
31	Y	613	CLA	CAA-CBA-CGA-O2A
31	6	611	CLA	O1A-CGA-O2A-C1
32	L	102	LHG	C11-C12-C13-C14
32	S	621	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
36	7	201	3PH	C21-C22-C23-C24
32	4	615	LHG	C15-C16-C17-C18
32	l	102	LHG	C14-C15-C16-C17
31	N	613	CLA	C6-C7-C8-C9
32	R	619	LHG	C23-C24-C25-C26
31	1	603	CLA	O1A-CGA-O2A-C1
31	Y	604	CLA	CBA-CGA-O2A-C1
31	Y	614	CLA	O2A-C1-C2-C3
32	L	102	LHG	C14-C15-C16-C17
30	13	609	CHL	O2A-C1-C2-C3
32	Y	618	LHG	C6-C5-O7-C7
31	3	611	CLA	CAA-CBA-CGA-O2A
31	r	614	CLA	C2-C3-C5-C6
30	1	605	CHL	C3C-C2C-CMC-OMC
30	2	609	CHL	C3C-C2C-CMC-OMC
30	5	609	CHL	C3C-C2C-CMC-OMC
30	11	605	CHL	C3C-C2C-CMC-OMC
30	13	609	CHL	C3C-C2C-CMC-OMC
30	G	609	CHL	C3C-C2C-CMC-OMC
30	g	606	CHL	C3C-C2C-CMC-OMC
30	g	609	CHL	C3C-C2C-CMC-OMC
30	2	609	CHL	C16-C17-C18-C20
31	N	611	CLA	C11-C12-C13-C14
31	b	604	CLA	C16-C17-C18-C19
31	b	609	CLA	C16-C17-C18-C20
32	a	414	LHG	O6-C4-C5-C6
32	D	408	LHG	C23-C24-C25-C26
31	6	613	CLA	O1A-CGA-O2A-C1
32	A	411	LHG	C10-C11-C12-C13
30	Y	609	CHL	C14-C13-C15-C16
30	y	607	CHL	C11-C10-C8-C9
30	y	609	CHL	C14-C13-C15-C16
31	1	602	CLA	C6-C7-C8-C9
31	1	602	CLA	C11-C10-C8-C9
31	3	604	CLA	C6-C7-C8-C9
31	6	604	CLA	C6-C7-C8-C9
31	B	604	CLA	C11-C10-C8-C9
31	B	612	CLA	C11-C12-C13-C14
31	S	614	CLA	C11-C12-C13-C14
31	c	503	CLA	C14-C13-C15-C16
31	r	603	CLA	C14-C13-C15-C16
31	R	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
31	S	602	CLA	C11-C10-C8-C7
31	d	402	CLA	C12-C13-C15-C16
31	r	610	CLA	C6-C7-C8-C10
31	s	604	CLA	C11-C10-C8-C7
32	a	414	LHG	O6-C4-C5-O7
32	R	621	LHG	C9-C10-C11-C12
32	S	621	LHG	C32-C33-C34-C35
30	2	609	CHL	C16-C17-C18-C19
30	N	607	CHL	C16-C17-C18-C20
30	r	605	CHL	C6-C7-C8-C10
30	r	606	CHL	C16-C17-C18-C20
40	L	101	SQD	C11-C10-C9-C8
30	g	609	CHL	O1A-CGA-O2A-C1
31	n	613	CLA	C2C-C3C-CAC-CBC
46	W	501	DGD	CAB-CBB-CCB-CDB
32	r	619	LHG	C13-C14-C15-C16
32	s	617	LHG	C10-C11-C12-C13
31	13	602	CLA	C5-C6-C7-C8
31	G	613	CLA	C4-C3-C5-C6
31	c	514	CLA	CAA-CBA-CGA-O2A
31	C	509	CLA	C4C-C3C-CAC-CBC
31	n	602	CLA	CBA-CGA-O2A-C1
31	3	610	CLA	C11-C12-C13-C14
31	12	602	CLA	C11-C12-C13-C14
31	N	613	CLA	C6-C7-C8-C10
32	S	617	LHG	C26-C27-C28-C29
32	d	409	LHG	C25-C26-C27-C28
32	r	621	LHG	C25-C26-C27-C28
31	c	509	CLA	C4C-C3C-CAC-CBC
41	w	501	LMG	C28-C29-C30-C31
40	D	411	SQD	O6-C44-C45-O47
40	d	414	SQD	O6-C44-C45-O47
30	4	607	CHL	CAA-CBA-CGA-O2A
43	Y	620	LNL	C15-C16-C17-C18
43	r	620	LNL	C15-C16-C17-C18
30	N	606	CHL	C8-C10-C11-C12
30	S	606	CHL	C5-C6-C7-C8
46	c	517	DGD	C9B-CAB-CBB-CCB
30	r	605	CHL	C6-C7-C8-C9
31	B	609	CLA	C16-C17-C18-C20
31	D	405	CLA	C16-C17-C18-C20
31	b	609	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	b	611	CLA	C16-C17-C18-C19
32	S	617	LHG	C10-C11-C12-C13
41	j	102	LMG	C33-C34-C35-C36
40	l	101	SQD	O47-C7-C8-C9
30	14	608	CHL	C2C-C3C-CAC-CBC
31	12	612	CLA	C2A-CAA-CBA-CGA
31	b	607	CLA	C2A-CAA-CBA-CGA
32	A	411	LHG	C14-C15-C16-C17
41	J	102	LMG	C33-C34-C35-C36
31	b	608	CLA	CBA-CGA-O2A-C1
31	16	603	CLA	C10-C11-C12-C13
32	16	616	LHG	C28-C29-C30-C31
31	a	407	CLA	C4-C3-C5-C6
31	y	615	CLA	C4-C3-C5-C6
32	A	411	LHG	C16-C17-C18-C19
32	l	102	LHG	C11-C12-C13-C14
31	R	601	CLA	O2A-C1-C2-C3
31	g	614	CLA	O2A-C1-C2-C3
31	B	611	CLA	C16-C17-C18-C19
31	15	604	CLA	CAA-CBA-CGA-O2A
31	C	510	CLA	CAA-CBA-CGA-O2A
31	C	514	CLA	CAA-CBA-CGA-O2A
31	s	609	CLA	CAA-CBA-CGA-O2A
31	y	613	CLA	CAA-CBA-CGA-O2A
32	L	102	LHG	C11-C10-C9-C8
32	a	414	LHG	C9-C10-C11-C12
32	r	621	LHG	C4-C5-C6-O8
30	13	601	CHL	C2C-C3C-CAC-CBC
31	S	604	CLA	CAA-CBA-CGA-O2A
31	n	613	CLA	CAA-CBA-CGA-O2A
32	A	415	LHG	O8-C23-C24-C25
30	13	606	CHL	C11-C12-C13-C15
31	C	506	CLA	C16-C17-C18-C20
31	y	612	CLA	C16-C17-C18-C19
30	2	609	CHL	C1C-C2C-CMC-OMC
30	5	609	CHL	C1C-C2C-CMC-OMC
30	11	605	CHL	C1C-C2C-CMC-OMC
30	g	609	CHL	C1C-C2C-CMC-OMC
31	15	603	CLA	CBA-CGA-O2A-C1
32	6	616	LHG	C7-C8-C9-C10
31	12	612	CLA	C2C-C3C-CAC-CBC
32	3	617	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
40	d	412	SQD	C45-C44-O6-C1
41	d	410	LMG	C8-C7-O1-C1
46	C	517	DGD	C9B-CAB-CBB-CCB
32	6	617	LHG	C14-C15-C16-C17
30	y	601	CHL	C2A-CAA-CBA-CGA
31	15	609	CLA	C2A-CAA-CBA-CGA
31	b	614	CLA	C2A-CAA-CBA-CGA
31	c	506	CLA	C2A-CAA-CBA-CGA
30	r	606	CHL	C16-C17-C18-C19
46	C	517	DGD	C1B-C2B-C3B-C4B
32	R	619	LHG	C9-C10-C11-C12
30	N	609	CHL	C4-C3-C5-C6
31	B	616	CLA	C4-C3-C5-C6
42	d	407	PL9	C30-C29-C31-C32
31	13	611	CLA	CBA-CGA-O2A-C1
40	l	101	SQD	C25-C26-C27-C28
31	n	603	CLA	C8-C10-C11-C12
32	1	615	LHG	C12-C13-C14-C15
32	d	409	LHG	C28-C29-C30-C31
31	3	613	CLA	O1A-CGA-O2A-C1
32	6	617	LHG	O1-C1-C2-O2
30	N	607	CHL	C16-C17-C18-C19
31	6	613	CLA	C6-C7-C8-C9
30	15	608	CHL	C11-C10-C8-C9
30	n	605	CHL	C6-C7-C8-C9
31	S	610	CLA	C11-C10-C8-C9
31	c	512	CLA	C11-C12-C13-C14
41	B	621	LMG	C35-C36-C37-C38
30	s	607	CHL	O1D-CGD-O2D-CED
31	S	609	CLA	CBA-CGA-O2A-C1
32	16	616	LHG	C5-C4-O6-P
32	Y	616	LHG	C5-C4-O6-P
31	d	402	CLA	O1D-CGD-O2D-CED
31	C	506	CLA	C13-C15-C16-C17
31	Y	604	CLA	O1A-CGA-O2A-C1
31	c	504	CLA	C16-C17-C18-C19
31	B	608	CLA	CBA-CGA-O2A-C1
32	A	415	LHG	C23-C24-C25-C26
31	b	615	CLA	C5-C6-C7-C8
31	r	603	CLA	C13-C15-C16-C17
30	g	609	CHL	C2A-CAA-CBA-CGA
31	2	612	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	B	601	CLA	C4-C3-C5-C6
31	16	611	CLA	C2-C3-C5-C6
31	R	610	CLA	C2-C3-C5-C6
31	R	613	CLA	C2-C3-C5-C6
31	r	610	CLA	C2-C3-C5-C6
43	a	412	LNL	C7-C8-C9-C10
32	a	411	LHG	C14-C15-C16-C17
32	D	412	LHG	C16-C17-C18-C19
31	16	604	CLA	CBA-CGA-O2A-C1
49	F	101	HEM	C4C-C3C-CAC-CBC
49	f	101	HEM	C4C-C3C-CAC-CBC
31	B	609	CLA	C16-C17-C18-C19
31	C	514	CLA	C16-C17-C18-C19
30	1	601	CHL	C11-C10-C8-C7
30	Y	609	CHL	C12-C13-C15-C16
30	y	609	CHL	C12-C13-C15-C16
31	B	606	CLA	C12-C13-C15-C16
31	B	612	CLA	C12-C13-C15-C16
31	N	602	CLA	C12-C13-C15-C16
31	N	611	CLA	C6-C7-C8-C10
31	S	611	CLA	C11-C12-C13-C15
31	b	606	CLA	C12-C13-C15-C16
31	b	612	CLA	C12-C13-C15-C16
31	s	611	CLA	C11-C12-C13-C15
30	n	607	CHL	C15-C16-C17-C18
41	K	102	LMG	C11-C12-C13-C14
32	13	616	LHG	C31-C32-C33-C34
32	D	408	LHG	C10-C11-C12-C13
31	C	504	CLA	C15-C16-C17-C18
36	b	623	3PH	C24-C25-C26-C27
30	13	606	CHL	O1A-CGA-O2A-C1
32	3	617	LHG	C26-C27-C28-C29
31	S	614	CLA	CBA-CGA-O2A-C1
40	L	101	SQD	C31-C32-C33-C34
30	13	601	CHL	C6-C7-C8-C9
31	6	613	CLA	C6-C7-C8-C10
30	n	607	CHL	O1D-CGD-O2D-CED
50	n	620	PAM	C7-C8-C9-C10
32	y	617	LHG	C23-C24-C25-C26
31	R	614	CLA	O1D-CGD-O2D-CED
30	n	606	CHL	C8-C10-C11-C12
31	B	615	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	R	610	CLA	C8-C10-C11-C12
32	a	401	LHG	O7-C5-C6-O8
32	g	615	LHG	C12-C13-C14-C15
30	4	608	CHL	C3A-C2A-CAA-CBA
30	G	608	CHL	C3A-C2A-CAA-CBA
30	R	605	CHL	C3A-C2A-CAA-CBA
30	Y	606	CHL	C3A-C2A-CAA-CBA
30	g	601	CHL	C3A-C2A-CAA-CBA
30	g	608	CHL	C3A-C2A-CAA-CBA
31	4	604	CLA	C3A-C2A-CAA-CBA
31	5	604	CLA	C3A-C2A-CAA-CBA
31	6	613	CLA	C3A-C2A-CAA-CBA
31	D	404	CLA	C3A-C2A-CAA-CBA
31	D	405	CLA	C3A-C2A-CAA-CBA
31	Y	611	CLA	C3A-C2A-CAA-CBA
31	b	605	CLA	C3A-C2A-CAA-CBA
31	b	609	CLA	C3A-C2A-CAA-CBA
31	n	613	CLA	C3A-C2A-CAA-CBA
31	r	601	CLA	C3A-C2A-CAA-CBA
31	y	611	CLA	C3A-C2A-CAA-CBA
42	D	407	PL9	C30-C29-C31-C32
30	N	609	CHL	C2C-C3C-CAC-CBC
32	r	621	LHG	O7-C7-C8-C9
32	S	617	LHG	C7-C8-C9-C10
46	c	517	DGD	C1B-C2B-C3B-C4B
41	B	621	LMG	C37-C38-C39-C40
33	5	614	LUT	C20-C13-C14-C15
34	2	616	NEX	C39-C29-C30-C31
34	3	621	NEX	C39-C29-C30-C31
34	5	616	NEX	C39-C29-C30-C31
34	6	621	NEX	C39-C29-C30-C31
34	12	616	NEX	C39-C29-C30-C31
34	13	619	NEX	C39-C29-C30-C31
34	15	616	NEX	C39-C29-C30-C31
34	16	619	NEX	C39-C29-C30-C31
34	G	618	NEX	C39-C29-C30-C31
34	N	619	NEX	C39-C29-C30-C31
34	R	617	NEX	C39-C29-C30-C31
34	S	620	NEX	C39-C29-C30-C31
34	Y	623	NEX	C39-C29-C30-C31
34	g	618	NEX	C39-C29-C30-C31
34	n	619	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
34	r	617	NEX	C39-C29-C30-C31
34	s	620	NEX	C39-C29-C30-C31
34	y	624	NEX	C39-C29-C30-C31
44	B	623	STE	C11-C12-C13-C14
32	d	409	LHG	C24-C25-C26-C27
41	s	616	LMG	C11-C12-C13-C14
43	Y	620	LNL	O1-C1-C2-C3
32	g	615	LHG	C9-C10-C11-C12
40	A	408	SQD	C10-C11-C12-C13
40	a	409	SQD	C10-C11-C12-C13
30	3	607	CHL	C2-C1-O2A-CGA
30	12	606	CHL	C2-C1-O2A-CGA
30	16	607	CHL	C2-C1-O2A-CGA
30	N	608	CHL	C2-C1-O2A-CGA
30	Y	607	CHL	C2-C1-O2A-CGA
31	3	611	CLA	C2-C1-O2A-CGA
31	Y	615	CLA	C2-C1-O2A-CGA
30	N	605	CHL	C3-C5-C6-C7
31	Y	612	CLA	C16-C17-C18-C19
30	13	606	CHL	C10-C11-C12-C13
32	n	616	LHG	C26-C27-C28-C29
32	a	401	LHG	C23-C24-C25-C26
31	c	502	CLA	C15-C16-C17-C18
32	3	617	LHG	C19-C20-C21-C22
31	r	613	CLA	C5-C6-C7-C8
31	y	610	CLA	C15-C16-C17-C18
30	13	605	CHL	C4-C3-C5-C6
42	d	407	PL9	C40-C39-C41-C42
31	c	510	CLA	CAA-CBA-CGA-O2A
31	12	603	CLA	C6-C7-C8-C9
31	Y	602	CLA	C16-C17-C18-C20
32	D	409	LHG	C1-C2-C3-O3
32	a	401	LHG	C1-C2-C3-O3
32	d	409	LHG	C1-C2-C3-O3
32	r	619	LHG	C12-C13-C14-C15
41	J	102	LMG	C20-C21-C22-C23
30	2	606	CHL	CAA-CBA-CGA-O2A
31	n	612	CLA	CAA-CBA-CGA-O2A
32	d	408	LHG	C34-C35-C36-C37
31	C	512	CLA	C5-C6-C7-C8
32	a	401	LHG	C4-C5-C6-O8
32	l	102	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
32	r	618	LHG	C4-C5-C6-O8
42	A	410	PL9	C19-C21-C22-C23
42	a	410	PL9	C19-C21-C22-C23
41	j	102	LMG	C20-C21-C22-C23
32	y	618	LHG	C35-C36-C37-C38
31	c	514	CLA	C3-C5-C6-C7
30	6	607	CHL	C15-C16-C17-C18
32	3	617	LHG	C24-C25-C26-C27
30	s	601	CHL	CAA-CBA-CGA-O2A
30	5	609	CHL	C6-C7-C8-C9
30	6	607	CHL	C6-C7-C8-C9
30	6	607	CHL	C11-C10-C8-C9
30	G	609	CHL	C6-C7-C8-C9
30	N	609	CHL	C14-C13-C15-C16
30	g	601	CHL	C11-C10-C8-C9
31	4	602	CLA	C11-C10-C8-C9
31	11	602	CLA	C11-C10-C8-C9
31	13	602	CLA	C11-C12-C13-C14
31	16	611	CLA	C6-C7-C8-C9
31	B	603	CLA	C11-C10-C8-C9
31	C	502	CLA	C11-C12-C13-C14
31	C	510	CLA	C6-C7-C8-C9
31	C	514	CLA	C14-C13-C15-C16
31	S	604	CLA	C6-C7-C8-C9
31	b	603	CLA	C11-C10-C8-C9
31	c	510	CLA	C6-C7-C8-C9
31	c	514	CLA	C6-C7-C8-C9
31	y	602	CLA	C11-C10-C8-C9
32	D	412	LHG	C29-C30-C31-C32
36	B	624	3PH	C22-C23-C24-C25
32	6	617	LHG	O1-C1-C2-C3
32	16	616	LHG	O1-C1-C2-C3
32	d	413	LHG	C29-C30-C31-C32
32	11	615	LHG	C26-C27-C28-C29
32	d	408	LHG	C11-C12-C13-C14
30	S	601	CHL	CAA-CBA-CGA-O2A
31	r	601	CLA	CAA-CBA-CGA-O2A
32	Y	618	LHG	C4-C5-O7-C7
36	B	624	3PH	C21-C22-C23-C24
31	A	403	CLA	C3-C5-C6-C7
30	1	609	CHL	C1-C2-C3-C4
30	2	609	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
30	3	606	CHL	C1A-C2A-CAA-CBA
30	3	609	CHL	C1A-C2A-CAA-CBA
30	5	605	CHL	C1A-C2A-CAA-CBA
30	5	609	CHL	C1A-C2A-CAA-CBA
30	6	608	CHL	C1A-C2A-CAA-CBA
30	6	609	CHL	C1A-C2A-CAA-CBA
30	12	606	CHL	C1A-C2A-CAA-CBA
30	14	607	CHL	C1A-C2A-CAA-CBA
30	14	608	CHL	C1A-C2A-CAA-CBA
30	15	606	CHL	C1A-C2A-CAA-CBA
30	G	606	CHL	C1A-C2A-CAA-CBA
30	Y	601	CHL	C1A-C2A-CAA-CBA
30	y	601	CHL	C1A-C2A-CAA-CBA
31	4	610	CLA	C1-C2-C3-C4
31	15	602	CLA	C1-C2-C3-C4
31	C	504	CLA	C1-C2-C3-C4
31	C	512	CLA	C1-C2-C3-C4
31	D	405	CLA	C1-C2-C3-C4
31	G	603	CLA	C1-C2-C3-C4
31	N	613	CLA	C1-C2-C3-C4
31	S	611	CLA	C1-C2-C3-C4
31	S	614	CLA	C1-C2-C3-C4
31	c	504	CLA	C1-C2-C3-C4
31	c	505	CLA	C1-C2-C3-C4
31	d	405	CLA	C1-C2-C3-C4
31	g	602	CLA	CBD-CGD-O2D-CED
31	g	603	CLA	C1-C2-C3-C4
31	n	603	CLA	C1-C2-C3-C4
31	r	614	CLA	C1-C2-C3-C4
31	s	610	CLA	C1-C2-C3-C4
31	s	614	CLA	C1-C2-C3-C4
38	D	402	PHO	C1-C2-C3-C4
32	n	616	LHG	C31-C32-C33-C34
32	16	616	LHG	C9-C10-C11-C12
31	12	611	CLA	CAA-CBA-CGA-O2A
31	15	611	CLA	CAA-CBA-CGA-O2A
32	16	616	LHG	C25-C26-C27-C28
42	D	407	PL9	C40-C39-C41-C42
31	R	609	CLA	C16-C17-C18-C20
31	4	613	CLA	CAA-CBA-CGA-O2A
30	16	606	CHL	C2-C3-C5-C6
46	w	502	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
43	Y	620	LNL	O2-C1-C2-C3
30	16	607	CHL	C2A-CAA-CBA-CGA
31	16	613	CLA	C2A-CAA-CBA-CGA
31	16	615	CLA	C2A-CAA-CBA-CGA
31	Y	615	CLA	C2A-CAA-CBA-CGA
31	4	611	CLA	C1A-C2A-CAA-CBA
31	5	612	CLA	C1A-C2A-CAA-CBA
31	12	604	CLA	C1A-C2A-CAA-CBA
31	14	603	CLA	C1A-C2A-CAA-CBA
31	16	611	CLA	C1A-C2A-CAA-CBA
31	B	605	CLA	C1A-C2A-CAA-CBA
31	C	510	CLA	C1A-C2A-CAA-CBA
31	D	404	CLA	C1A-C2A-CAA-CBA
31	D	405	CLA	C1A-C2A-CAA-CBA
31	R	604	CLA	C1A-C2A-CAA-CBA
31	Y	611	CLA	C1A-C2A-CAA-CBA
31	b	605	CLA	C1A-C2A-CAA-CBA
31	c	510	CLA	C1A-C2A-CAA-CBA
31	r	601	CLA	C1A-C2A-CAA-CBA
31	r	604	CLA	C1A-C2A-CAA-CBA
33	5	614	LUT	C12-C13-C14-C15
34	2	616	NEX	C28-C29-C30-C31
34	3	621	NEX	C28-C29-C30-C31
34	5	616	NEX	C28-C29-C30-C31
34	6	621	NEX	C28-C29-C30-C31
34	12	616	NEX	C28-C29-C30-C31
34	13	619	NEX	C28-C29-C30-C31
34	15	616	NEX	C28-C29-C30-C31
34	16	619	NEX	C28-C29-C30-C31
34	G	618	NEX	C28-C29-C30-C31
34	N	619	NEX	C28-C29-C30-C31
34	R	617	NEX	C28-C29-C30-C31
34	S	620	NEX	C28-C29-C30-C31
34	Y	623	NEX	C28-C29-C30-C31
34	g	618	NEX	C28-C29-C30-C31
34	n	619	NEX	C28-C29-C30-C31
34	r	617	NEX	C28-C29-C30-C31
34	s	620	NEX	C28-C29-C30-C31
34	y	624	NEX	C28-C29-C30-C31
32	3	617	LHG	C28-C29-C30-C31
30	5	606	CHL	CAA-CBA-CGA-O2A
43	Y	619	LNL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
41	K	102	LMG	C10-C11-C12-C13
31	r	602	CLA	C4C-C3C-CAC-CBC
32	s	617	LHG	O6-C4-C5-O7
32	C	521	LHG	C24-C25-C26-C27
31	S	604	CLA	C5-C6-C7-C8
31	2	604	CLA	C2B-C3B-CAB-CBB
31	A	404	CLA	C2B-C3B-CAB-CBB
31	Y	610	CLA	C2B-C3B-CAB-CBB
31	a	404	CLA	C2B-C3B-CAB-CBB
31	y	610	CLA	C2B-C3B-CAB-CBB
33	Y	621	LUT	C1-C6-C7-C8
33	s	618	LUT	C5-C6-C7-C8
33	y	622	LUT	C1-C6-C7-C8
39	C	515	BCR	C5-C6-C7-C8
39	c	515	BCR	C5-C6-C7-C8
39	c	516	BCR	C1-C6-C7-C8
39	h	102	BCR	C1-C6-C7-C8
32	c	521	LHG	C34-C35-C36-C37
32	l	102	LHG	C7-C8-C9-C10
30	11	607	CHL	CAA-CBA-CGA-O1A
32	d	408	LHG	C24-C23-O8-C6
31	s	604	CLA	C5-C6-C7-C8
32	1	615	LHG	C5-C4-O6-P
32	3	616	LHG	C5-C4-O6-P
32	D	409	LHG	C2-C3-O3-P
32	d	409	LHG	C2-C3-O3-P
31	d	402	CLA	C3-C5-C6-C7
30	2	606	CHL	CAA-CBA-CGA-O1A
43	Y	619	LNL	O2-C1-C2-C3
30	6	605	CHL	C4-C3-C5-C6
32	N	616	LHG	O6-C4-C5-C6
30	16	607	CHL	C2-C3-C5-C6
31	11	614	CLA	O2A-C1-C2-C3
31	14	614	CLA	O2A-C1-C2-C3
31	G	614	CLA	O2A-C1-C2-C3
30	2	609	CHL	C6-C7-C8-C10
30	3	609	CHL	C11-C12-C13-C15
30	4	609	CHL	C12-C13-C15-C16
30	11	601	CHL	C11-C10-C8-C7
30	13	609	CHL	C11-C10-C8-C7
30	S	606	CHL	C11-C10-C8-C7
30	s	606	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	3	602	CLA	C11-C10-C8-C7
31	4	602	CLA	C6-C7-C8-C10
31	6	602	CLA	C11-C10-C8-C7
31	11	602	CLA	C11-C10-C8-C7
31	C	512	CLA	C11-C12-C13-C15
31	D	404	CLA	C12-C13-C15-C16
31	Y	612	CLA	C11-C10-C8-C7
31	b	609	CLA	C11-C10-C8-C7
31	c	503	CLA	C12-C13-C15-C16
31	d	404	CLA	C6-C7-C8-C10
31	r	603	CLA	C12-C13-C15-C16
38	A	405	PHO	C12-C13-C15-C16
30	3	609	CHL	C16-C17-C18-C19
31	b	602	CLA	C16-C17-C18-C20
31	s	611	CLA	C16-C17-C18-C19
30	2	607	CHL	C2A-CAA-CBA-CGA
31	2	602	CLA	C2A-CAA-CBA-CGA
31	6	612	CLA	C2A-CAA-CBA-CGA
31	S	610	CLA	C2A-CAA-CBA-CGA
31	y	615	CLA	C2A-CAA-CBA-CGA
41	s	616	LMG	C15-C16-C17-C18
32	16	616	LHG	O7-C5-C6-O8
32	l	102	LHG	O7-C5-C6-O8
46	W	501	DGD	O1G-C1G-C2G-O2G
43	R	620	LNL	O2-C1-C2-C3
43	r	620	LNL	O2-C1-C2-C3
42	A	410	PL9	C4-C3-C7-C8
43	C	523	LNL	C10-C11-C12-C13
43	C	524	LNL	C10-C11-C12-C13
43	I	101	LNL	C10-C11-C12-C13
43	c	523	LNL	C10-C11-C12-C13
43	c	524	LNL	C10-C11-C12-C13
43	i	101	LNL	C10-C11-C12-C13
43	r	620	LNL	C10-C11-C12-C13
43	r	620	LNL	C13-C14-C15-C16
43	x	201	LNL	C13-C14-C15-C16
31	C	511	CLA	C13-C15-C16-C17
31	b	608	CLA	C8-C10-C11-C12
32	Y	618	LHG	C16-C17-C18-C19
31	15	603	CLA	C3-C5-C6-C7
31	12	611	CLA	CAA-CBA-CGA-O1A
30	3	601	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
31	13	613	CLA	C2C-C3C-CAC-CBC
31	A	403	CLA	O1D-CGD-O2D-CED
31	6	610	CLA	C11-C12-C13-C15
32	d	409	LHG	C31-C32-C33-C34
31	n	610	CLA	C10-C11-C12-C13
30	6	601	CHL	C2C-C3C-CAC-CBC
40	L	101	SQD	C10-C11-C12-C13
31	15	611	CLA	CAA-CBA-CGA-O1A
31	N	612	CLA	CAA-CBA-CGA-O2A
30	N	606	CHL	C4-C3-C5-C6
31	N	613	CLA	C4-C3-C5-C6
31	b	616	CLA	C4-C3-C5-C6
31	d	404	CLA	C4-C3-C5-C6
42	a	410	PL9	C12-C11-C9-C10
40	D	413	SQD	C30-C31-C32-C33
42	d	407	PL9	C38-C39-C41-C42
41	v	101	LMG	C11-C12-C13-C14
30	6	607	CHL	C2-C1-O2A-CGA
30	14	609	CHL	C1-C2-C3-C5
30	R	605	CHL	C1-C2-C3-C5
30	n	601	CHL	C1-C2-C3-C5
31	1	610	CLA	C1-C2-C3-C5
31	2	602	CLA	C1-C2-C3-C5
31	11	613	CLA	C1-C2-C3-C5
31	12	609	CLA	C1-C2-C3-C5
31	13	611	CLA	C1-C2-C3-C5
31	14	613	CLA	C1-C2-C3-C5
31	15	602	CLA	C1-C2-C3-C5
31	16	602	CLA	C1-C2-C3-C5
31	B	604	CLA	C1-C2-C3-C5
31	C	505	CLA	C2-C1-O2A-CGA
31	G	603	CLA	C1-C2-C3-C5
31	S	605	CLA	C2-C1-O2A-CGA
31	S	611	CLA	C1-C2-C3-C5
31	y	603	CLA	C1-C2-C3-C5
31	B	615	CLA	C13-C15-C16-C17
31	B	606	CLA	C16-C17-C18-C20
31	6	604	CLA	C5-C6-C7-C8
36	b	623	3PH	O21-C21-C22-C23
32	y	618	LHG	C23-C24-C25-C26
31	r	612	CLA	C1-C2-C3-C5
30	11	601	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	13	602	CLA	C2A-CAA-CBA-CGA
31	C	511	CLA	C2A-CAA-CBA-CGA
31	n	614	CLA	CAA-CBA-CGA-O1A
30	6	607	CHL	C14-C13-C15-C16
30	13	607	CHL	C11-C10-C8-C9
30	Y	607	CHL	C6-C7-C8-C9
31	B	613	CLA	C11-C10-C8-C9
31	G	613	CLA	C14-C13-C15-C16
31	N	611	CLA	C6-C7-C8-C9
31	a	404	CLA	C14-C13-C15-C16
32	16	616	LHG	C24-C25-C26-C27
43	R	620	LNL	O1-C1-C2-C3
30	y	609	CHL	C2C-C3C-CAC-CBC
30	g	607	CHL	C1-C2-C3-C4
30	Y	607	CHL	C4-C3-C5-C6
30	y	609	CHL	C4-C3-C5-C6
31	S	602	CLA	C4-C3-C5-C6
31	S	611	CLA	C4-C3-C5-C6
32	6	616	LHG	C5-C4-O6-P
32	R	621	LHG	C5-C4-O6-P
32	y	618	LHG	C5-C4-O6-P
40	L	101	SQD	O47-C7-C8-C9
31	B	601	CLA	C2-C3-C5-C6
31	N	610	CLA	C2-C3-C5-C6
31	Y	610	CLA	C2-C3-C5-C6
42	D	407	PL9	C38-C39-C41-C42
32	d	408	LHG	O10-C23-O8-C6
31	c	512	CLA	C5-C6-C7-C8
31	B	610	CLA	C16-C17-C18-C19
31	b	610	CLA	C16-C17-C18-C19
30	15	605	CHL	CAA-CBA-CGA-O2A
32	d	413	LHG	C24-C25-C26-C27
31	r	601	CLA	O2A-C1-C2-C3
30	y	601	CHL	C10-C11-C12-C13
31	c	507	CLA	C13-C15-C16-C17
32	R	619	LHG	C27-C28-C29-C30
32	g	615	LHG	C18-C19-C20-C21
32	16	616	LHG	C4-C5-C6-O8
32	r	619	LHG	C4-C5-C6-O8
30	3	601	CHL	C5-C6-C7-C8
32	s	621	LHG	C13-C14-C15-C16
31	n	614	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	g	605	CHL	C2-C1-O2A-CGA
31	3	602	CLA	C2A-CAA-CBA-CGA
31	5	610	CLA	C2A-CAA-CBA-CGA
31	c	511	CLA	C2A-CAA-CBA-CGA
30	13	609	CHL	C11-C12-C13-C14
31	B	603	CLA	C16-C17-C18-C20
31	b	602	CLA	C16-C17-C18-C19
32	D	408	LHG	C34-C35-C36-C37
49	F	101	HEM	CAD-CBD-CGD-O2D
49	f	101	HEM	CAD-CBD-CGD-O2D
32	D	412	LHG	C24-C25-C26-C27
32	Y	616	LHG	C29-C30-C31-C32
31	R	611	CLA	O1D-CGD-O2D-CED
31	3	610	CLA	C8-C10-C11-C12
32	D	408	LHG	O1-C1-C2-O2
32	N	616	LHG	O6-C4-C5-O7
30	Y	609	CHL	C4-C3-C5-C6
30	y	607	CHL	C4-C3-C5-C6
31	D	404	CLA	C4-C3-C5-C6
31	y	612	CLA	C4-C3-C5-C6
31	S	604	CLA	CAA-CBA-CGA-O1A
31	y	613	CLA	CAA-CBA-CGA-O1A
42	D	407	PL9	C28-C29-C31-C32
42	d	407	PL9	C28-C29-C31-C32
30	3	609	CHL	C16-C17-C18-C20
31	b	603	CLA	C16-C17-C18-C20
32	16	616	LHG	C32-C33-C34-C35
31	3	604	CLA	C5-C6-C7-C8
31	A	403	CLA	O1A-CGA-O2A-C1
31	d	402	CLA	O1A-CGA-O2A-C1
41	J	102	LMG	C19-C20-C21-C22
31	C	514	CLA	CAA-CBA-CGA-O1A
43	W	502	LNL	C7-C8-C9-C10
43	w	503	LNL	C7-C8-C9-C10
43	y	620	LNL	C7-C8-C9-C10
50	N	621	PAM	C9-C10-C11-C12
50	n	620	PAM	C9-C10-C11-C12
31	R	608	CLA	CAA-CBA-CGA-O2A
32	Y	618	LHG	O8-C23-C24-C25
41	H	102	LMG	O7-C10-C11-C12
31	11	603	CLA	C5-C6-C7-C8
41	j	102	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
41	d	410	LMG	C17-C18-C19-C20
31	3	613	CLA	C6-C7-C8-C10
31	B	602	CLA	C16-C17-C18-C19
31	B	602	CLA	C16-C17-C18-C20
31	B	616	CLA	C11-C12-C13-C14
31	Y	602	CLA	C16-C17-C18-C19
31	c	506	CLA	C16-C17-C18-C20
31	S	615	CLA	C2-C1-O2A-CGA
30	3	605	CHL	CHA-CBD-CGD-O1D
30	6	605	CHL	CHA-CBD-CGD-O1D
30	11	606	CHL	CHA-CBD-CGD-O2D
30	12	608	CHL	CHA-CBD-CGD-O1D
30	13	601	CHL	CHA-CBD-CGD-O2D
30	13	609	CHL	CHA-CBD-CGD-O1D
30	14	605	CHL	CHA-CBD-CGD-O1D
30	14	606	CHL	CHA-CBD-CGD-O2D
30	14	609	CHL	CHA-CBD-CGD-O1D
30	15	608	CHL	CHA-CBD-CGD-O1D
30	16	601	CHL	CHA-CBD-CGD-O2D
30	N	605	CHL	CHA-CBD-CGD-O1D
30	n	601	CHL	CHA-CBD-CGD-O1D
30	n	601	CHL	CHA-CBD-CGD-O2D
31	G	602	CLA	CAA-CBA-CGA-O2A
31	2	602	CLA	O1D-CGD-O2D-CED
30	11	607	CHL	CAA-CBA-CGA-O2A
31	13	614	CLA	CAA-CBA-CGA-O1A
31	Y	614	CLA	O1A-CGA-O2A-C1
41	D	414	LMG	C36-C37-C38-C39
41	d	415	LMG	C36-C37-C38-C39
32	6	616	LHG	O6-C4-C5-C6
30	n	606	CHL	C11-C12-C13-C14
31	b	611	CLA	C4-C3-C5-C6
46	C	519	DGD	C5B-C6B-C7B-C8B
32	r	619	LHG	O7-C5-C6-O8
41	A	409	LMG	O1-C7-C8-O7
41	c	522	LMG	O1-C7-C8-O7
41	s	616	LMG	O7-C8-C9-O8
31	B	616	CLA	C10-C11-C12-C13
32	r	621	LHG	C7-C8-C9-C10
30	5	606	CHL	CAA-CBA-CGA-O1A
31	13	614	CLA	CAA-CBA-CGA-O2A
31	S	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
43	y	620	LNL	O1-C1-C2-C3
46	w	502	DGD	O6D-C1D-O3G-C3G
31	b	616	CLA	C5-C6-C7-C8
32	D	409	LHG	C31-C32-C33-C34
32	S	621	LHG	C24-C25-C26-C27
30	n	605	CHL	C11-C10-C8-C7
31	B	609	CLA	C11-C10-C8-C7
31	S	612	CLA	CAA-CBA-CGA-O2A
43	r	620	LNL	O1-C1-C2-C3
31	c	514	CLA	CAA-CBA-CGA-O1A
31	16	613	CLA	C2C-C3C-CAC-CBC
31	B	613	CLA	C13-C15-C16-C17
32	a	401	LHG	O8-C23-C24-C25
32	C	521	LHG	C10-C11-C12-C13
30	G	605	CHL	C2-C1-O2A-CGA
31	12	613	CLA	CAA-CBA-CGA-O1A
30	3	601	CHL	C6-C7-C8-C9
30	N	606	CHL	C11-C10-C8-C9
30	N	607	CHL	C6-C7-C8-C9
30	n	609	CHL	C14-C13-C15-C16
31	4	610	CLA	C6-C7-C8-C9
31	A	404	CLA	C14-C13-C15-C16
31	D	404	CLA	C6-C7-C8-C9
31	D	405	CLA	C14-C13-C15-C16
31	N	602	CLA	C11-C12-C13-C14
31	R	609	CLA	C11-C12-C13-C14
31	b	607	CLA	C11-C10-C8-C9
31	b	613	CLA	C11-C10-C8-C9
31	c	502	CLA	C11-C10-C8-C9
31	d	405	CLA	C14-C13-C15-C16
31	s	614	CLA	C11-C10-C8-C9
31	12	612	CLA	C4C-C3C-CAC-CBC
31	C	505	CLA	O1A-CGA-O2A-C1
30	3	607	CHL	C8-C10-C11-C12
31	b	615	CLA	C13-C15-C16-C17
40	d	414	SQD	C5-C6-S-O8
41	C	522	LMG	C8-C7-O1-C1
41	S	616	LMG	C8-C7-O1-C1
41	c	522	LMG	C8-C7-O1-C1
36	B	624	3PH	C27-C28-C29-C2A
32	L	102	LHG	C7-C8-C9-C10
32	6	617	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
32	S	621	LHG	C12-C13-C14-C15
31	16	614	CLA	CAA-CBA-CGA-O1A
31	16	614	CLA	CAA-CBA-CGA-O2A
30	12	607	CHL	C2A-CAA-CBA-CGA
31	15	602	CLA	C2A-CAA-CBA-CGA
31	B	603	CLA	C2A-CAA-CBA-CGA
31	Y	602	CLA	C2A-CAA-CBA-CGA
31	b	603	CLA	C2A-CAA-CBA-CGA
30	3	605	CHL	C2-C1-O2A-CGA
30	4	607	CHL	C2-C1-O2A-CGA
30	5	601	CHL	C2-C1-O2A-CGA
30	11	601	CHL	C2-C1-O2A-CGA
30	14	601	CHL	C2-C1-O2A-CGA
30	14	609	CHL	C2-C1-O2A-CGA
30	g	608	CHL	C2-C1-O2A-CGA
30	n	608	CHL	C2-C1-O2A-CGA
30	y	607	CHL	C2-C1-O2A-CGA
31	6	611	CLA	C2-C1-O2A-CGA
31	6	615	CLA	C2-C1-O2A-CGA
31	11	611	CLA	C2-C1-O2A-CGA
31	D	404	CLA	C2-C1-O2A-CGA
31	c	503	CLA	C2-C1-O2A-CGA
31	d	404	CLA	C2-C1-O2A-CGA
31	r	601	CLA	C2-C1-O2A-CGA
32	6	617	LHG	C26-C27-C28-C29
31	3	610	CLA	C11-C12-C13-C15
31	3	613	CLA	C6-C7-C8-C9
31	C	502	CLA	C16-C17-C18-C20
31	b	608	CLA	C16-C17-C18-C20
41	b	620	LMG	C14-C15-C16-C17
30	y	606	CHL	C10-C11-C12-C13
31	n	602	CLA	C15-C16-C17-C18
32	S	617	LHG	C23-C24-C25-C26
32	g	615	LHG	C17-C18-C19-C20
30	1	601	CHL	C3A-C2A-CAA-CBA
30	5	608	CHL	C3A-C2A-CAA-CBA
30	11	609	CHL	C3A-C2A-CAA-CBA
31	2	611	CLA	C3A-C2A-CAA-CBA
31	3	613	CLA	C3A-C2A-CAA-CBA
31	5	612	CLA	C3A-C2A-CAA-CBA
31	11	603	CLA	C3A-C2A-CAA-CBA
31	14	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	14	614	CLA	C3A-C2A-CAA-CBA
31	15	602	CLA	C3A-C2A-CAA-CBA
31	B	609	CLA	C3A-C2A-CAA-CBA
31	C	512	CLA	C3A-C2A-CAA-CBA
31	N	604	CLA	C3A-C2A-CAA-CBA
31	b	604	CLA	C3A-C2A-CAA-CBA
31	c	505	CLA	C3A-C2A-CAA-CBA
31	d	405	CLA	C3A-C2A-CAA-CBA
31	n	604	CLA	C3A-C2A-CAA-CBA
31	y	614	CLA	C3A-C2A-CAA-CBA
31	y	615	CLA	C3A-C2A-CAA-CBA
32	6	616	LHG	C13-C14-C15-C16
41	D	414	LMG	C13-C14-C15-C16
31	r	608	CLA	CAA-CBA-CGA-O2A
31	y	610	CLA	C2-C3-C5-C6
41	d	415	LMG	C13-C14-C15-C16
36	7	201	3PH	C3A-C3B-C3C-C3D
43	C	524	LNL	O1-C1-C2-C3
43	c	524	LNL	O1-C1-C2-C3
41	d	415	LMG	C31-C32-C33-C34
30	13	607	CHL	O2A-C1-C2-C3
31	2	603	CLA	O2A-C1-C2-C3
31	5	603	CLA	O2A-C1-C2-C3
31	6	615	CLA	O2A-C1-C2-C3
30	12	605	CHL	CAA-CBA-CGA-O2A
32	14	615	LHG	C33-C34-C35-C36
43	a	412	LNL	C4-C5-C6-C7
31	n	613	CLA	C4C-C3C-CAC-CBC
32	13	616	LHG	C24-C25-C26-C27
31	n	612	CLA	CAA-CBA-CGA-O1A
49	F	101	HEM	CAD-CBD-CGD-O1D
31	a	404	CLA	C2A-CAA-CBA-CGA
31	y	602	CLA	C2A-CAA-CBA-CGA
30	Y	606	CHL	C4-C3-C5-C6
31	G	610	CLA	C5-C6-C7-C8
31	y	603	CLA	C8-C10-C11-C12
41	D	414	LMG	C31-C32-C33-C34
30	13	609	CHL	C8-C10-C11-C12
31	c	506	CLA	C13-C15-C16-C17
32	A	411	LHG	C25-C26-C27-C28
31	Y	604	CLA	C6-C7-C8-C10
43	C	524	LNL	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
43	c	524	LNL	O2-C1-C2-C3
30	4	601	CHL	C8-C10-C11-C12
31	b	616	CLA	C10-C11-C12-C13
32	l	102	LHG	O6-C4-C5-O7
30	5	608	CHL	O2A-C1-C2-C3
30	S	601	CHL	CAA-CBA-CGA-O1A
30	s	601	CHL	CAA-CBA-CGA-O1A
43	i	101	LNL	O1-C1-C2-C3
43	i	101	LNL	O2-C1-C2-C3
32	L	102	LHG	C4-C5-C6-O8
32	R	618	LHG	C4-C5-C6-O8
36	b	623	3PH	C1-C2-C3-O31
32	d	408	LHG	O1-C1-C2-O2
43	I	101	LNL	O1-C1-C2-C3
32	y	618	LHG	C15-C16-C17-C18
31	S	604	CLA	CBA-CGA-O2A-C1
41	B	622	LMG	C31-C32-C33-C34
30	6	606	CHL	C4-C3-C5-C6
30	16	606	CHL	C4-C3-C5-C6
31	R	602	CLA	C4-C3-C5-C6
31	G	604	CLA	C2A-CAA-CBA-CGA
32	g	615	LHG	O8-C23-C24-C25
31	N	612	CLA	CAA-CBA-CGA-O1A
43	I	101	LNL	O2-C1-C2-C3
43	y	620	LNL	O2-C1-C2-C3
49	f	101	HEM	CAD-CBD-CGD-O1D
30	n	606	CHL	C2-C3-C5-C6
32	A	414	LHG	C27-C28-C29-C30
32	r	619	LHG	C24-C25-C26-C27
30	13	607	CHL	C8-C10-C11-C12
31	s	602	CLA	C13-C15-C16-C17
30	3	607	CHL	CAA-CBA-CGA-O2A
32	L	102	LHG	C28-C29-C30-C31
30	1	607	CHL	C1-C2-C3-C5
31	3	612	CLA	CBD-CGD-O2D-CED
30	G	601	CHL	C11-C10-C8-C9
31	4	610	CLA	C11-C12-C13-C14
31	C	509	CLA	C11-C10-C8-C9
31	S	604	CLA	C14-C13-C15-C16
31	b	607	CLA	C6-C7-C8-C9
31	b	613	CLA	C11-C12-C13-C14
31	s	614	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	C	502	CLA	C16-C17-C18-C19
31	b	608	CLA	C16-C17-C18-C19
31	r	602	CLA	C16-C17-C18-C20
31	y	604	CLA	C6-C7-C8-C10
43	r	620	LNL	C7-C8-C9-C10
30	3	609	CHL	CBD-CGD-O2D-CED
30	6	607	CHL	CAA-CBA-CGA-O2A
31	12	602	CLA	CAA-CBA-CGA-O2A
31	C	507	CLA	CAA-CBA-CGA-O2A
31	R	603	CLA	CAA-CBA-CGA-O2A
32	3	616	LHG	O8-C23-C24-C25
32	G	615	LHG	O8-C23-C24-C25
30	14	605	CHL	C2-C1-O2A-CGA
31	C	506	CLA	C4-C3-C5-C6
30	6	605	CHL	O1A-CGA-O2A-C1
30	n	607	CHL	C10-C11-C12-C13
31	R	613	CLA	CAA-CBA-CGA-O2A
32	A	413	LHG	O8-C23-C24-C25
32	S	617	LHG	O8-C23-C24-C25
40	A	408	SQD	O47-C7-C8-C9
40	a	409	SQD	O47-C7-C8-C9
31	b	616	CLA	C11-C12-C13-C14
31	12	610	CLA	CAA-CBA-CGA-O2A
32	l	102	LHG	C27-C28-C29-C30
40	d	414	SQD	C11-C10-C9-C8
30	r	606	CHL	C2A-CAA-CBA-CGA
30	6	605	CHL	C6-C7-C8-C10
30	6	607	CHL	C11-C10-C8-C7
30	6	607	CHL	C12-C13-C15-C16
30	n	605	CHL	C6-C7-C8-C10
31	3	610	CLA	C11-C10-C8-C7
31	3	611	CLA	C11-C12-C13-C15
31	4	610	CLA	C6-C7-C8-C10
31	16	611	CLA	C11-C12-C13-C15
31	B	614	CLA	C12-C13-C15-C16
31	C	514	CLA	C12-C13-C15-C16
31	D	405	CLA	C12-C13-C15-C16
31	G	613	CLA	C12-C13-C15-C16
31	S	604	CLA	C11-C12-C13-C15
31	S	614	CLA	C11-C10-C8-C7
31	a	404	CLA	C12-C13-C15-C16
31	b	607	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	b	609	CLA	C11-C12-C13-C15
31	c	502	CLA	C11-C10-C8-C7
31	d	405	CLA	C11-C10-C8-C7
38	a	405	PHO	C12-C13-C15-C16
30	5	609	CHL	O1D-CGD-O2D-CED
32	13	616	LHG	C26-C27-C28-C29
30	1	606	CHL	C2C-C3C-CAC-CBC
32	a	401	LHG	C32-C33-C34-C35
30	15	605	CHL	CAA-CBA-CGA-O1A
44	b	622	STE	O2-C1-C2-C3
33	12	614	LUT	C1-C6-C7-C8
33	12	614	LUT	C5-C6-C7-C8
33	Y	621	LUT	C5-C6-C7-C8
33	y	622	LUT	C5-C6-C7-C8
39	C	516	BCR	C23-C24-C25-C30
39	H	103	BCR	C23-C24-C25-C26
39	H	103	BCR	C23-C24-C25-C30
39	c	516	BCR	C5-C6-C7-C8
39	c	516	BCR	C23-C24-C25-C30
39	h	102	BCR	C5-C6-C7-C8
40	D	411	SQD	C24-C25-C26-C27
30	15	607	CHL	CAA-CBA-CGA-O2A
32	c	521	LHG	O7-C7-C8-C9
43	W	503	LNL	C7-C8-C9-C10
43	y	621	LNL	C7-C8-C9-C10
41	s	616	LMG	C12-C13-C14-C15
30	1	601	CHL	C2-C1-O2A-CGA
30	1	608	CHL	C2-C1-O2A-CGA
30	11	609	CHL	C2-C1-O2A-CGA
30	13	607	CHL	C2-C1-O2A-CGA
30	13	608	CHL	C2-C1-O2A-CGA
30	14	607	CHL	C2-C1-O2A-CGA
30	16	608	CHL	C2-C1-O2A-CGA
30	G	608	CHL	C2-C1-O2A-CGA
31	11	613	CLA	C2-C1-O2A-CGA
31	13	604	CLA	C2-C1-O2A-CGA
31	13	611	CLA	C2-C1-O2A-CGA
31	14	613	CLA	C2-C1-O2A-CGA
31	15	609	CLA	C2-C1-O2A-CGA
31	A	403	CLA	C2-C1-O2A-CGA
31	R	611	CLA	C2-C1-O2A-CGA
31	b	609	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	b	612	CLA	C2-C1-O2A-CGA
31	b	613	CLA	C2-C1-O2A-CGA
31	d	402	CLA	C2-C1-O2A-CGA
31	s	614	CLA	C2-C1-O2A-CGA
31	y	615	CLA	C2-C1-O2A-CGA
32	S	617	LHG	C11-C12-C13-C14
46	w	502	DGD	C2D-C1D-O3G-C3G
30	n	605	CHL	C11-C12-C13-C14
31	R	603	CLA	C16-C17-C18-C20
36	7	201	3PH	C3D-C3E-C3F-C3G
30	14	601	CHL	CAA-CBA-CGA-O2A
31	N	603	CLA	CAA-CBA-CGA-O2A
31	R	614	CLA	CAA-CBA-CGA-O2A
31	r	603	CLA	CAA-CBA-CGA-O2A
32	1	615	LHG	O8-C23-C24-C25
43	x	201	LNL	O2-C1-C2-C3
32	d	409	LHG	O10-C23-O8-C6
30	13	601	CHL	C4-C3-C5-C6
30	g	609	CHL	C4-C3-C5-C6
31	16	611	CLA	C4-C3-C5-C6
31	14	611	CLA	C3-C5-C6-C7
30	11	608	CHL	CAA-CBA-CGA-O2A
30	y	605	CHL	CAA-CBA-CGA-O2A
31	15	609	CLA	CAA-CBA-CGA-O2A
32	16	616	LHG	O8-C23-C24-C25
32	s	617	LHG	O8-C23-C24-C25
31	G	613	CLA	C2-C3-C5-C6
31	r	608	CLA	C2-C3-C5-C6
30	6	609	CHL	C2A-CAA-CBA-CGA
31	A	404	CLA	C2A-CAA-CBA-CGA
31	B	608	CLA	C2A-CAA-CBA-CGA
31	G	602	CLA	C2A-CAA-CBA-CGA
31	R	609	CLA	C2A-CAA-CBA-CGA
32	s	621	LHG	C32-C33-C34-C35
31	11	602	CLA	C8-C10-C11-C12
31	B	608	CLA	C8-C10-C11-C12
32	d	409	LHG	C24-C23-O8-C6
30	12	608	CHL	CAA-CBA-CGA-O2A
31	2	602	CLA	CAA-CBA-CGA-O2A
31	r	613	CLA	CAA-CBA-CGA-O2A
32	13	616	LHG	O8-C23-C24-C25
32	d	408	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
32	d	409	LHG	O8-C23-C24-C25
41	K	102	LMG	O7-C10-C11-C12
32	6	616	LHG	C14-C15-C16-C17
41	B	621	LMG	C14-C15-C16-C17
42	a	410	PL9	C4-C3-C7-C8
30	6	609	CHL	C2C-C3C-CAC-CBC
41	C	522	LMG	C20-C21-C22-C23
31	S	614	CLA	C5-C6-C7-C8
31	r	602	CLA	C15-C16-C17-C18
30	1	601	CHL	CAA-CBA-CGA-O2A
30	Y	601	CHL	CAA-CBA-CGA-O2A
30	Y	605	CHL	CAA-CBA-CGA-O2A
30	Y	606	CHL	CAA-CBA-CGA-O2A
30	y	601	CHL	CAA-CBA-CGA-O2A
31	g	602	CLA	CAA-CBA-CGA-O2A
32	D	408	LHG	O8-C23-C24-C25
32	D	409	LHG	O8-C23-C24-C25
32	a	414	LHG	O8-C23-C24-C25
41	v	101	LMG	O7-C10-C11-C12
40	D	413	SQD	C29-C30-C31-C32
31	s	615	CLA	C2-C1-O2A-CGA
50	N	621	PAM	O1-C1-C2-C3
31	11	613	CLA	C4-C3-C5-C6
31	B	611	CLA	C4-C3-C5-C6
32	s	617	LHG	C13-C14-C15-C16
31	1	613	CLA	CAA-CBA-CGA-O2A
32	S	617	LHG	O7-C7-C8-C9
31	S	609	CLA	C2-C3-C5-C6
31	r	609	CLA	C2-C3-C5-C6
30	15	608	CHL	C2C-C3C-CAC-CBC
32	l	102	LHG	C30-C31-C32-C33
31	B	607	CLA	C2A-CAA-CBA-CGA
31	R	601	CLA	C2A-CAA-CBA-CGA
31	g	602	CLA	C2A-CAA-CBA-CGA
32	y	616	LHG	C29-C30-C31-C32
30	12	605	CHL	CAA-CBA-CGA-O1A
43	y	619	LNL	O2-C1-C2-C3
30	11	601	CHL	CAA-CBA-CGA-O2A
30	N	608	CHL	CAA-CBA-CGA-O2A
31	S	602	CLA	CAA-CBA-CGA-O2A
40	L	101	SQD	C25-C26-C27-C28
31	B	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	4	609	CHL	C11-C12-C13-C14
30	16	607	CHL	C6-C7-C8-C9
30	y	607	CHL	C6-C7-C8-C9
31	6	602	CLA	C11-C10-C8-C9
31	13	602	CLA	C11-C10-C8-C9
31	B	604	CLA	C6-C7-C8-C9
31	B	609	CLA	C11-C10-C8-C9
31	C	512	CLA	C11-C12-C13-C14
31	G	611	CLA	C11-C10-C8-C9
31	R	603	CLA	C6-C7-C8-C9
31	d	404	CLA	C6-C7-C8-C9
36	7	201	3PH	C3C-C3D-C3E-C3F
41	c	522	LMG	C20-C21-C22-C23
31	r	609	CLA	O1D-CGD-O2D-CED
32	N	616	LHG	C7-C8-C9-C10
30	1	608	CHL	CAA-CBA-CGA-O2A
31	5	602	CLA	CAA-CBA-CGA-O2A
31	S	605	CLA	CAA-CBA-CGA-O2A
46	C	517	DGD	O2G-C1B-C2B-C3B
32	4	615	LHG	C11-C10-C9-C8
32	A	415	LHG	C32-C33-C34-C35
32	C	521	LHG	C33-C34-C35-C36
40	l	101	SQD	C9-C10-C11-C12
31	Y	613	CLA	C13-C15-C16-C17
31	1	610	CLA	C4B-C3B-CAB-CBB
31	5	604	CLA	C1A-C2A-CAA-CBA
31	6	613	CLA	C1A-C2A-CAA-CBA
31	11	603	CLA	C1A-C2A-CAA-CBA
31	12	611	CLA	C1A-C2A-CAA-CBA
31	15	611	CLA	C1A-C2A-CAA-CBA
31	Y	613	CLA	C1A-C2A-CAA-CBA
31	b	609	CLA	C1A-C2A-CAA-CBA
31	d	404	CLA	C1A-C2A-CAA-CBA
31	d	405	CLA	C1A-C2A-CAA-CBA
31	y	611	CLA	C1A-C2A-CAA-CBA
43	y	619	LNL	O1-C1-C2-C3
32	R	619	LHG	C12-C13-C14-C15
30	12	608	CHL	C2C-C3C-CAC-CBC
30	16	609	CHL	C4-C3-C5-C6
31	S	604	CLA	C4-C3-C5-C6
31	n	611	CLA	C5-C6-C7-C8
30	3	606	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	16	609	CHL	CAA-CBA-CGA-O2A
30	R	607	CHL	CAA-CBA-CGA-O2A
30	n	608	CHL	CAA-CBA-CGA-O2A
31	4	602	CLA	CAA-CBA-CGA-O2A
31	6	614	CLA	CAA-CBA-CGA-O2A
31	11	604	CLA	CAA-CBA-CGA-O2A
32	6	616	LHG	O8-C23-C24-C25
32	L	102	LHG	O7-C5-C6-O8
32	y	618	LHG	O7-C5-C6-O8
41	C	522	LMG	O1-C7-C8-O7
32	l	102	LHG	C28-C29-C30-C31
30	3	609	CHL	C13-C15-C16-C17
30	11	609	CHL	C5-C6-C7-C8
40	d	412	SQD	C24-C25-C26-C27
31	1	610	CLA	C6-C7-C8-C9
31	R	603	CLA	C16-C17-C18-C19
30	5	601	CHL	CBA-CGA-O2A-C1
32	Y	616	LHG	C26-C27-C28-C29
31	R	613	CLA	O1D-CGD-O2D-CED
30	4	608	CHL	CAA-CBA-CGA-O2A
30	n	607	CHL	CAA-CBA-CGA-O2A
31	1	612	CLA	CAA-CBA-CGA-O2A
31	5	603	CLA	CAA-CBA-CGA-O2A
31	16	603	CLA	CAA-CBA-CGA-O2A
31	b	613	CLA	CAA-CBA-CGA-O2A
41	D	410	LMG	O7-C10-C11-C12
41	d	411	LMG	O8-C28-C29-C30
46	C	519	DGD	O2G-C1B-C2B-C3B
30	g	601	CHL	C2A-CAA-CBA-CGA
31	4	610	CLA	C2A-CAA-CBA-CGA
31	b	608	CLA	C2A-CAA-CBA-CGA
31	n	614	CLA	C2A-CAA-CBA-CGA
32	c	521	LHG	C32-C33-C34-C35
43	r	620	LNL	C3-C4-C5-C6
30	G	609	CHL	C2C-C3C-CAC-CBC
32	L	102	LHG	C30-C31-C32-C33
41	C	520	LMG	C29-C30-C31-C32
31	N	602	CLA	C2C-C3C-CAC-CBC
30	12	607	CHL	CAA-CBA-CGA-O2A
31	3	602	CLA	CAA-CBA-CGA-O2A
31	6	603	CLA	CAA-CBA-CGA-O2A
31	16	602	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	B	613	CLA	CAA-CBA-CGA-O2A
31	R	612	CLA	CAA-CBA-CGA-O2A
46	c	517	DGD	O2G-C1B-C2B-C3B
46	c	519	DGD	O2G-C1B-C2B-C3B
31	b	606	CLA	O1D-CGD-O2D-CED
32	l	102	LHG	C1-C2-C3-O3
40	D	411	SQD	C5-C6-S-O7
40	d	412	SQD	C5-C6-S-O7
40	d	414	SQD	C5-C6-S-O7
41	v	101	LMG	C10-C11-C12-C13
31	g	611	CLA	C10-C11-C12-C13
31	y	613	CLA	C13-C15-C16-C17
30	5	609	CHL	C4-C3-C5-C6
30	4	608	CHL	C2-C1-O2A-CGA
30	15	606	CHL	C2-C1-O2A-CGA
30	R	607	CHL	C2-C1-O2A-CGA
30	Y	605	CHL	C2-C1-O2A-CGA
31	1	611	CLA	C2-C1-O2A-CGA
31	B	612	CLA	C2-C1-O2A-CGA
31	B	613	CLA	C2-C1-O2A-CGA
31	C	503	CLA	C2-C1-O2A-CGA
31	R	609	CLA	C2-C1-O2A-CGA
31	R	610	CLA	C2-C1-O2A-CGA
31	S	614	CLA	C2-C1-O2A-CGA
31	r	611	CLA	C2-C1-O2A-CGA
30	S	608	CHL	CAA-CBA-CGA-O2A
31	2	603	CLA	CAA-CBA-CGA-O2A
30	2	609	CHL	C11-C12-C13-C15
30	3	605	CHL	C11-C10-C8-C7
30	13	607	CHL	C11-C10-C8-C7
30	16	606	CHL	C6-C7-C8-C10
30	16	609	CHL	C11-C10-C8-C7
30	n	606	CHL	C6-C7-C8-C10
31	D	405	CLA	C11-C10-C8-C7
31	R	603	CLA	C6-C7-C8-C10
31	R	609	CLA	C11-C10-C8-C7
31	R	609	CLA	C11-C12-C13-C15
31	S	611	CLA	C6-C7-C8-C10
32	L	102	LHG	C27-C28-C29-C30
30	G	601	CHL	C16-C17-C18-C20
30	n	607	CHL	C16-C17-C18-C19
31	C	508	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
40	d	412	SQD	C23-C24-C25-C26
41	b	621	LMG	C10-C11-C12-C13
32	Y	618	LHG	C31-C32-C33-C34
31	3	603	CLA	O2A-C1-C2-C3
31	6	603	CLA	O2A-C1-C2-C3
31	14	611	CLA	O2A-C1-C2-C3
32	A	415	LHG	C26-C27-C28-C29
43	X	201	LNL	C15-C16-C17-C18
30	g	609	CHL	C2C-C3C-CAC-CBC
31	3	603	CLA	CAA-CBA-CGA-O2A
31	15	602	CLA	CAA-CBA-CGA-O2A
41	J	102	LMG	O7-C10-C11-C12
41	j	102	LMG	O7-C10-C11-C12
31	s	603	CLA	C3A-C2A-CAA-CBA
32	A	411	LHG	C15-C16-C17-C18
41	K	102	LMG	C12-C13-C14-C15
30	Y	607	CHL	C2A-CAA-CBA-CGA
30	y	607	CHL	C2A-CAA-CBA-CGA
31	1	602	CLA	C2A-CAA-CBA-CGA
31	r	602	CLA	C2A-CAA-CBA-CGA
30	g	601	CHL	C16-C17-C18-C20
31	3	611	CLA	C16-C17-C18-C20
31	3	612	CLA	C16-C17-C18-C19
31	c	508	CLA	C16-C17-C18-C20
31	s	614	CLA	C16-C17-C18-C19
32	d	413	LHG	C17-C18-C19-C20
44	b	622	STE	O1-C1-C2-C3
31	b	607	CLA	C13-C15-C16-C17
32	A	414	LHG	C11-C10-C9-C8
32	a	411	LHG	C10-C11-C12-C13
41	c	520	LMG	C29-C30-C31-C32
32	y	617	LHG	O8-C23-C24-C25
30	6	606	CHL	CAA-CBA-CGA-O1A
31	G	603	CLA	CAA-CBA-CGA-O1A
31	r	612	CLA	O1A-CGA-O2A-C1
42	d	407	PL9	C44-C46-C47-C48
31	14	604	CLA	C5-C6-C7-C8
36	B	620	3PH	C2-C1-O11-P
31	N	602	CLA	C4C-C3C-CAC-CBC
30	14	609	CHL	C3A-C2A-CAA-CBA
30	r	605	CHL	C3A-C2A-CAA-CBA
31	1	604	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	2	613	CLA	C3A-C2A-CAA-CBA
31	4	613	CLA	C3A-C2A-CAA-CBA
31	12	611	CLA	C3A-C2A-CAA-CBA
31	15	611	CLA	C3A-C2A-CAA-CBA
31	C	514	CLA	C3A-C2A-CAA-CBA
31	Y	615	CLA	C3A-C2A-CAA-CBA
31	c	514	CLA	C3A-C2A-CAA-CBA
31	d	404	CLA	C3A-C2A-CAA-CBA
31	y	613	CLA	C3A-C2A-CAA-CBA
31	1	612	CLA	CAA-CBA-CGA-O1A
31	B	606	CLA	C8-C10-C11-C12
38	A	405	PHO	C13-C15-C16-C17
31	Y	602	CLA	C2-C3-C5-C6
31	13	613	CLA	C4C-C3C-CAC-CBC
30	y	606	CHL	CAA-CBA-CGA-O1A
31	5	603	CLA	CAA-CBA-CGA-O1A
31	6	603	CLA	CAA-CBA-CGA-O1A
31	16	603	CLA	CAA-CBA-CGA-O1A
32	3	617	LHG	C14-C15-C16-C17
41	d	415	LMG	C35-C36-C37-C38
31	R	602	CLA	C15-C16-C17-C18
41	D	414	LMG	C35-C36-C37-C38
31	D	405	CLA	CAA-CBA-CGA-O2A
31	s	605	CLA	CAA-CBA-CGA-O2A
41	s	616	LMG	O7-C10-C11-C12
30	12	608	CHL	CAA-CBA-CGA-O1A
30	16	609	CHL	CAA-CBA-CGA-O1A
30	S	608	CHL	CAA-CBA-CGA-O1A
31	2	603	CLA	CAA-CBA-CGA-O1A
31	g	603	CLA	CAA-CBA-CGA-O1A
32	1	615	LHG	O10-C23-C24-C25
32	16	616	LHG	O10-C23-C24-C25
32	D	408	LHG	O10-C23-C24-C25
32	G	615	LHG	O10-C23-C24-C25
32	s	617	LHG	O10-C23-C24-C25
41	K	102	LMG	O9-C10-C11-C12
31	4	603	CLA	C3-C5-C6-C7
32	Y	618	LHG	C28-C29-C30-C31
31	Y	611	CLA	C2A-CAA-CBA-CGA
30	15	608	CHL	CBA-CGA-O2A-C1
31	1	602	CLA	CBA-CGA-O2A-C1
50	N	621	PAM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	2	609	CHL	C11-C10-C8-C9
30	5	609	CHL	C11-C10-C8-C9
30	14	601	CHL	C11-C12-C13-C14
30	n	606	CHL	C11-C10-C8-C9
31	3	602	CLA	C11-C10-C8-C9
31	6	611	CLA	C11-C10-C8-C9
31	b	609	CLA	C11-C10-C8-C9
31	c	509	CLA	C11-C10-C8-C9
31	y	612	CLA	C11-C12-C13-C14
38	A	405	PHO	C14-C13-C15-C16
32	A	411	LHG	C27-C28-C29-C30
32	a	413	LHG	O8-C23-C24-C25
31	3	603	CLA	CAA-CBA-CGA-O1A
31	3	612	CLA	CAA-CBA-CGA-O1A
31	R	614	CLA	CAA-CBA-CGA-O1A
32	13	616	LHG	O10-C23-C24-C25
32	a	414	LHG	O10-C23-C24-C25
32	y	617	LHG	C25-C26-C27-C28
41	J	102	LMG	C32-C33-C34-C35
41	v	101	LMG	C12-C13-C14-C15
46	W	501	DGD	CEB-CFB-CGB-CHB
30	N	607	CHL	C10-C11-C12-C13
32	D	412	LHG	C12-C13-C14-C15
46	c	519	DGD	C5B-C6B-C7B-C8B
38	a	405	PHO	C13-C15-C16-C17
31	N	602	CLA	C4-C3-C5-C6
42	A	410	PL9	C12-C11-C9-C10
31	1	611	CLA	CAA-CBA-CGA-O1A
31	11	604	CLA	CAA-CBA-CGA-O1A
31	b	606	CLA	CAA-CBA-CGA-O1A
31	s	605	CLA	CAA-CBA-CGA-O1A
32	11	615	LHG	O8-C23-C24-C25
31	g	602	CLA	C2-C3-C5-C6
42	a	410	PL9	C12-C11-C9-C8
31	B	616	CLA	C5-C6-C7-C8
35	3	620	XAT	C1-C6-C7-C8
35	6	620	XAT	C1-C6-C7-C8
40	D	411	SQD	O5-C5-C6-S
40	d	412	SQD	O5-C5-C6-S
31	c	510	CLA	CAA-CBA-CGA-O1A
31	r	603	CLA	CAA-CBA-CGA-O1A
32	d	408	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
40	A	408	SQD	O49-C7-C8-C9
31	c	511	CLA	C8-C10-C11-C12
32	Y	616	LHG	O1-C1-C2-O2
32	6	617	LHG	C11-C12-C13-C14
31	2	613	CLA	CAA-CBA-CGA-O2A
31	3	614	CLA	CAA-CBA-CGA-O2A
31	c	507	CLA	CAA-CBA-CGA-O2A
31	s	611	CLA	C16-C17-C18-C20
43	x	201	LNL	O1-C1-C2-C3
30	12	607	CHL	CAA-CBA-CGA-O1A
30	n	607	CHL	CAA-CBA-CGA-O1A
31	12	602	CLA	CAA-CBA-CGA-O1A
31	13	603	CLA	CAA-CBA-CGA-O1A
31	C	511	CLA	CAA-CBA-CGA-O1A
31	R	603	CLA	CAA-CBA-CGA-O1A
31	c	511	CLA	CAA-CBA-CGA-O1A
31	d	404	CLA	CAA-CBA-CGA-O1A
32	3	616	LHG	O10-C23-C24-C25
32	6	616	LHG	O10-C23-C24-C25
32	S	617	LHG	O10-C23-C24-C25
32	g	615	LHG	O10-C23-C24-C25
40	a	409	SQD	O49-C7-C8-C9
46	c	519	DGD	O1B-C1B-C2B-C3B
41	D	410	LMG	C8-C7-O1-C1
32	4	615	LHG	O9-C7-O7-C5
31	16	613	CLA	C4C-C3C-CAC-CBC
32	A	414	LHG	C10-C11-C12-C13
31	R	611	CLA	O2A-C1-C2-C3
31	S	613	CLA	O2A-C1-C2-C3
31	r	611	CLA	O2A-C1-C2-C3
31	14	604	CLA	CAA-CBA-CGA-O1A
31	A	403	CLA	CAA-CBA-CGA-O1A
31	D	404	CLA	CAA-CBA-CGA-O1A
32	D	409	LHG	O10-C23-C24-C25
46	C	519	DGD	O1B-C1B-C2B-C3B
30	Y	607	CHL	CAA-CBA-CGA-O2A
31	N	613	CLA	CAA-CBA-CGA-O2A
31	d	405	CLA	CAA-CBA-CGA-O2A
31	g	610	CLA	CAA-CBA-CGA-O2A
31	n	610	CLA	CAA-CBA-CGA-O2A
31	s	602	CLA	CAA-CBA-CGA-O2A
32	13	616	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	y	603	CLA	C5-C6-C7-C8
30	G	601	CHL	C2A-CAA-CBA-CGA
31	3	612	CLA	C2A-CAA-CBA-CGA
31	16	612	CLA	C2A-CAA-CBA-CGA
31	B	610	CLA	C2A-CAA-CBA-CGA
31	b	610	CLA	C2A-CAA-CBA-CGA
41	j	102	LMG	C32-C33-C34-C35
31	s	614	CLA	C16-C17-C18-C20
30	3	609	CHL	C2C-C3C-CAC-CBC
41	C	522	LMG	C23-C24-C25-C26
41	S	616	LMG	C7-C8-C9-O8
42	D	407	PL9	C44-C46-C47-C48
46	W	501	DGD	O1G-C1G-C2G-C3G
31	N	603	CLA	CAA-CBA-CGA-O1A
31	g	602	CLA	CAA-CBA-CGA-O1A
41	d	411	LMG	O10-C28-C29-C30
46	c	517	DGD	O1B-C1B-C2B-C3B
32	a	414	LHG	C27-C28-C29-C30
30	y	607	CHL	CAA-CBA-CGA-O2A
31	G	603	CLA	CAA-CBA-CGA-O2A
31	g	603	CLA	CAA-CBA-CGA-O2A
32	Y	617	LHG	O8-C23-C24-C25
32	a	411	LHG	C34-C35-C36-C37
31	B	608	CLA	C13-C15-C16-C17
31	1	602	CLA	CAA-CBA-CGA-O1A
31	S	605	CLA	CAA-CBA-CGA-O1A
32	S	617	LHG	O9-C7-C8-C9
32	d	409	LHG	O10-C23-C24-C25
41	v	101	LMG	O9-C10-C11-C12
32	Y	618	LHG	C23-C24-C25-C26
30	2	601	CHL	CAD-CBD-CGD-O2D
30	2	608	CHL	CAD-CBD-CGD-O2D
30	2	607	CHL	CAD-CBD-CGD-O2D
30	6	606	CHL	CAD-CBD-CGD-O2D
30	12	605	CHL	CAD-CBD-CGD-O2D
30	N	601	CHL	CAD-CBD-CGD-O2D
30	s	608	CHL	CAD-CBD-CGD-O2D
31	1	602	CLA	CAD-CBD-CGD-O2D
31	3	615	CLA	CAD-CBD-CGD-O2D
31	6	615	CLA	CAD-CBD-CGD-O2D
31	11	611	CLA	CAD-CBD-CGD-O2D
31	13	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	13	614	CLA	CAD-CBD-CGD-O2D
31	B	607	CLA	CAD-CBD-CGD-O2D
31	R	609	CLA	CAD-CBD-CGD-O2D
31	R	612	CLA	CAD-CBD-CGD-O2D
31	R	614	CLA	CAD-CBD-CGD-O2D
31	S	612	CLA	CAD-CBD-CGD-O2D
31	Y	615	CLA	CAD-CBD-CGD-O2D
31	r	609	CLA	CAD-CBD-CGD-O2D
31	s	603	CLA	CAD-CBD-CGD-O2D
31	s	614	CLA	CAD-CBD-CGD-O2D
32	3	617	LHG	C32-C33-C34-C35
43	C	524	LNL	C2-C3-C4-C5
30	y	606	CHL	CAA-CBA-CGA-O2A
31	3	612	CLA	CAA-CBA-CGA-O2A
32	r	618	LHG	O8-C23-C24-C25
30	4	601	CHL	C3-C5-C6-C7
31	5	612	CLA	CAA-CBA-CGA-O1A
31	6	612	CLA	CAA-CBA-CGA-O1A
31	d	402	CLA	CAA-CBA-CGA-O1A
31	r	613	CLA	CAA-CBA-CGA-O1A
41	D	410	LMG	O9-C10-C11-C12
46	C	517	DGD	O1B-C1B-C2B-C3B
30	13	605	CHL	C5-C6-C7-C8
31	s	604	CLA	C13-C15-C16-C17
31	4	602	CLA	O1D-CGD-O2D-CED
31	B	613	CLA	O1D-CGD-O2D-CED
43	c	524	LNL	C2-C3-C4-C5
30	n	607	CHL	C2-C1-O2A-CGA
31	15	603	CLA	C2-C1-O2A-CGA
31	B	609	CLA	C2-C1-O2A-CGA
30	5	601	CHL	CAA-CBA-CGA-O2A
32	y	618	LHG	O8-C23-C24-C25
30	6	601	CHL	C1-C2-C3-C4
30	11	609	CHL	C1-C2-C3-C4
30	13	601	CHL	C1-C2-C3-C4
30	13	605	CHL	C1-C2-C3-C4
30	13	608	CHL	C1A-C2A-CAA-CBA
30	15	605	CHL	C1A-C2A-CAA-CBA
30	16	606	CHL	C1-C2-C3-C4
30	16	608	CHL	C1A-C2A-CAA-CBA
30	Y	606	CHL	C1-C2-C3-C4
30	g	601	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	n	605	CHL	C1-C2-C3-C4
30	n	609	CHL	C1-C2-C3-C4
30	s	606	CHL	C1-C2-C3-C4
31	16	603	CLA	C1-C2-C3-C4
31	B	613	CLA	C1-C2-C3-C4
31	B	616	CLA	C1-C2-C3-C4
31	C	511	CLA	C1-C2-C3-C4
31	N	603	CLA	C1-C2-C3-C4
31	R	603	CLA	C1-C2-C3-C4
31	b	613	CLA	C1-C2-C3-C4
31	b	616	CLA	C1-C2-C3-C4
31	c	502	CLA	C1-C2-C3-C4
31	c	511	CLA	C1-C2-C3-C4
30	y	606	CHL	C16-C17-C18-C20
31	g	613	CLA	C16-C17-C18-C20
41	c	522	LMG	C23-C24-C25-C26
31	R	602	CLA	C2A-CAA-CBA-CGA
41	c	520	LMG	C14-C15-C16-C17
41	C	522	LMG	C35-C36-C37-C38
30	6	605	CHL	C5-C6-C7-C8
30	G	601	CHL	C10-C11-C12-C13
31	5	603	CLA	C5-C6-C7-C8
31	g	613	CLA	C8-C10-C11-C12
32	14	615	LHG	O8-C23-C24-C25
32	A	414	LHG	O8-C23-C24-C25
32	n	616	LHG	O7-C7-C8-C9
32	n	616	LHG	O8-C23-C24-C25
46	w	502	DGD	O2G-C1B-C2B-C3B
31	S	612	CLA	O1D-CGD-O2D-CED
32	14	615	LHG	C28-C29-C30-C31
41	C	520	LMG	C14-C15-C16-C17
31	n	604	CLA	C6-C7-C8-C9
30	3	607	CHL	CAA-CBA-CGA-O1A
30	s	606	CHL	CAA-CBA-CGA-O1A
31	B	613	CLA	CAA-CBA-CGA-O1A
31	n	603	CLA	CAA-CBA-CGA-O1A
32	11	615	LHG	O10-C23-C24-C25
32	13	616	LHG	O9-C7-C8-C9
36	B	620	3PH	C24-C25-C26-C27
36	B	620	3PH	C2A-C2B-C2C-C2D
40	d	412	SQD	C13-C14-C15-C16
32	n	616	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
32	1	615	LHG	C24-C25-C26-C27
41	d	410	LMG	C30-C31-C32-C33
41	d	410	LMG	O7-C10-C11-C12
46	W	501	DGD	O2G-C1B-C2B-C3B
46	w	502	DGD	C3B-C4B-C5B-C6B
31	16	602	CLA	C8-C10-C11-C12
30	6	607	CHL	CAA-CBA-CGA-O1A
30	R	606	CHL	CAA-CBA-CGA-O1A
31	C	507	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

521 monomers are involved in 1093 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	2	603	CLA	5	0
31	n	613	CLA	4	0
35	r	616	XAT	1	0
30	G	605	CHL	1	0
31	11	610	CLA	3	0
32	d	409	LHG	1	0
33	N	618	LUT	1	0
30	3	608	CHL	1	0
30	S	606	CHL	4	0
30	y	605	CHL	2	0
31	n	604	CLA	2	0
31	13	615	CLA	1	0
31	Y	612	CLA	4	0
33	14	617	LUT	1	0
30	15	606	CHL	1	0
31	13	604	CLA	1	0
31	A	404	CLA	1	0
39	B	619	BCR	1	0
32	y	616	LHG	5	0
31	c	509	CLA	2	0
31	b	602	CLA	4	0
31	14	604	CLA	1	0
34	G	618	NEX	1	0
33	13	618	LUT	1	0
36	b	623	3PH	1	0
31	B	601	CLA	2	0
31	S	615	CLA	1	0
31	Y	602	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	c	526	BCR	3	0
32	a	411	LHG	1	0
33	n	618	LUT	1	0
31	B	602	CLA	3	0
43	h	101	LNL	2	0
31	S	612	CLA	2	0
31	d	402	CLA	5	0
33	S	618	LUT	4	0
30	r	605	CHL	2	0
33	2	614	LUT	5	0
30	n	609	CHL	1	0
39	b	619	BCR	1	0
32	a	414	LHG	3	0
30	1	609	CHL	2	0
30	R	606	CHL	7	0
31	r	611	CLA	2	0
33	G	616	LUT	3	0
41	w	501	LMG	3	0
31	5	611	CLA	2	0
31	C	503	CLA	1	0
31	S	611	CLA	3	0
31	b	601	CLA	2	0
31	b	616	CLA	3	0
30	16	606	CHL	1	0
30	Y	601	CHL	1	0
32	S	621	LHG	3	0
42	A	410	PL9	2	0
30	g	606	CHL	2	0
31	b	615	CLA	4	0
39	a	408	BCR	1	0
31	14	610	CLA	5	0
31	S	603	CLA	2	0
38	a	406	PHO	1	0
41	d	410	LMG	1	0
30	14	601	CHL	3	0
30	6	607	CHL	5	0
31	B	615	CLA	3	0
30	2	609	CHL	7	0
31	R	613	CLA	3	0
30	3	609	CHL	1	0
30	12	607	CHL	2	0
31	r	610	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	2	602	CLA	2	0
33	n	617	LUT	7	0
30	6	605	CHL	5	0
41	D	414	LMG	1	0
30	1	605	CHL	1	0
31	B	607	CLA	1	0
30	3	606	CHL	2	0
31	G	613	CLA	1	0
33	11	617	LUT	2	0
31	S	602	CLA	1	0
32	D	408	LHG	3	0
31	1	612	CLA	1	0
31	c	502	CLA	4	0
31	B	604	CLA	3	0
31	B	611	CLA	1	0
32	a	413	LHG	2	0
31	12	611	CLA	5	0
39	B	618	BCR	3	0
31	c	507	CLA	3	0
31	b	606	CLA	1	0
31	n	610	CLA	4	0
31	1	611	CLA	1	0
31	12	609	CLA	13	0
31	C	512	CLA	4	0
33	16	617	LUT	2	0
46	c	518	DGD	5	0
30	14	607	CHL	1	0
43	w	503	LNL	1	0
33	12	615	LUT	2	0
31	4	610	CLA	3	0
31	15	611	CLA	4	0
32	y	618	LHG	2	0
30	16	607	CHL	2	0
31	3	604	CLA	1	0
31	13	614	CLA	4	0
31	s	613	CLA	1	0
41	j	102	LMG	5	0
31	14	603	CLA	6	0
31	r	613	CLA	2	0
31	d	404	CLA	3	0
33	13	617	LUT	2	0
30	11	607	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	12	602	CLA	7	0
31	B	613	CLA	3	0
46	C	517	DGD	2	0
39	h	102	BCR	4	0
46	C	519	DGD	3	0
30	14	608	CHL	1	0
31	g	602	CLA	1	0
43	W	502	LNL	1	0
32	s	617	LHG	3	0
39	B	617	BCR	3	0
39	C	526	BCR	3	0
31	Y	614	CLA	2	0
31	6	611	CLA	1	0
31	Y	610	CLA	2	0
31	B	614	CLA	2	0
31	c	508	CLA	1	0
31	s	611	CLA	4	0
32	r	621	LHG	4	0
31	3	610	CLA	2	0
30	12	606	CHL	1	0
31	15	603	CLA	12	0
31	c	503	CLA	2	0
33	6	618	LUT	3	0
31	r	609	CLA	4	0
33	1	616	LUT	4	0
31	n	615	CLA	2	0
31	3	614	CLA	3	0
39	b	618	BCR	1	0
31	12	612	CLA	27	0
41	C	522	LMG	1	0
32	3	616	LHG	1	0
33	Y	621	LUT	3	0
30	13	607	CHL	3	0
31	r	603	CLA	3	0
43	x	201	LNL	1	0
40	l	101	SQD	2	0
31	1	602	CLA	2	0
31	C	504	CLA	4	0
30	2	605	CHL	1	0
33	3	618	LUT	2	0
31	13	610	CLA	3	0
41	B	621	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	y	613	CLA	5	0
31	s	612	CLA	2	0
31	12	603	CLA	3	0
31	R	601	CLA	1	0
31	r	612	CLA	1	0
33	12	614	LUT	33	0
43	Y	619	LNL	1	0
31	S	614	CLA	2	0
43	c	523	LNL	1	0
31	C	506	CLA	3	0
30	G	601	CHL	1	0
31	1	613	CLA	1	0
30	y	601	CHL	3	0
39	c	515	BCR	1	0
30	2	608	CHL	5	0
30	15	607	CHL	2	0
31	D	404	CLA	4	0
31	16	615	CLA	4	0
31	3	613	CLA	1	0
32	13	616	LHG	3	0
30	s	606	CHL	7	0
31	c	513	CLA	2	0
30	r	606	CHL	3	0
33	3	619	LUT	1	0
31	n	603	CLA	1	0
30	11	606	CHL	1	0
30	14	609	CHL	2	0
32	G	615	LHG	2	0
44	B	623	STE	1	0
32	r	618	LHG	3	0
41	C	520	LMG	1	0
31	14	602	CLA	7	0
31	n	612	CLA	2	0
31	C	507	CLA	1	0
30	N	606	CHL	3	0
30	13	609	CHL	4	0
30	G	607	CHL	2	0
32	R	618	LHG	2	0
31	16	603	CLA	5	0
35	g	619	XAT	2	0
31	r	608	CLA	3	0
42	d	407	PL9	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	D	402	PHO	4	0
31	11	612	CLA	3	0
33	N	617	LUT	5	0
30	n	606	CHL	2	0
43	Y	620	LNL	1	0
31	C	511	CLA	2	0
31	G	602	CLA	2	0
32	L	102	LHG	4	0
32	14	615	LHG	3	0
32	S	617	LHG	4	0
32	s	621	LHG	4	0
30	14	606	CHL	1	0
33	y	623	LUT	2	0
31	13	603	CLA	8	0
31	C	510	CLA	1	0
31	Y	613	CLA	3	0
31	5	610	CLA	3	0
31	G	610	CLA	4	0
31	c	506	CLA	4	0
31	d	405	CLA	2	0
43	H	101	LNL	4	0
43	X	201	LNL	1	0
33	s	618	LUT	7	0
30	5	609	CHL	2	0
31	y	611	CLA	4	0
31	5	613	CLA	3	0
33	r	615	LUT	4	0
30	G	606	CHL	1	0
32	a	401	LHG	2	0
33	5	615	LUT	1	0
35	14	619	XAT	1	0
35	6	620	XAT	4	0
32	c	521	LHG	3	0
31	r	602	CLA	5	0
33	15	614	LUT	9	0
30	16	601	CHL	2	0
34	S	620	NEX	1	0
31	n	614	CLA	1	0
39	C	515	BCR	2	0
34	Y	623	NEX	1	0
31	11	602	CLA	5	0
31	11	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	5	607	CHL	1	0
31	b	604	CLA	4	0
31	13	611	CLA	1	0
31	16	613	CLA	3	0
32	4	615	LHG	2	0
46	C	518	DGD	6	0
30	Y	609	CHL	1	0
31	2	612	CLA	1	0
30	1	601	CHL	3	0
31	2	604	CLA	3	0
31	y	612	CLA	5	0
43	W	503	LNL	1	0
34	3	621	NEX	3	0
30	4	608	CHL	5	0
30	3	601	CHL	1	0
31	b	611	CLA	3	0
30	g	609	CHL	3	0
31	R	609	CLA	1	0
43	y	621	LNL	1	0
31	Y	611	CLA	4	0
31	16	604	CLA	1	0
30	n	605	CHL	3	0
31	3	612	CLA	3	0
31	g	604	CLA	2	0
30	N	601	CHL	1	0
42	a	410	PL9	4	0
30	11	609	CHL	2	0
31	N	610	CLA	3	0
41	v	101	LMG	1	0
32	n	616	LHG	5	0
33	15	615	LUT	4	0
31	1	604	CLA	3	0
41	D	410	LMG	1	0
31	R	608	CLA	2	0
30	s	607	CHL	1	0
30	1	607	CHL	3	0
32	R	621	LHG	3	0
34	12	616	NEX	2	0
41	s	616	LMG	2	0
30	11	601	CHL	1	0
32	r	619	LHG	4	0
31	R	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	S	608	CHL	4	0
32	N	616	LHG	2	0
34	s	620	NEX	1	0
32	D	409	LHG	2	0
35	G	619	XAT	1	0
30	6	609	CHL	1	0
30	r	607	CHL	1	0
31	B	610	CLA	4	0
30	R	605	CHL	3	0
31	S	613	CLA	1	0
32	11	615	LHG	3	0
39	J	101	BCR	3	0
31	C	505	CLA	3	0
40	d	414	SQD	4	0
31	B	609	CLA	2	0
33	g	616	LUT	3	0
31	11	611	CLA	1	0
32	Y	616	LHG	5	0
30	13	605	CHL	2	0
30	n	601	CHL	2	0
31	6	603	CLA	1	0
34	n	619	NEX	1	0
50	N	621	PAM	1	0
31	b	613	CLA	3	0
39	b	617	BCR	3	0
43	C	523	LNL	1	0
32	6	617	LHG	3	0
31	B	603	CLA	1	0
31	A	406	CLA	1	0
32	A	413	LHG	2	0
30	5	608	CHL	3	0
30	g	608	CHL	4	0
30	16	609	CHL	1	0
41	d	415	LMG	1	0
31	B	612	CLA	4	0
39	A	407	BCR	2	0
31	R	614	CLA	2	0
30	g	607	CHL	2	0
31	6	604	CLA	1	0
32	16	616	LHG	3	0
31	16	614	CLA	2	0
31	4	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	a	403	CLA	5	0
30	N	608	CHL	4	0
36	8	201	3PH	2	0
31	s	610	CLA	3	0
31	N	604	CLA	3	0
49	F	101	HEM	2	0
30	4	609	CHL	4	0
32	Y	618	LHG	4	0
30	g	605	CHL	1	0
31	G	611	CLA	1	0
40	D	411	SQD	2	0
32	A	414	LHG	5	0
30	4	601	CHL	4	0
39	H	103	BCR	3	0
31	b	608	CLA	1	0
31	5	602	CLA	2	0
31	b	609	CLA	2	0
31	C	514	CLA	2	0
36	T	101	3PH	4	0
41	K	102	LMG	3	0
31	14	612	CLA	3	0
30	1	608	CHL	4	0
39	d	406	BCR	1	0
31	A	403	CLA	3	0
31	B	608	CLA	1	0
31	13	613	CLA	2	0
33	2	615	LUT	4	0
34	6	621	NEX	4	0
31	N	615	CLA	1	0
41	S	616	LMG	3	0
30	y	607	CHL	4	0
31	c	505	CLA	2	0
31	n	611	CLA	3	0
41	d	411	LMG	2	0
32	A	411	LHG	2	0
31	11	604	CLA	2	0
41	b	621	LMG	1	0
31	4	604	CLA	2	0
31	6	615	CLA	3	0
31	s	609	CLA	2	0
33	16	618	LUT	4	0
31	B	616	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	b	620	LMG	1	0
31	N	611	CLA	1	0
31	s	615	CLA	2	0
30	6	608	CHL	4	0
31	c	512	CLA	3	0
33	5	614	LUT	2	0
46	W	501	DGD	4	0
31	s	603	CLA	1	0
30	12	608	CHL	1	0
31	s	602	CLA	2	0
31	15	602	CLA	6	0
31	12	604	CLA	5	0
31	15	613	CLA	4	0
31	5	604	CLA	2	0
30	Y	606	CHL	4	0
31	6	613	CLA	3	0
31	S	604	CLA	4	0
41	c	522	LMG	1	0
31	4	613	CLA	2	0
34	r	617	NEX	1	0
30	Y	605	CHL	1	0
31	c	514	CLA	3	0
33	6	619	LUT	1	0
31	14	611	CLA	3	0
46	c	519	DGD	3	0
31	15	604	CLA	7	0
43	y	619	LNL	3	0
31	R	610	CLA	2	0
31	N	602	CLA	2	0
31	N	613	CLA	2	0
32	6	616	LHG	2	0
31	3	602	CLA	2	0
31	B	605	CLA	2	0
30	1	606	CHL	2	0
31	16	602	CLA	3	0
41	J	102	LMG	5	0
31	g	603	CLA	2	0
32	d	413	LHG	1	0
30	15	605	CHL	3	0
31	B	606	CLA	3	0
39	j	101	BCR	3	0
33	11	616	LUT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	16	608	CHL	2	0
32	A	415	LHG	2	0
31	s	614	CLA	1	0
33	4	616	LUT	5	0
41	B	622	LMG	1	0
30	G	609	CHL	2	0
31	n	602	CLA	4	0
31	1	603	CLA	2	0
41	A	409	LMG	1	0
30	y	609	CHL	1	0
33	1	617	LUT	2	0
30	11	608	CHL	3	0
36	B	620	3PH	5	0
31	r	614	CLA	3	0
34	N	619	NEX	1	0
31	R	603	CLA	6	0
30	s	608	CHL	5	0
31	C	513	CLA	1	0
31	4	612	CLA	1	0
30	16	605	CHL	3	0
30	R	607	CHL	2	0
31	b	605	CLA	4	0
40	L	101	SQD	3	0
41	c	520	LMG	1	0
31	R	612	CLA	1	0
30	n	607	CHL	8	0
30	12	605	CHL	4	0
30	13	601	CHL	2	0
30	5	605	CHL	2	0
32	1	615	LHG	1	0
31	y	603	CLA	1	0
31	c	504	CLA	3	0
33	14	616	LUT	4	0
30	4	606	CHL	4	0
31	A	402	CLA	4	0
34	15	616	NEX	3	0
30	15	608	CHL	10	0
46	w	502	DGD	2	0
39	D	406	BCR	2	0
31	S	610	CLA	4	0
36	7	201	3PH	1	0
30	11	605	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	y	610	CLA	2	0
30	3	607	CHL	3	0
30	4	605	CHL	1	0
33	R	615	LUT	1	0
32	R	619	LHG	4	0
42	D	407	PL9	2	0
30	n	608	CHL	2	0
31	14	613	CLA	3	0
32	3	617	LHG	2	0
30	N	605	CHL	2	0
30	13	608	CHL	2	0
31	b	614	CLA	2	0
31	r	601	CLA	2	0
31	16	611	CLA	2	0
30	6	606	CHL	1	0
32	g	615	LHG	5	0
50	n	620	PAM	1	0
33	S	619	LUT	4	0
31	b	607	CLA	3	0
30	g	601	CHL	1	0
31	1	610	CLA	8	0
31	b	612	CLA	4	0
31	y	615	CLA	2	0
33	g	617	LUT	1	0
31	S	609	CLA	1	0
31	b	610	CLA	6	0
34	R	617	NEX	1	0
31	2	613	CLA	4	0
46	c	517	DGD	2	0
35	11	619	XAT	1	0
30	S	607	CHL	1	0
31	y	602	CLA	2	0
31	G	604	CLA	2	0
31	16	610	CLA	3	0
32	C	521	LHG	4	0
30	3	605	CHL	4	0
36	B	624	3PH	2	0
40	d	412	SQD	3	0
32	d	408	LHG	3	0
32	l	102	LHG	4	0
31	Y	603	CLA	1	0
31	13	602	CLA	5	0

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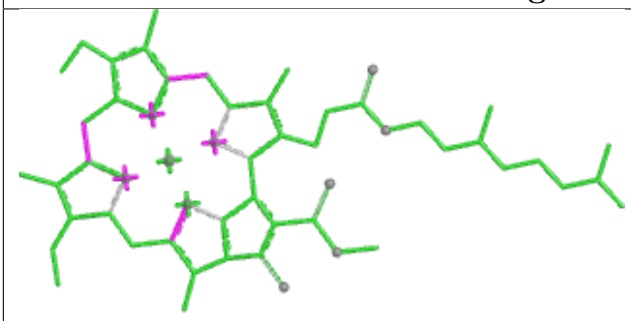
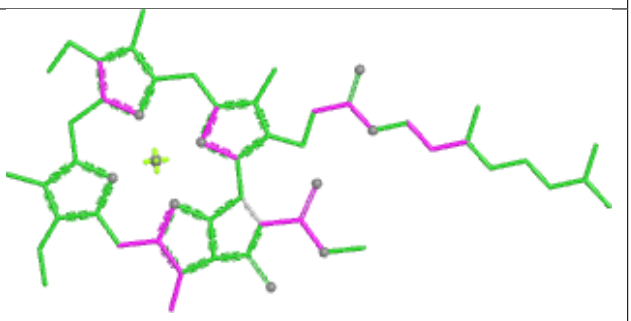
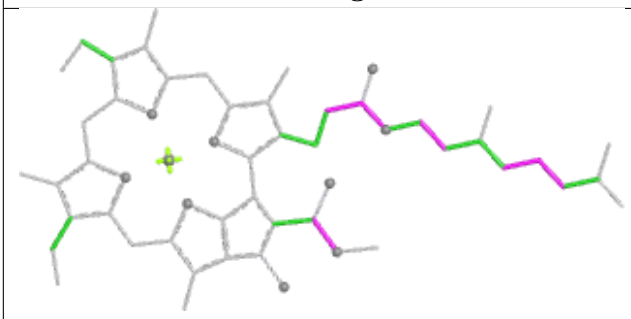
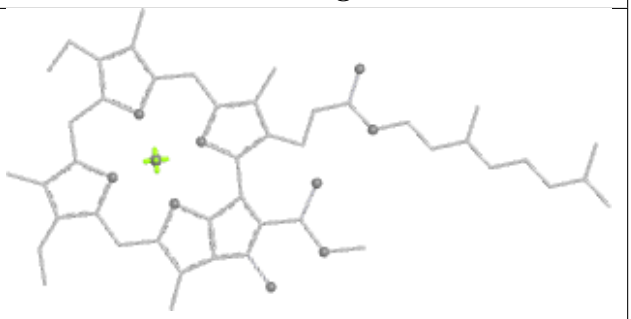
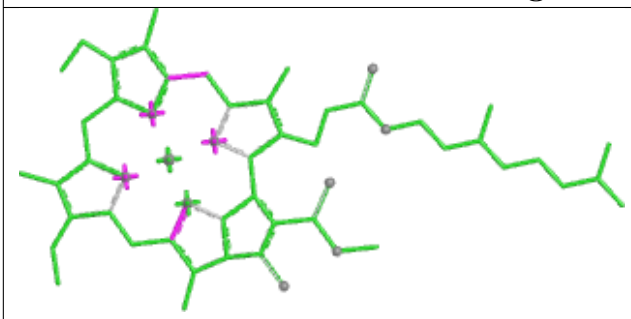
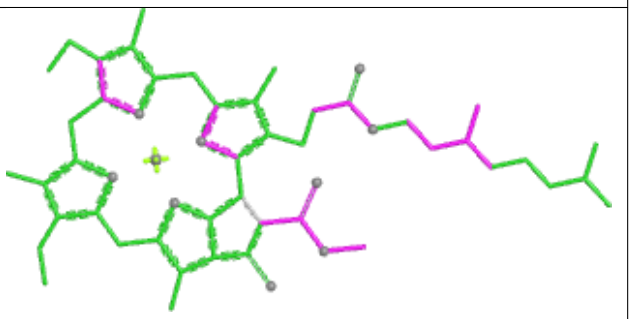
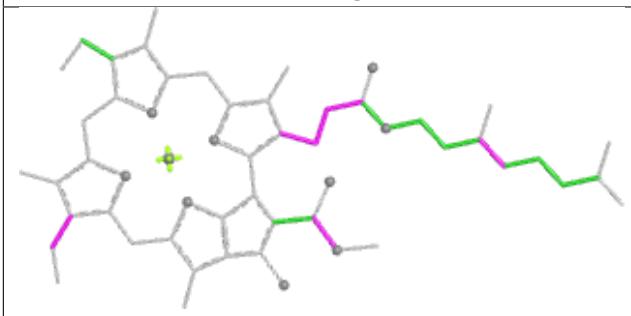
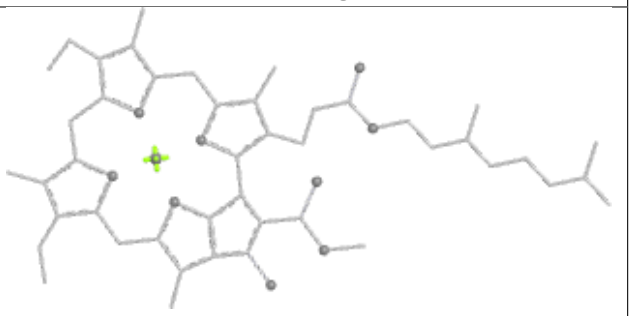
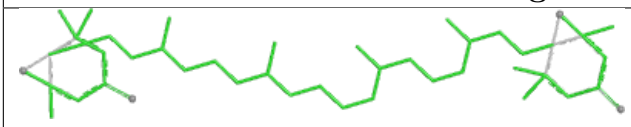
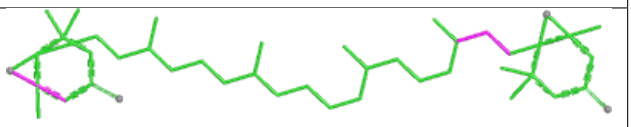
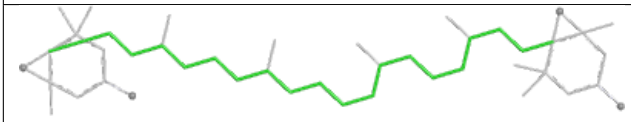
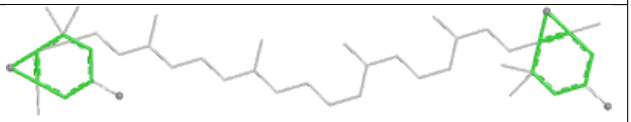
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	6	614	CLA	1	0
31	g	610	CLA	2	0
31	y	614	CLA	2	0
31	c	510	CLA	1	0
31	g	613	CLA	3	0
49	f	101	HEM	2	0
30	Y	607	CHL	4	0
31	Y	615	CLA	2	0
33	s	619	LUT	3	0
31	5	603	CLA	2	0
31	D	405	CLA	2	0
31	s	604	CLA	9	0
30	N	609	CHL	1	0
31	R	602	CLA	5	0
35	3	620	XAT	3	0
31	C	502	CLA	3	0
30	G	608	CHL	4	0
30	13	606	CHL	2	0
31	c	511	CLA	1	0
33	Y	622	LUT	1	0
31	11	603	CLA	4	0
30	4	607	CHL	2	0
31	4	603	CLA	1	0
31	C	509	CLA	2	0
33	y	622	LUT	4	0
33	4	617	LUT	2	0
35	R	616	XAT	2	0
31	2	610	CLA	2	0
31	15	612	CLA	8	0
30	N	607	CHL	8	0
31	6	610	CLA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand CLA 2 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT r 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

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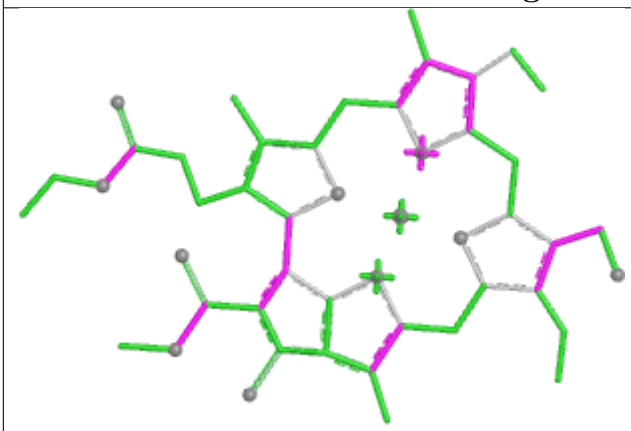
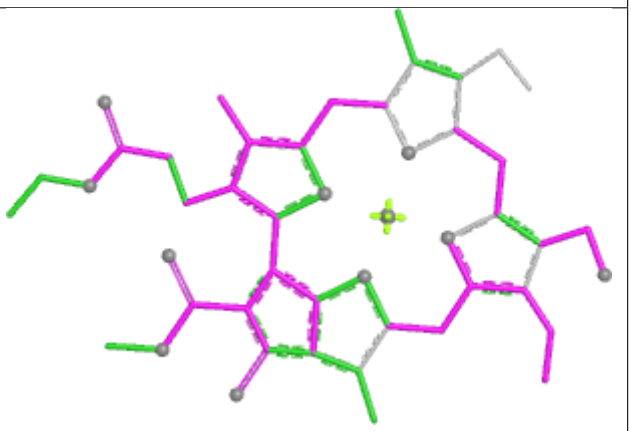
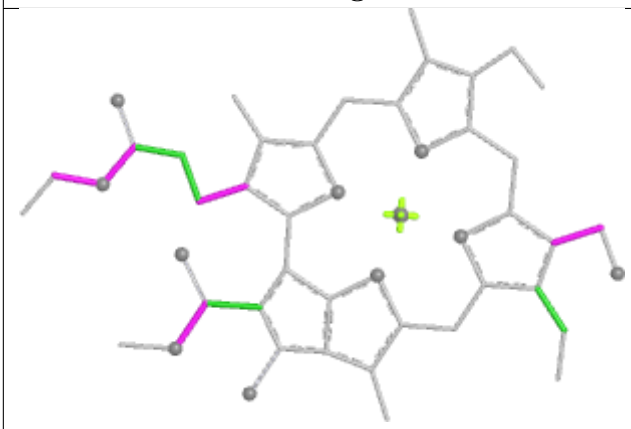
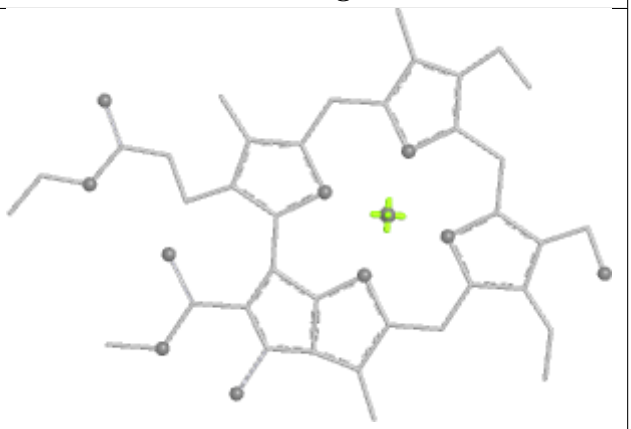
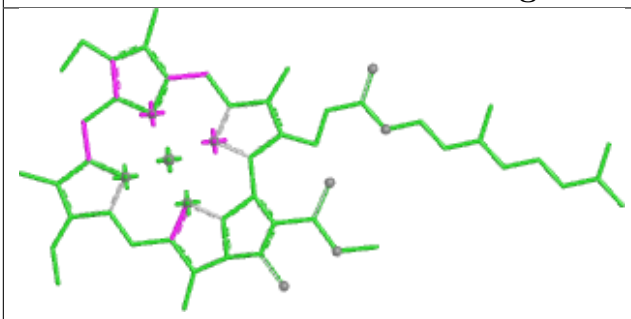
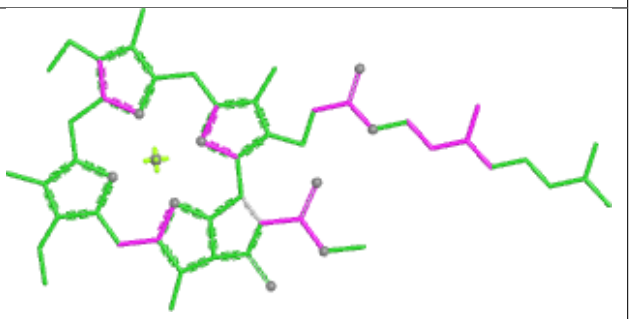
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 11 610



Bond lengths



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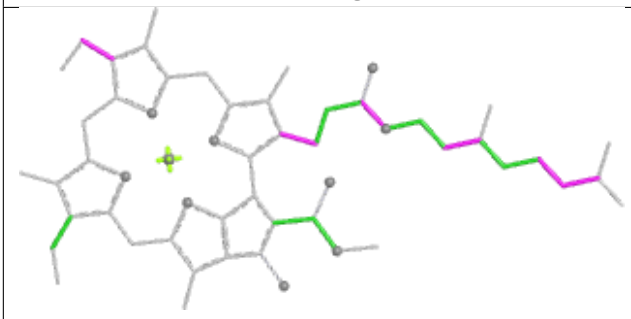

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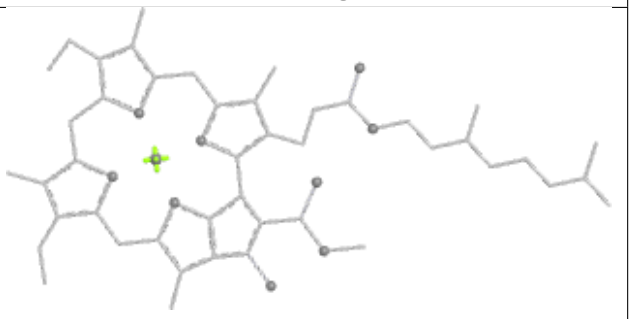

Rings

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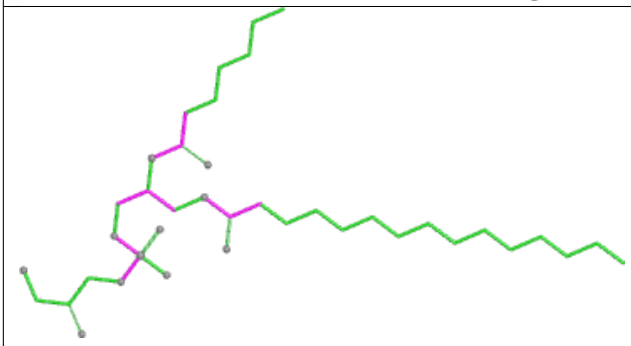

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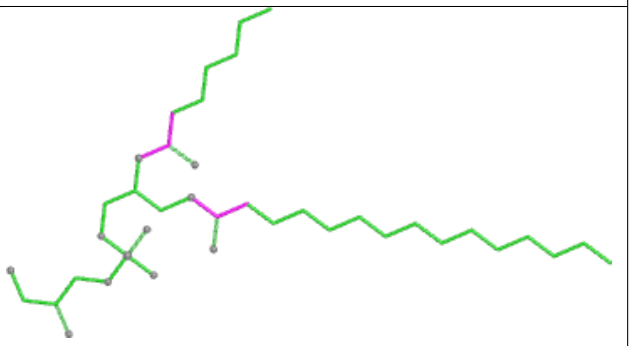

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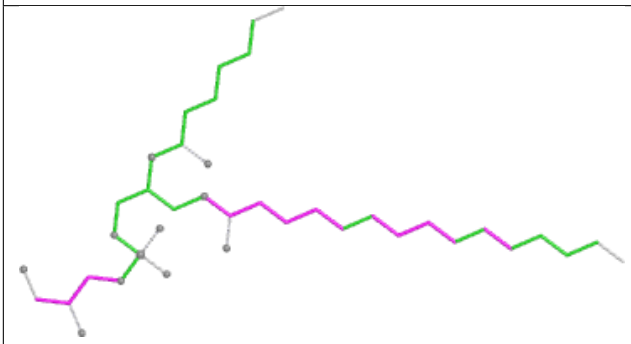

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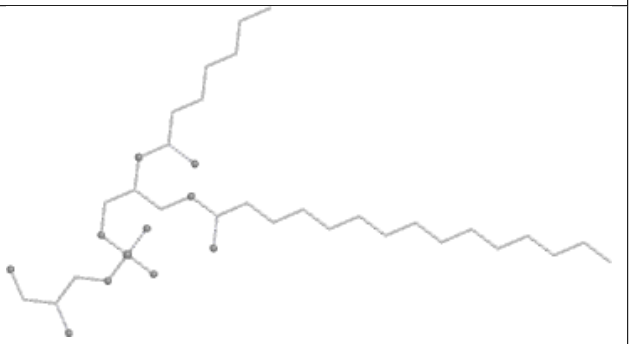

Rings

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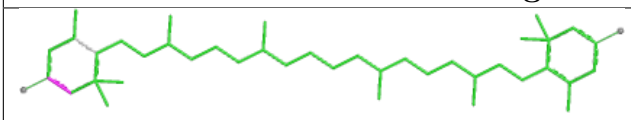
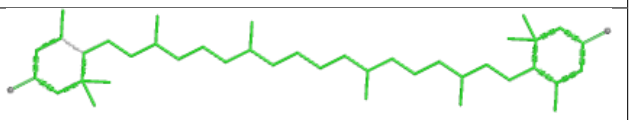
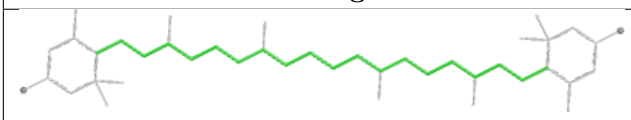
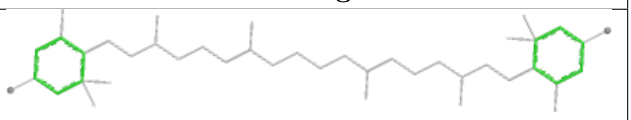
 Bond lengths	 Bond angles
 Torsions	 Rings

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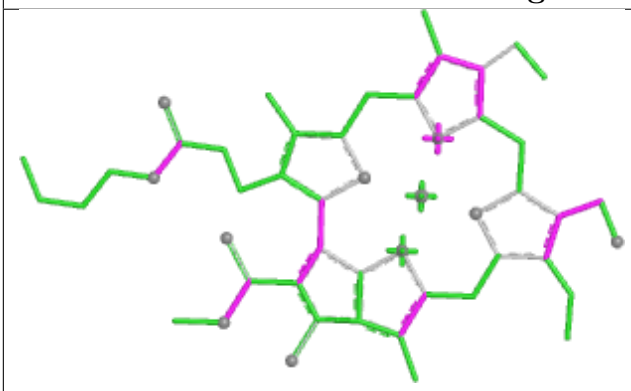
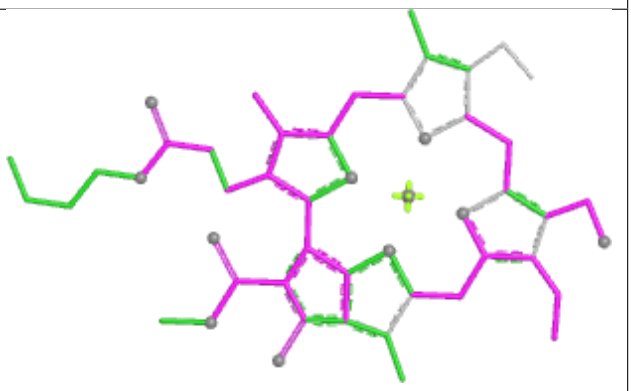
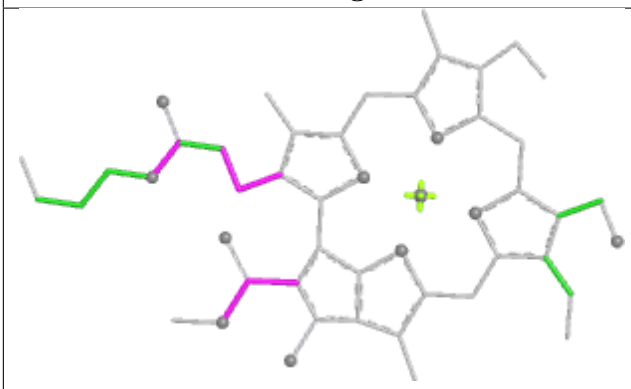
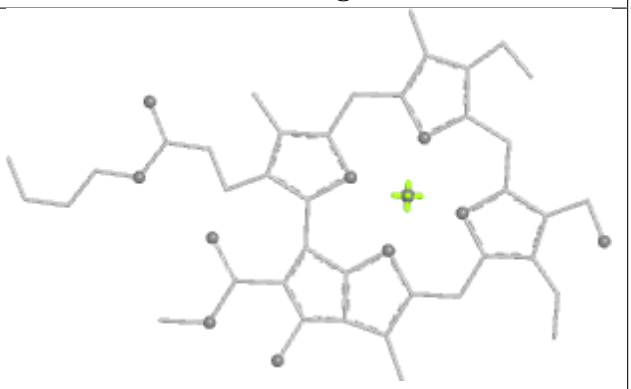
 Bond lengths	 Bond angles
 Torsions	 Rings

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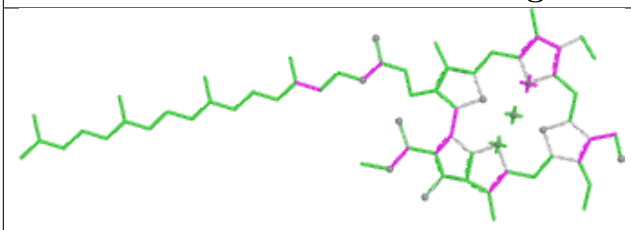
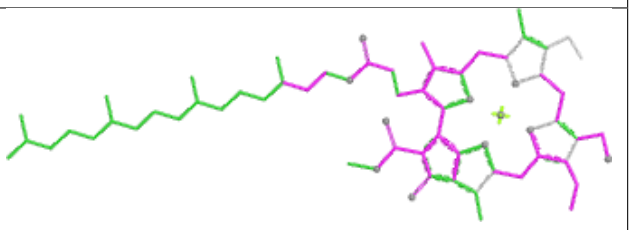
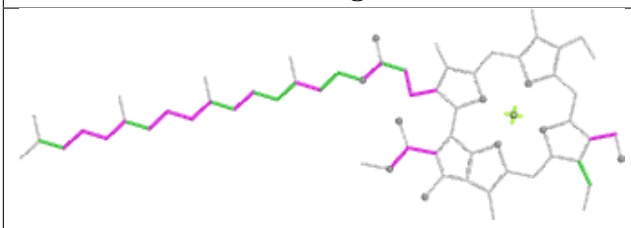
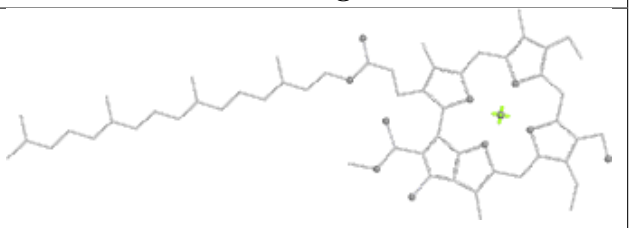
 Bond lengths	 Bond angles
 Torsions	 Rings

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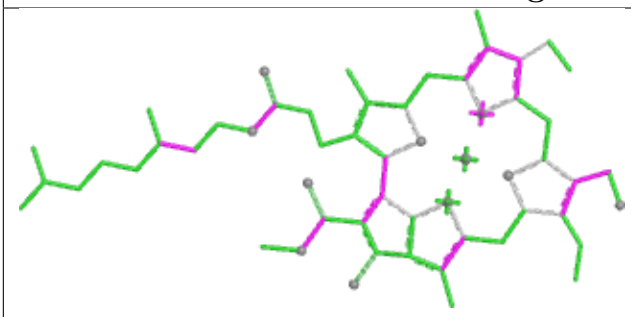
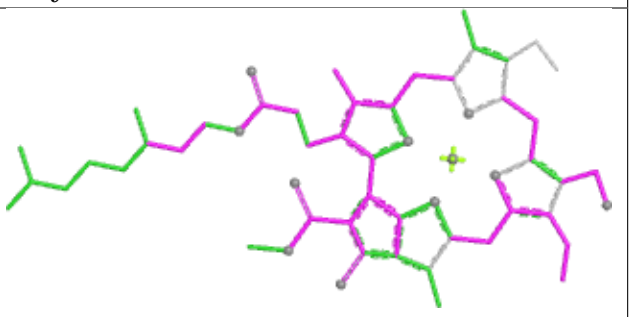
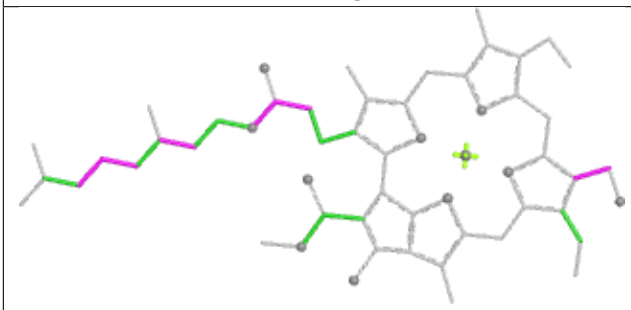
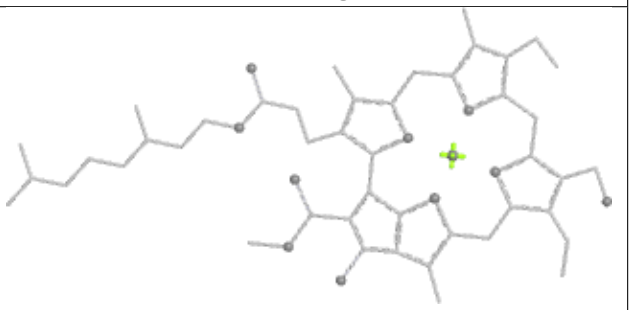
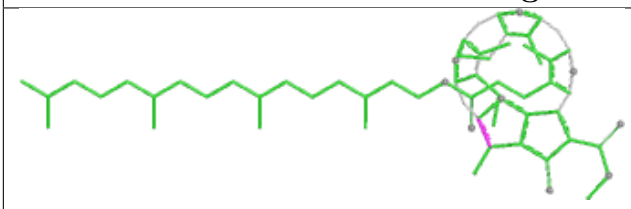
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO A 405



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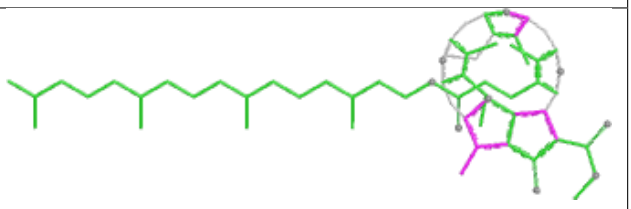
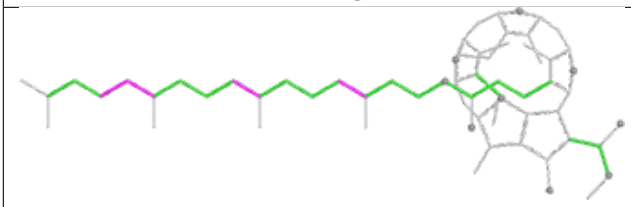


Bond angles



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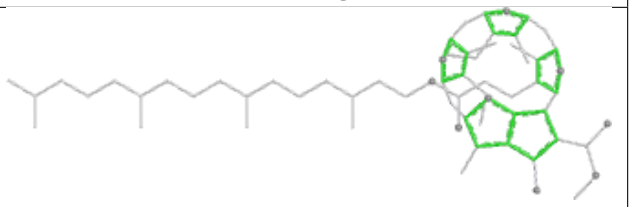
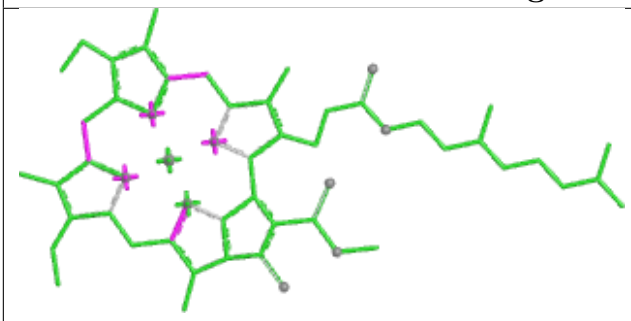


Rings

Ligand CLA n 604



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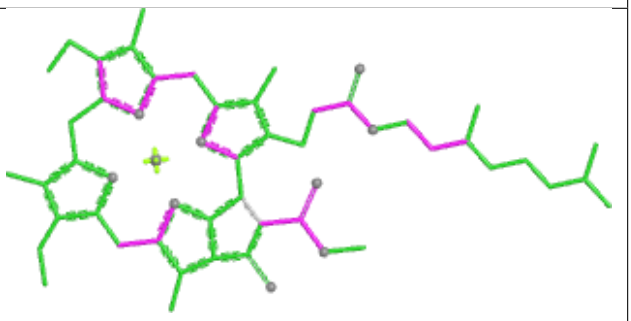
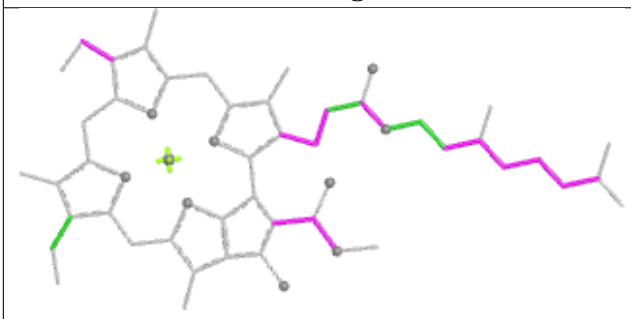


Bond angles



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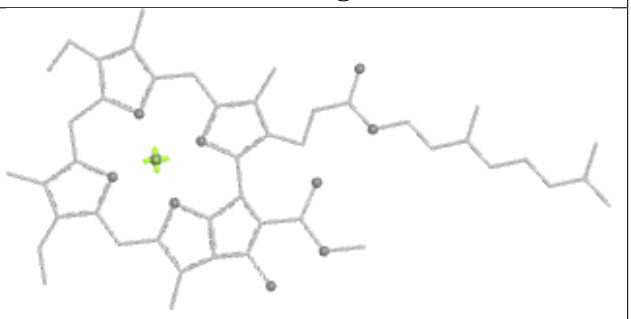

Rings

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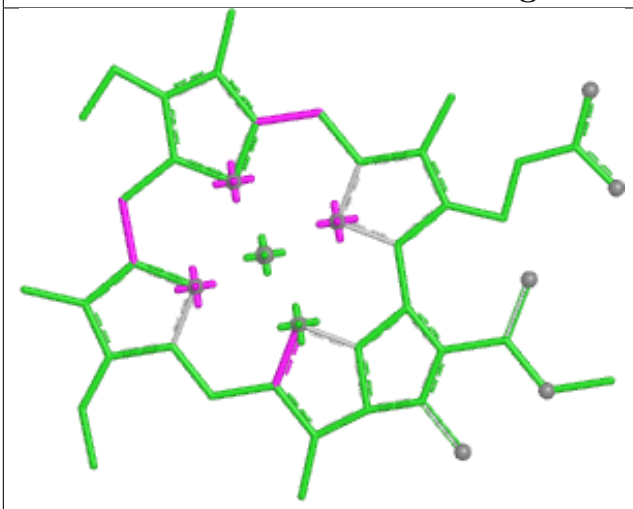

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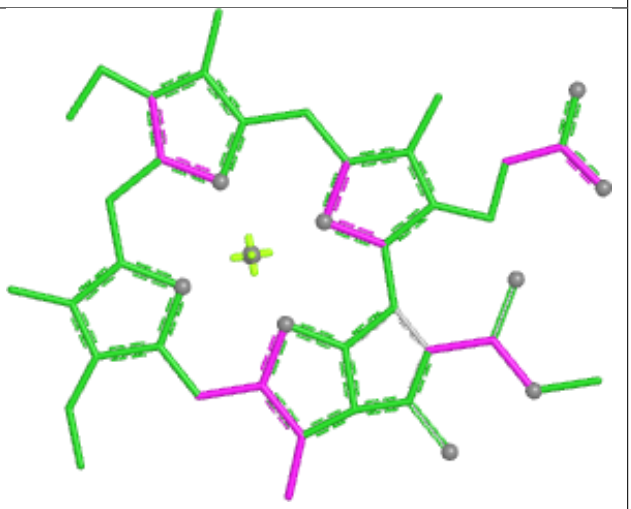
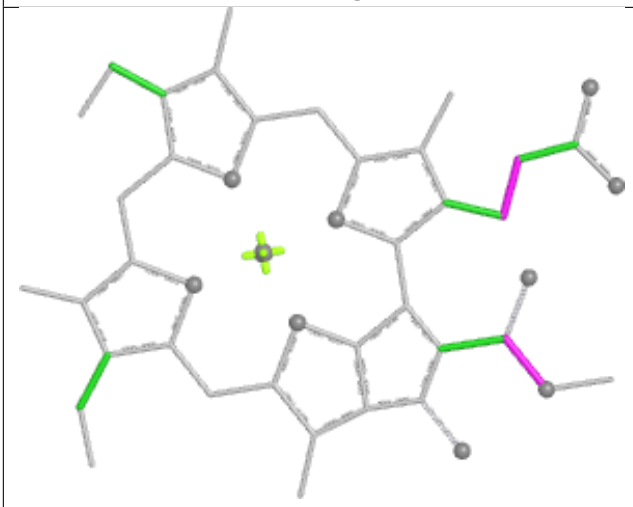


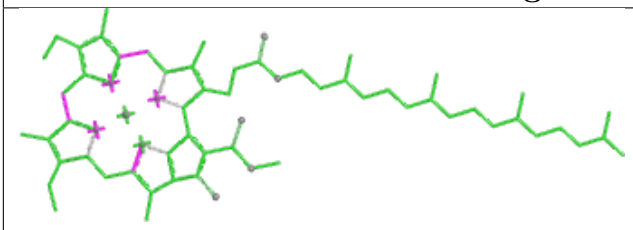
Bond angles



Torsions

Rings

Ligand CLA Y 612



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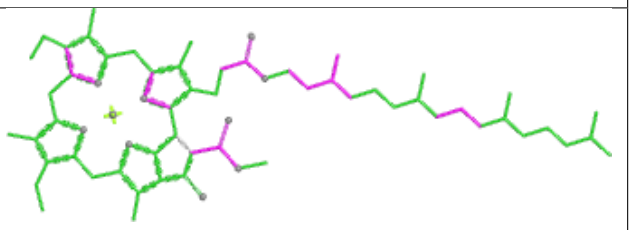

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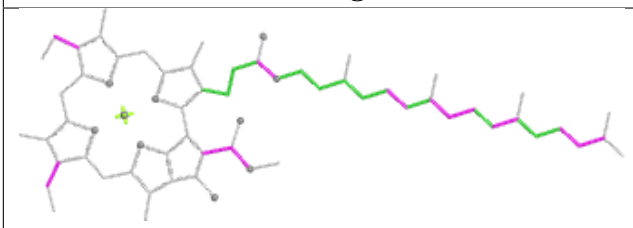
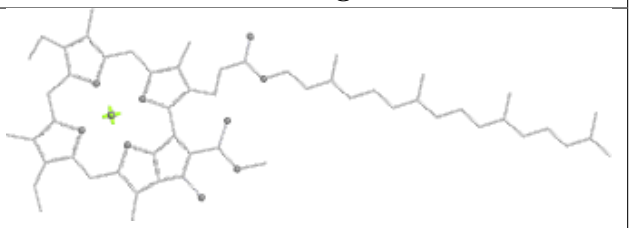
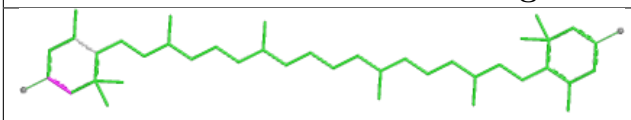
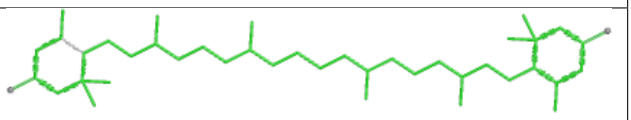
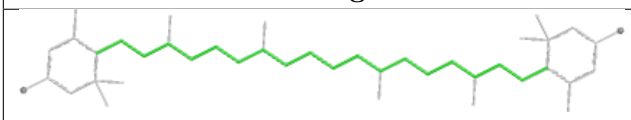
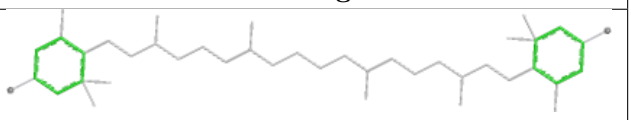


Torsions



Rings

Ligand LUT 14 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

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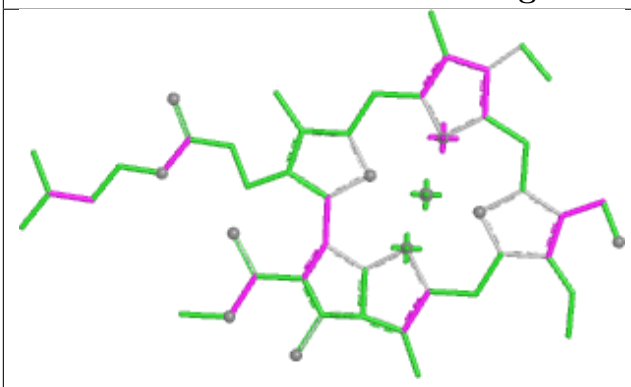
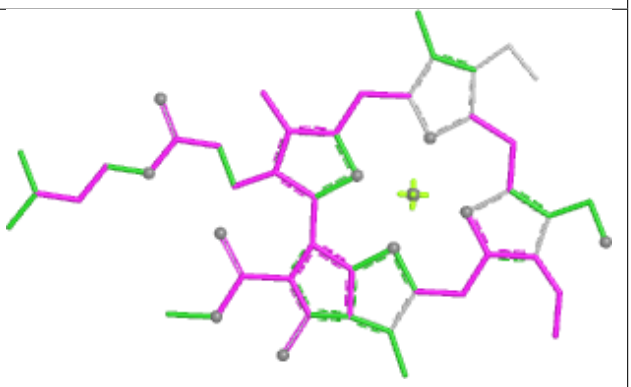
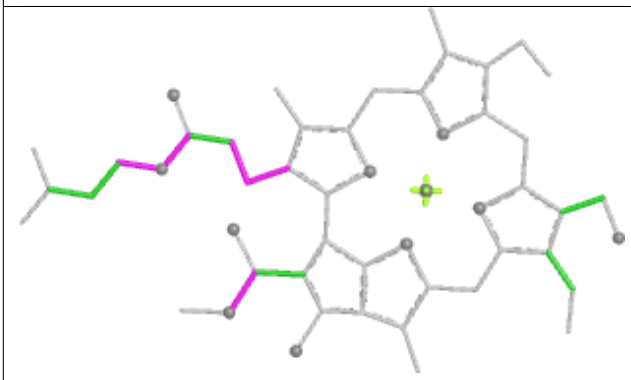
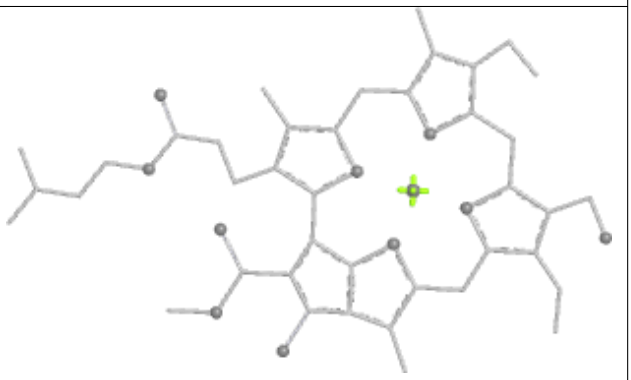
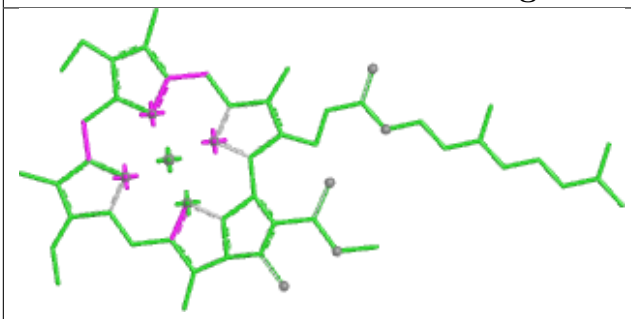
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 13 604



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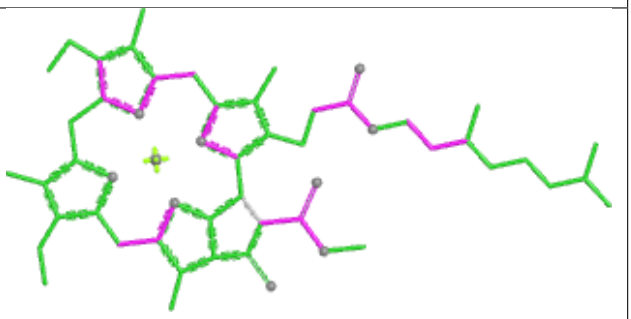

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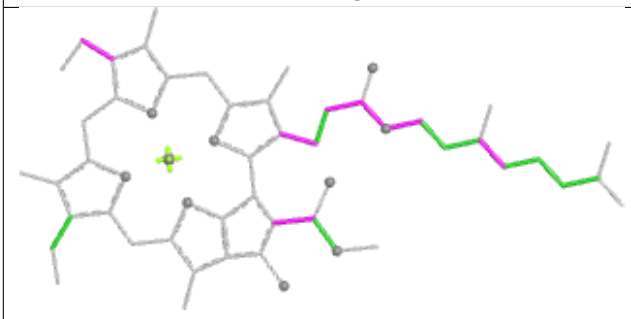

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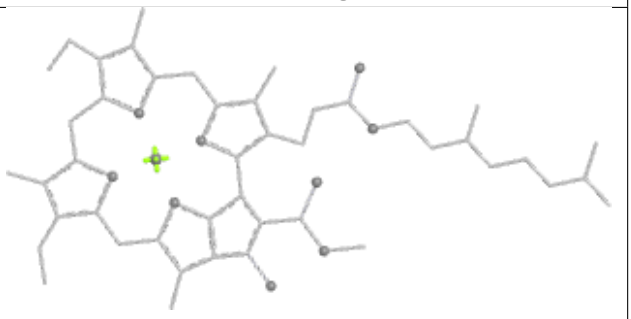
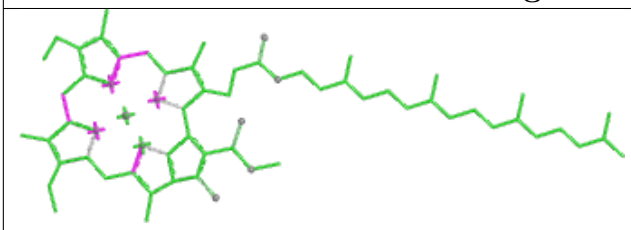


Rings

Ligand CLA A 404



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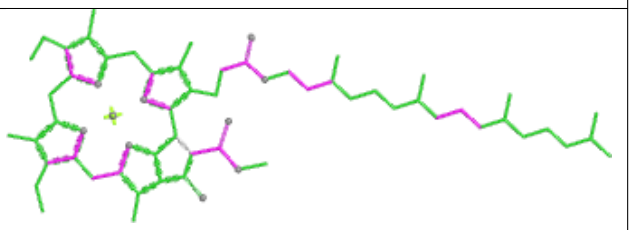

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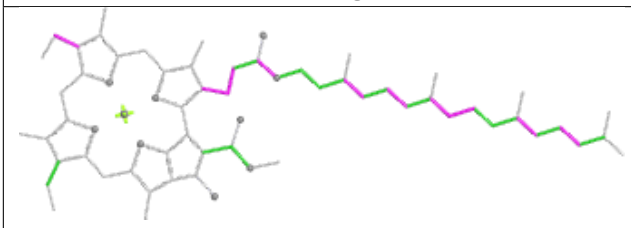

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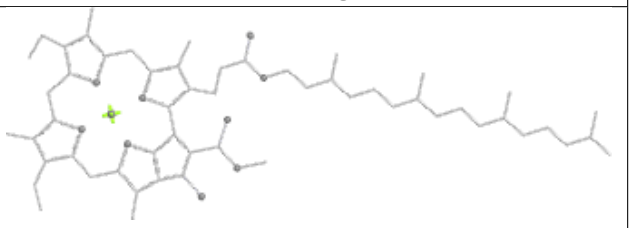
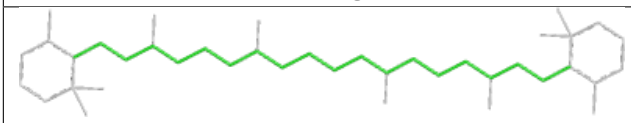


Rings

Ligand BCR B 619

Bond lengths

Bond angles



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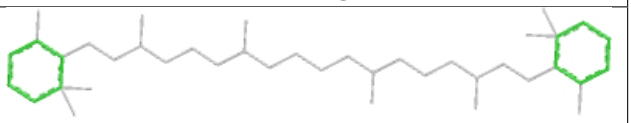
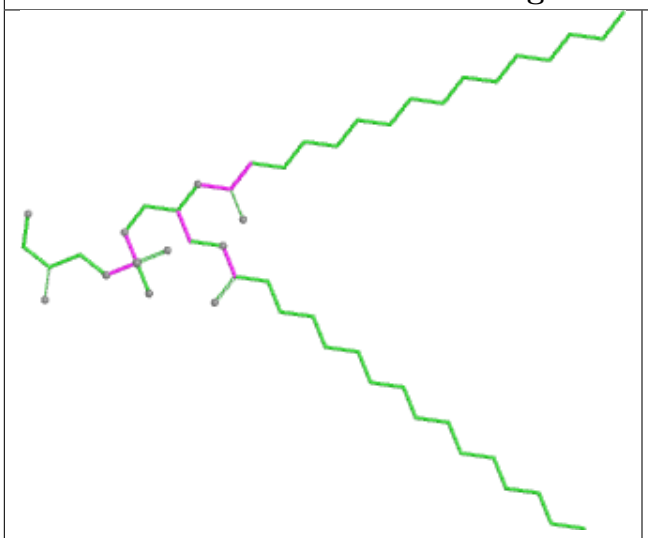


Rings

Ligand LHG y 616



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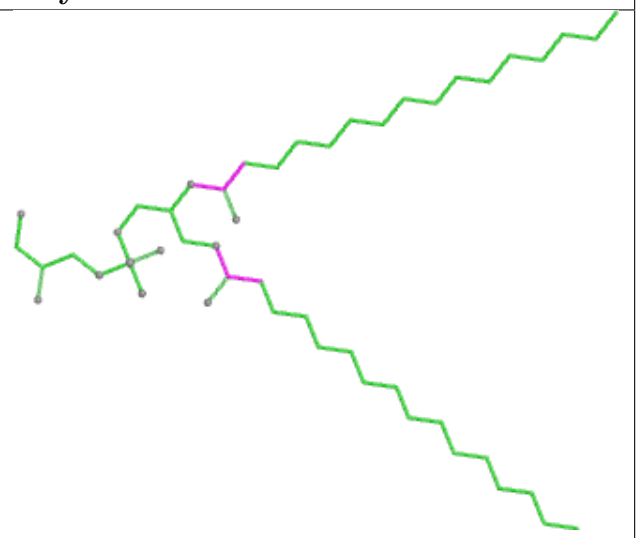

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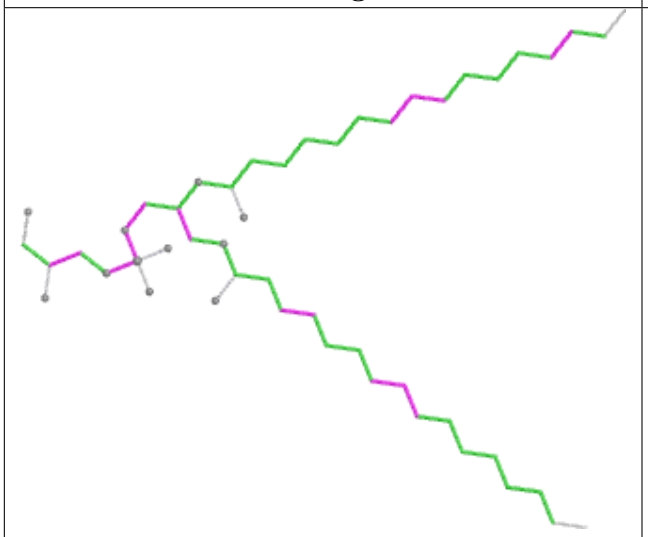

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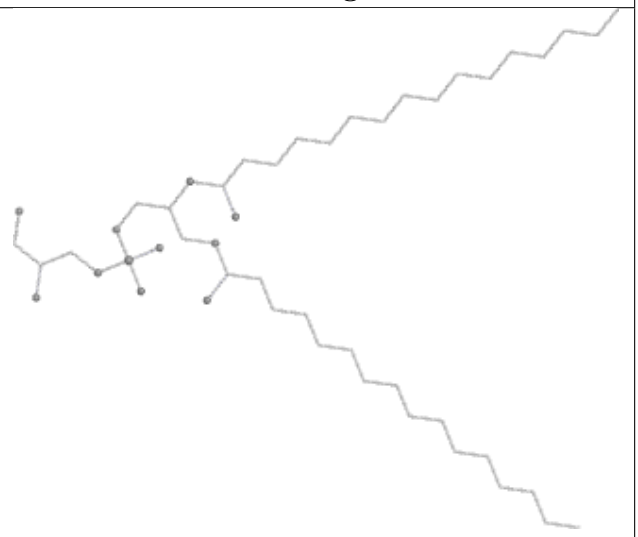
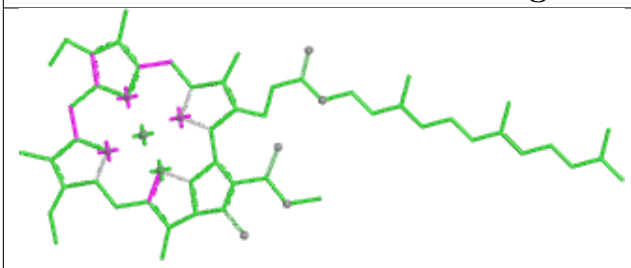
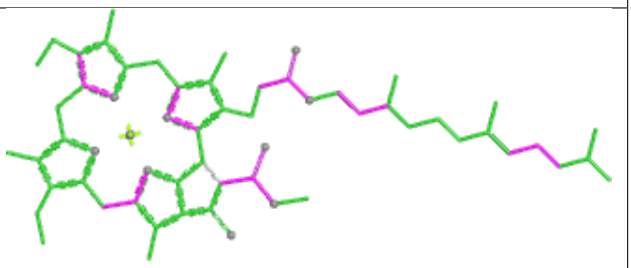
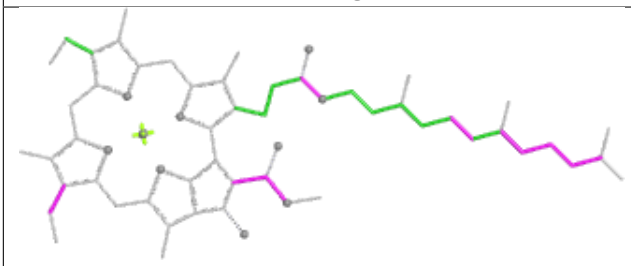
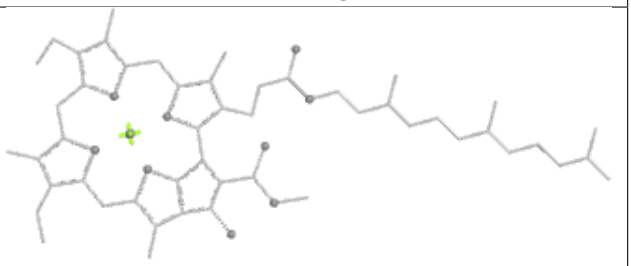
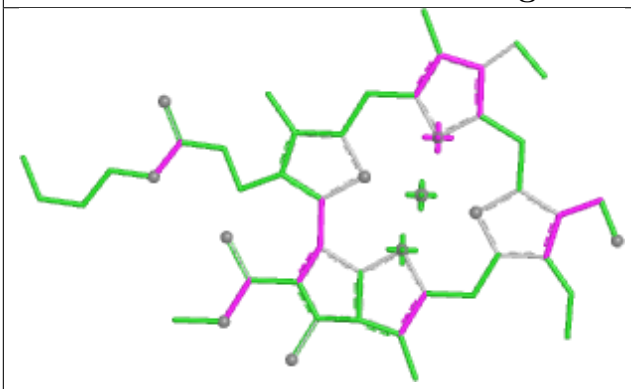
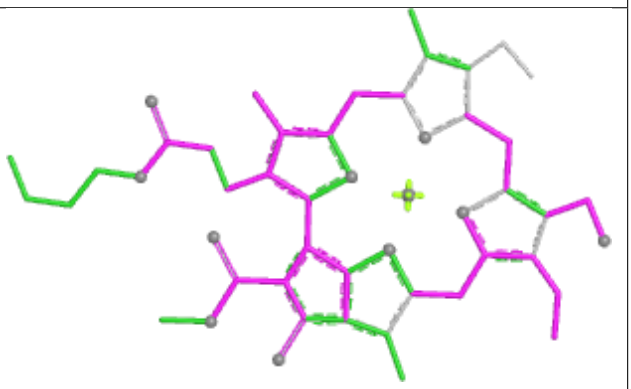
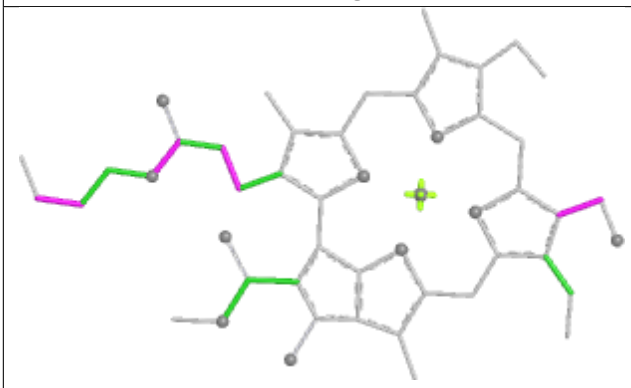
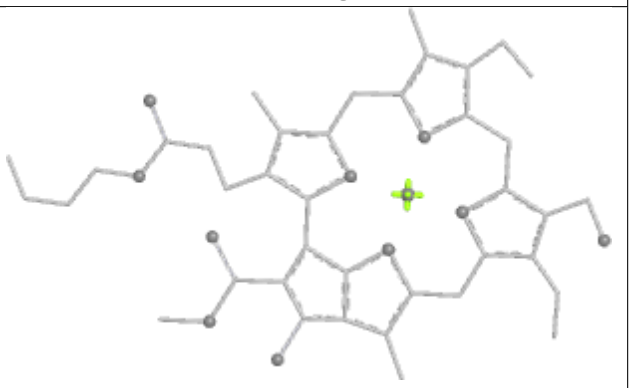
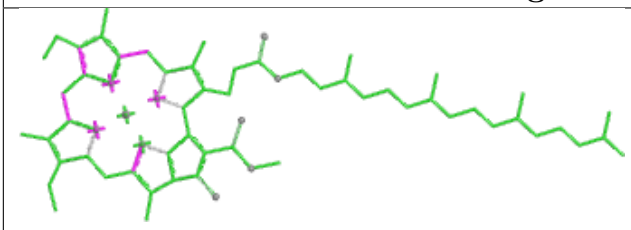
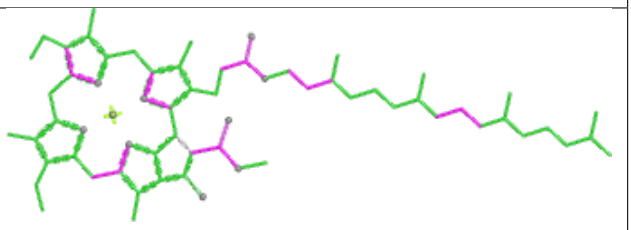
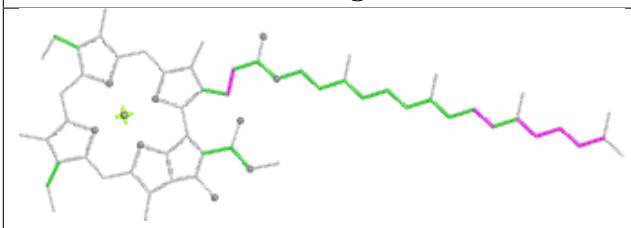
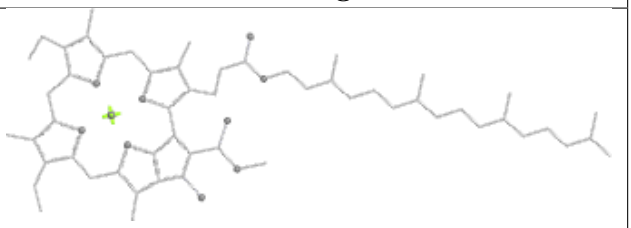


Rings

Ligand CLA c 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 12 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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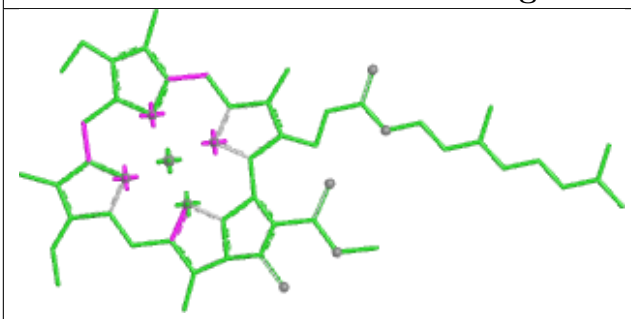
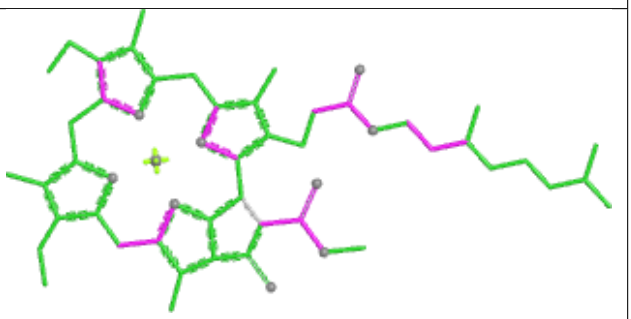
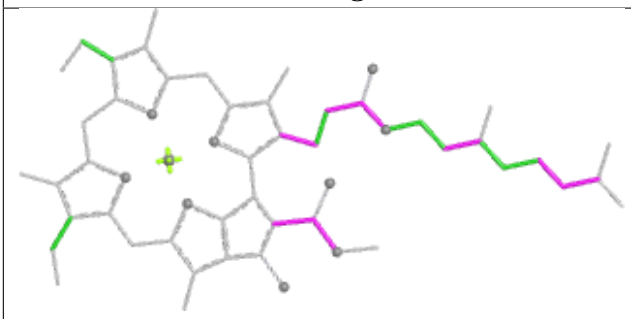
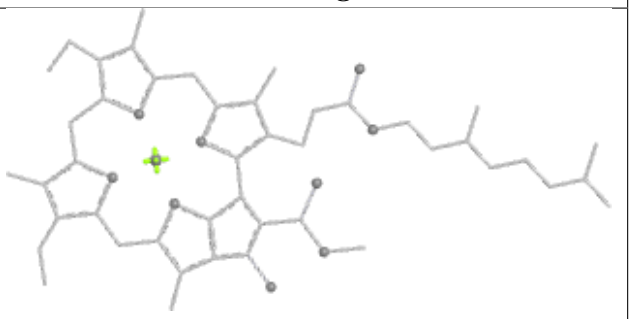
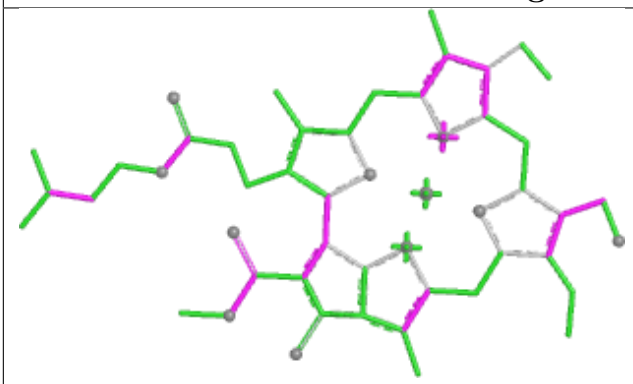
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 5 601



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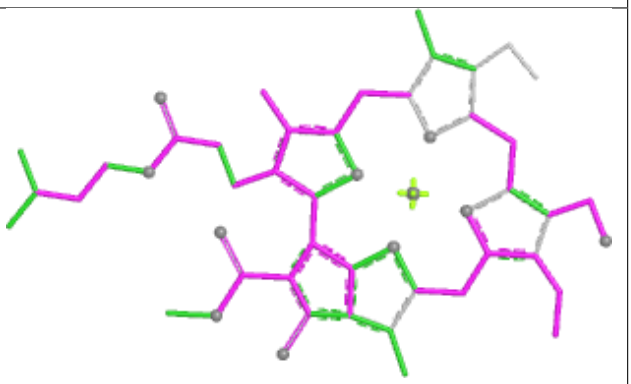
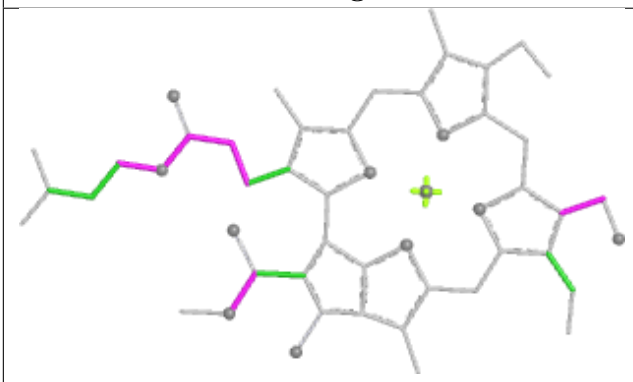


Bond angles



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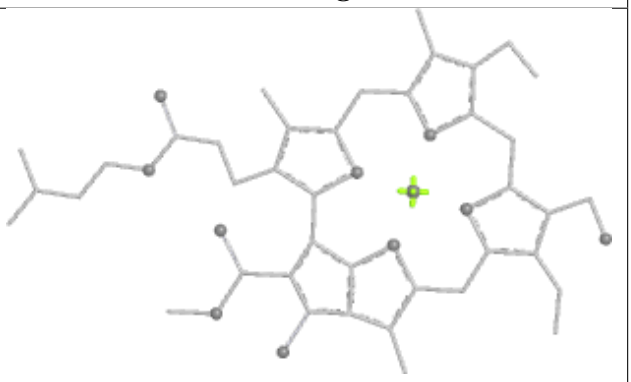
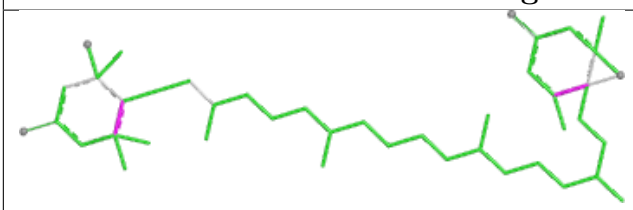


Rings

Ligand NEX G 618



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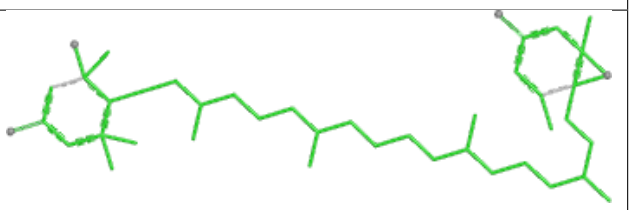

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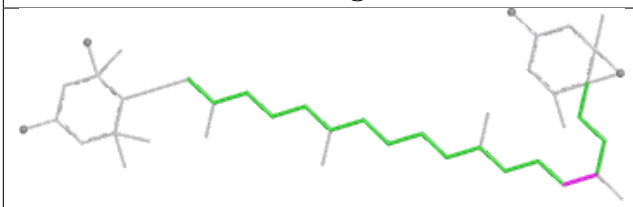

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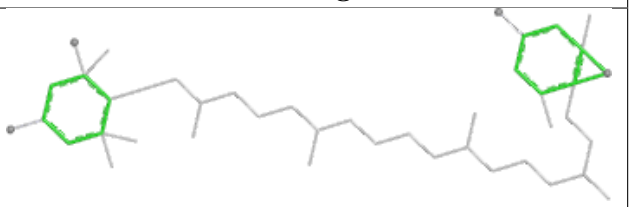
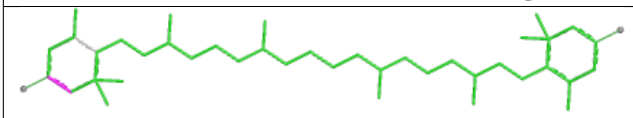


Rings

Ligand LUT 13 618



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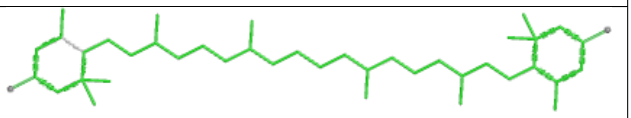
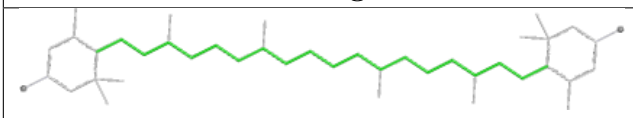
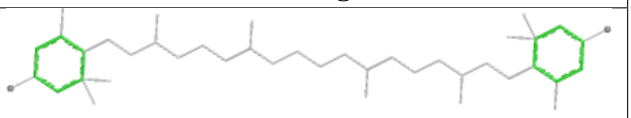


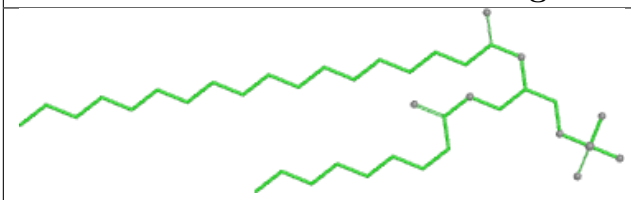
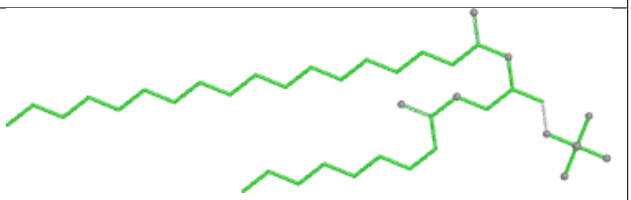
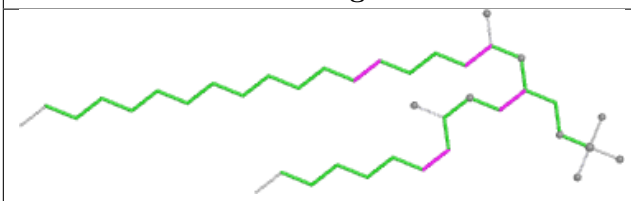
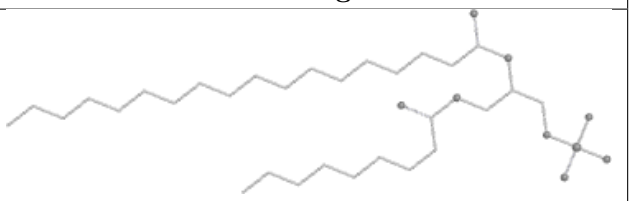
Bond angles

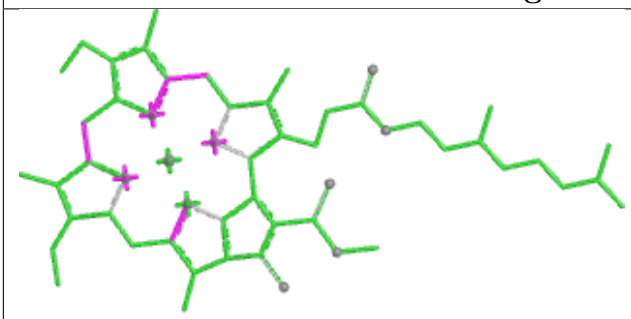
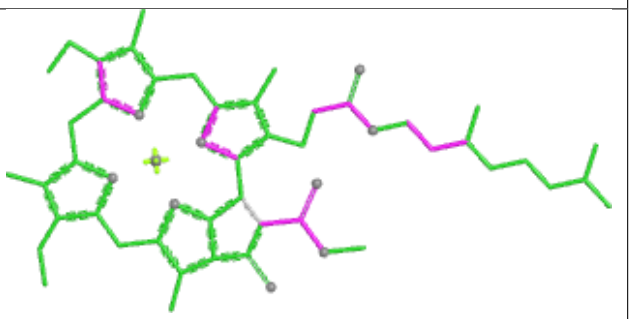
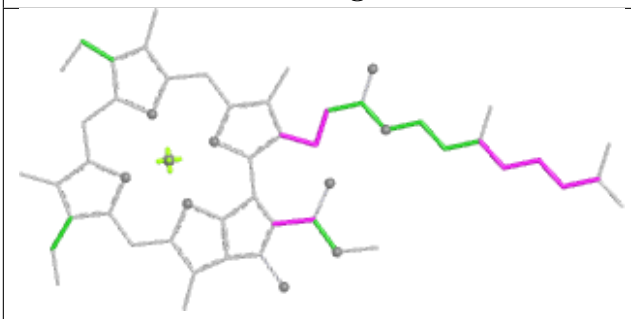
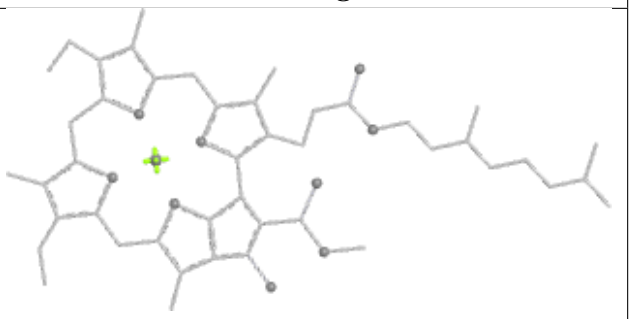


Torsions

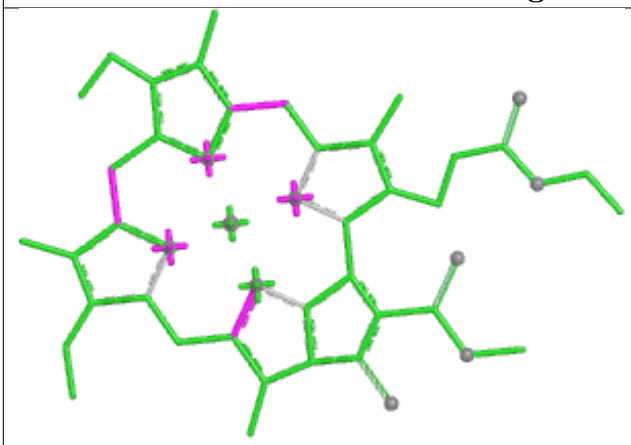


Rings

Ligand 3PH b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 615



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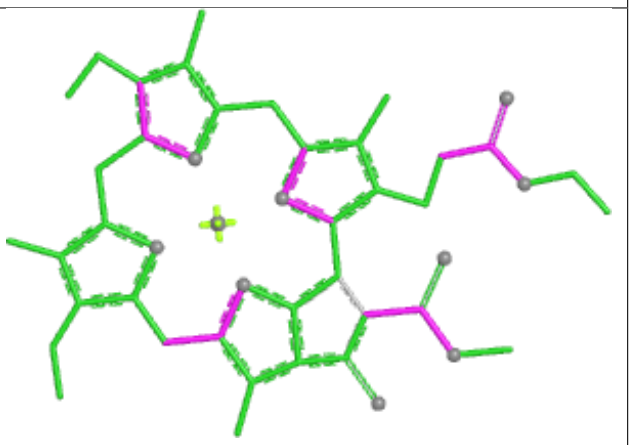
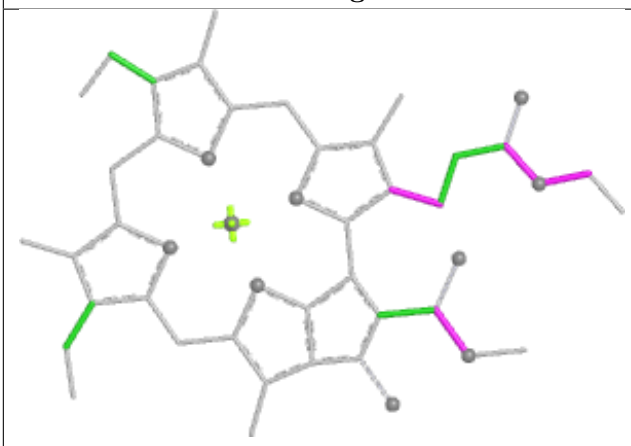


Bond angles



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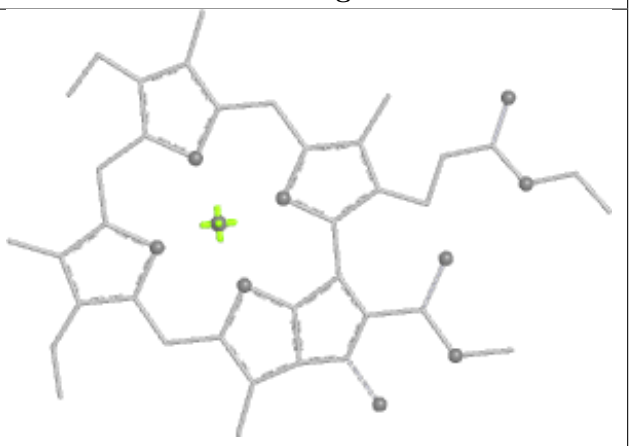
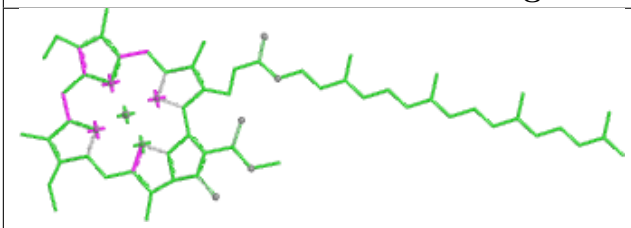


Rings

Ligand CLA Y 602



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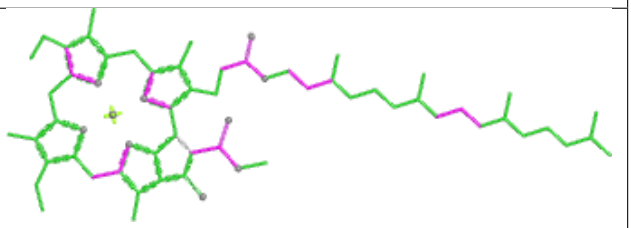
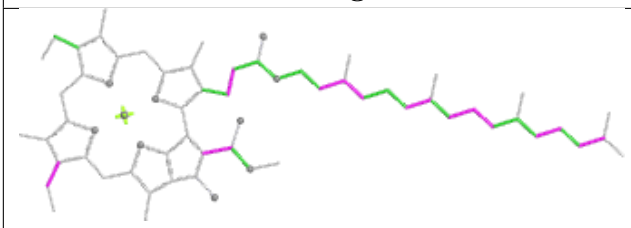


Bond angles



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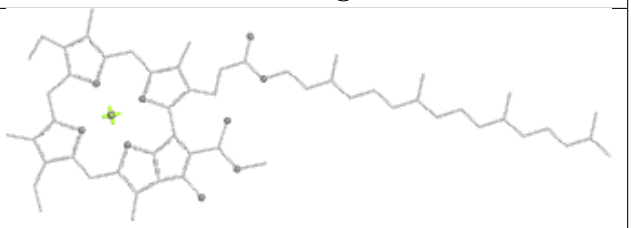
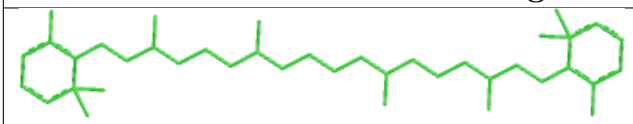


Rings

Ligand BCR c 526



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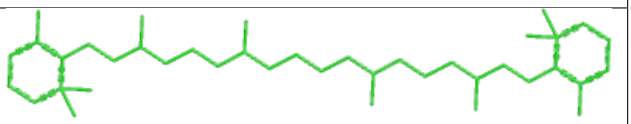
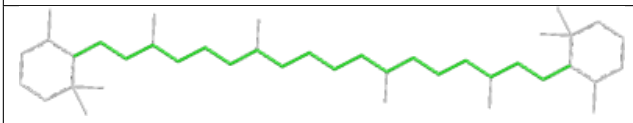


Bond angles



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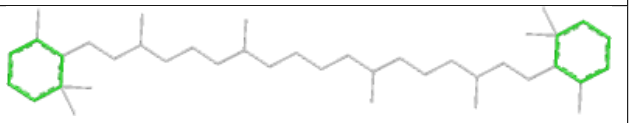
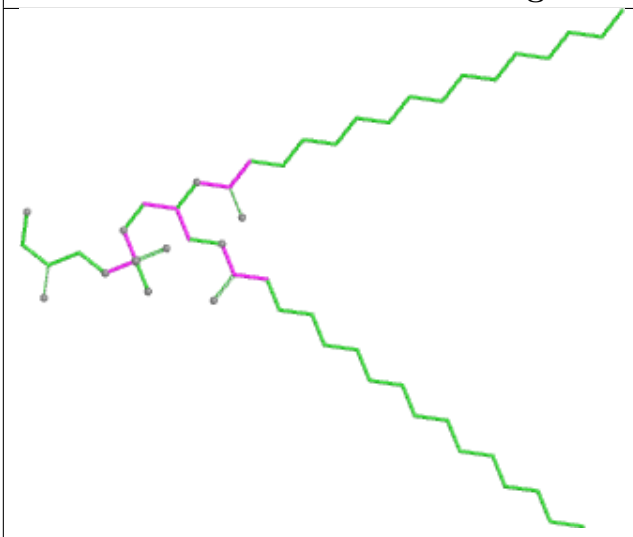


Rings

Ligand LHG a 411



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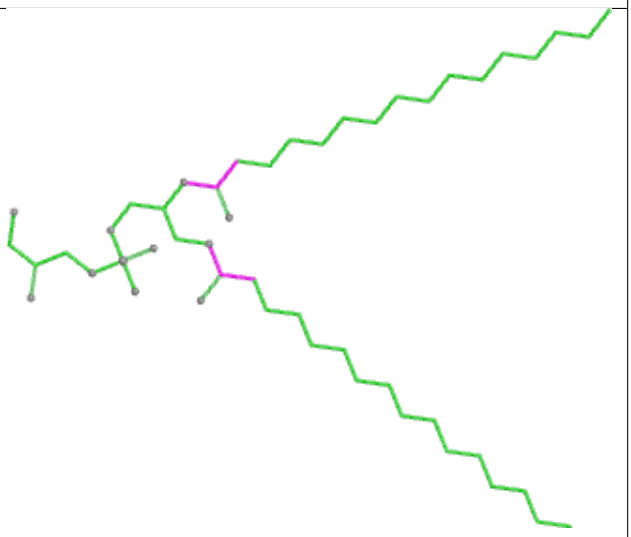
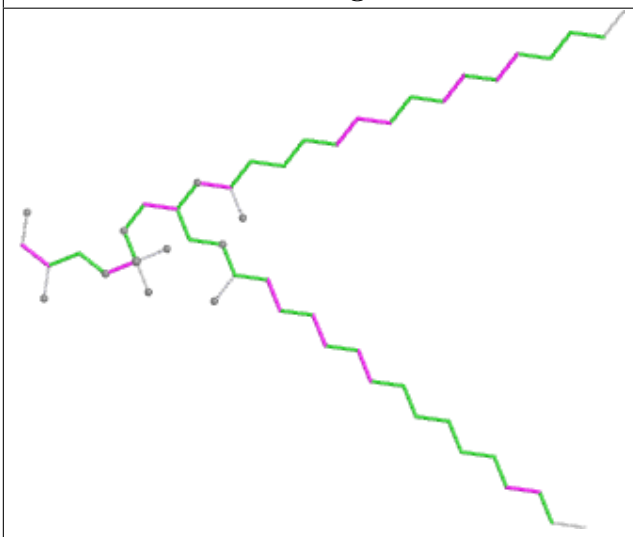


Bond angles



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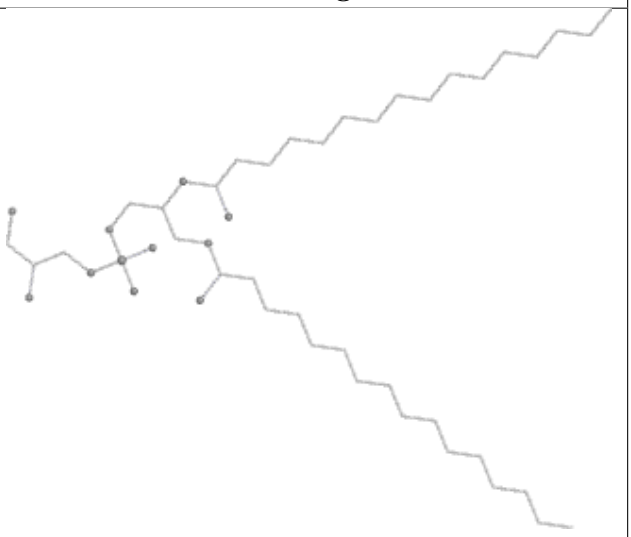
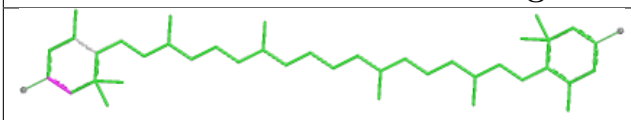


Rings

Ligand LUT n 618



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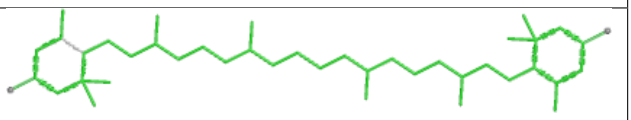

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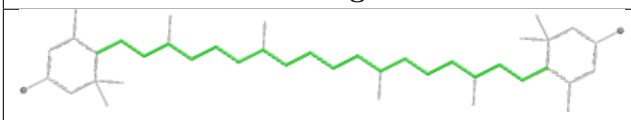

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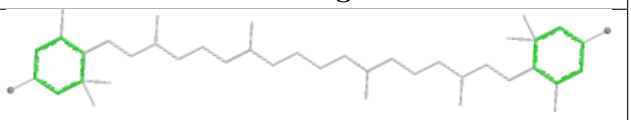
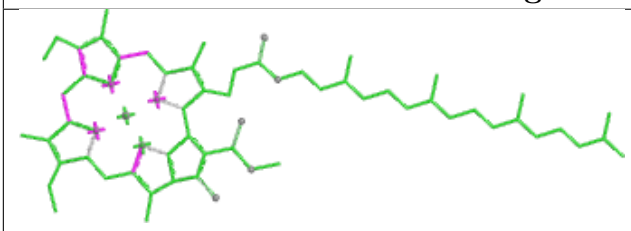


Rings

Ligand CLA B 602



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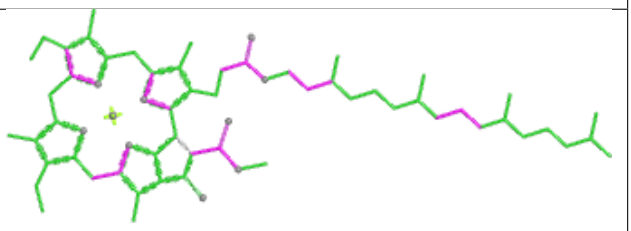

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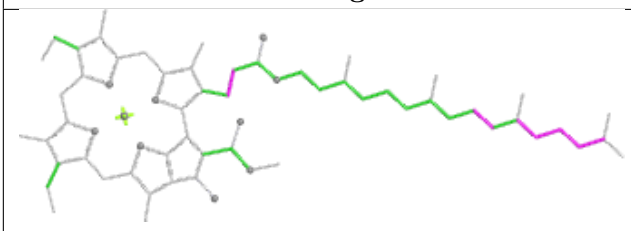

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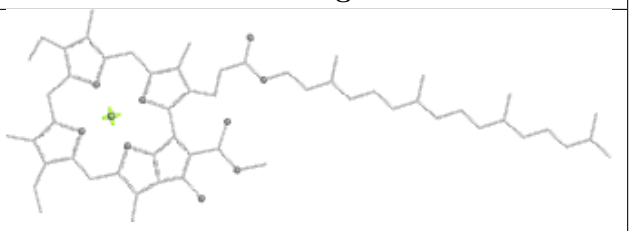
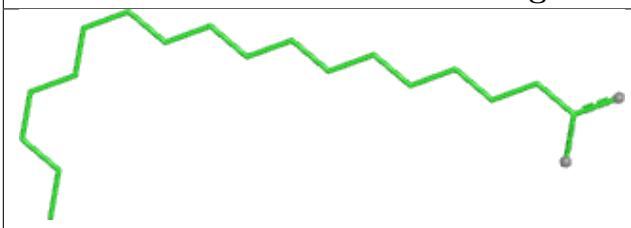


Rings

Ligand LNL h 101



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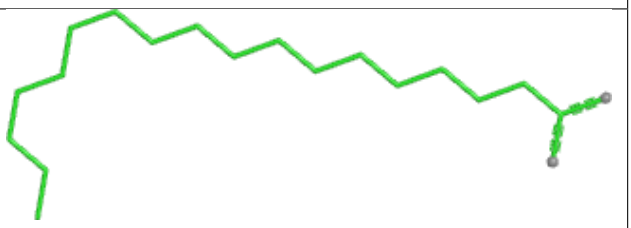
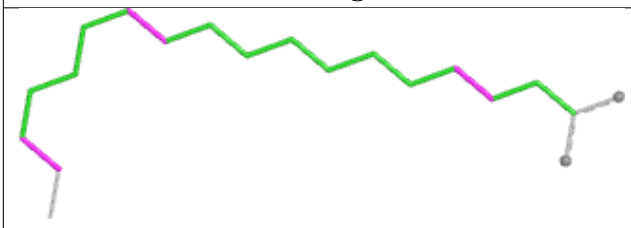


Bond angles



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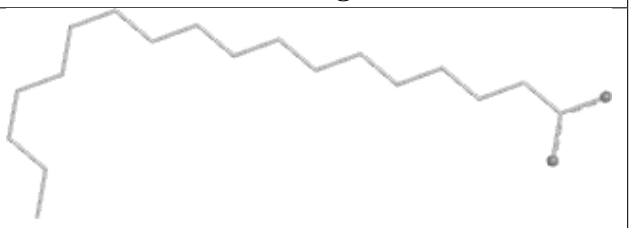
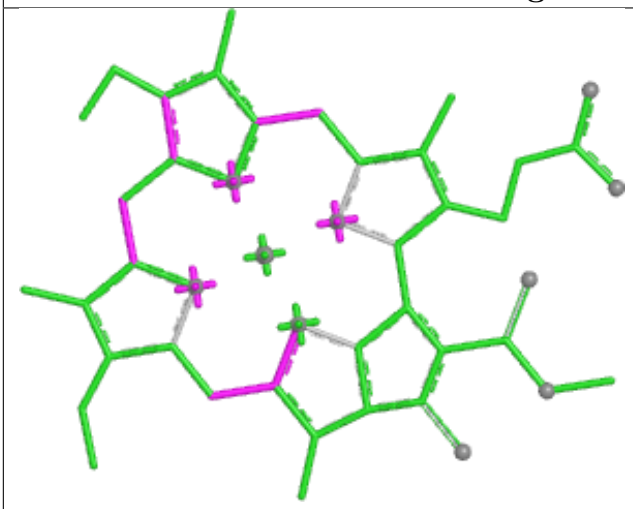


Rings

Ligand CLA S 612



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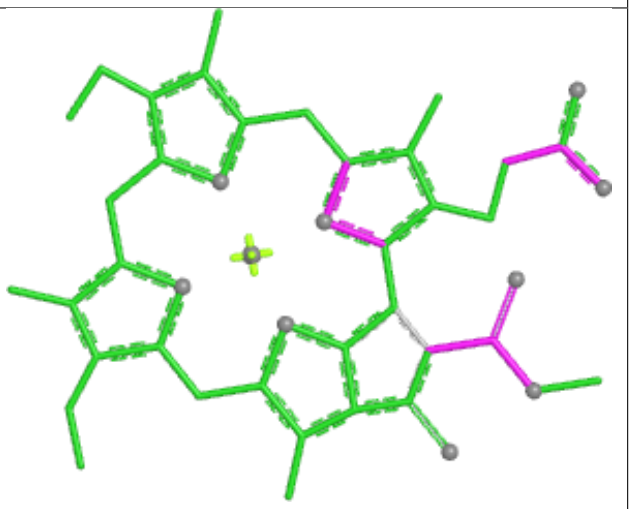
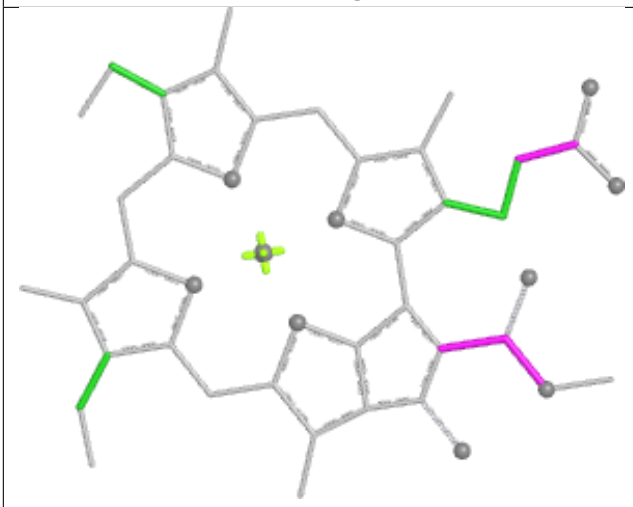


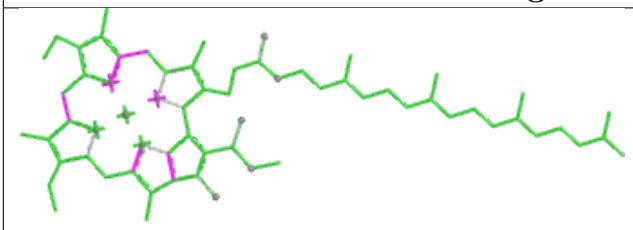
Bond angles



Torsions

Rings

Ligand CLA d 402



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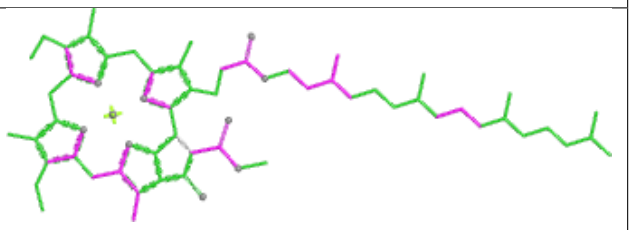
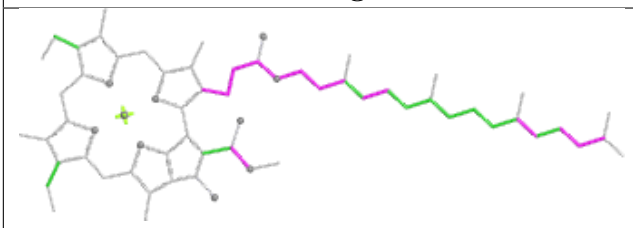
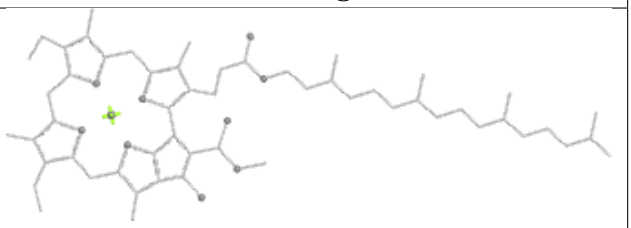


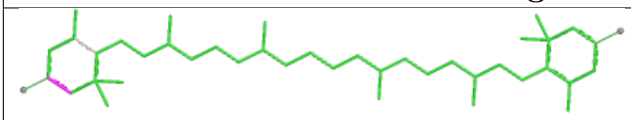
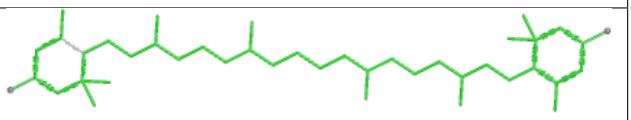
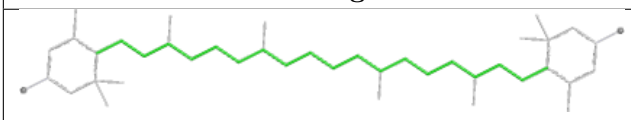
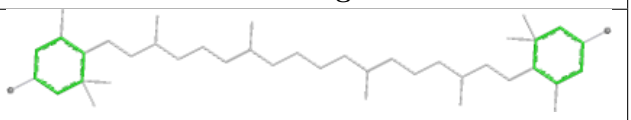
Bond angles

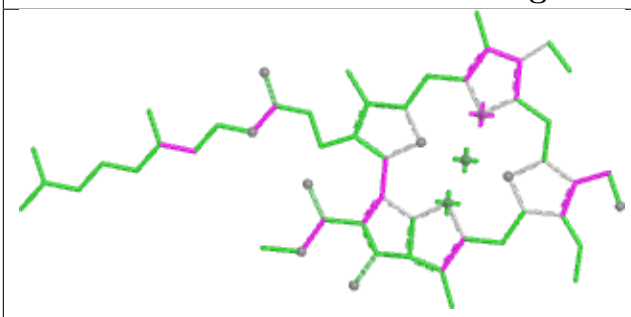
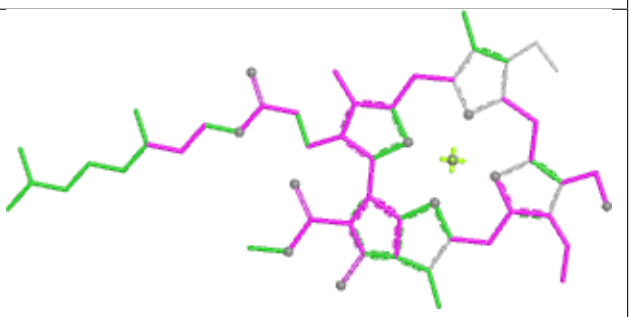
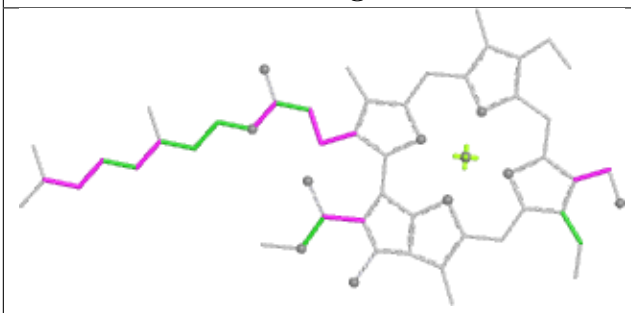
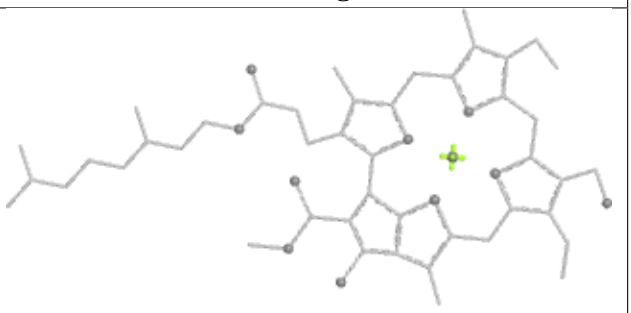


Torsions

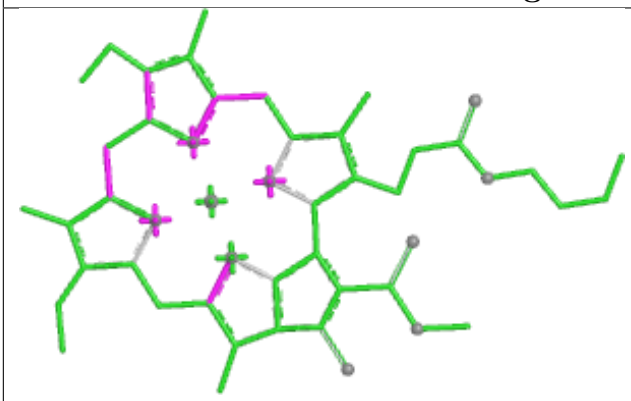


Rings

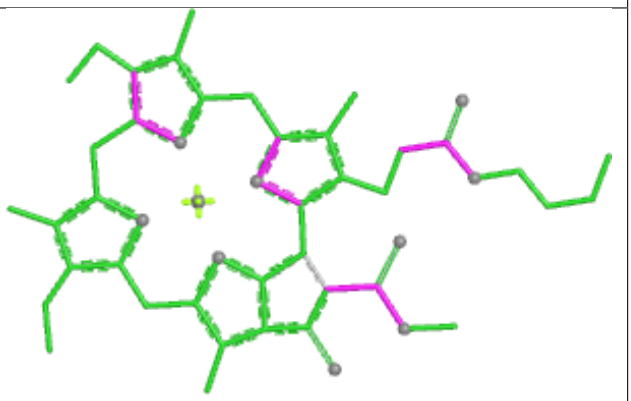
Ligand LUT S 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

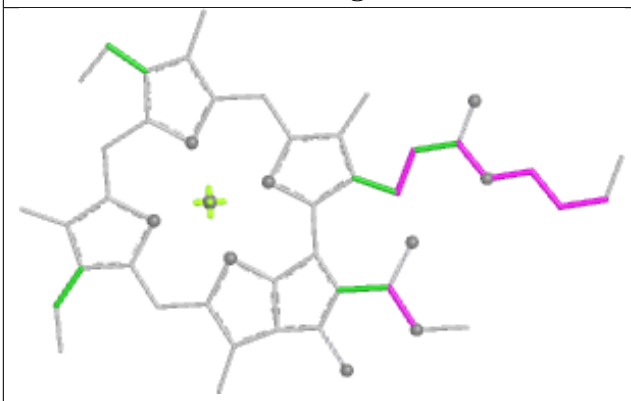
Ligand CLA R 611



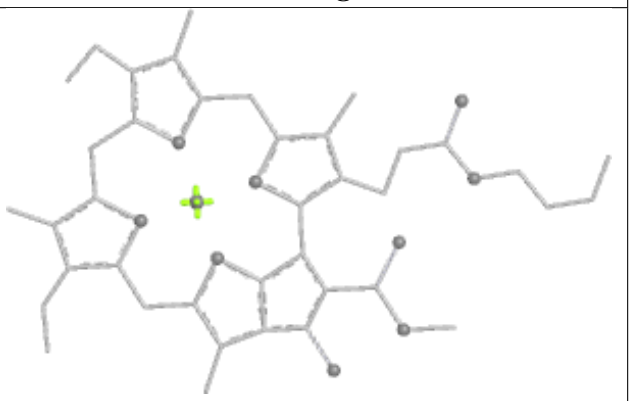
Bond lengths



Bond angles



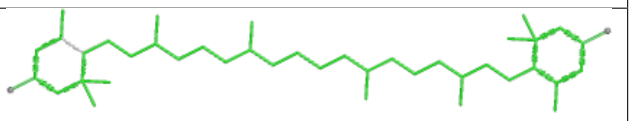
Torsions



Rings

Ligand LUT 2 614

Bond lengths



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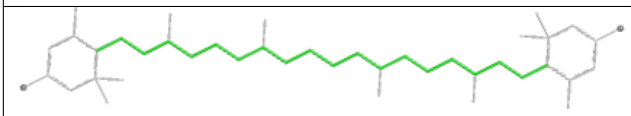
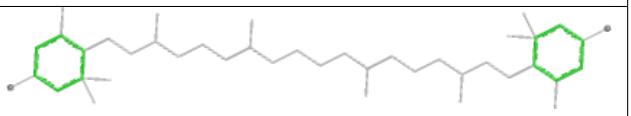
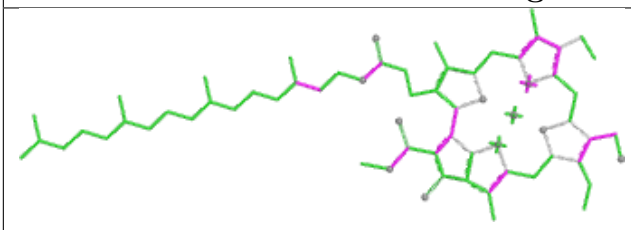
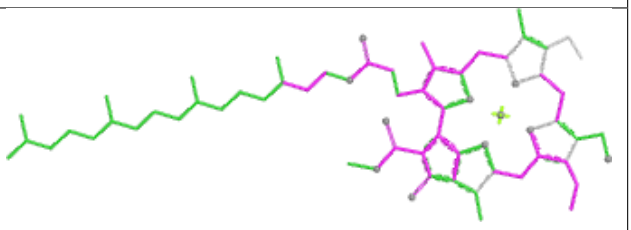
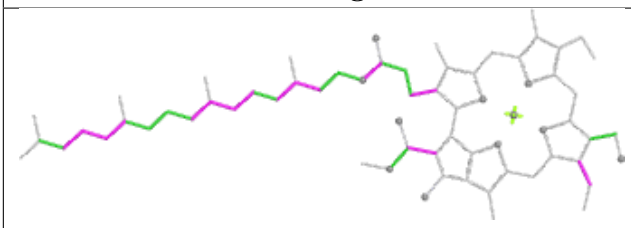
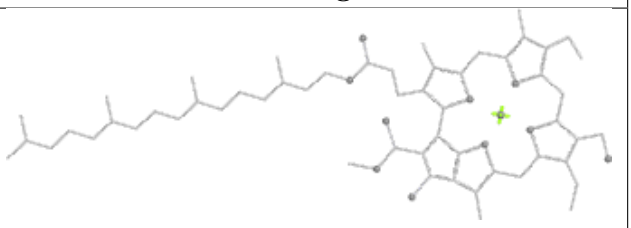
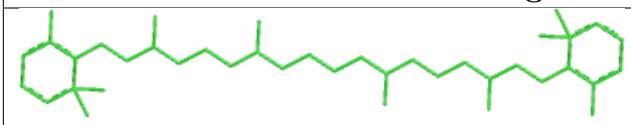
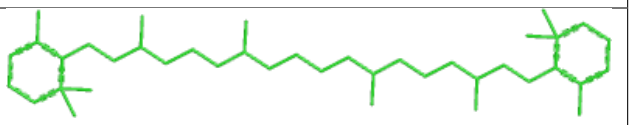
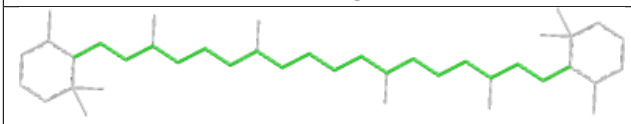
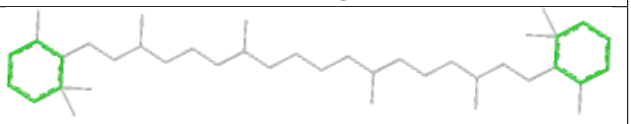


Torsions

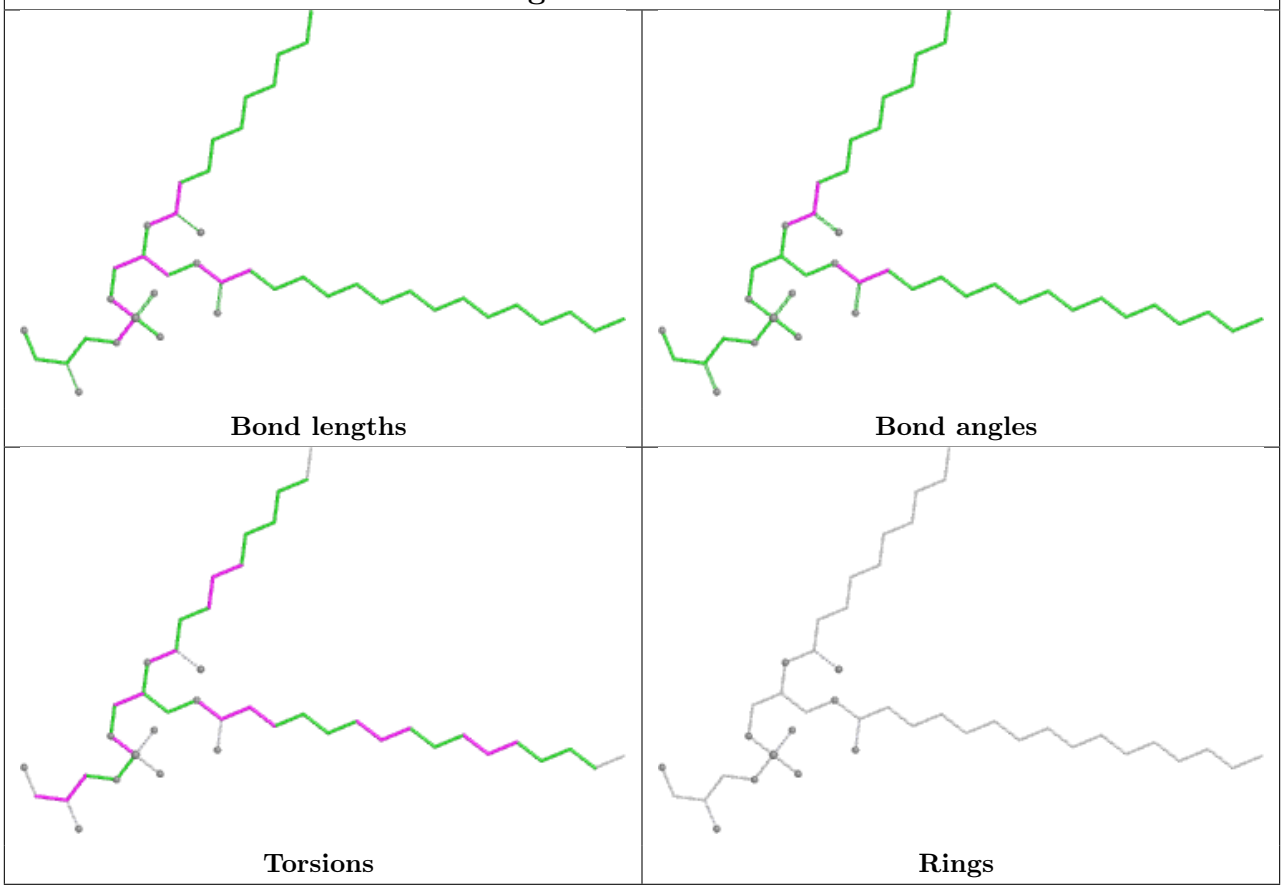


Rings

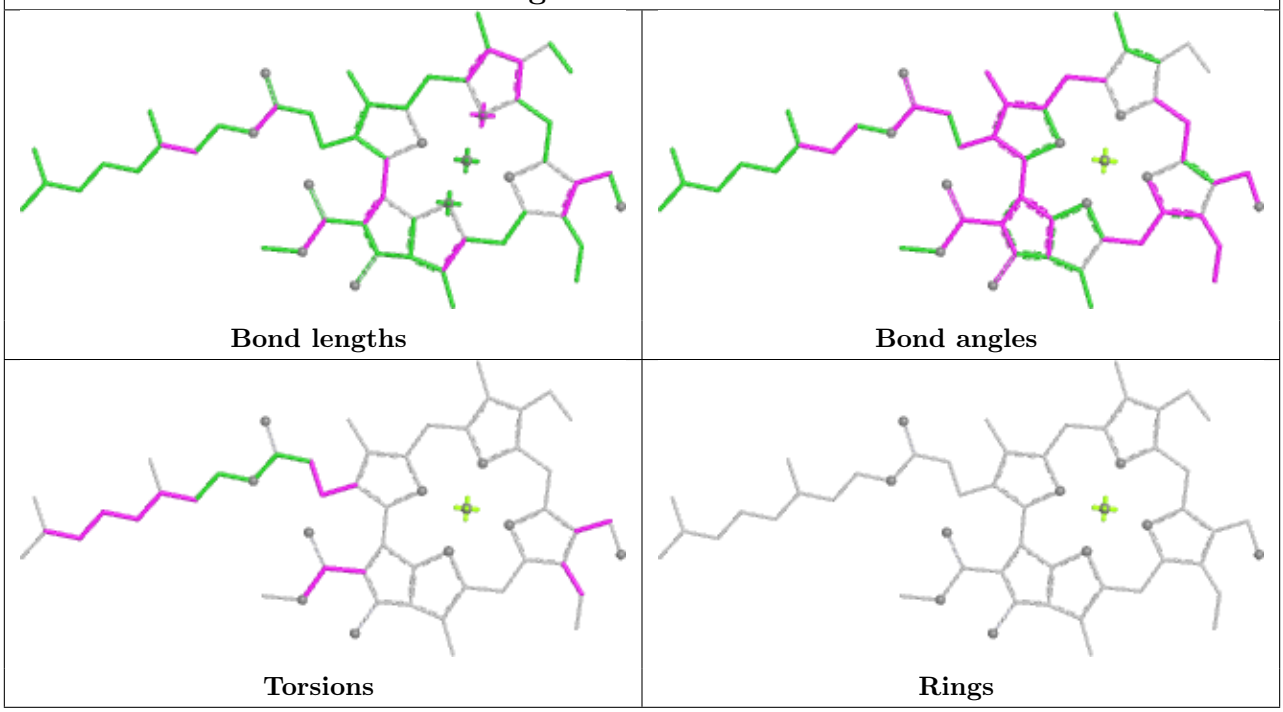
Ligand CHL n 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG a 414



Ligand CHL 1 609



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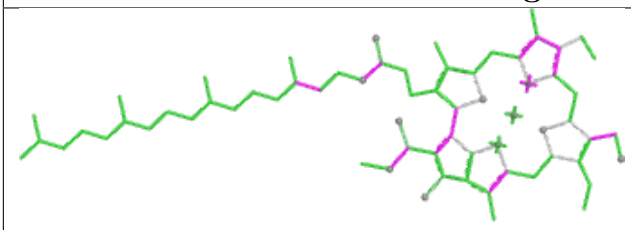
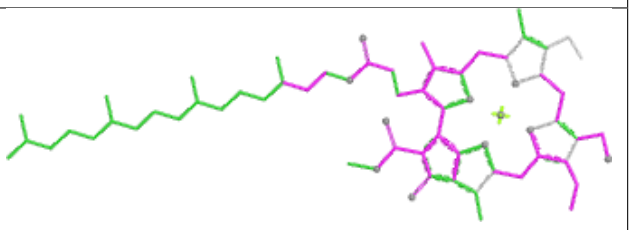
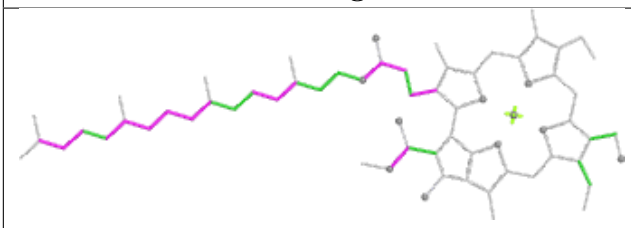
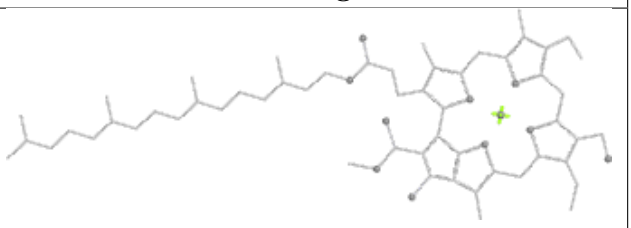
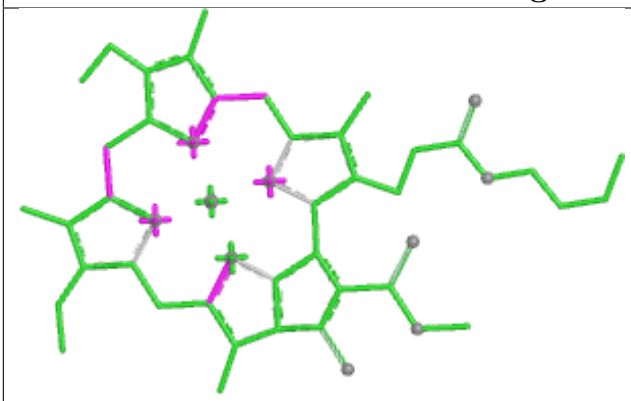
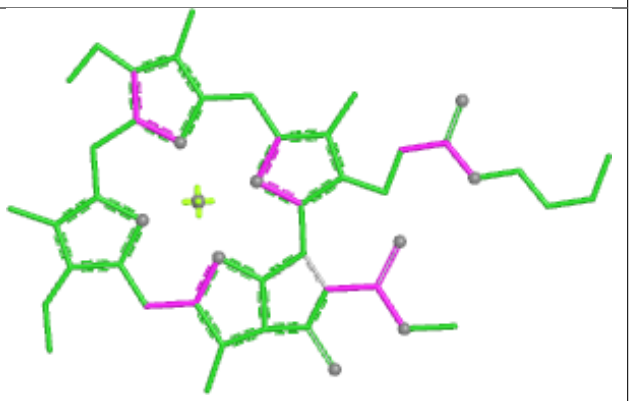
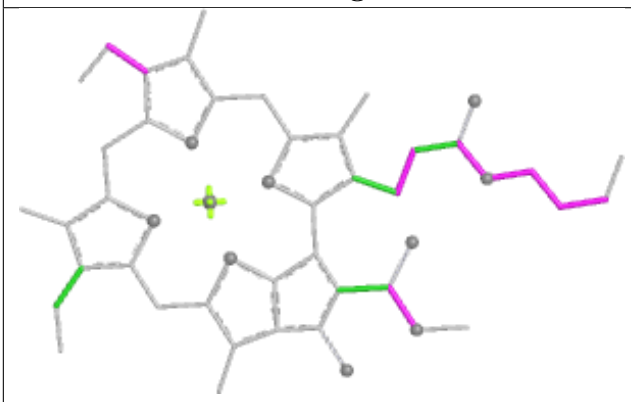
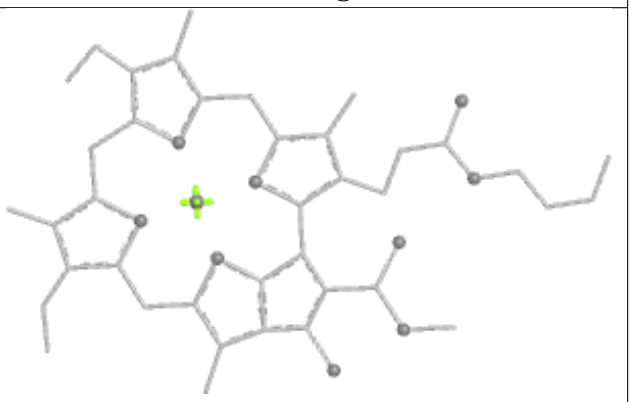
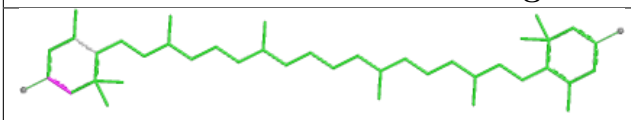
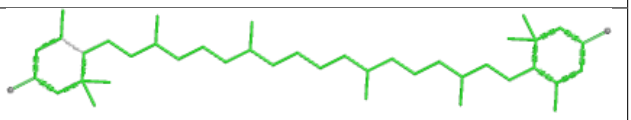
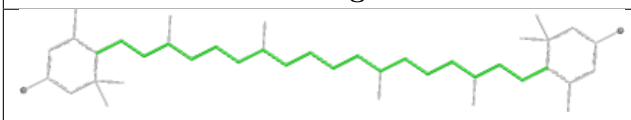
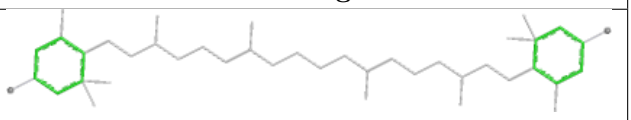
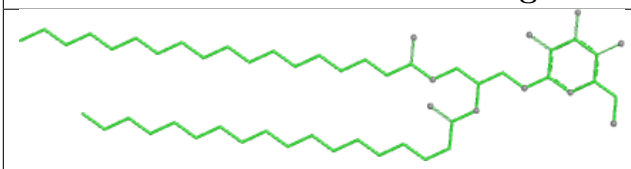
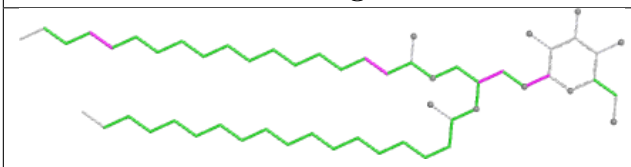
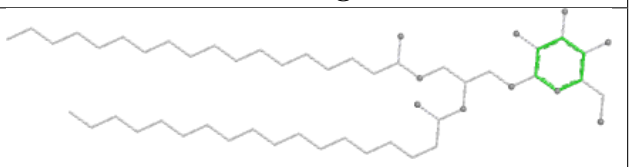
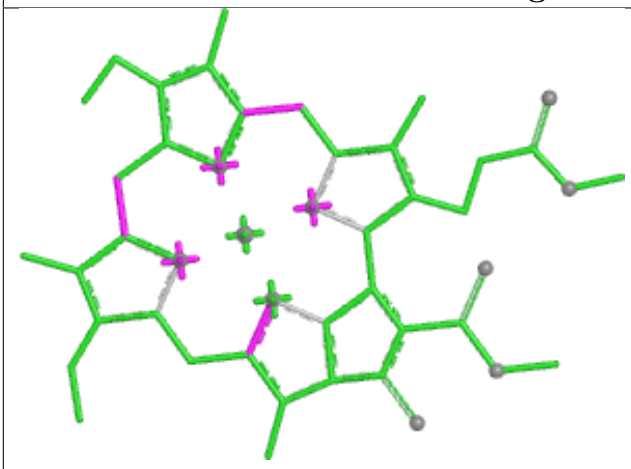
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

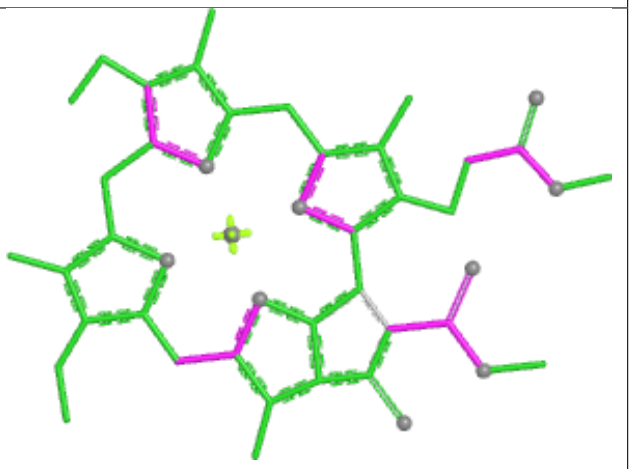
Ligand LUT G 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG w 501	
 Bond lengths	Bond angles
 Torsions	 Rings

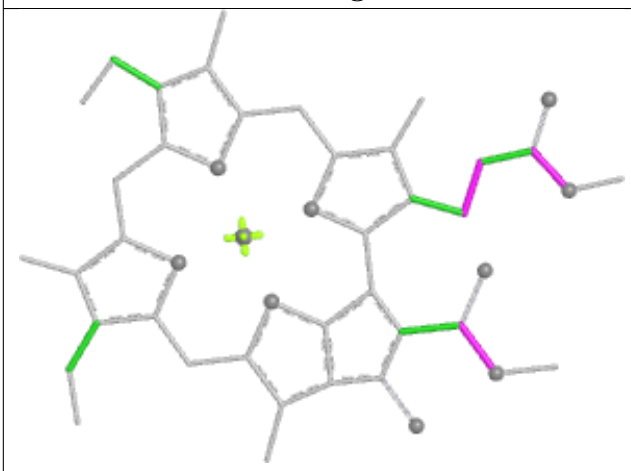
Ligand CLA 5 611



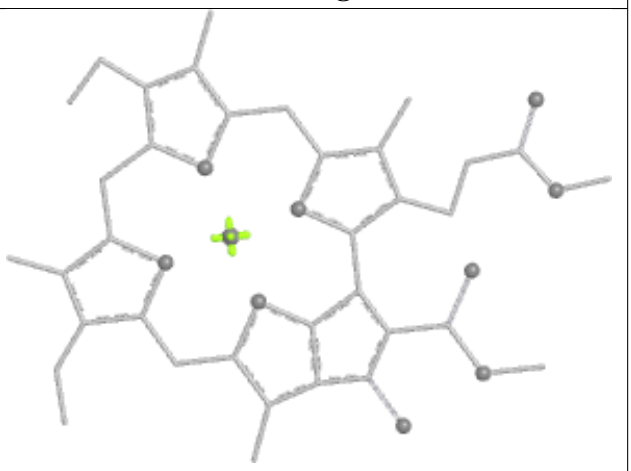
Bond lengths



Bond angles

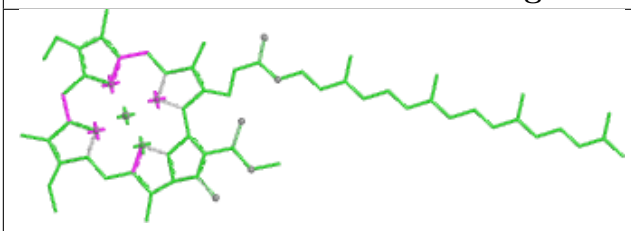


Torsions

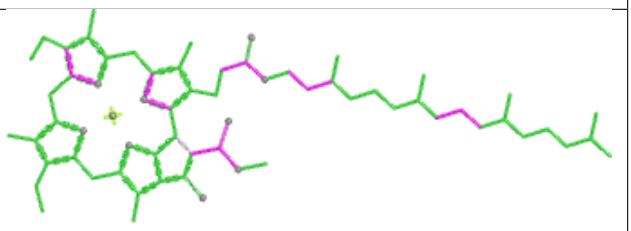


Rings

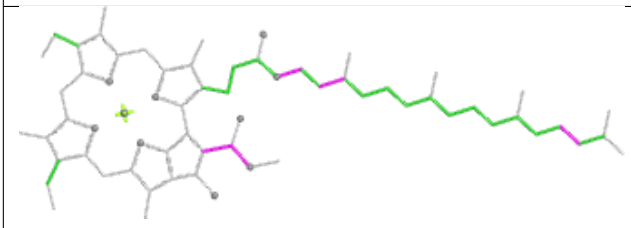
Ligand CLA C 503



Bond lengths



Bond angles



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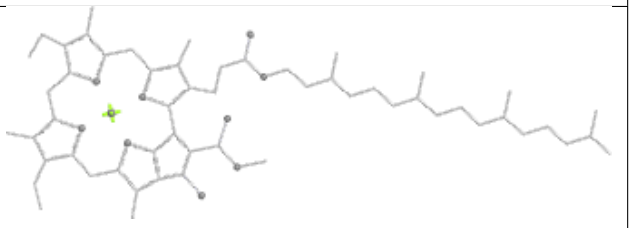
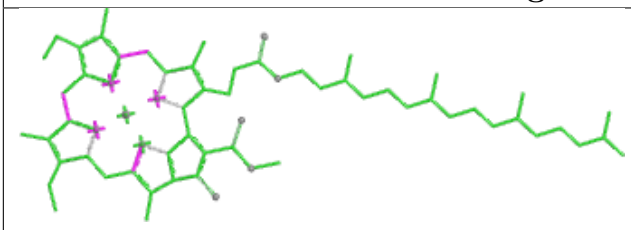
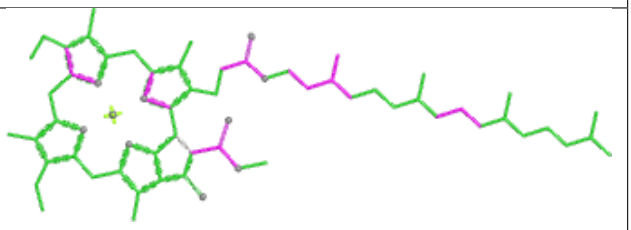
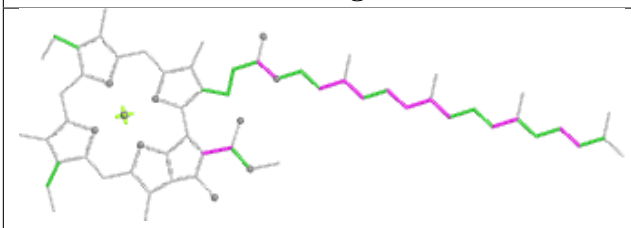
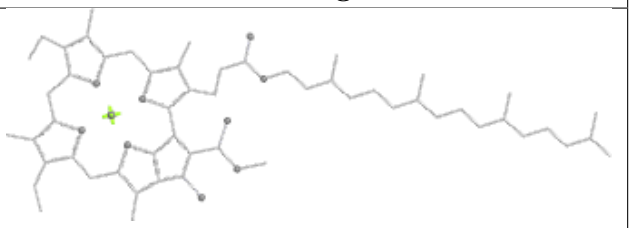
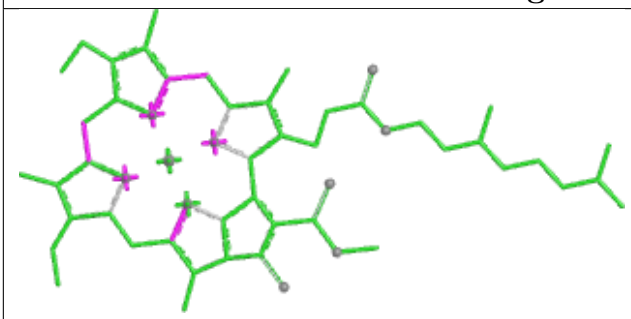
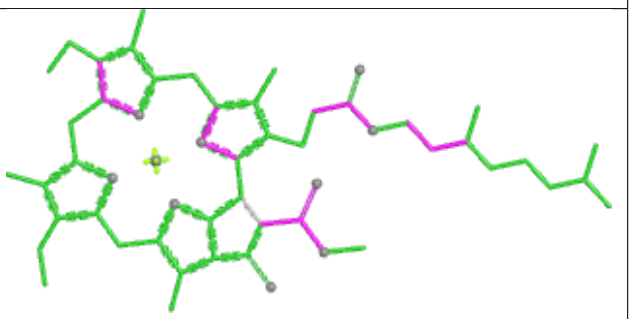
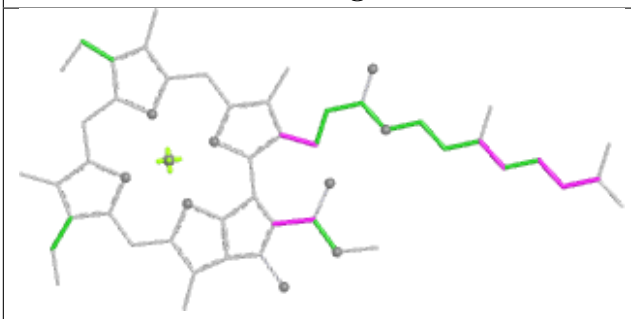
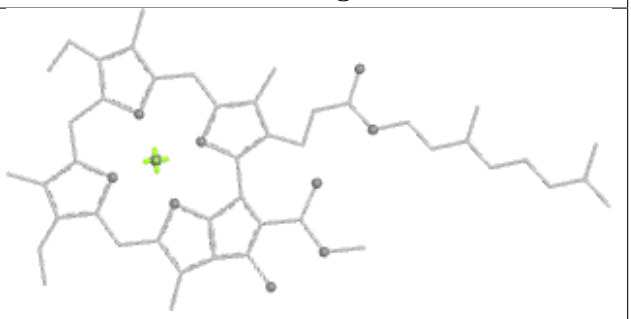
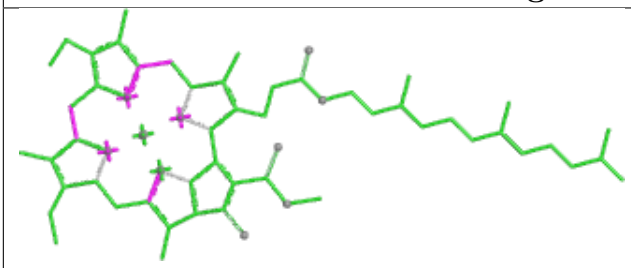
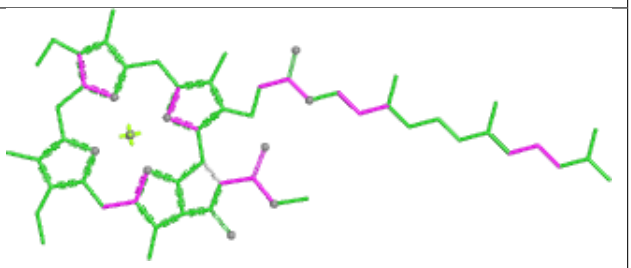
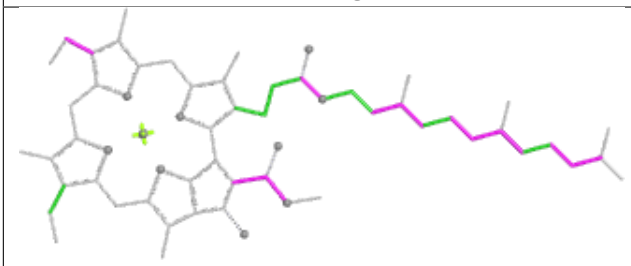
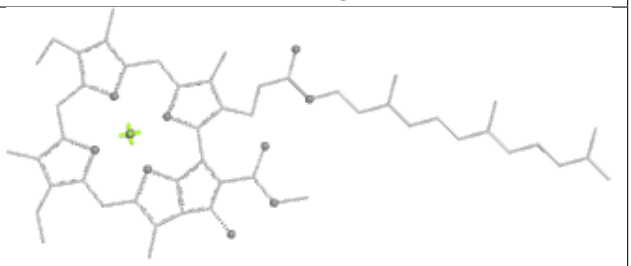
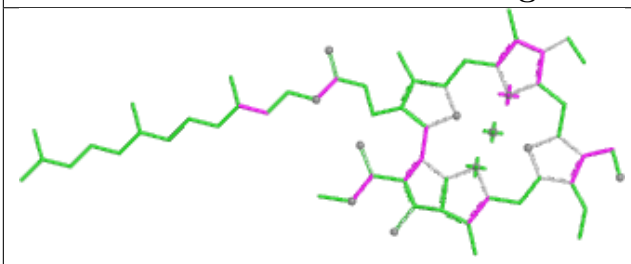
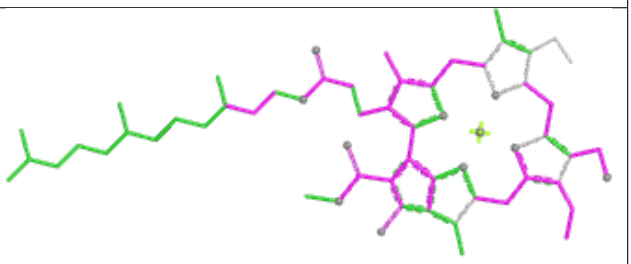
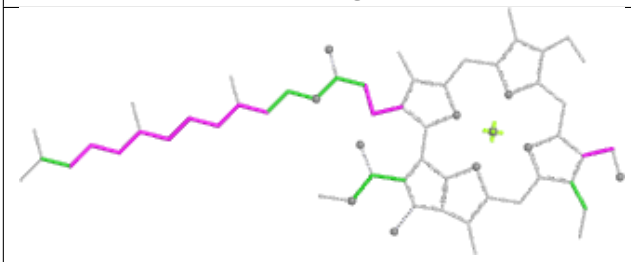
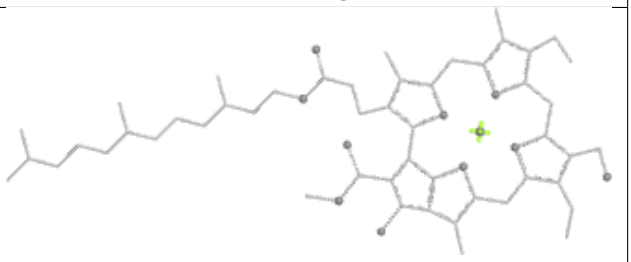


Rings

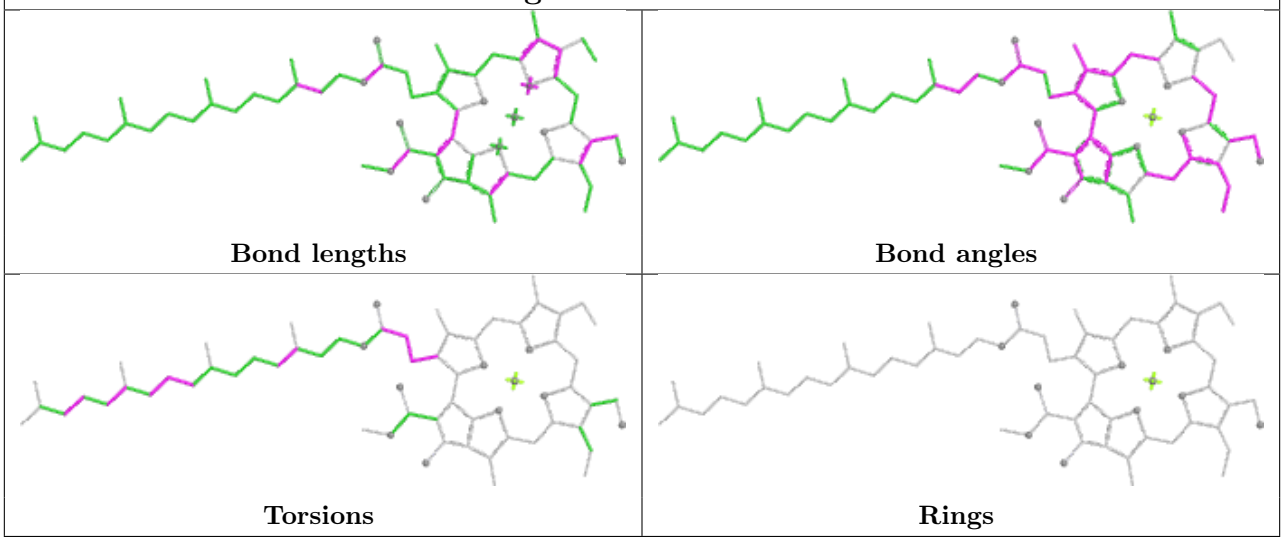
Ligand CLA S 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

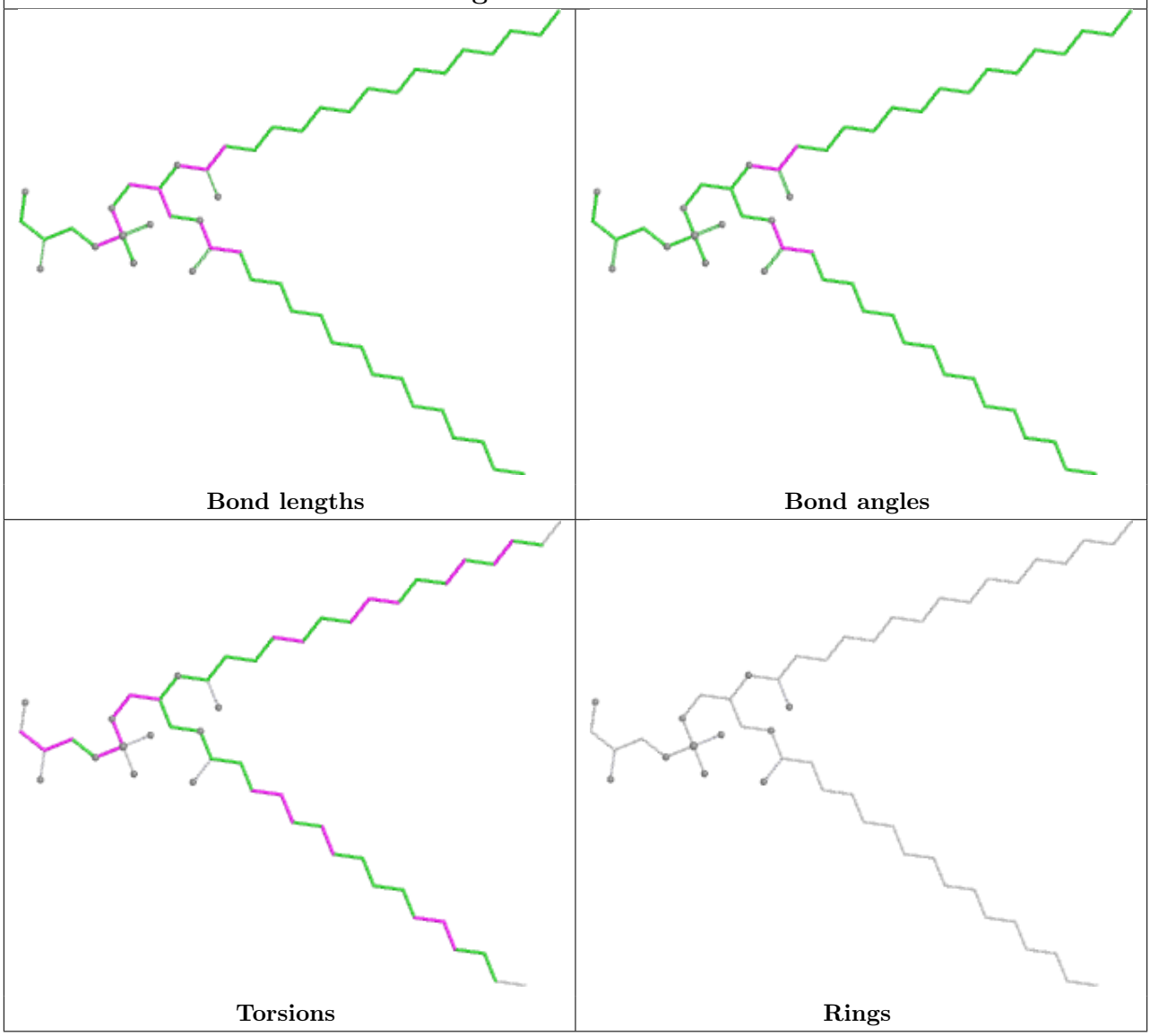
Ligand CLA b 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 16 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

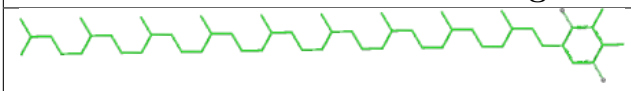
Ligand CHL Y 601



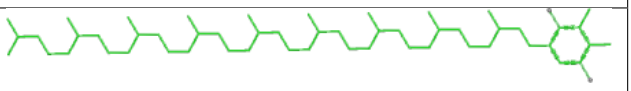
Ligand LHG S 621



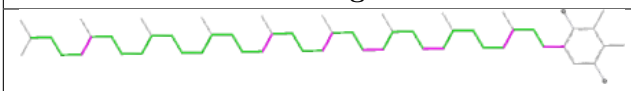
Ligand PL9 A 410



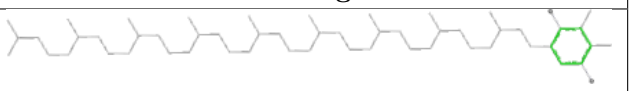
Bond lengths



Bond angles

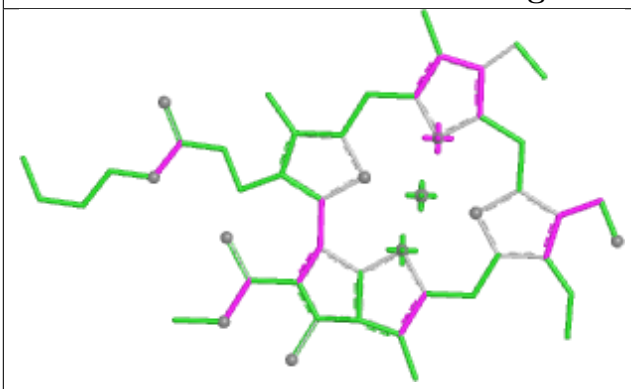


Torsions



Rings

Ligand CHL g 606



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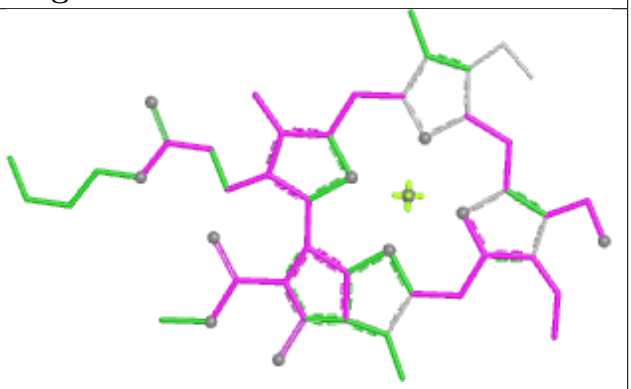
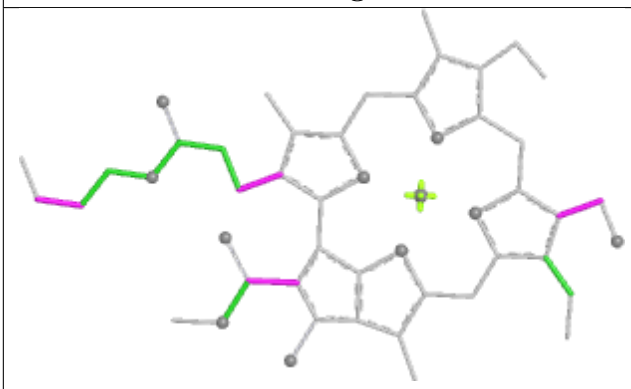


Bond angles



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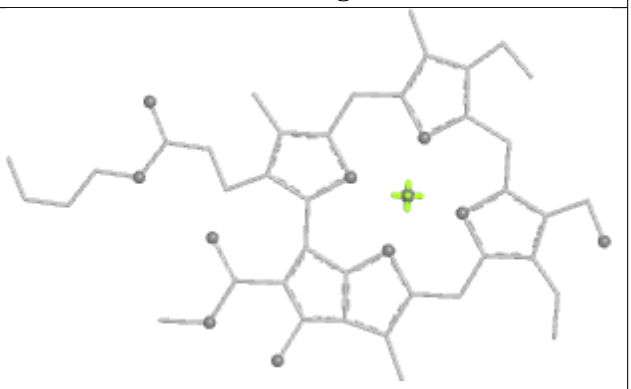
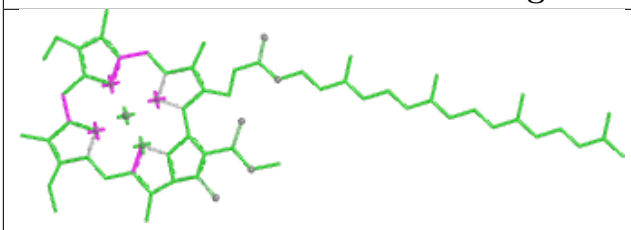
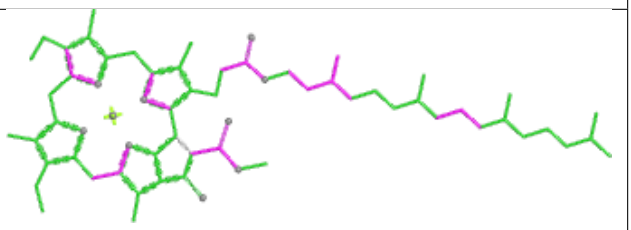


Rings

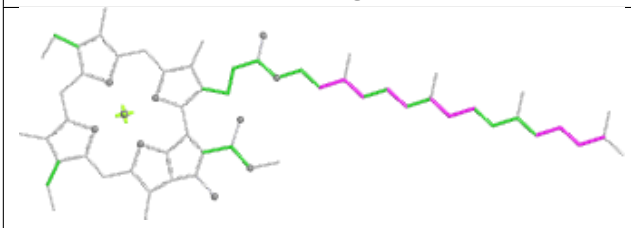
Ligand CLA b 615



Bond lengths



Bond angles



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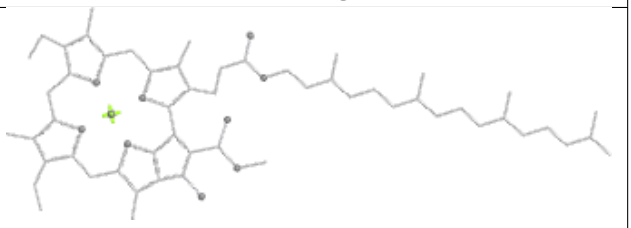
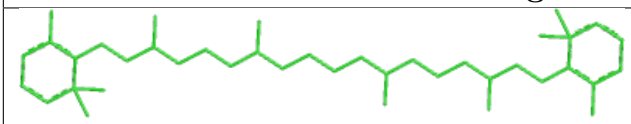
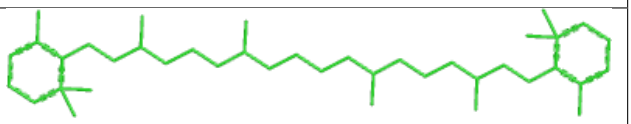
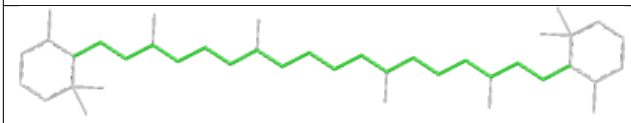
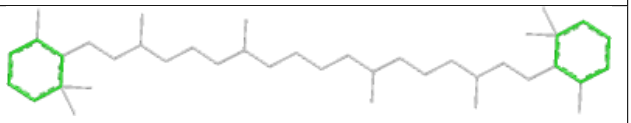
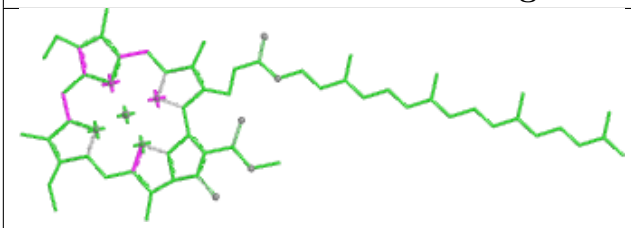
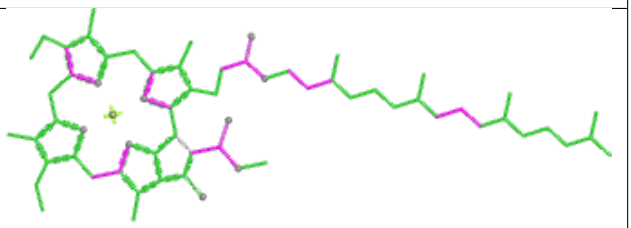
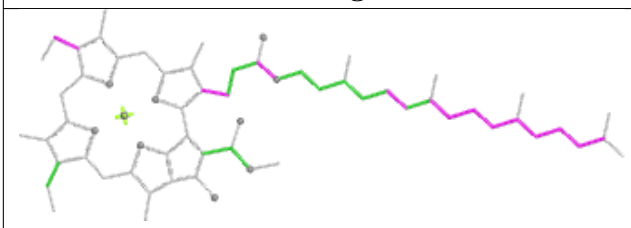
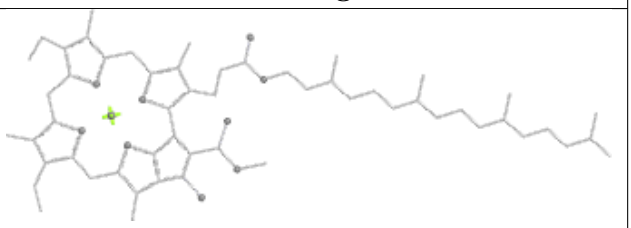
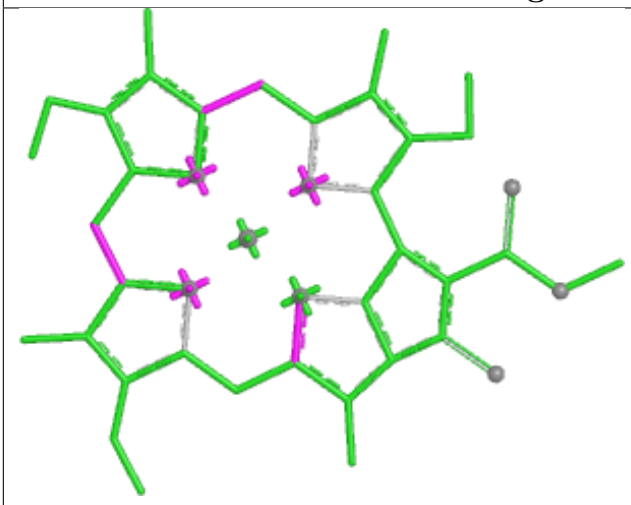


Rings

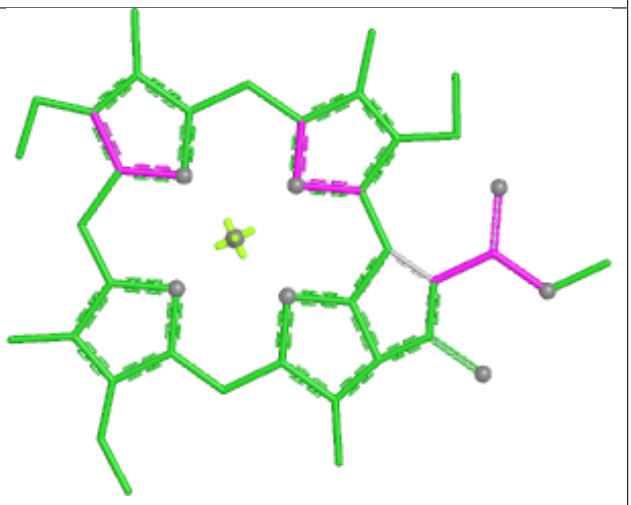
Ligand BCR a 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 14 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

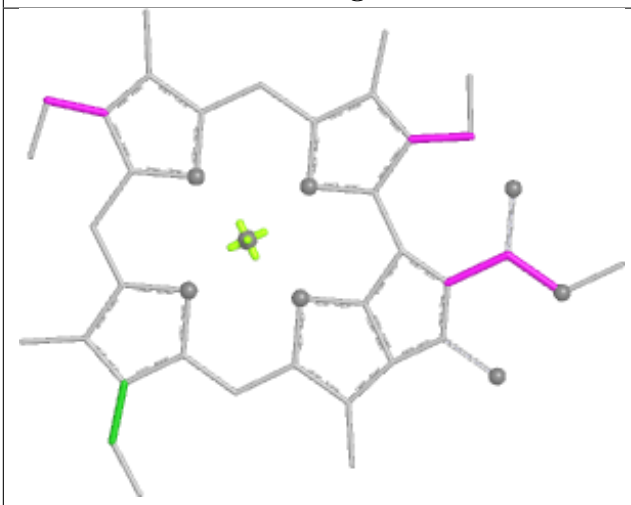
Ligand CLA S 603



Bond lengths



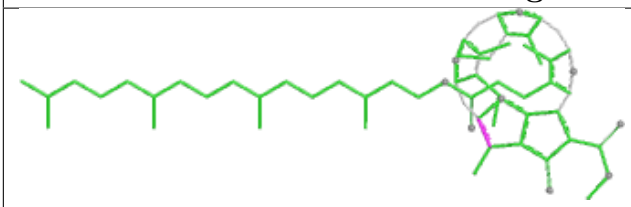
Bond angles



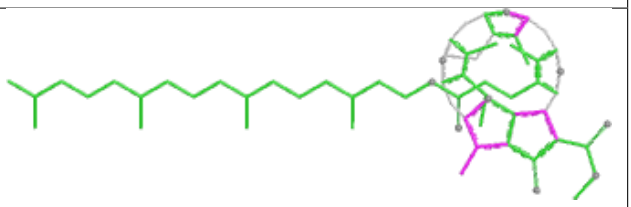
Torsions

Rings

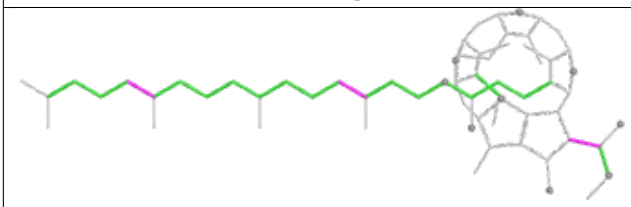
Ligand PHO a 406



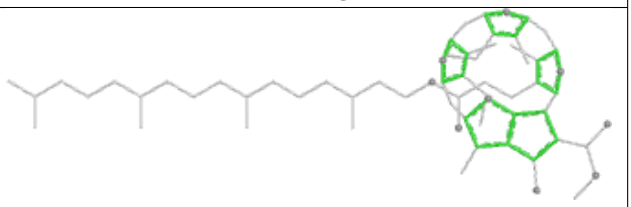
Bond lengths



Bond angles

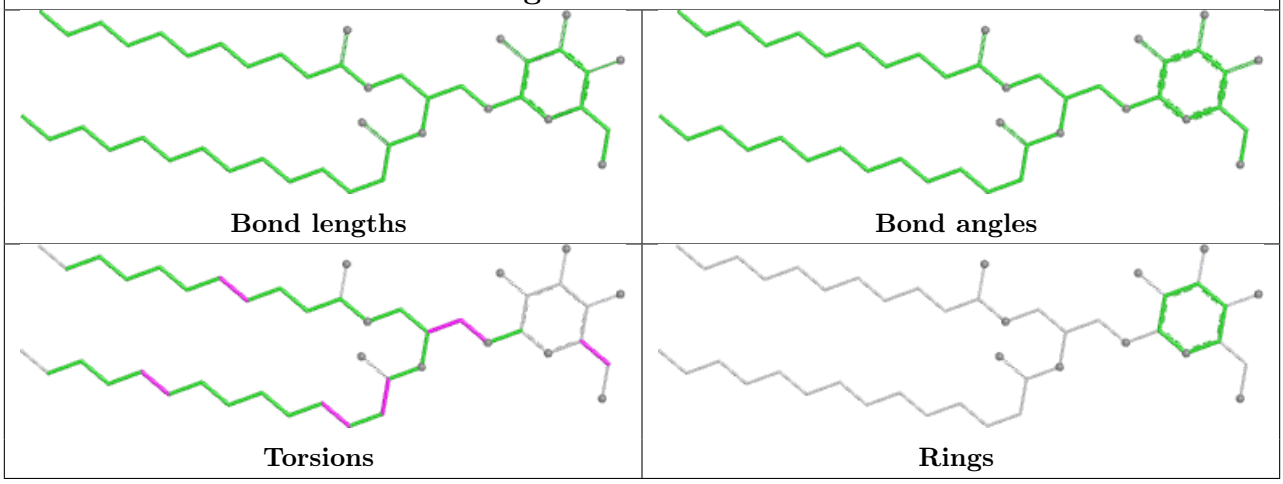


Torsions



Rings

Ligand LMG d 410



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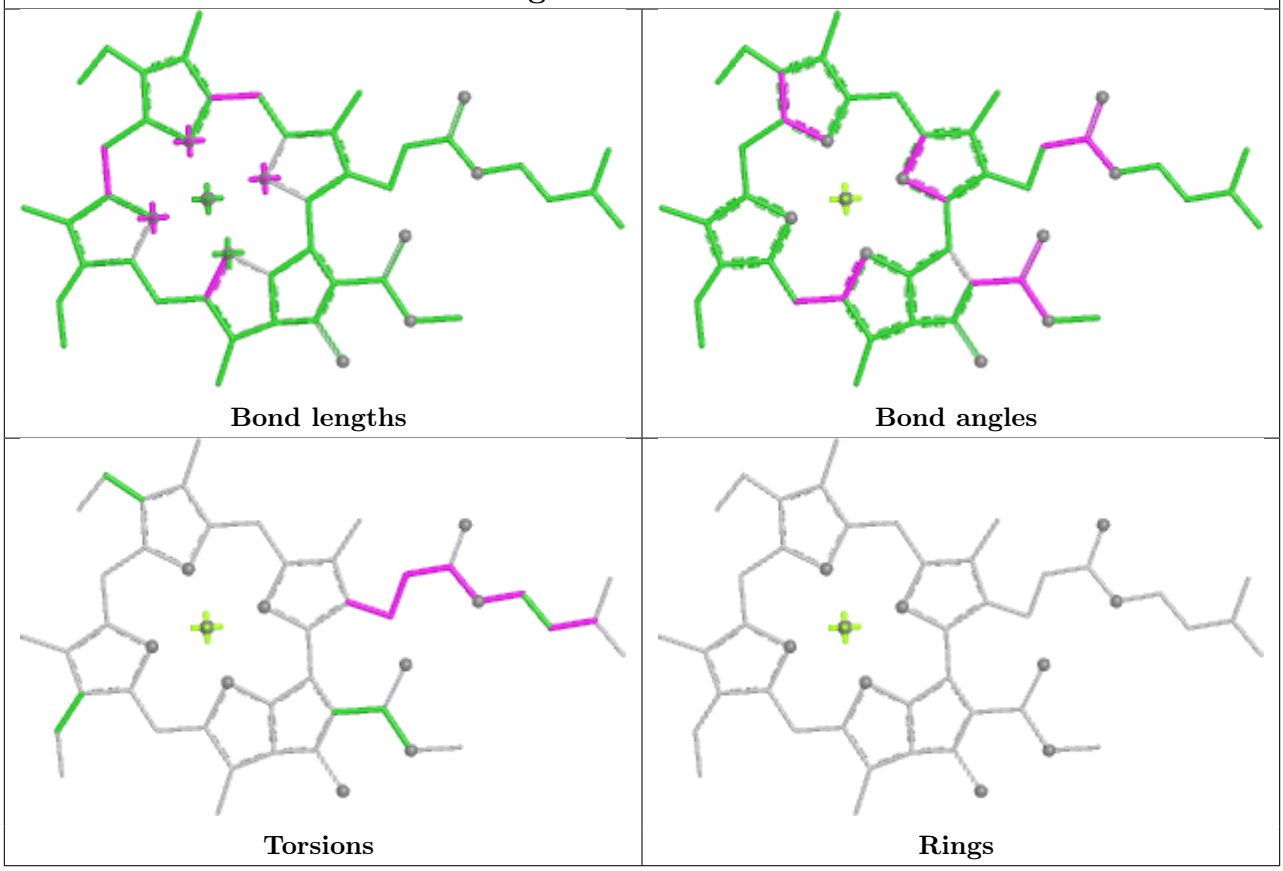
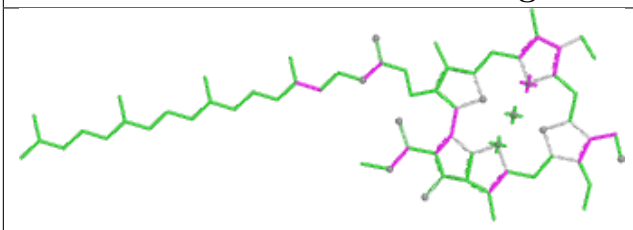
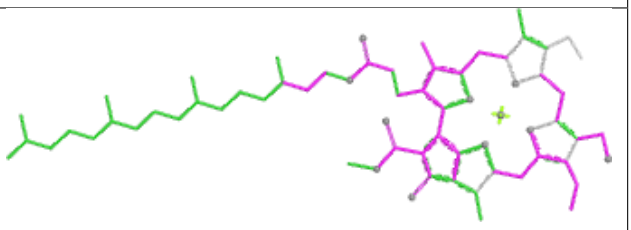


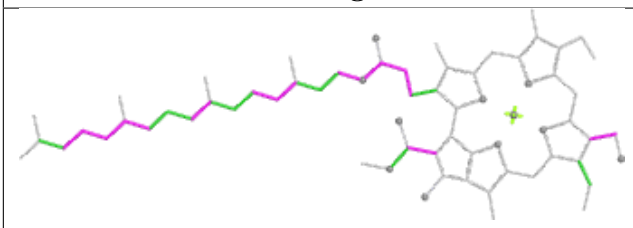
Ligand CHL 14 601



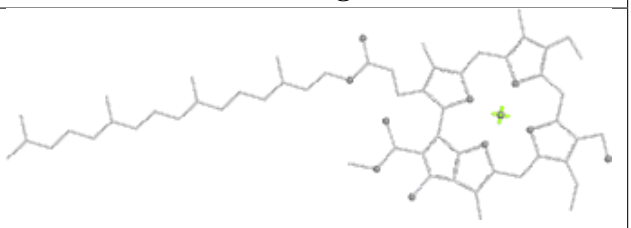
Bond lengths



Bond angles

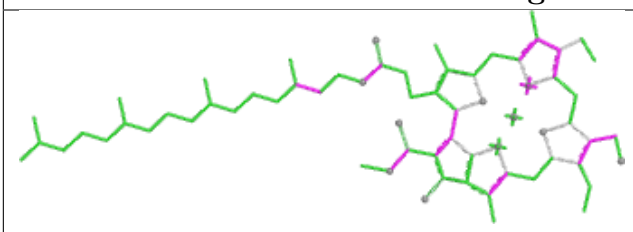


Torsions



Rings

Ligand CHL 6 607



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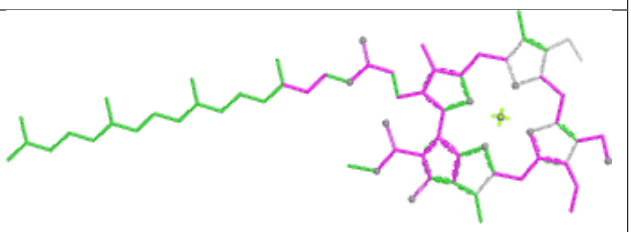
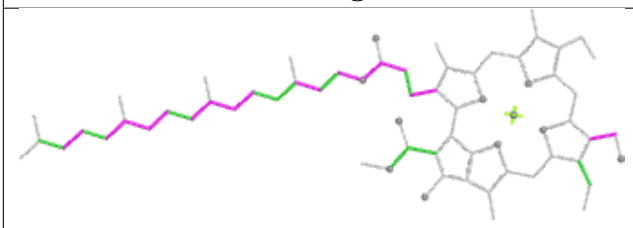


Bond angles



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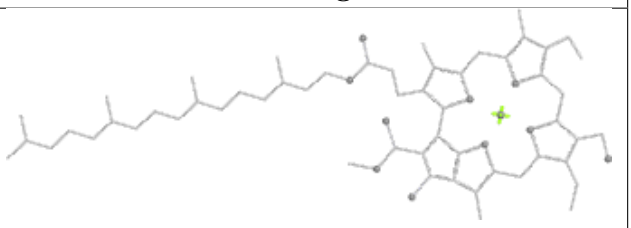
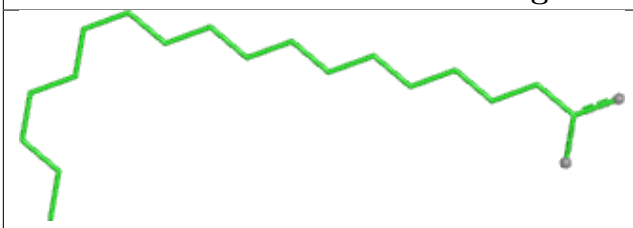


Rings

Ligand LNL c 524



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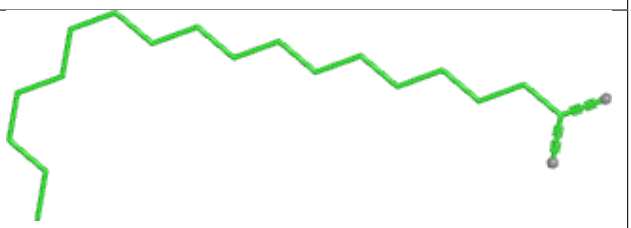

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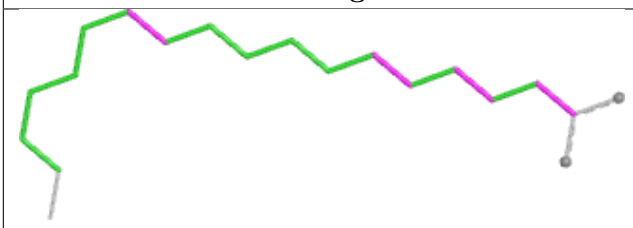

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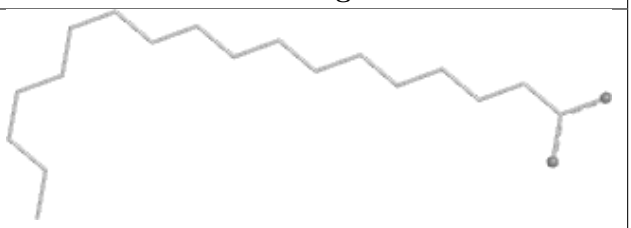
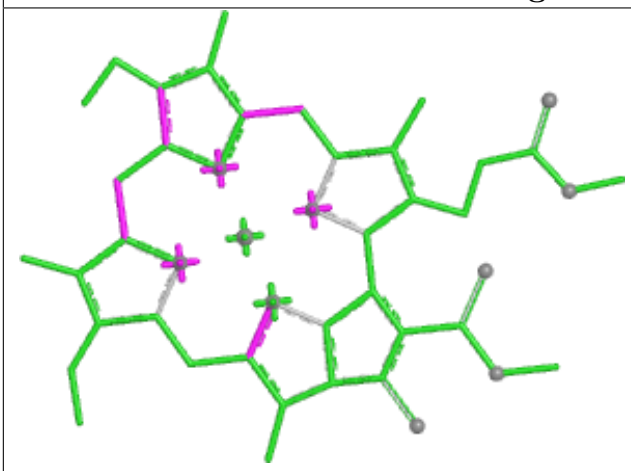


Rings

Ligand CLA 4 614



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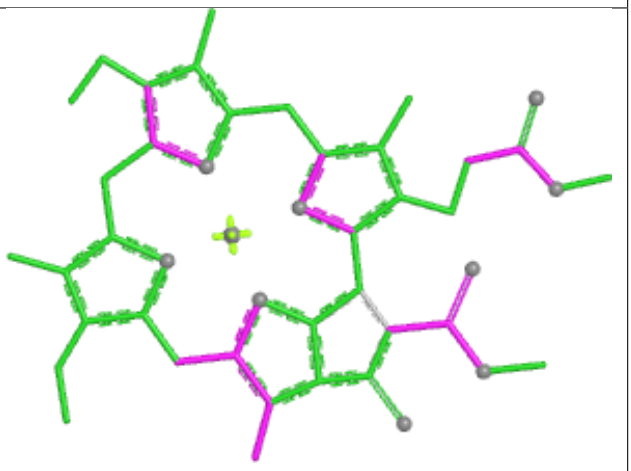
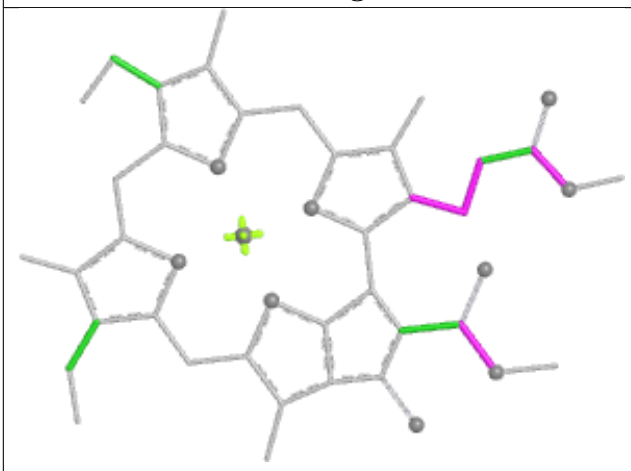


Bond angles



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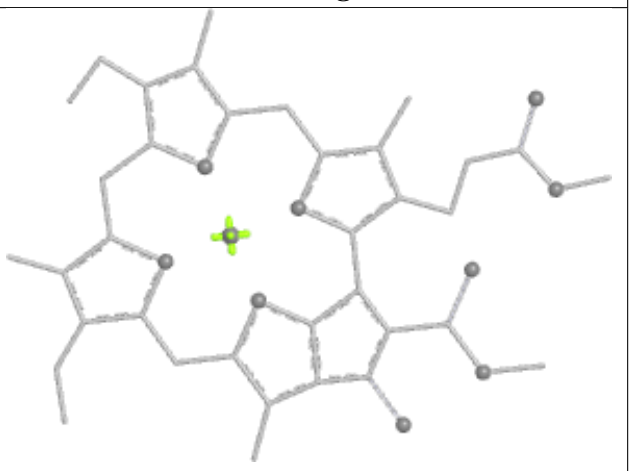
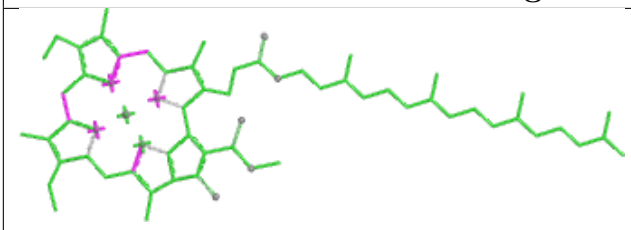


Rings

Ligand CLA B 615



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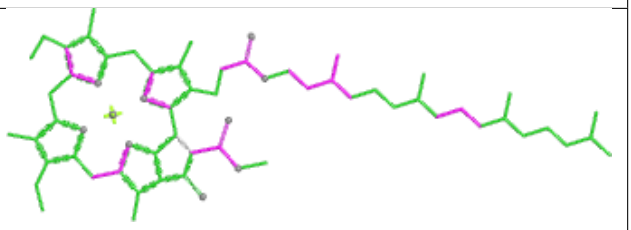
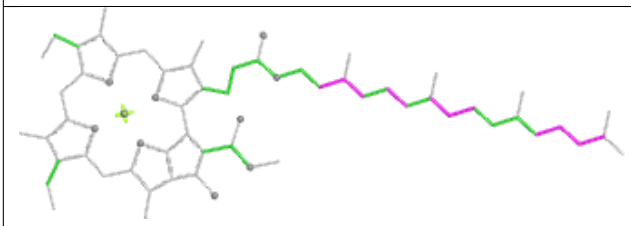


Bond angles



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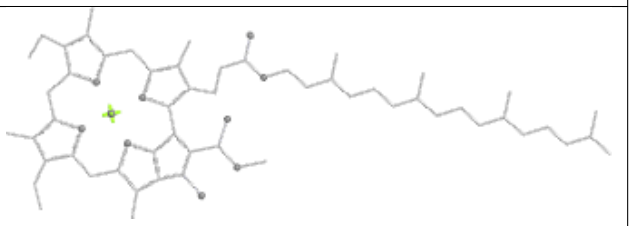
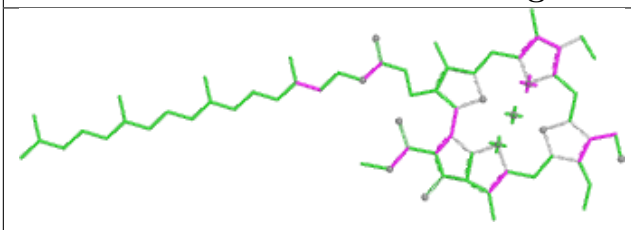
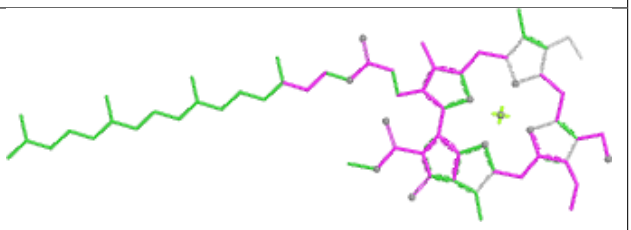
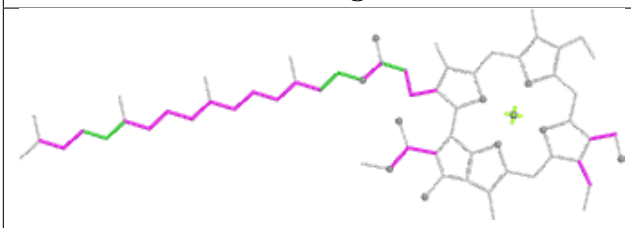
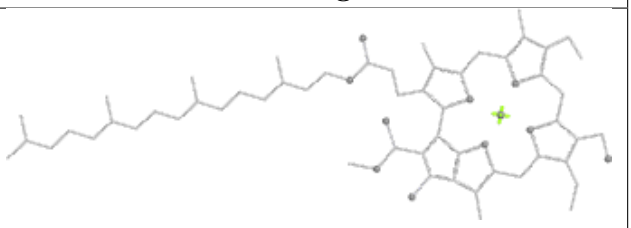
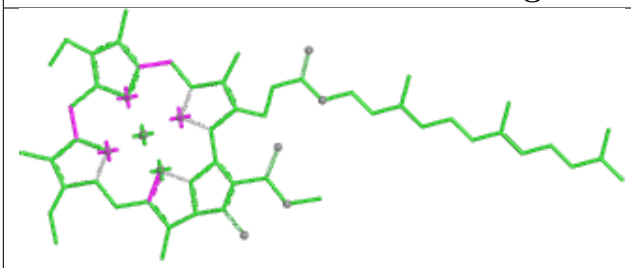
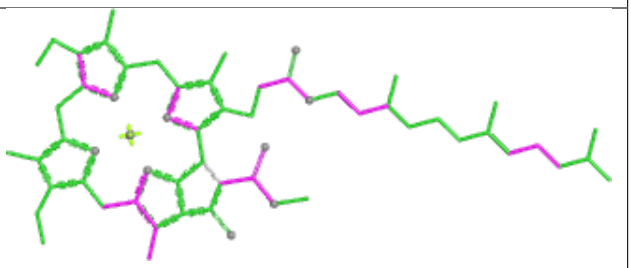
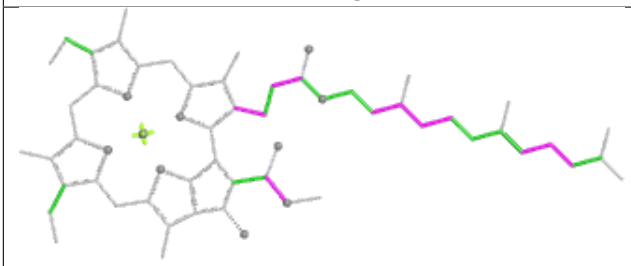
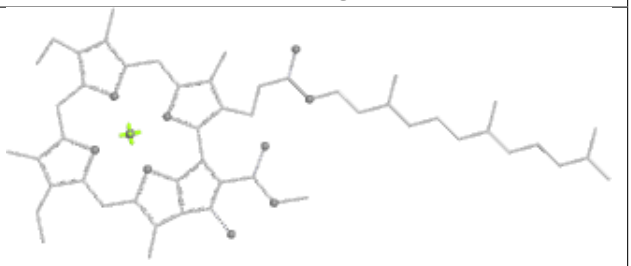


Rings

Ligand CHL 2 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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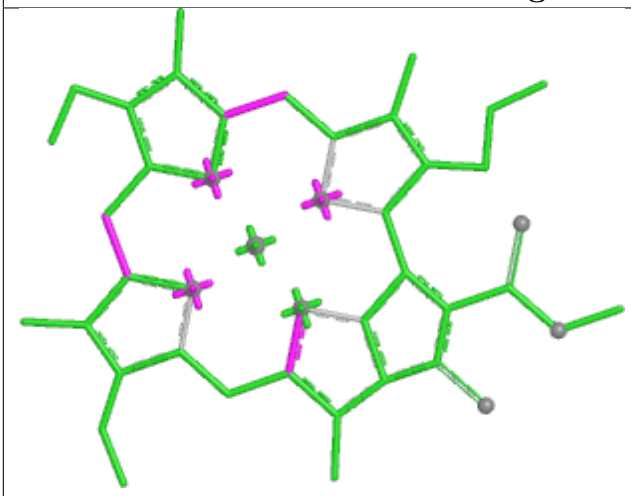

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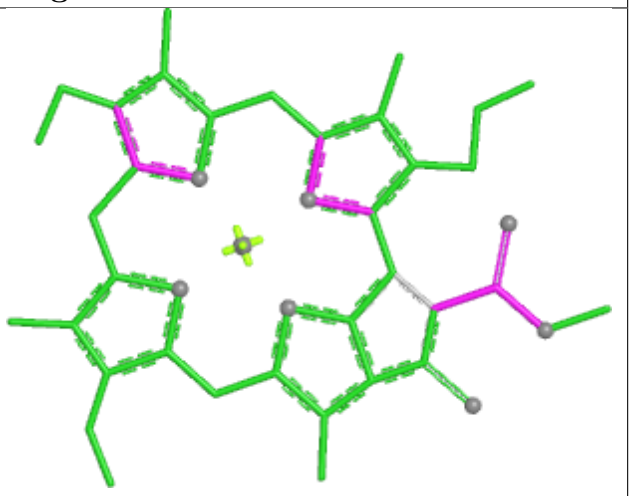

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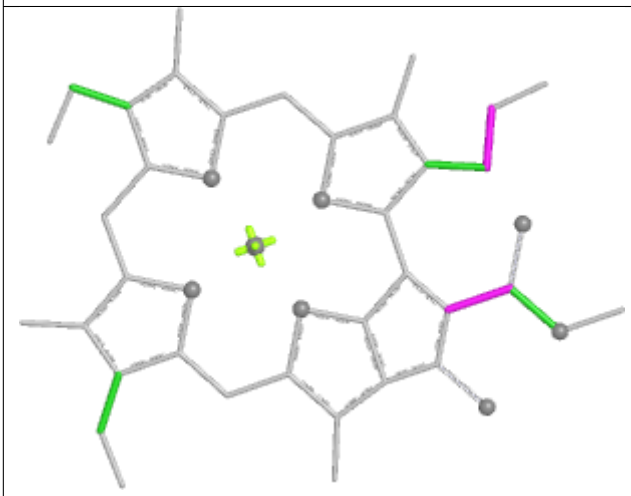

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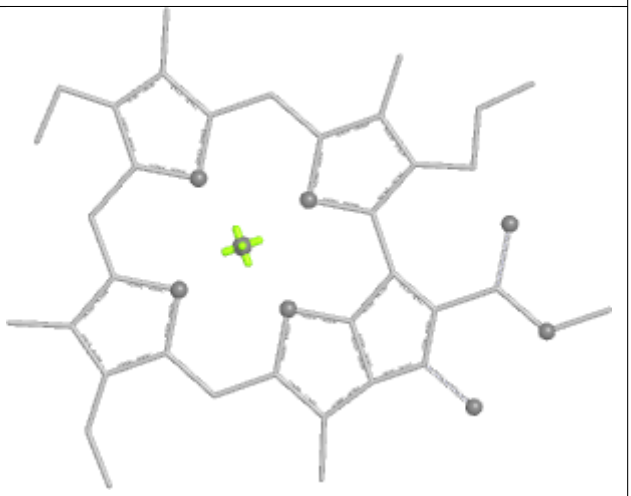
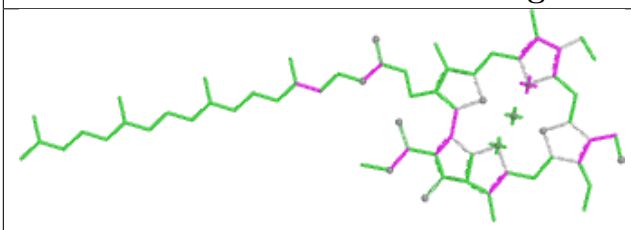


Rings

Ligand CHL 3 609



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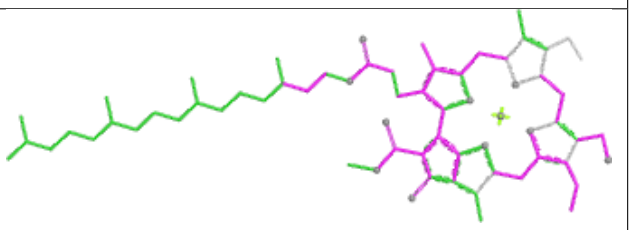

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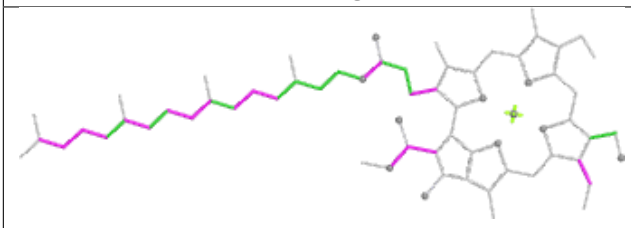

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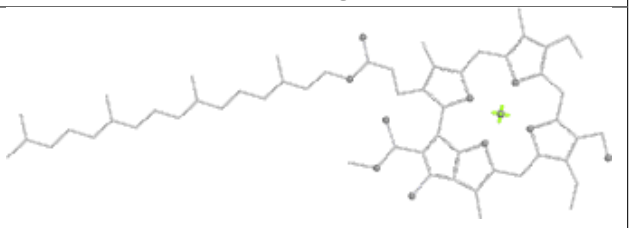

Rings

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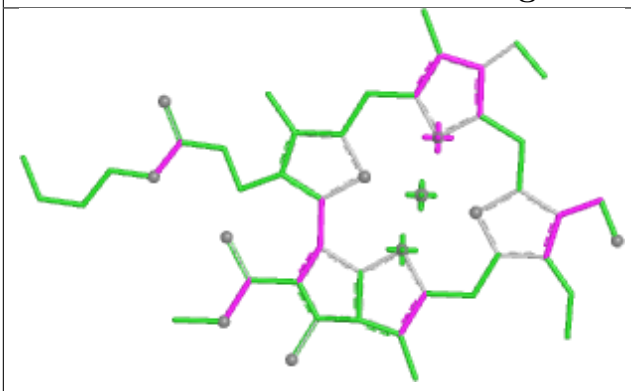
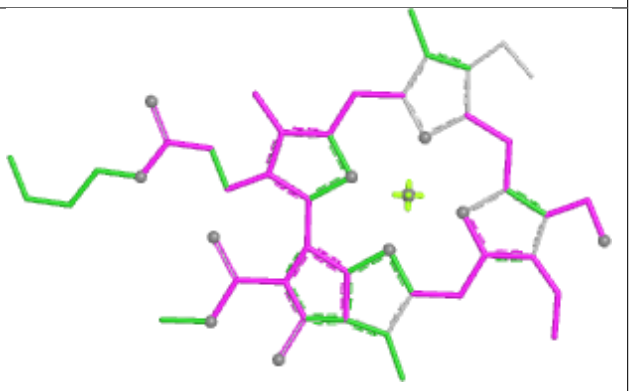
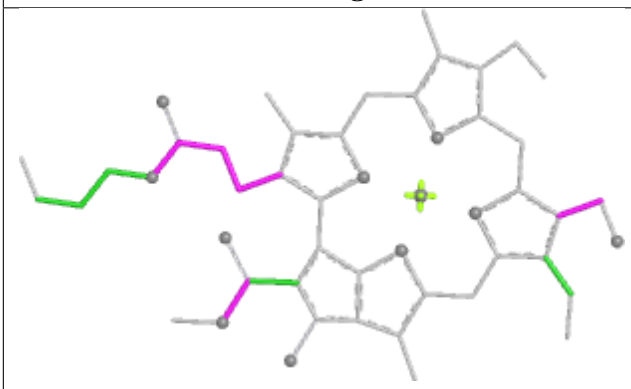
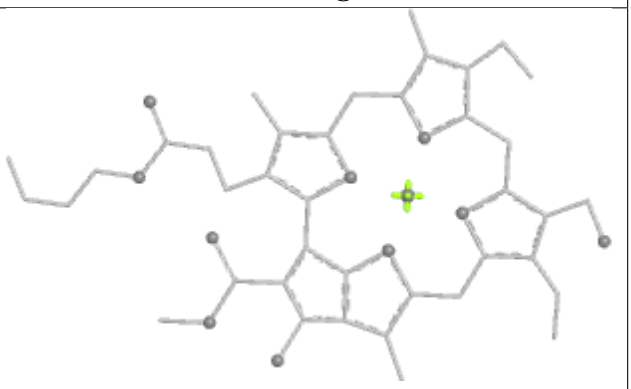
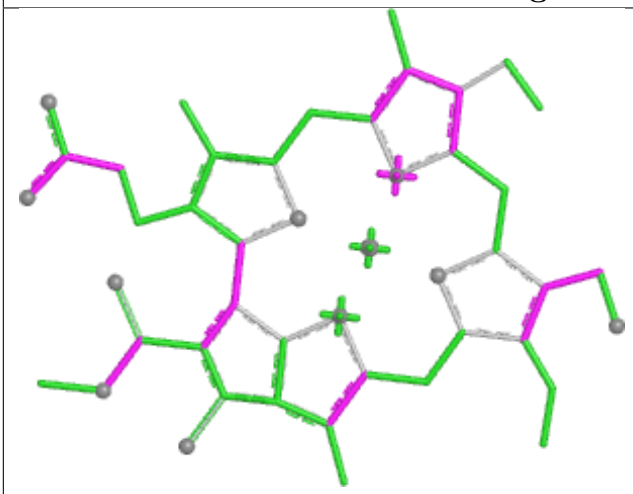
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL s 601



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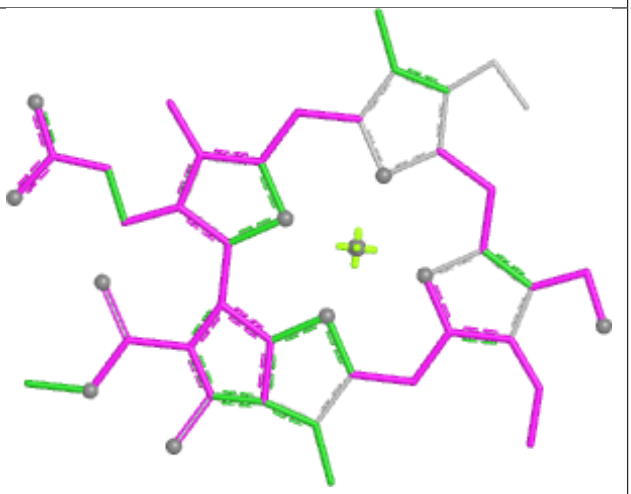

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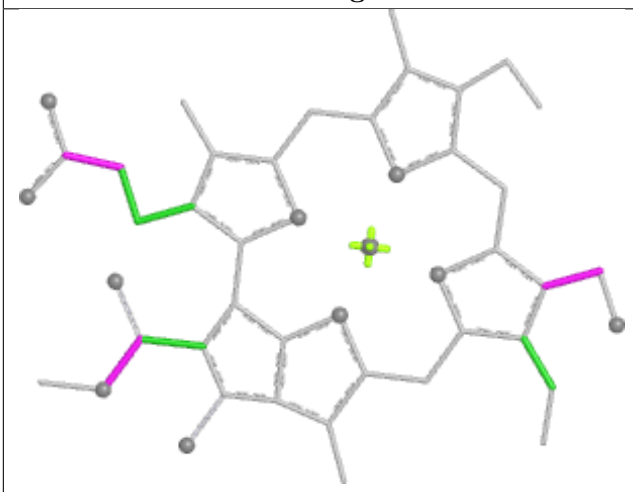

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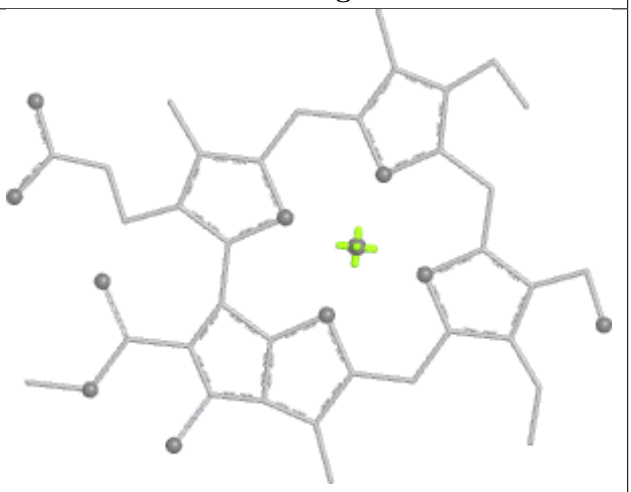
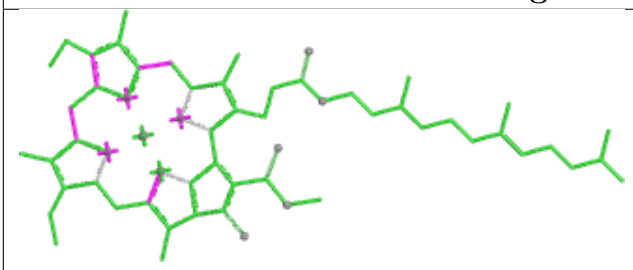


Rings

Ligand CLA r 610



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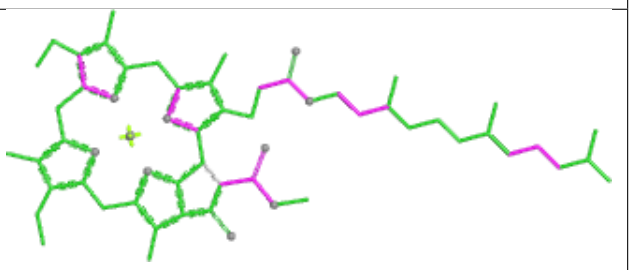

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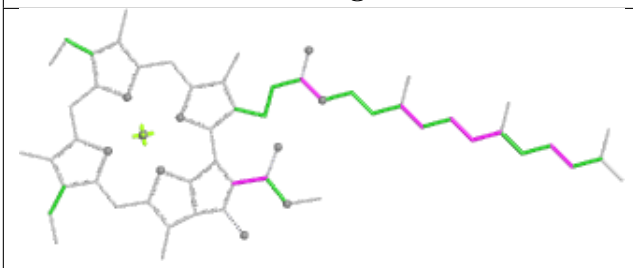

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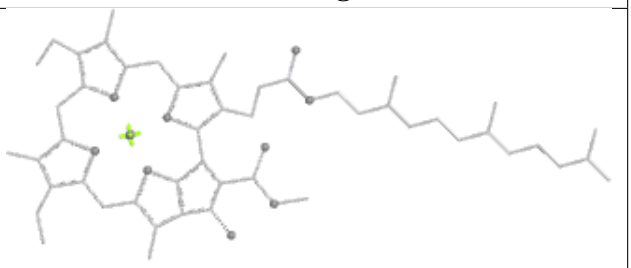

Rings

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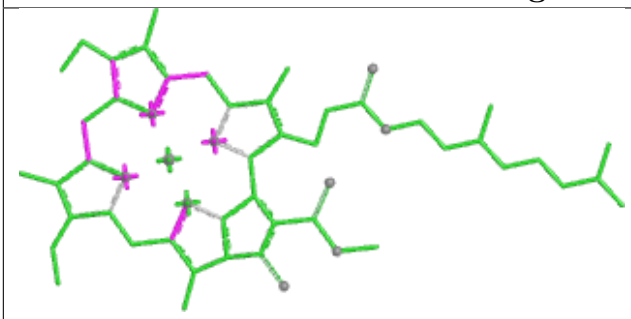

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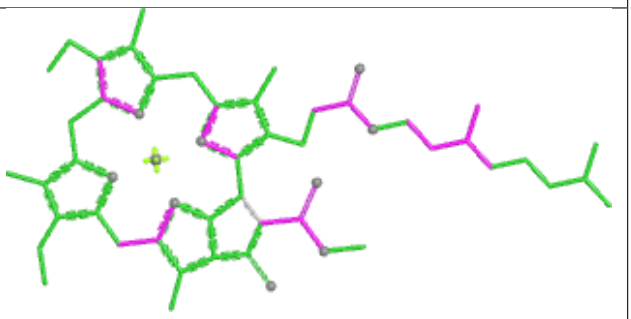

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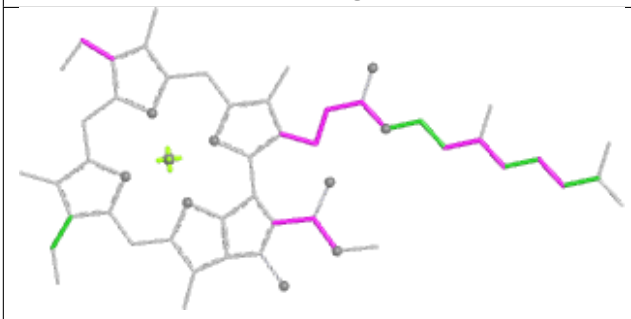

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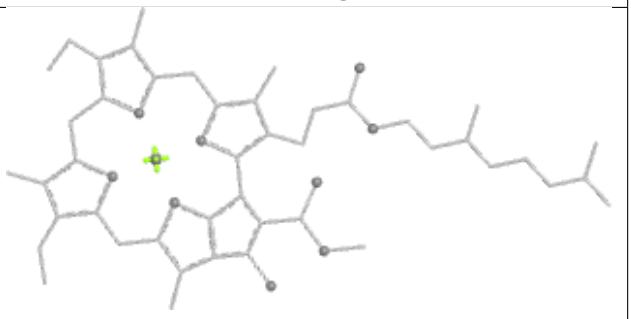
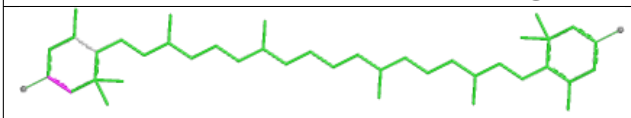


Rings

Ligand LUT n 617



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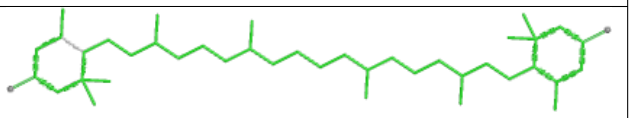

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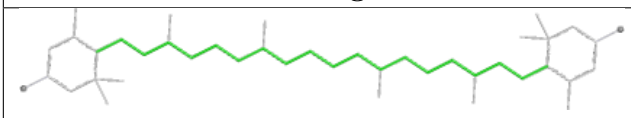

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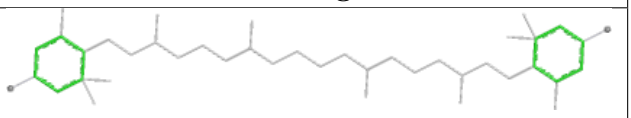

Rings

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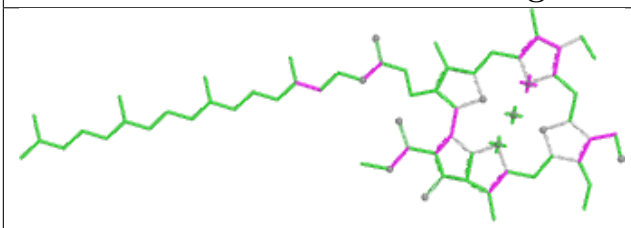

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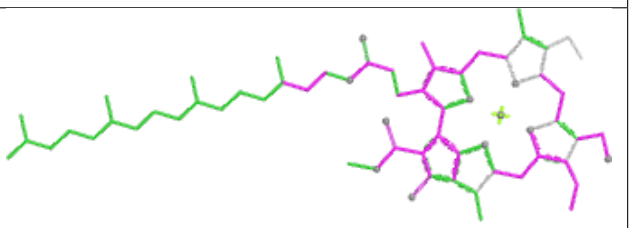

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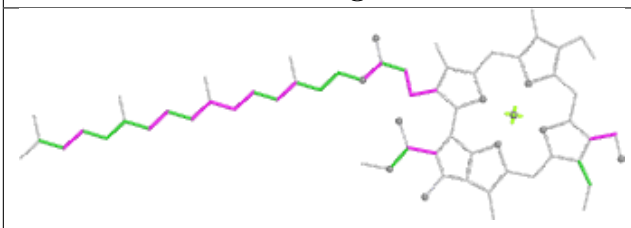

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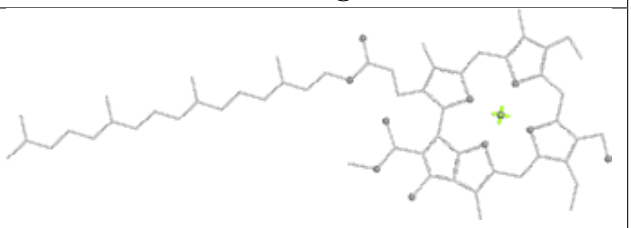

Rings

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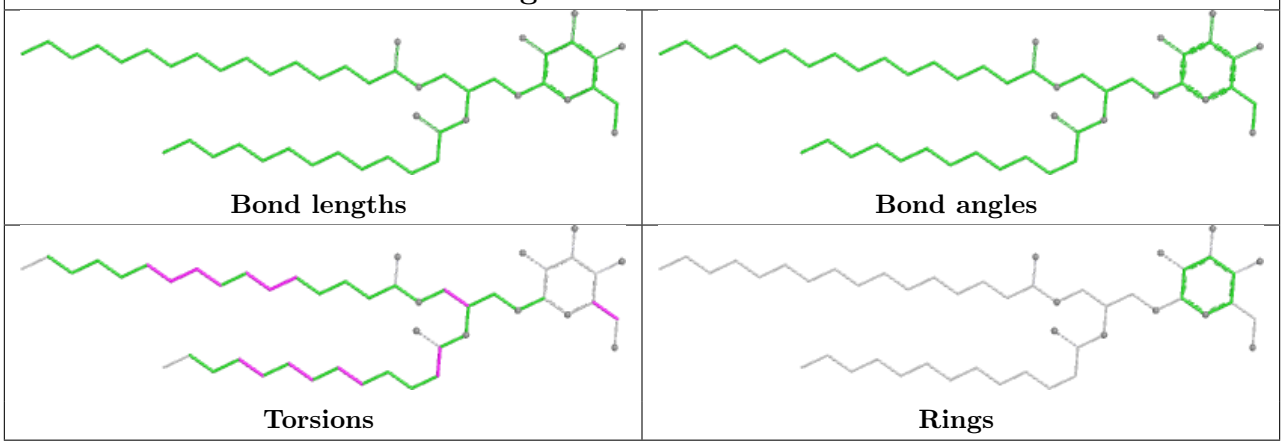

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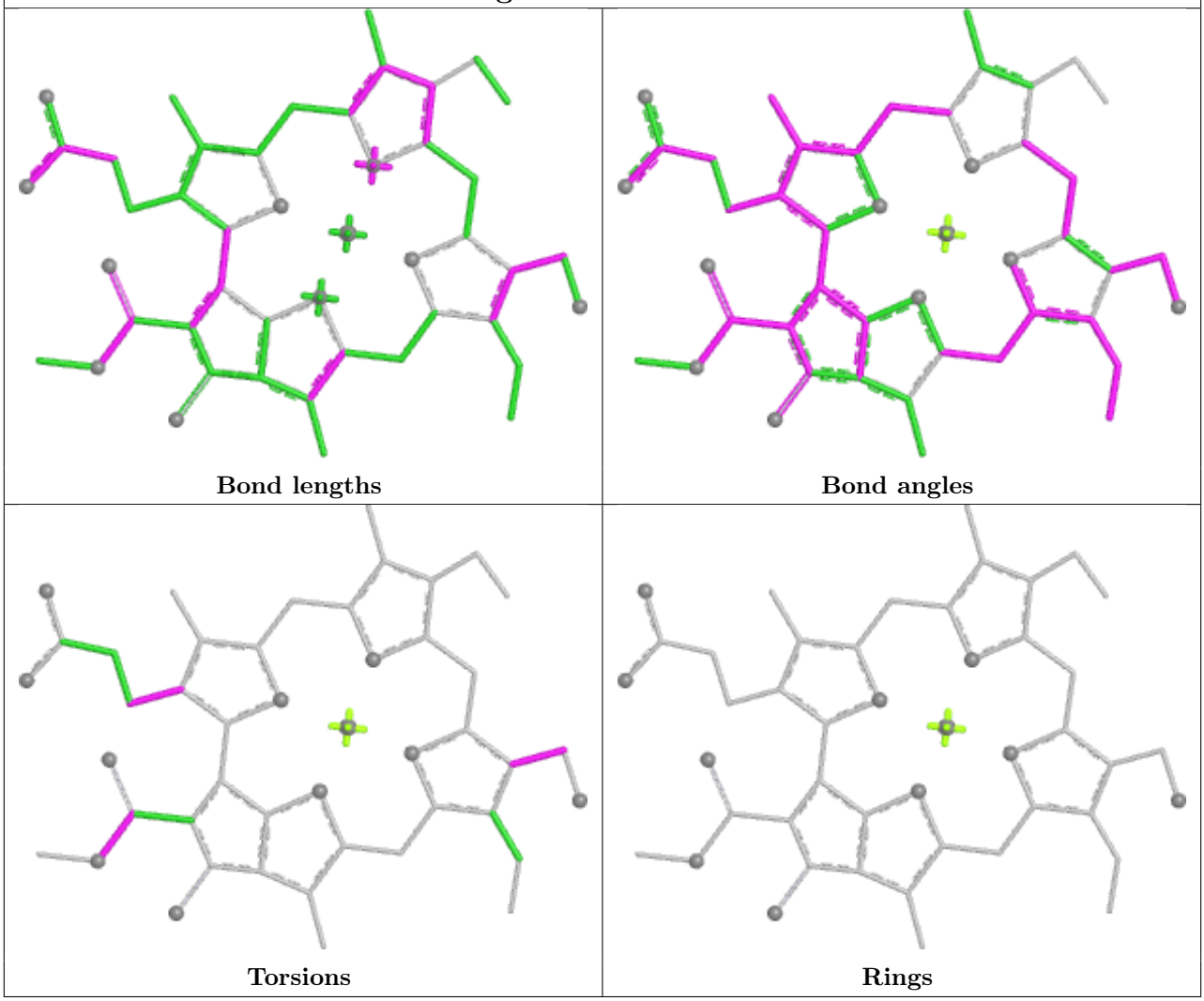
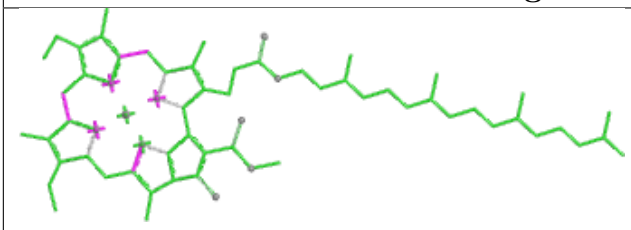
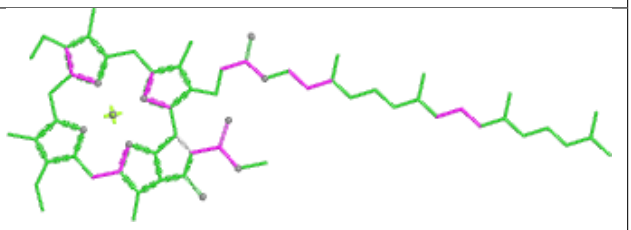
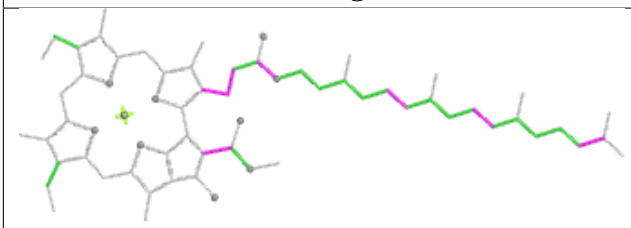
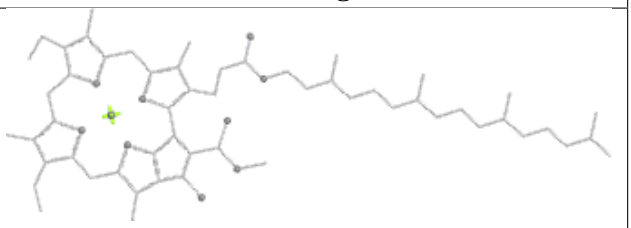


Ligand CLA B 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

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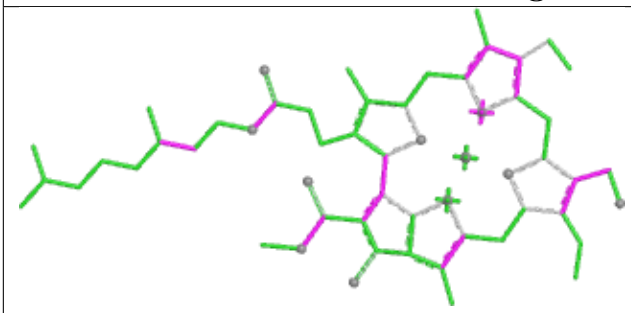
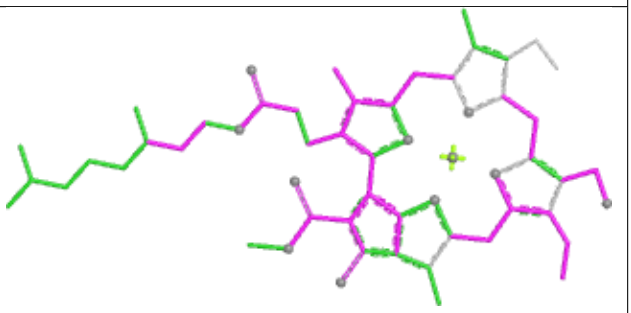
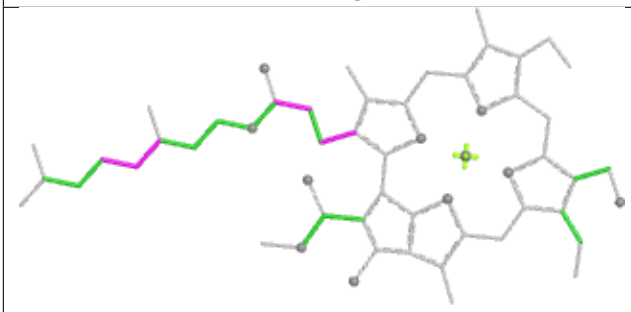
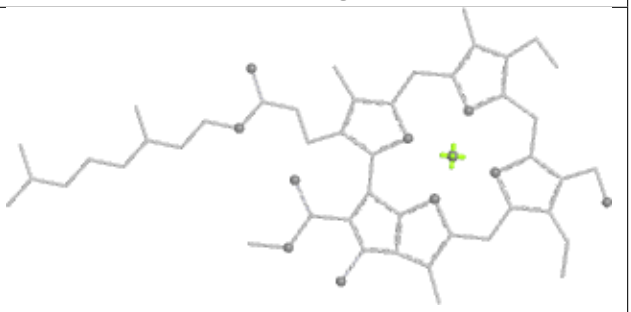
 Bond lengths	 Bond angles
 Torsions	 Rings

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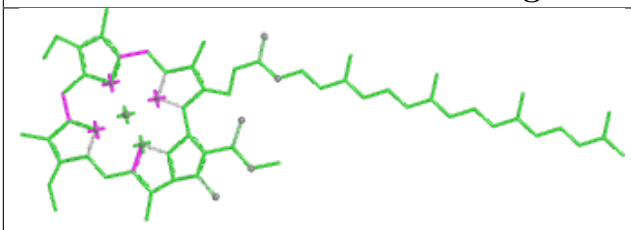
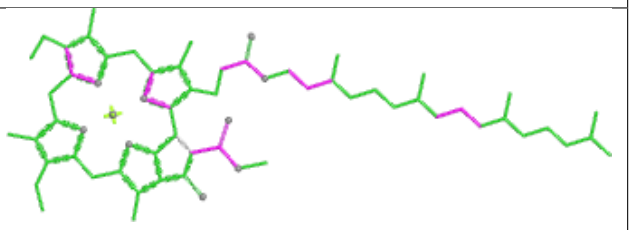
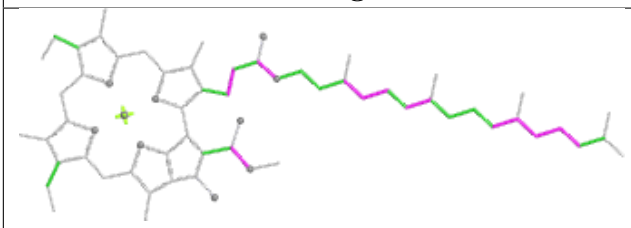
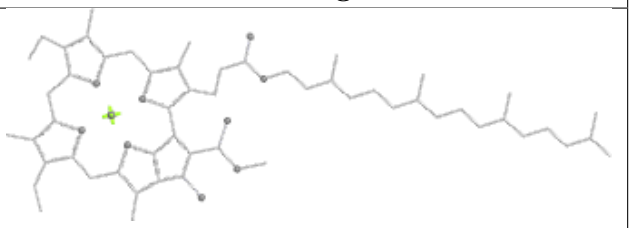
 Bond lengths	 Bond angles
 Torsions	 Rings

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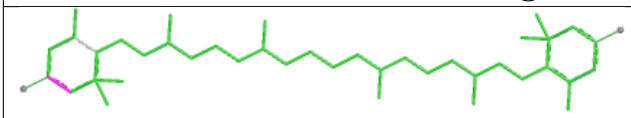
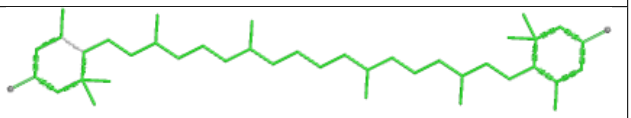
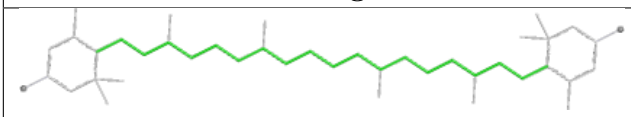
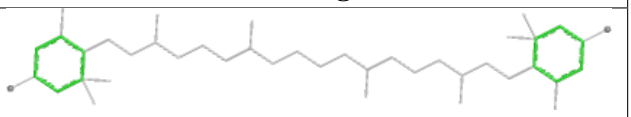
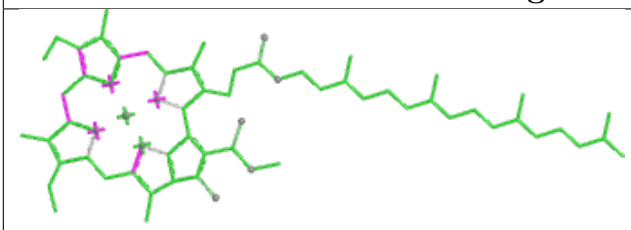
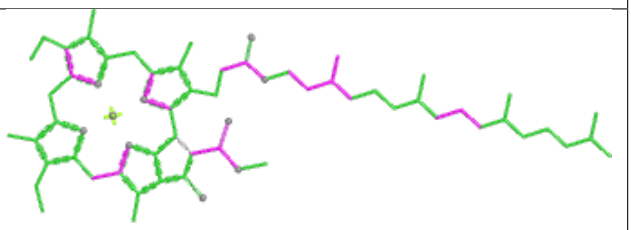
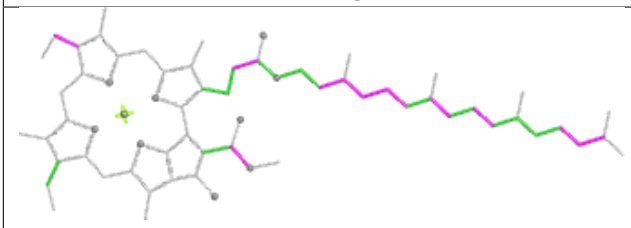
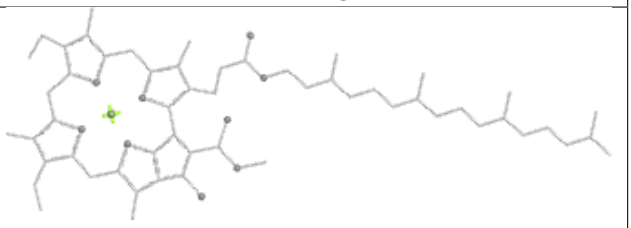
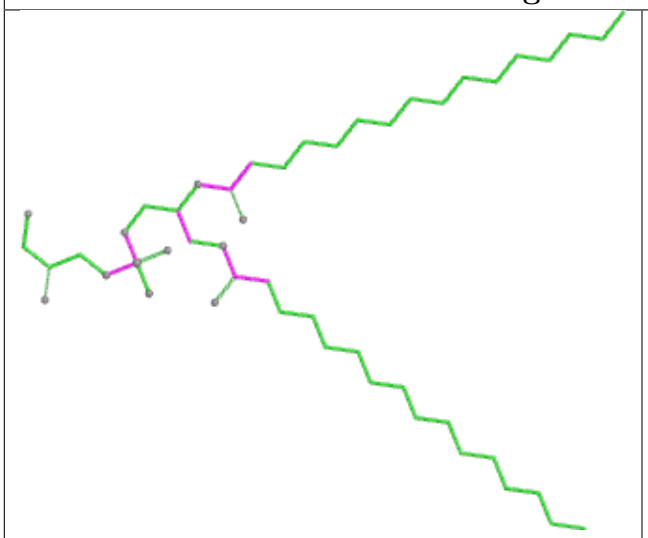
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG D 408



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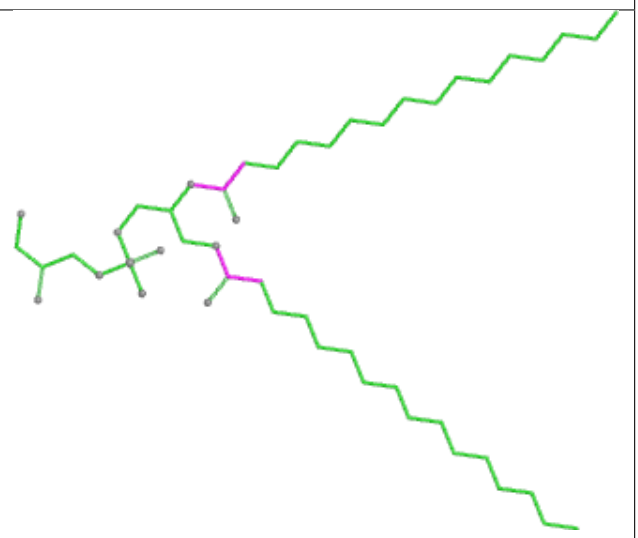

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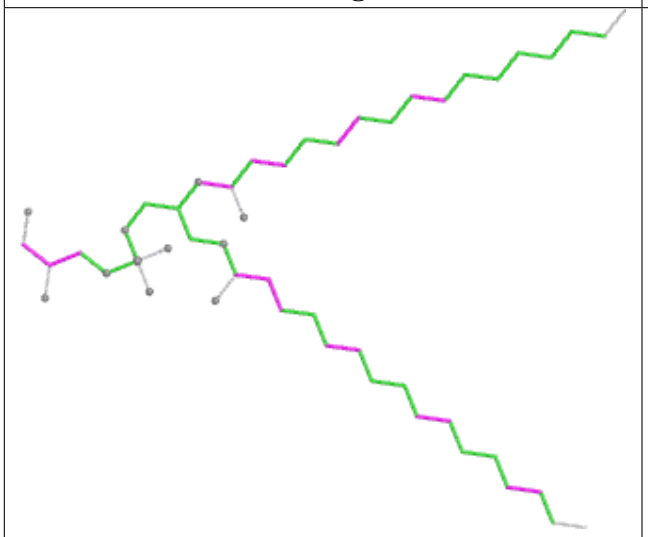

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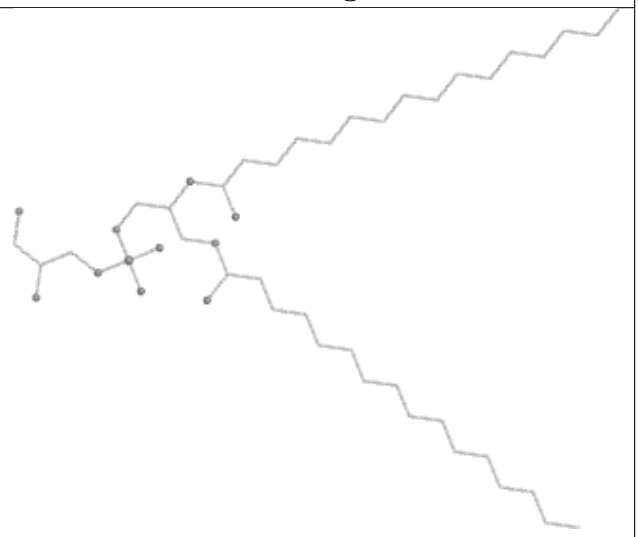
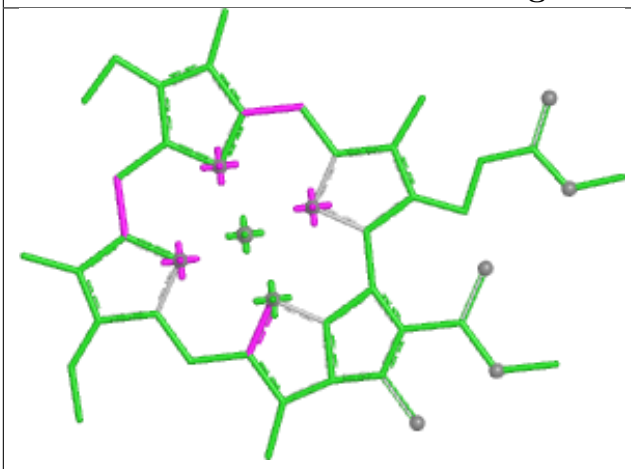


Rings

Ligand CLA 1 612



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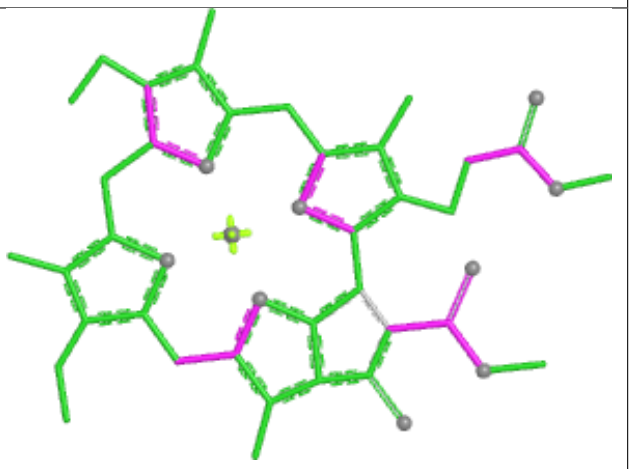

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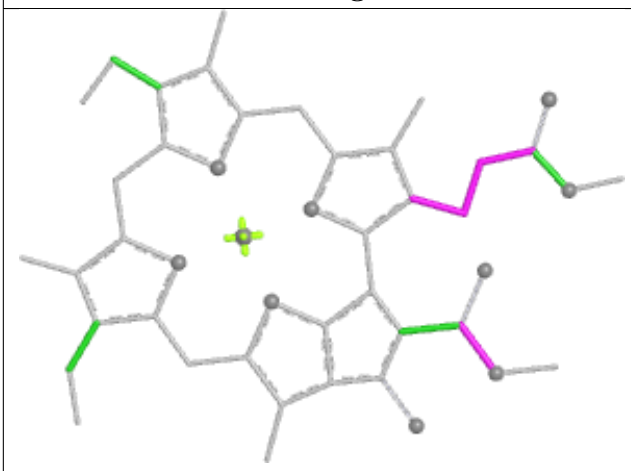

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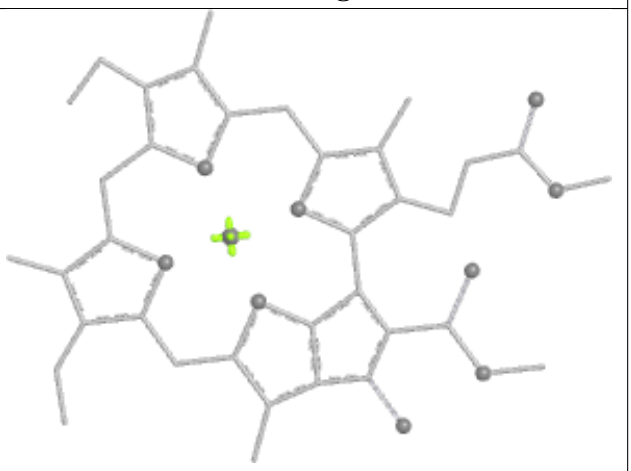
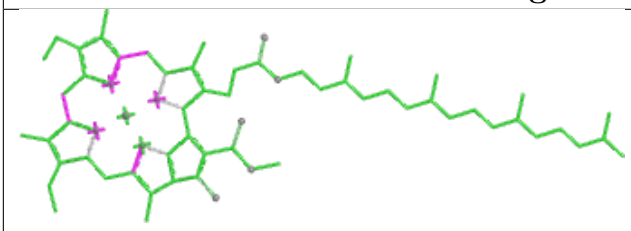


Rings

Ligand CLA c 502



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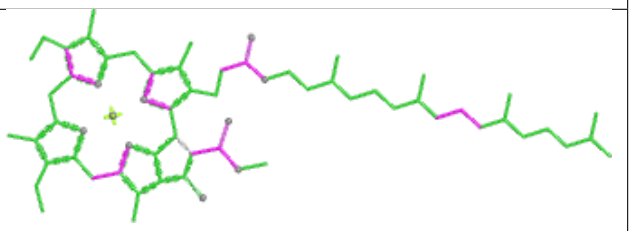

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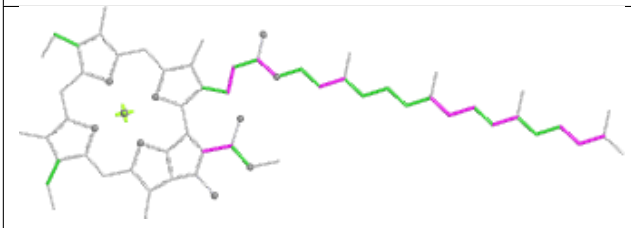

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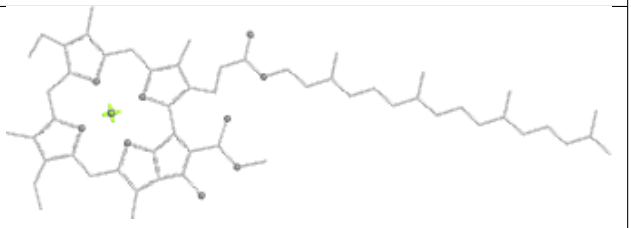
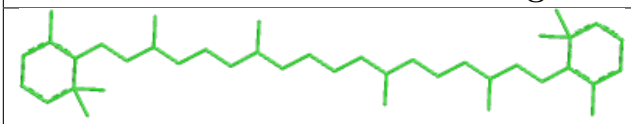


Rings

Ligand BCR c 516



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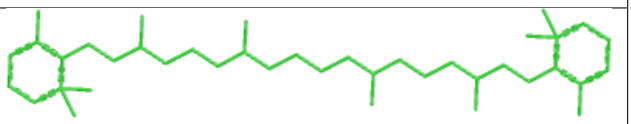

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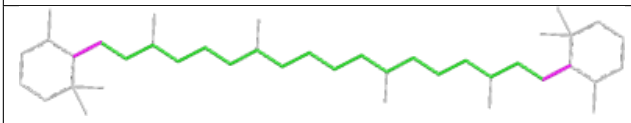

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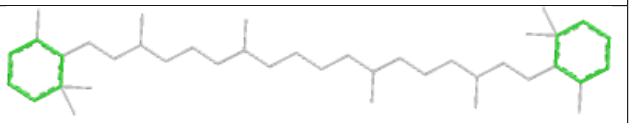
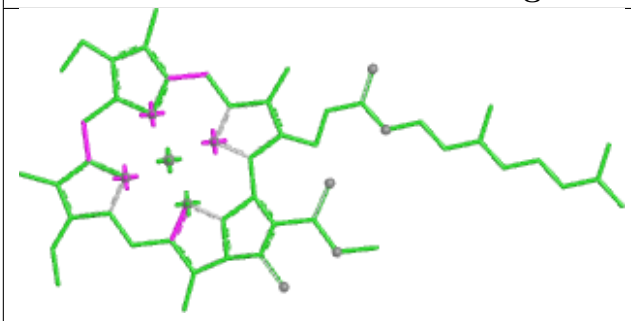


Rings

Ligand CLA Y 604



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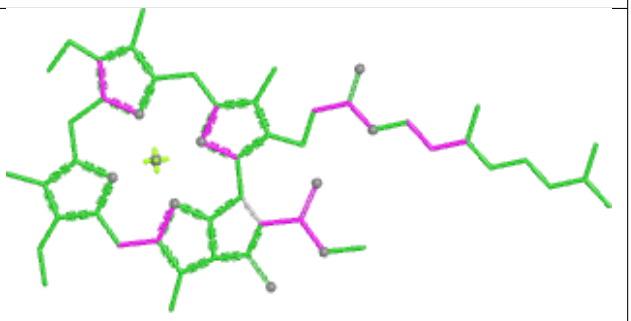

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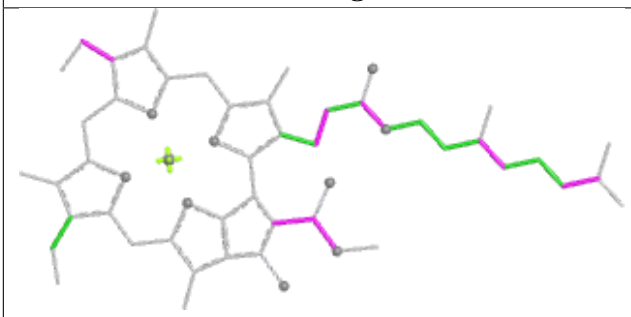

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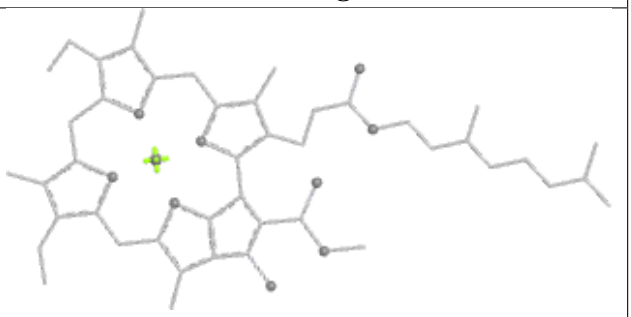
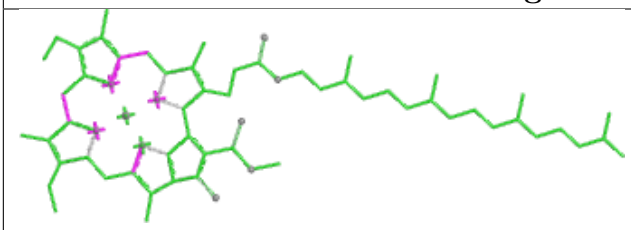


Rings

Ligand CLA B 604



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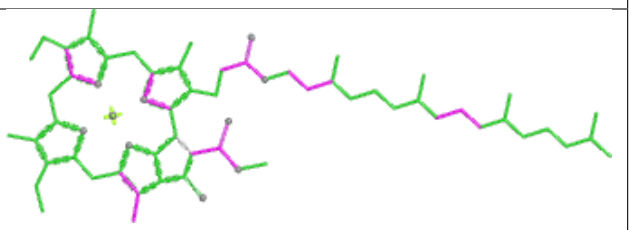

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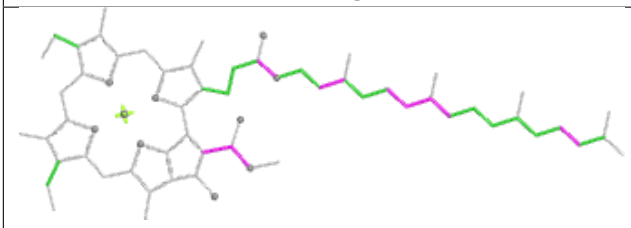

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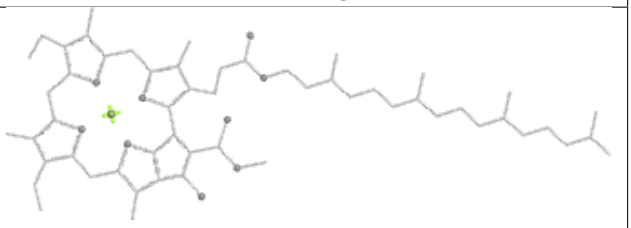
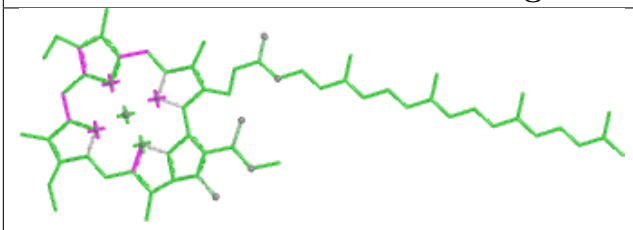


Rings

Ligand CLA B 611



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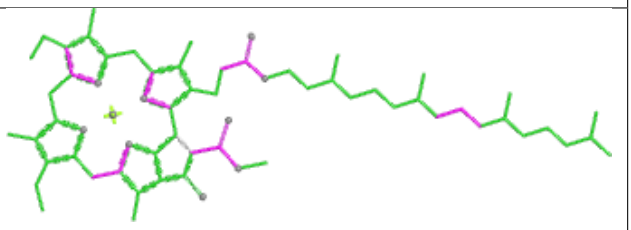

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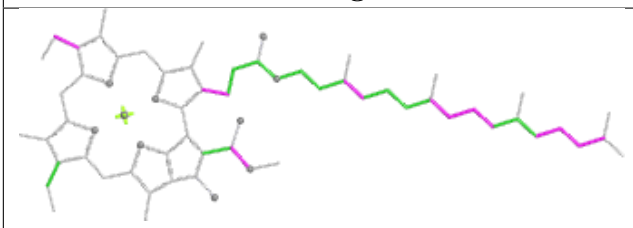

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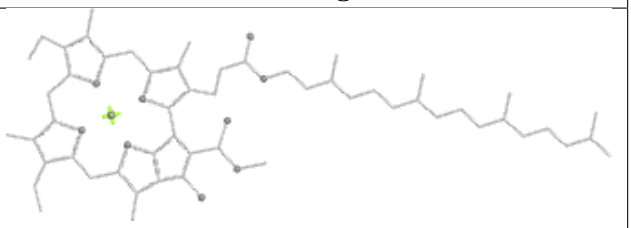
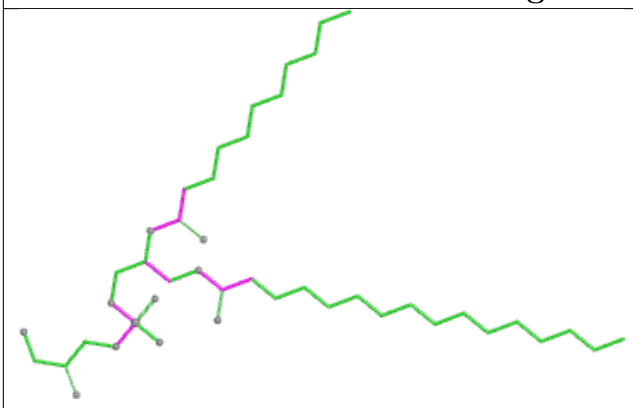


Rings

Ligand LHG a 413



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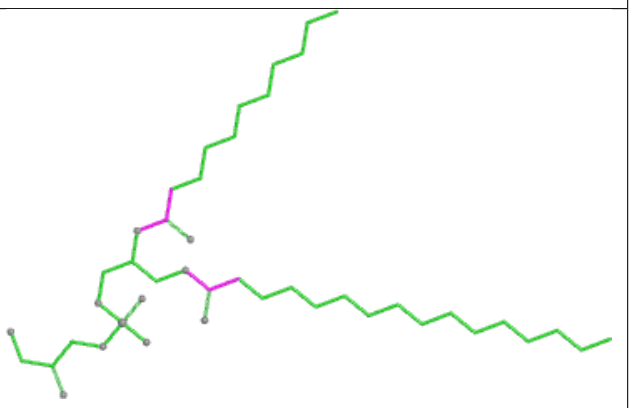

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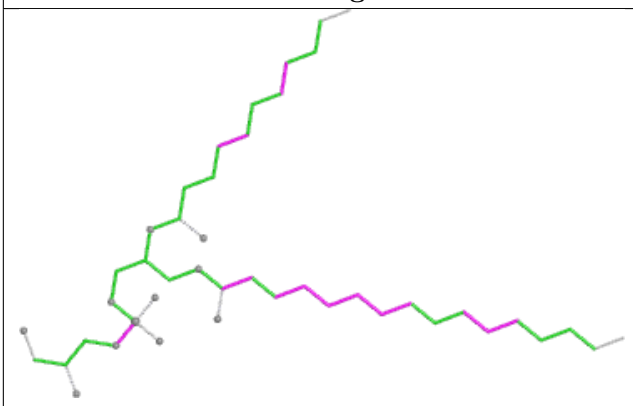

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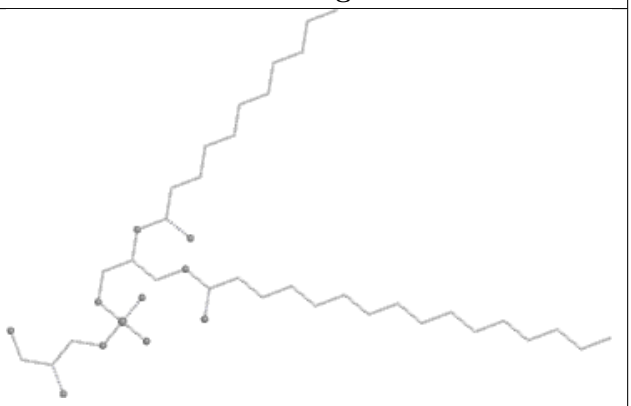

Rings

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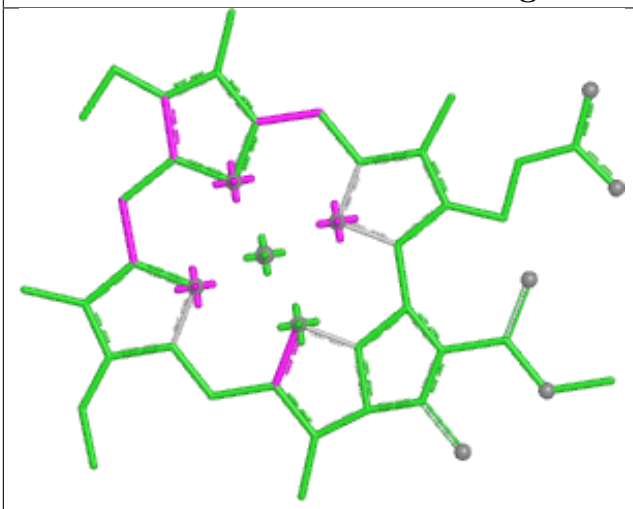

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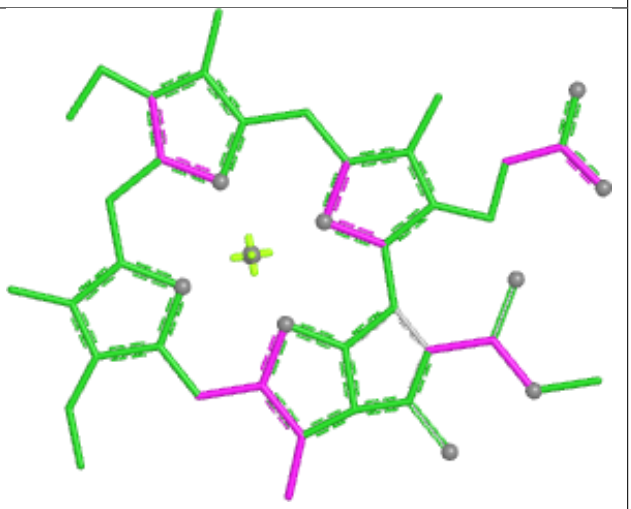

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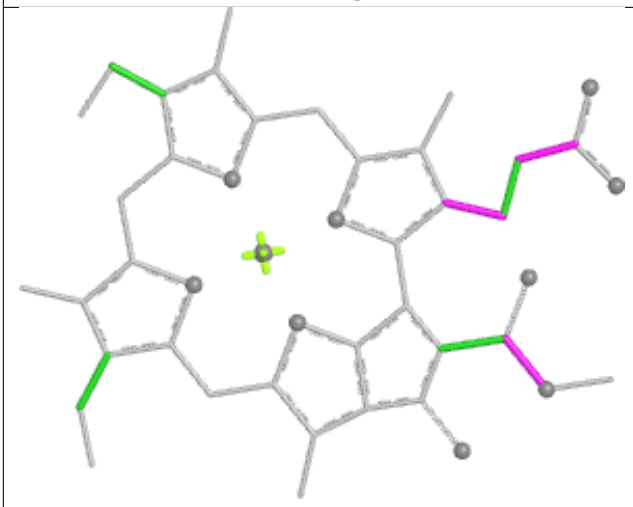
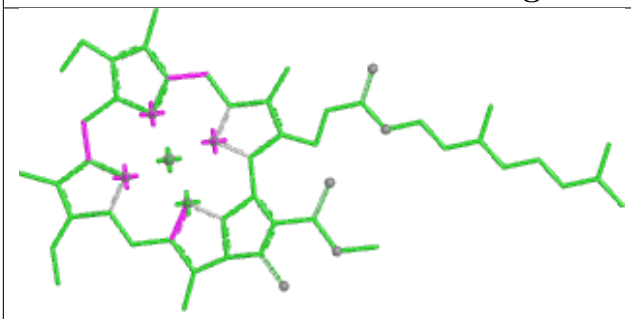
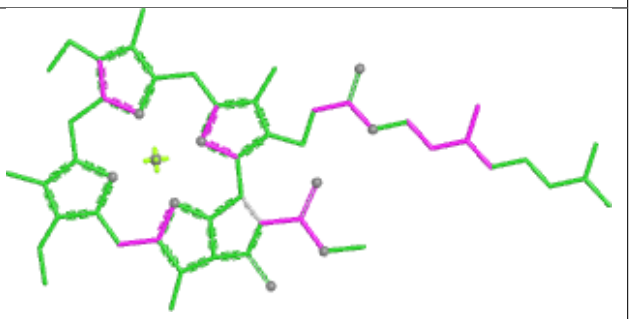
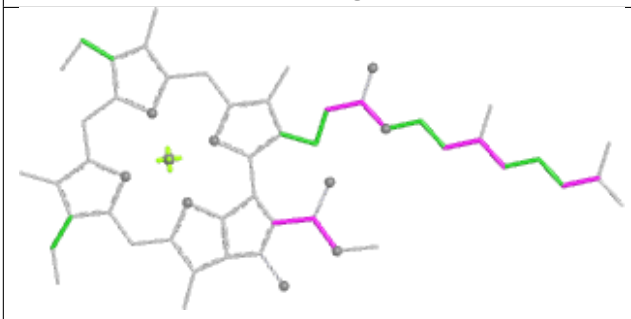
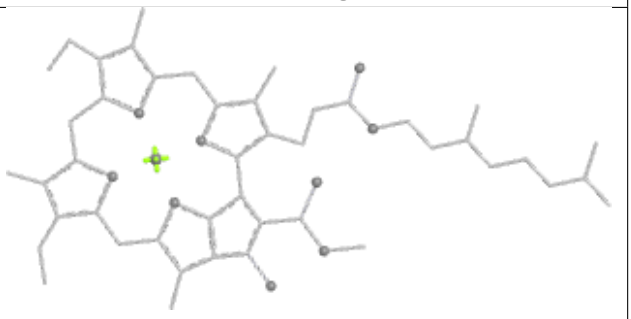
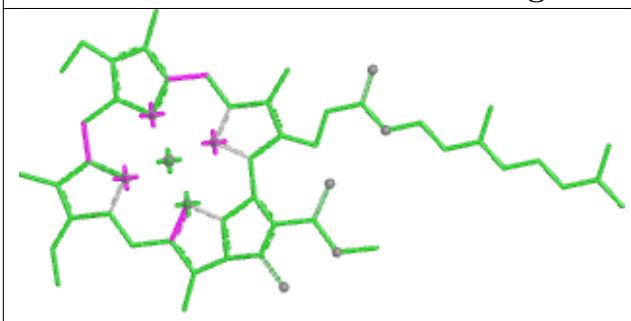
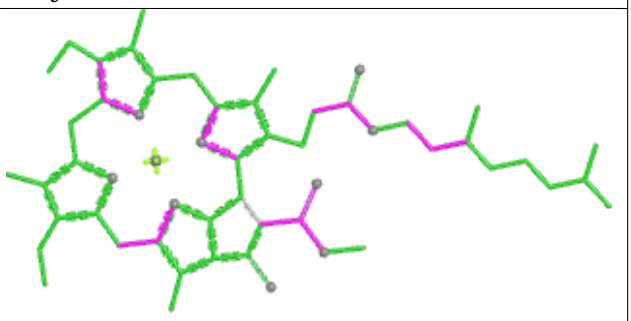
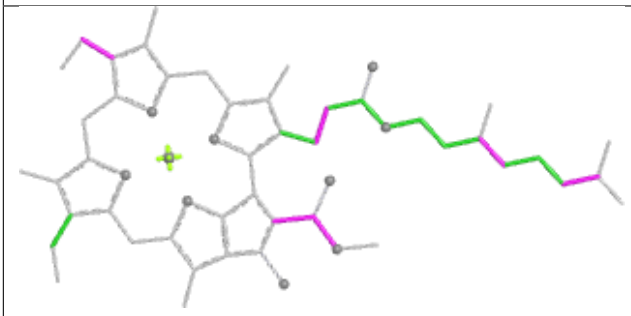
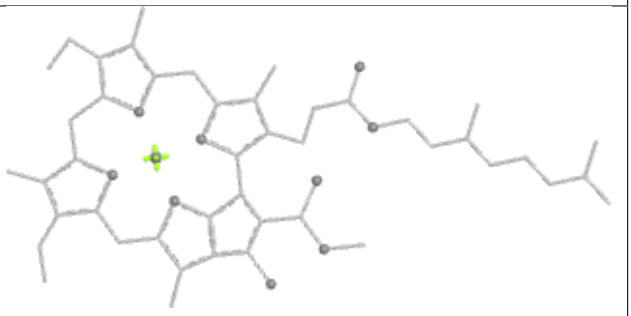


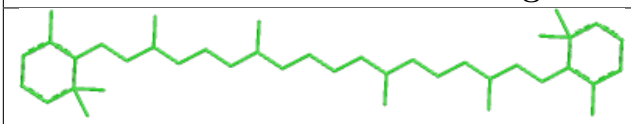
Torsions

Rings

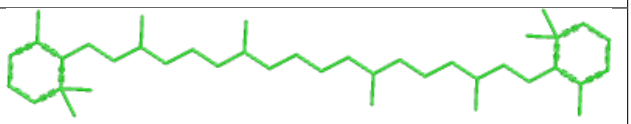
Ligand CLA G 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

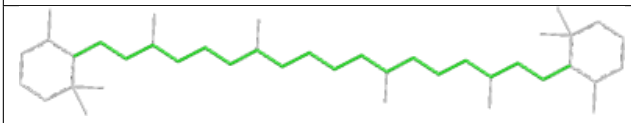
Ligand BCR B 618



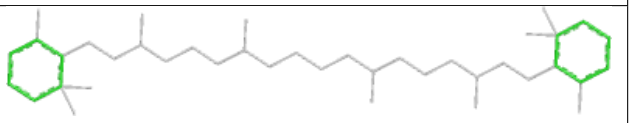
Bond lengths



Bond angles

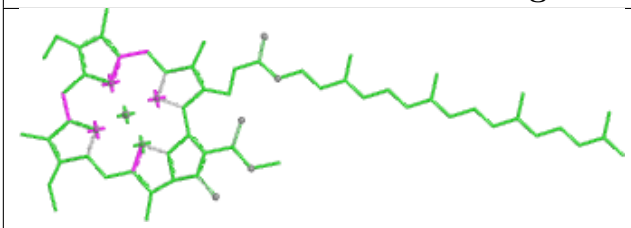


Torsions

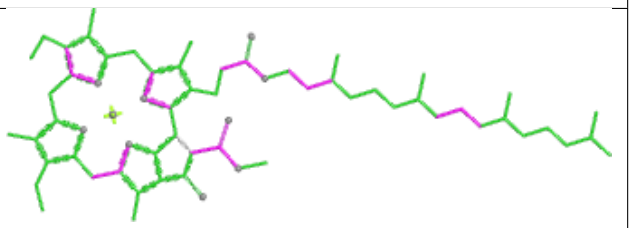


Rings

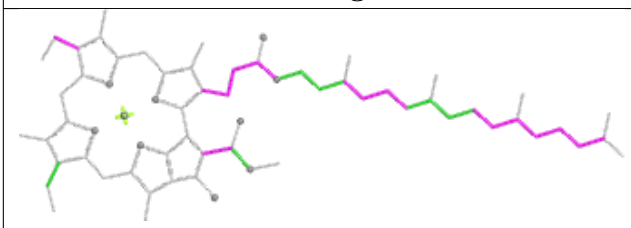
Ligand CLA c 507



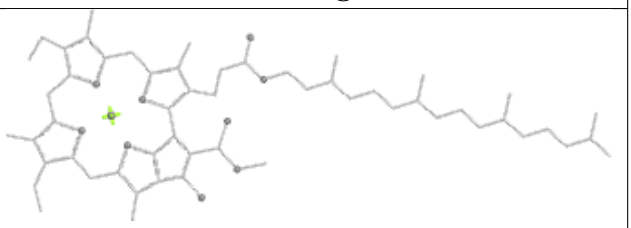
Bond lengths



Bond angles

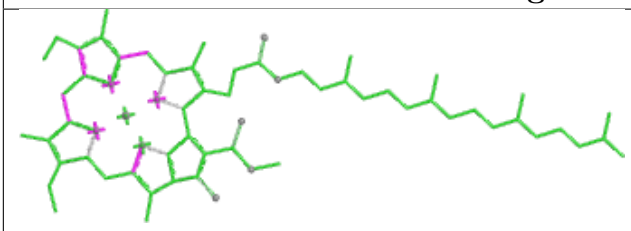


Torsions

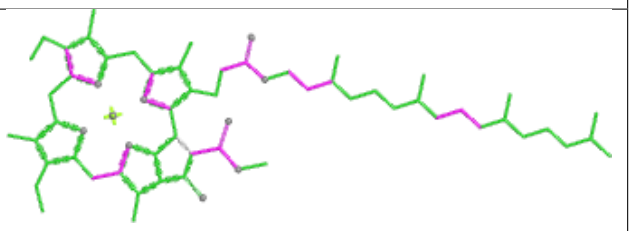


Rings

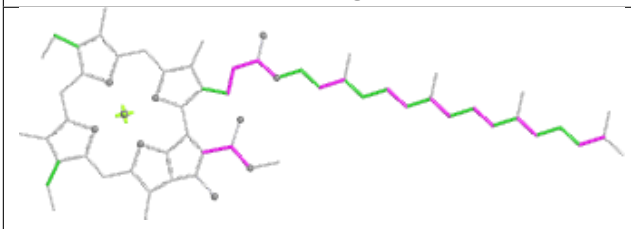
Ligand CLA b 606



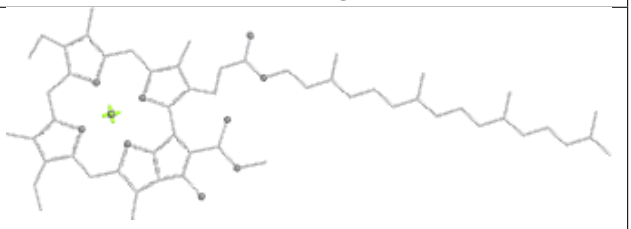
Bond lengths



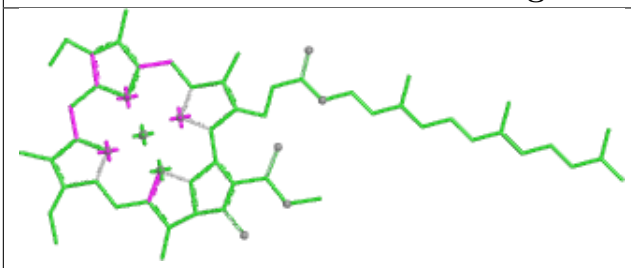
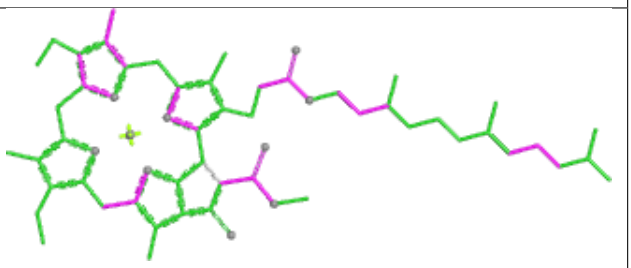
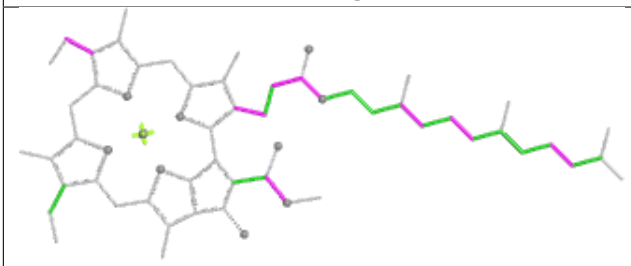
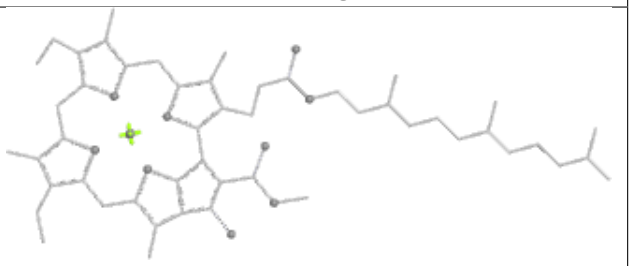
Bond angles

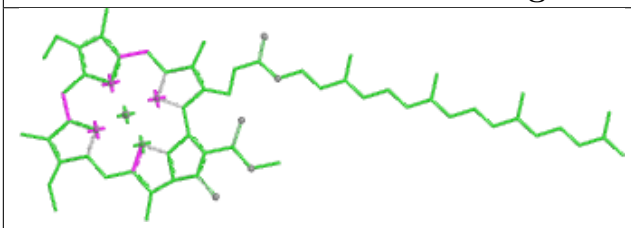
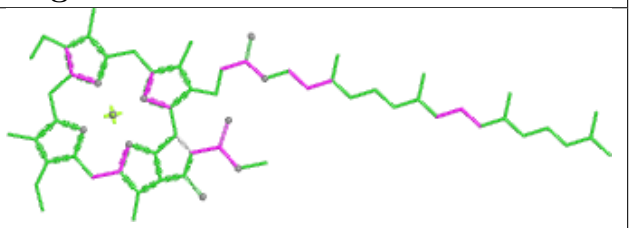
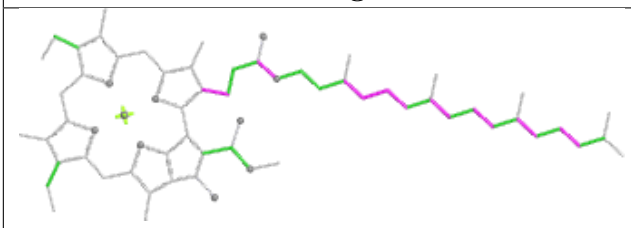
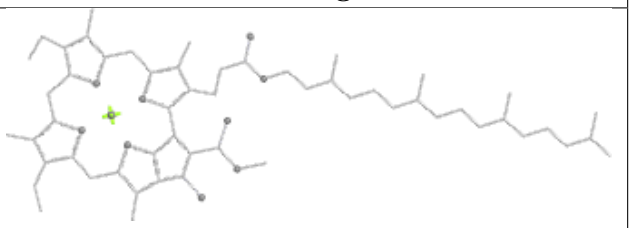


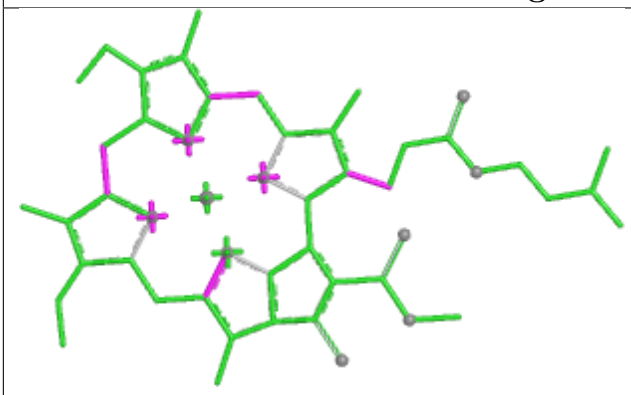
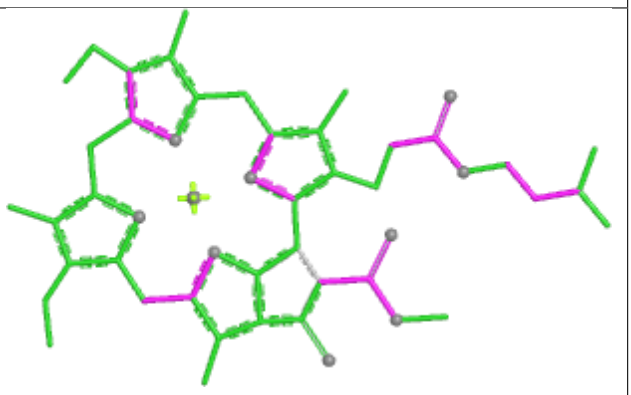
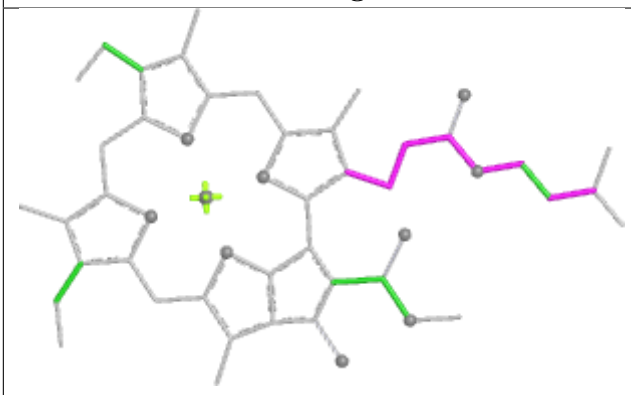
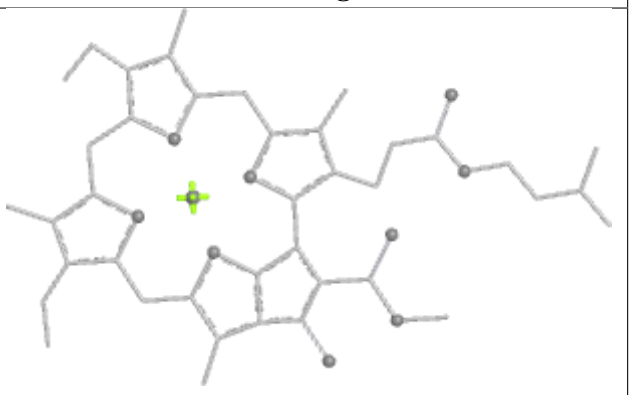
Torsions



Rings

Ligand CLA n 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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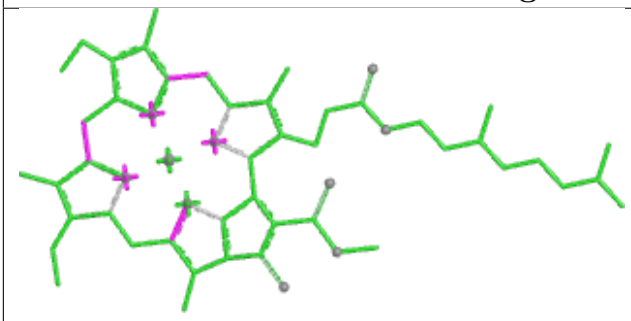
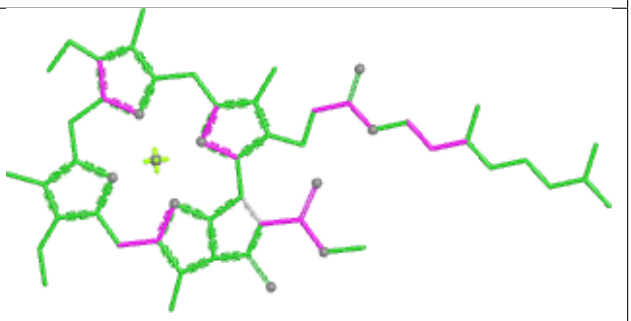
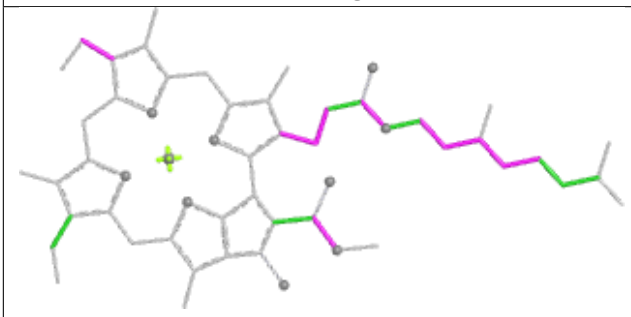
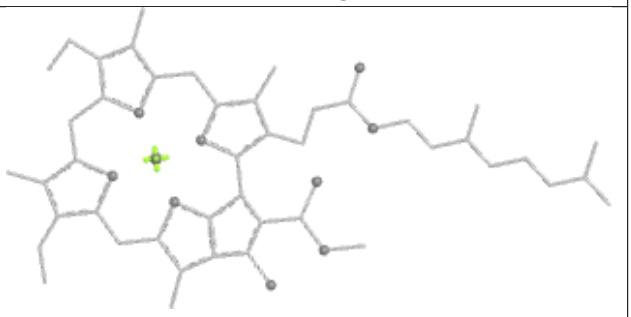
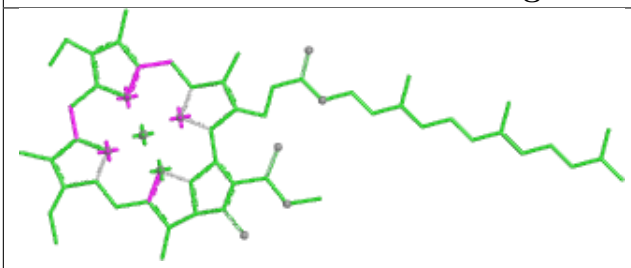
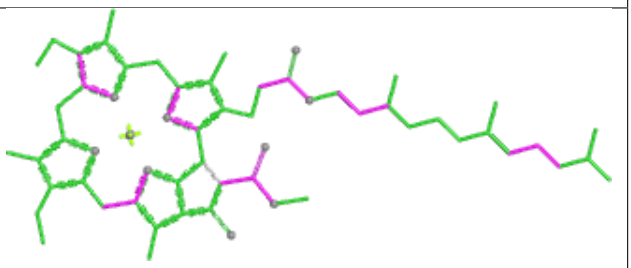
 Bond lengths	 Bond angles
 Torsions	 Rings

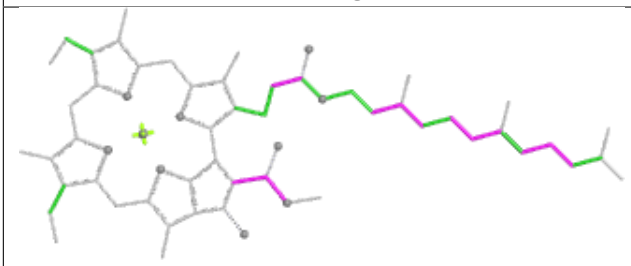
Ligand CLA N 603



Bond lengths



Bond angles



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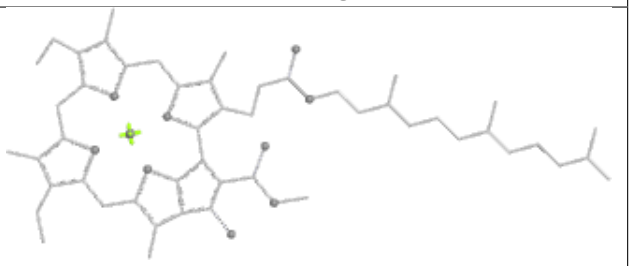
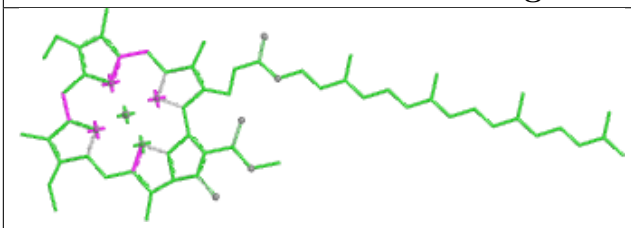
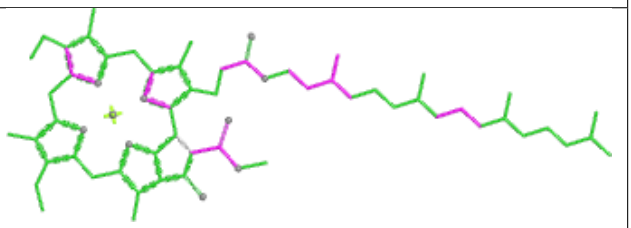


Rings

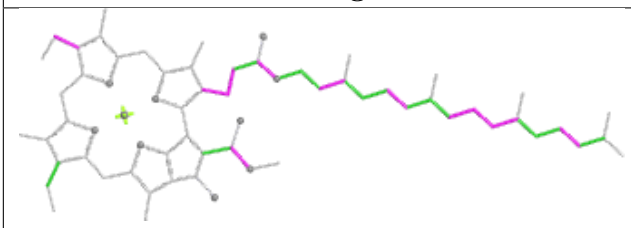
Ligand CLA C 512



Bond lengths



Bond angles



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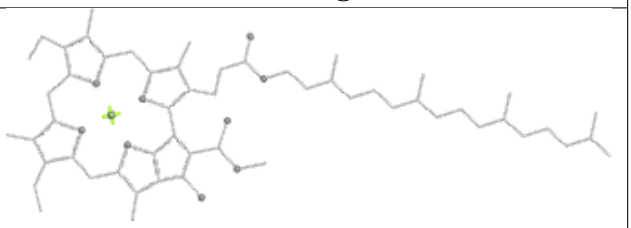
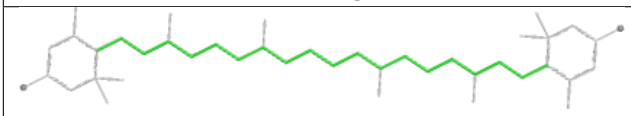


Rings

Ligand LUT 16 617

Bond lengths

Bond angles



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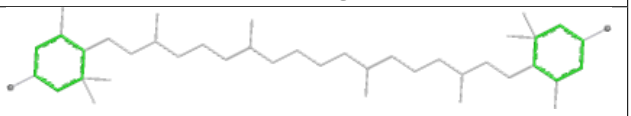
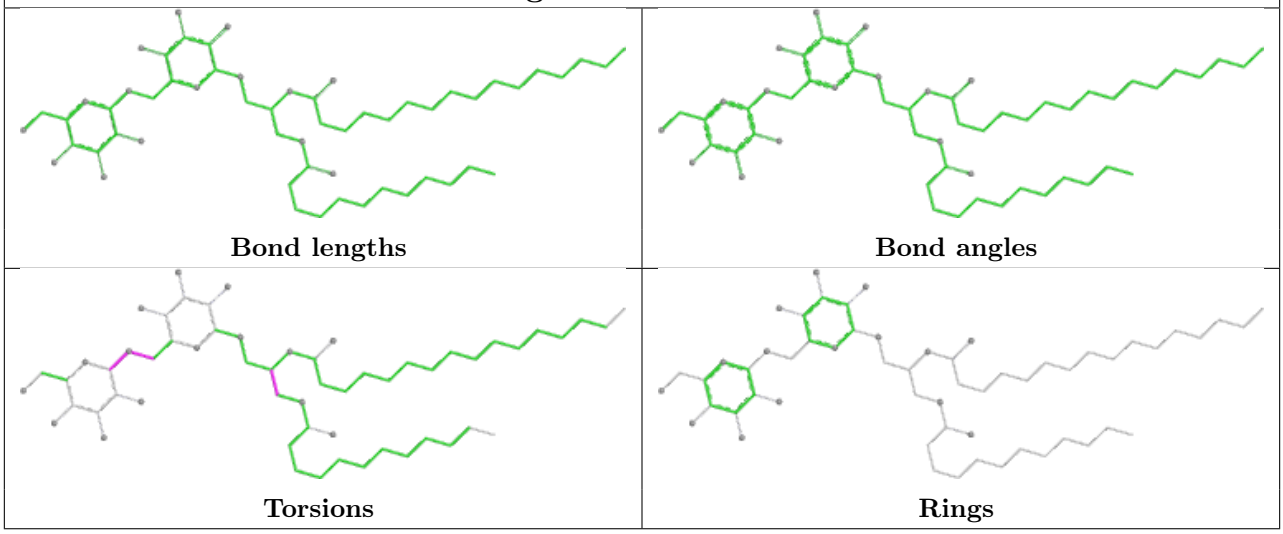
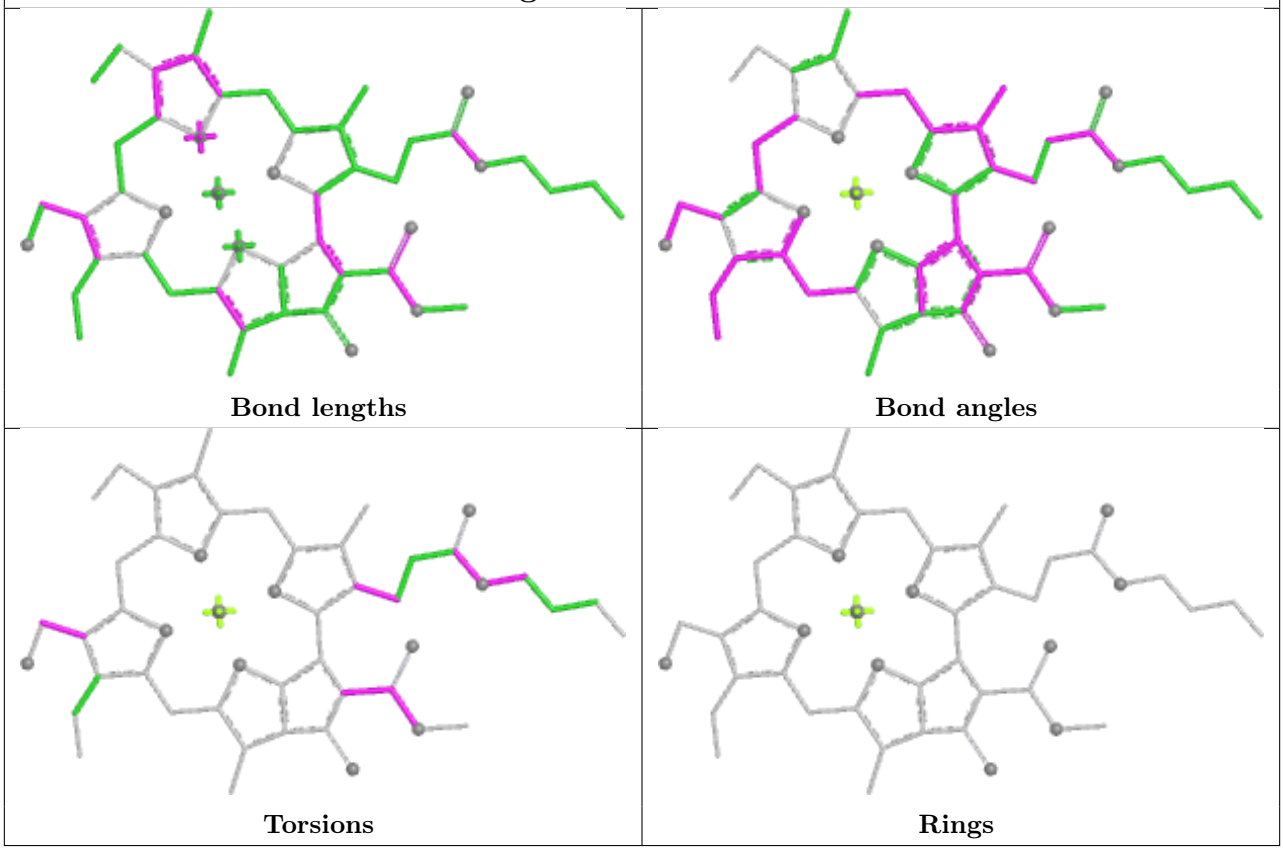


Rings

Ligand DGD c 518



Ligand CHL 14 607



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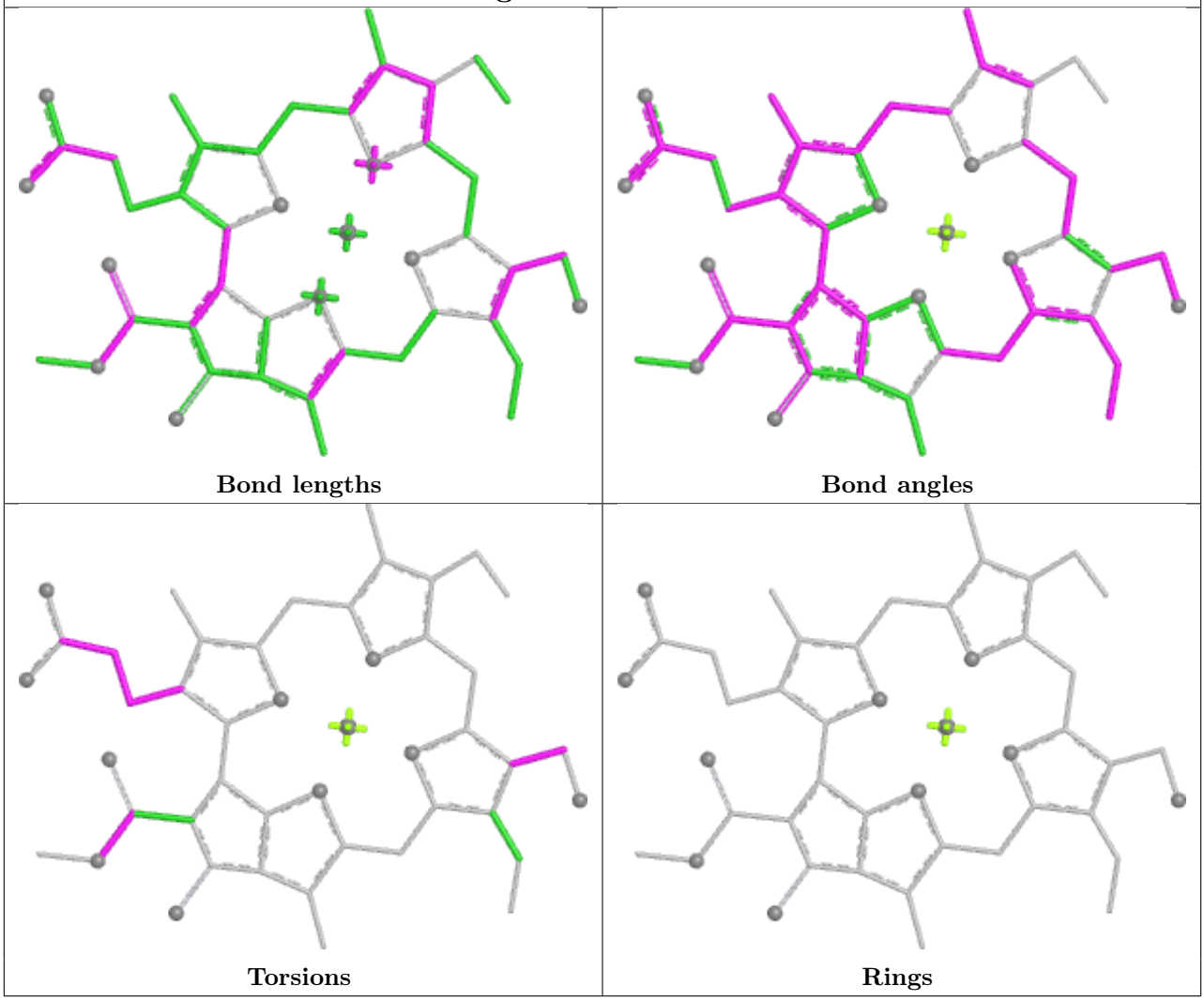
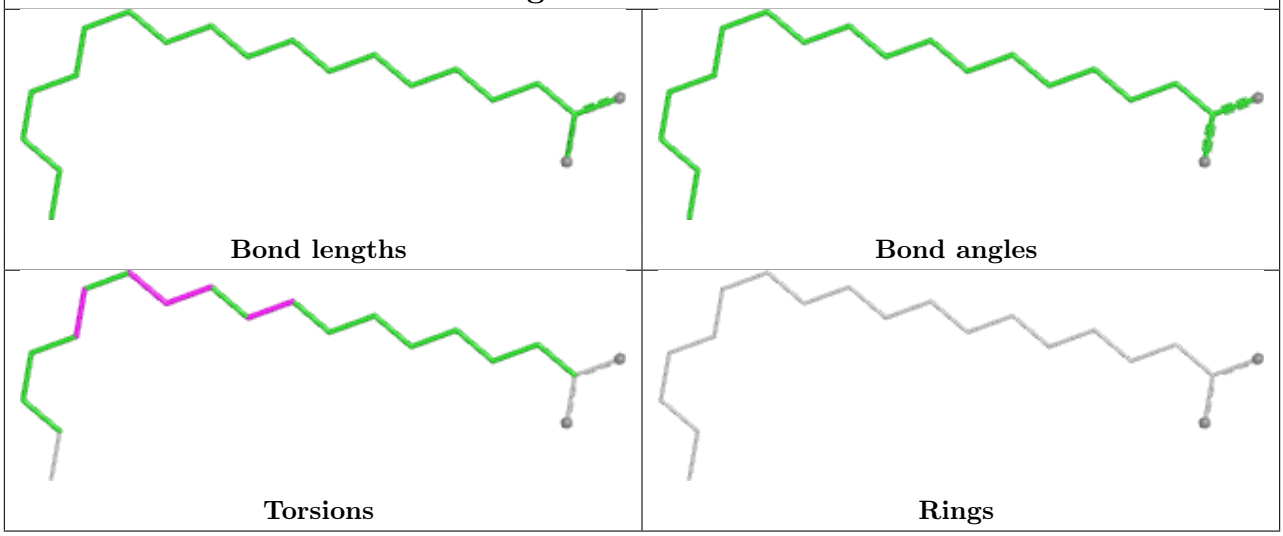
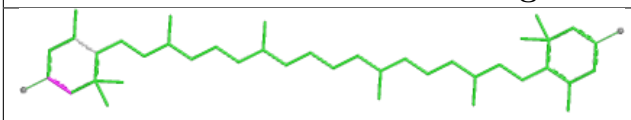
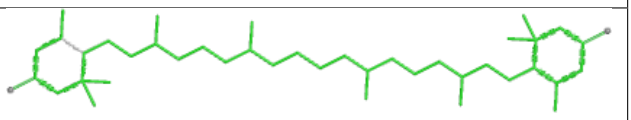
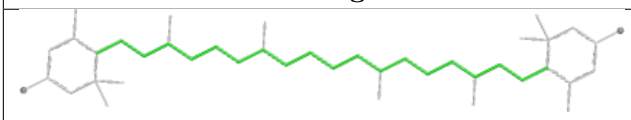
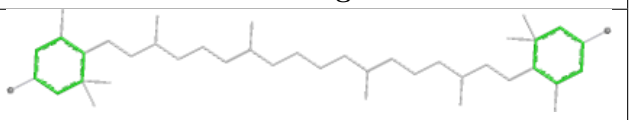
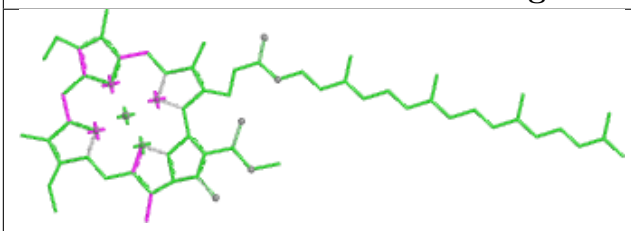
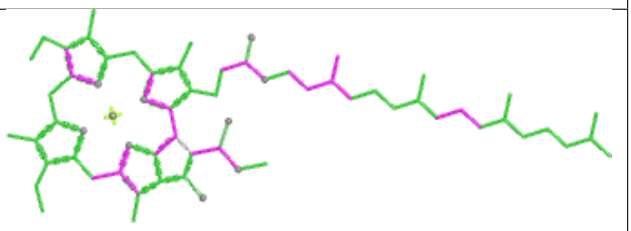
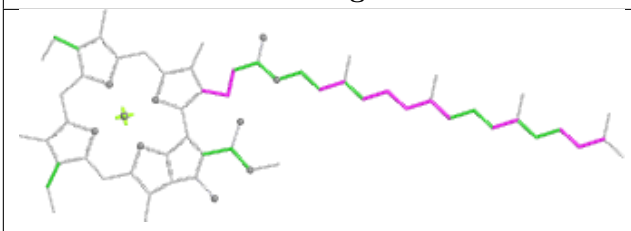
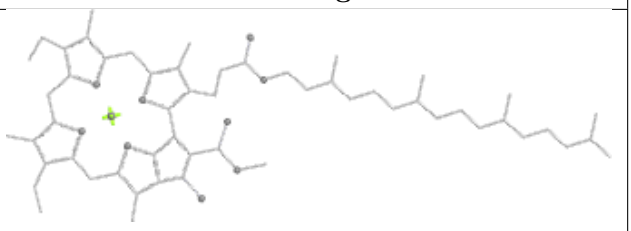


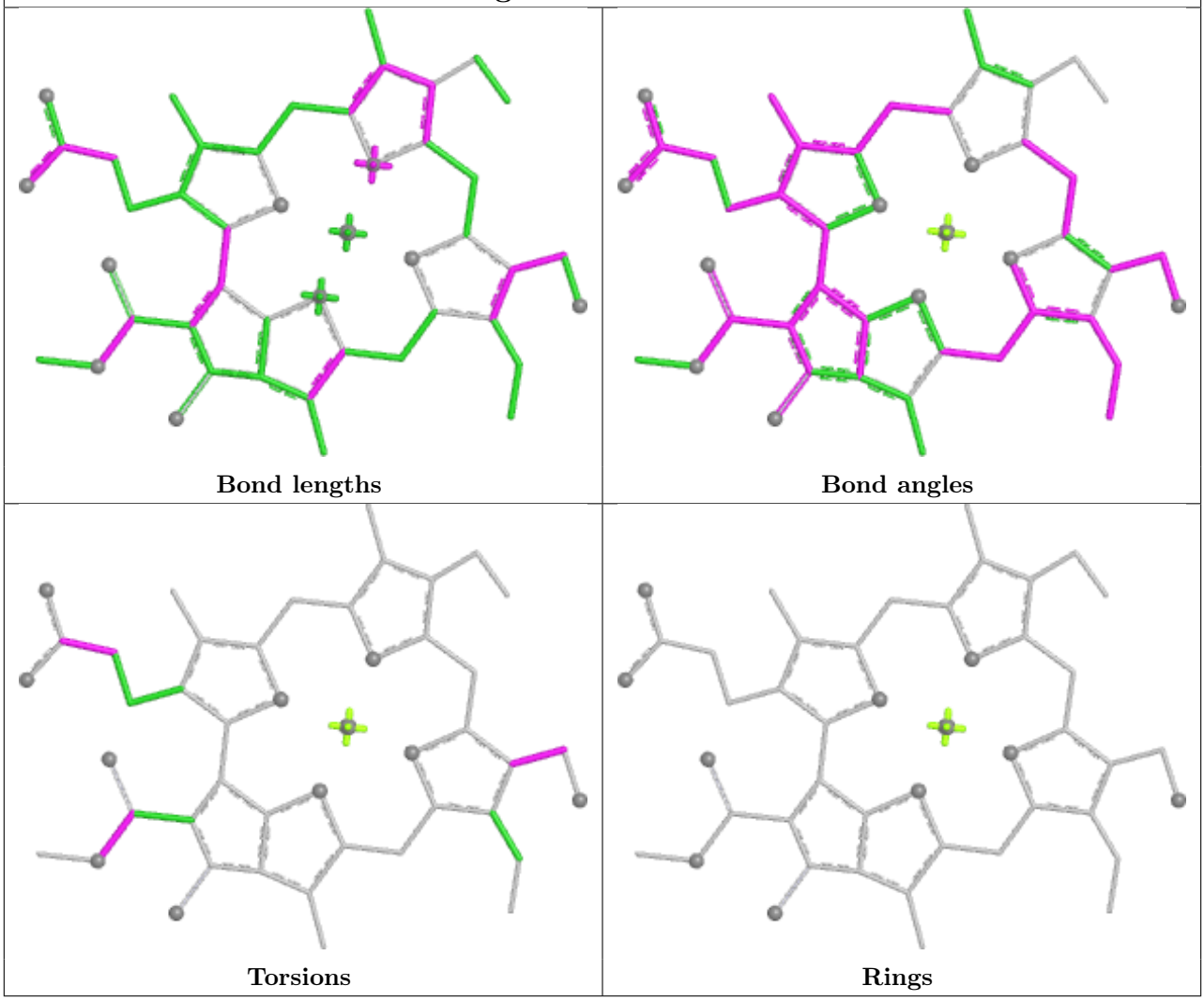
Ligand LNL w 503



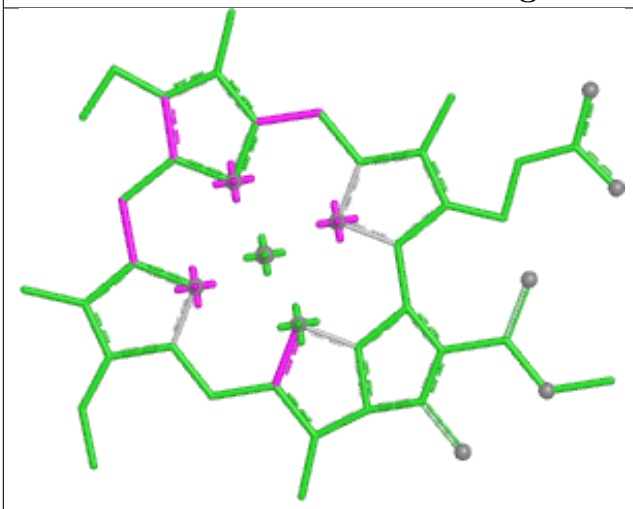
Ligand LUT 12 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

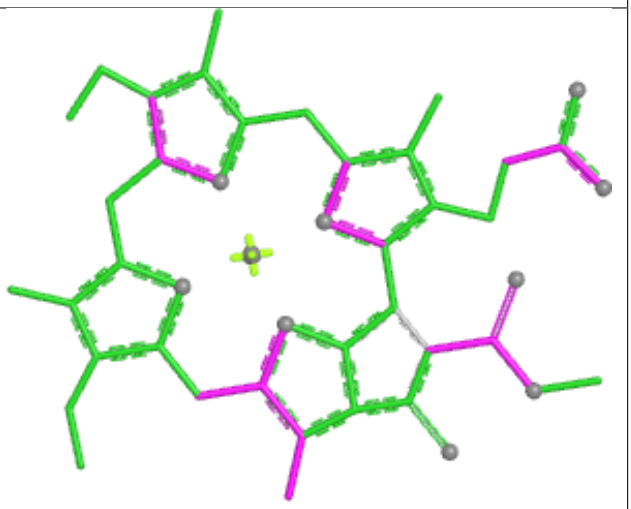
Ligand CHL S 601



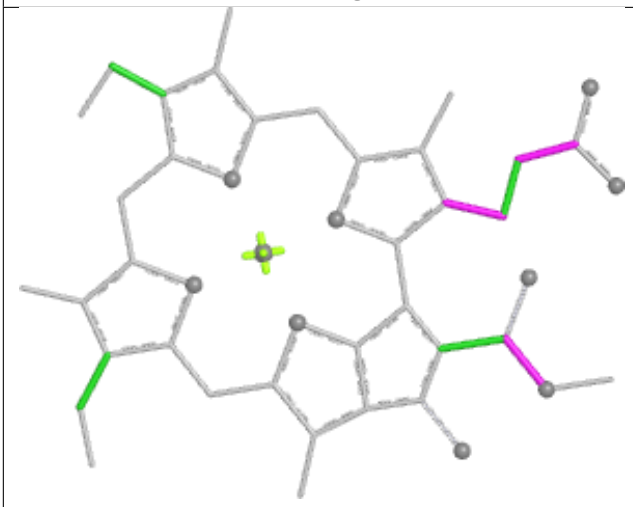
Ligand CLA 15 611



Bond lengths

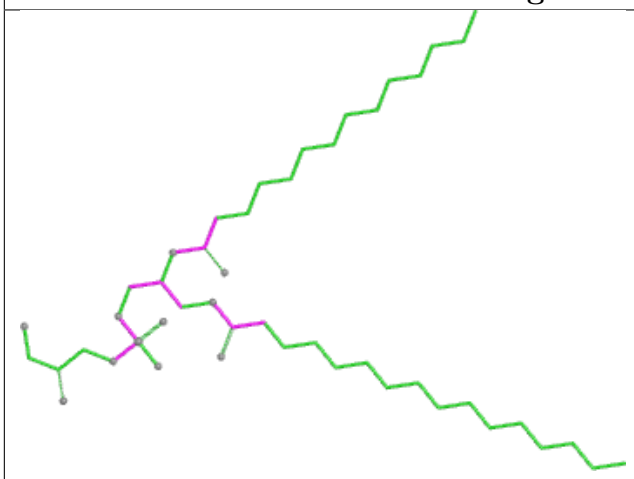
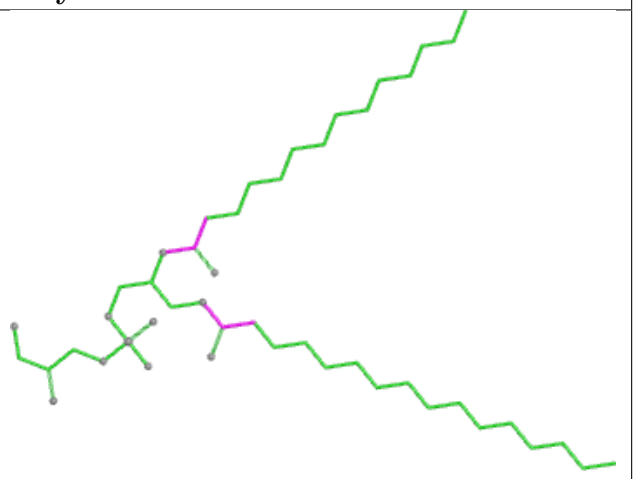
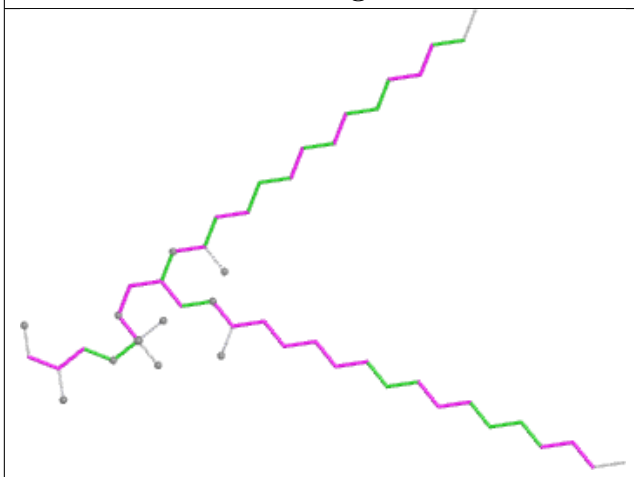
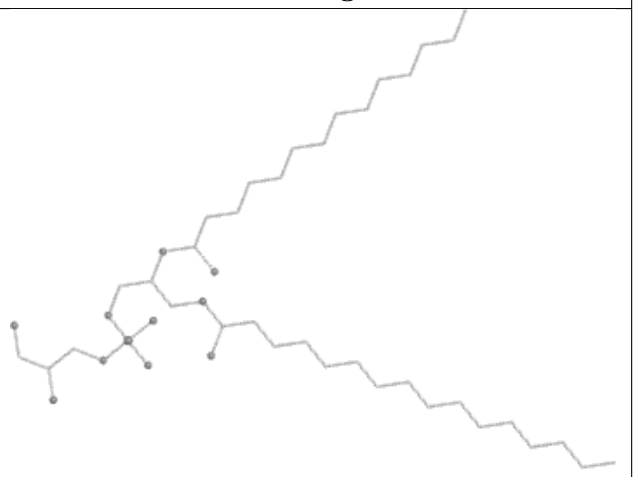


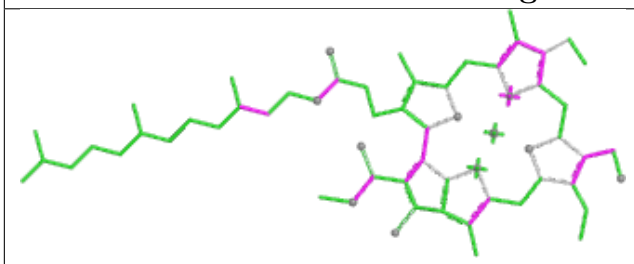
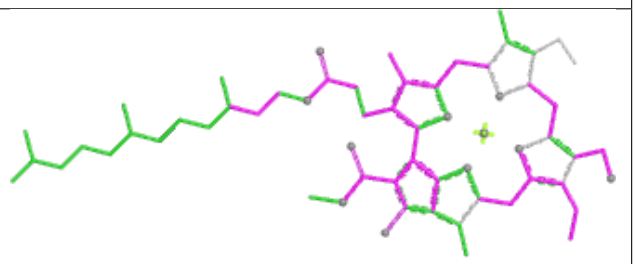
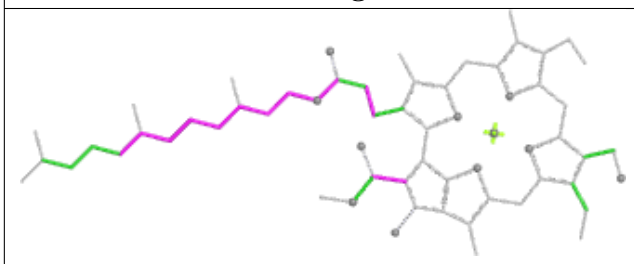
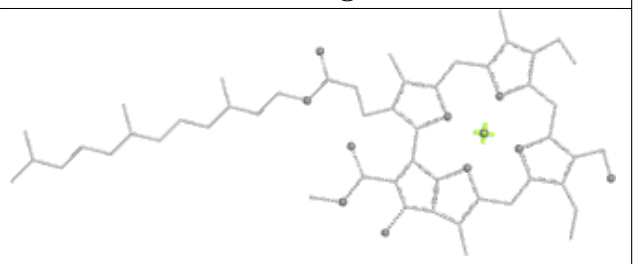
Bond angles



Torsions

Rings

Ligand LHG y 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 16 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

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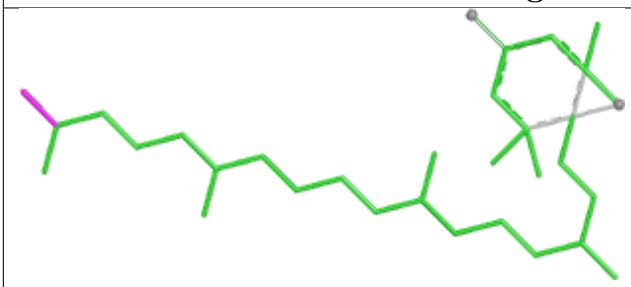
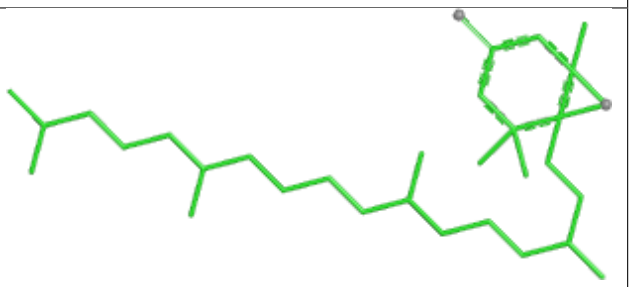
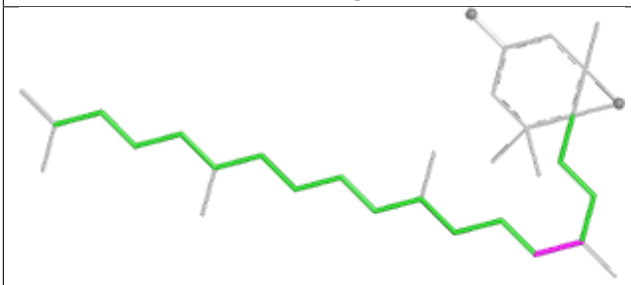
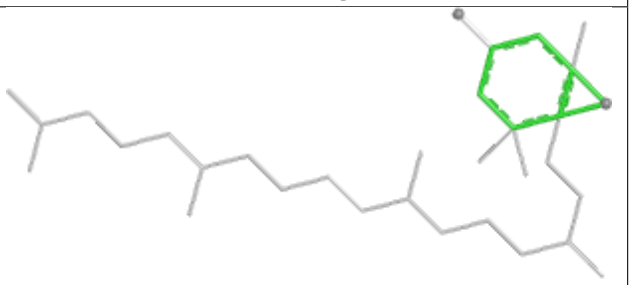
 Bond lengths	 Bond angles
 Torsions	 Rings

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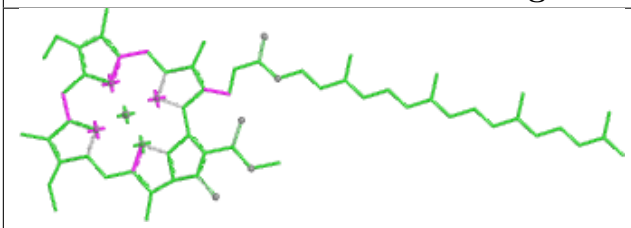
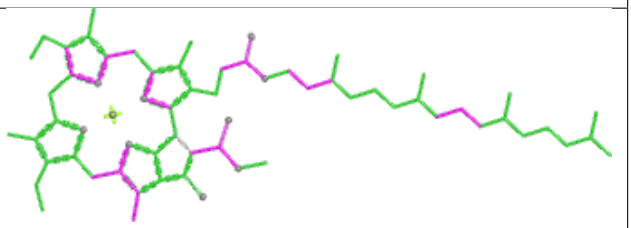
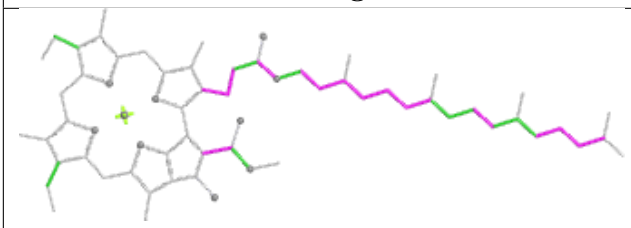
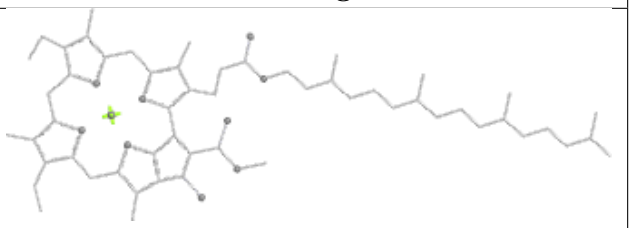
 Bond lengths	 Bond angles
 Torsions	 Rings

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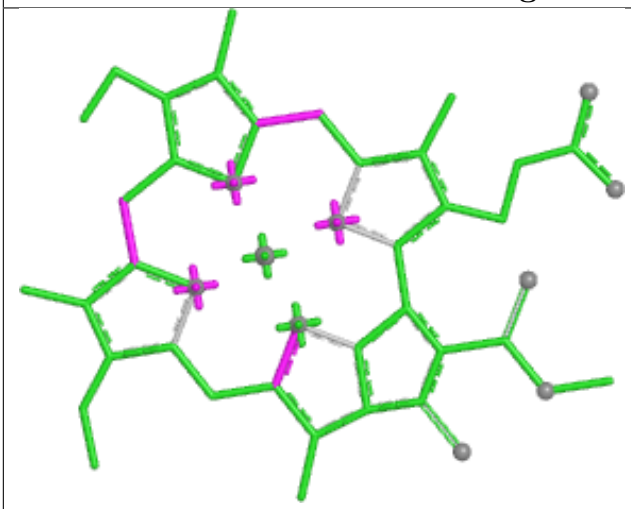

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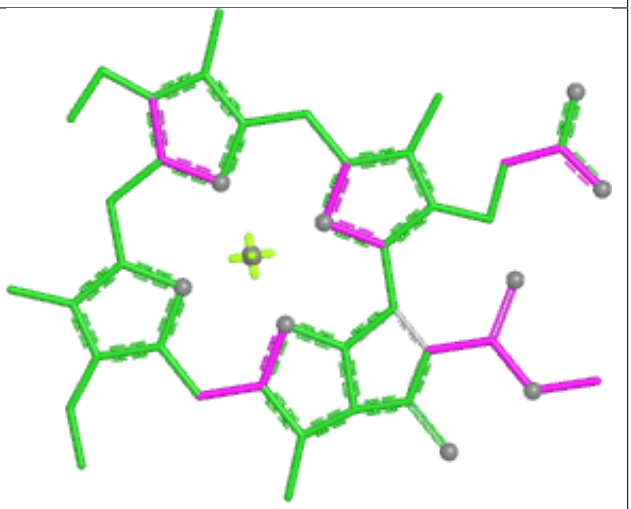

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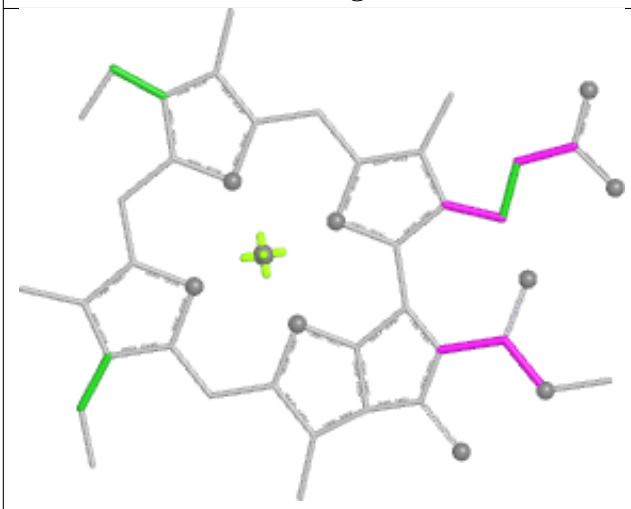

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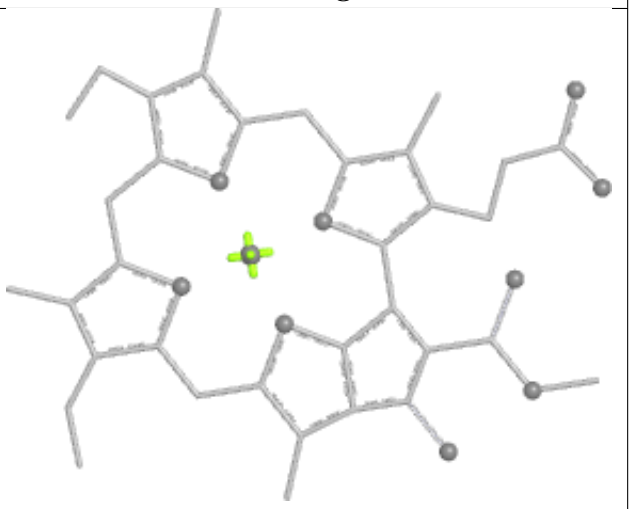

Rings

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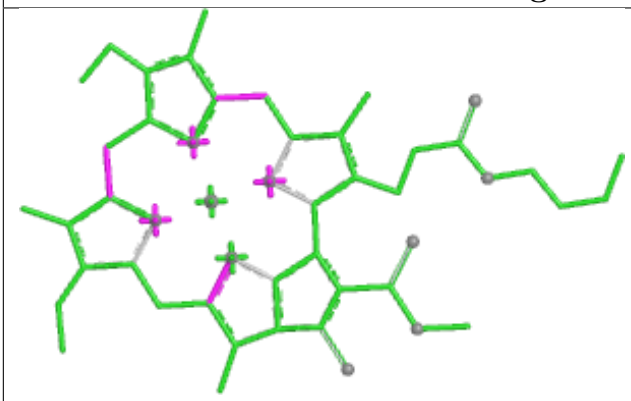

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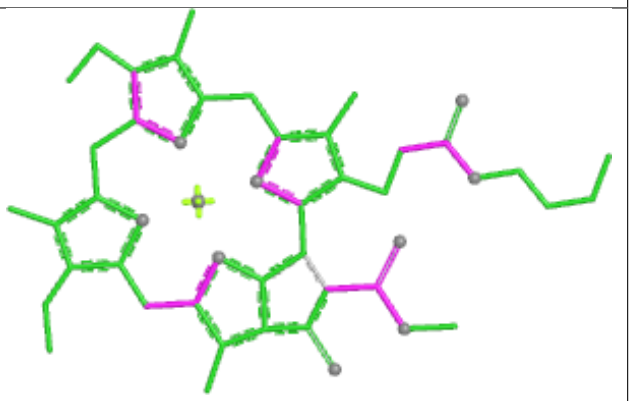

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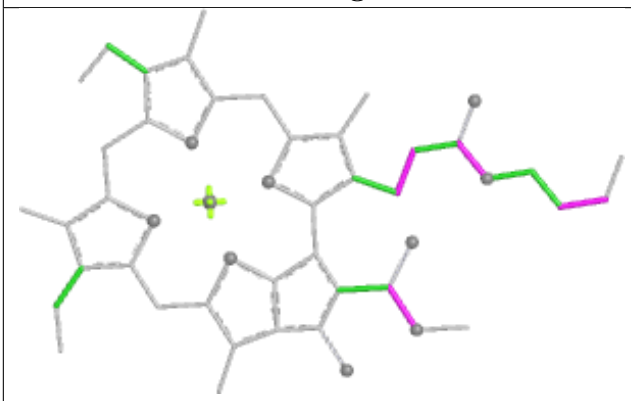

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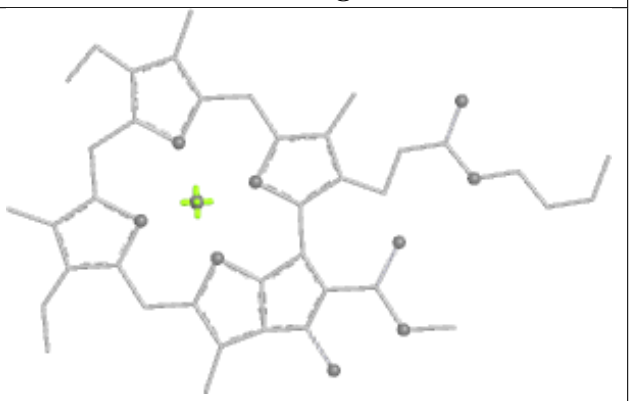
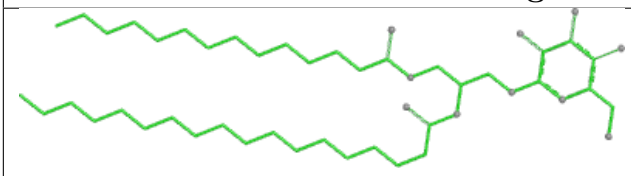


Rings

Ligand LMG j 102



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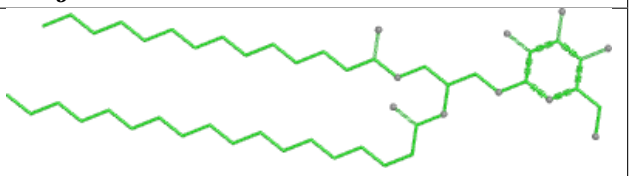

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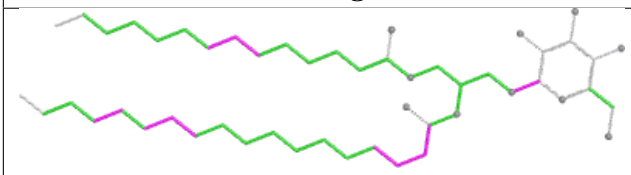

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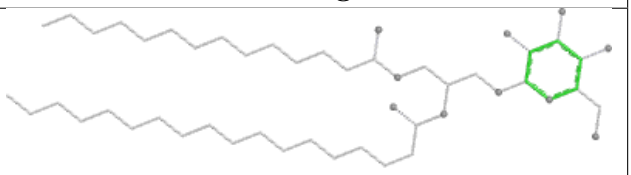

Rings

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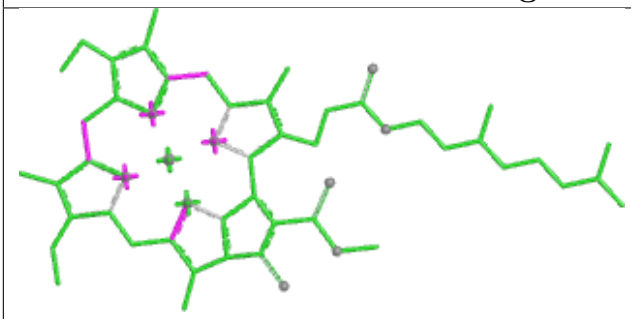
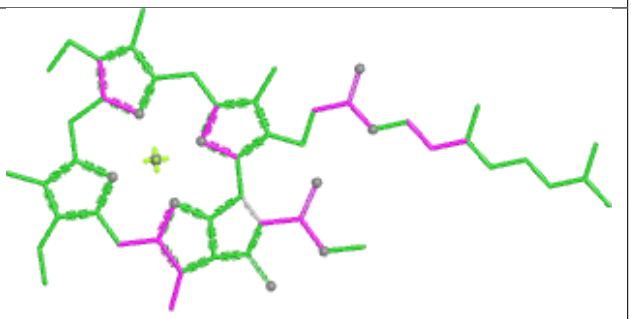
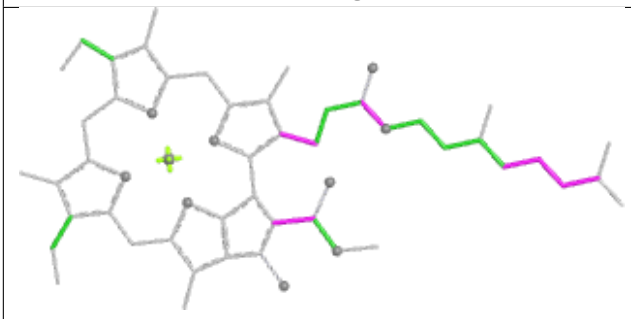
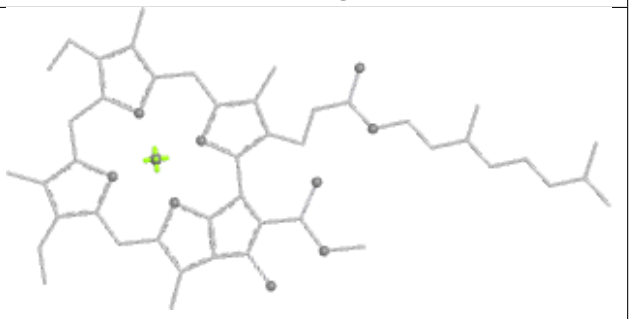
 Bond lengths	 Bond angles
 Torsions	 Rings

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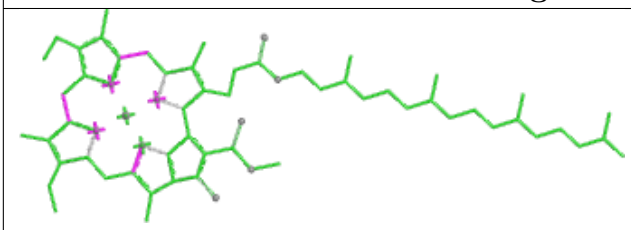
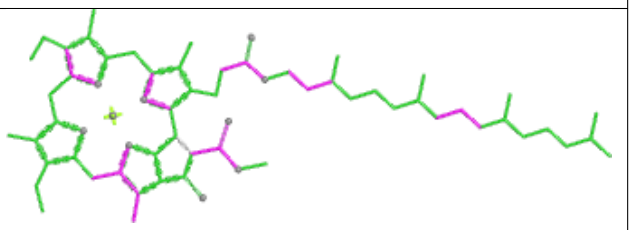
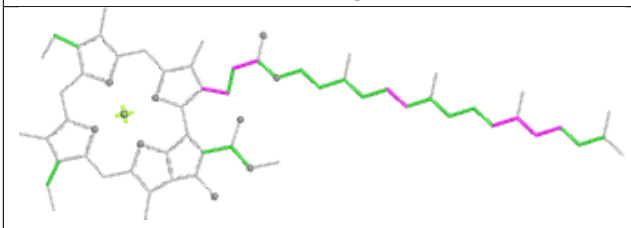
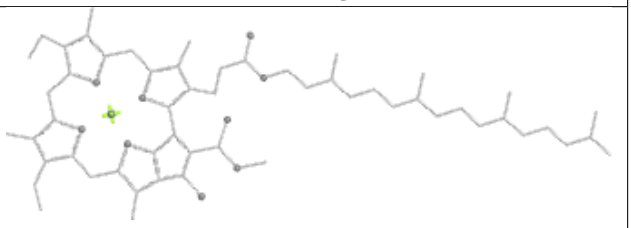
 Bond lengths	 Bond angles
 Torsions	 Rings

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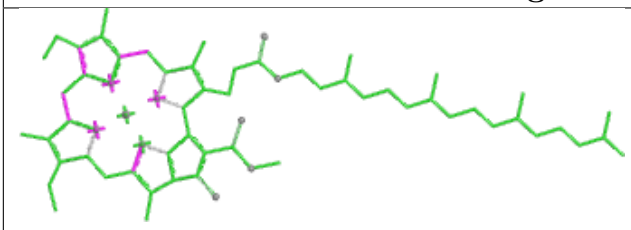
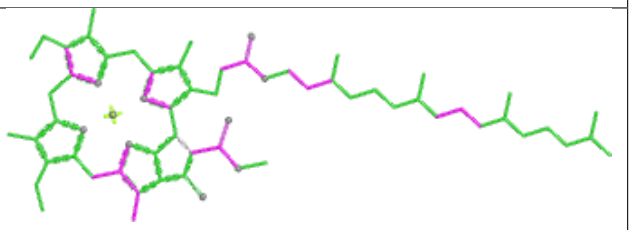
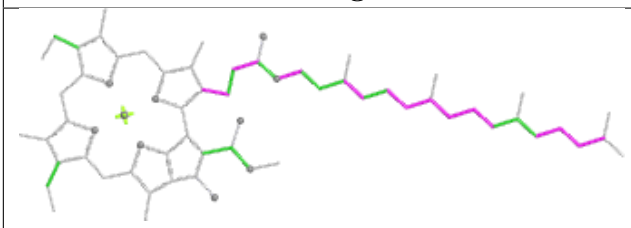
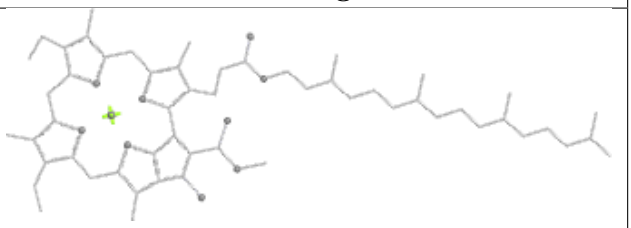
 Bond lengths	 Bond angles
 Torsions	 Rings

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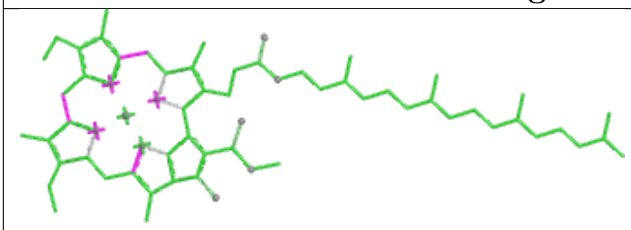
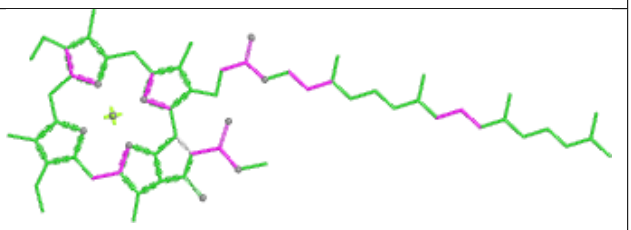
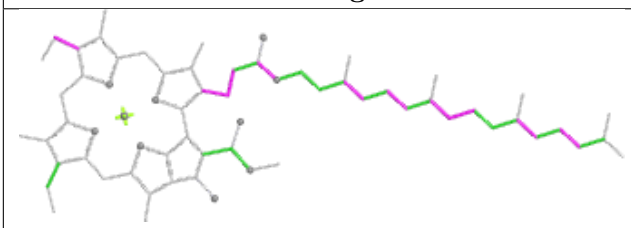
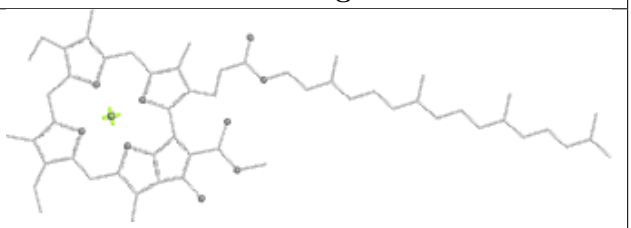
 Bond lengths	 Bond angles
 Torsions	 Rings

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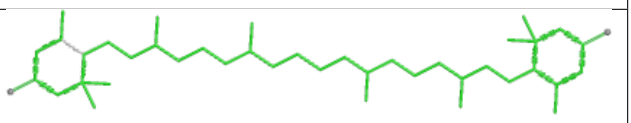
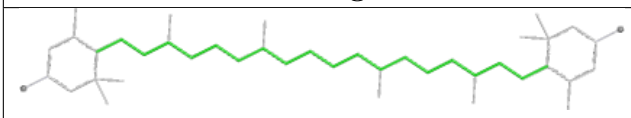
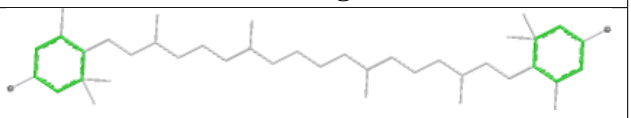
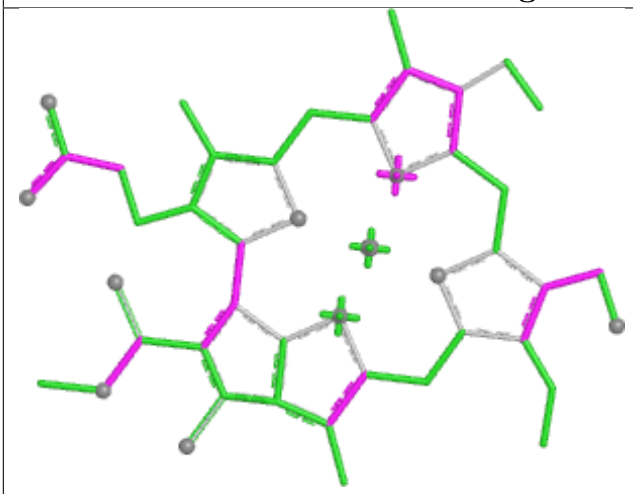
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 11 607



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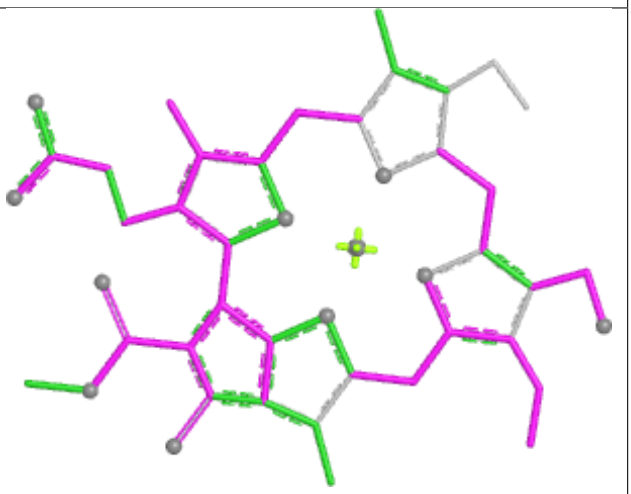

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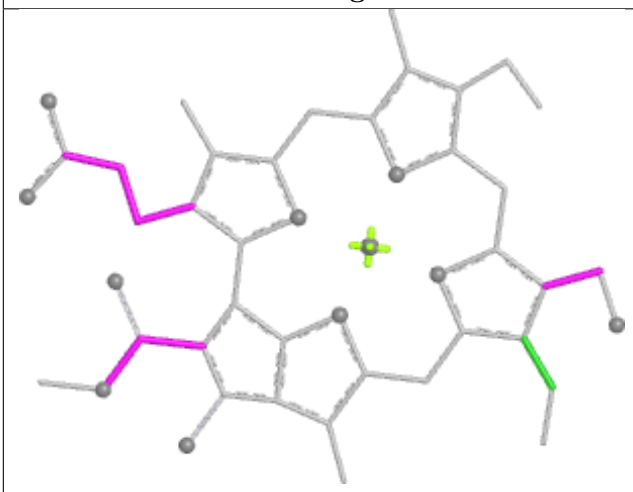

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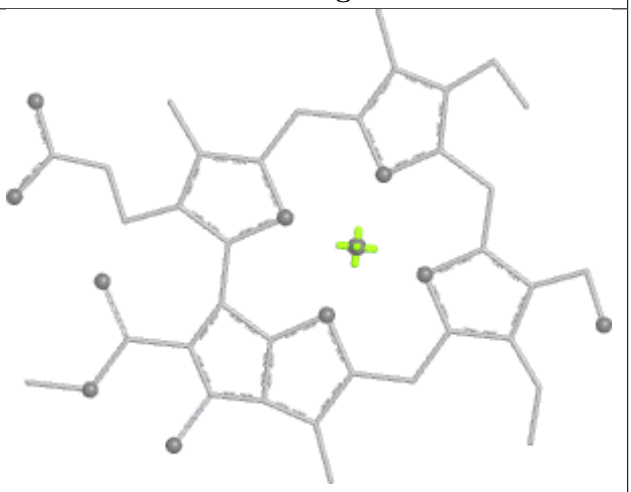
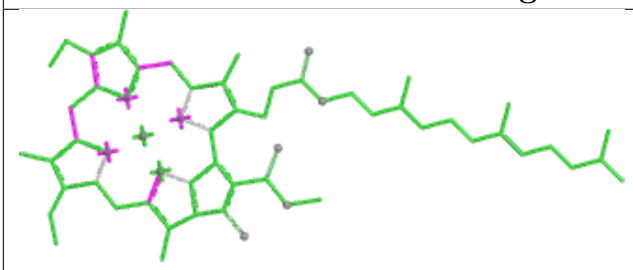


Rings

Ligand CLA 12 602



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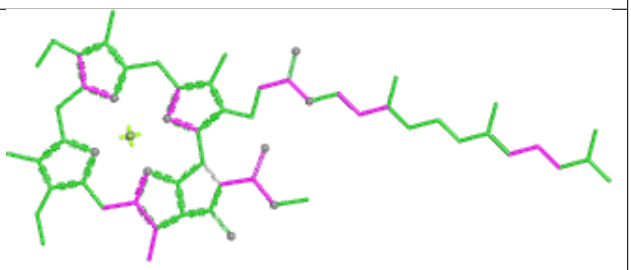

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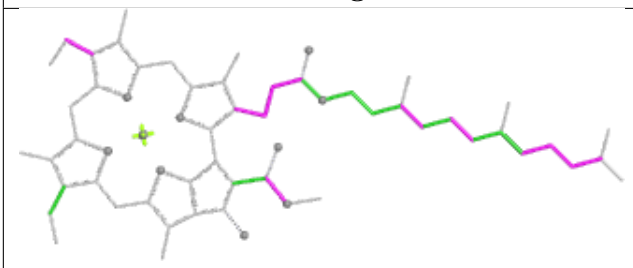

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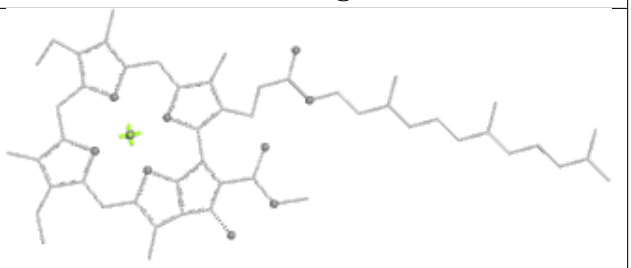

Rings

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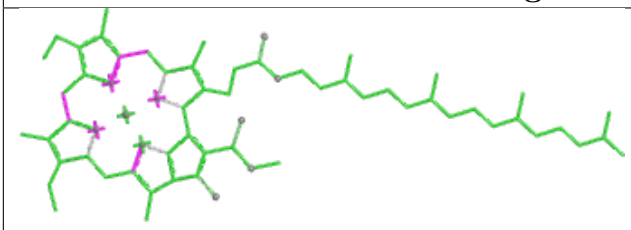

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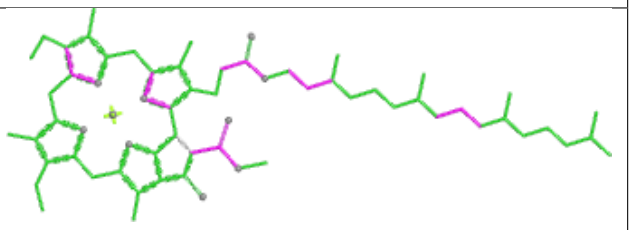
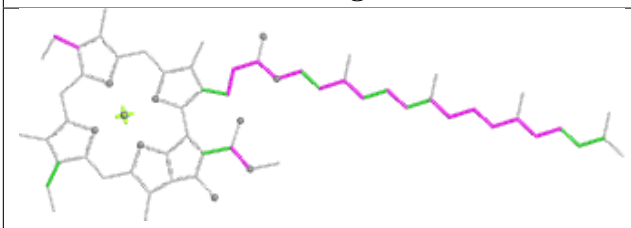
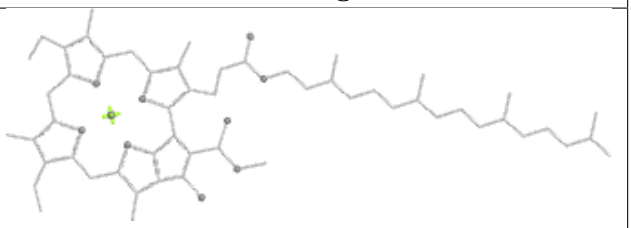


Bond angles

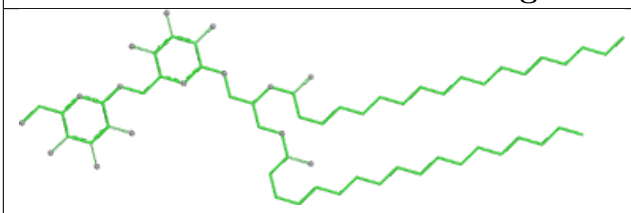


Torsions

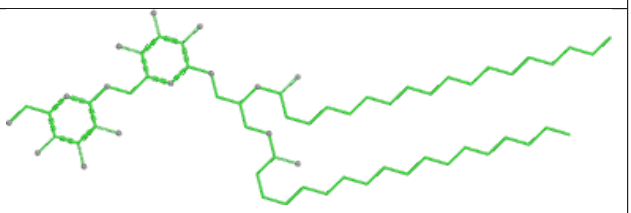


Rings

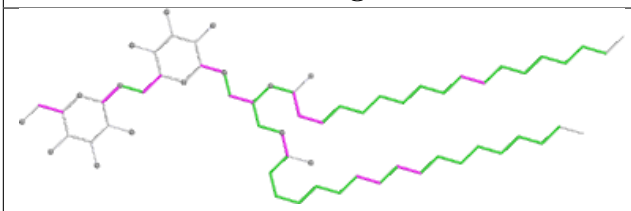
Ligand DGD C 517



Bond lengths



Bond angles



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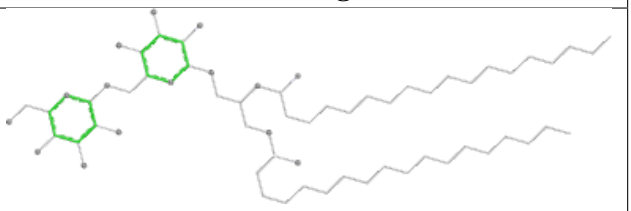
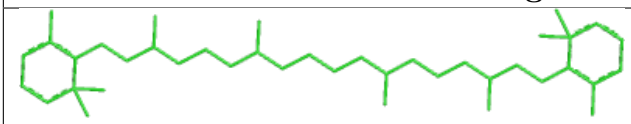


Rings

Ligand BCR h 102



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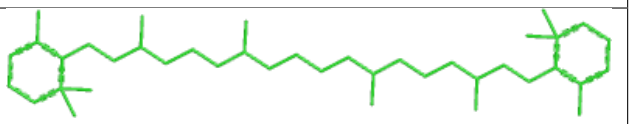

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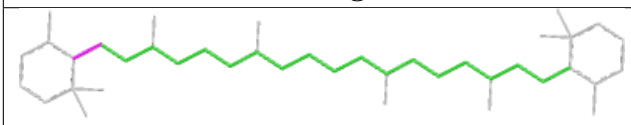

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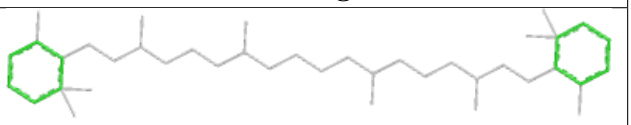
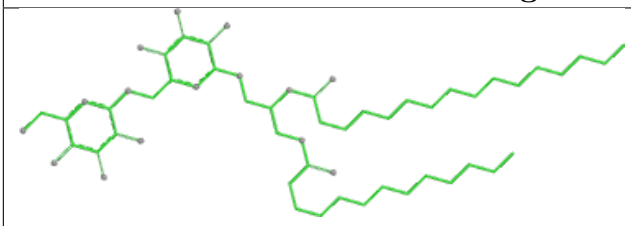
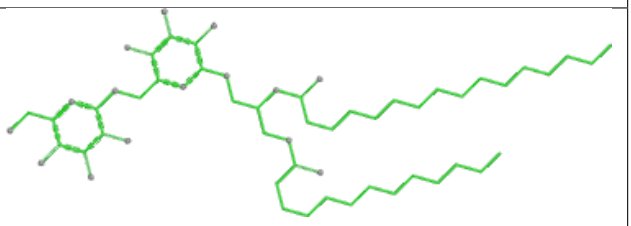
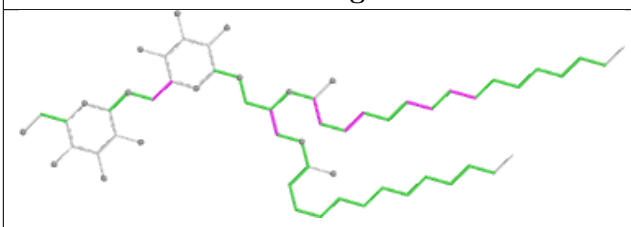
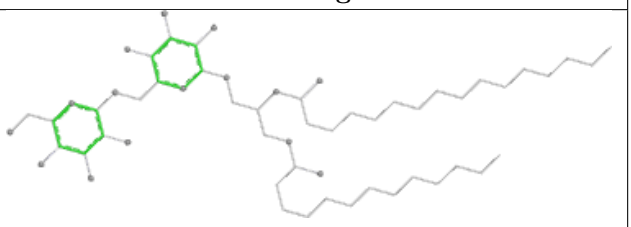


Rings

Ligand DGD C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

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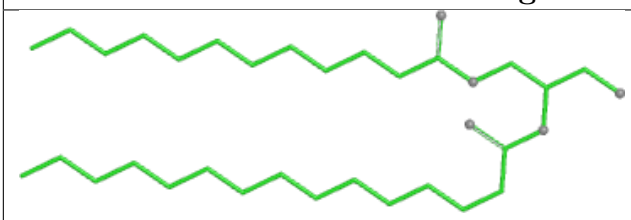
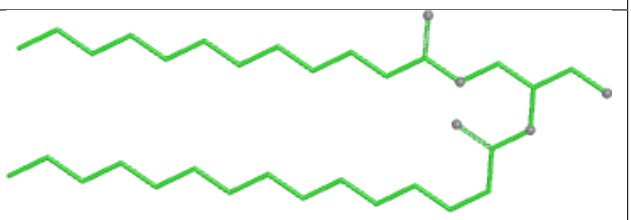
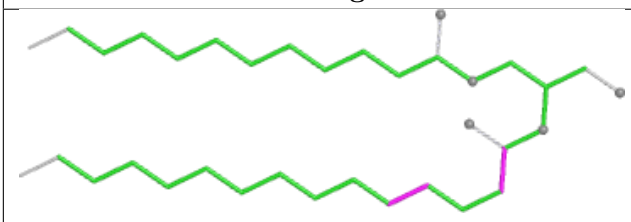
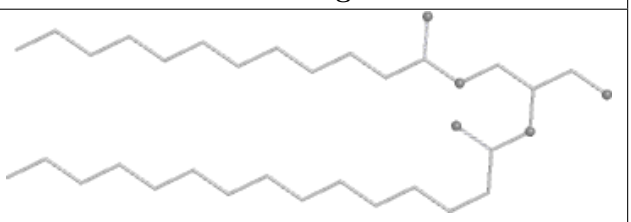
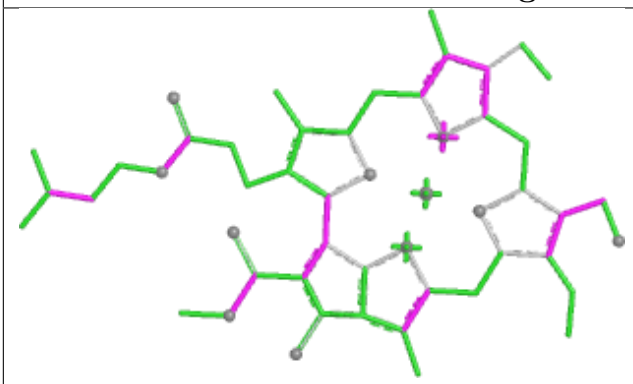
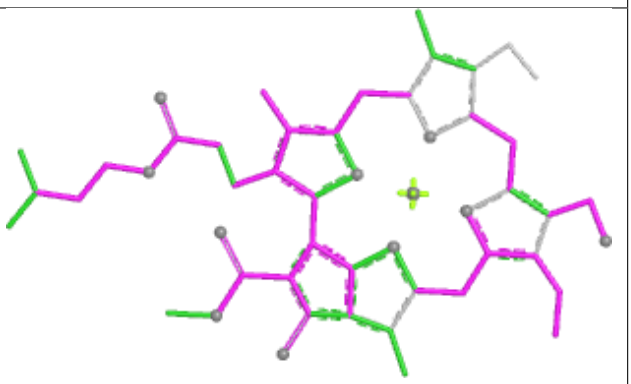
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 14 608



Bond lengths



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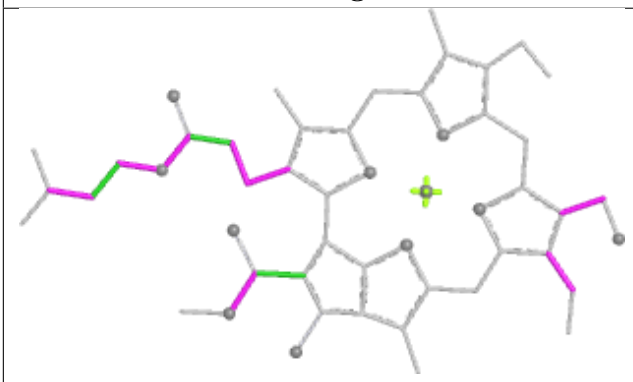

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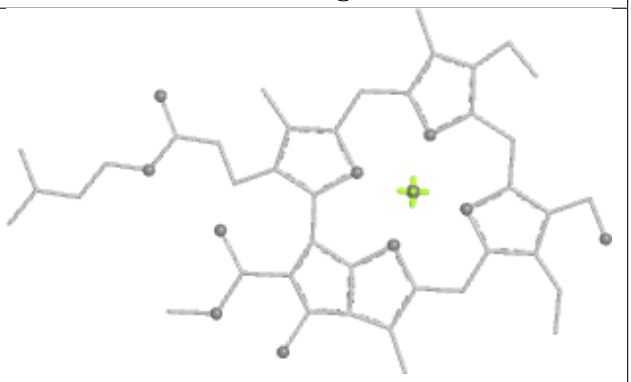
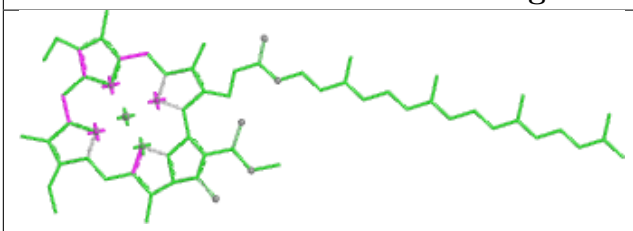


Rings

Ligand CLA g 602



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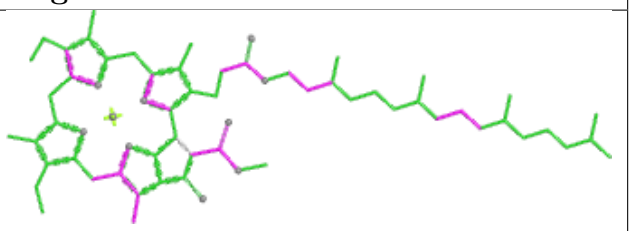

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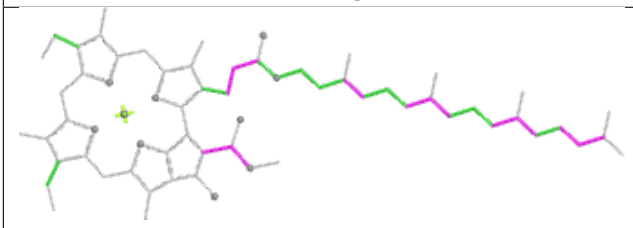

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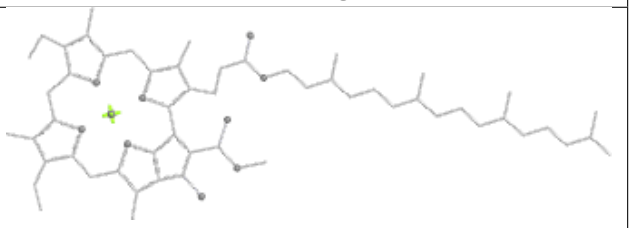
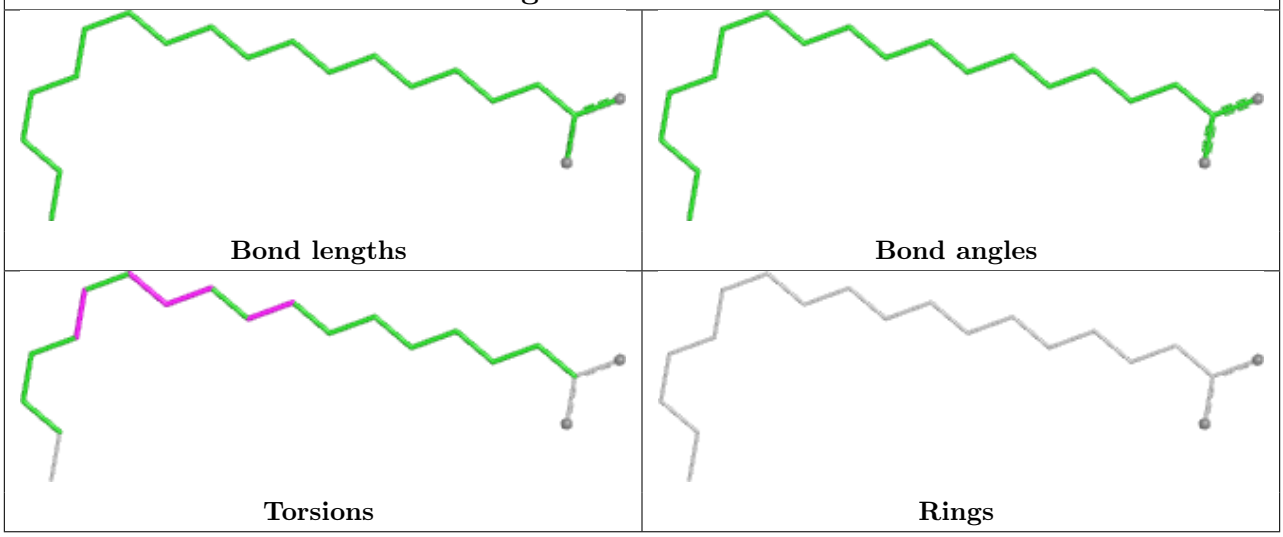
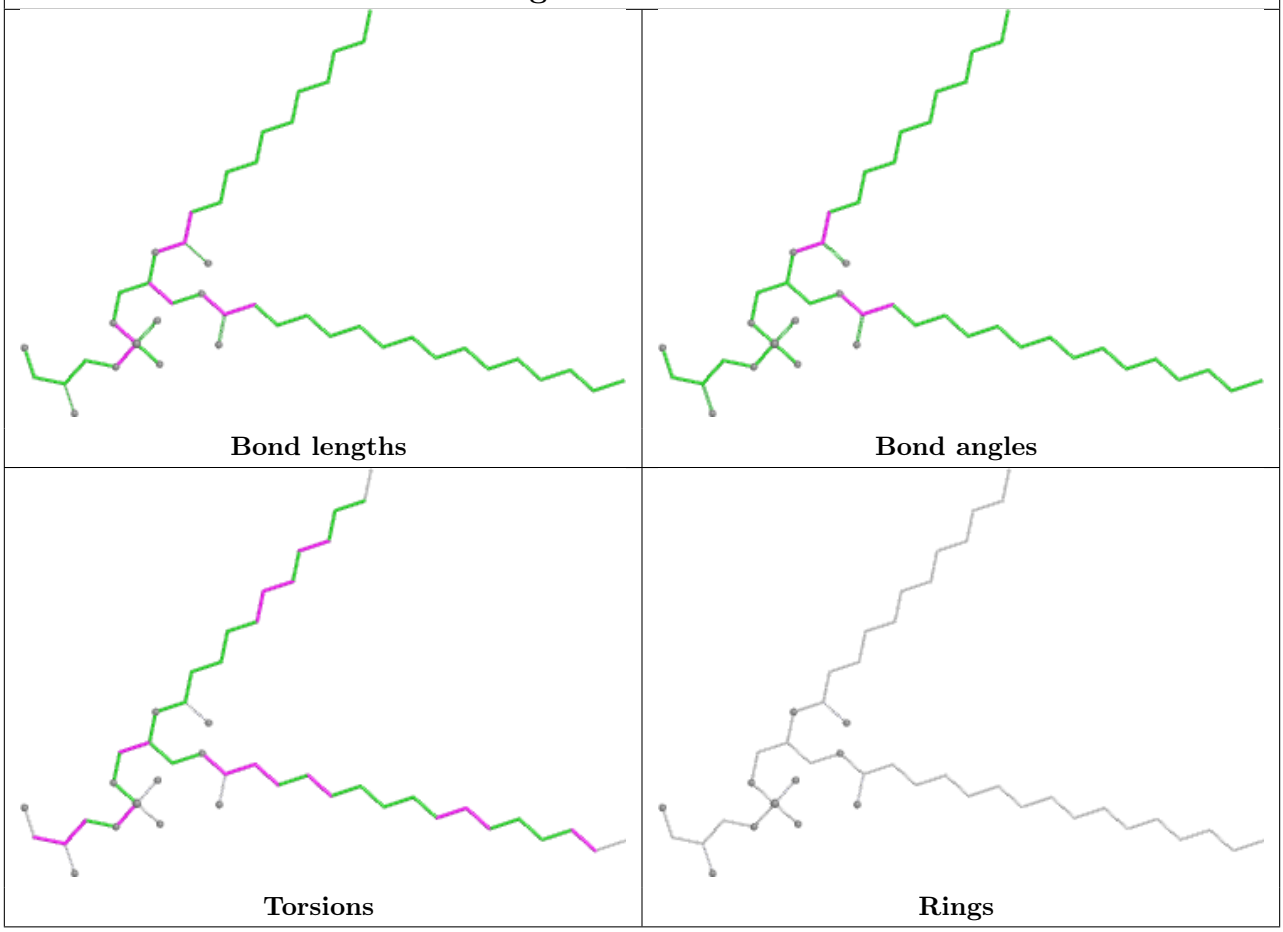


Rings

Ligand LNL W 502



Ligand LHG s 617



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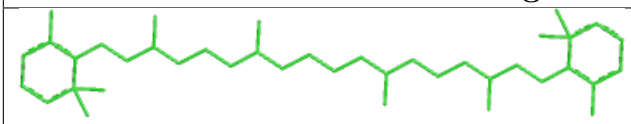
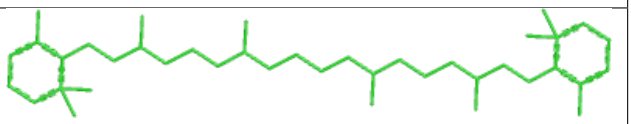


Bond lengths



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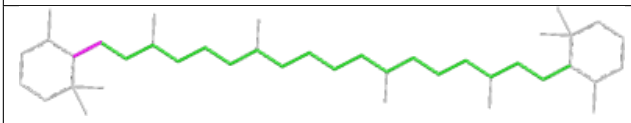

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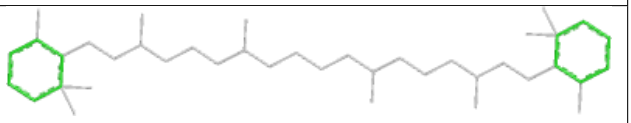
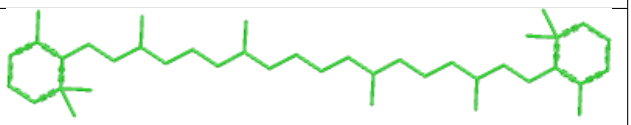


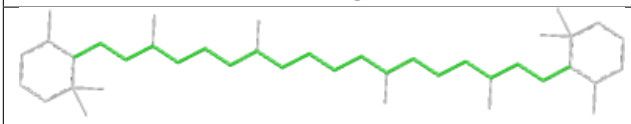
Rings

Ligand BCR C 526

Bond lengths



Bond angles



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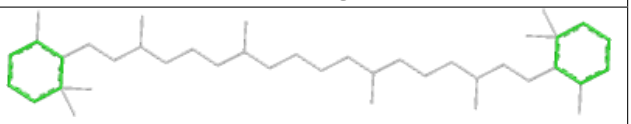
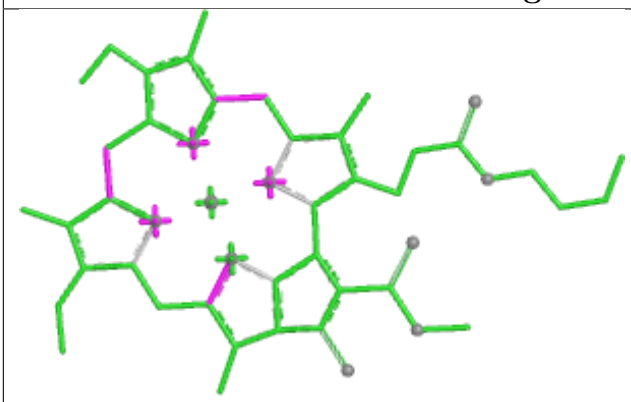


Rings

Ligand CLA Y 614



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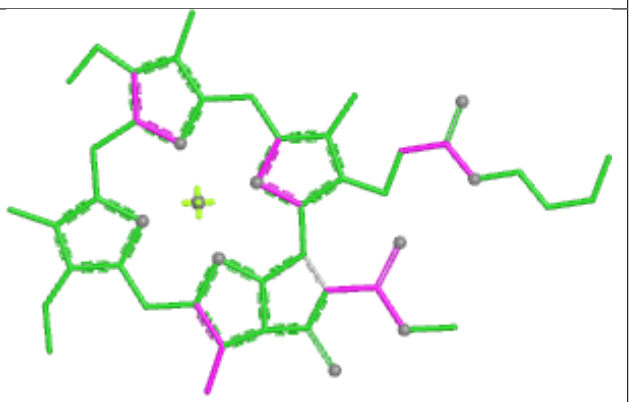

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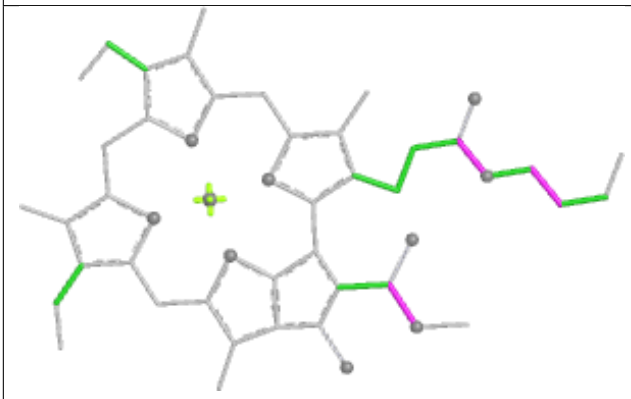

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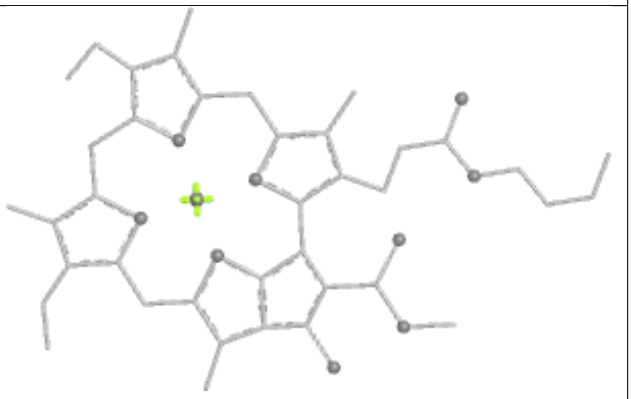
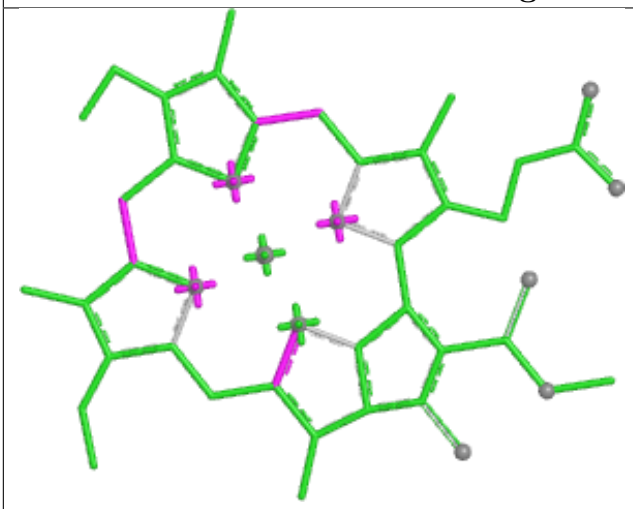


Rings

Ligand CLA 15 610



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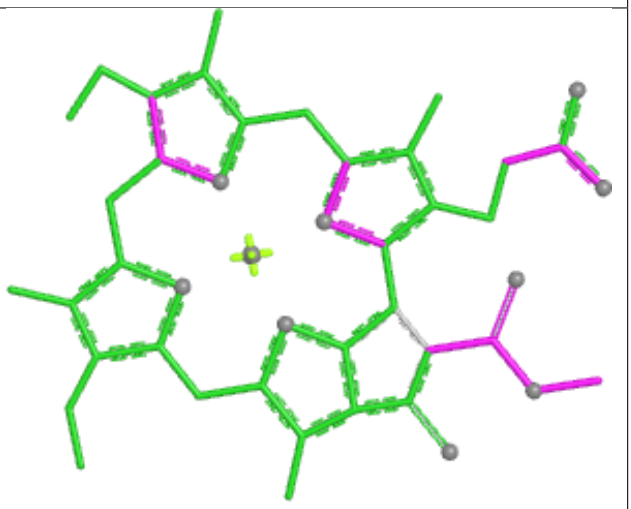

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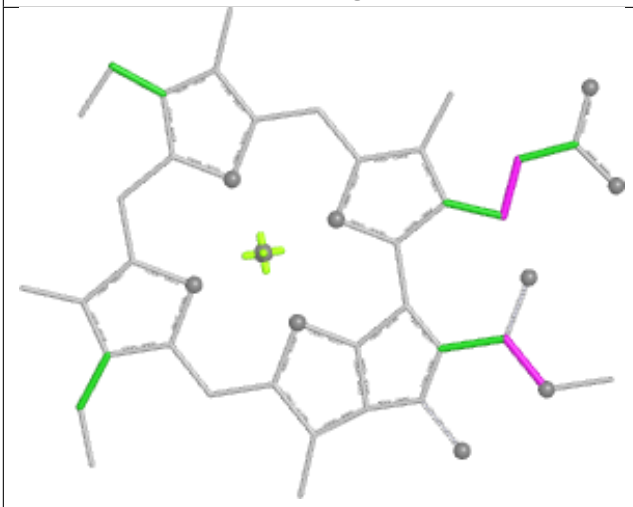
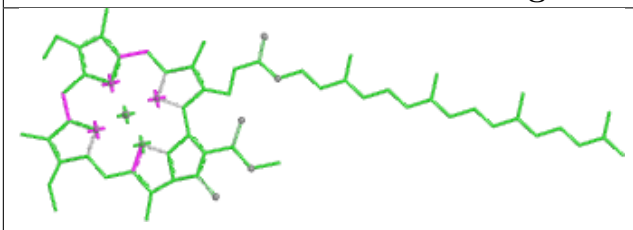


Torsions

Rings

Ligand CLA 6 611



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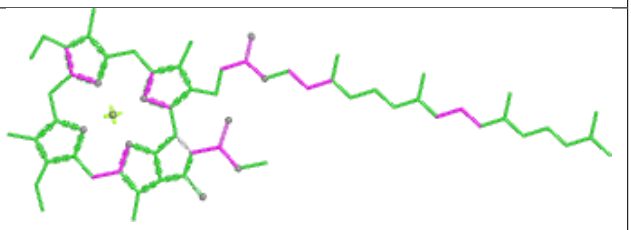
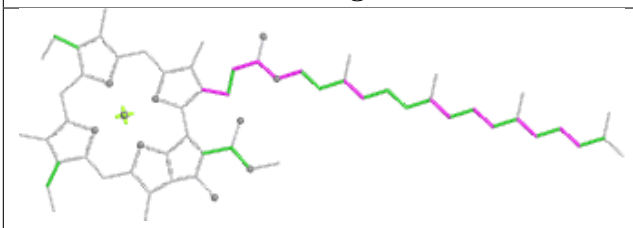


Bond angles



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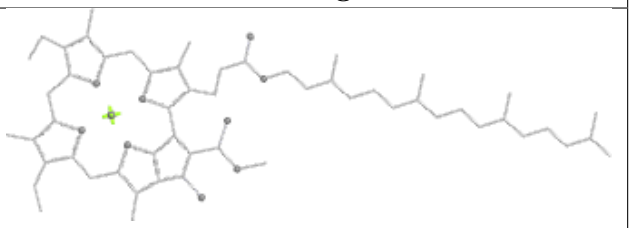
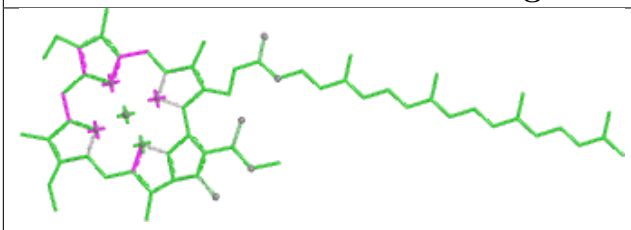
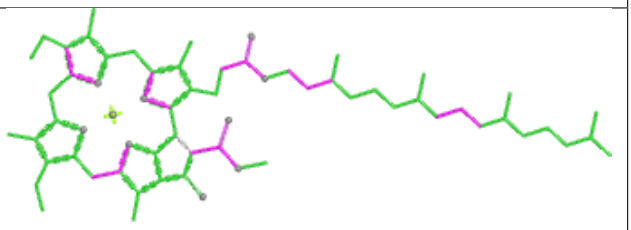
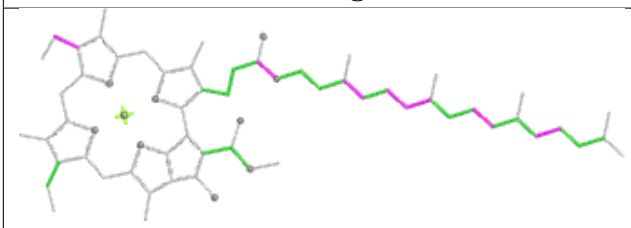
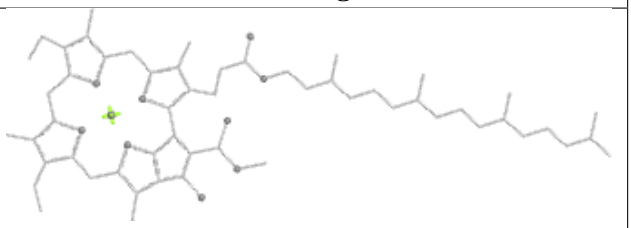


Rings

Ligand CLA Y 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

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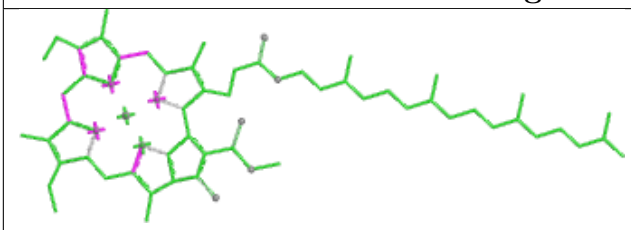
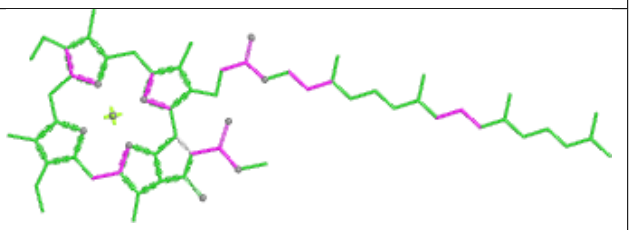
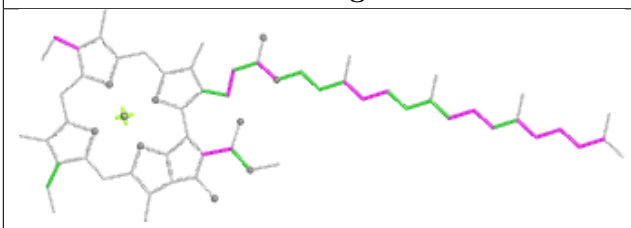
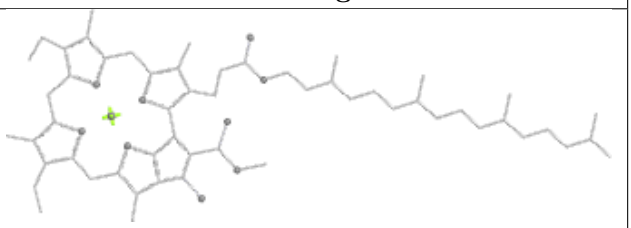
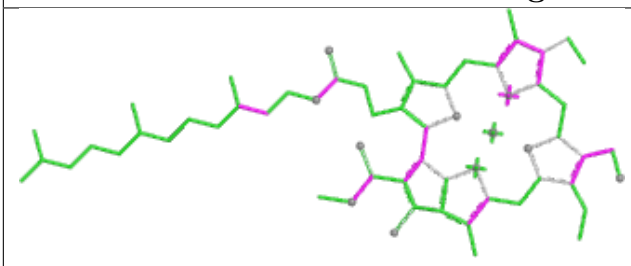
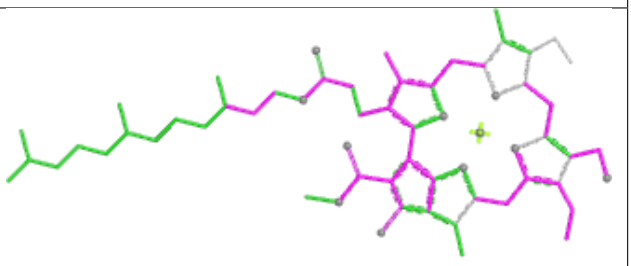
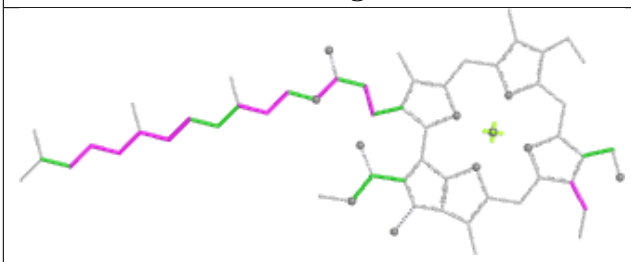
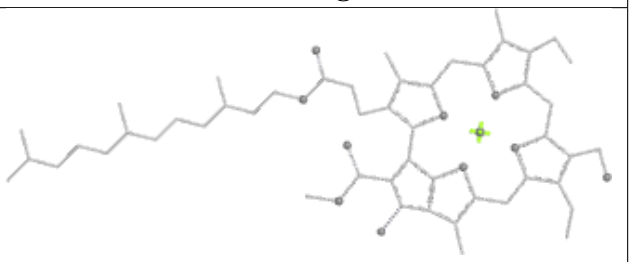
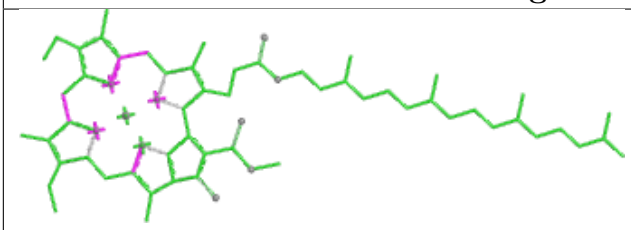
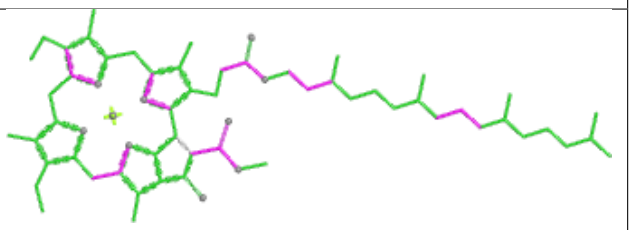
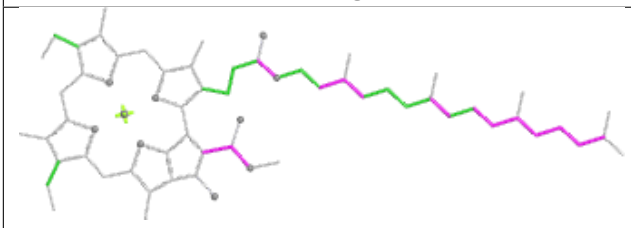
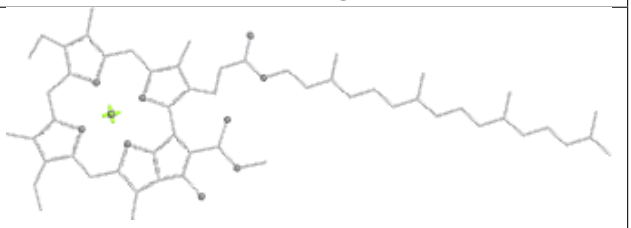
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

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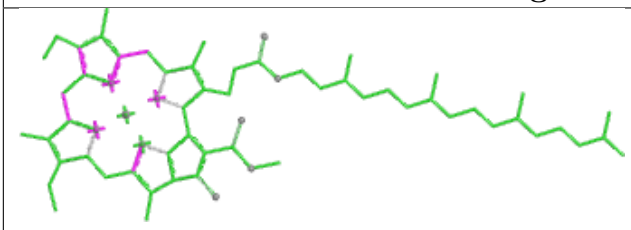
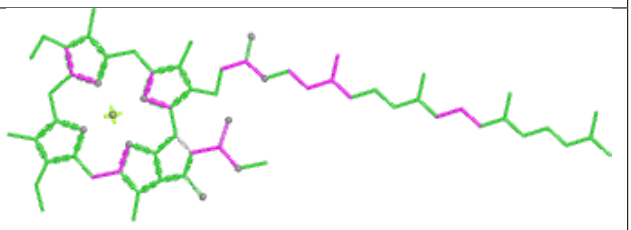
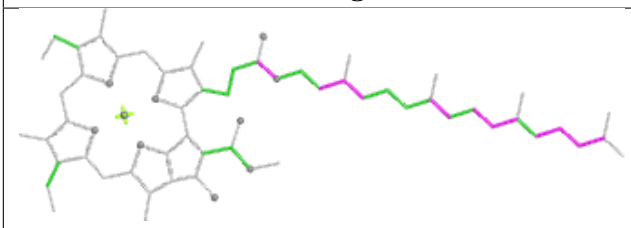
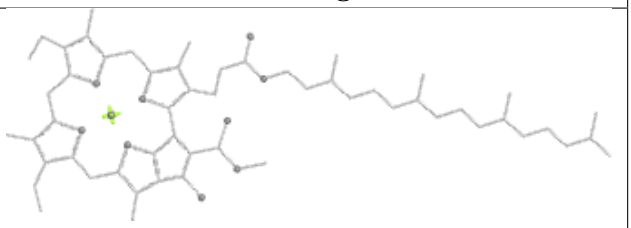
 Bond lengths	 Bond angles
 Torsions	 Rings

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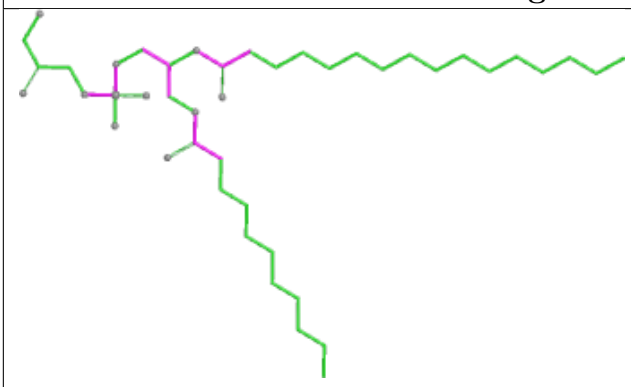
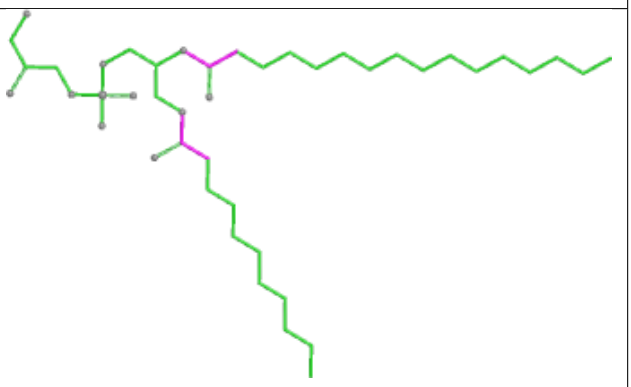
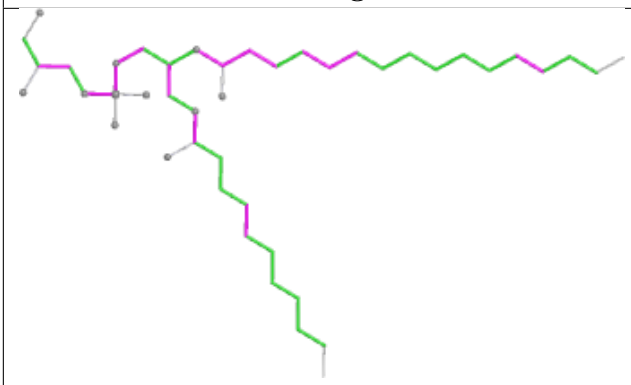
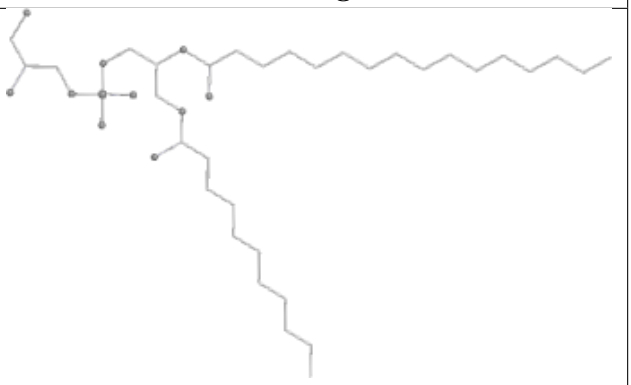
 Bond lengths	 Bond angles
 Torsions	 Rings

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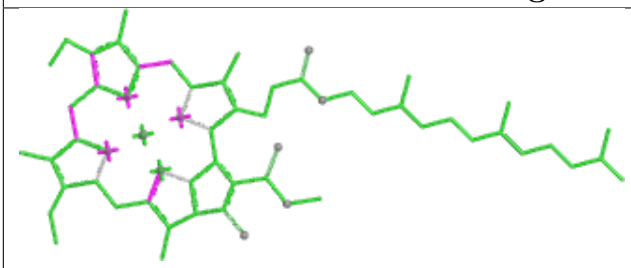
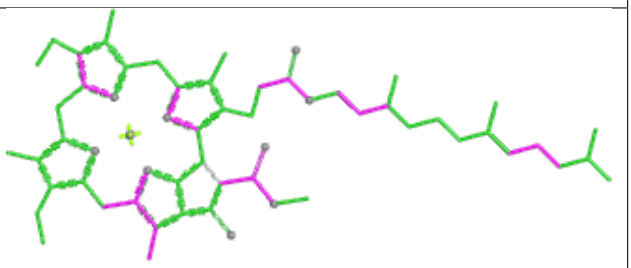
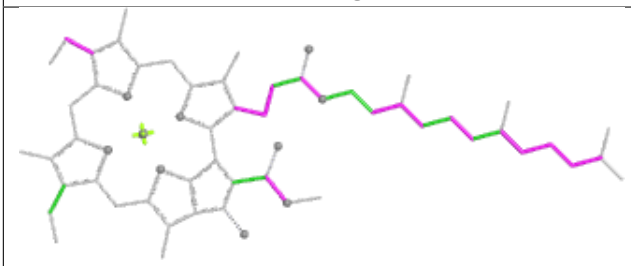
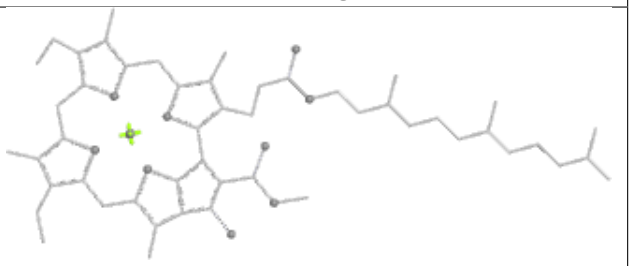
 Bond lengths	 Bond angles
 Torsions	 Rings

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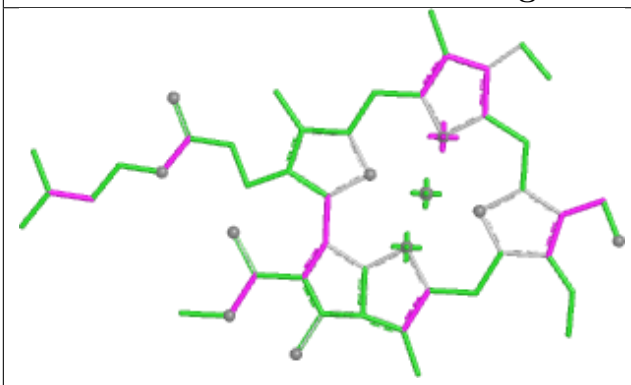
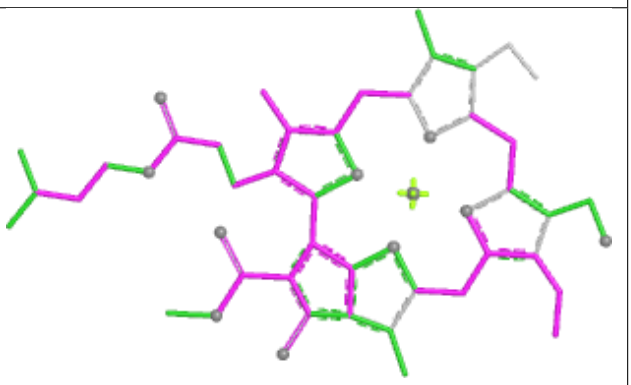
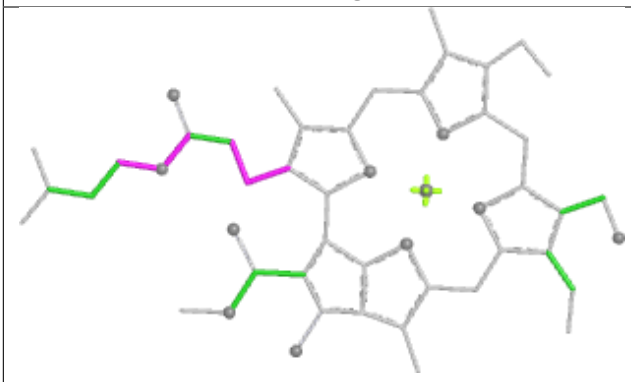
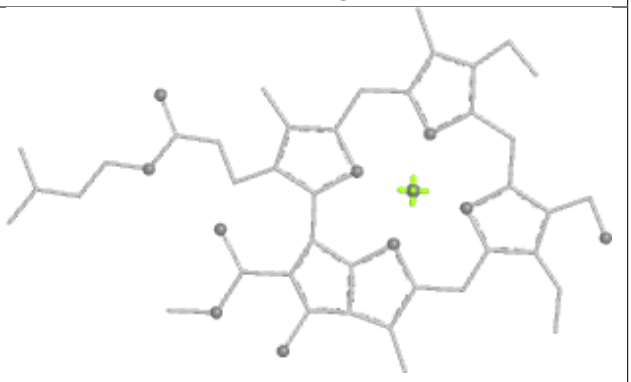
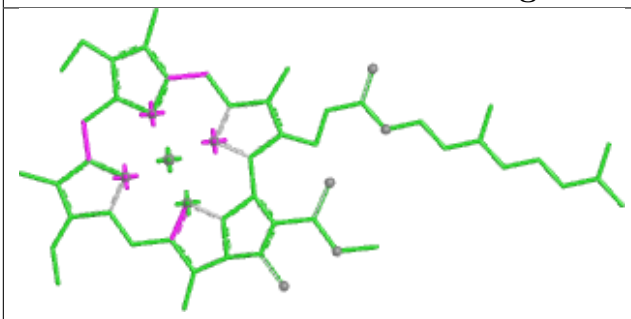
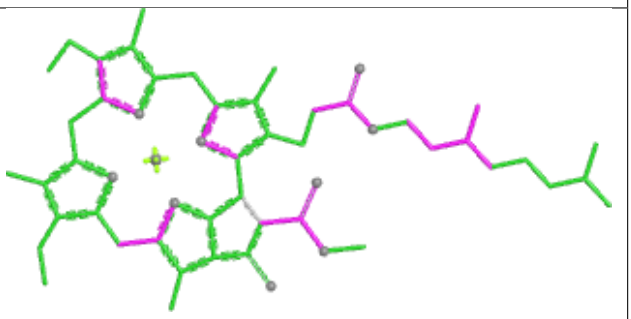
 Bond lengths	 Bond angles
 Torsions	 Rings

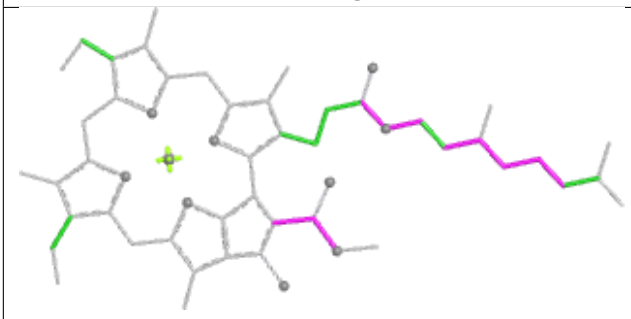
Ligand CLA 15 603



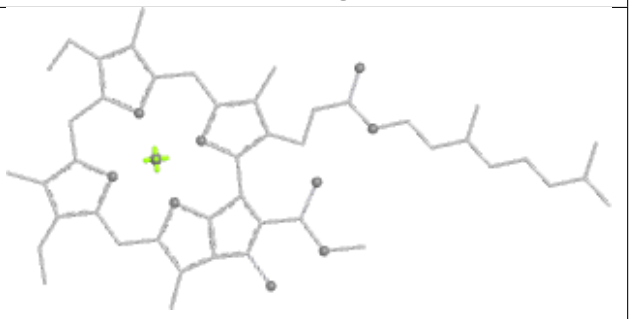
Bond lengths



Bond angles

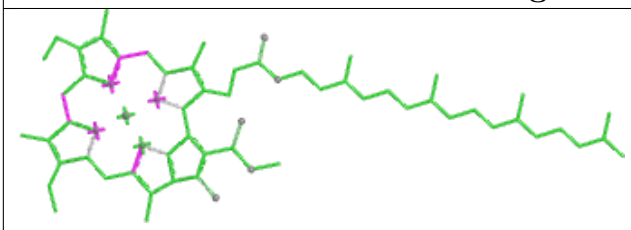


Torsions

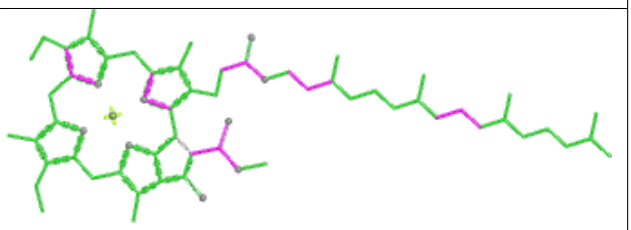


Rings

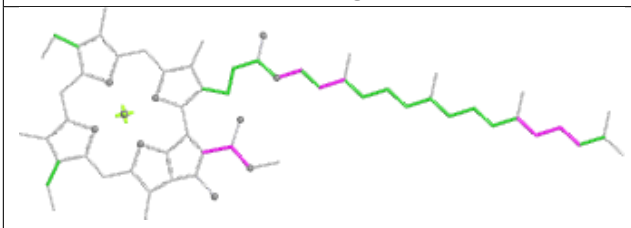
Ligand CLA c 503



Bond lengths



Bond angles



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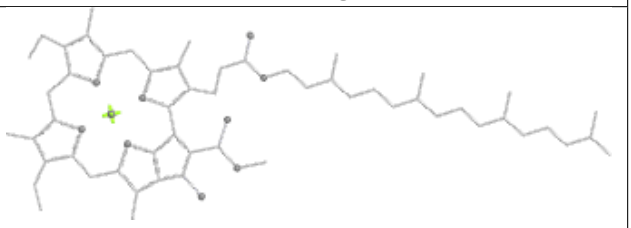
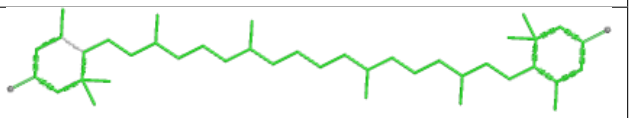


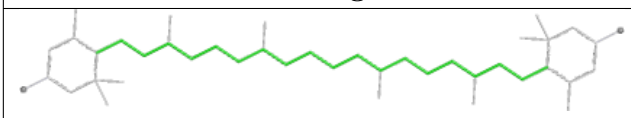
Rings

Ligand LUT 6 618

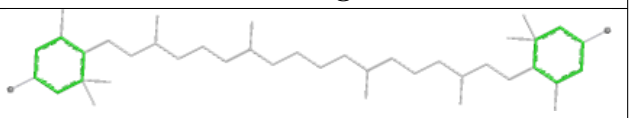
Bond lengths



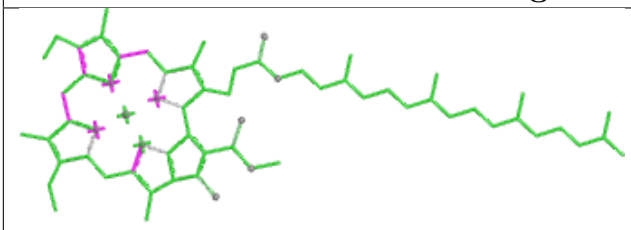
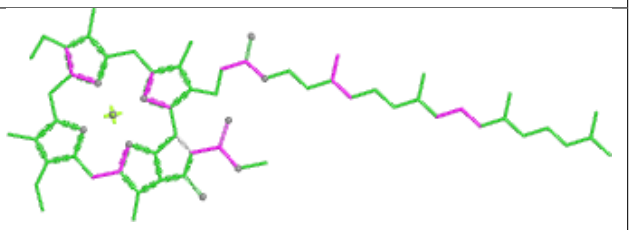
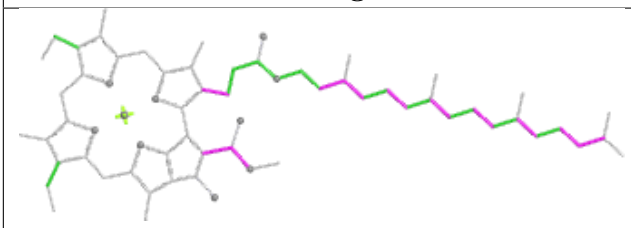
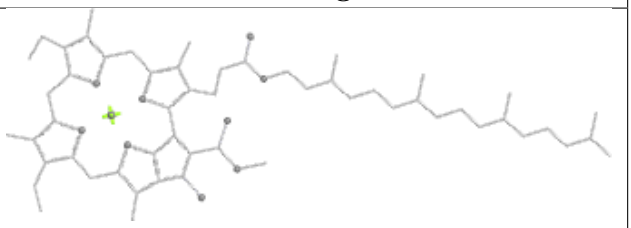
Bond angles

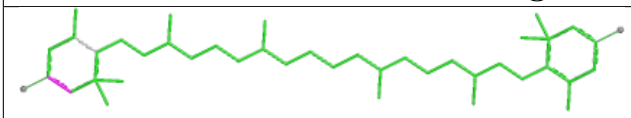
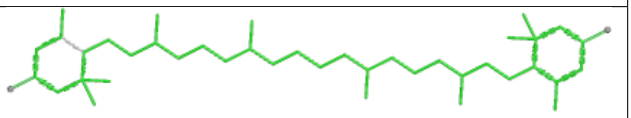
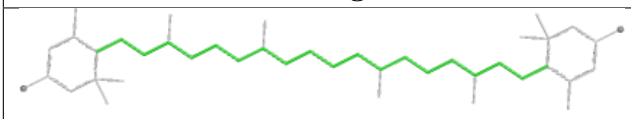
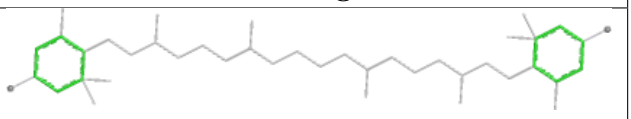


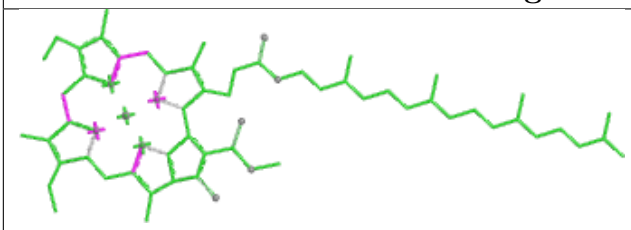
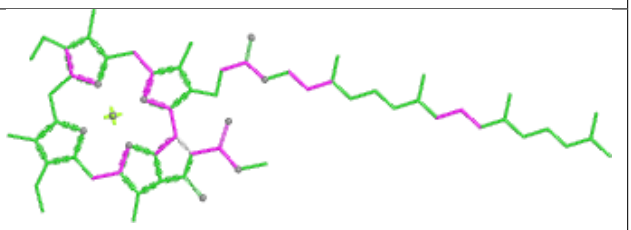
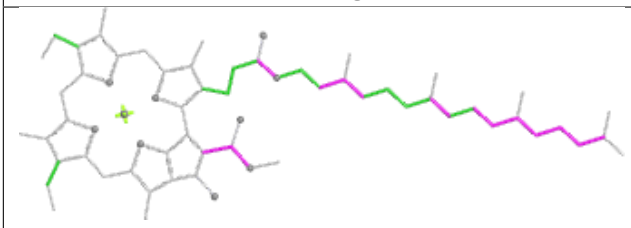
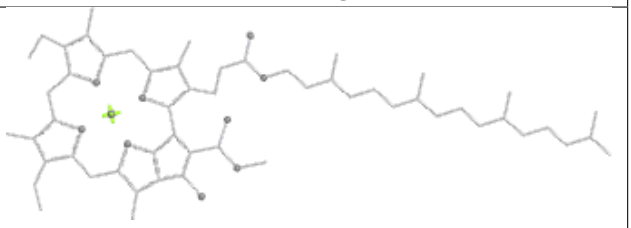
Torsions



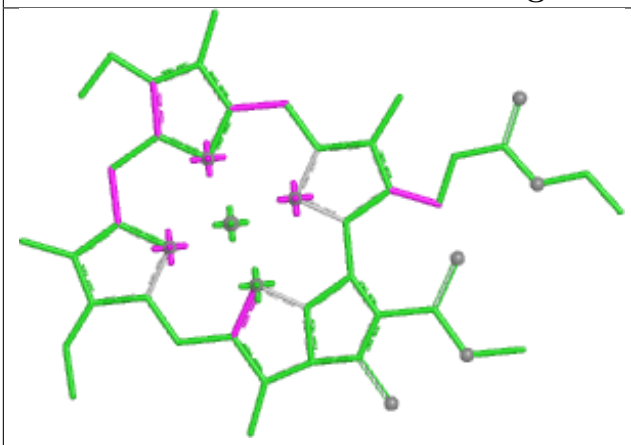
Rings

Ligand CLA r 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

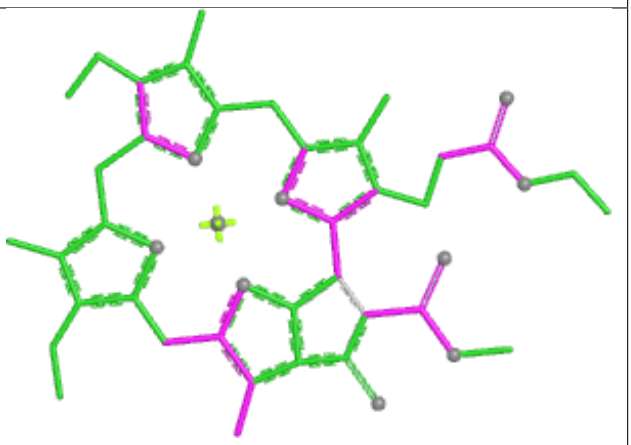
Ligand LUT 1 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

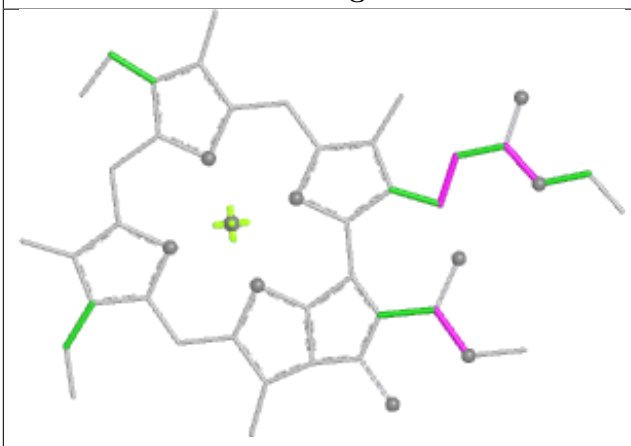
Ligand CLA n 615



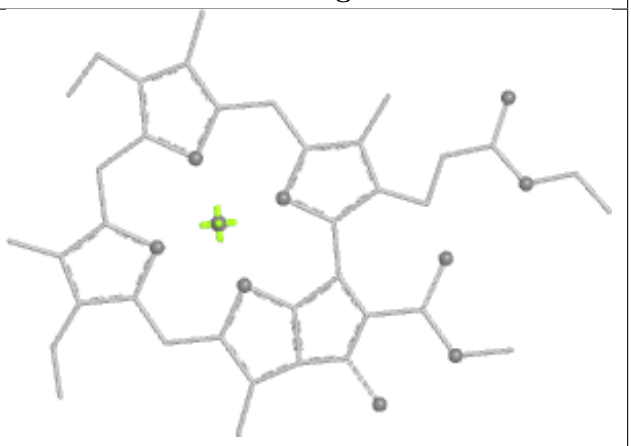
Bond lengths



Bond angles

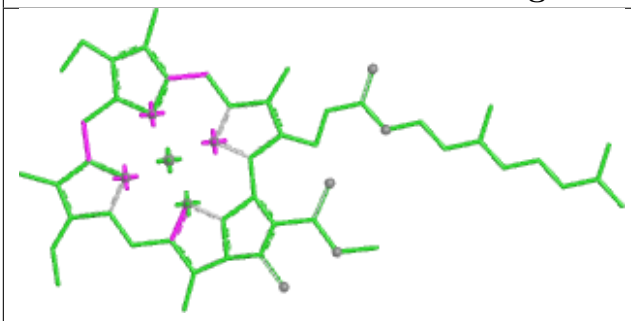


Torsions



Rings

Ligand CLA 6 612



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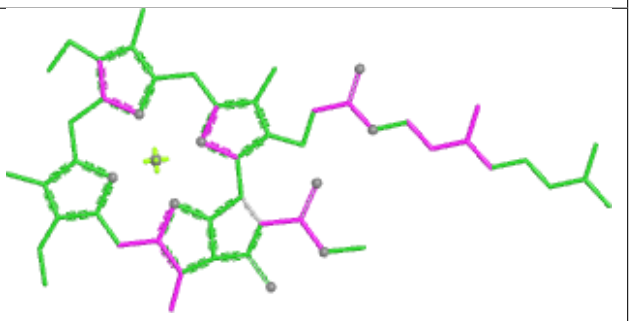
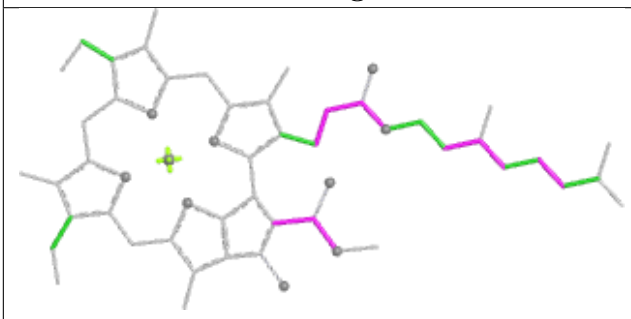
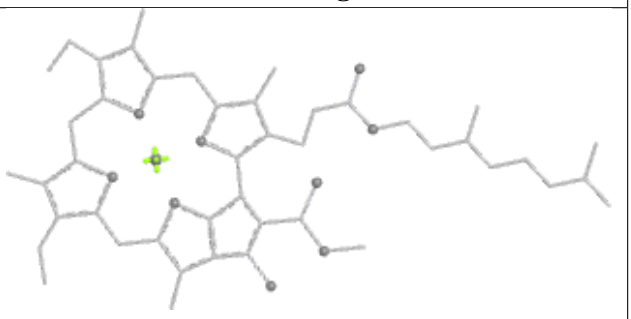


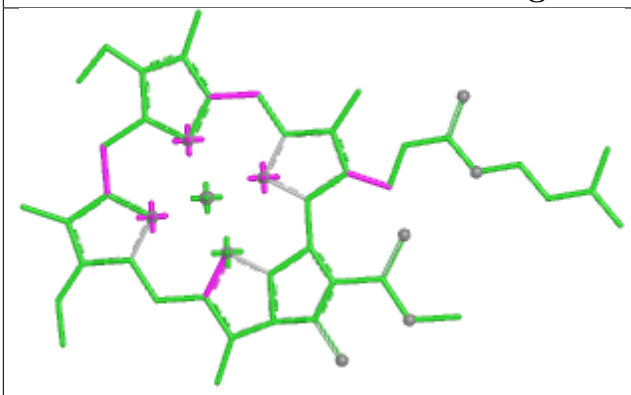
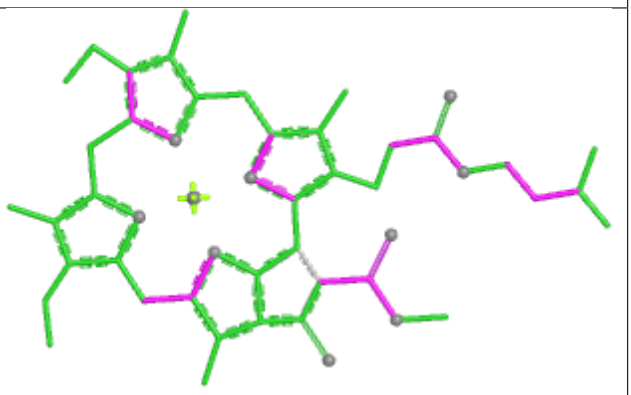
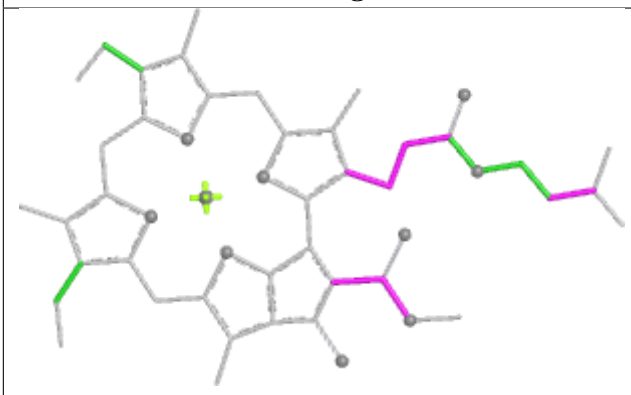
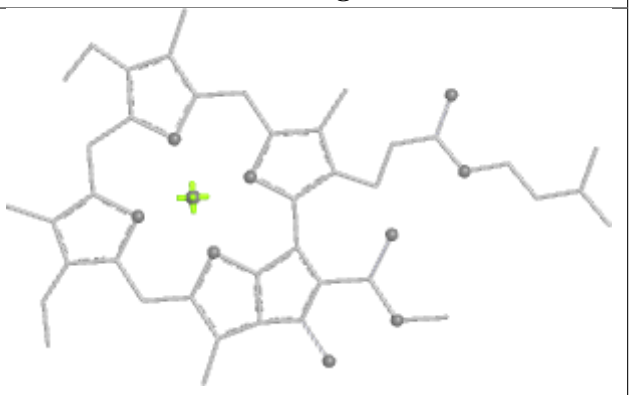
Bond angles

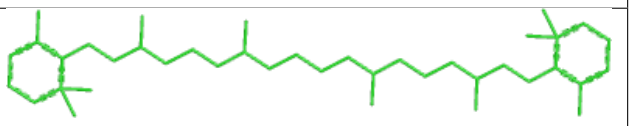
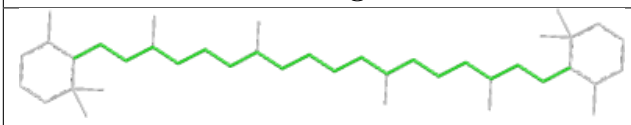
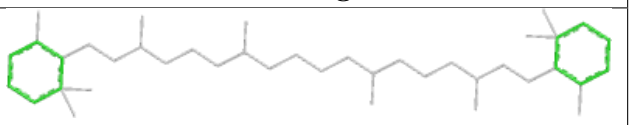


Torsions

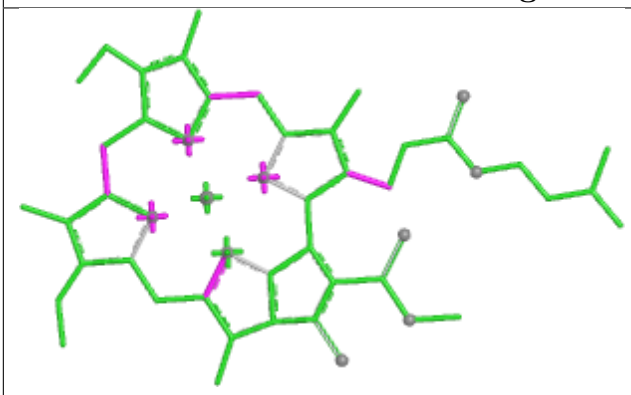


Rings

Ligand CLA 3 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 618	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 12 612



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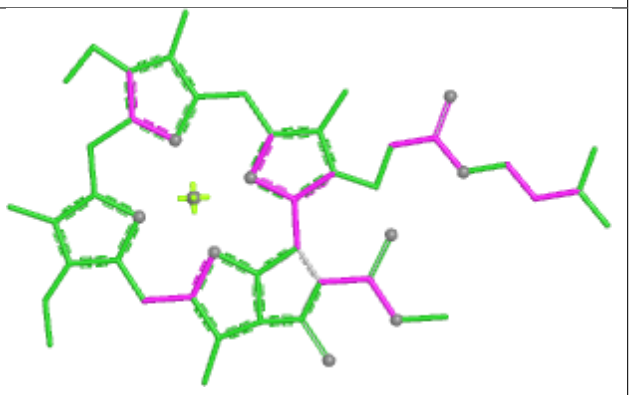

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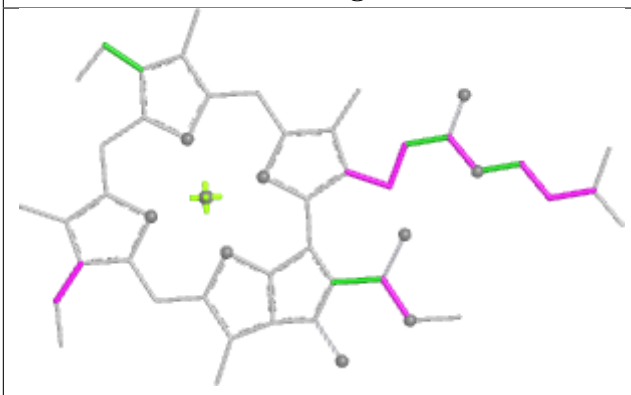

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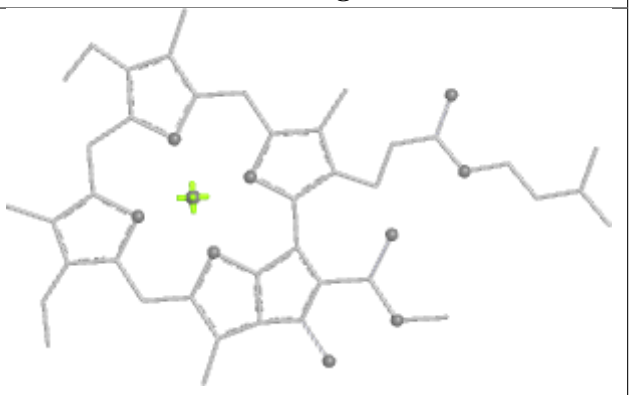
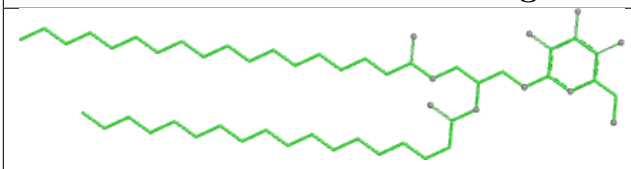


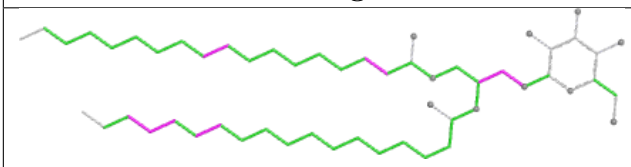
Rings

Ligand LMG C 522



Bond lengths

Bond angles



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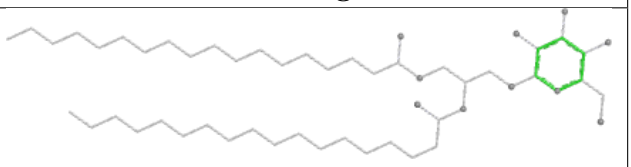
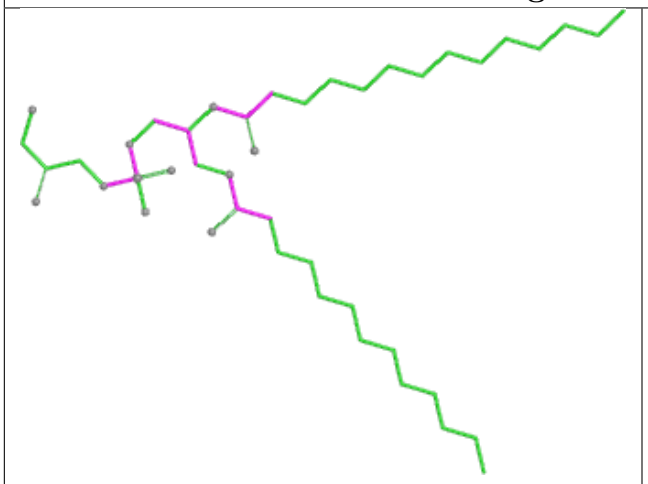


Rings

Ligand LHG 3 616



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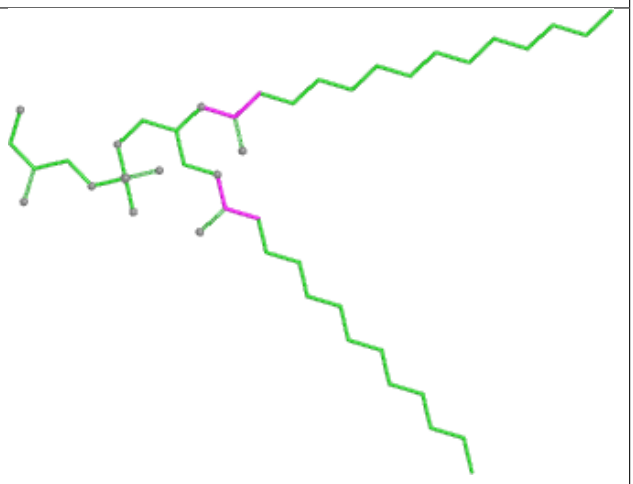
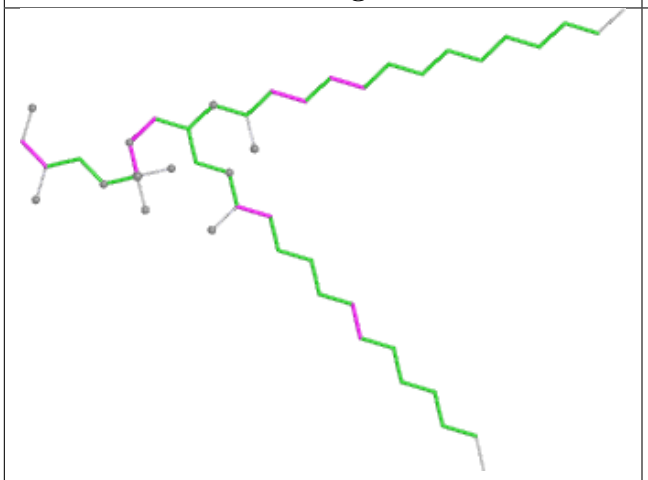


Bond angles



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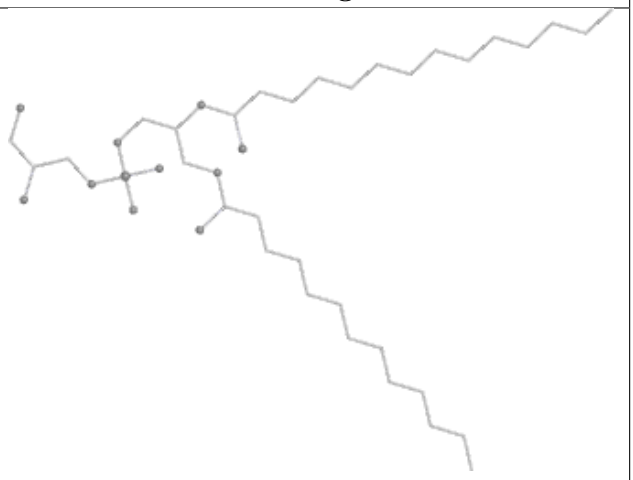
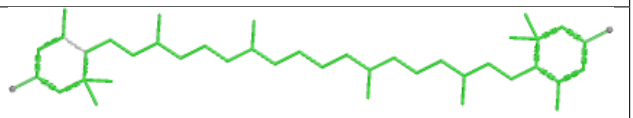


Rings

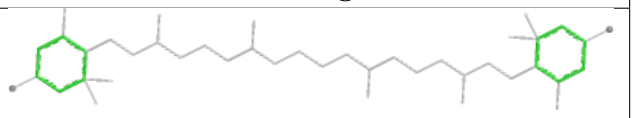
Ligand LUT Y 621

Bond lengths



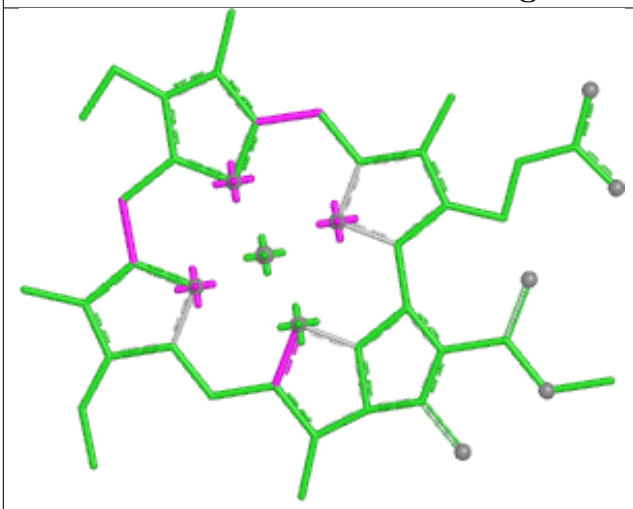
Bond angles

Torsions

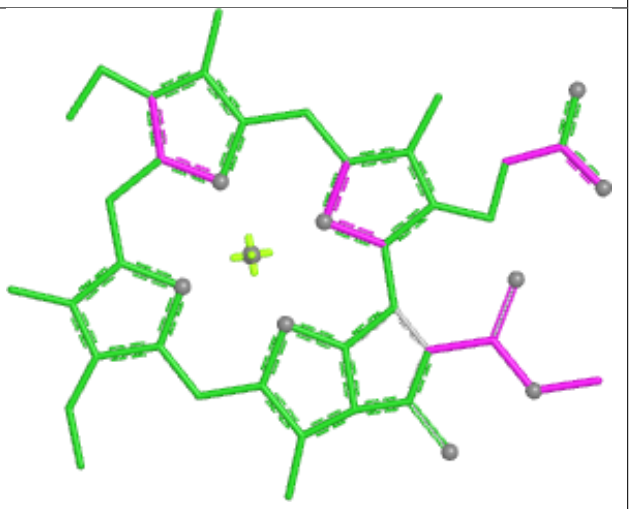


Rings

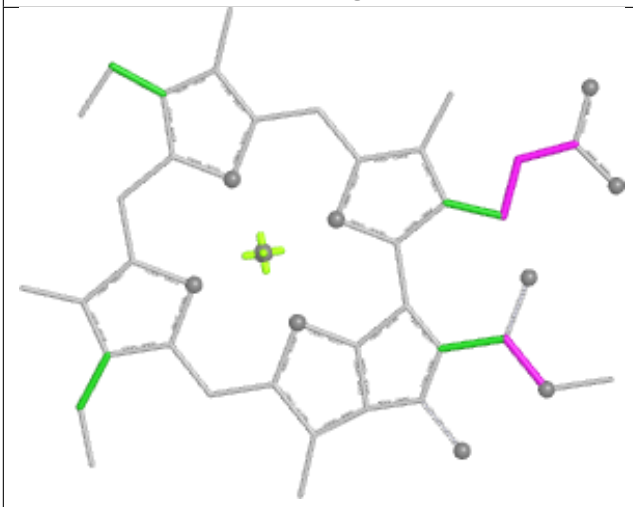
Ligand CLA 12 610



Bond lengths



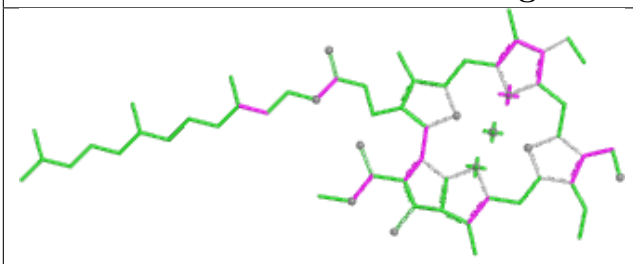
Bond angles



Torsions

Rings

Ligand CHL 13 607



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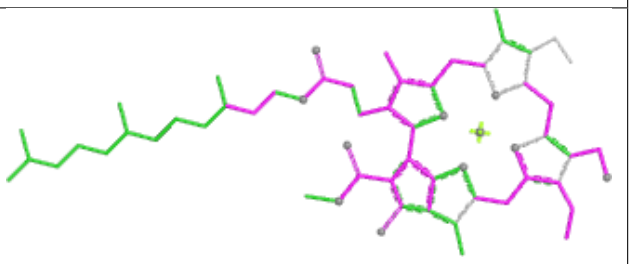
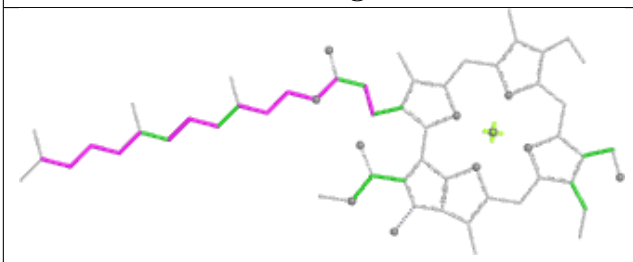


Bond angles



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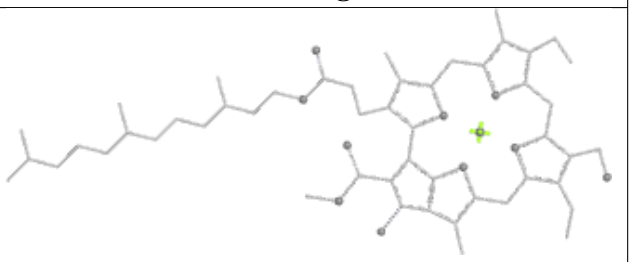
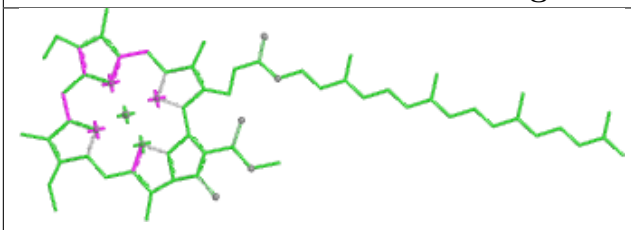
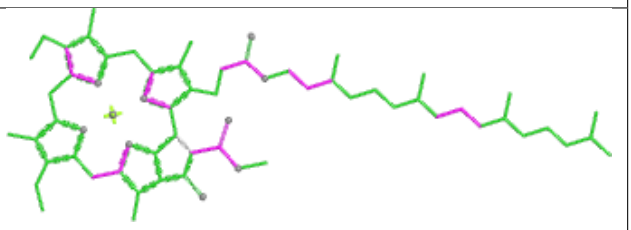
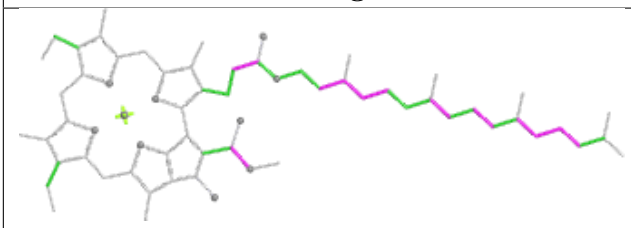
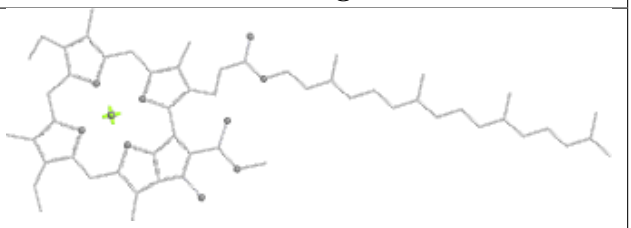


Rings

Ligand CLA r 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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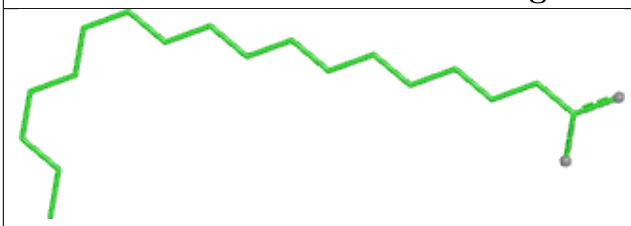
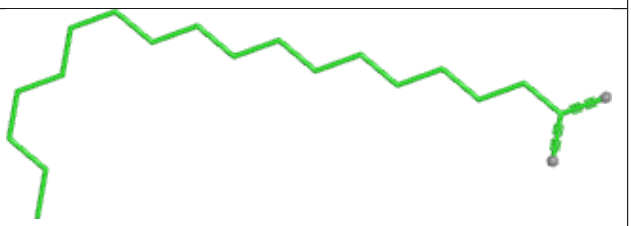
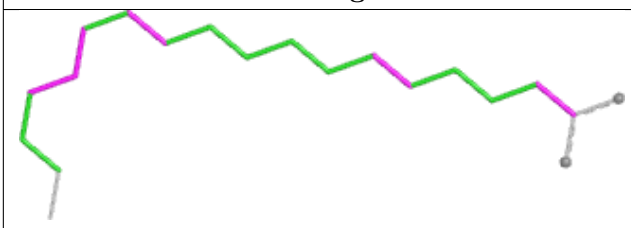
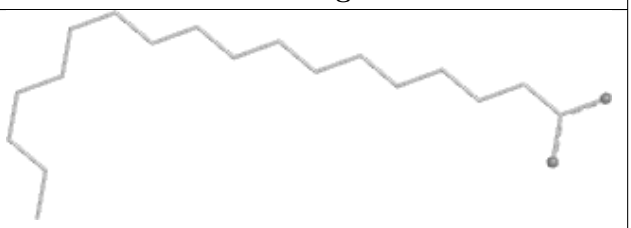
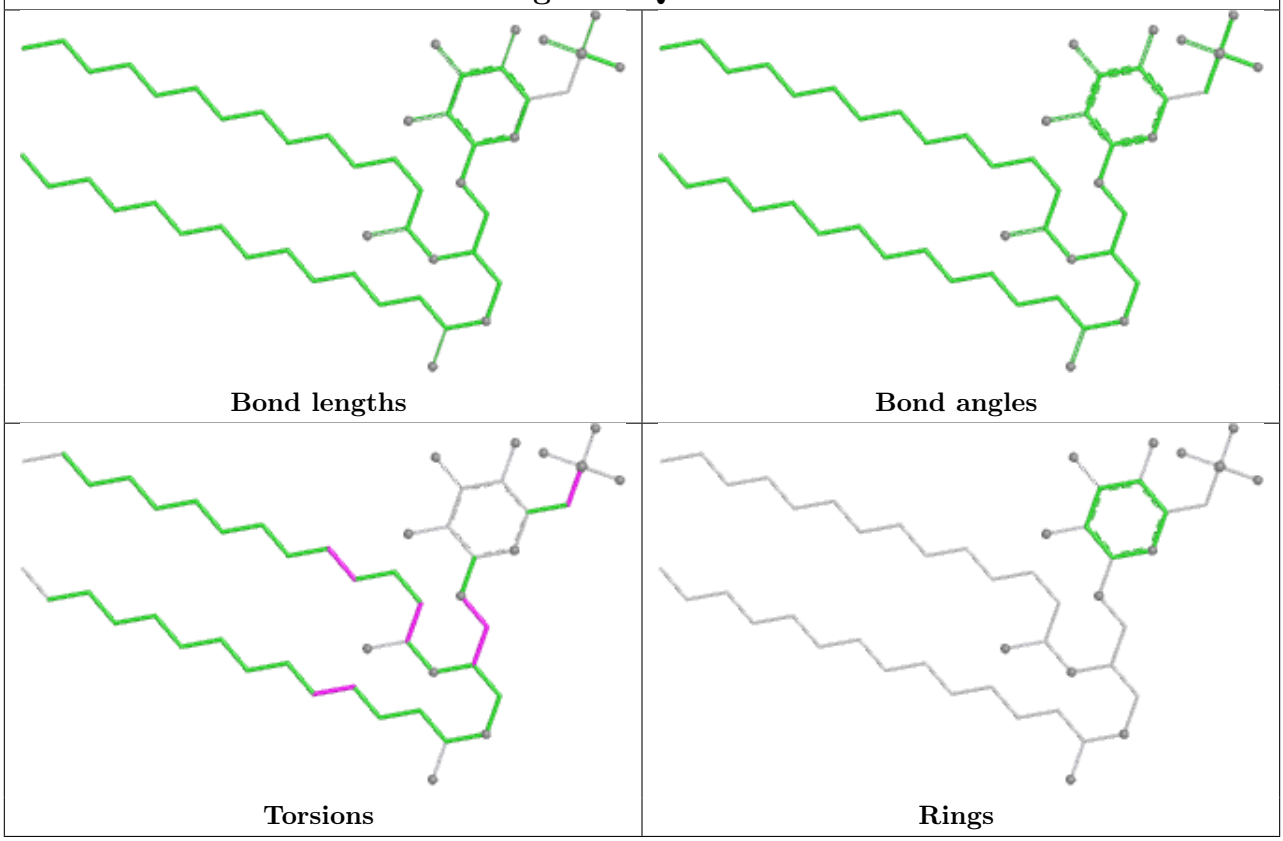
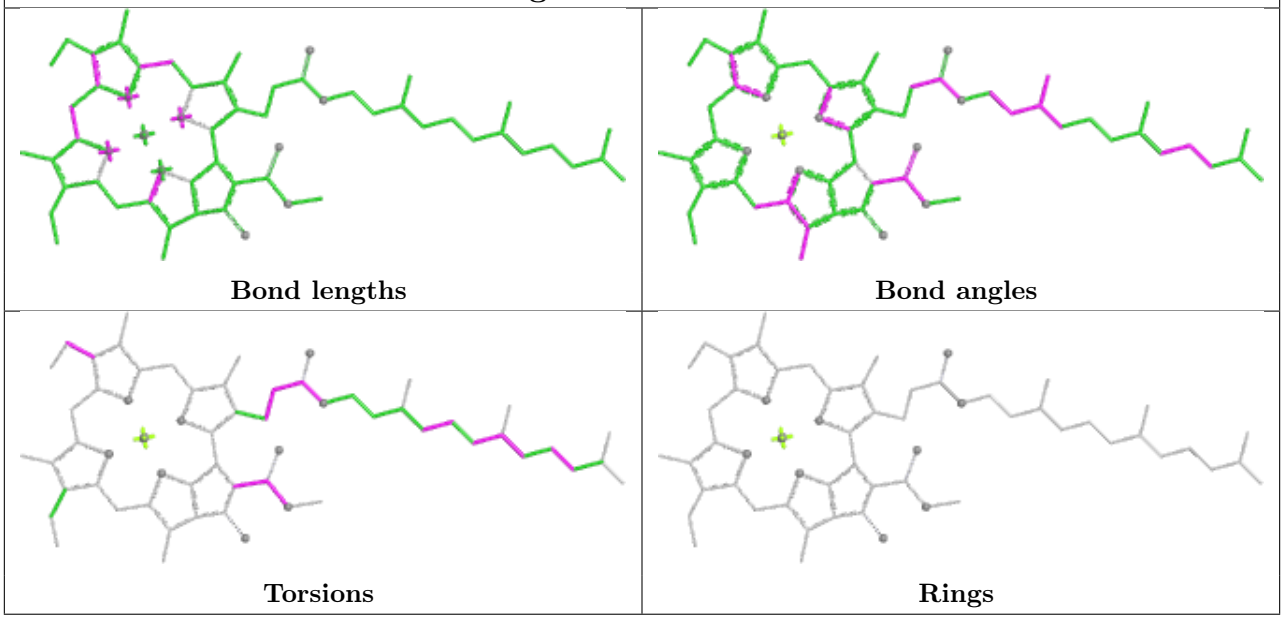
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD l 101



Ligand CLA 1 602



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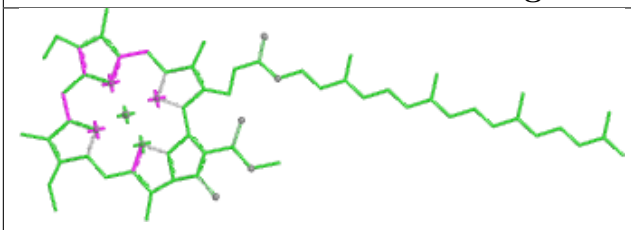
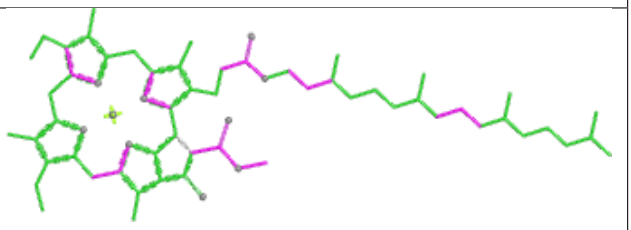
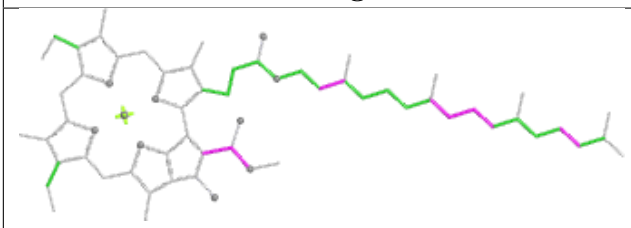
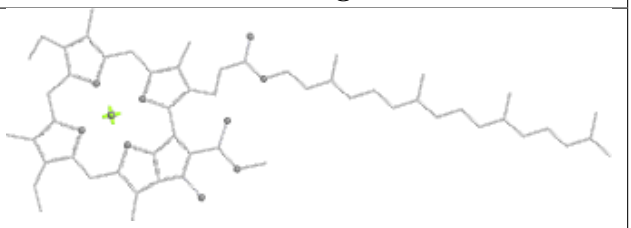
 Bond lengths	 Bond angles
 Torsions	 Rings

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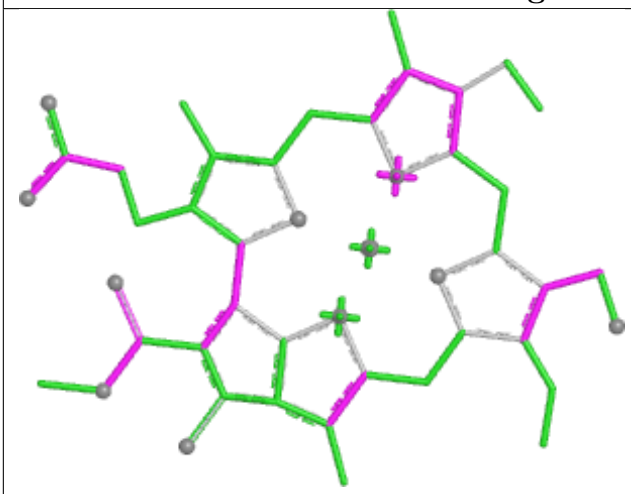
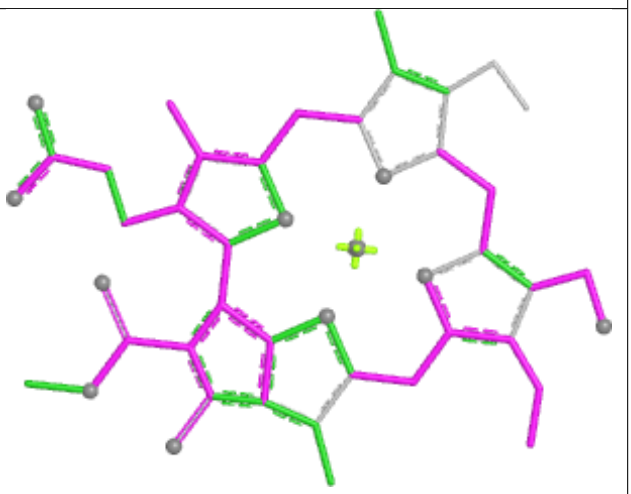
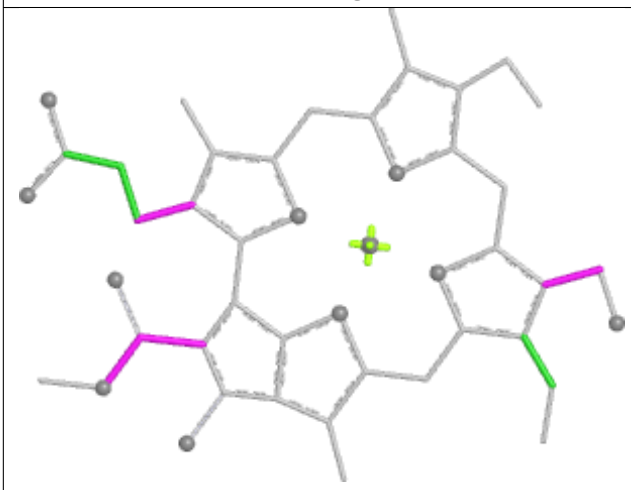
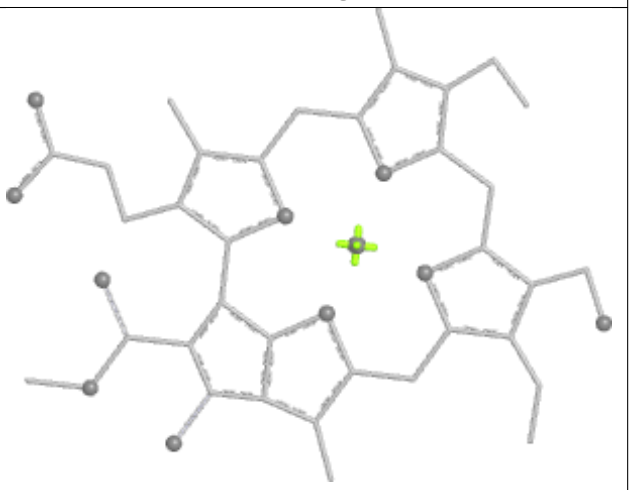
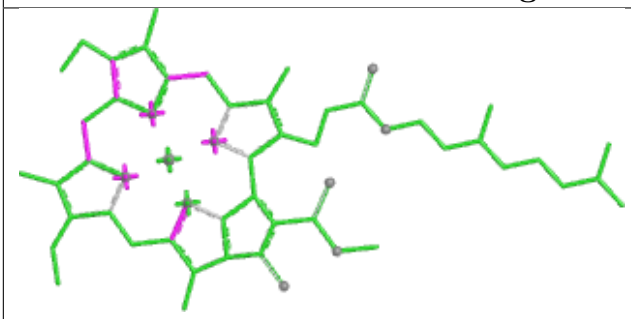
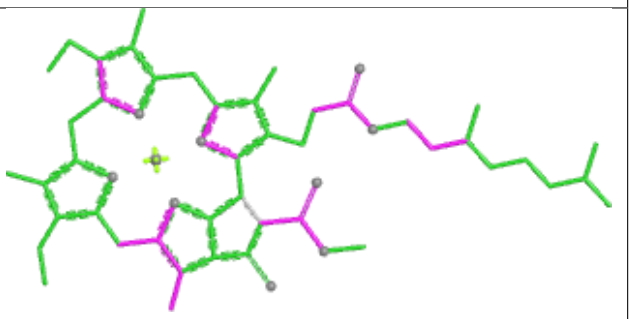
 Bond lengths	 Bond angles
 Torsions	 Rings

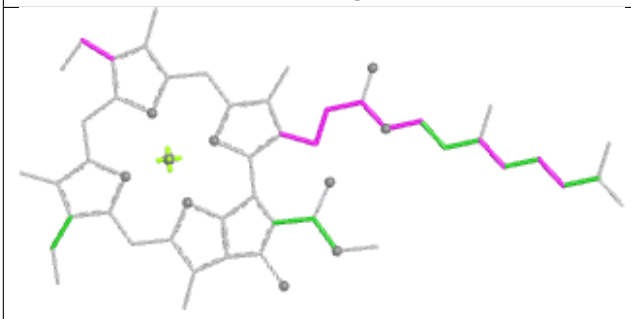
Ligand CLA 15 609



Bond lengths



Bond angles



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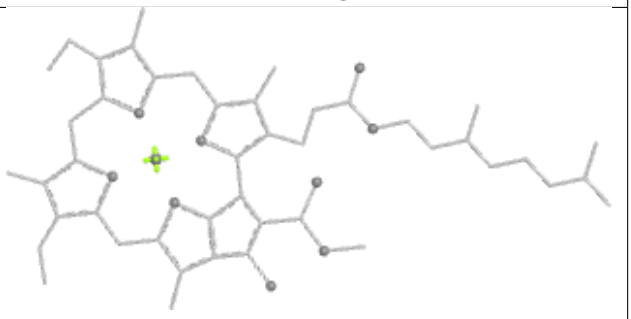
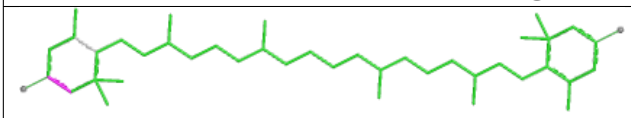
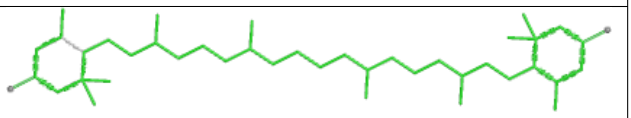


Rings

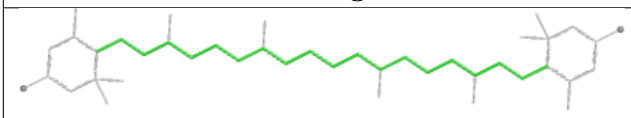
Ligand LUT 3 618



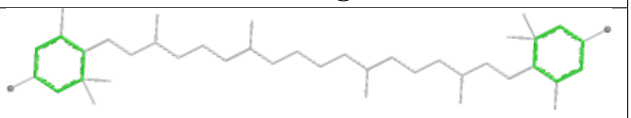
Bond lengths



Bond angles

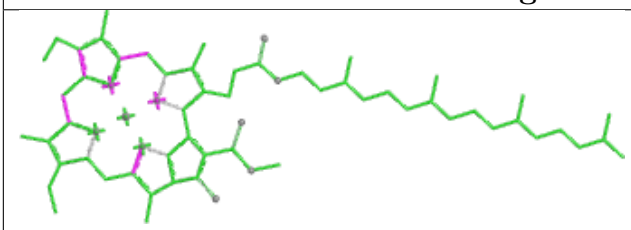


Torsions

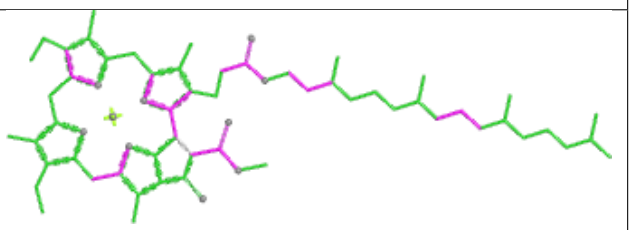


Rings

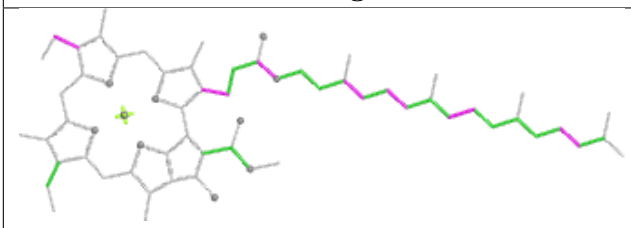
Ligand CLA 13 610



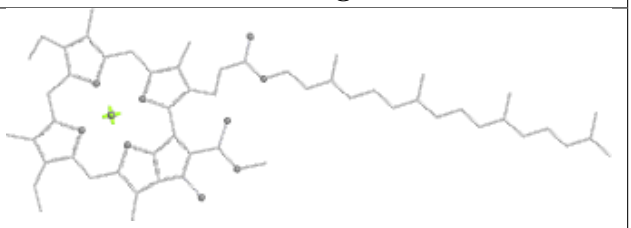
Bond lengths



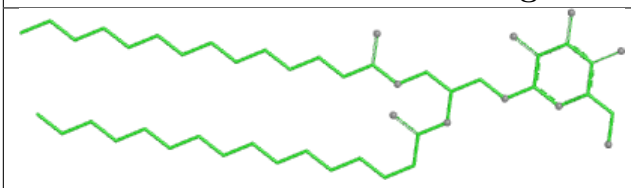
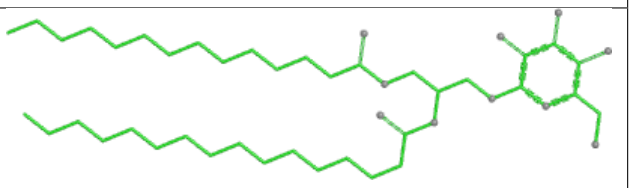
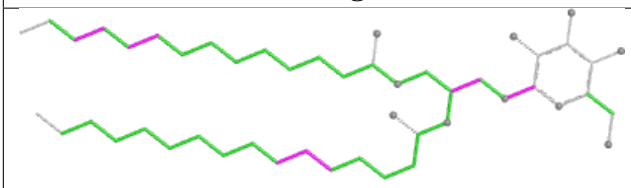
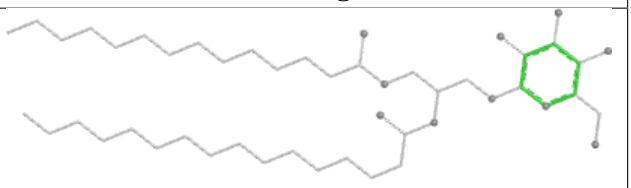
Bond angles



Torsions



Rings

Ligand LMG B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

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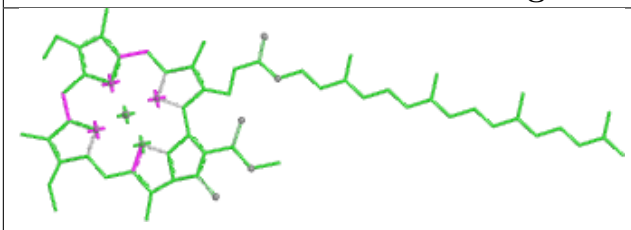
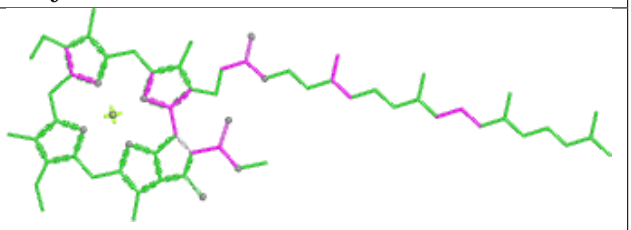
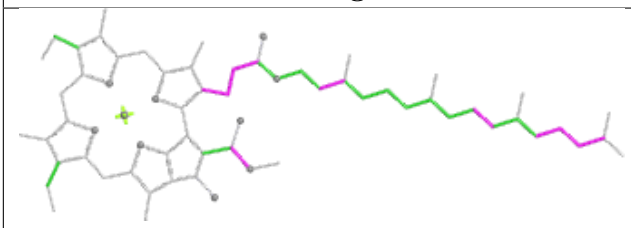
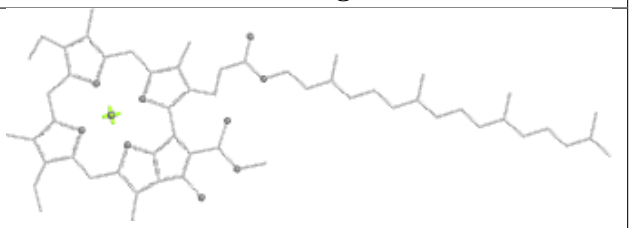
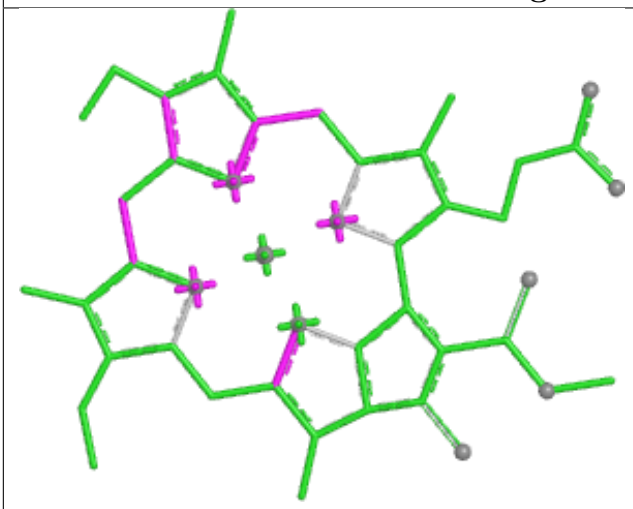
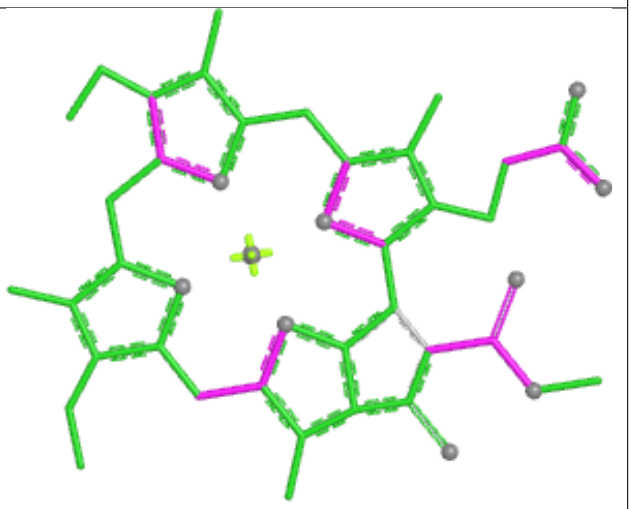
 Bond lengths	 Bond angles
 Torsions	 Rings

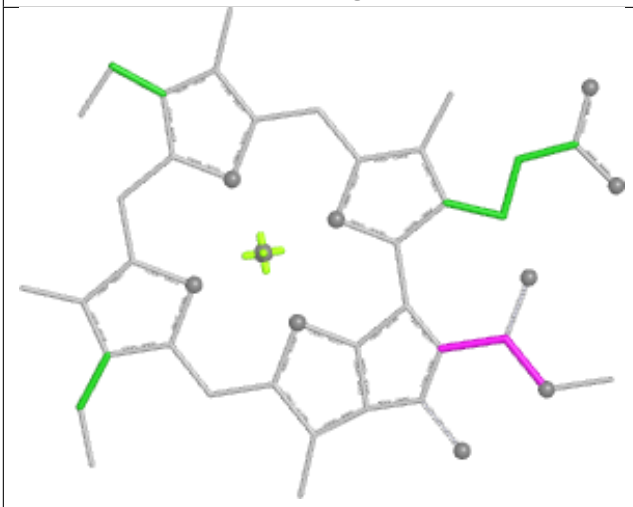
Ligand CLA s 612



Bond lengths

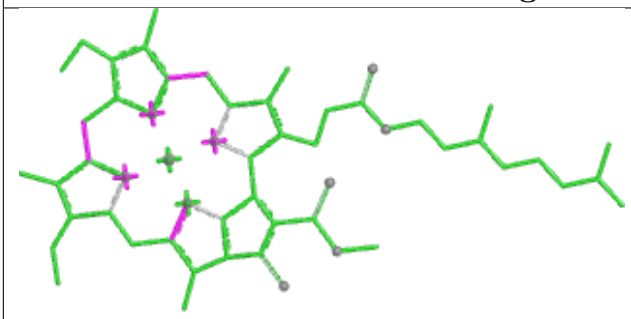
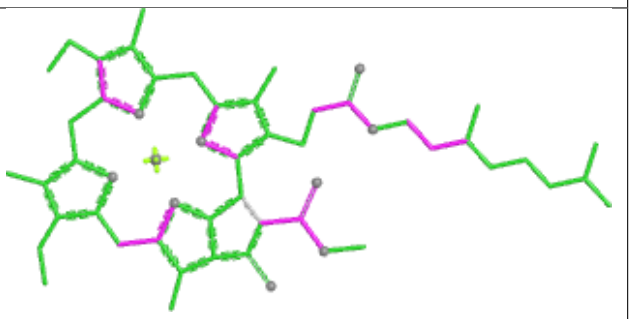
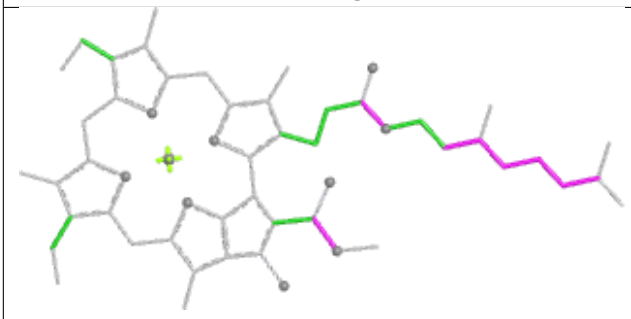
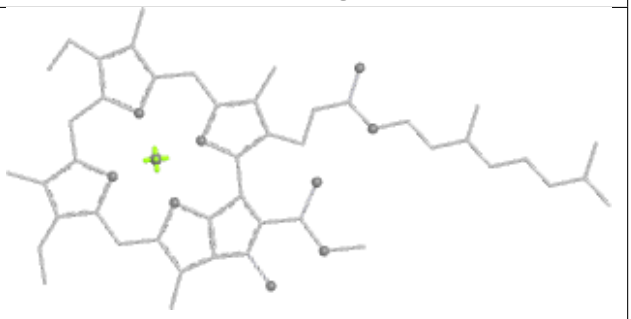


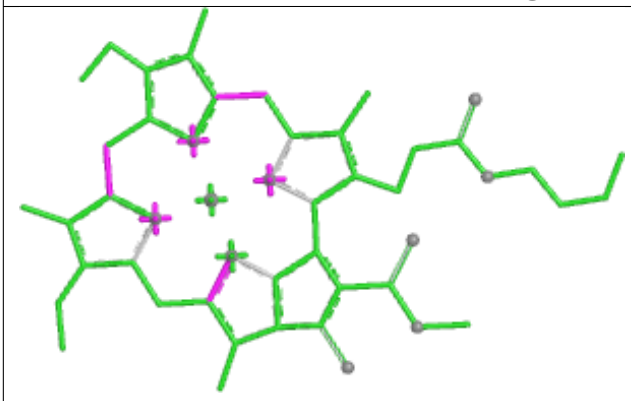
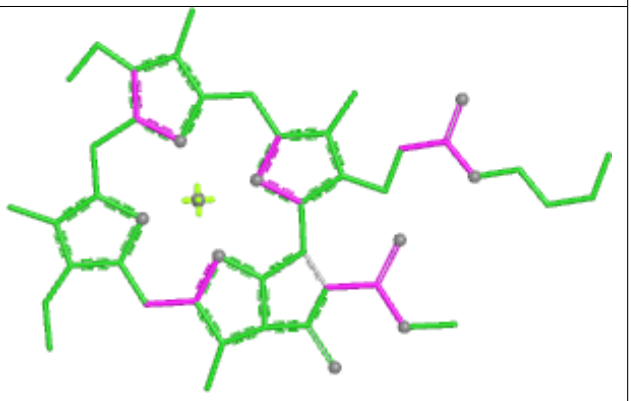
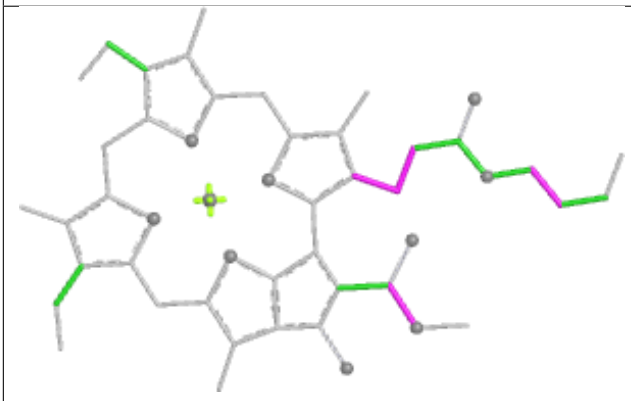
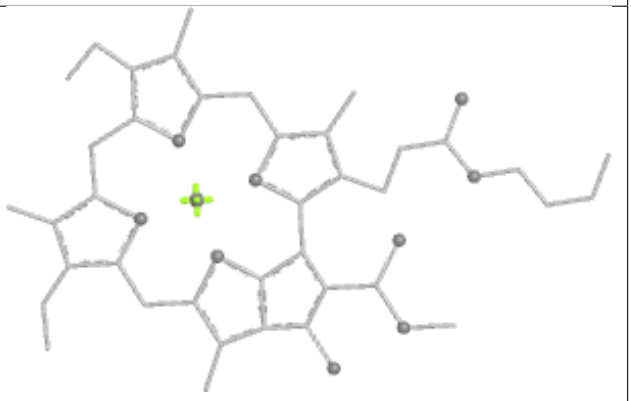
Bond angles

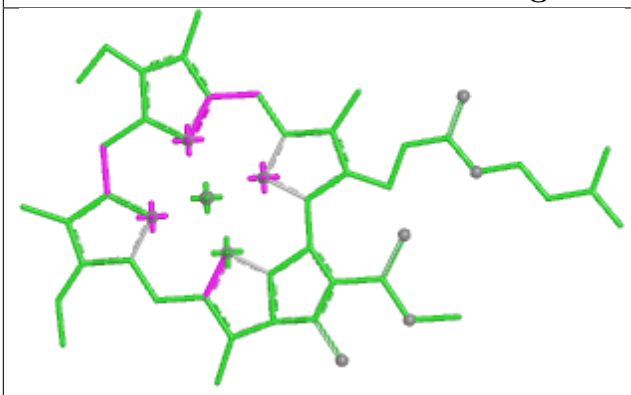
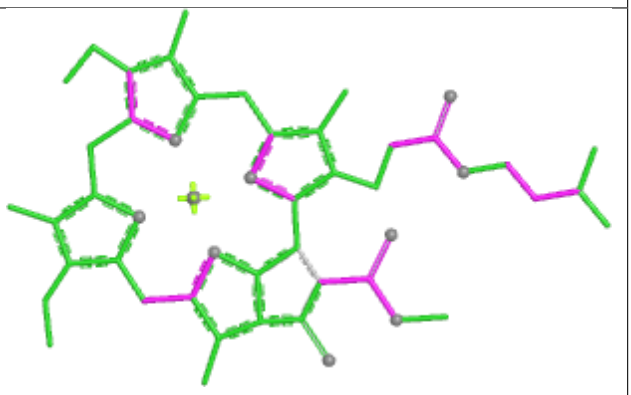
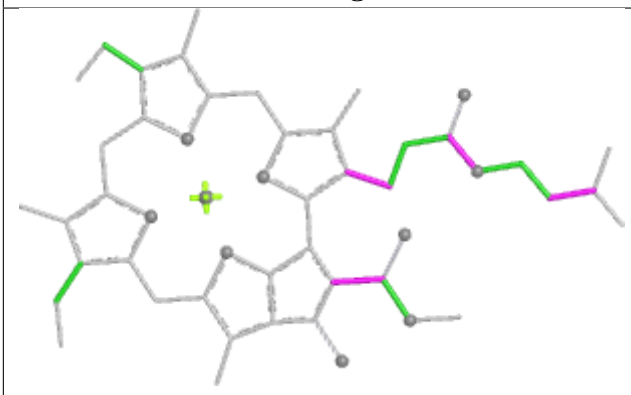
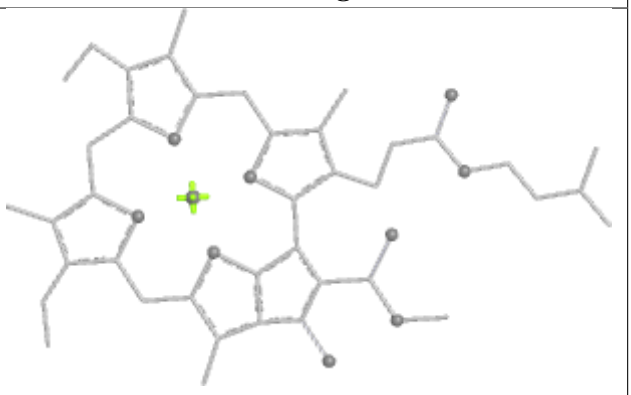


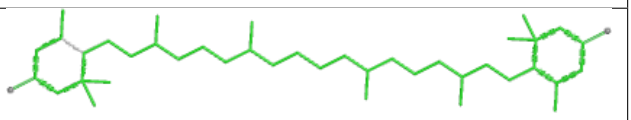
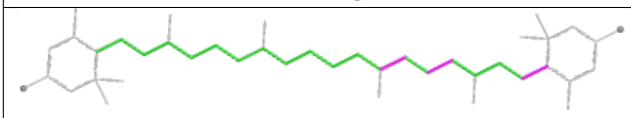
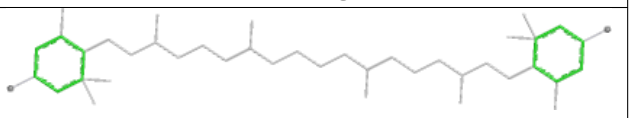
Torsions

Rings

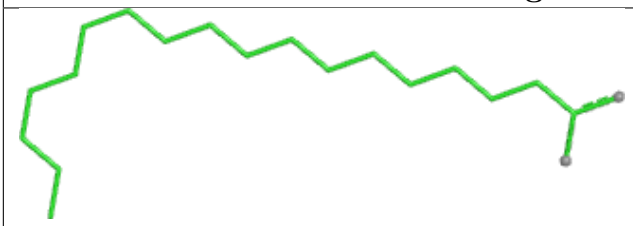
Ligand CLA 12 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

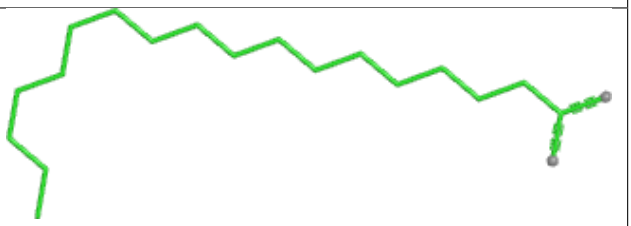
Ligand CLA r 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 12 614	
Bond lengths	 Bond angles
 Torsions	 Rings

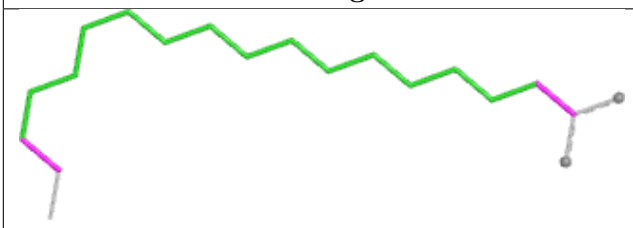
Ligand LNL Y 619



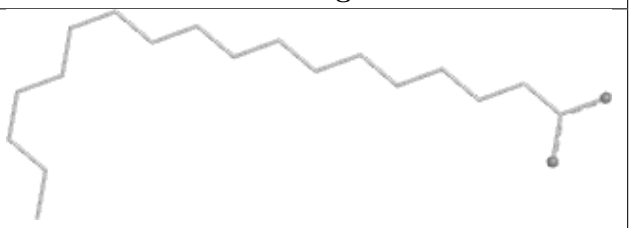
Bond lengths



Bond angles

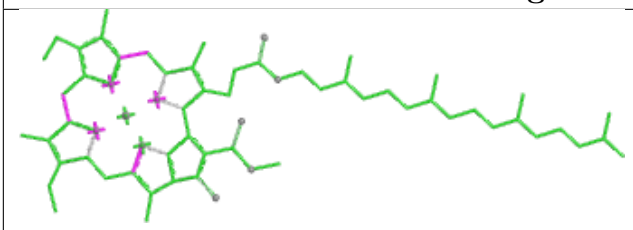


Torsions



Rings

Ligand CLA S 614



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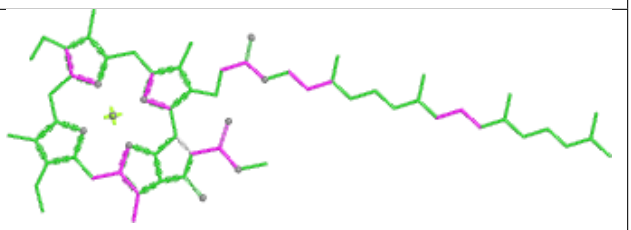
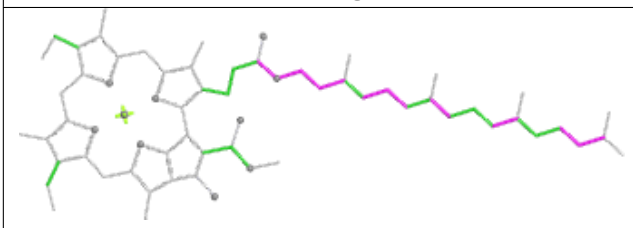


Bond angles



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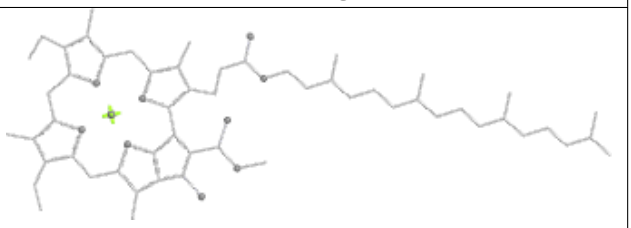
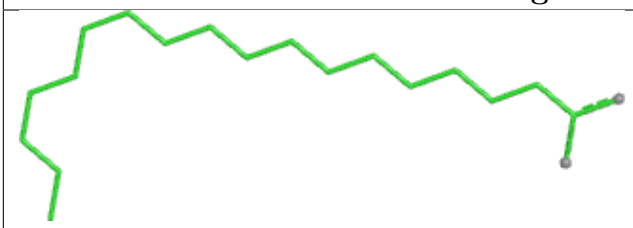


Rings

Ligand LNL c 523



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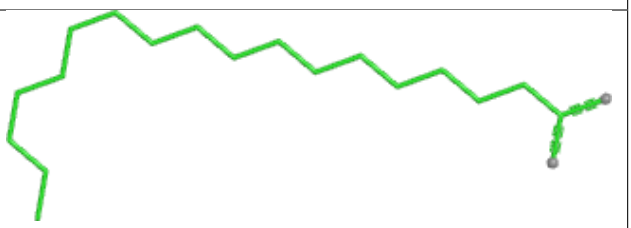

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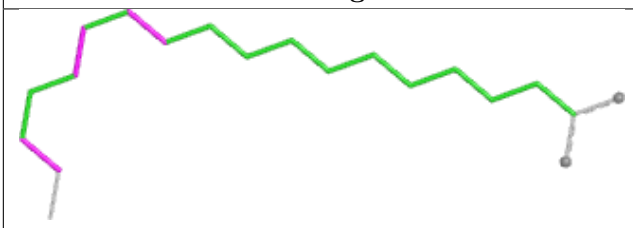

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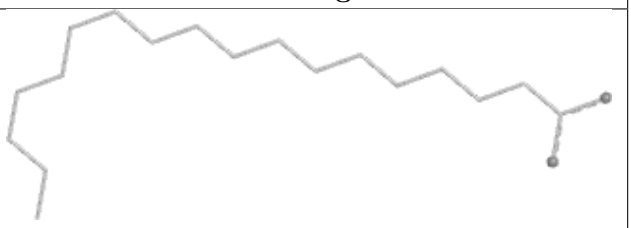
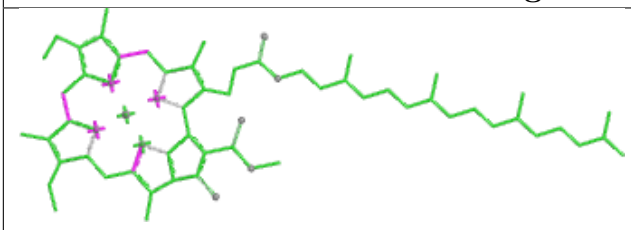


Rings

Ligand CLA C 506



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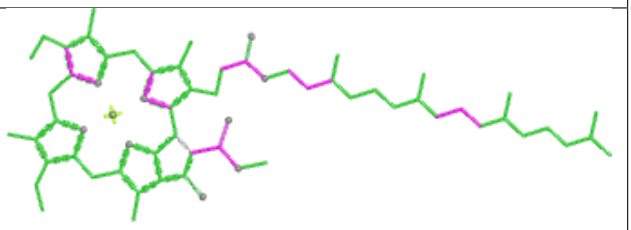
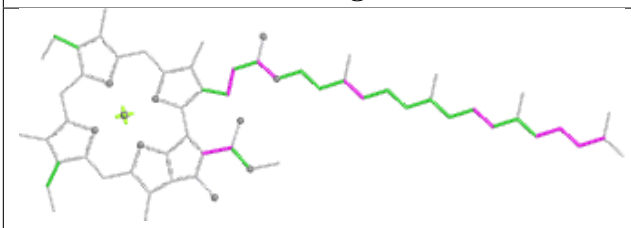


Bond angles



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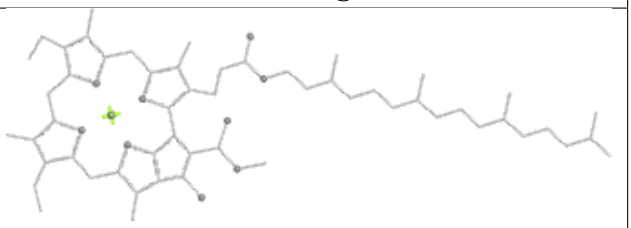
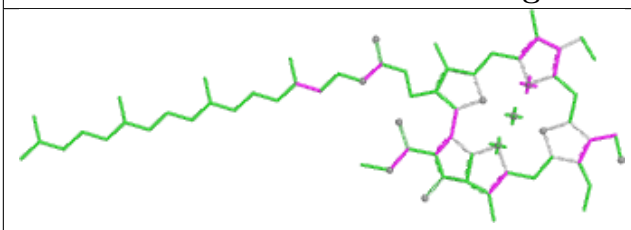


Rings

Ligand CHL G 601



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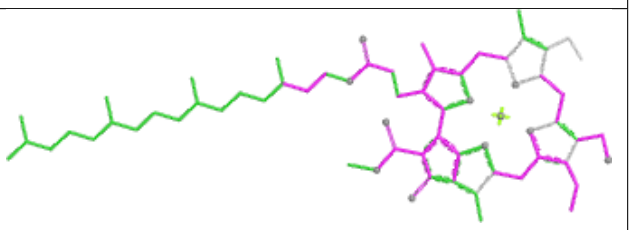
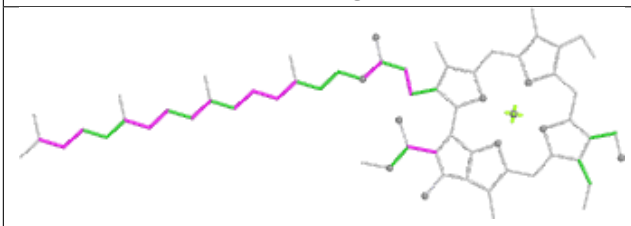


Bond angles



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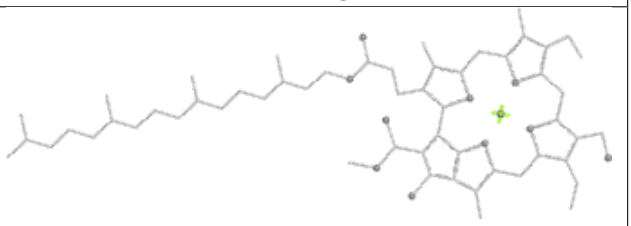
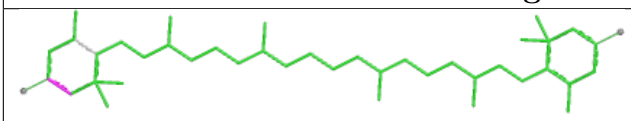


Rings

Ligand LUT G 617



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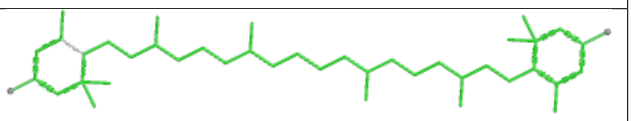
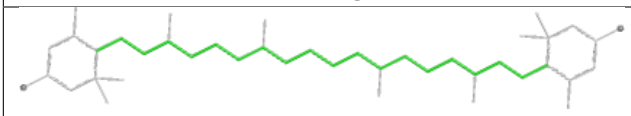
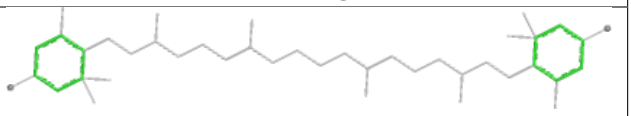


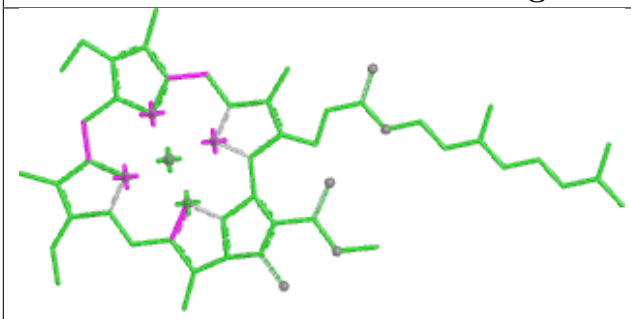
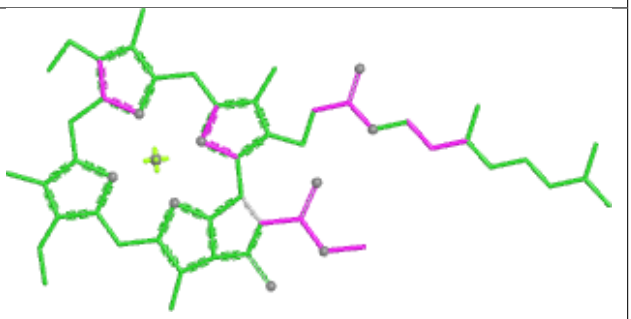
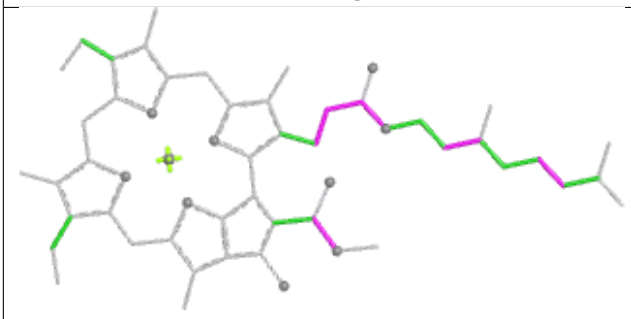
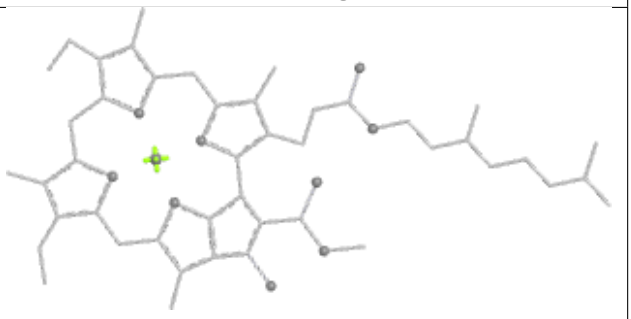
Bond angles



Torsions



Rings

Ligand CLA 1 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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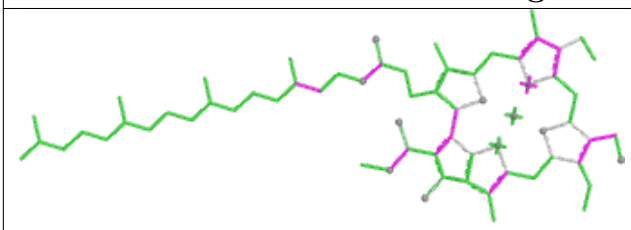
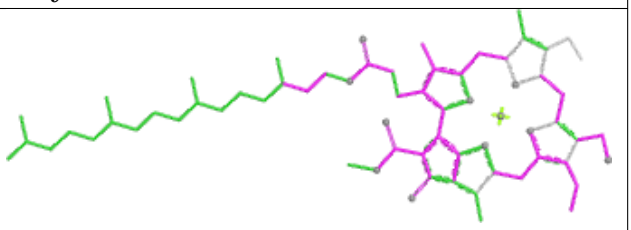
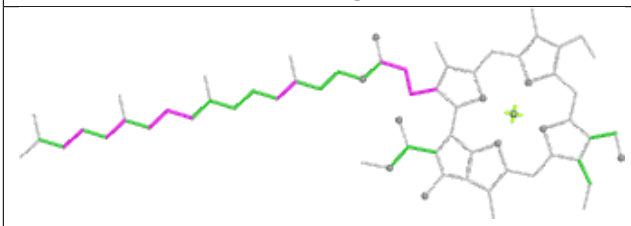
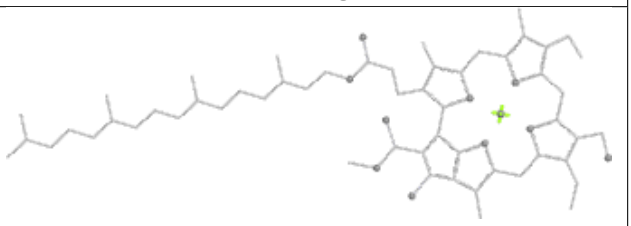
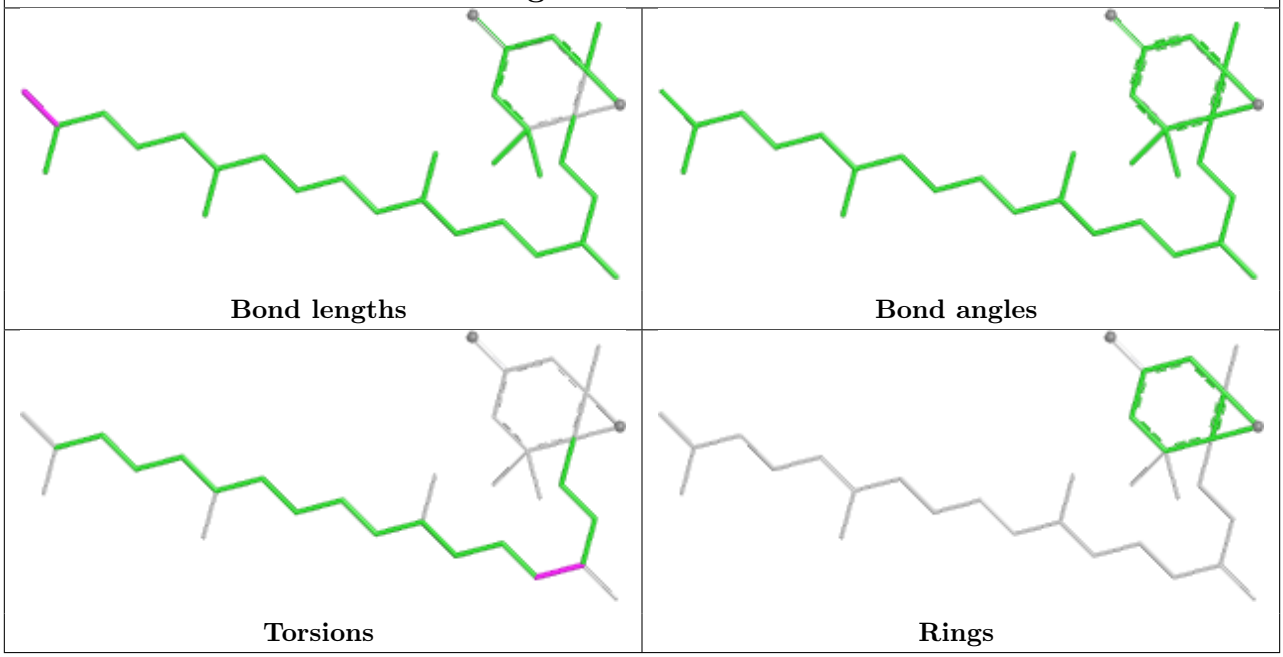
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX 5 616



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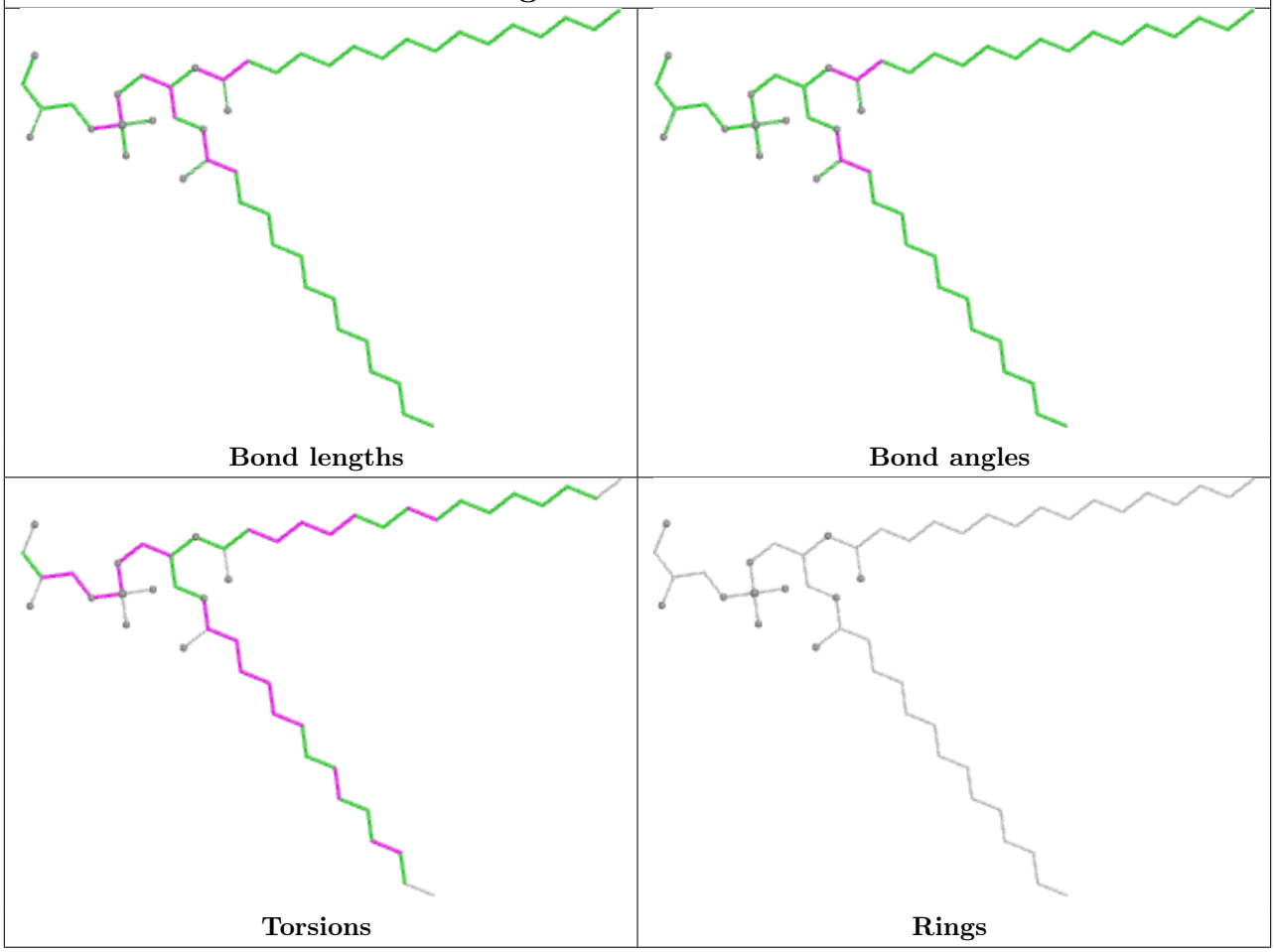

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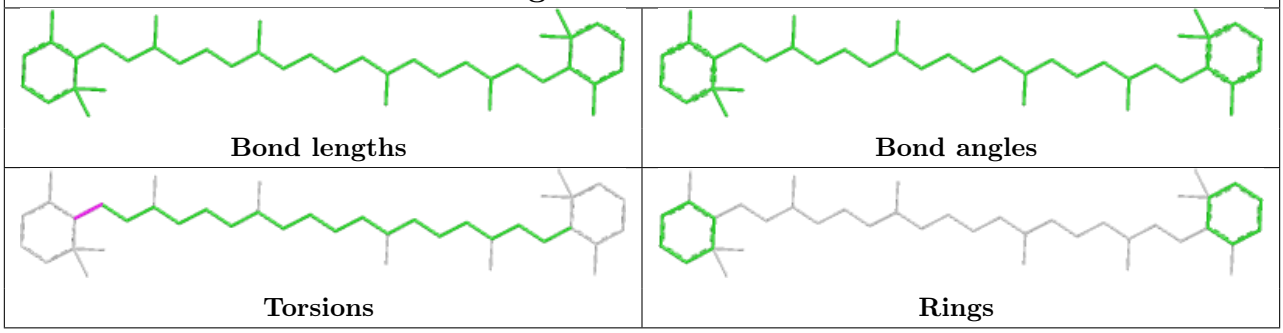

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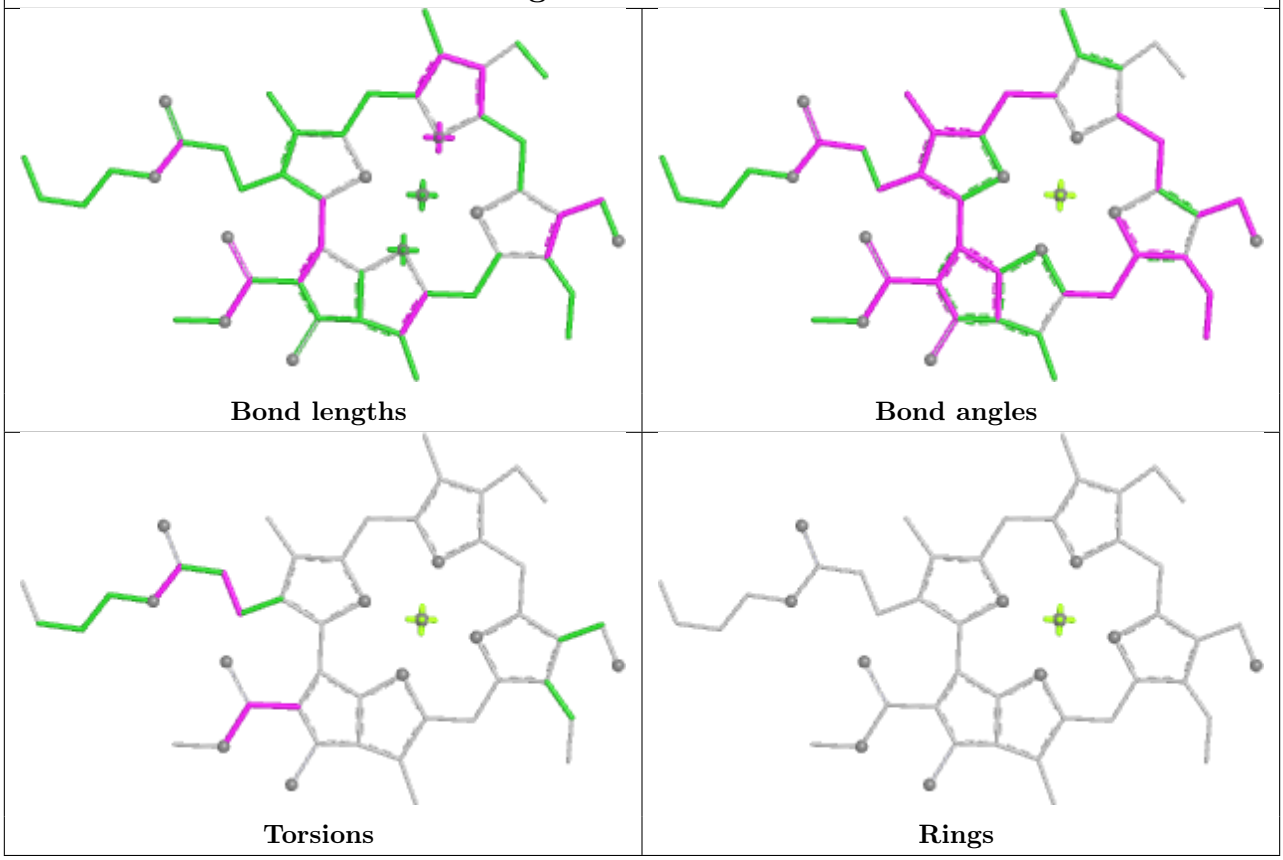

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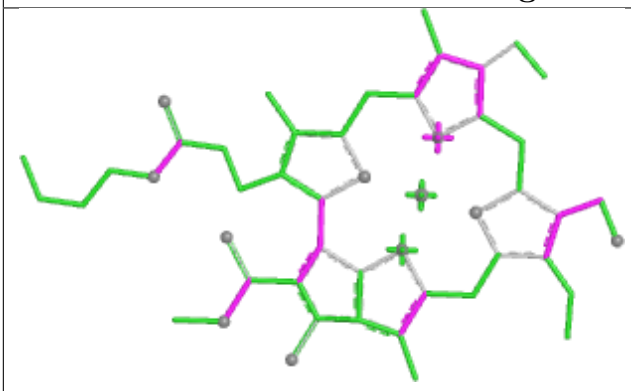
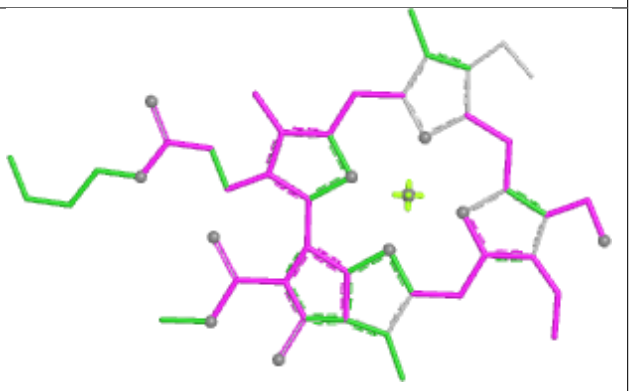
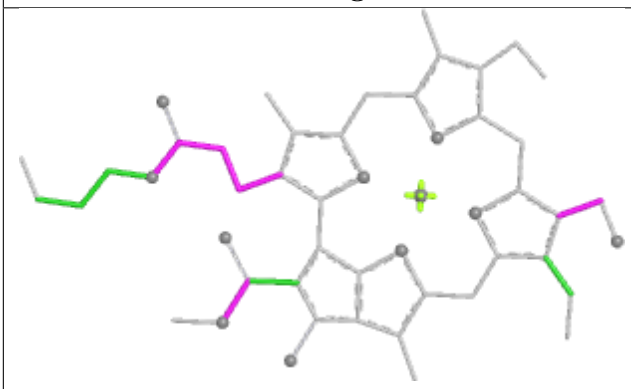
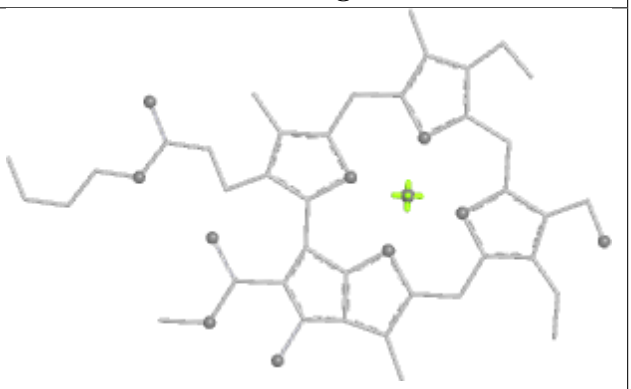
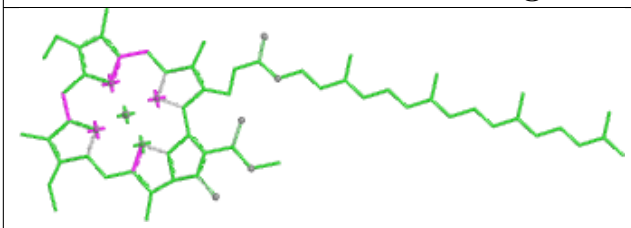
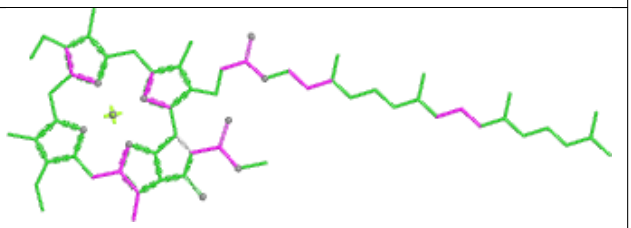
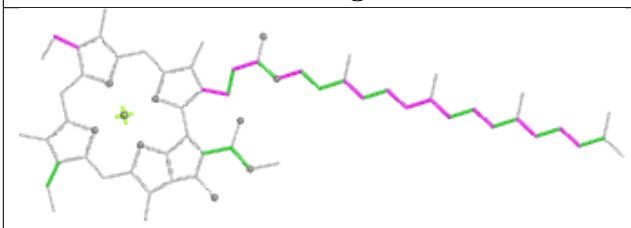
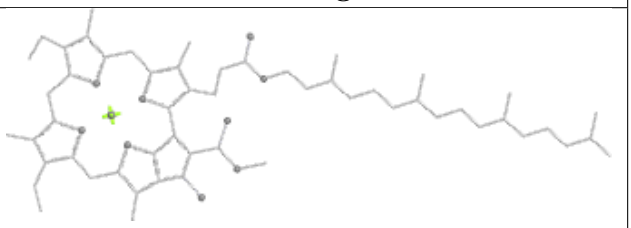
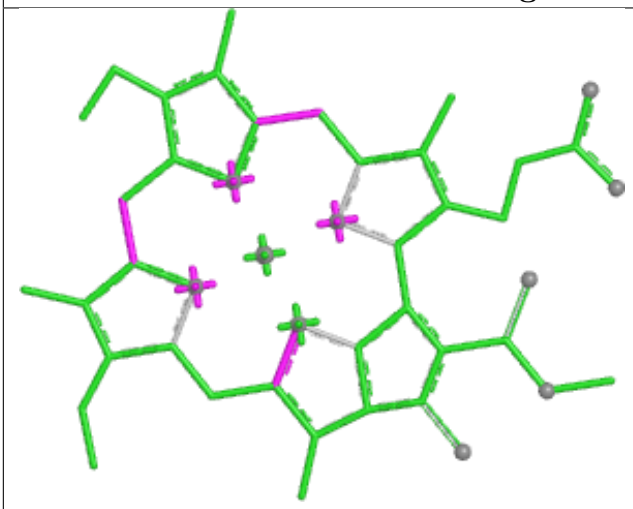
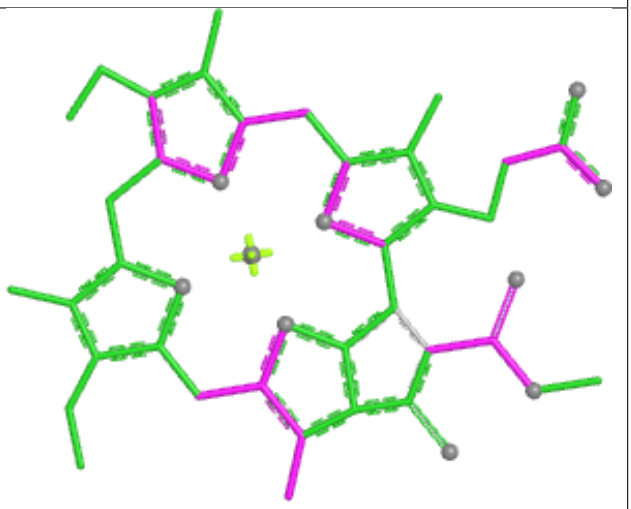
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

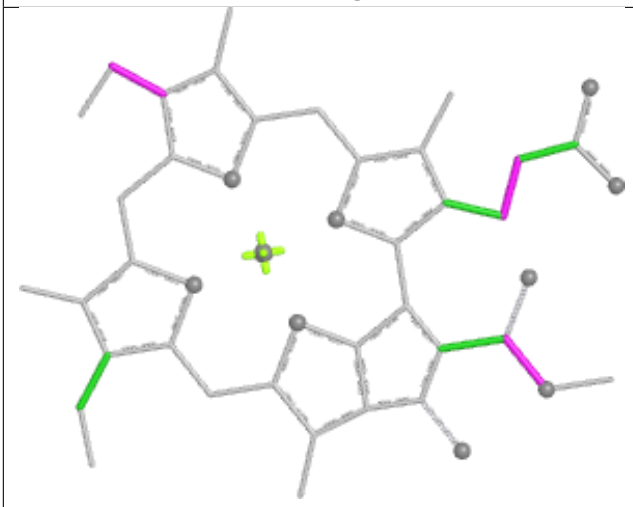
Ligand CLA 16 615



Bond lengths



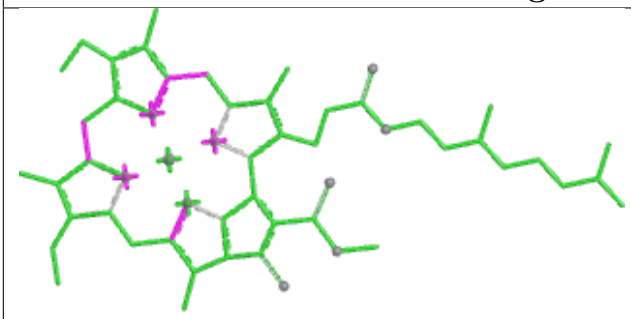
Bond angles



Torsions

Rings

Ligand CLA 3 613



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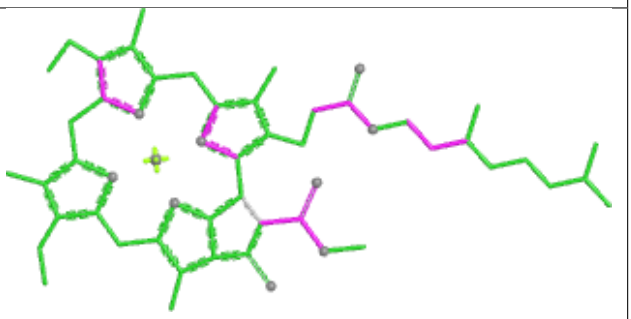

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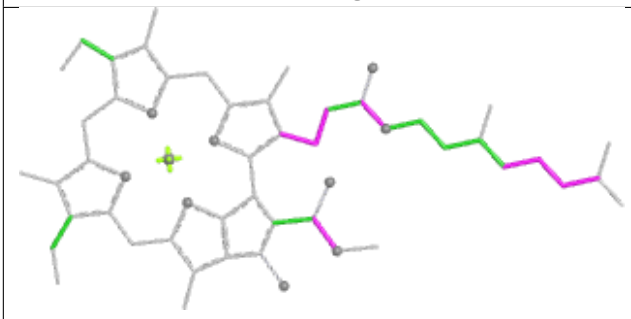

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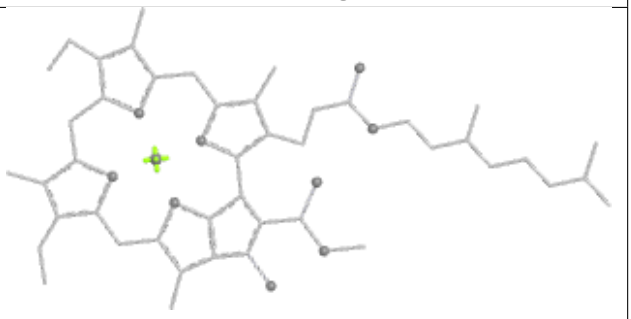
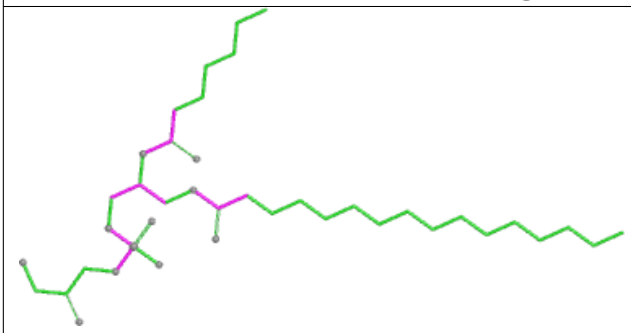


Rings

Ligand LHG 13 616



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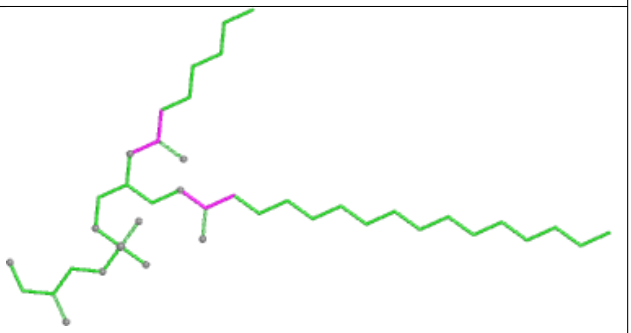

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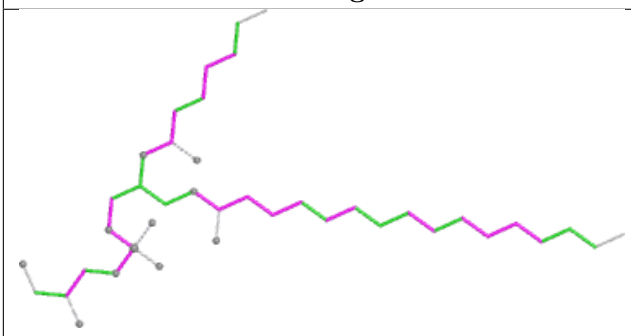

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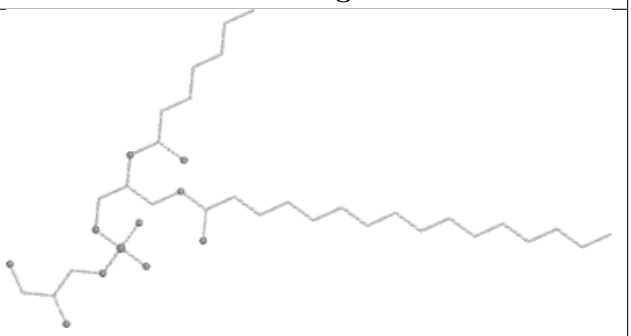
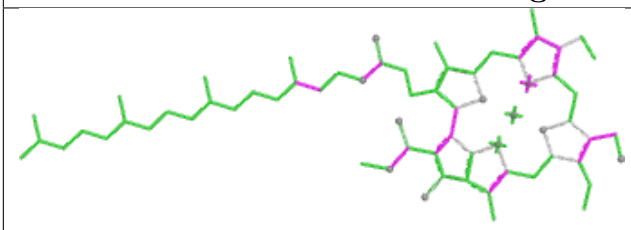
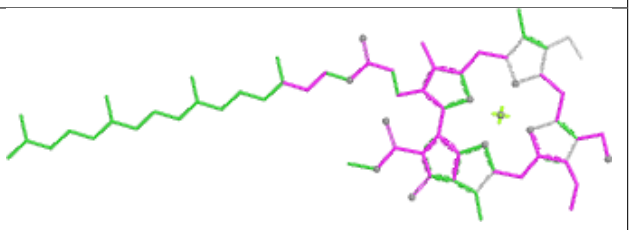
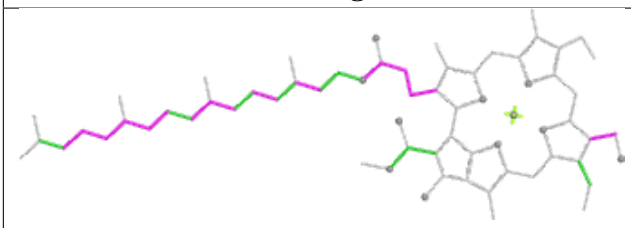
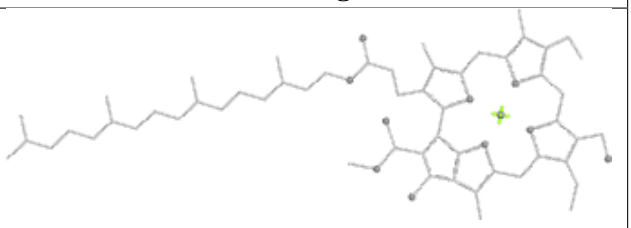


Rings

Ligand CHL s 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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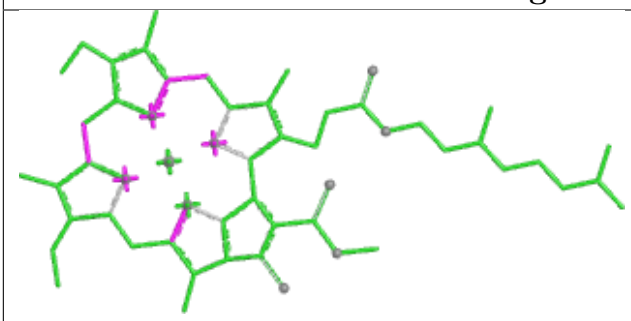
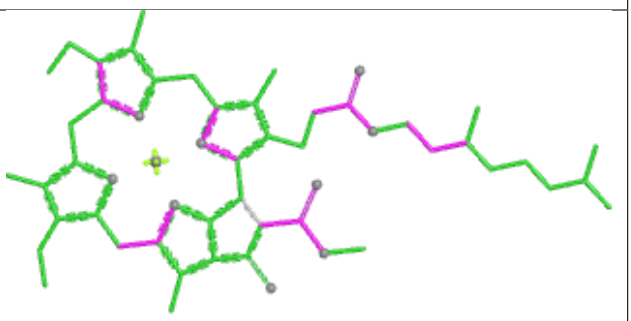
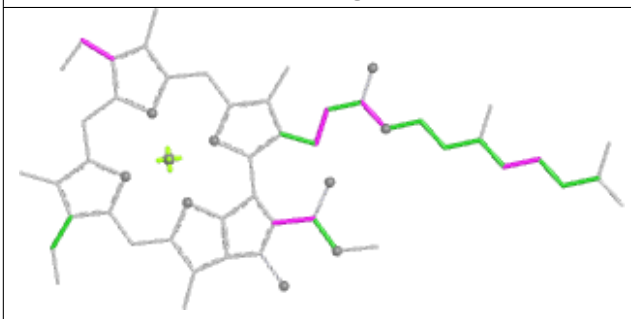
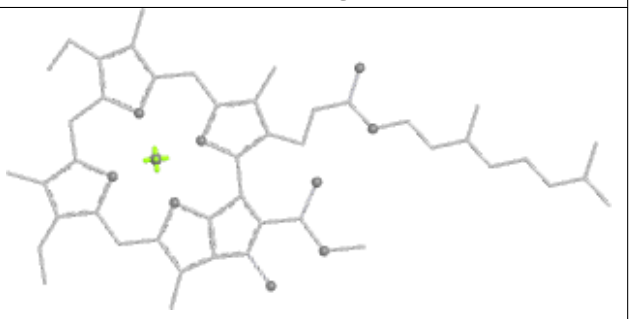
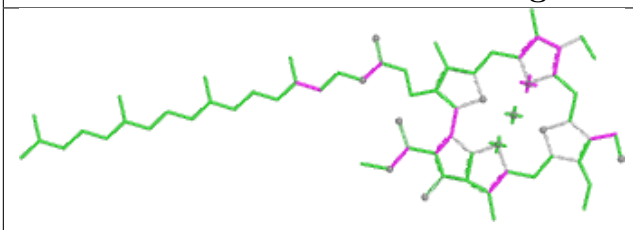
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 606



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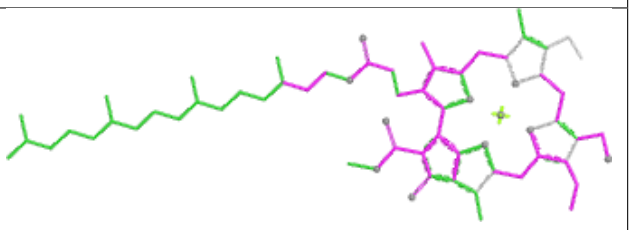
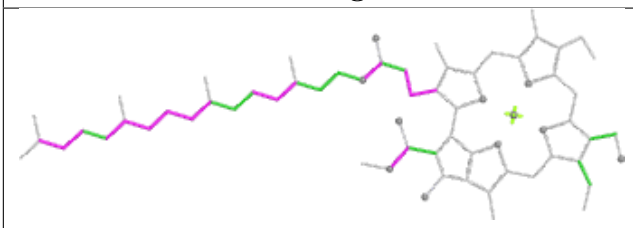


Bond angles



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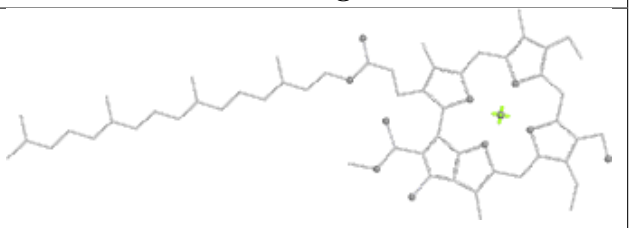
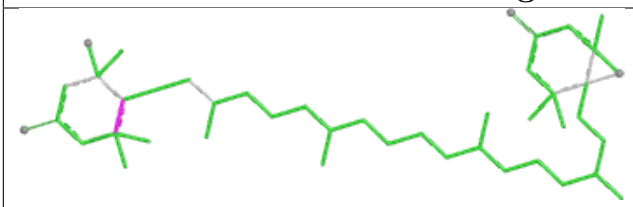


Rings

Ligand NEX 13 619



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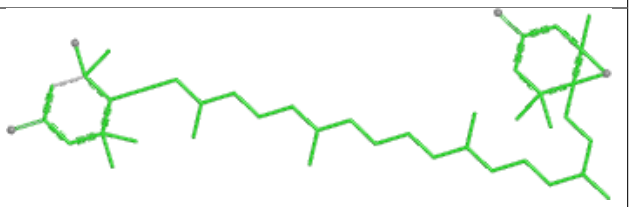
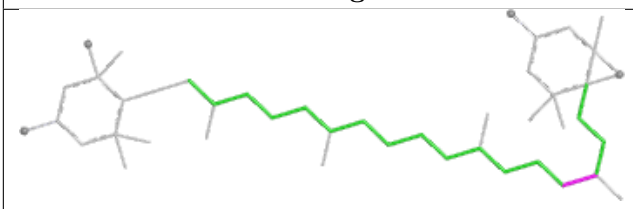


Bond angles



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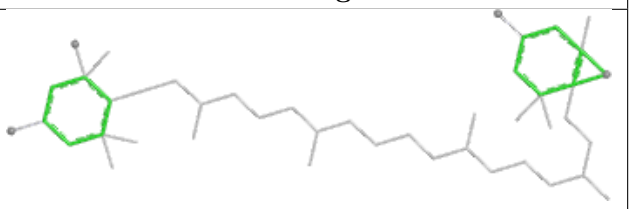
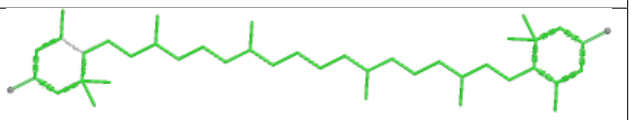


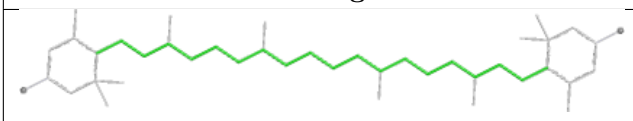
Rings

Ligand LUT 3 619

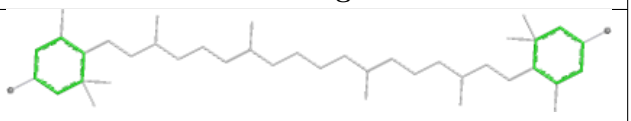
Bond lengths



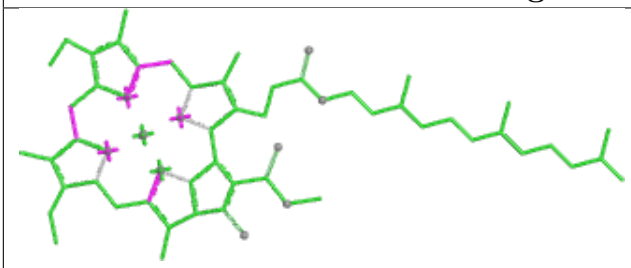
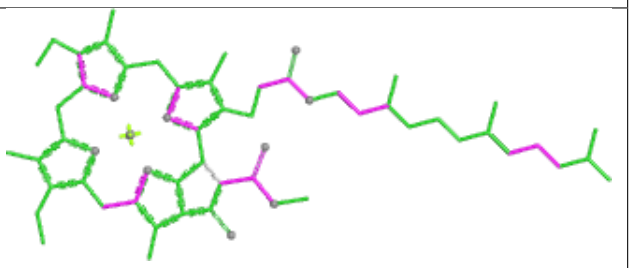
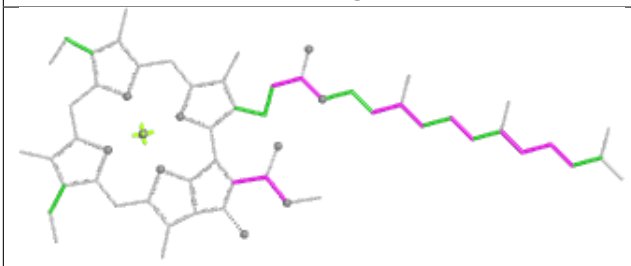
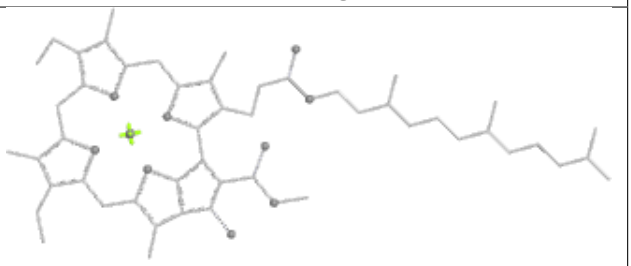
Bond angles

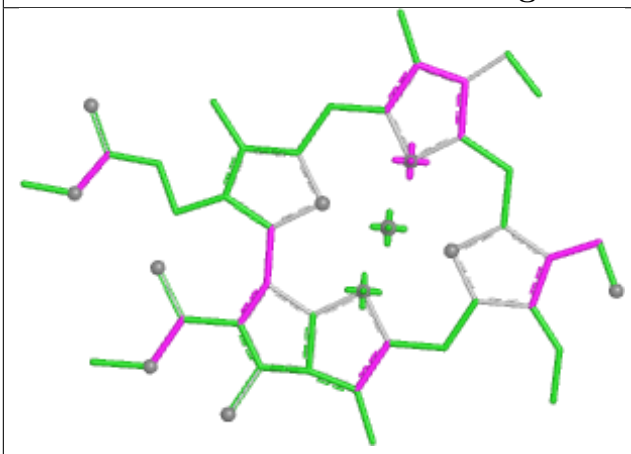
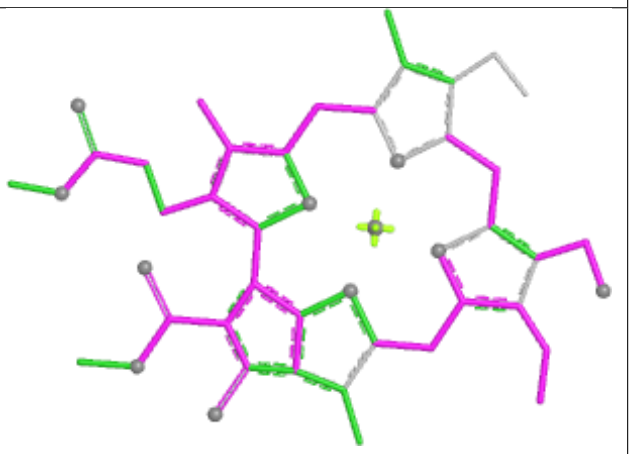
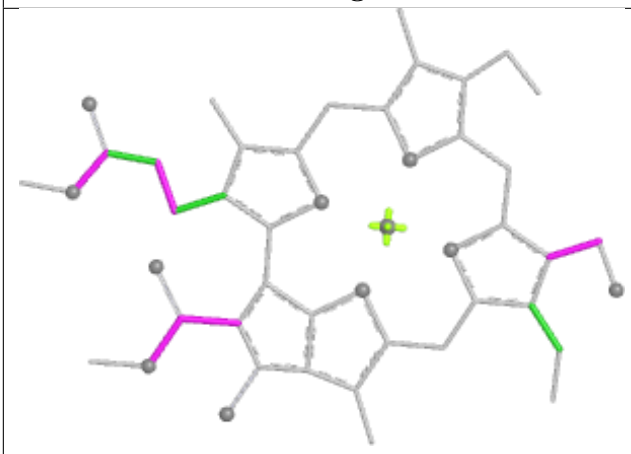


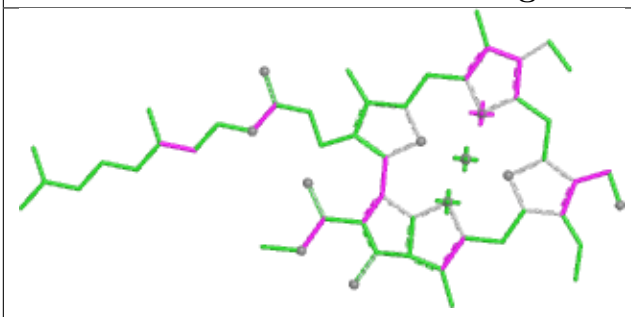
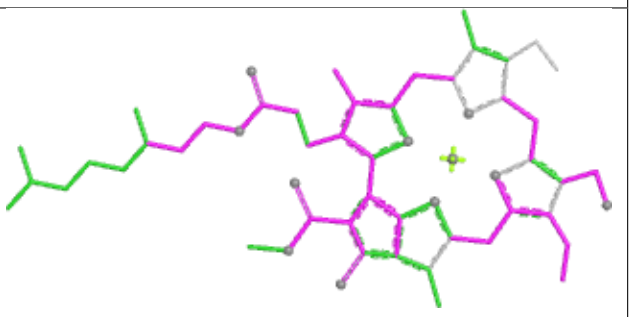
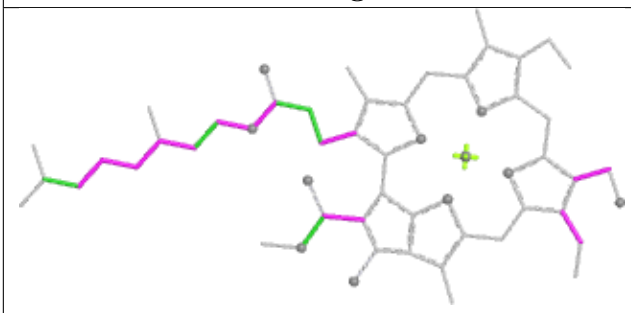
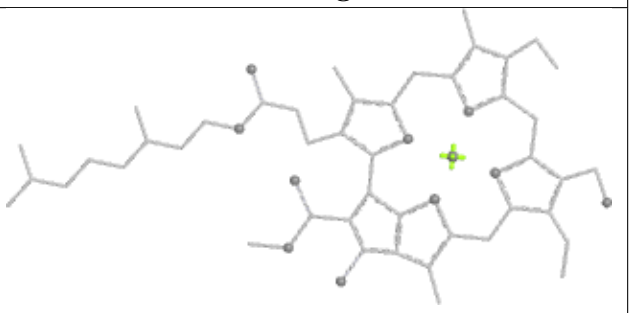
Torsions



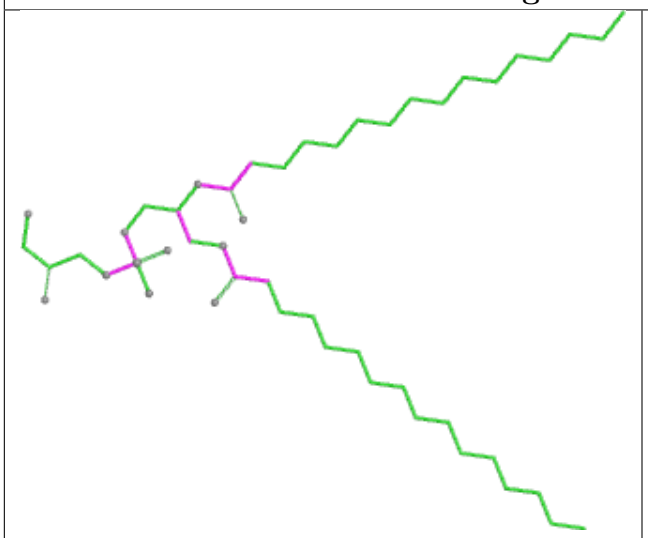
Rings

Ligand CLA n 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 11 606	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CHL 14 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG G 615



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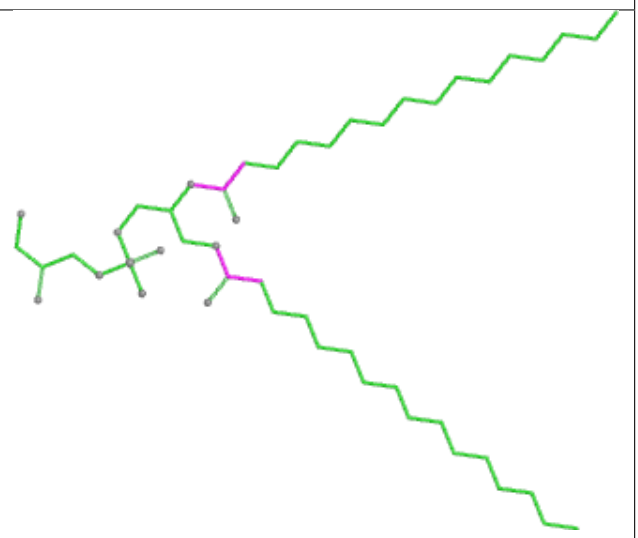
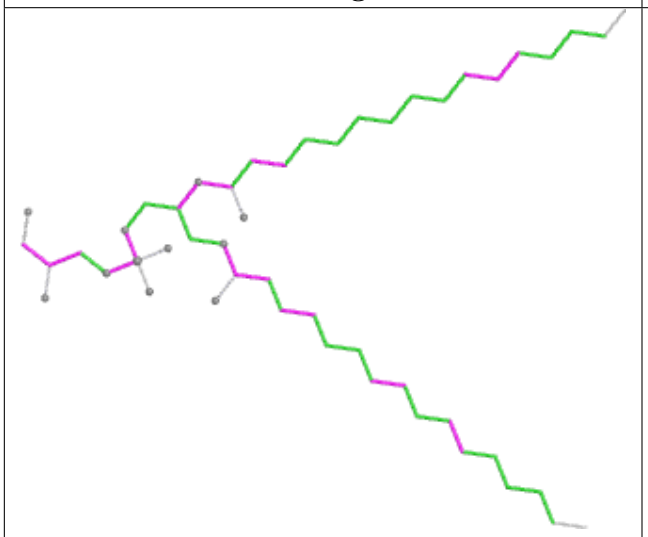


Bond angles



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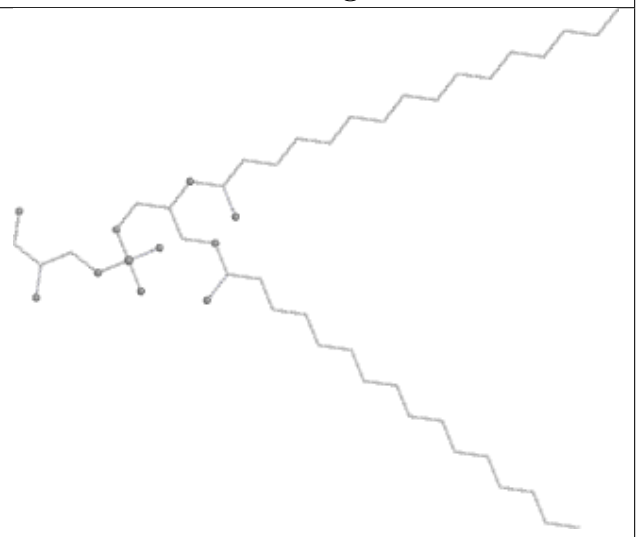
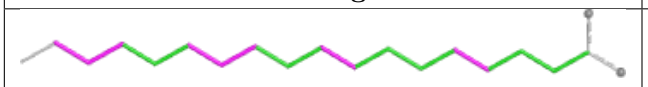


Rings

Ligand STE B 623

Bond lengths

Bond angles



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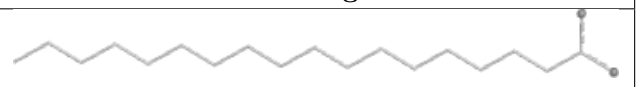
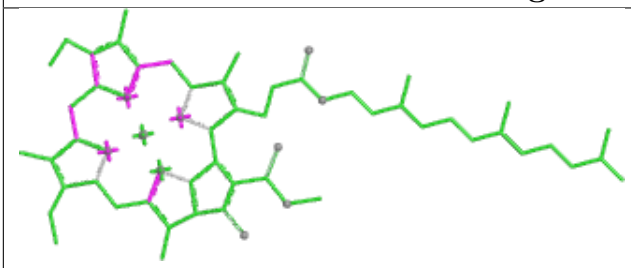


Rings

Ligand CLA 6 602



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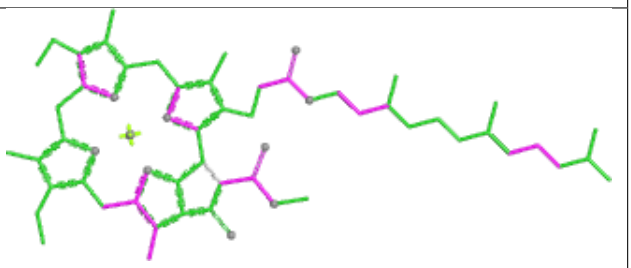

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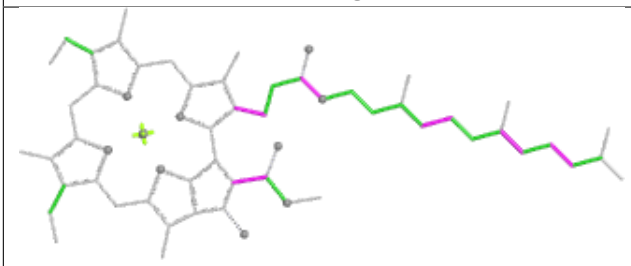

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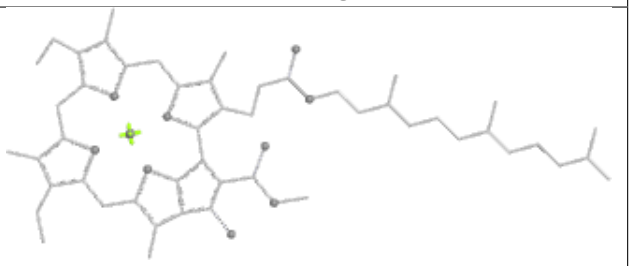
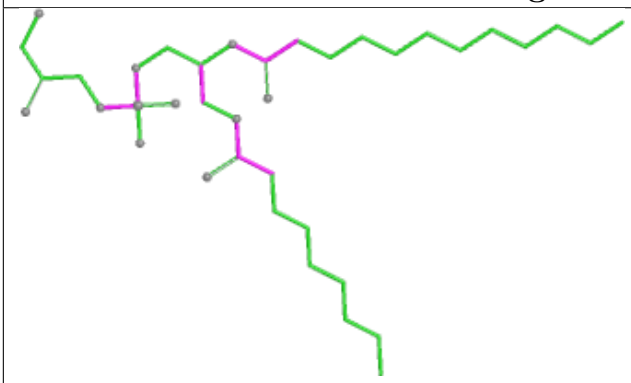


Rings

Ligand LHG r 618



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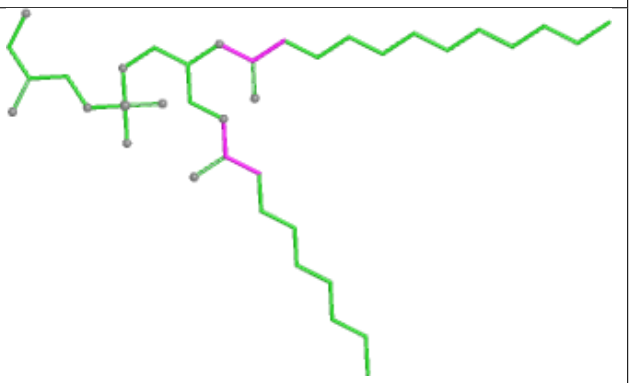

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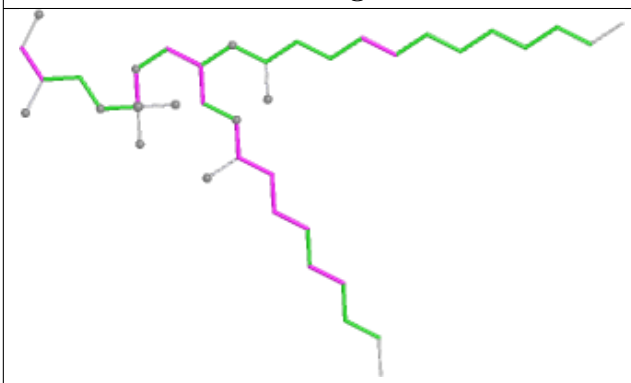

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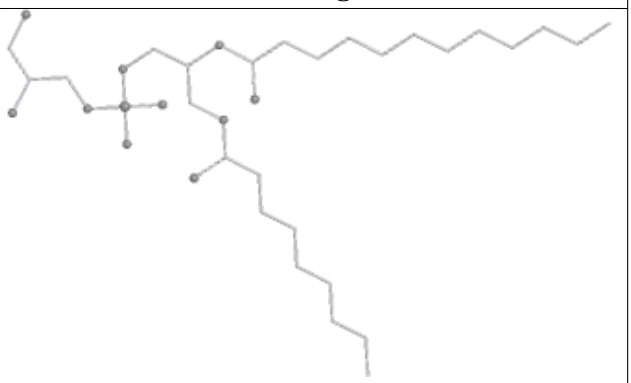
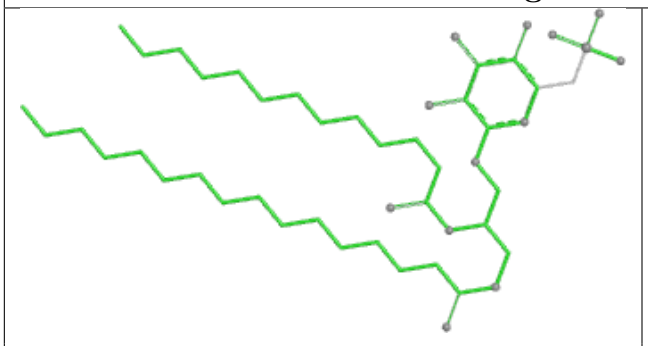


Rings

Ligand SQD A 408



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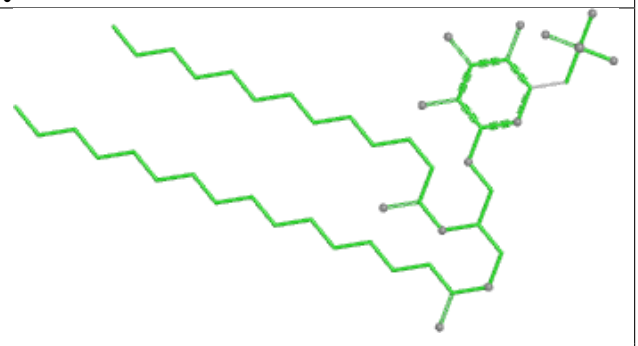

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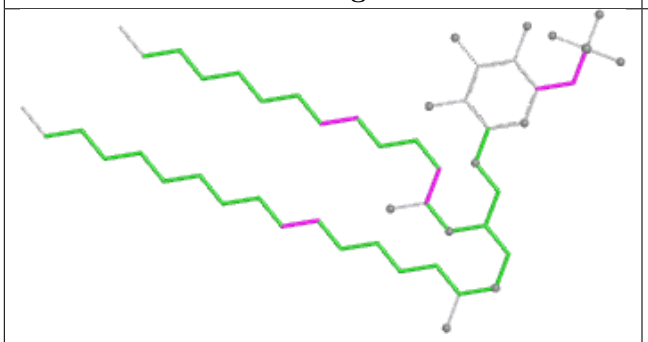

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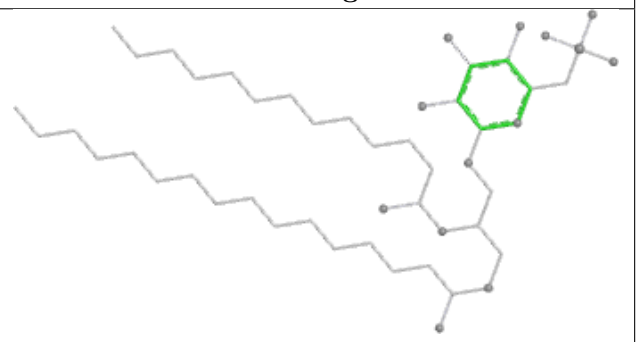
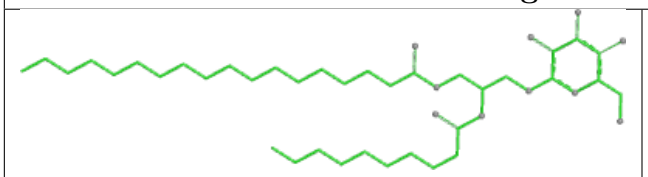


Rings

Ligand LMG C 520



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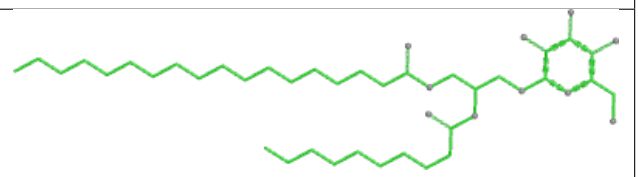

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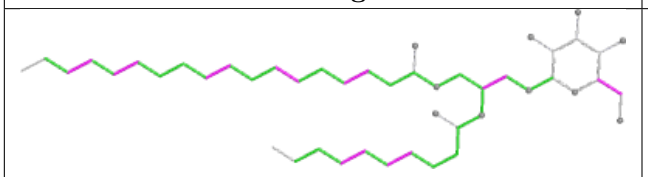

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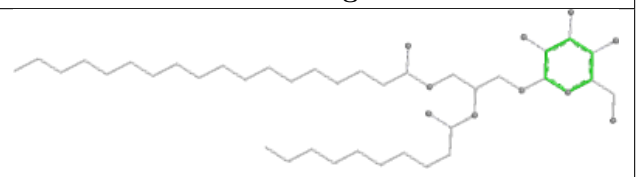
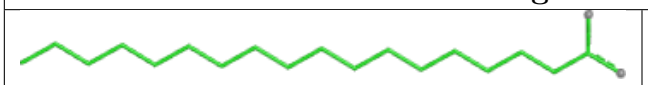


Rings

Ligand STE b 622



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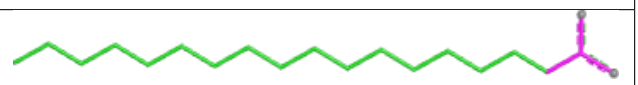
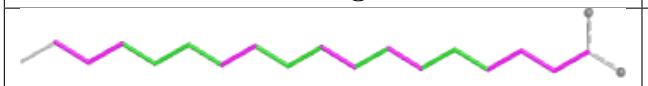


Bond angles



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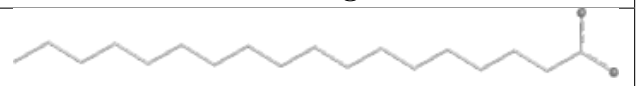
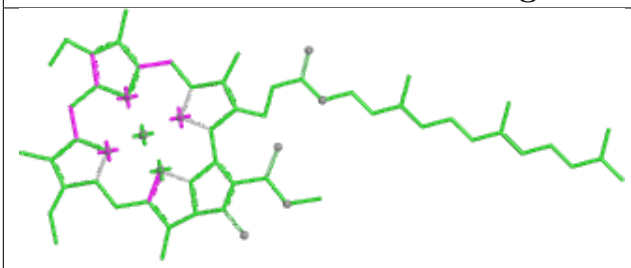
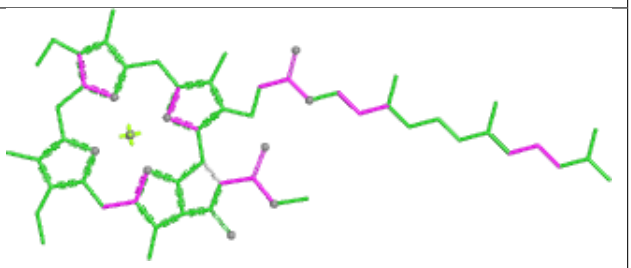
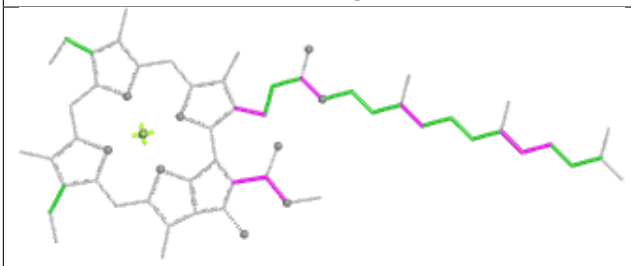
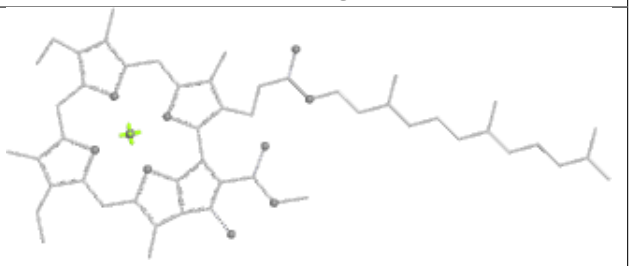


Rings

Ligand CLA 14 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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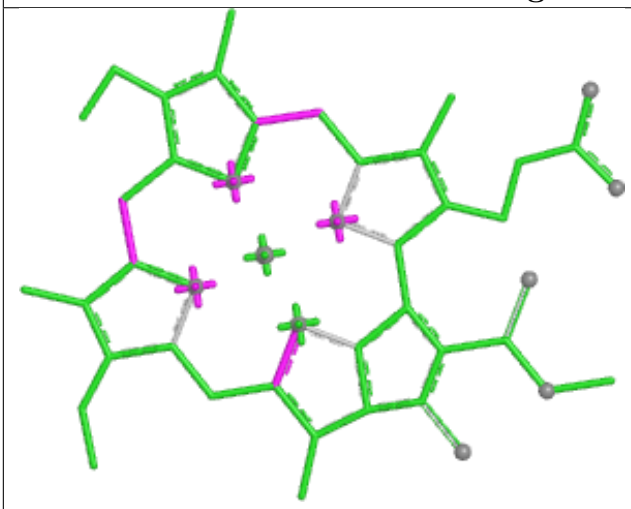
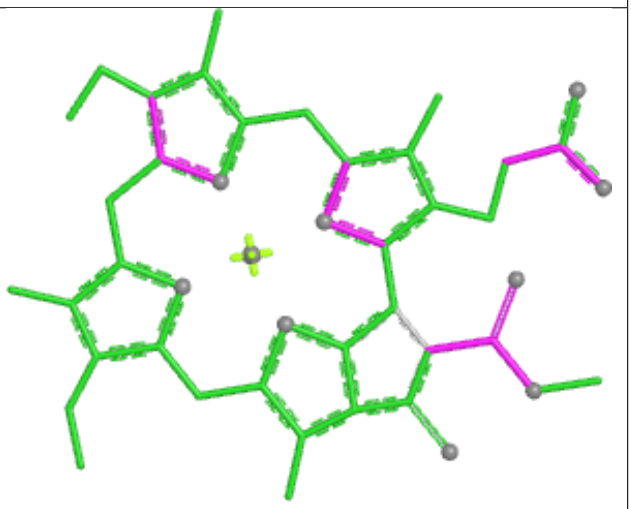
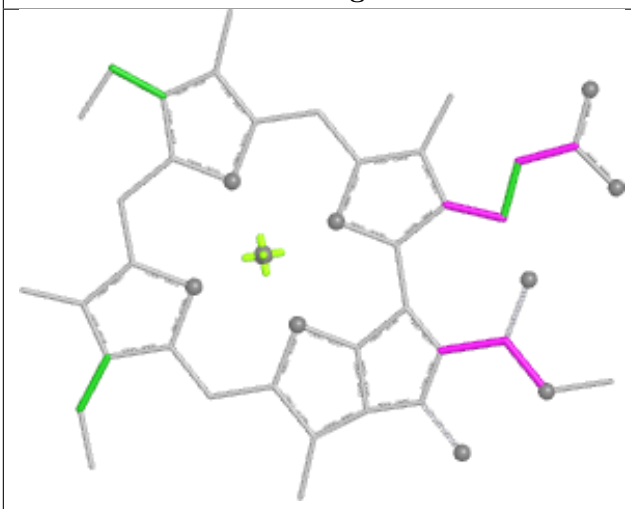
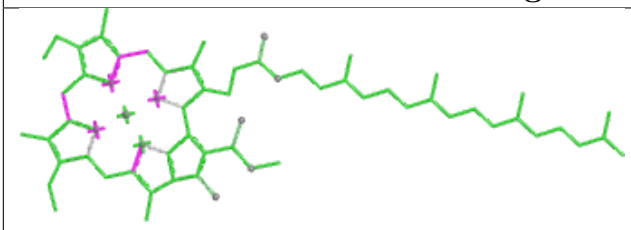
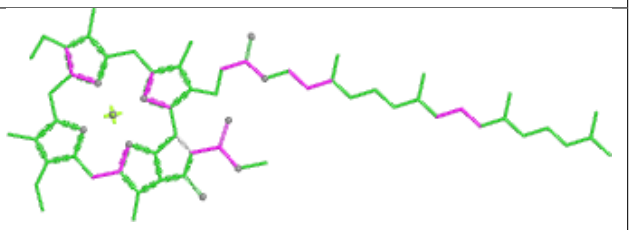
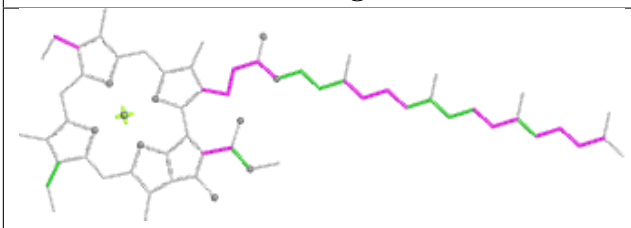
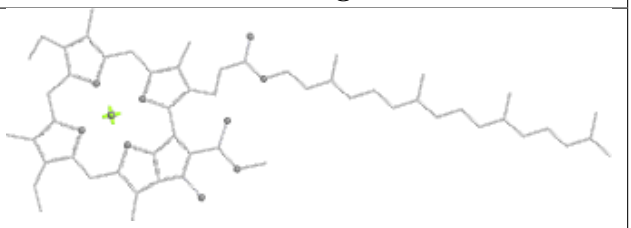
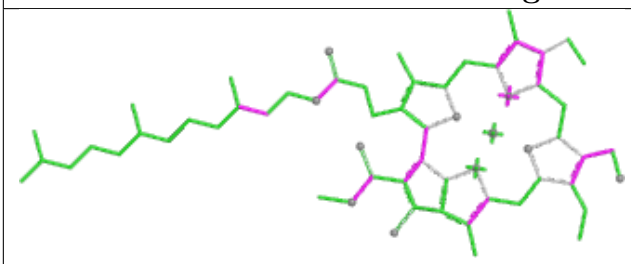
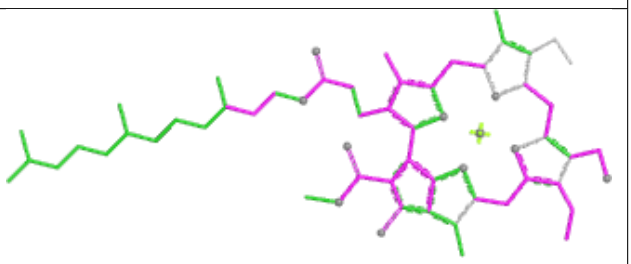
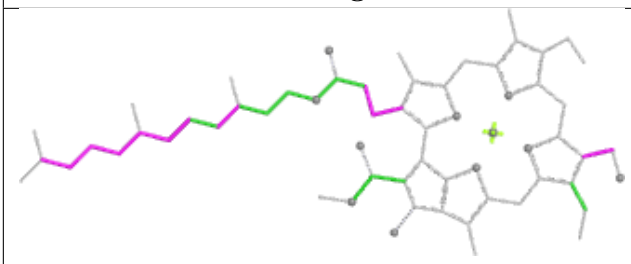
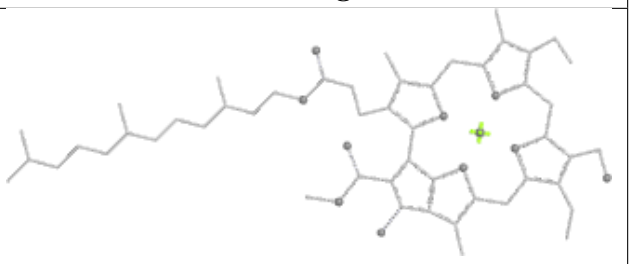
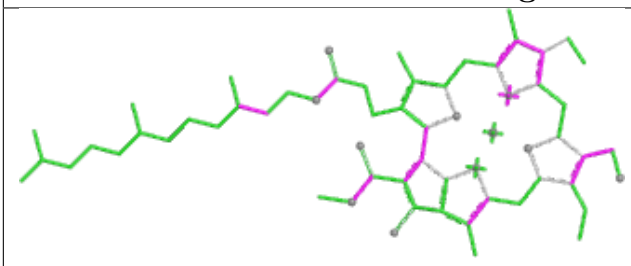
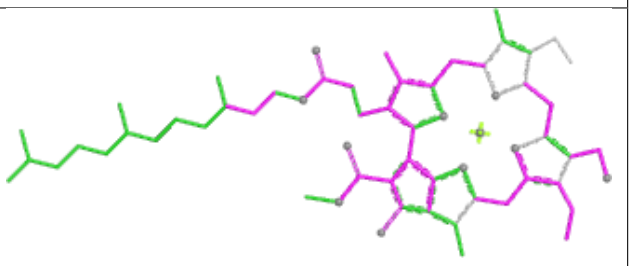
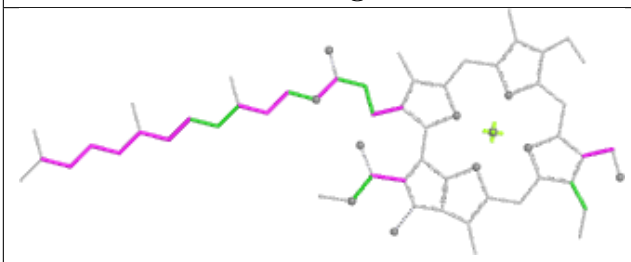
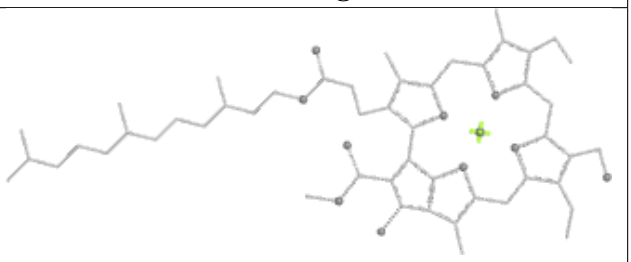
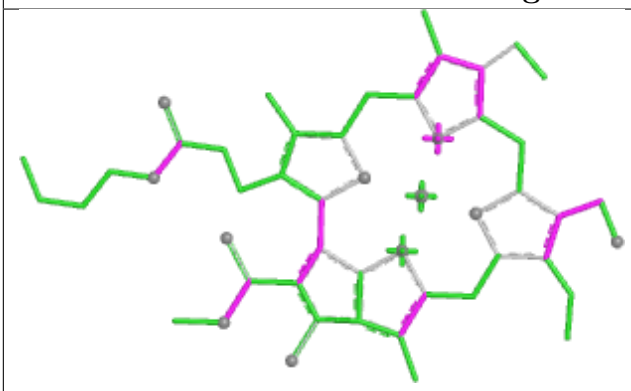
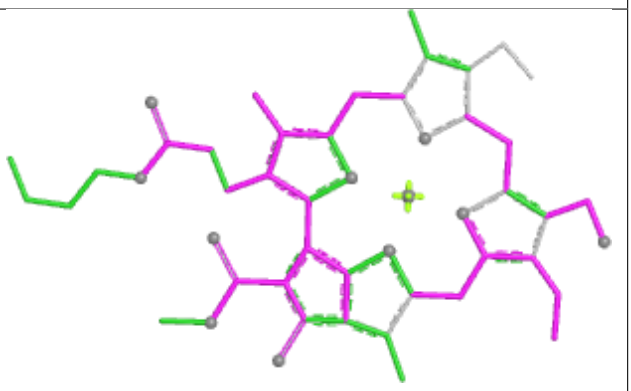
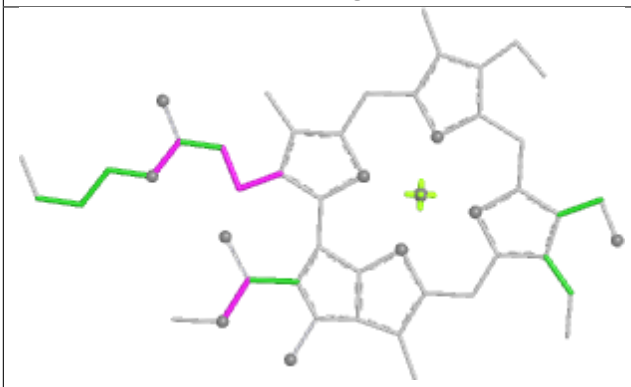
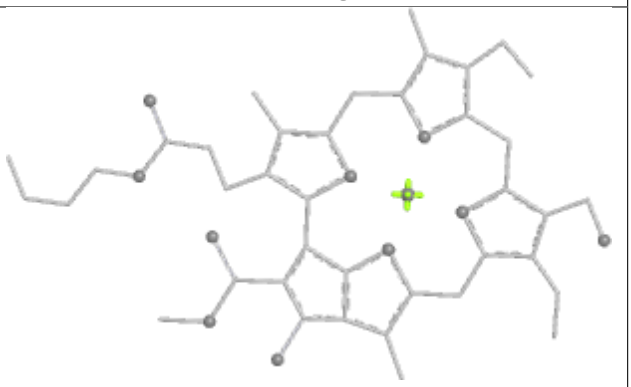
 Bond lengths	 Bond angles
 Torsions	Rings

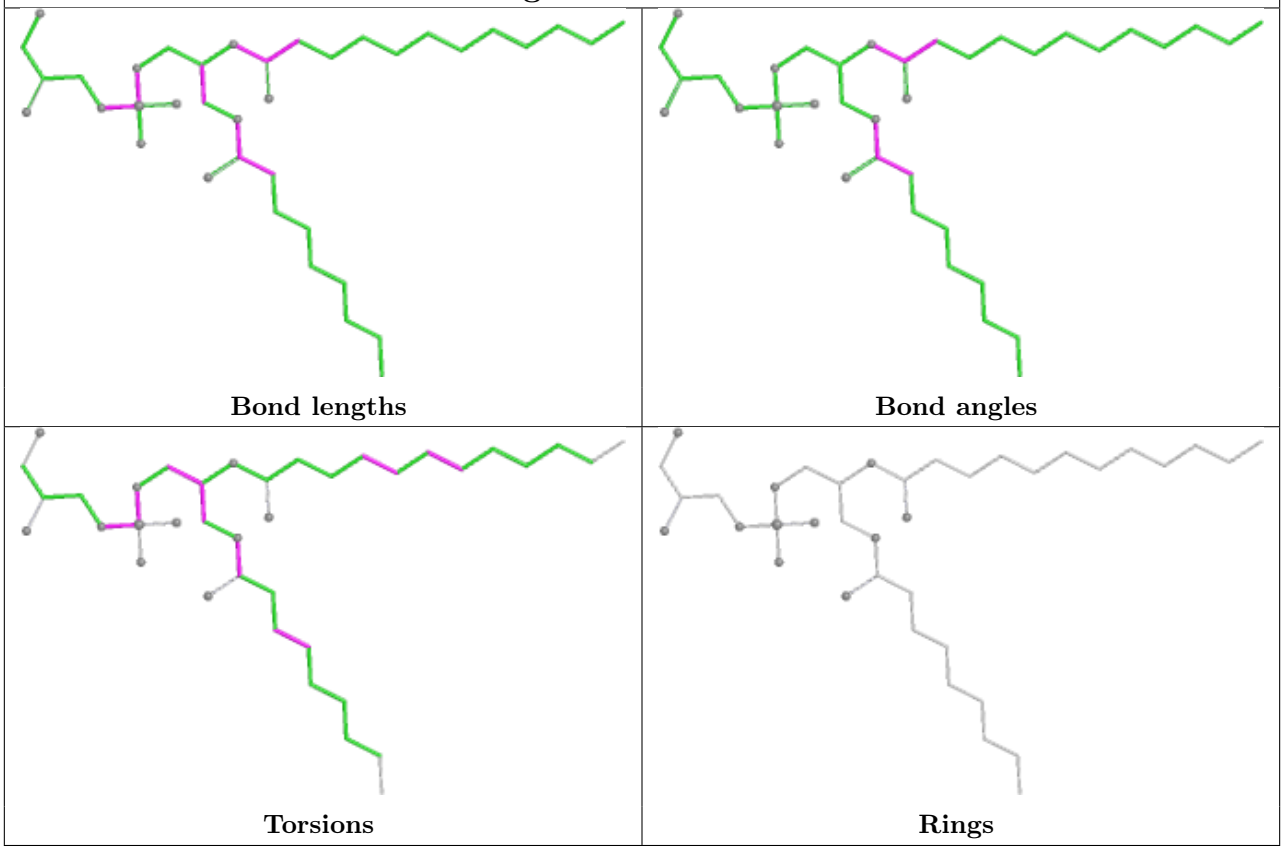
Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

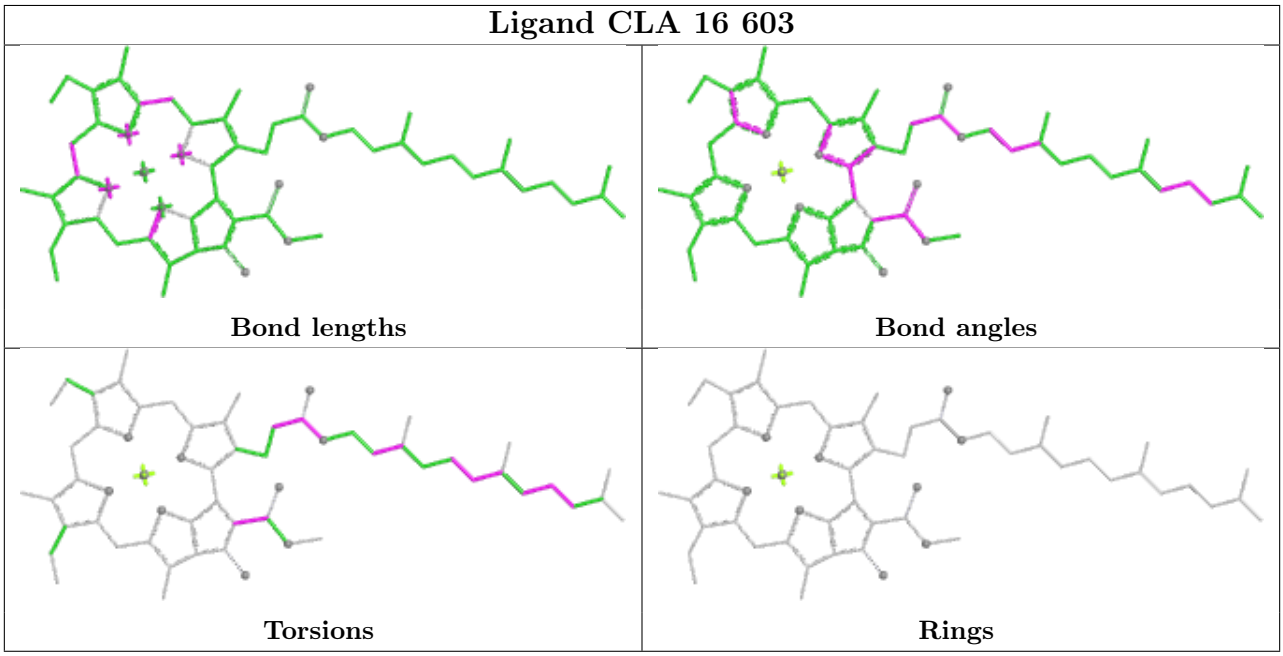
Ligand CHL 13 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG R 618



Ligand CLA 16 603



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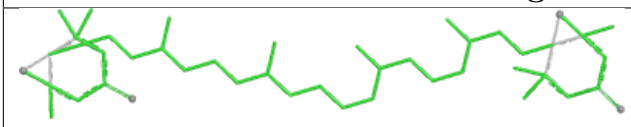
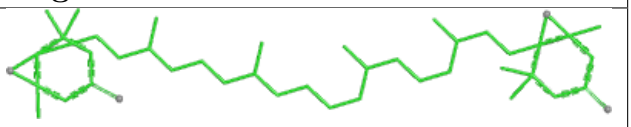
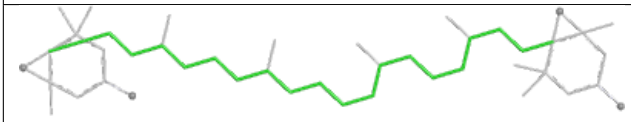
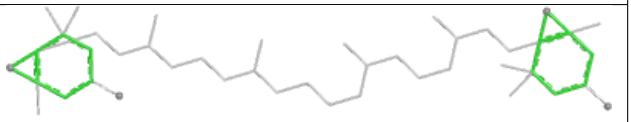
 Bond lengths	 Bond angles
 Torsions	 Rings

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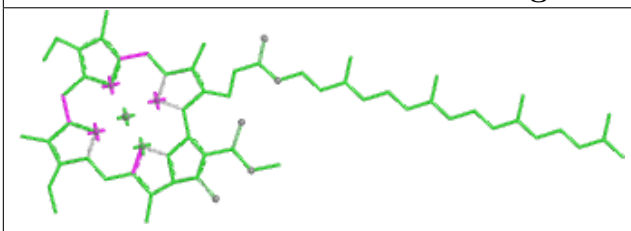
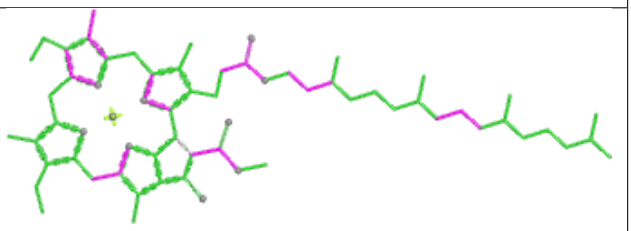
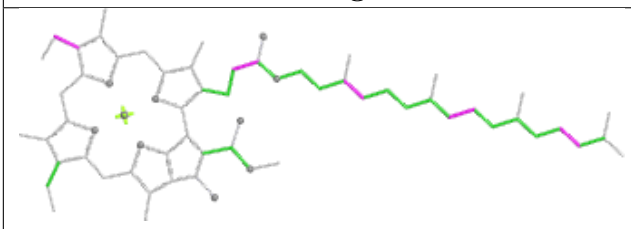
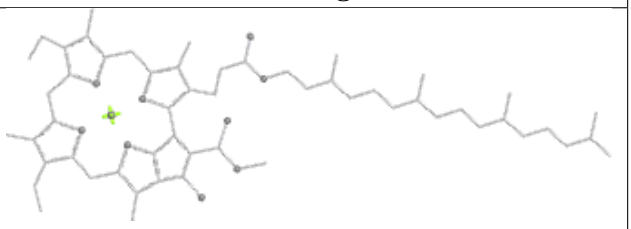
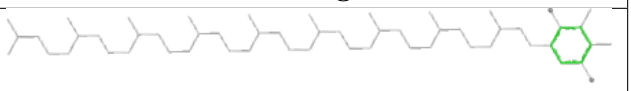
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 d 407	
Bond lengths	Bond angles
Torsions	 Rings

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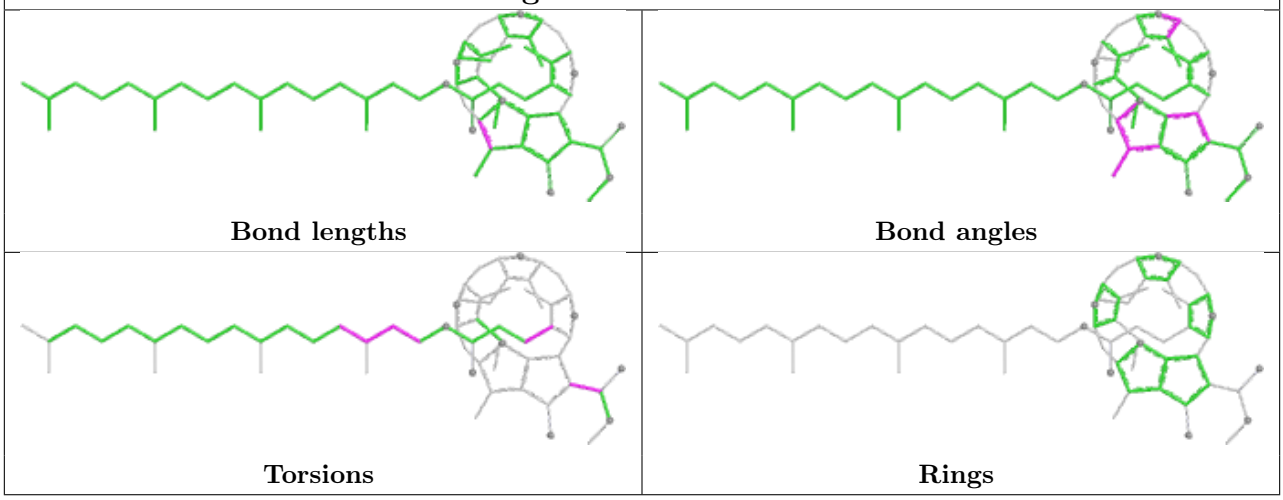

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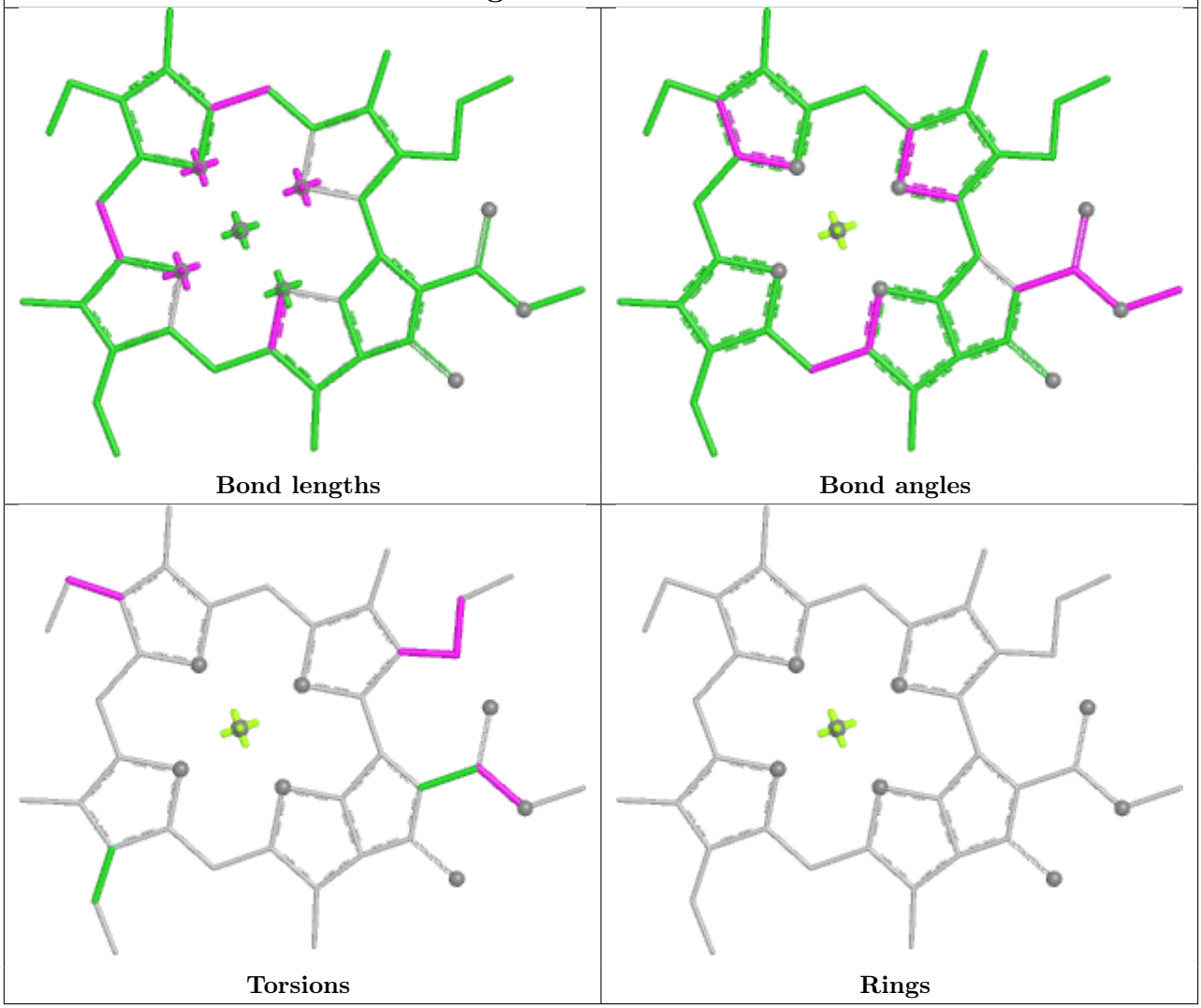

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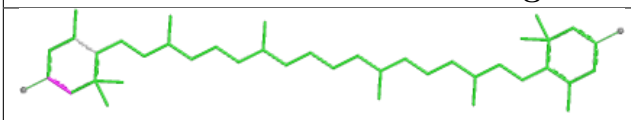
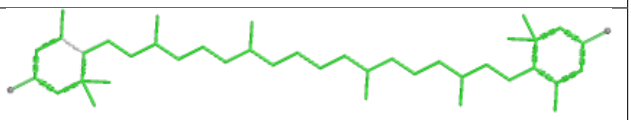
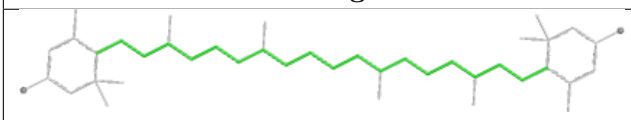


Bond lengths



Bond angles



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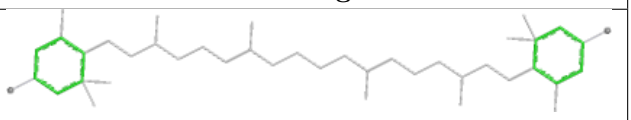
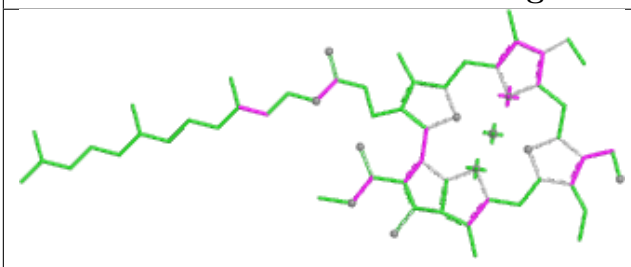
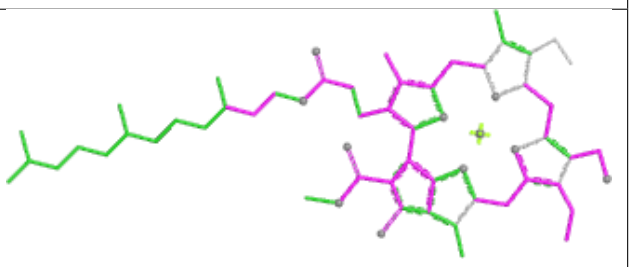


Rings

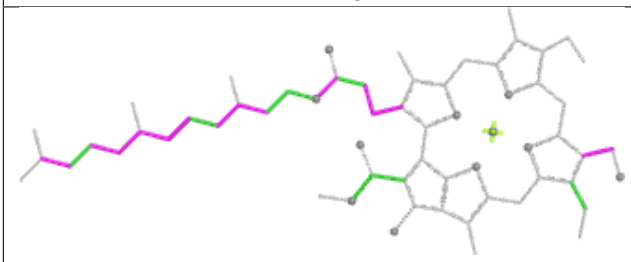
Ligand CHL n 606



Bond lengths



Bond angles



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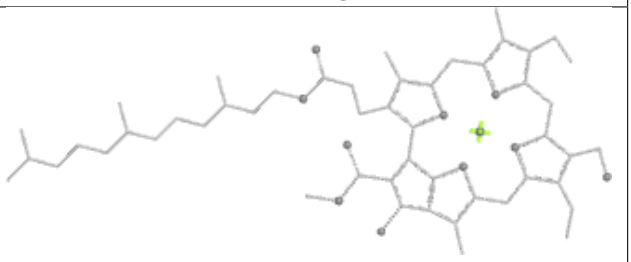
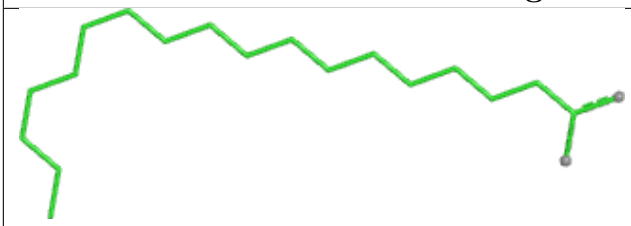


Rings

Ligand LNL Y 620



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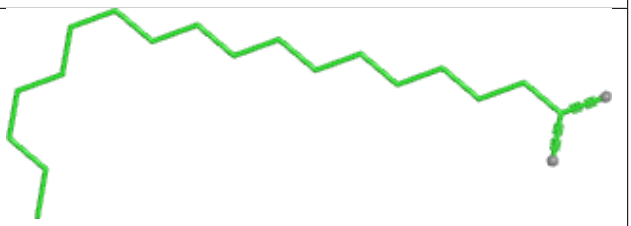
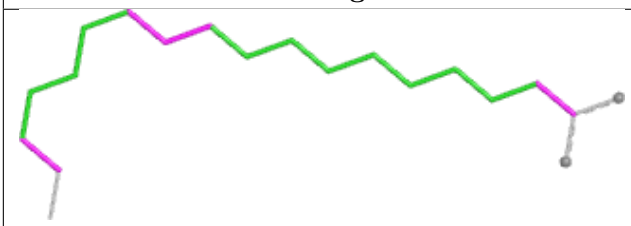


Bond angles



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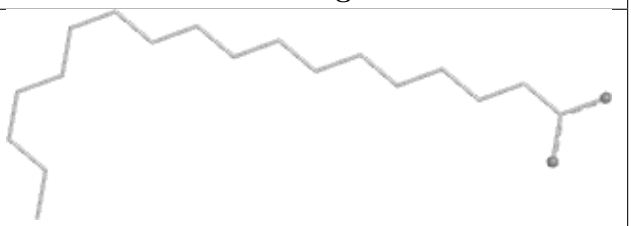
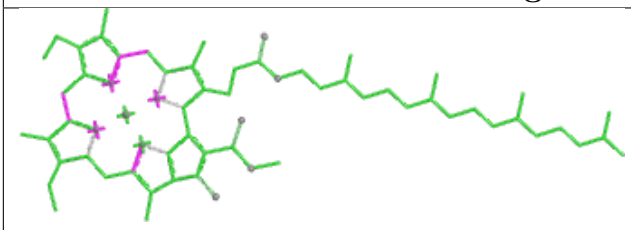
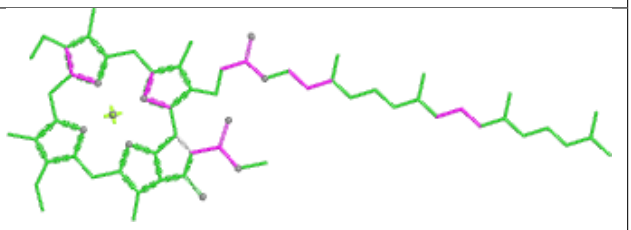
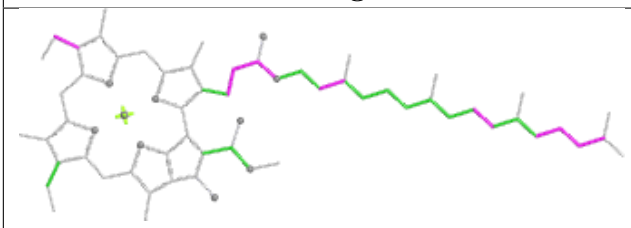
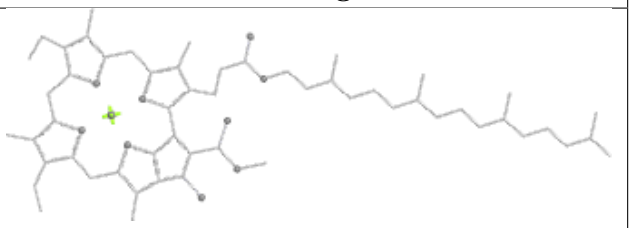


Rings

Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

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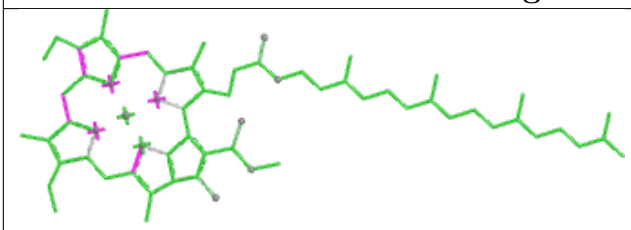
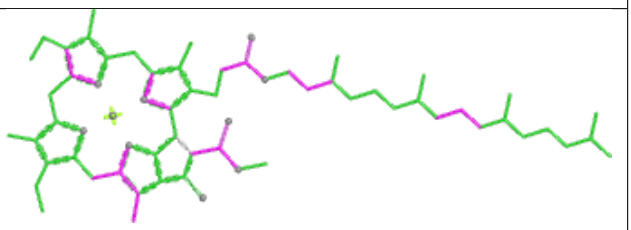
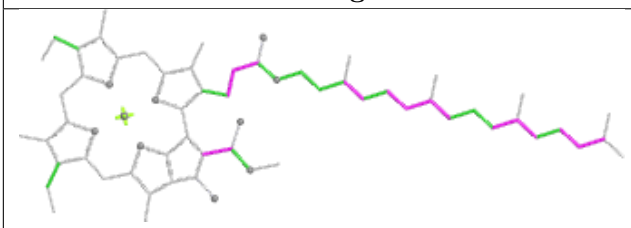
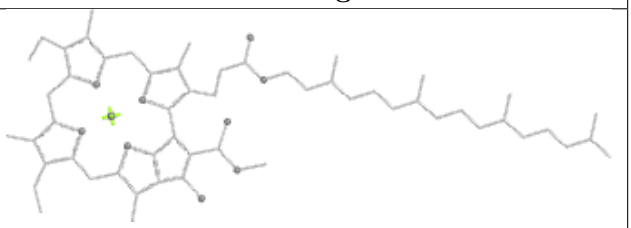
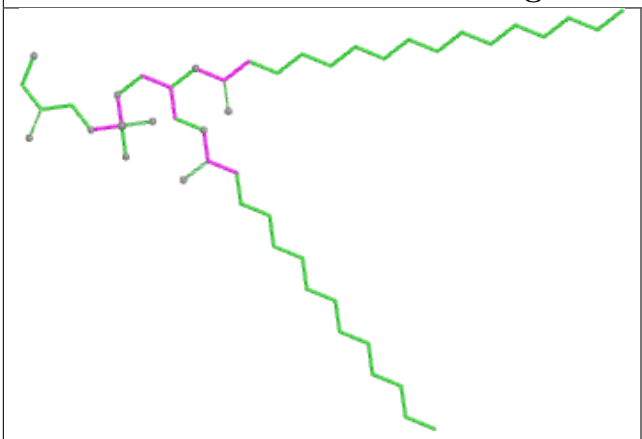
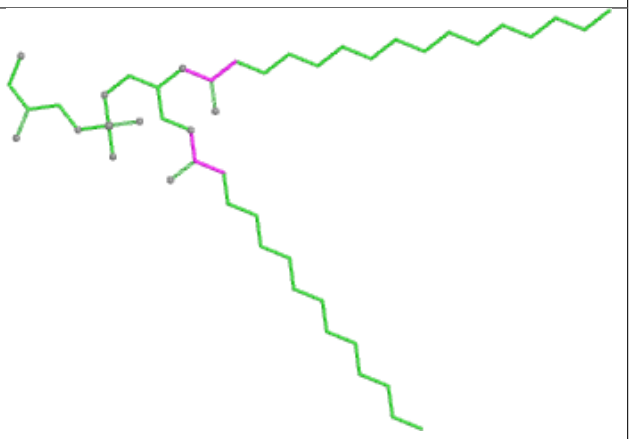
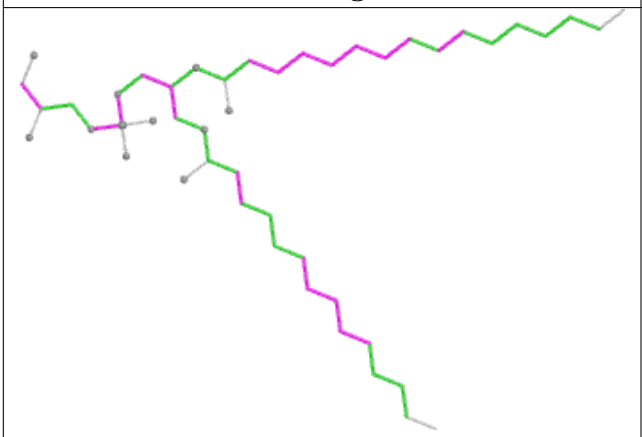
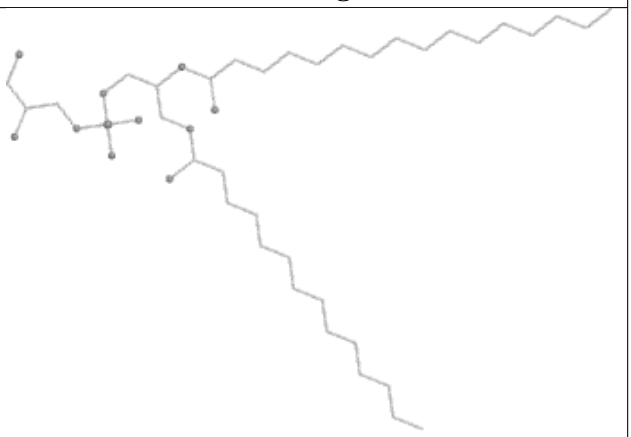
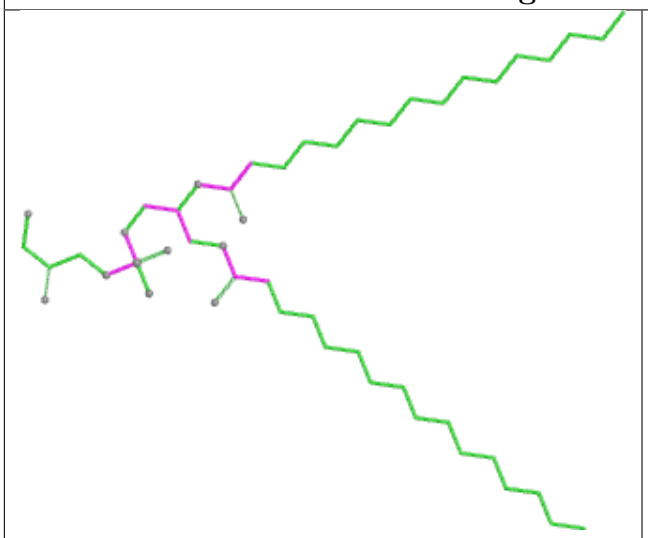
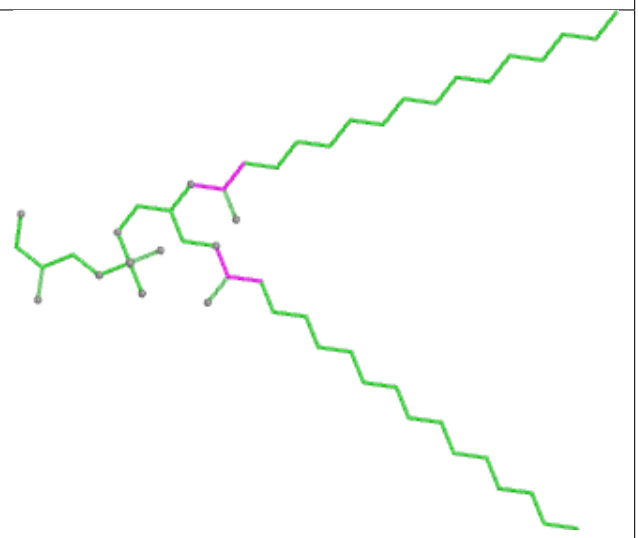
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG L 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

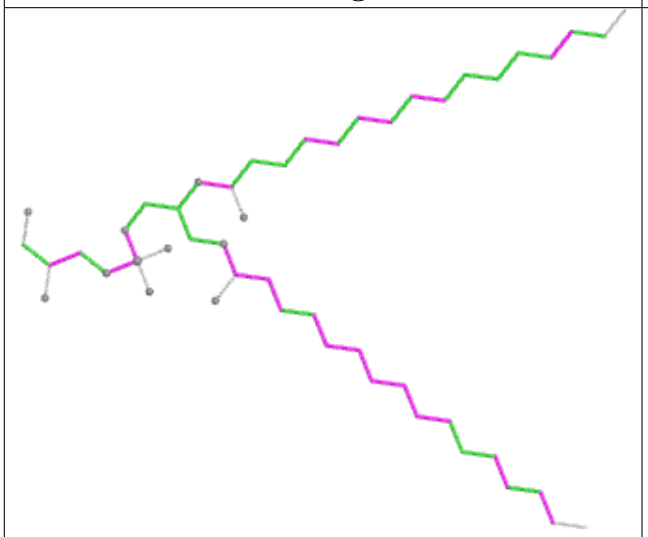
Ligand LHG 14 615



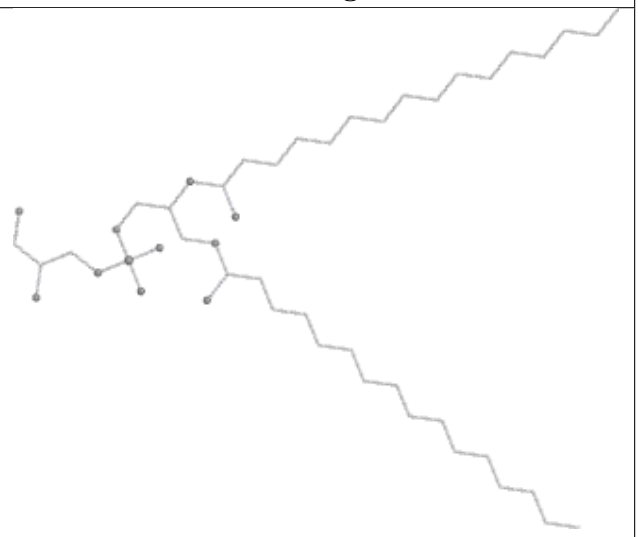
Bond lengths



Bond angles



Torsions



Rings

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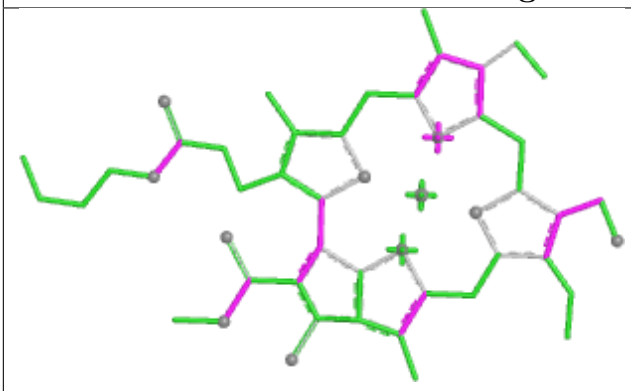
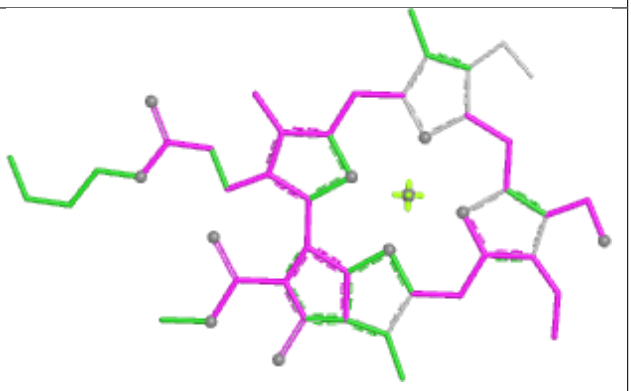
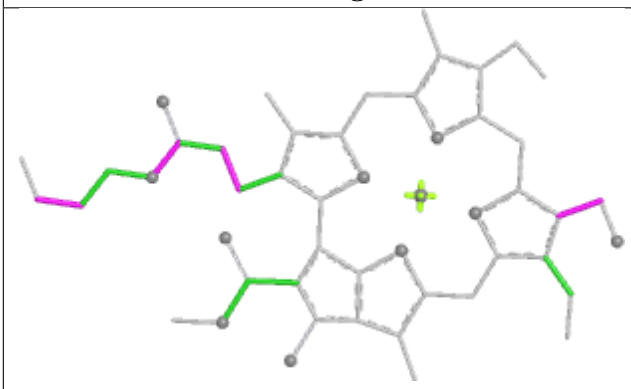
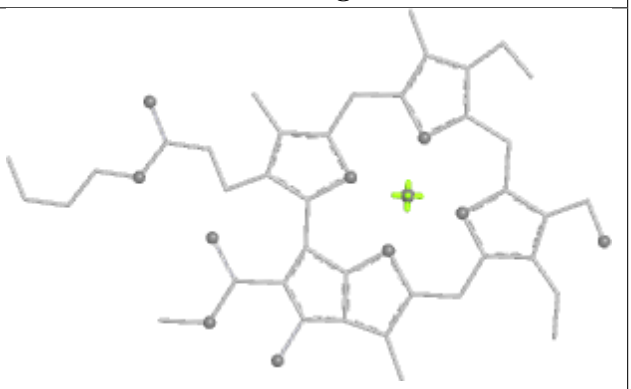
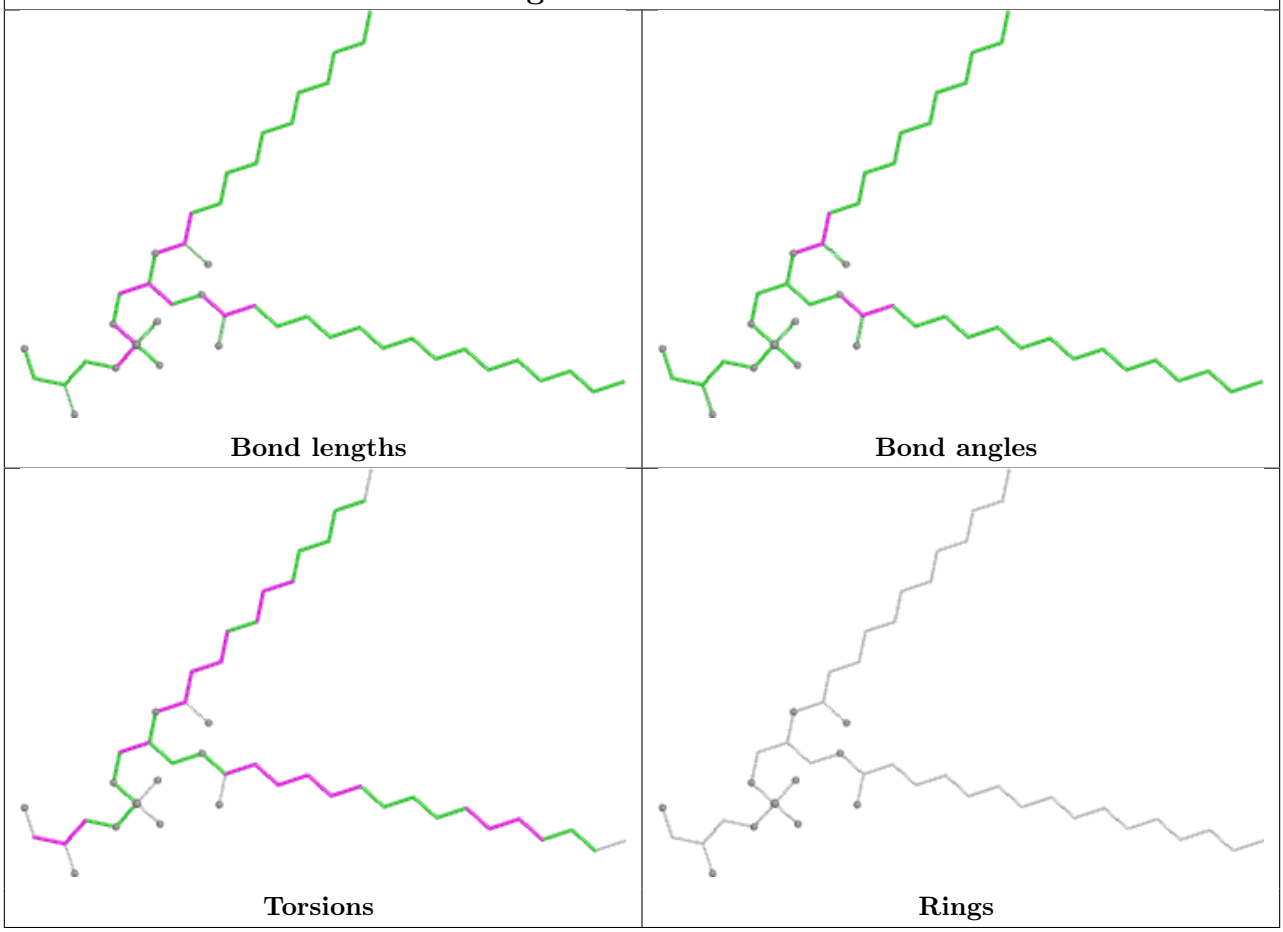
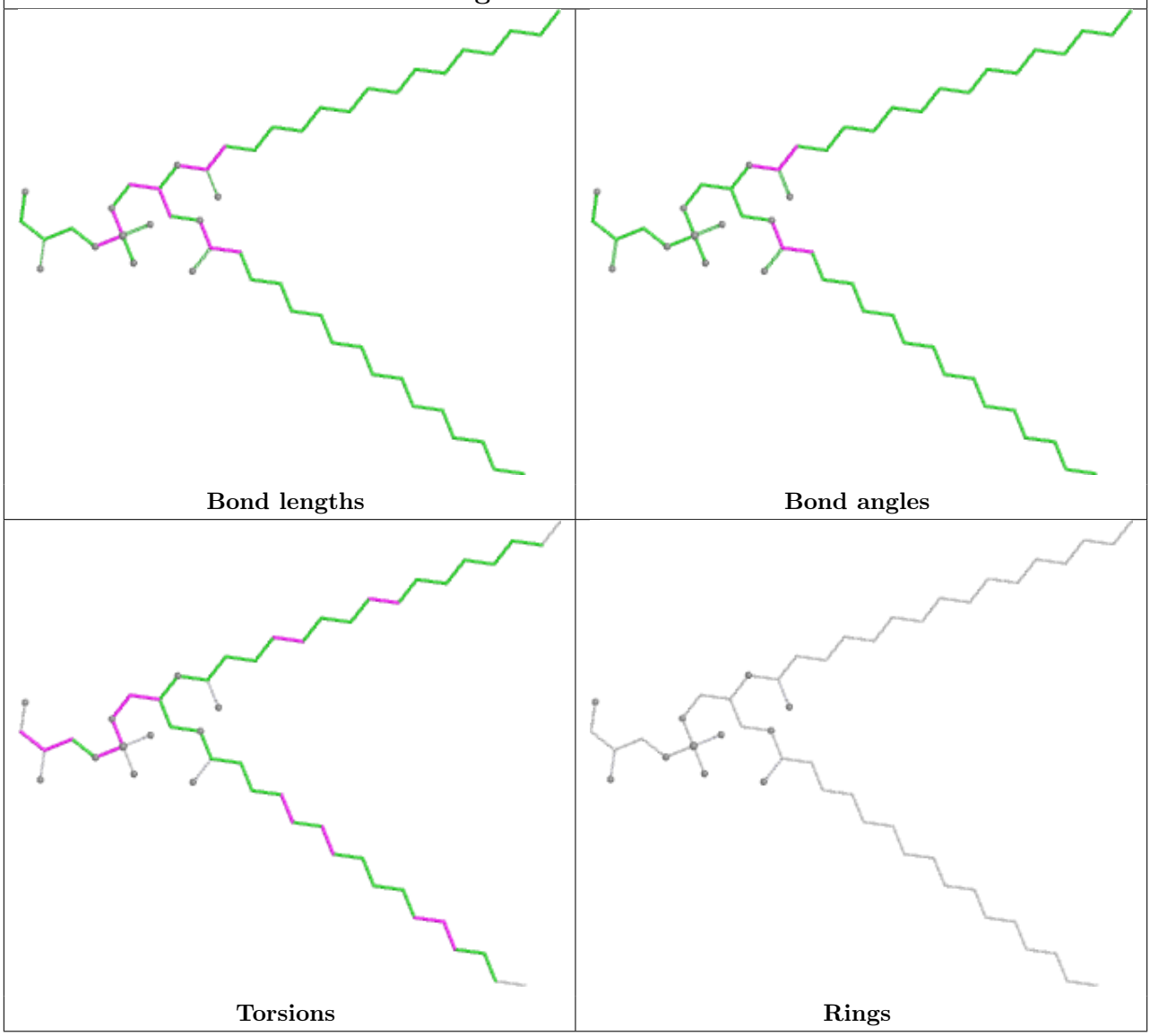
 Bond lengths	 Bond angles
 Torsions	 Rings

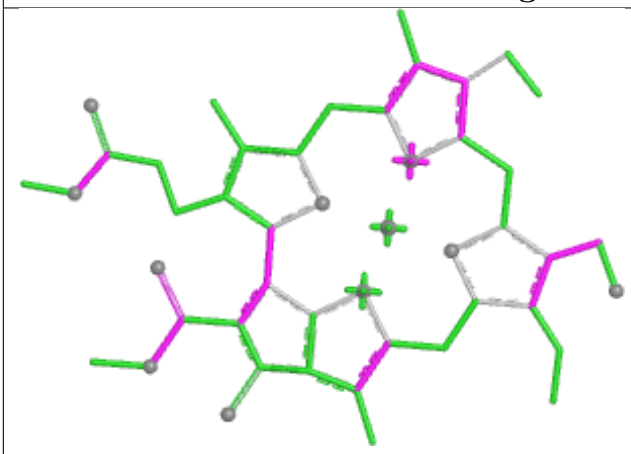
Ligand LHG S 617



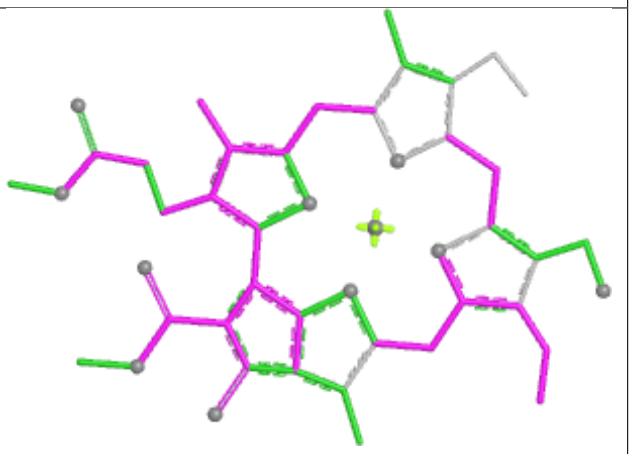
Ligand LHG s 621



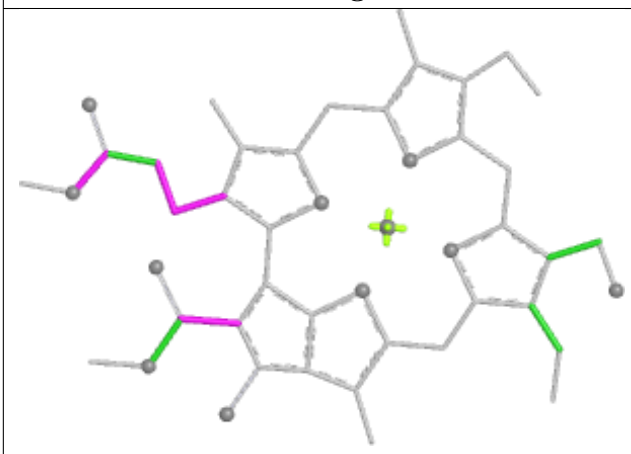
Ligand CHL 14 606



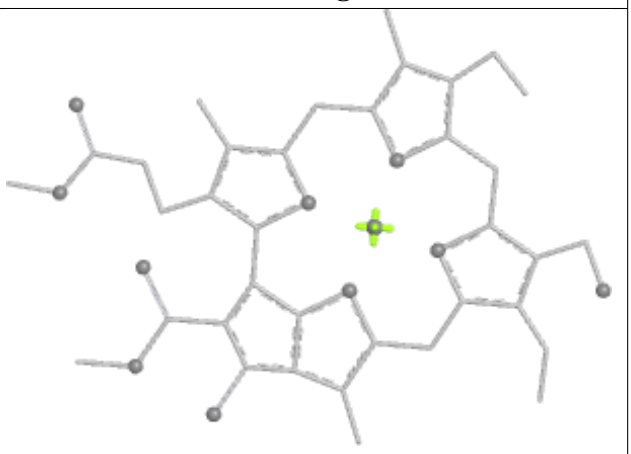
Bond lengths



Bond angles



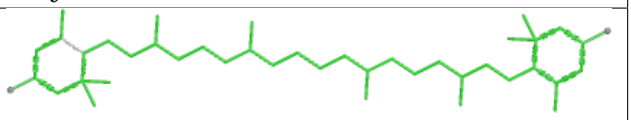
Torsions



Rings

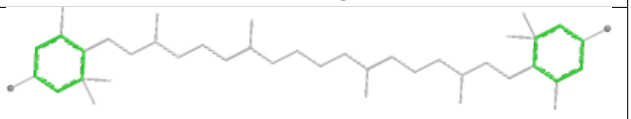
Ligand LUT y 623

Bond lengths

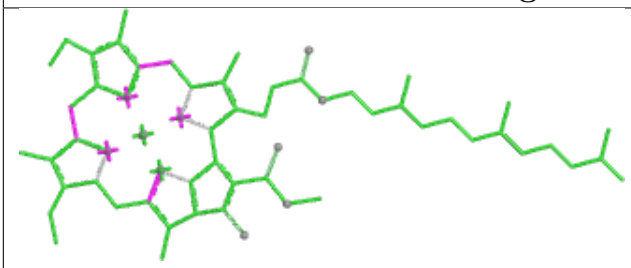
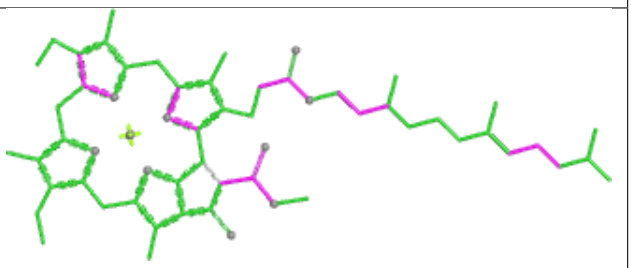
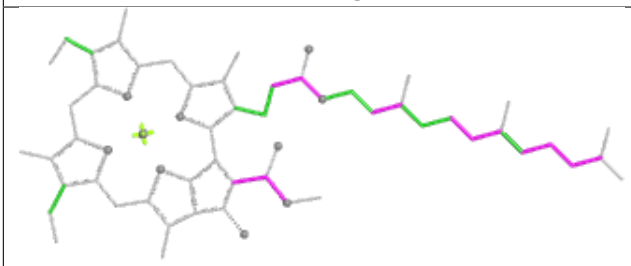
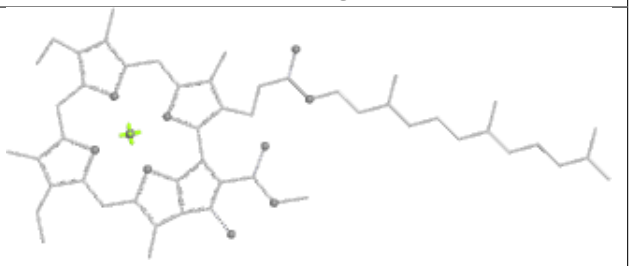


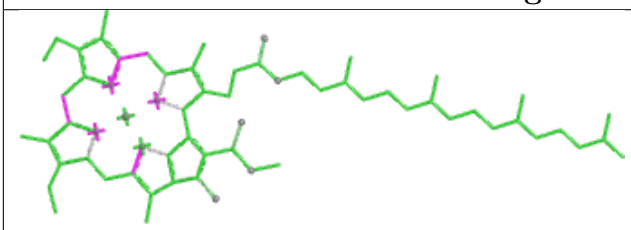
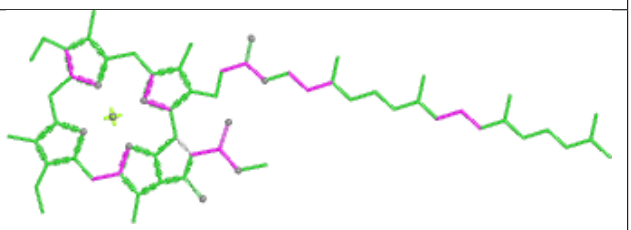
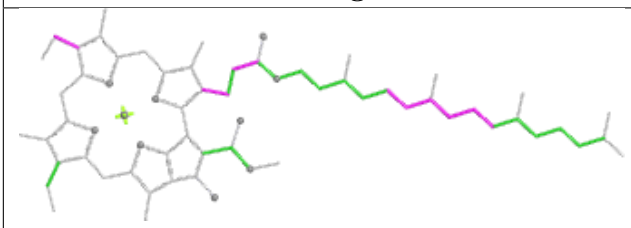
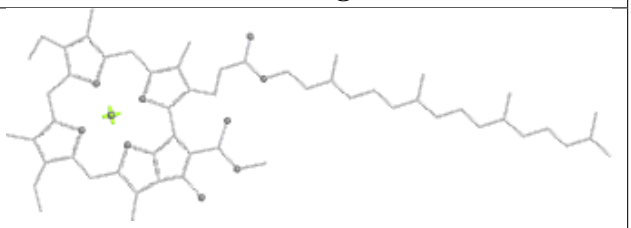
Bond angles

Torsions



Rings

Ligand CLA 13 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

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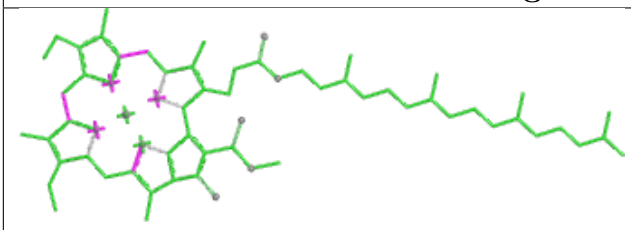
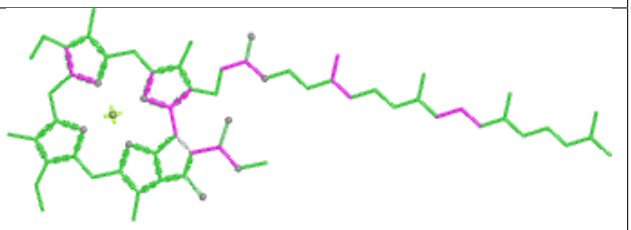
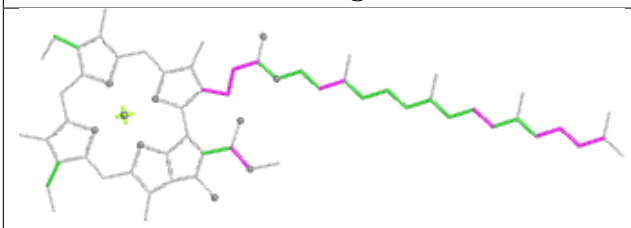
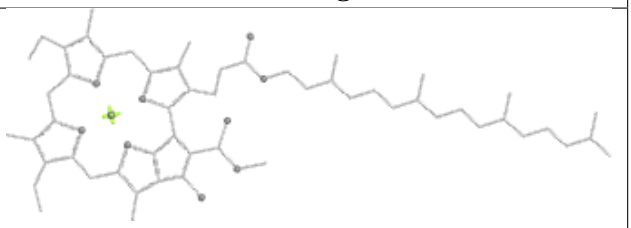
 Bond lengths	 Bond angles
 Torsions	 Rings

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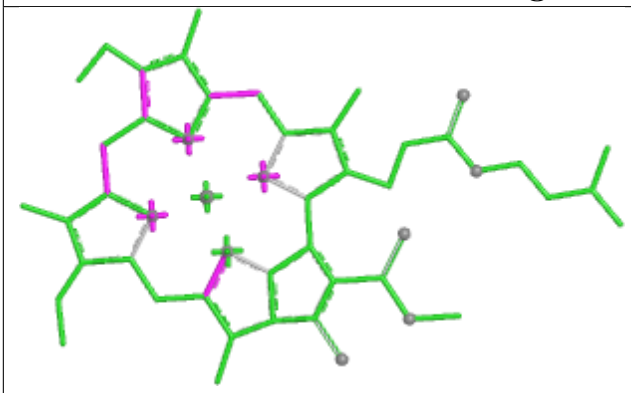
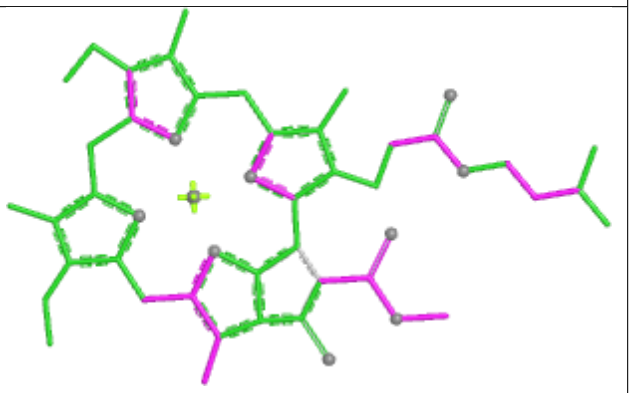
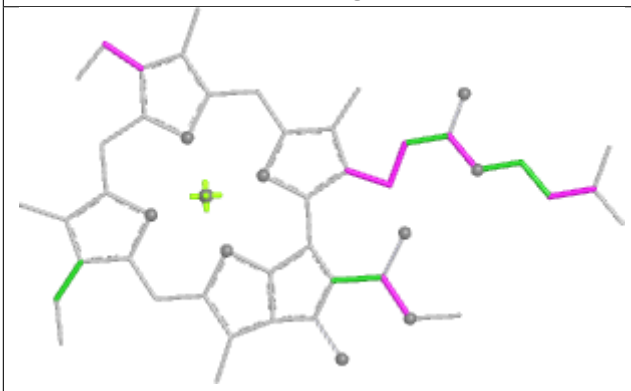
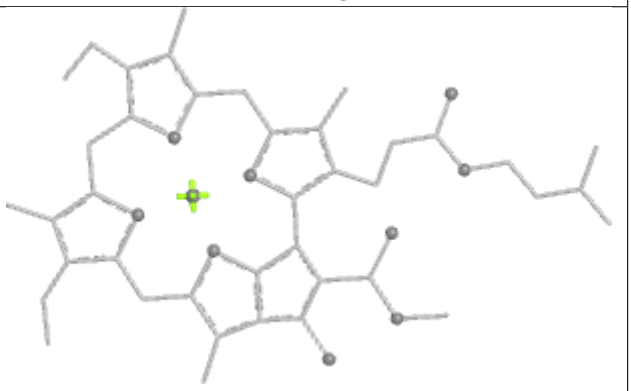
 Bond lengths	 Bond angles
 Torsions	 Rings

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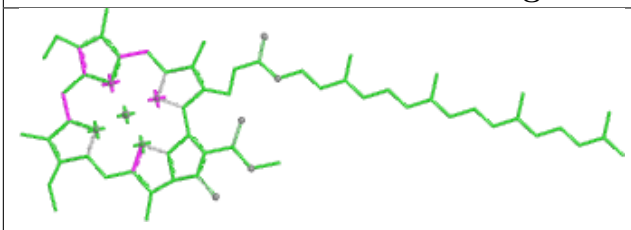

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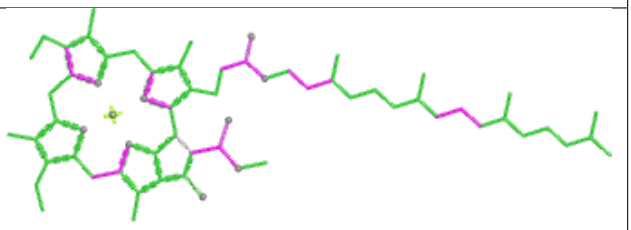
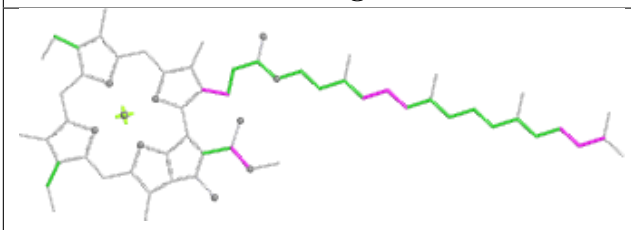


Bond angles



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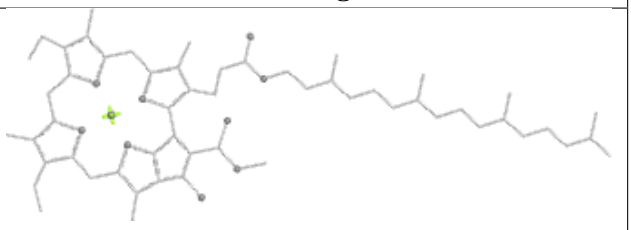
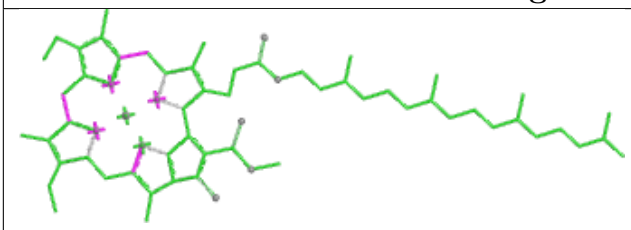


Rings

Ligand CLA c 506



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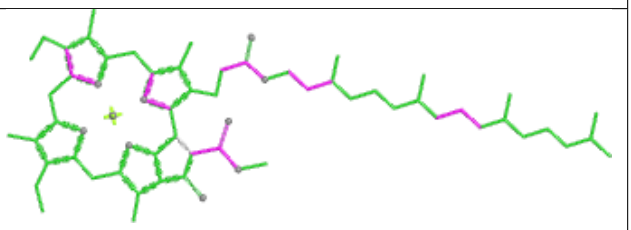
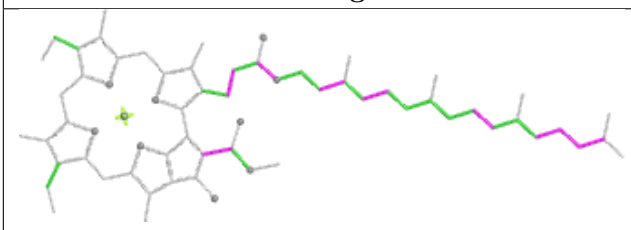


Bond angles



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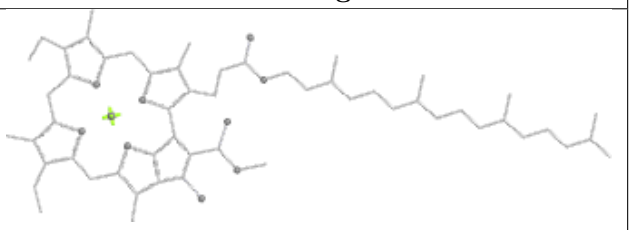
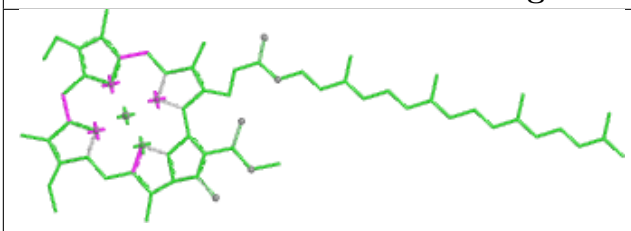


Rings

Ligand CLA d 405



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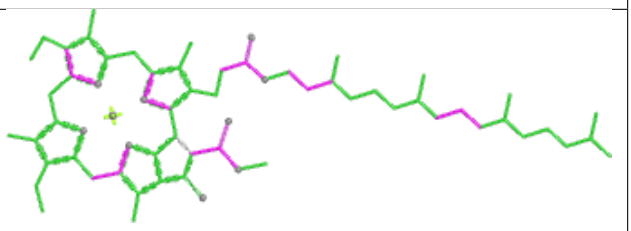

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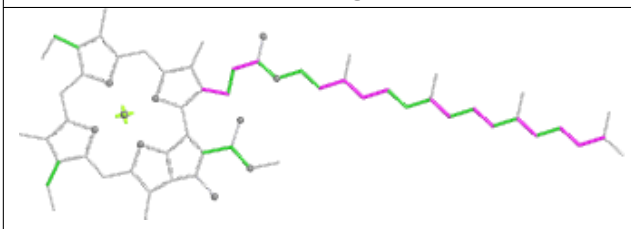

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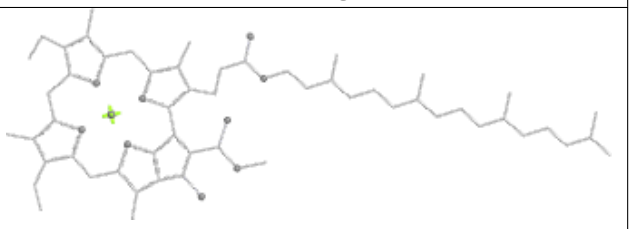
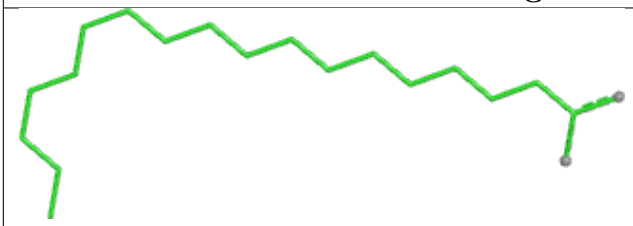


Rings

Ligand LNL H 101



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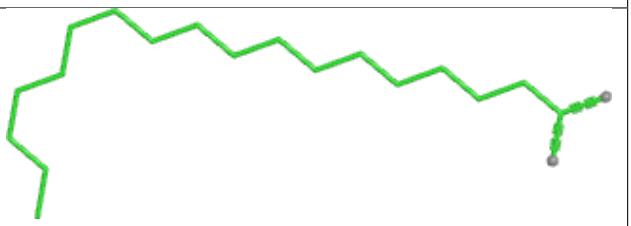
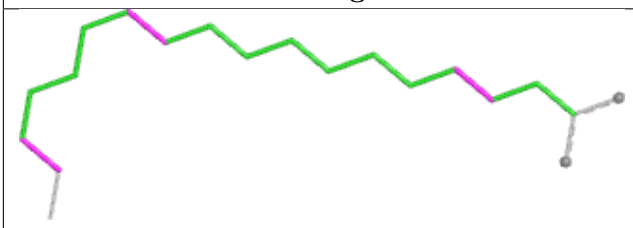


Bond angles



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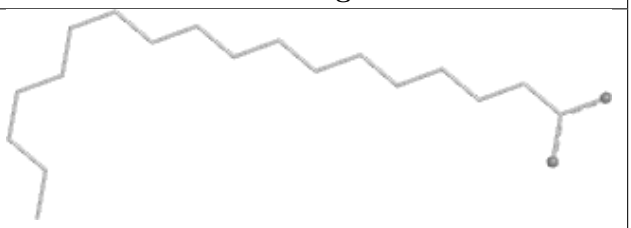
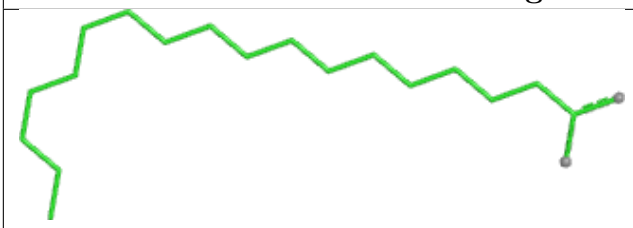


Rings

Ligand LNL X 201



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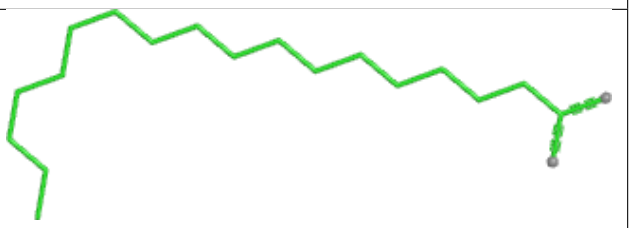

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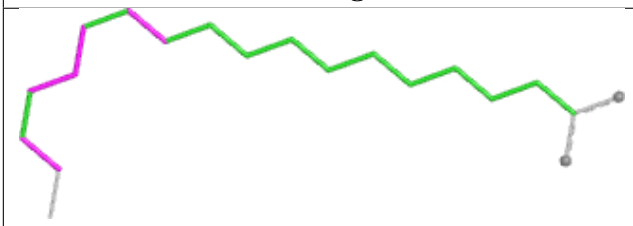

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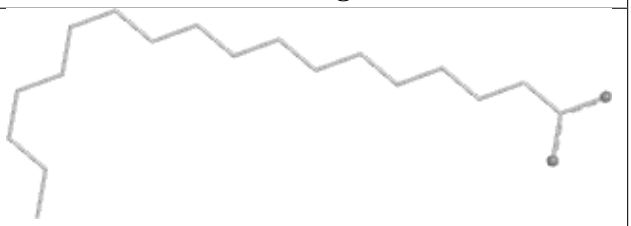
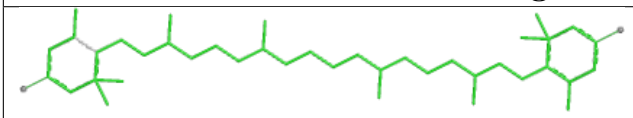


Rings

Ligand LUT s 618



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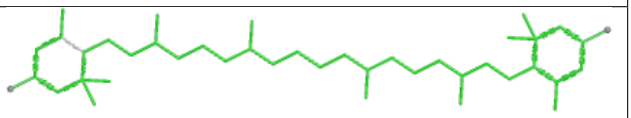

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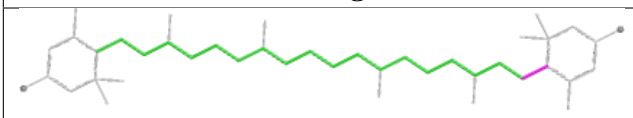

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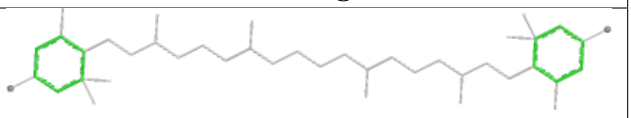

Rings

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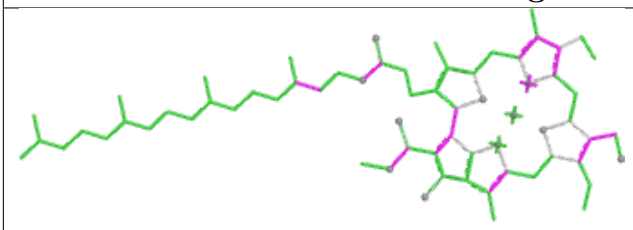

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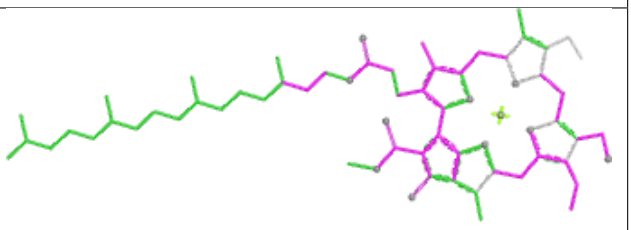
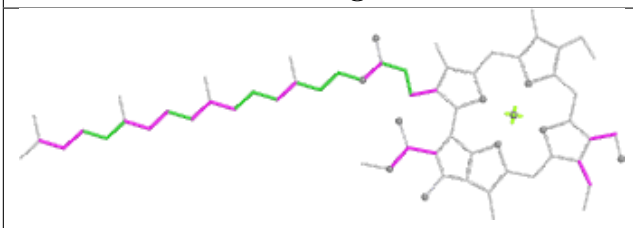


Bond angles



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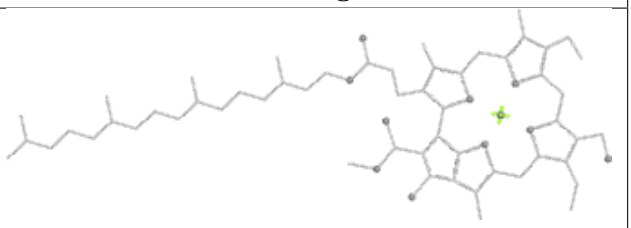

Rings

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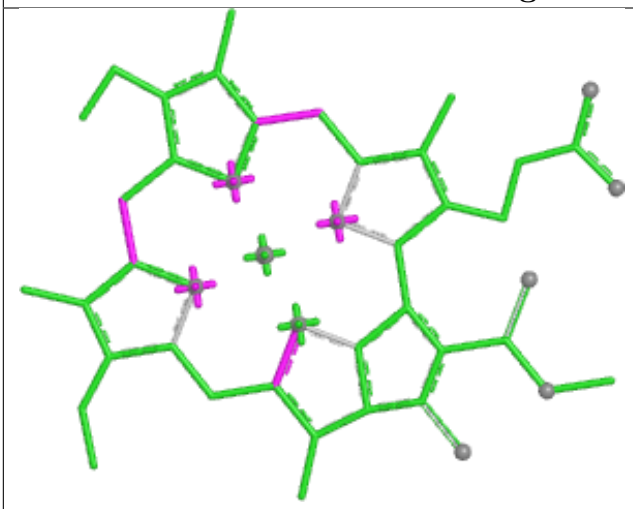

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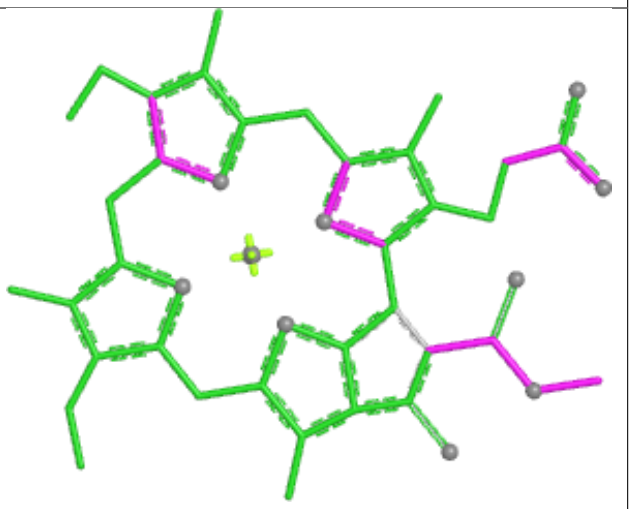
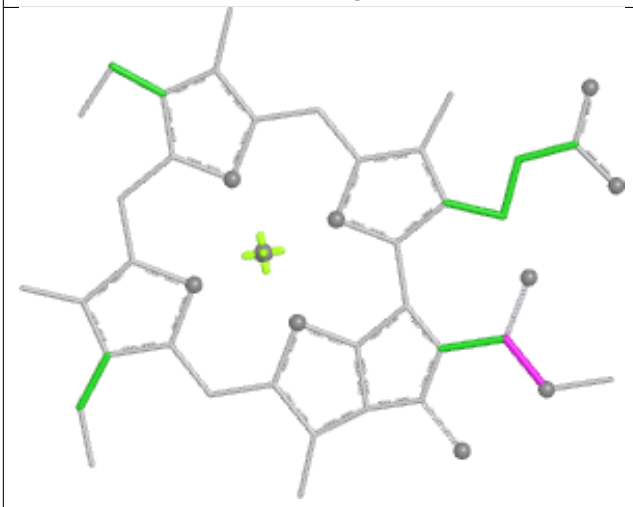


Bond angles



Torsions

Rings

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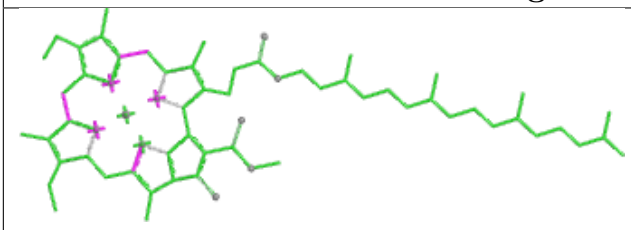
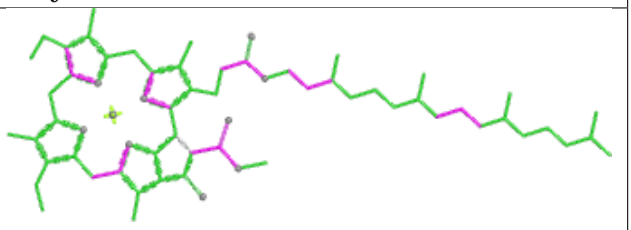
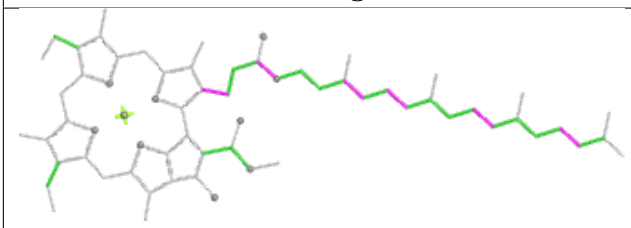
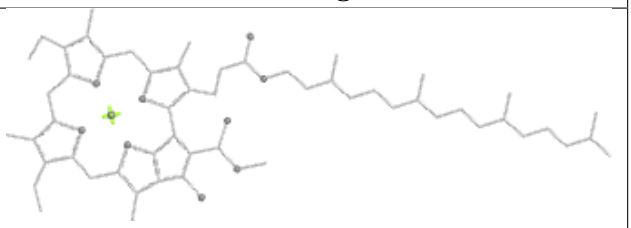
 Bond lengths	 Bond angles
 Torsions	 Rings

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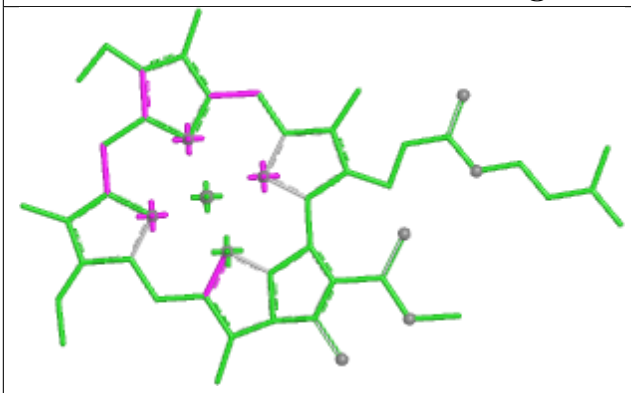
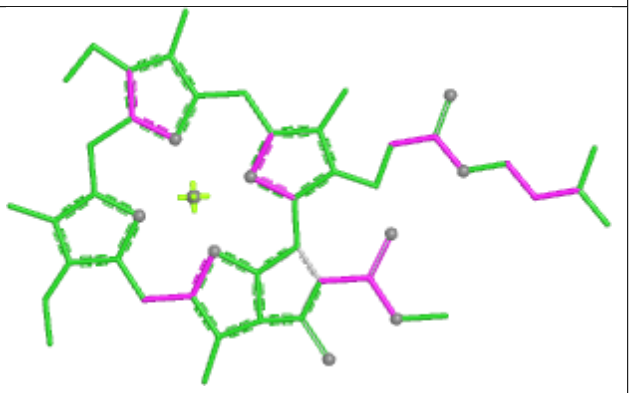
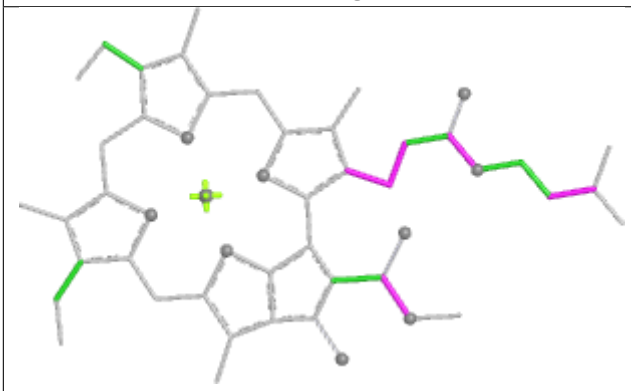
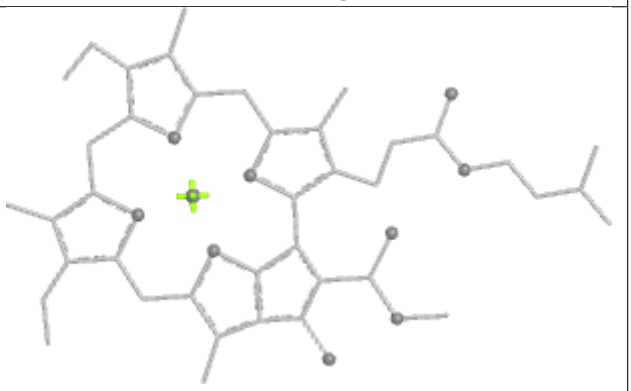
 Bond lengths	 Bond angles
 Torsions	 Rings

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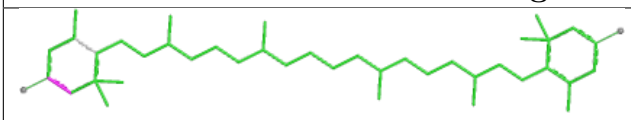
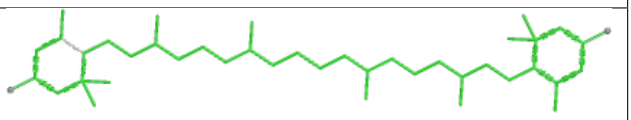
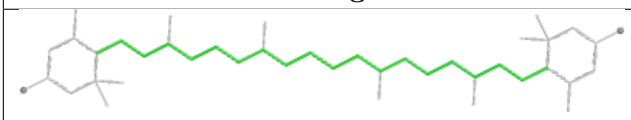
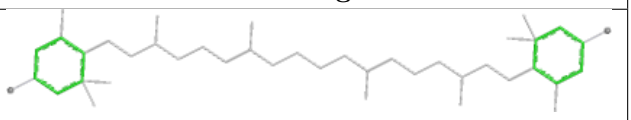
 Bond lengths	 Bond angles
 Torsions	 Rings

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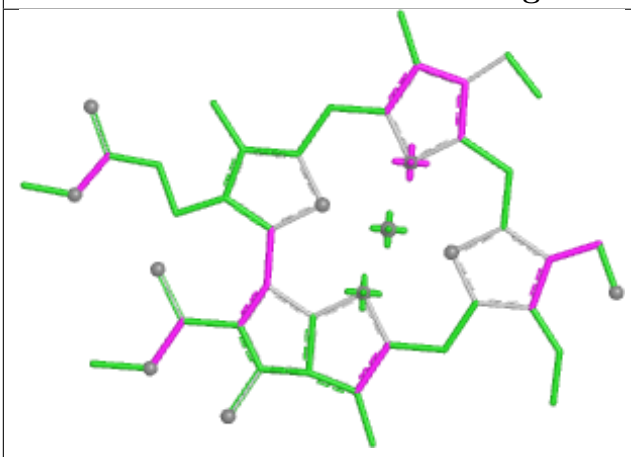
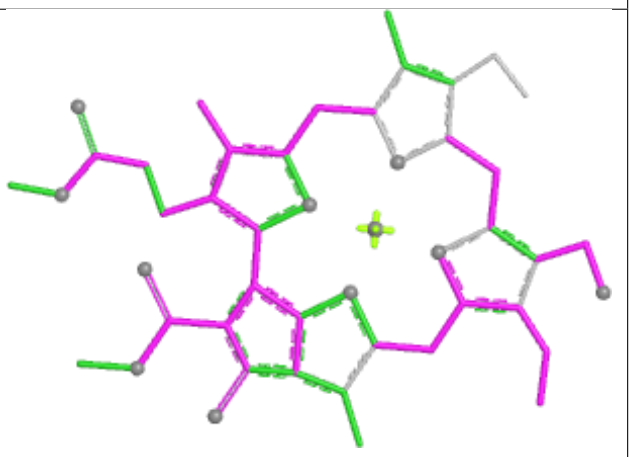
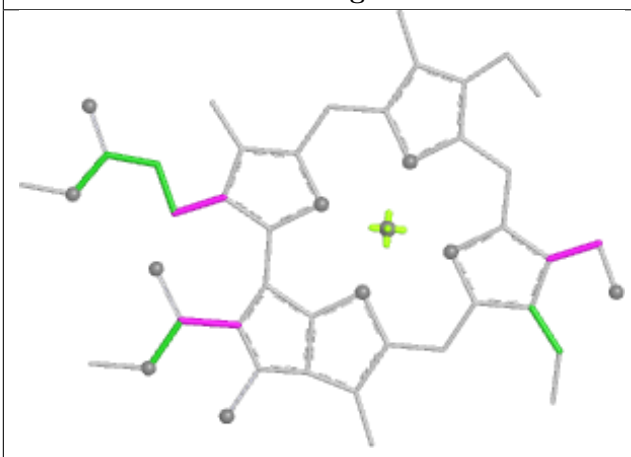
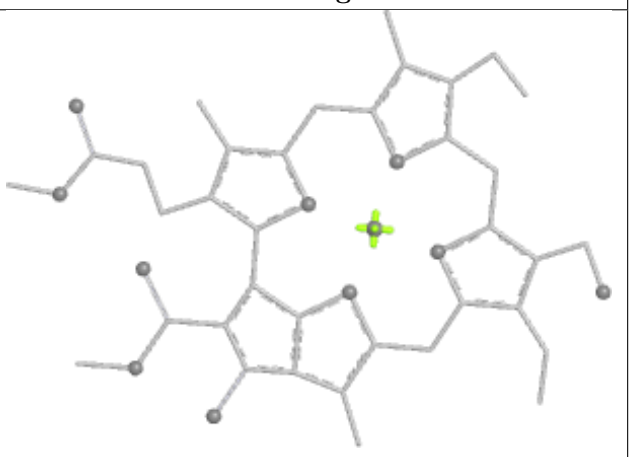
 Bond lengths	 Bond angles
 Torsions	 Rings

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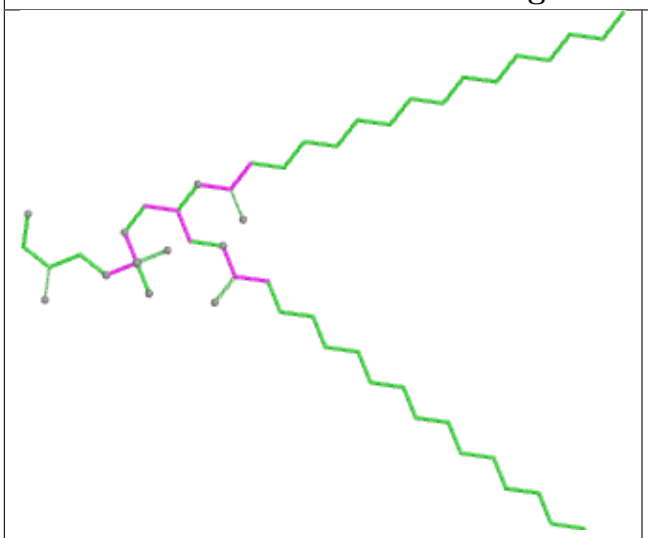

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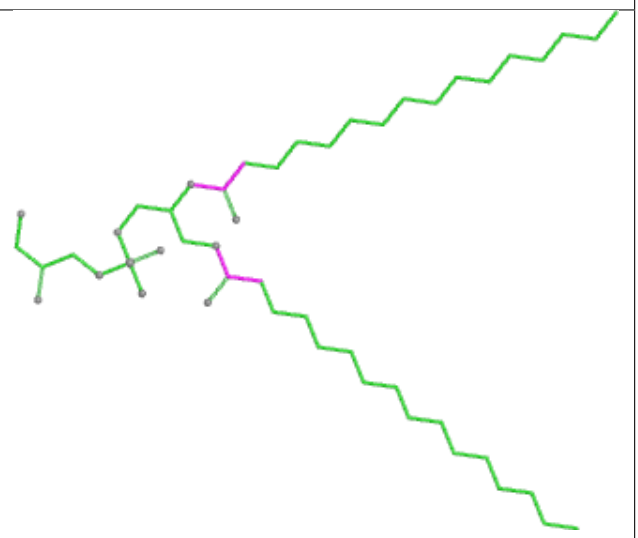

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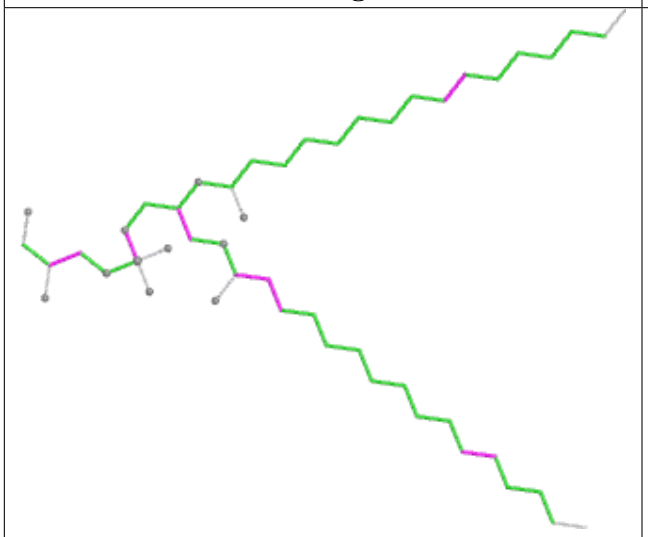

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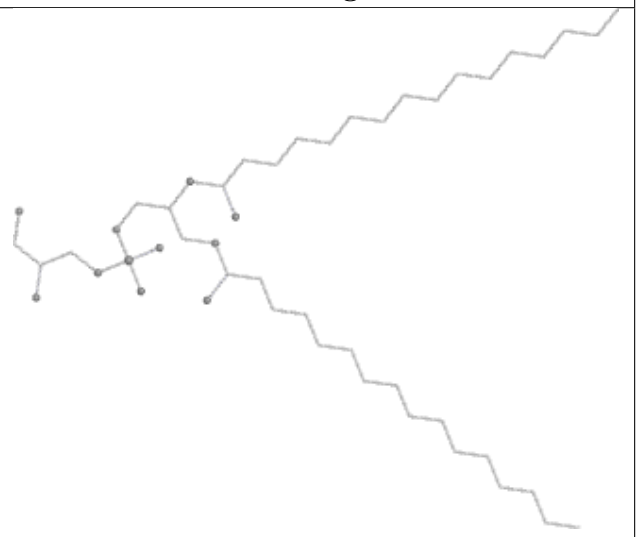


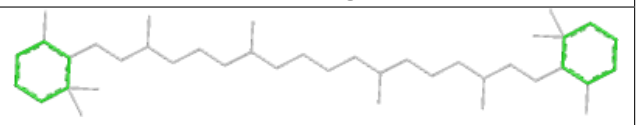
Rings

Ligand BCR C 516

Bond lengths

Bond angles

Torsions



Rings

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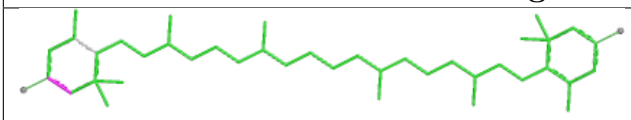

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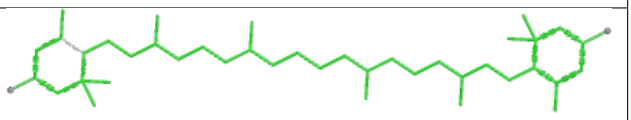

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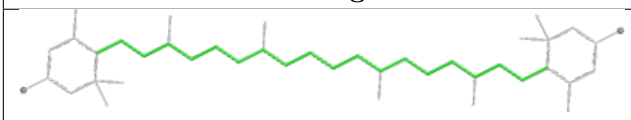

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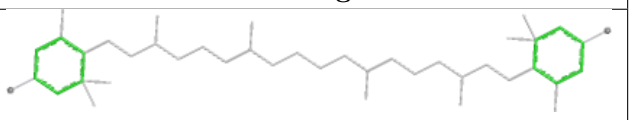

Rings

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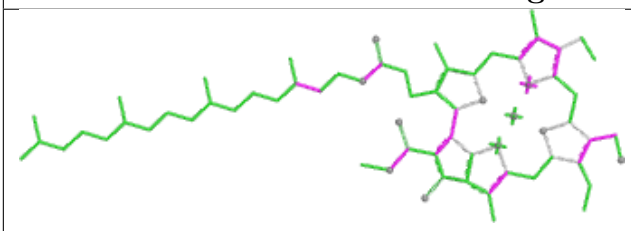

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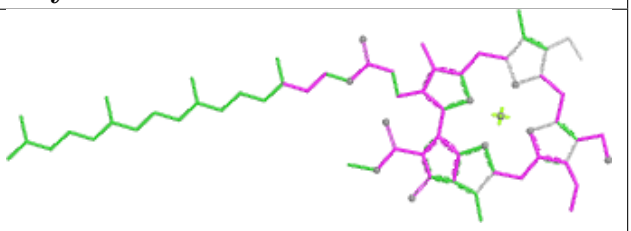

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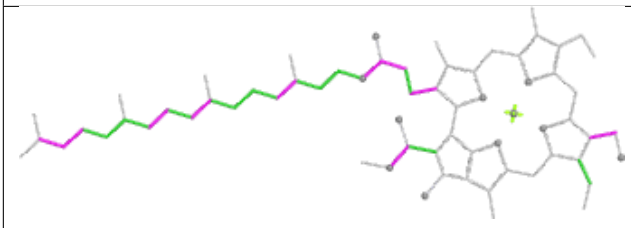

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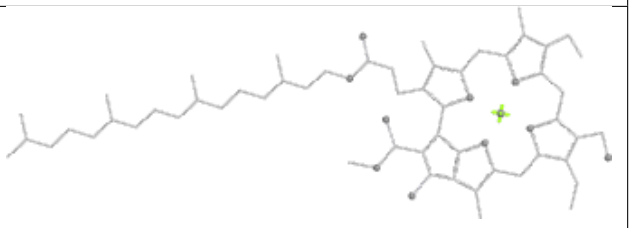

Rings

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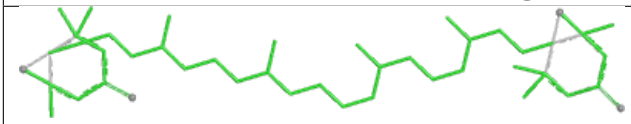

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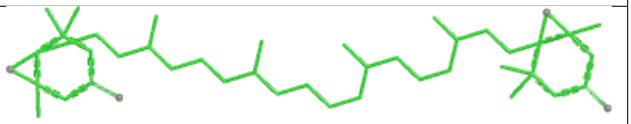

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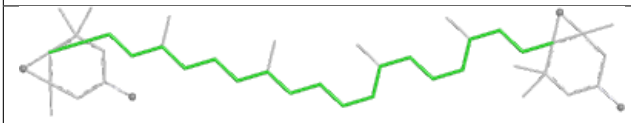

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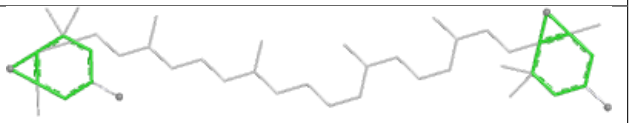

Rings

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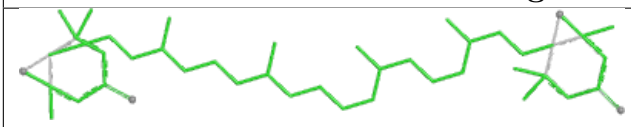

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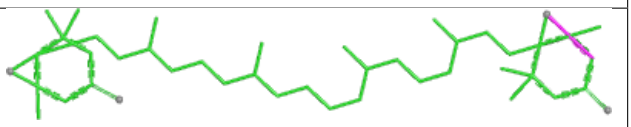

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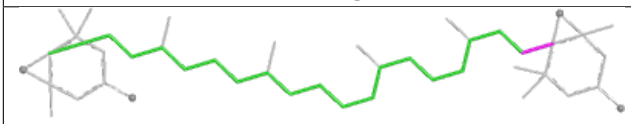

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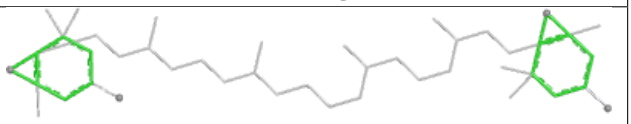

Rings

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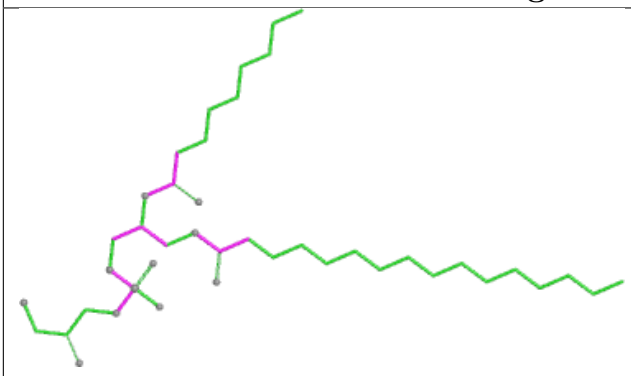
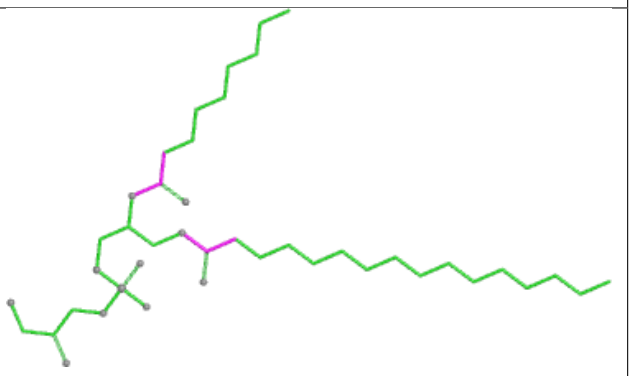
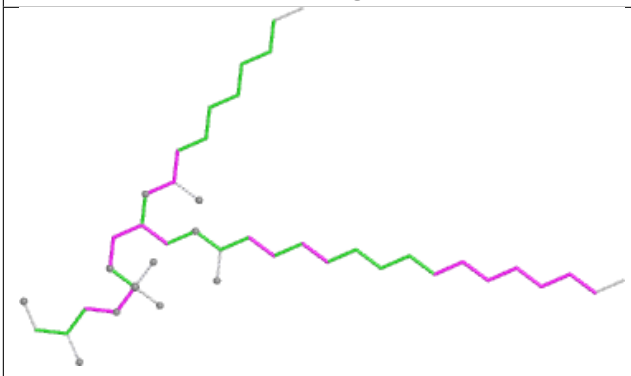
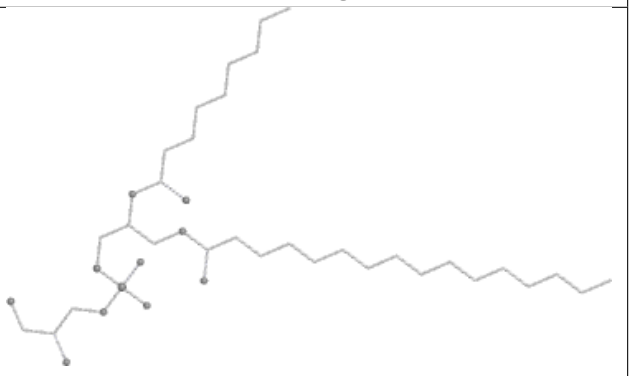
 Bond lengths	 Bond angles
 Torsions	 Rings

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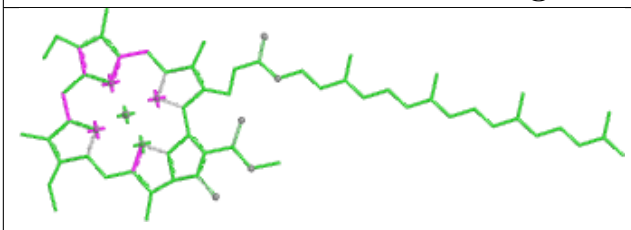
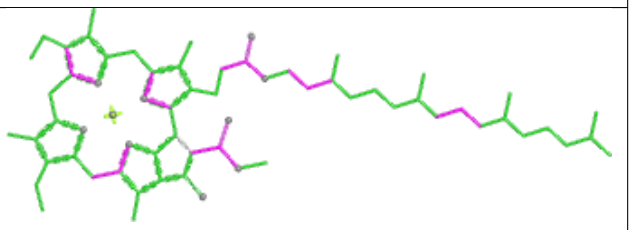
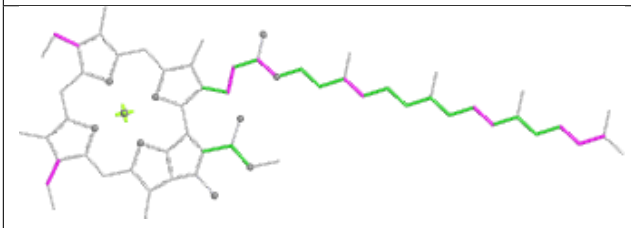
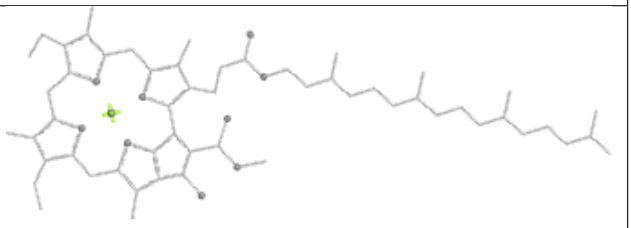
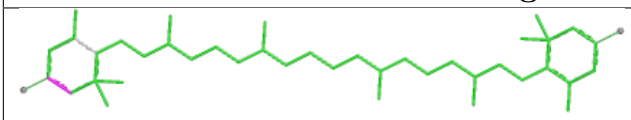
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 15 614



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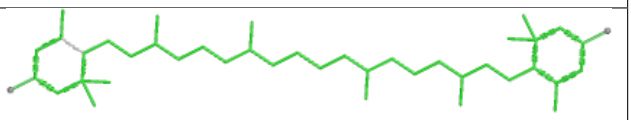

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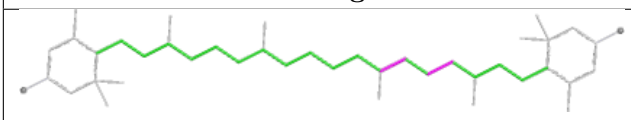

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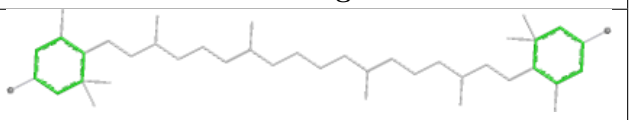

Rings

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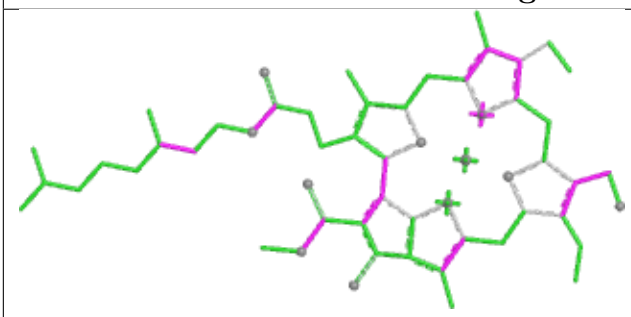

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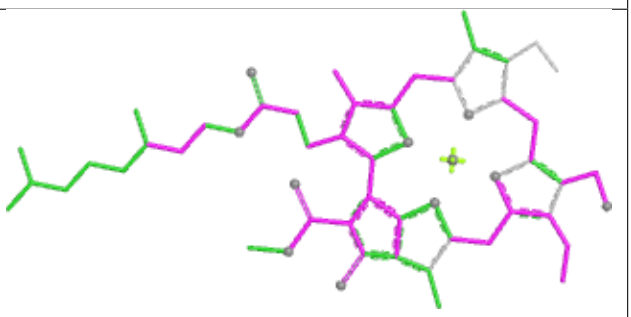

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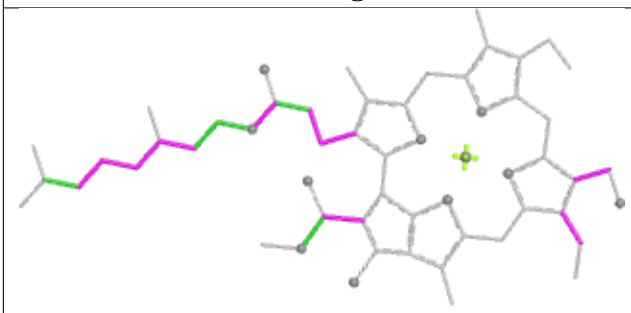

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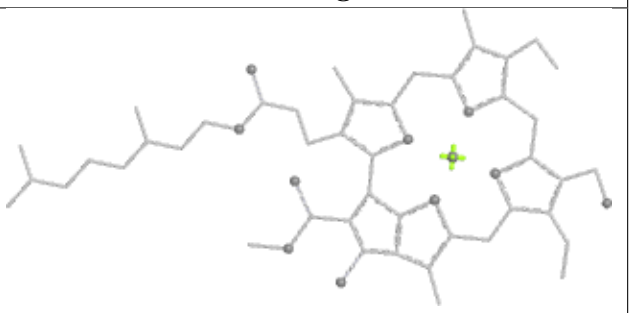
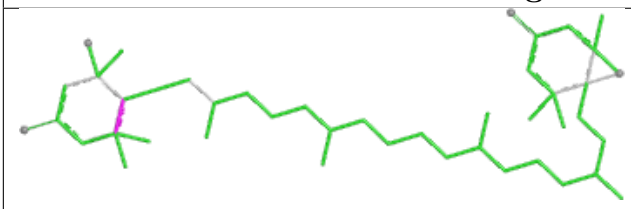


Rings

Ligand NEX S 620



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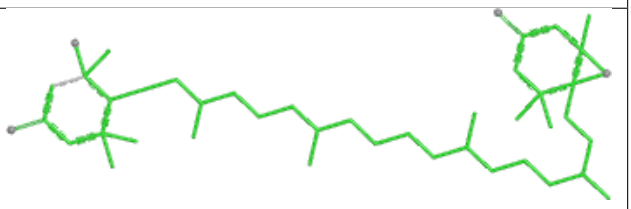
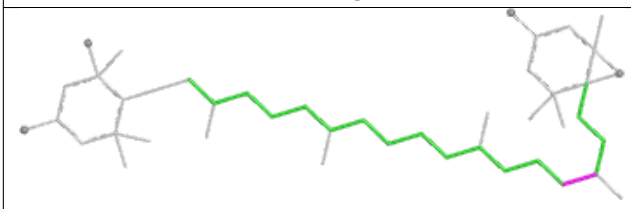
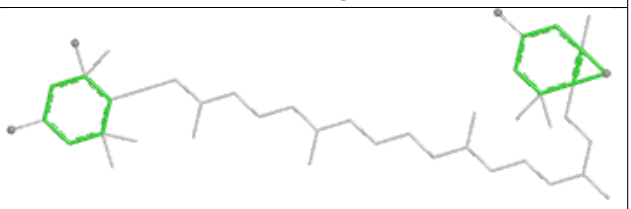


Bond angles

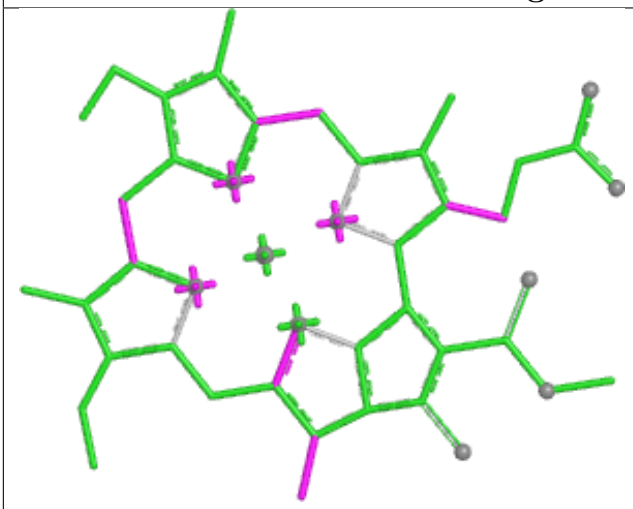


Torsions

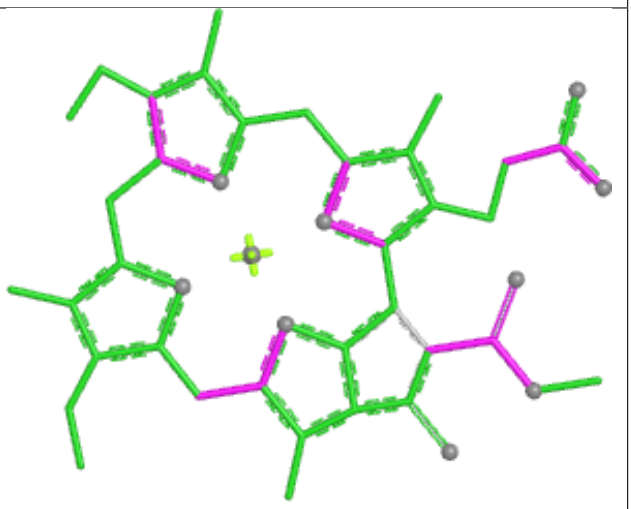


Rings

Ligand CLA n 614



Bond lengths



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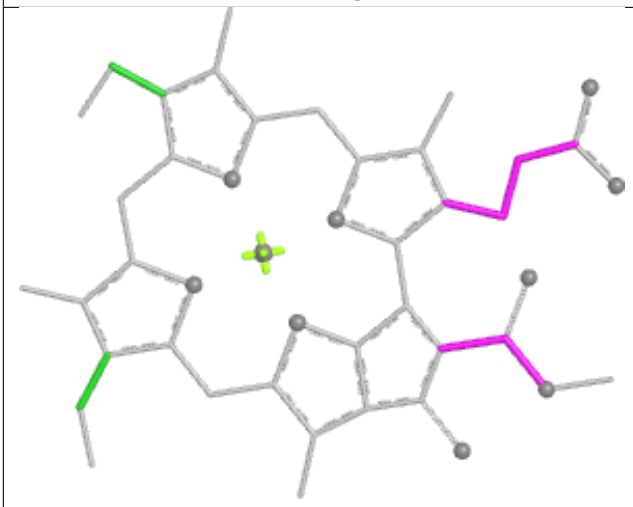
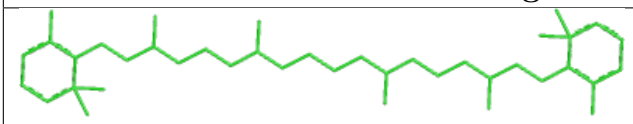


Torsions

Rings

Ligand BCR C 515



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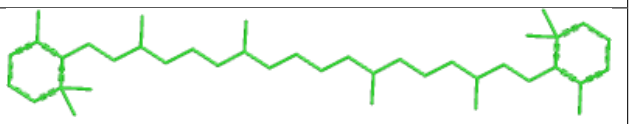
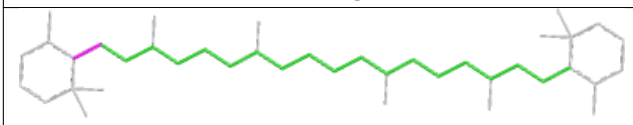
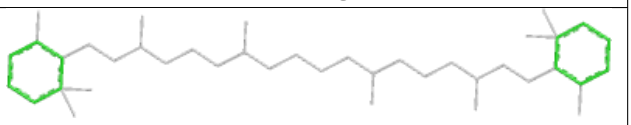


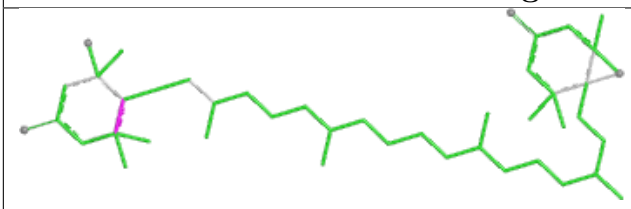
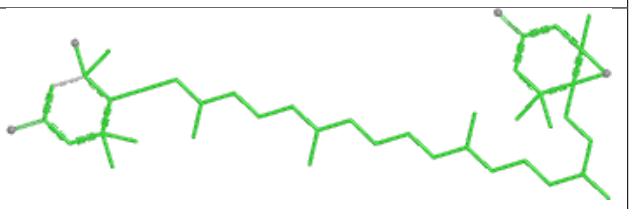
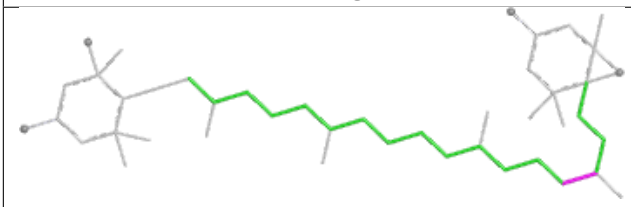
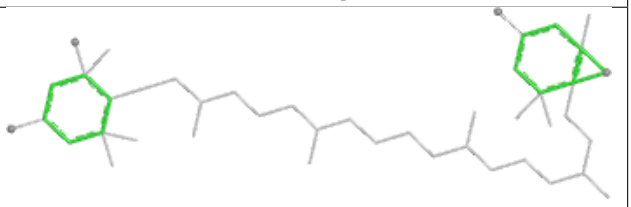
Bond angles

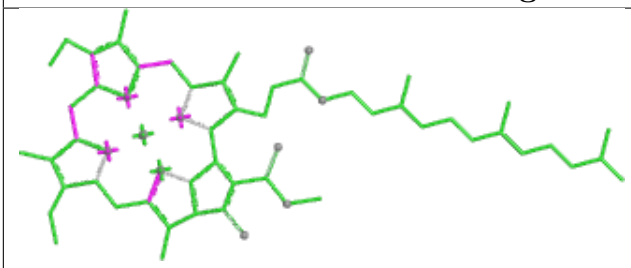
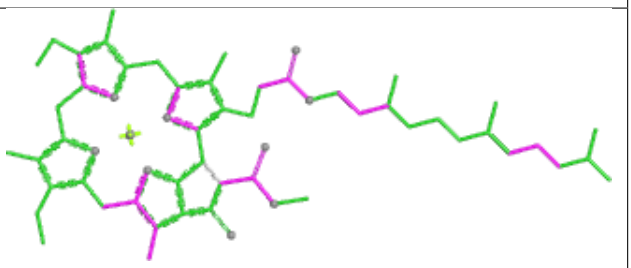
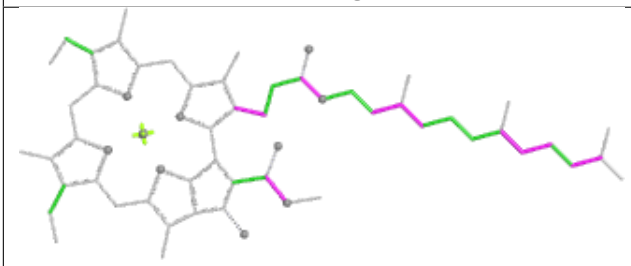
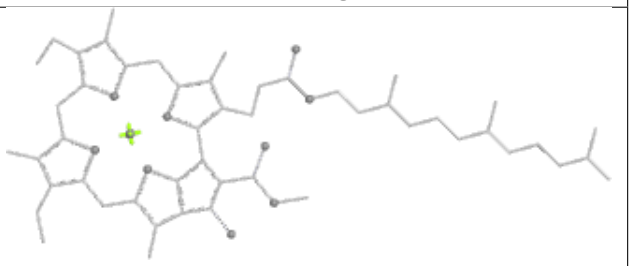


Torsions

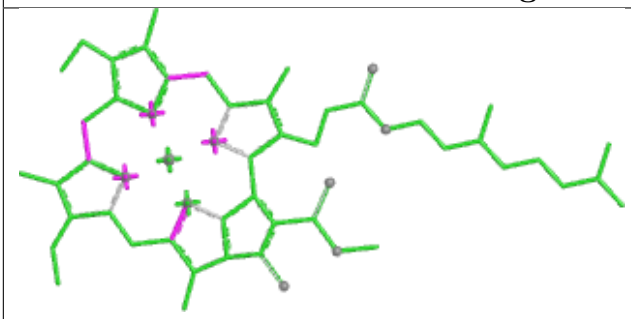


Rings

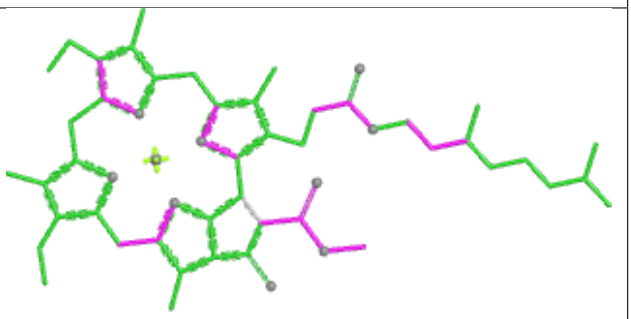
Ligand NEX Y 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 11 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

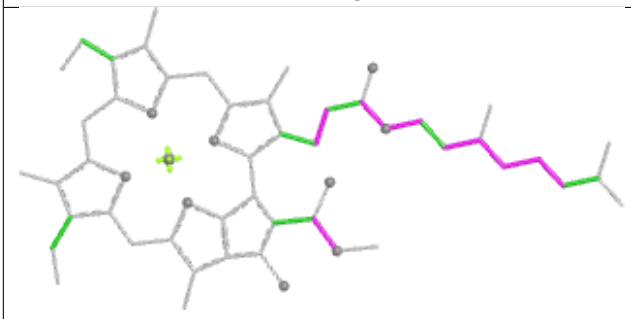
Ligand CLA 11 613



Bond lengths



Bond angles



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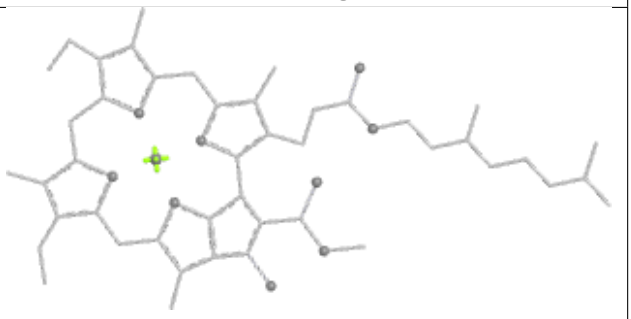
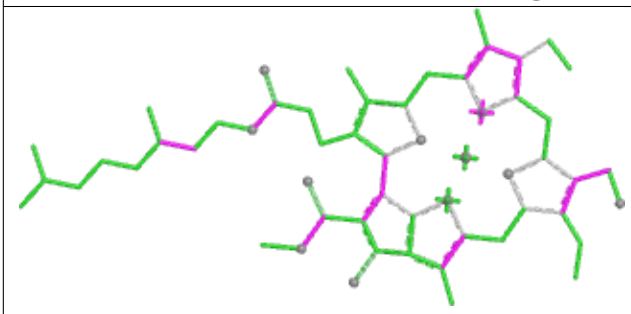


Rings

Ligand CHL 5 607



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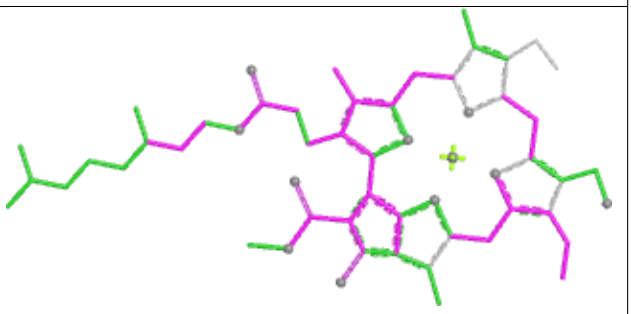
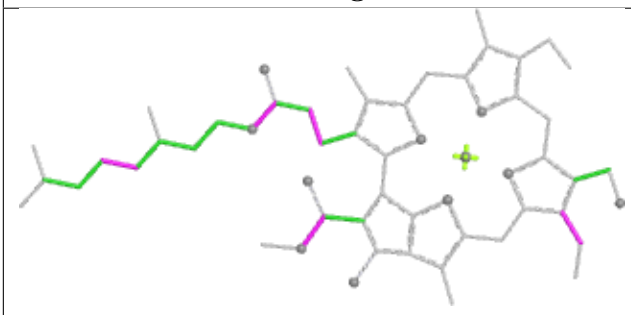


Bond angles



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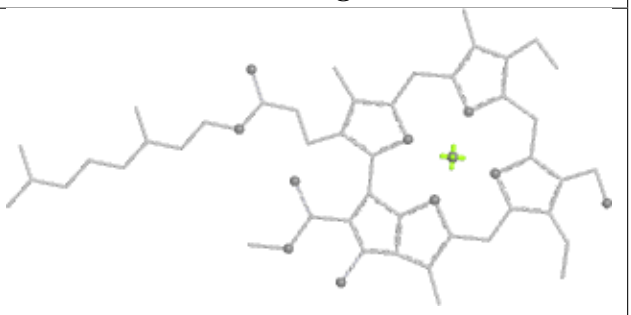
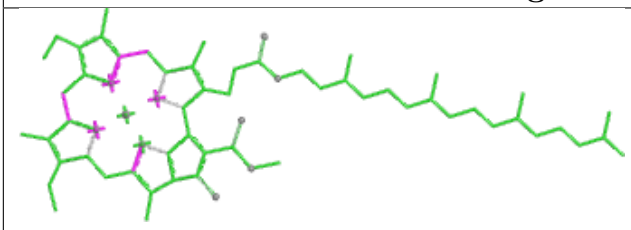
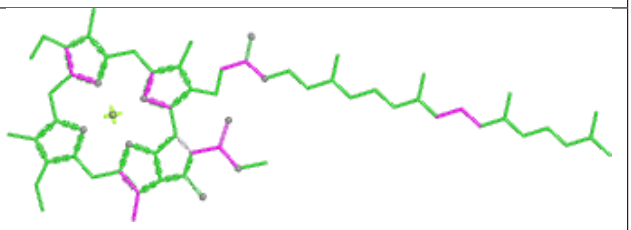
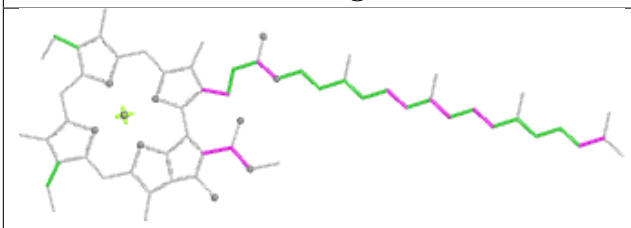
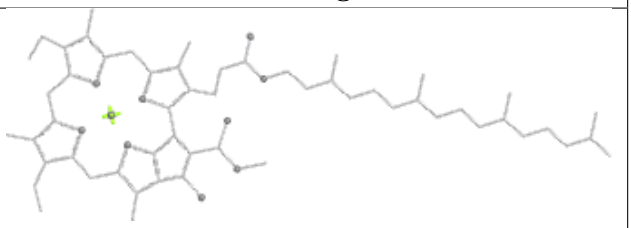


Rings

Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

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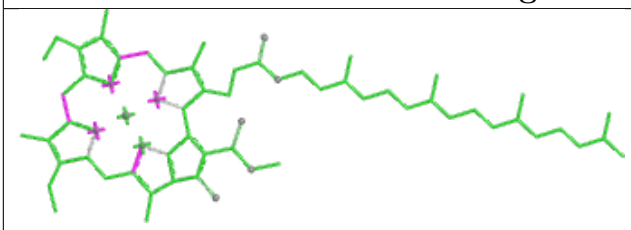
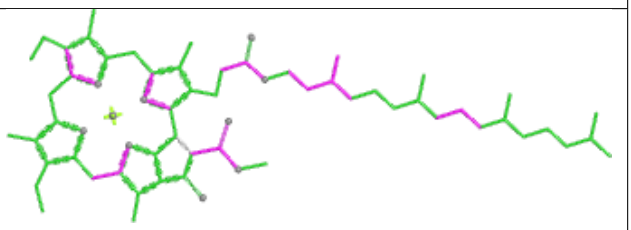
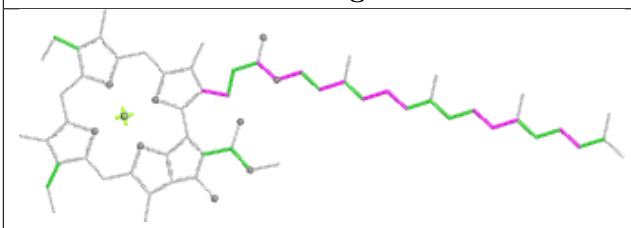
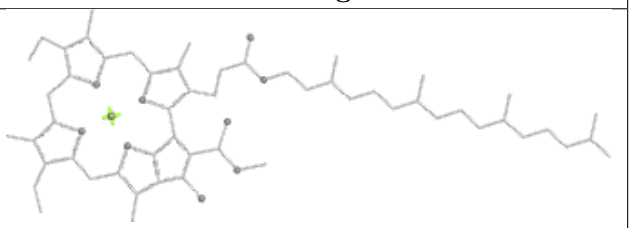
 Bond lengths	 Bond angles
 Torsions	 Rings

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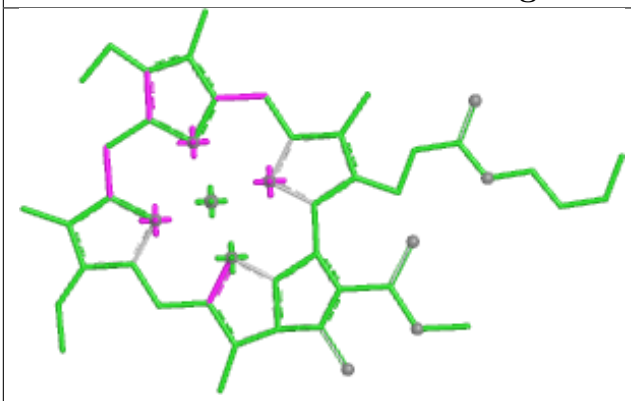
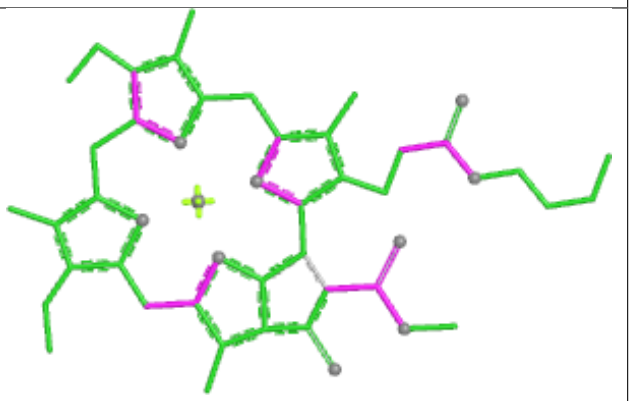
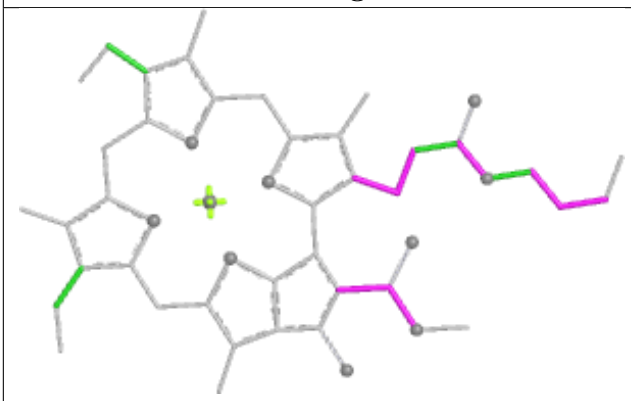
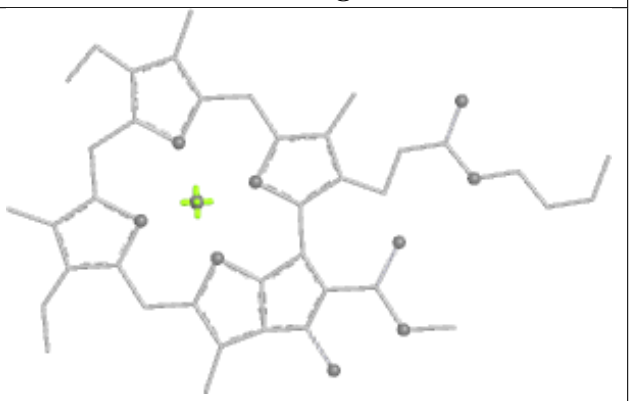
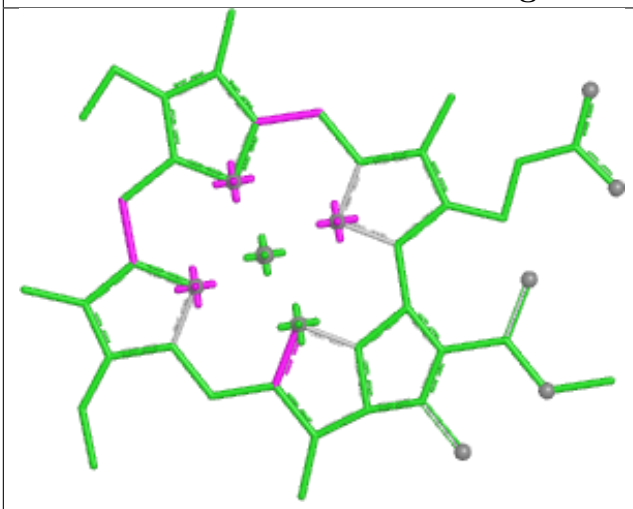
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 16 612



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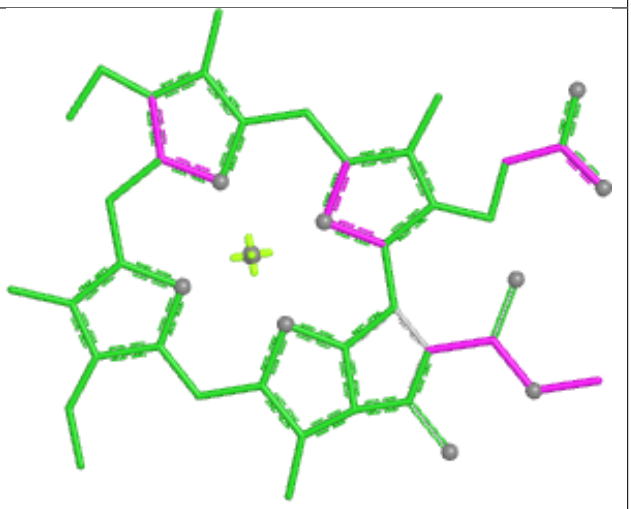
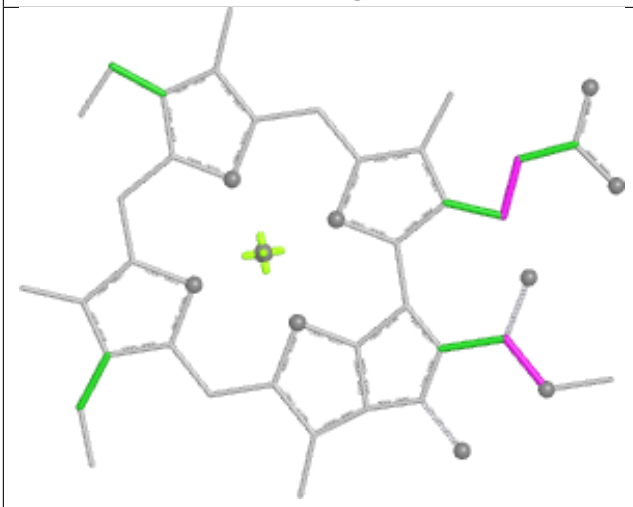
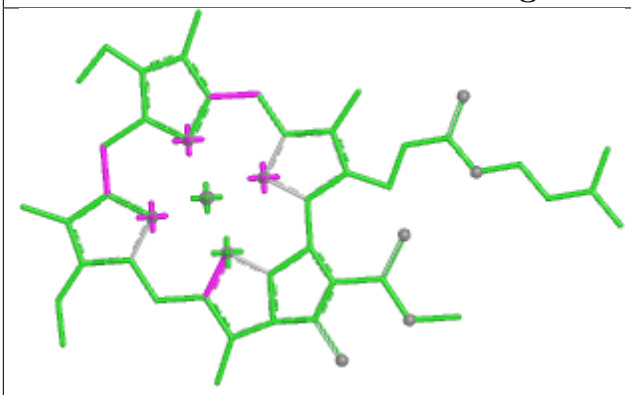
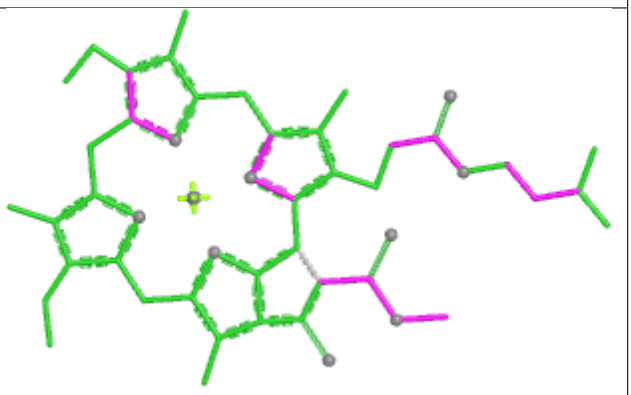
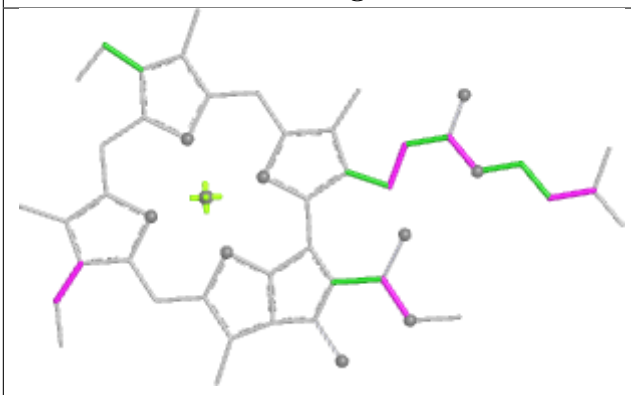
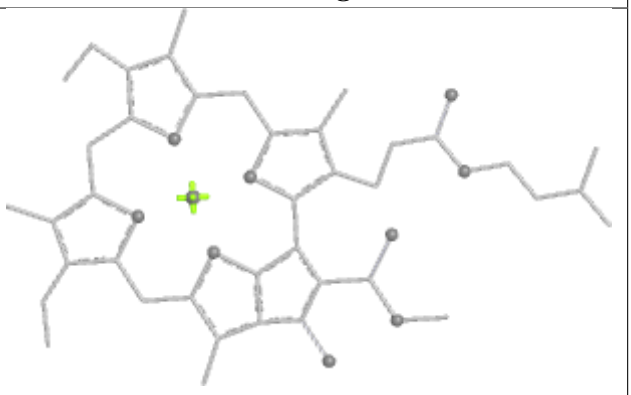


Bond angles

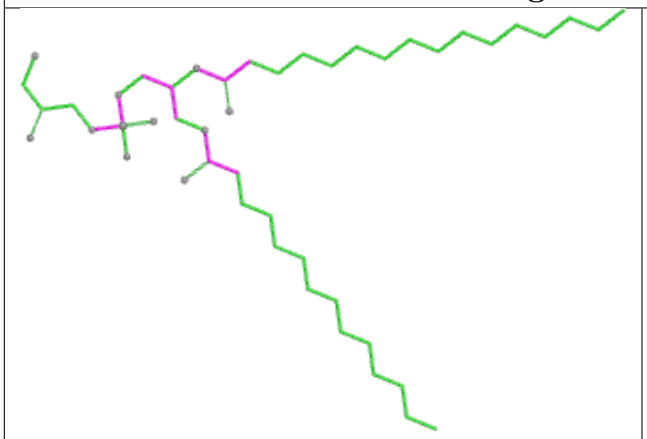


Torsions

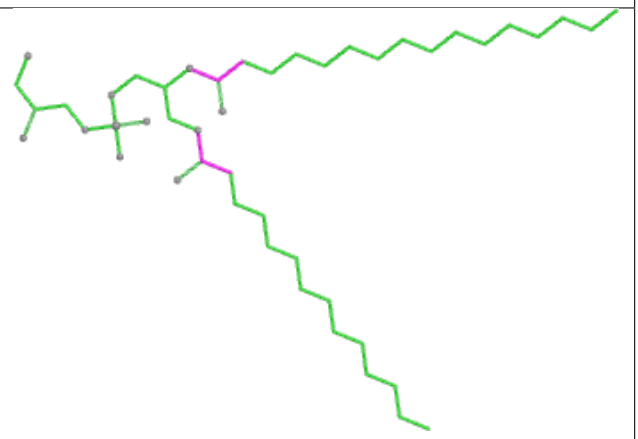
Rings

Ligand CLA 16 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

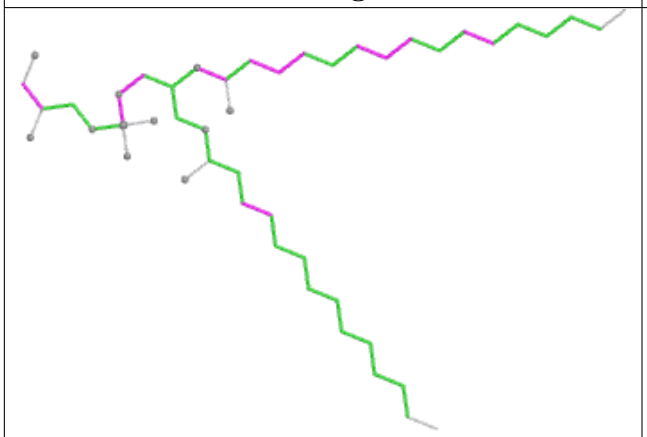
Ligand LHG 4 615



Bond lengths



Bond angles



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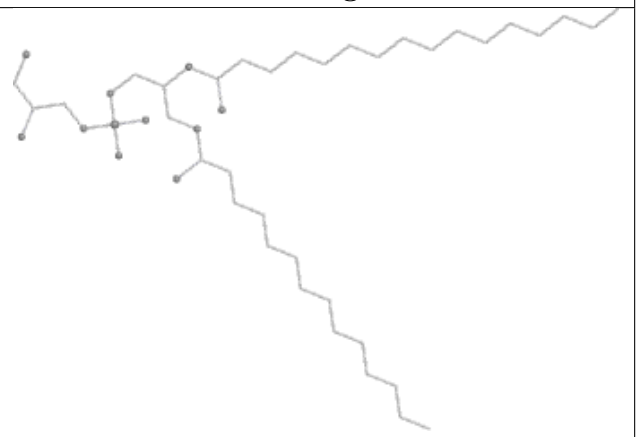
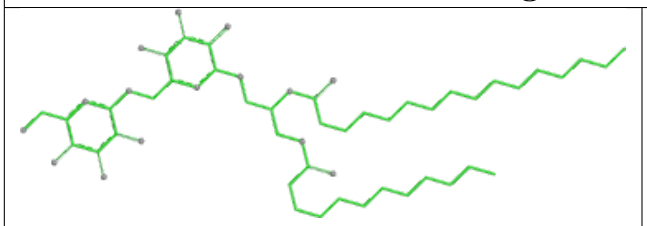


Rings

Ligand DGD C 518



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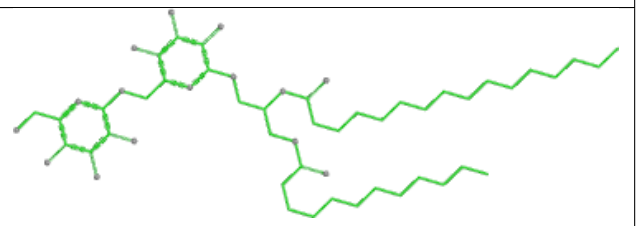
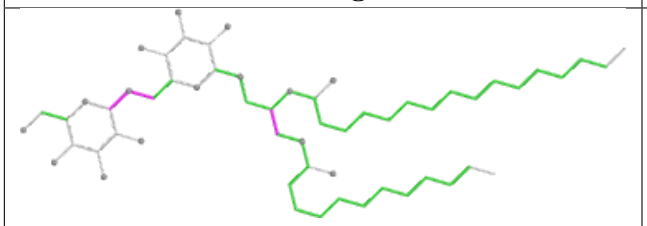
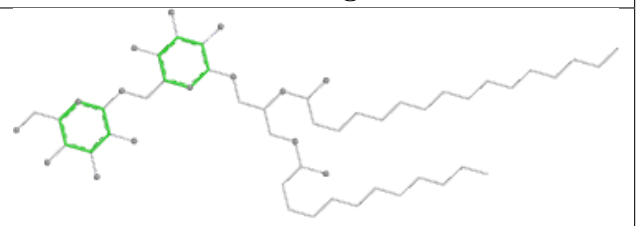


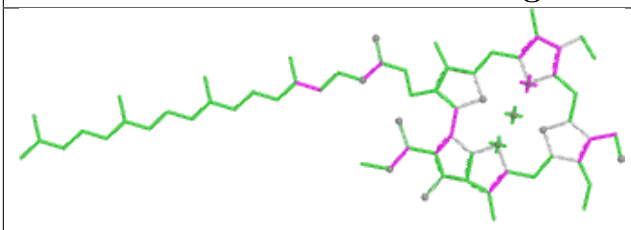
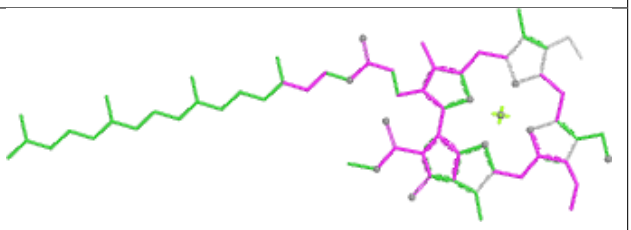
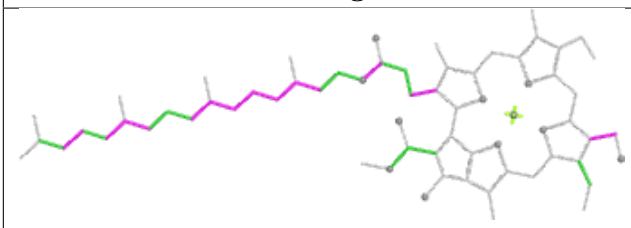
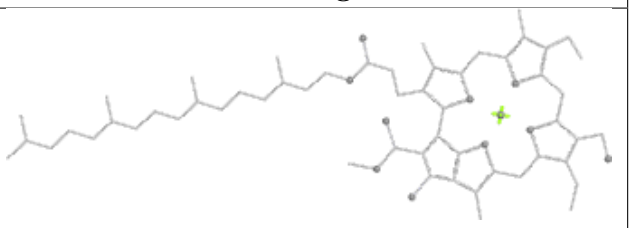
Bond angles

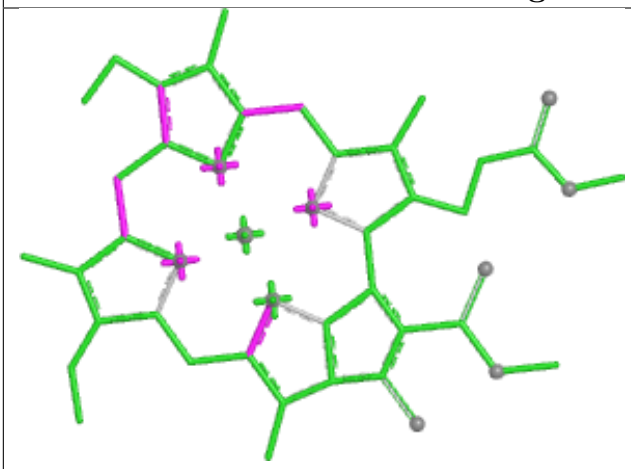
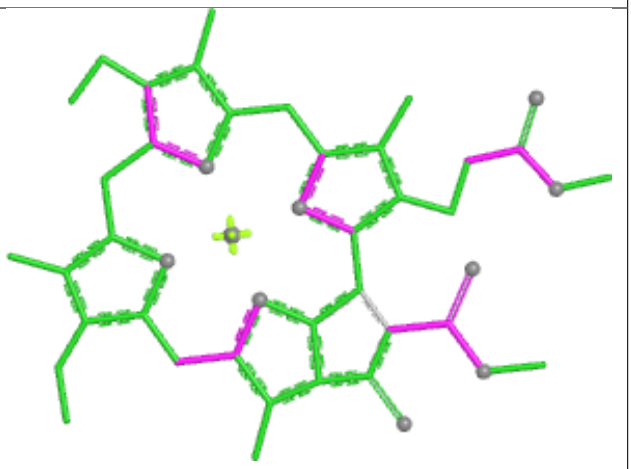
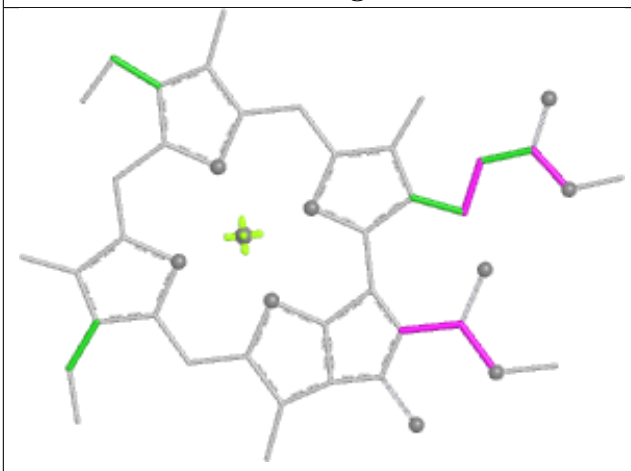
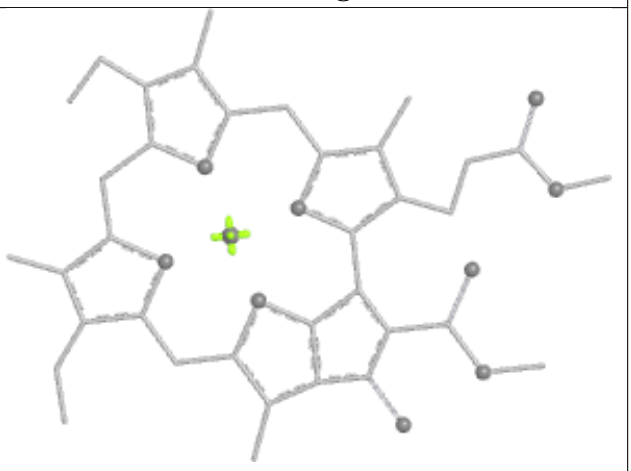


Torsions

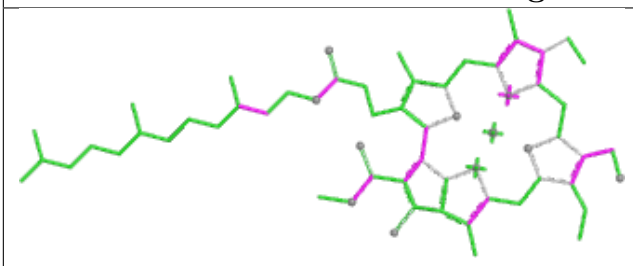


Rings

Ligand CHL Y 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 1 601



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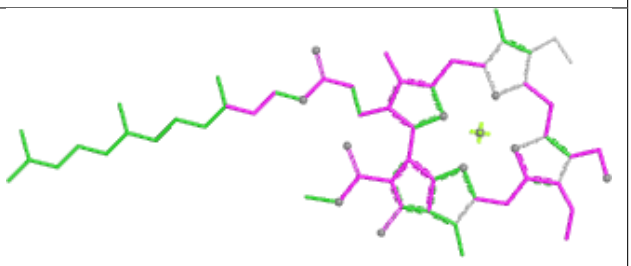

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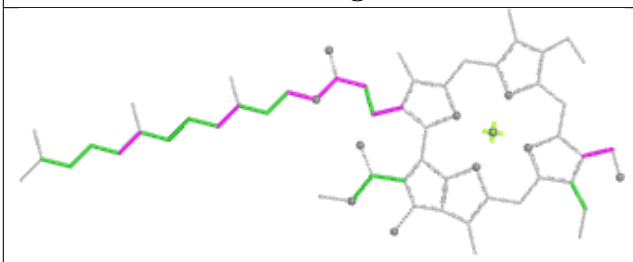

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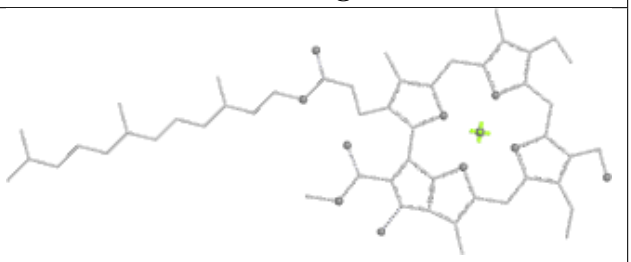

Rings

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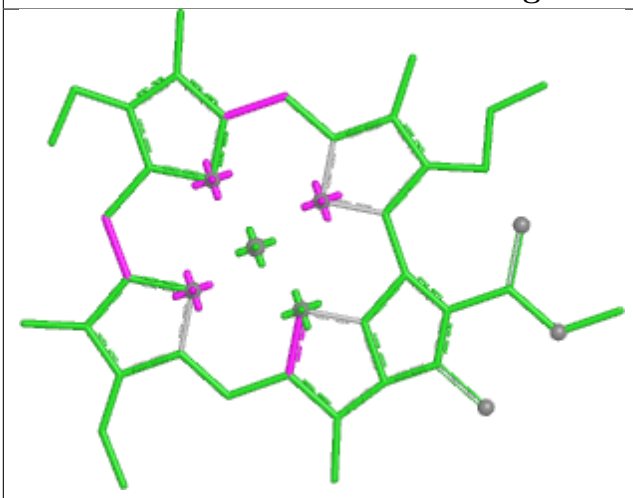

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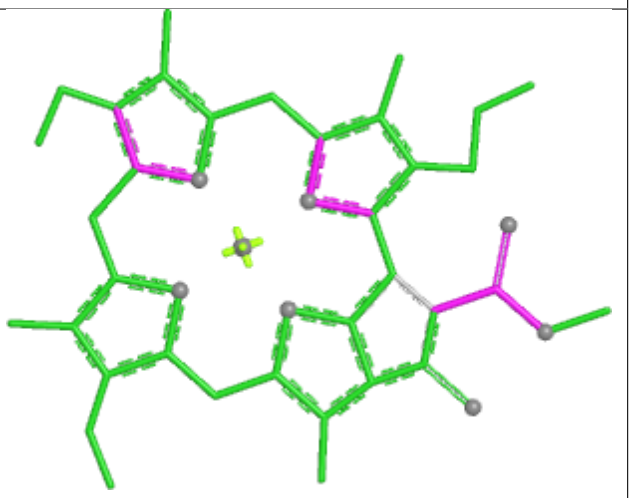

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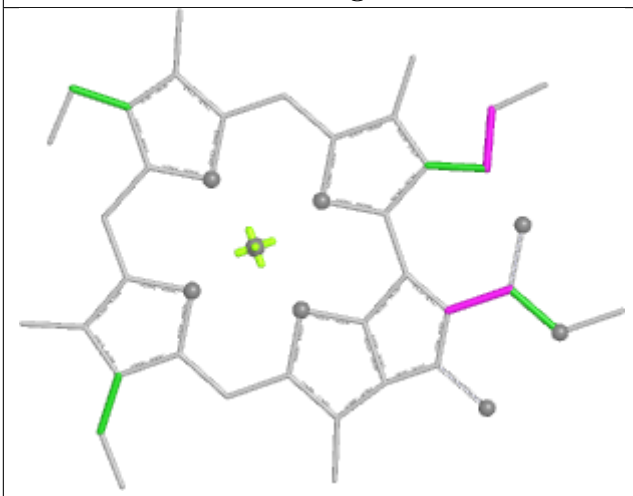

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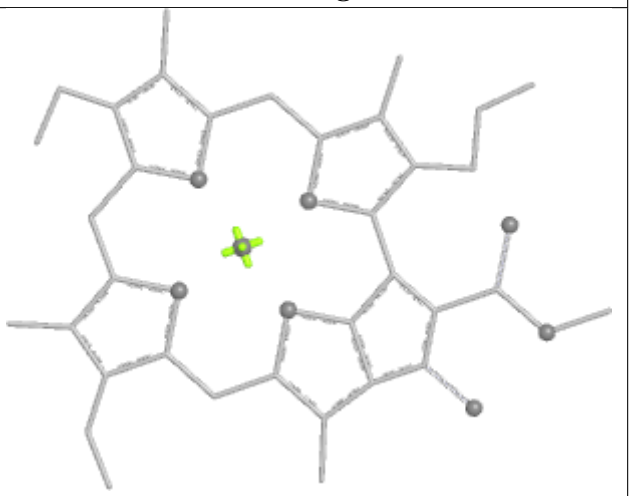

Rings

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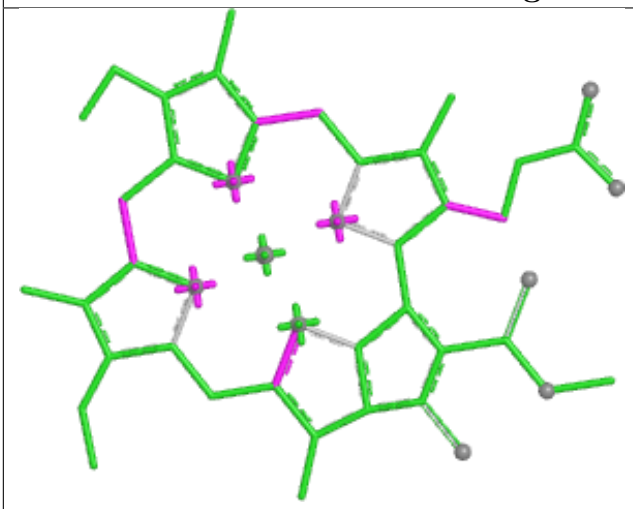

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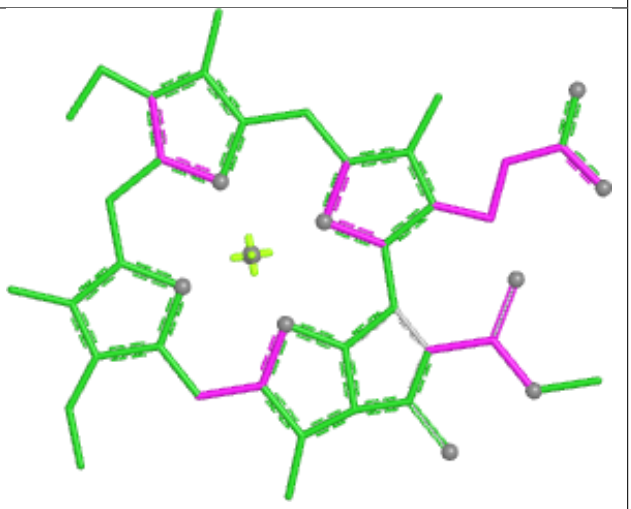

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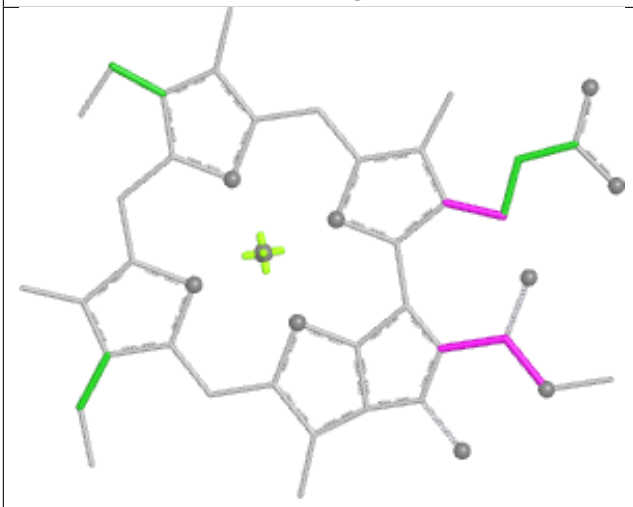

Torsions

Rings

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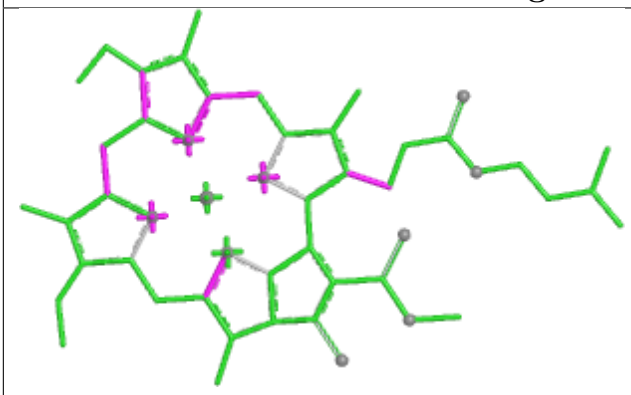
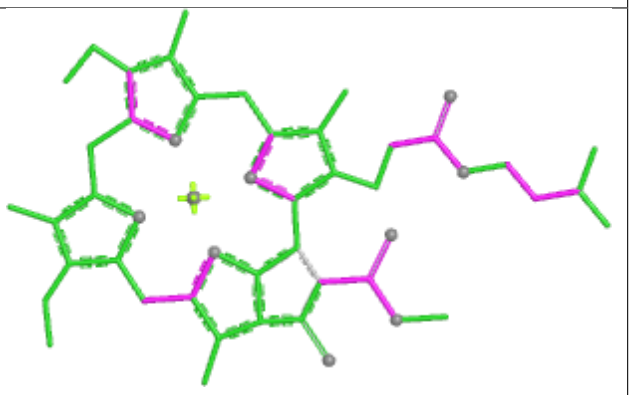
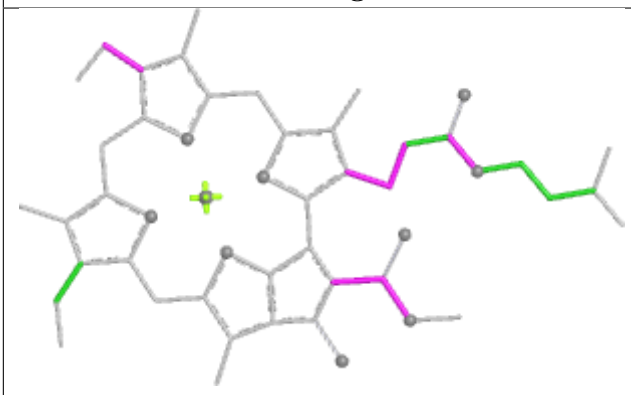
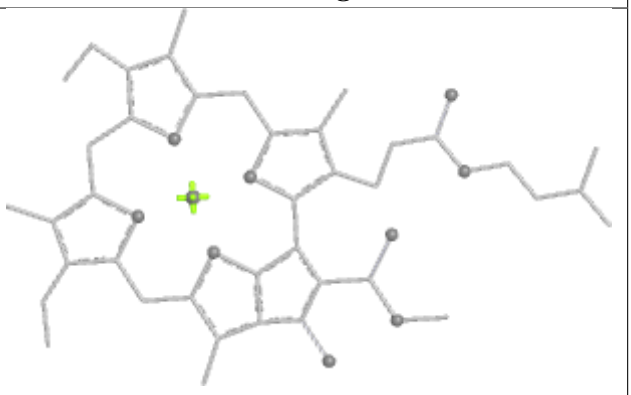
 Bond lengths	 Bond angles
 Torsions	 Rings

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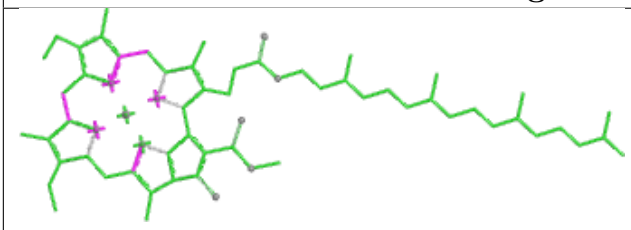
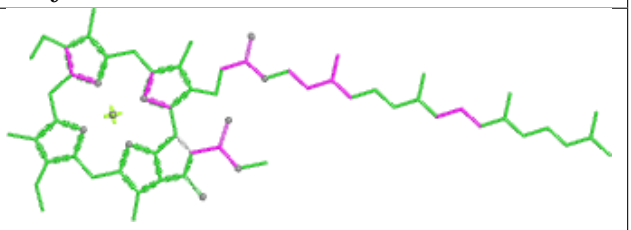
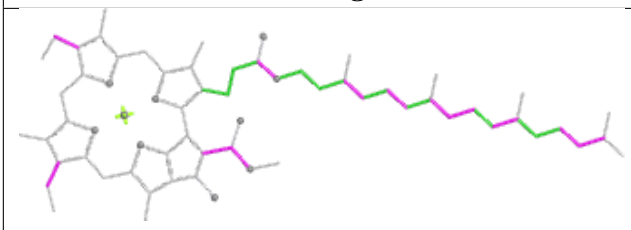
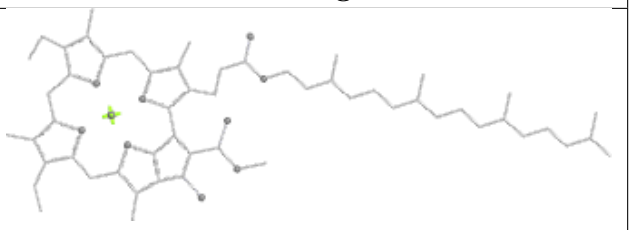
 Bond lengths	 Bond angles
 Torsions	 Rings

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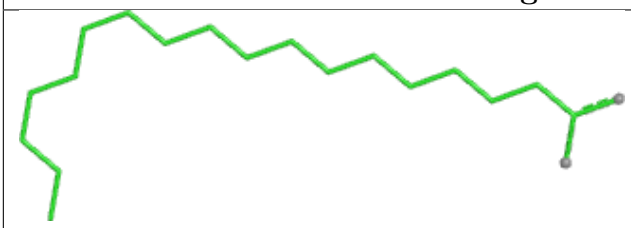
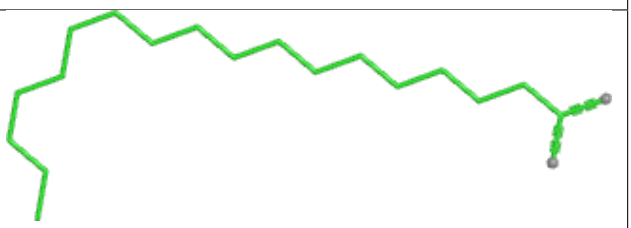
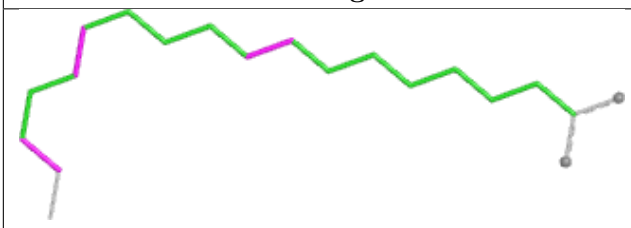
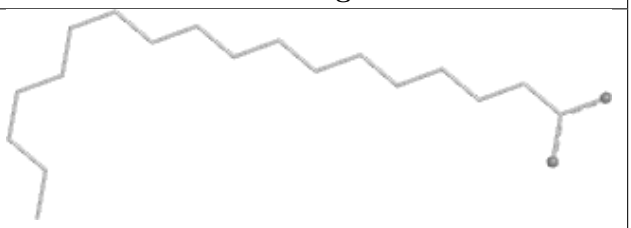
 Bond lengths	 Bond angles
 Torsions	 Rings

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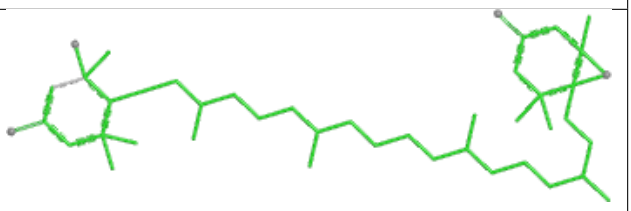
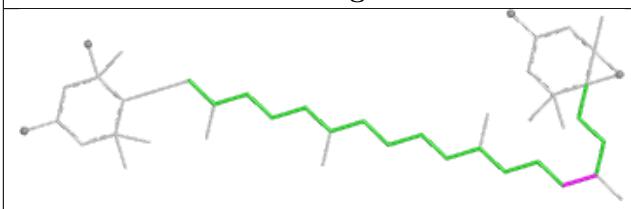
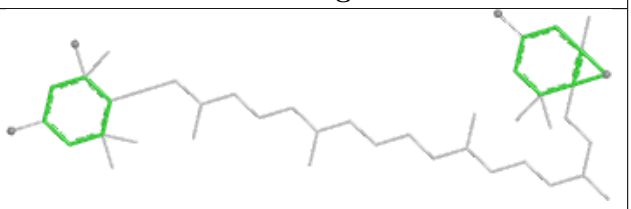
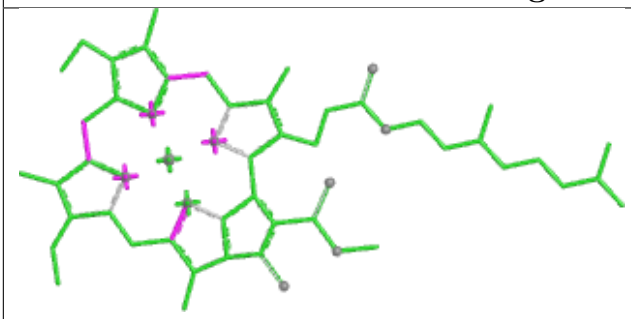
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 407



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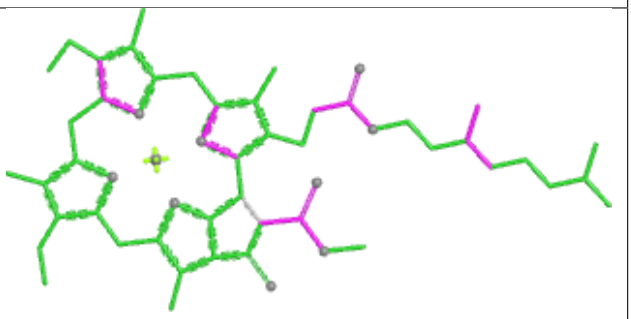

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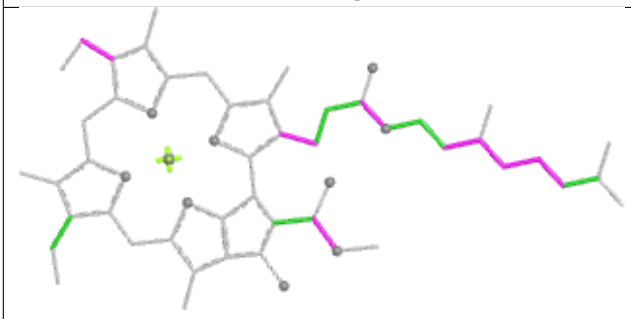

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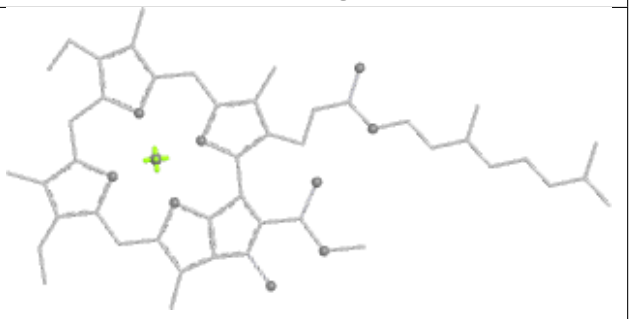
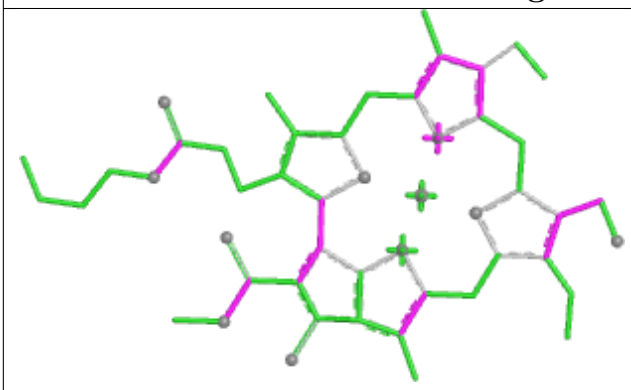


Rings

Ligand CHL 4 608



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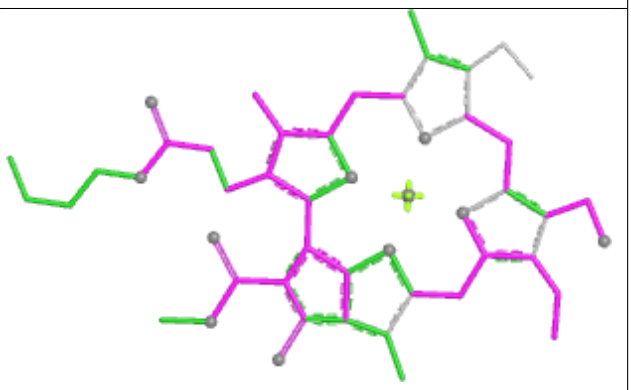
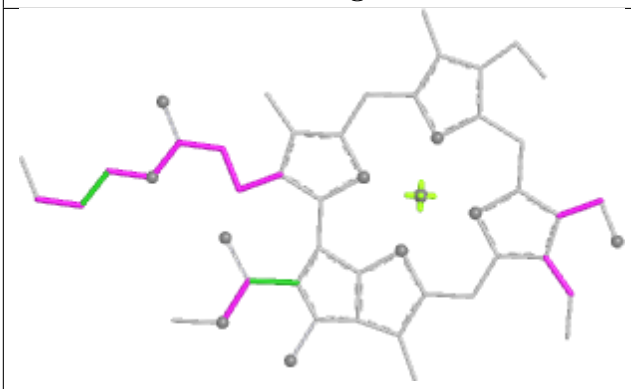


Bond angles



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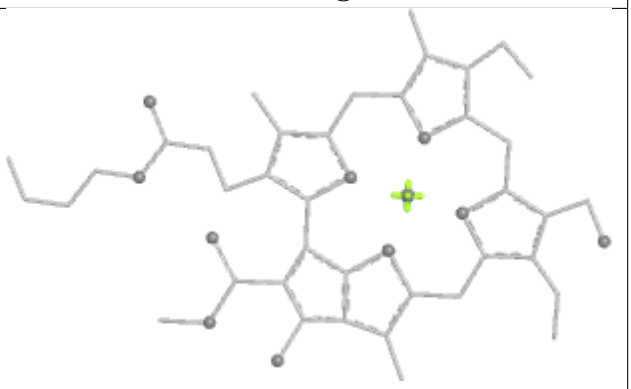

Rings

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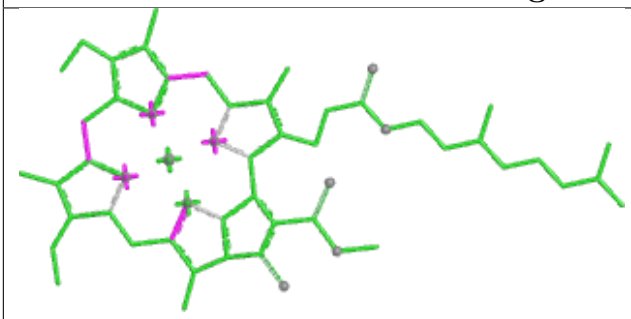
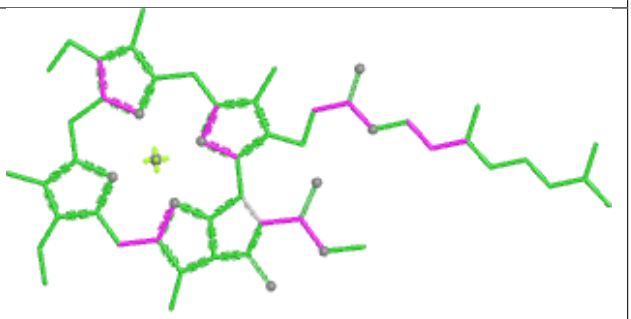
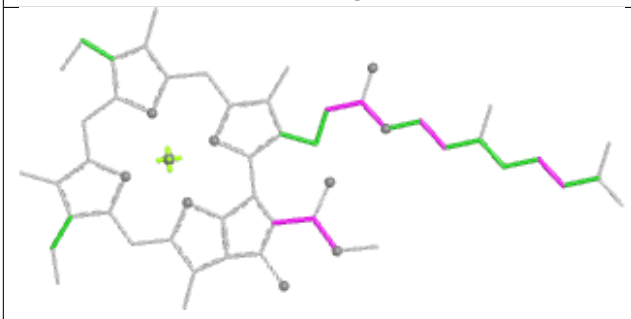
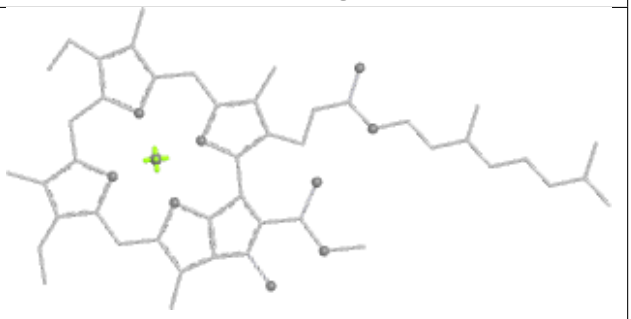
 Bond lengths	 Bond angles
 Torsions	 Rings

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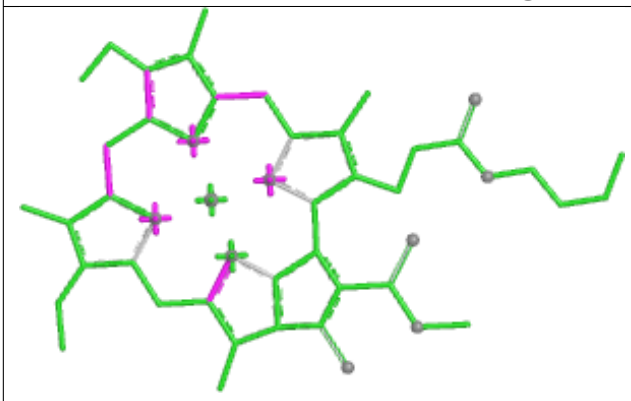
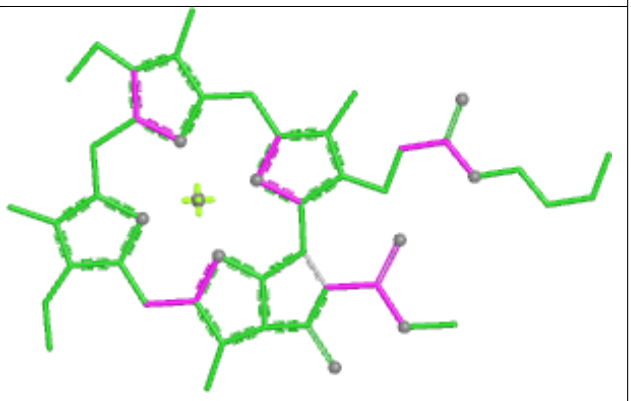
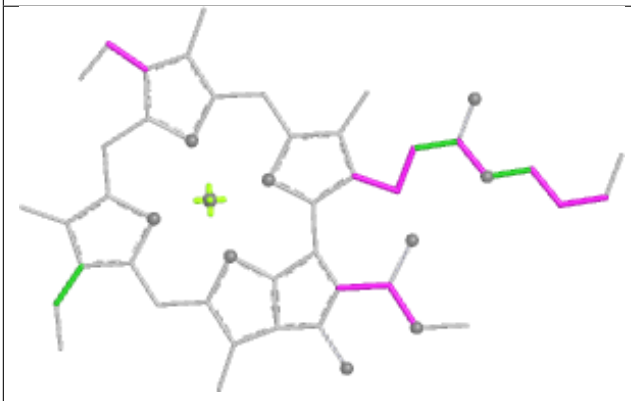
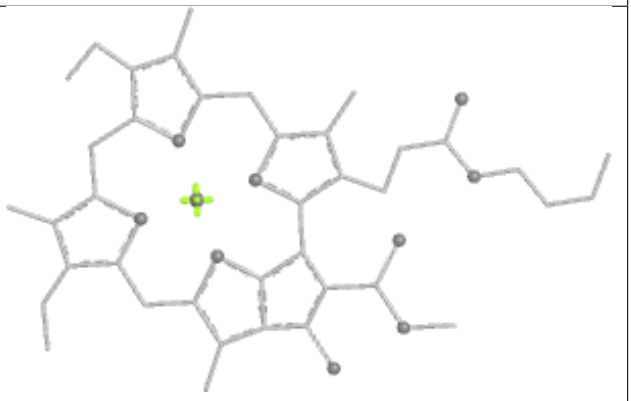
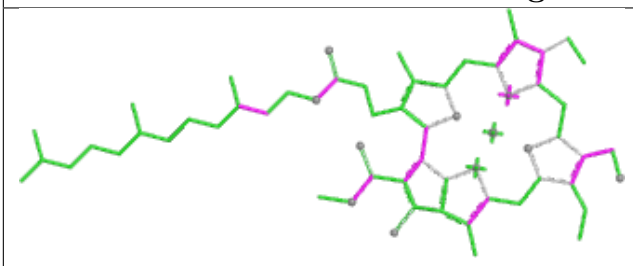
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 3 601



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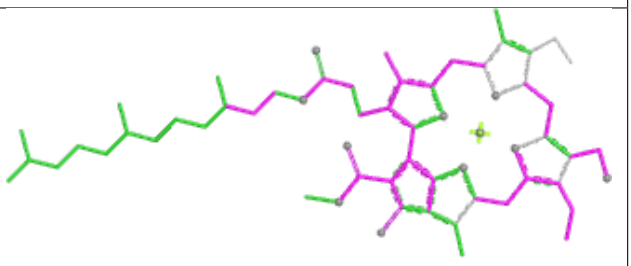

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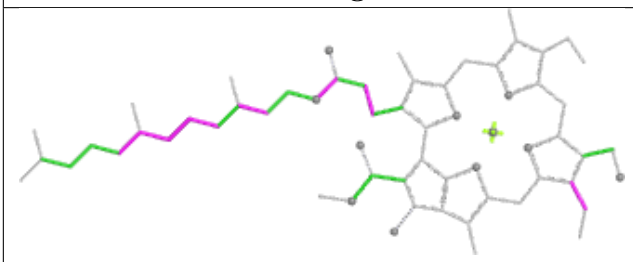
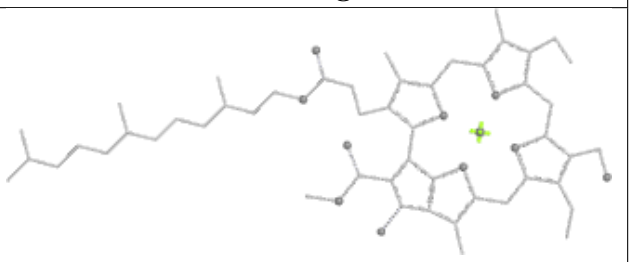
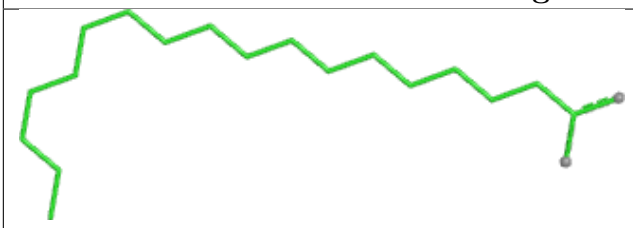


Torsions

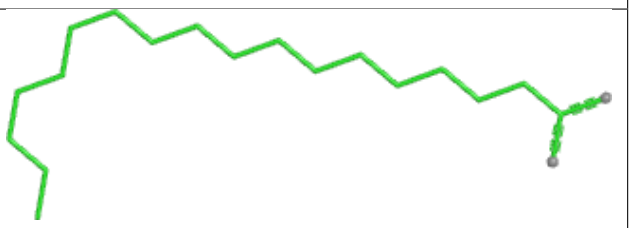


Rings

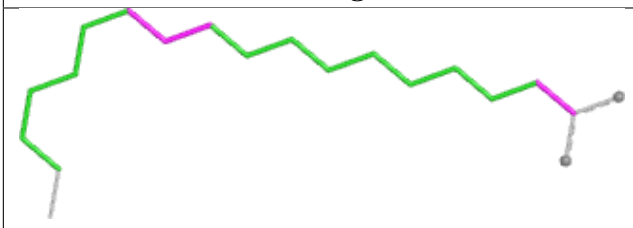
Ligand LNL I 101



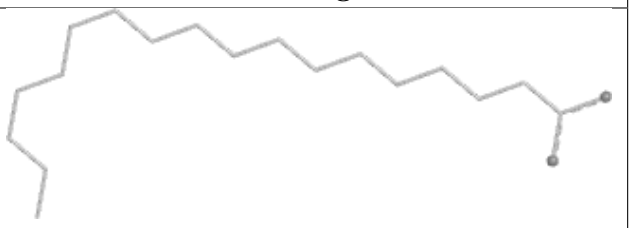
Bond lengths



Bond angles

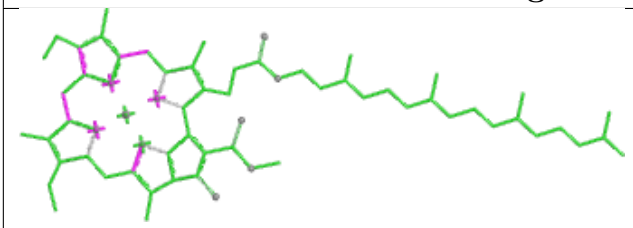


Torsions



Rings

Ligand CLA b 611



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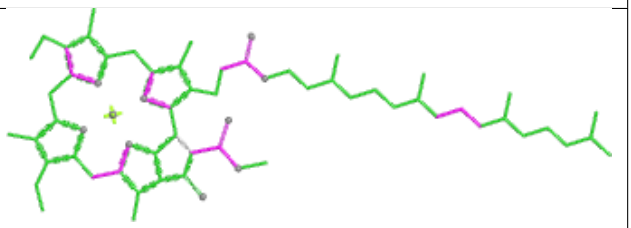

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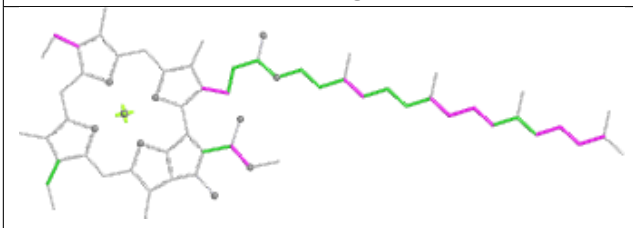

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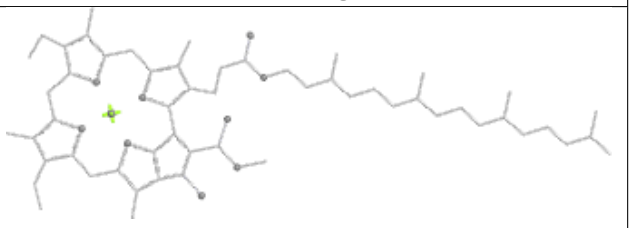
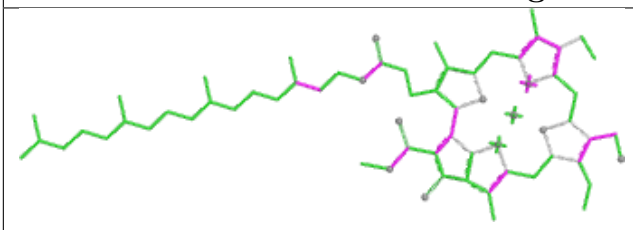


Rings

Ligand CHL g 609



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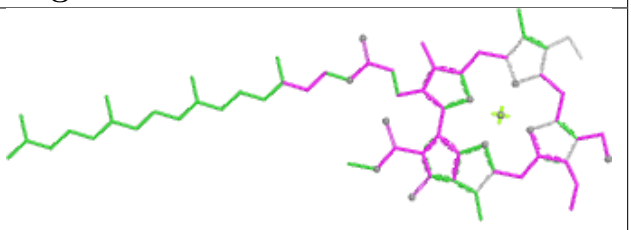

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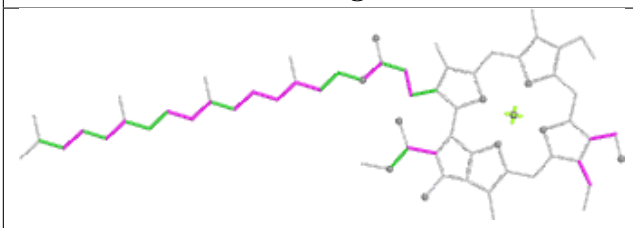

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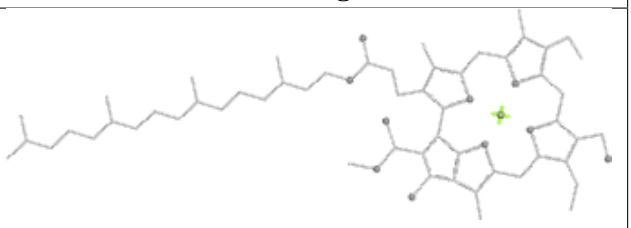
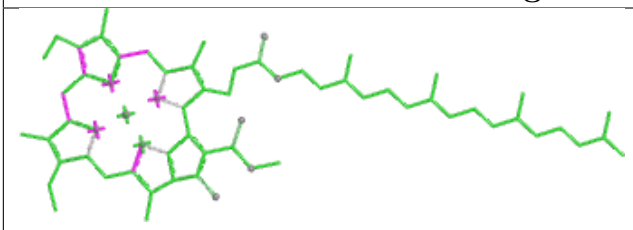


Rings

Ligand CLA R 609



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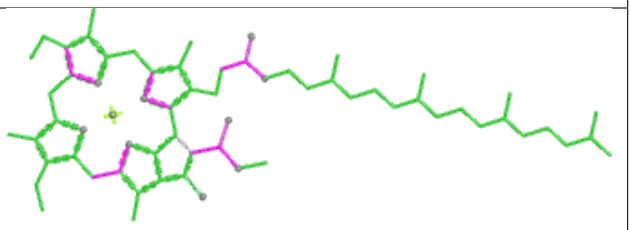

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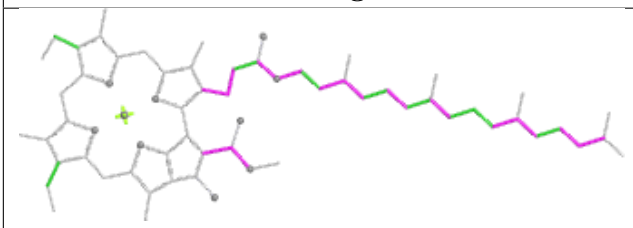

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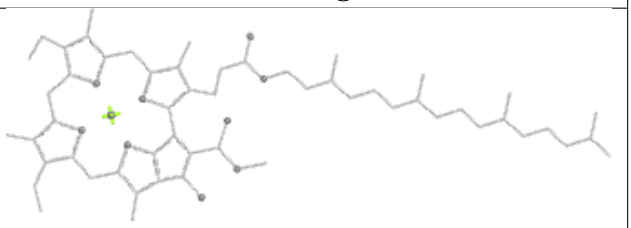
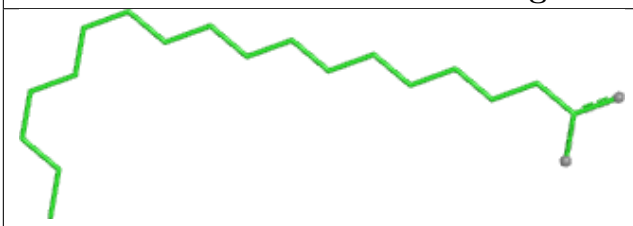


Rings

Ligand LNL y 621



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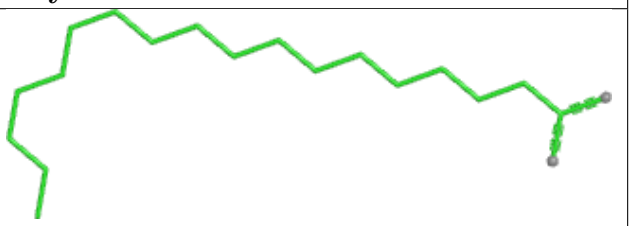
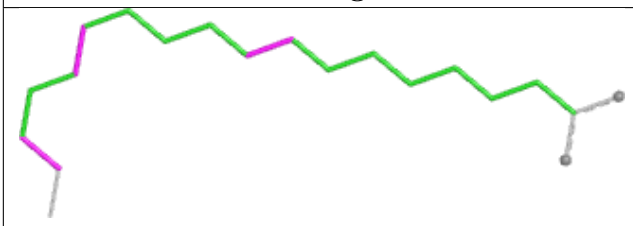


Bond angles



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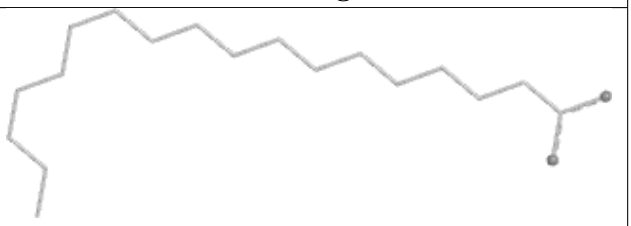
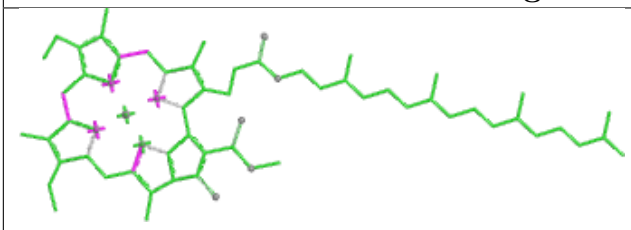
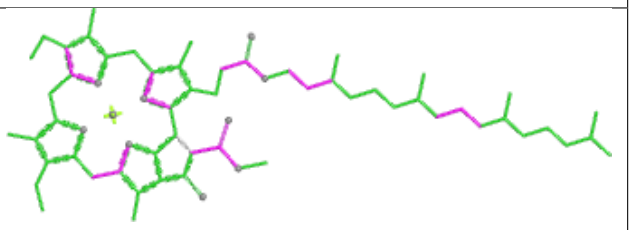
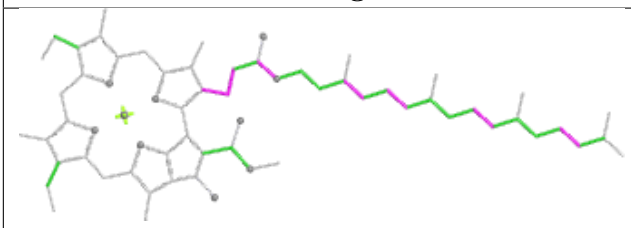
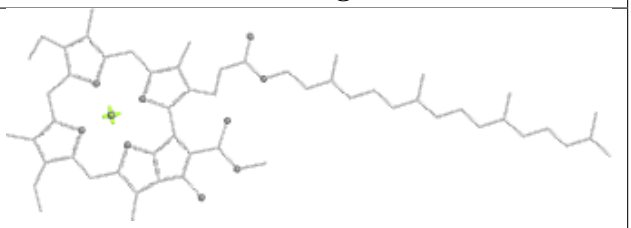
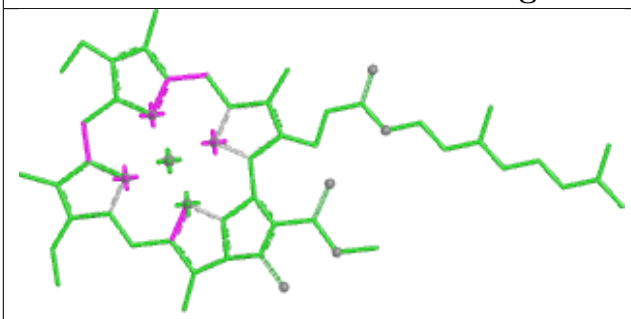
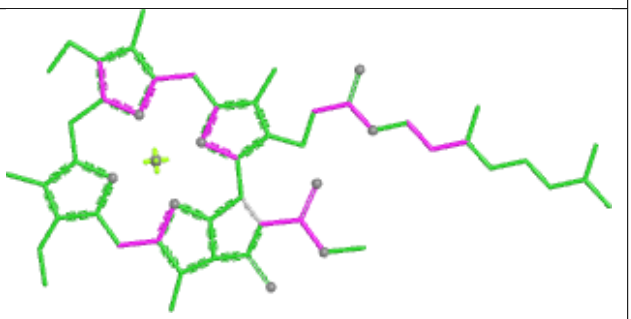
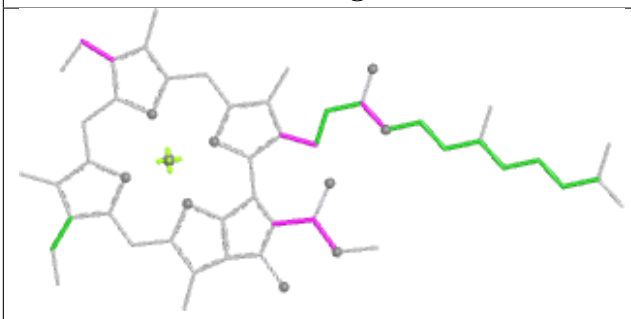
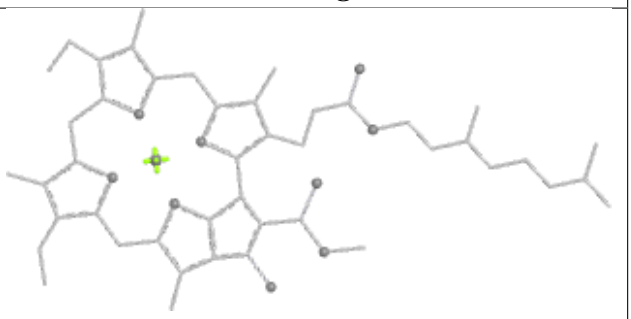
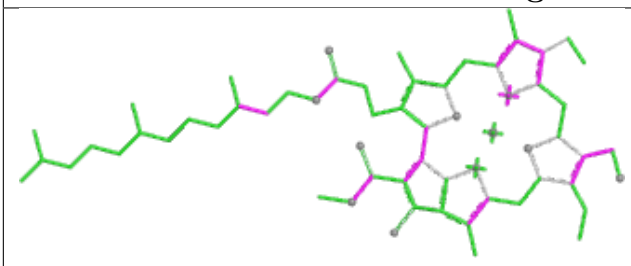


Rings

Ligand CLA Y 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 16 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL n 605



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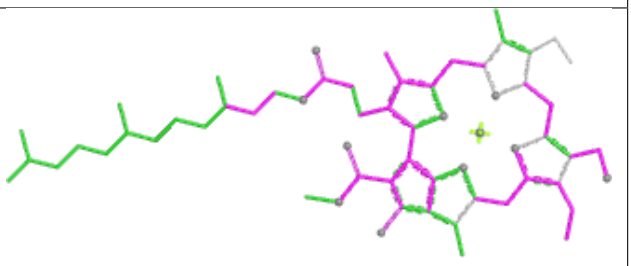
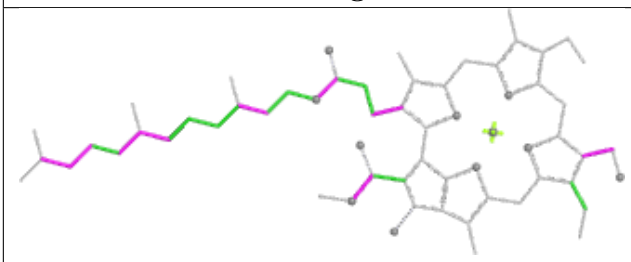
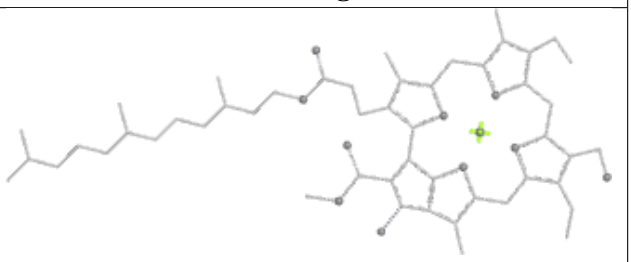


Bond angles

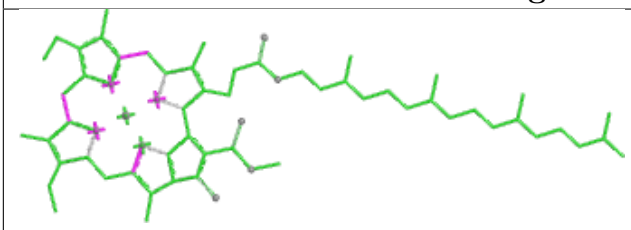


Torsions



Rings

Ligand CLA 3 612



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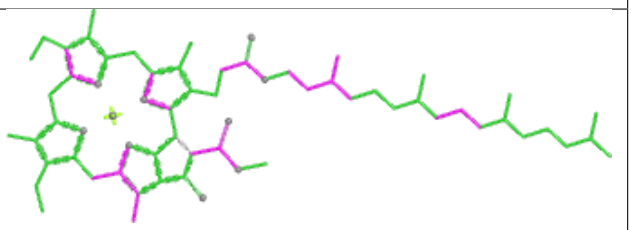
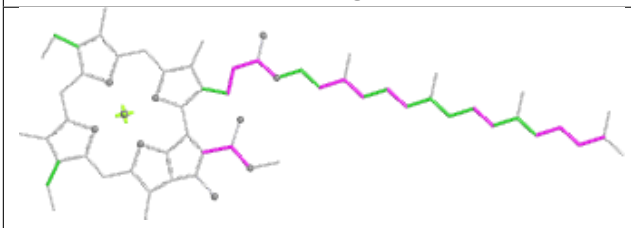


Bond angles



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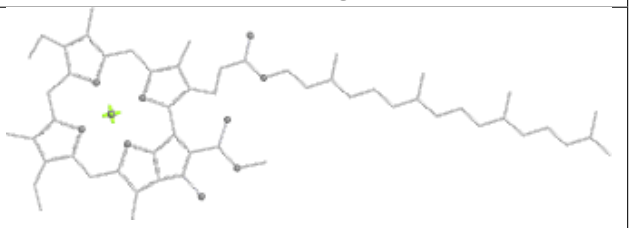
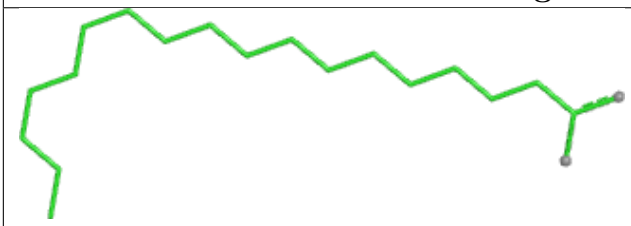


Rings

Ligand LNL i 101



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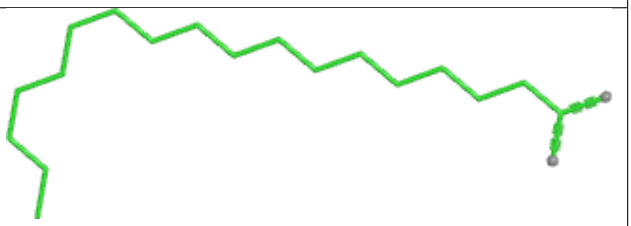

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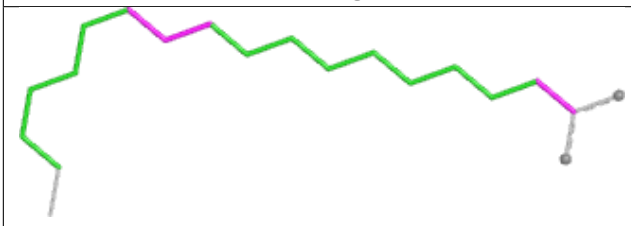

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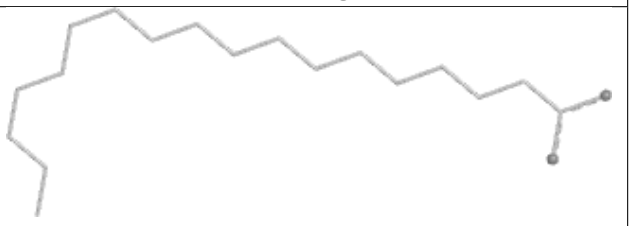
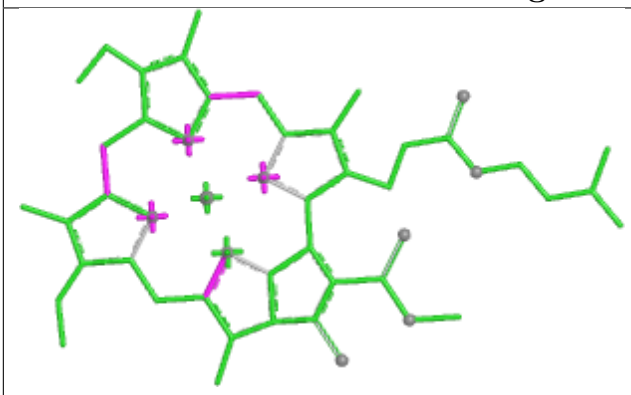


Rings

Ligand CLA g 604



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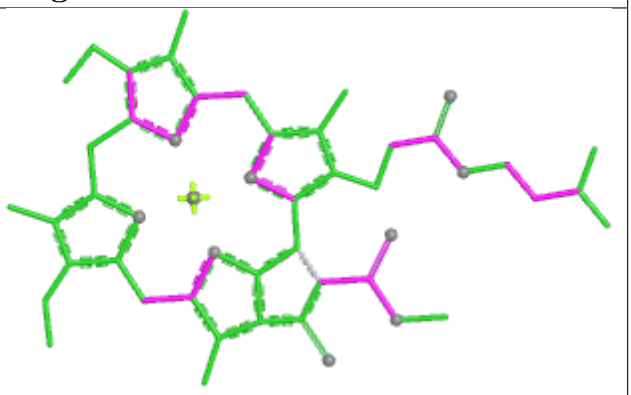
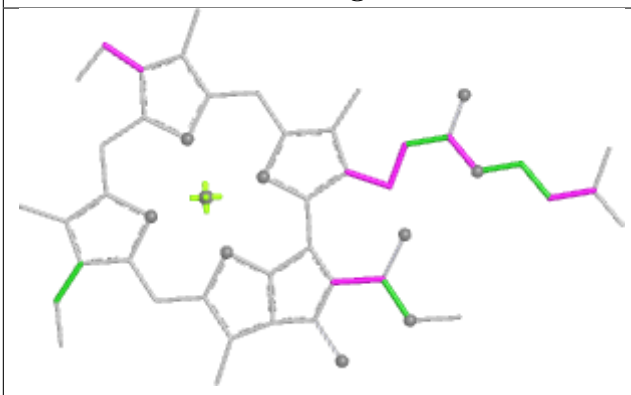


Bond angles



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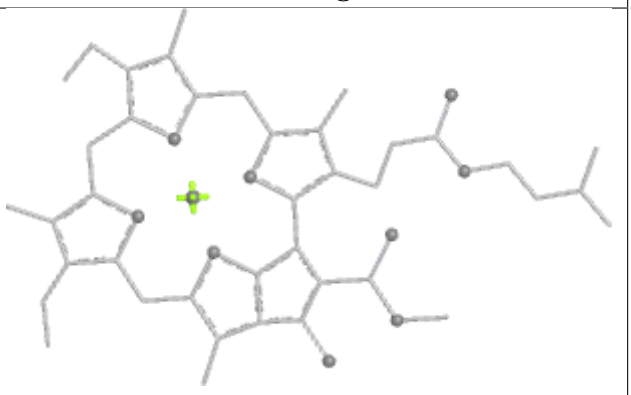
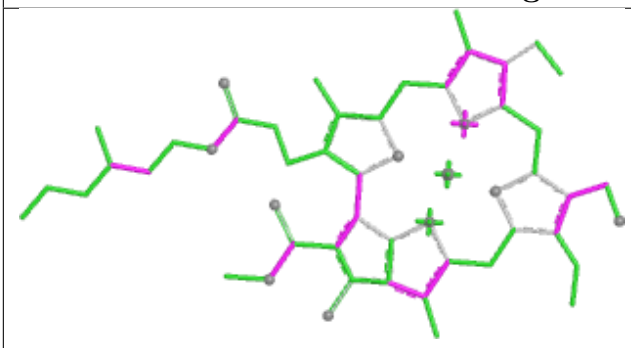


Rings

Ligand CHL N 601



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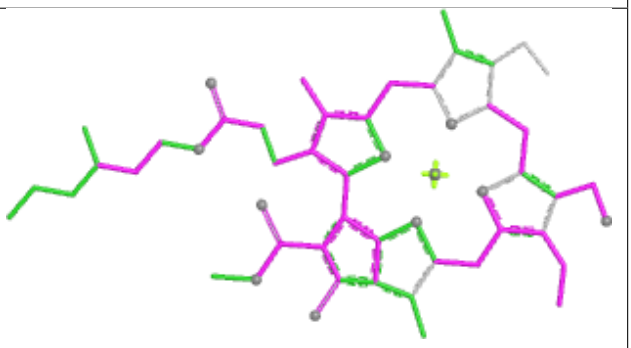
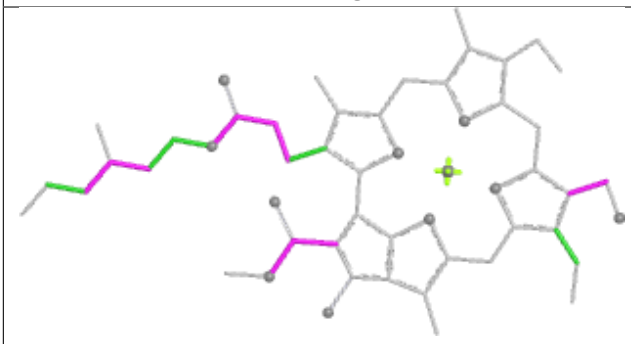


Bond angles



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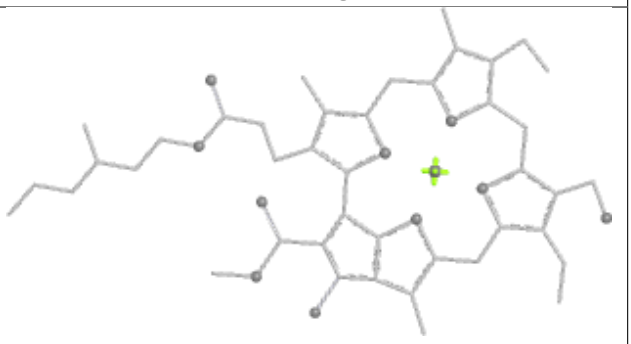
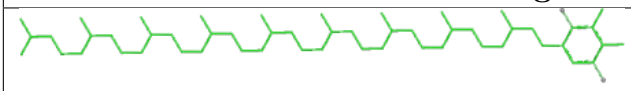


Rings

Ligand PL9 a 410



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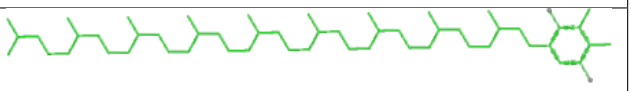
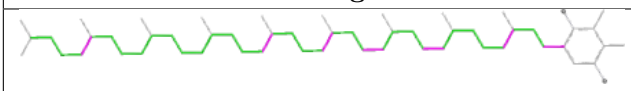


Bond angles



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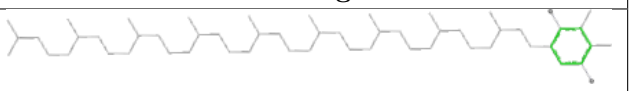
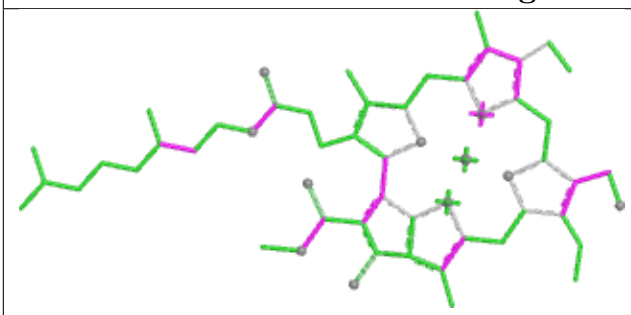


Rings

Ligand CHL 11 609



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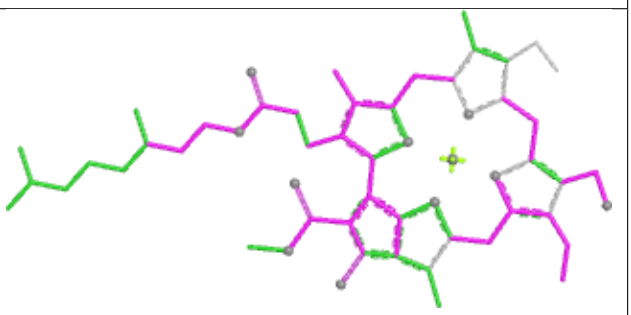
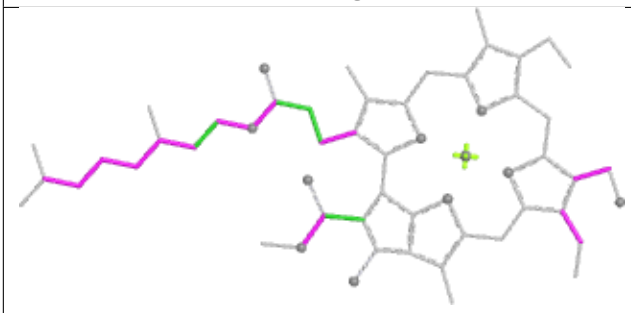
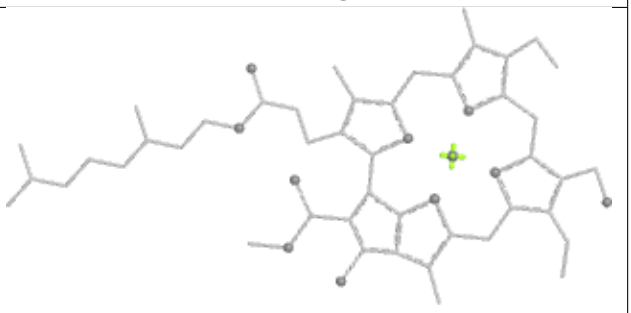


Bond angles

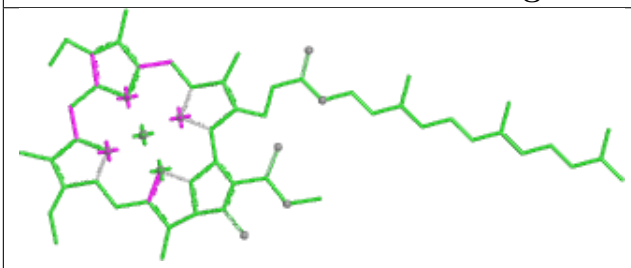


Torsions

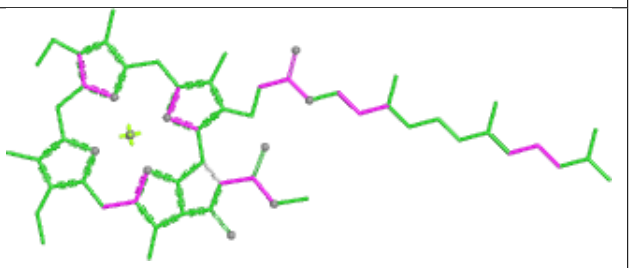


Rings

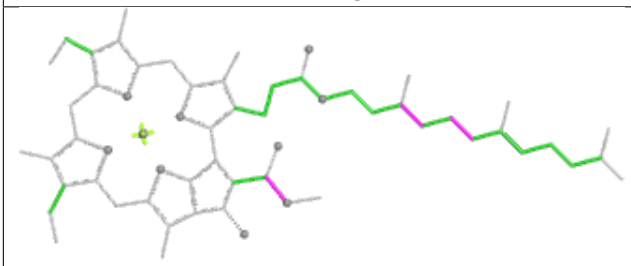
Ligand CLA N 610



Bond lengths



Bond angles



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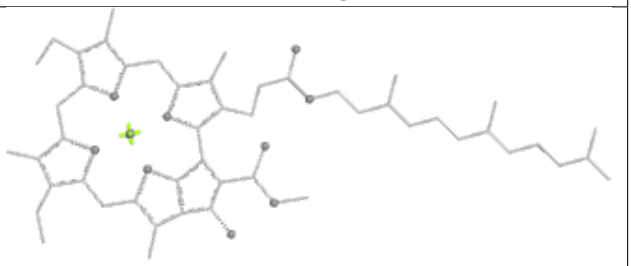
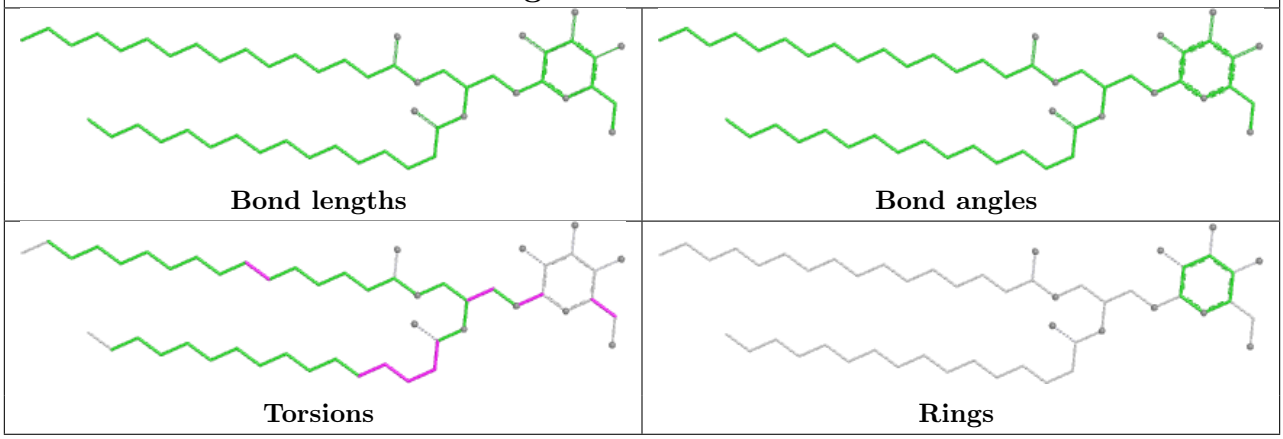
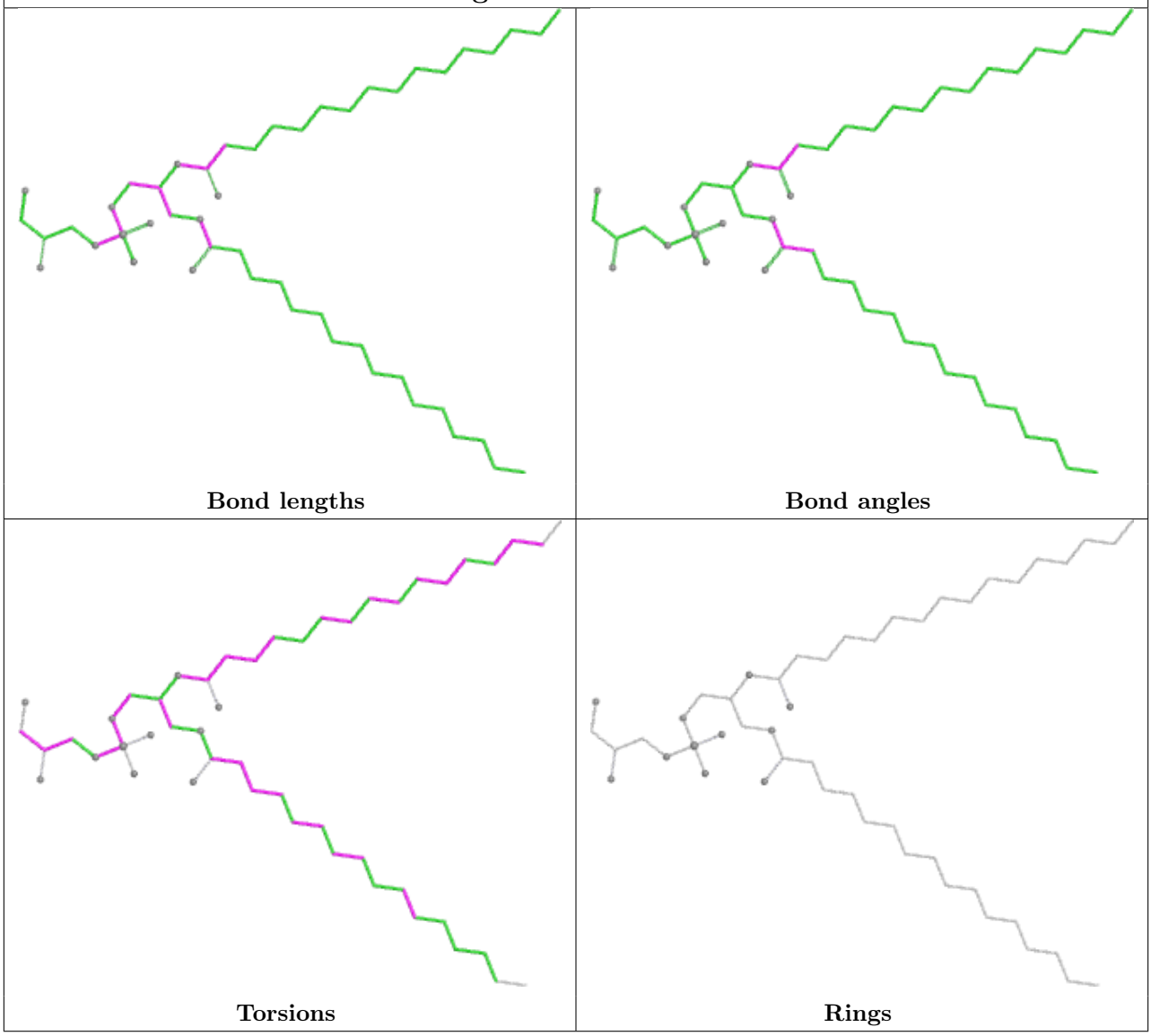


Rings

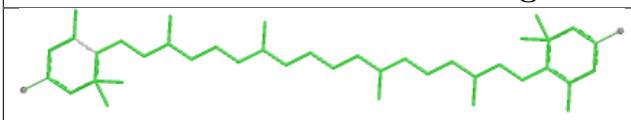
Ligand LMG v 101



Ligand LHG n 616



Ligand LUT 15 615



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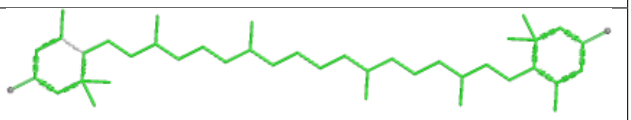
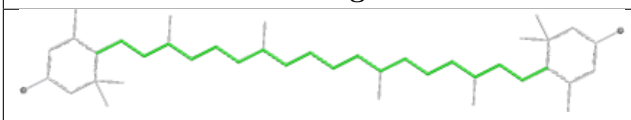


Bond angles



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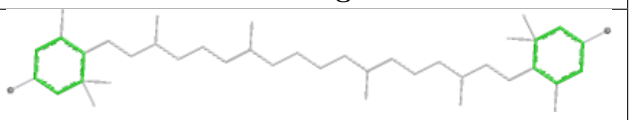
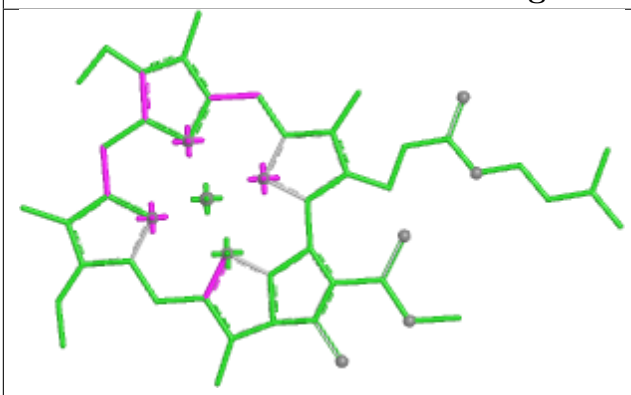


Rings

Ligand CLA 1 604



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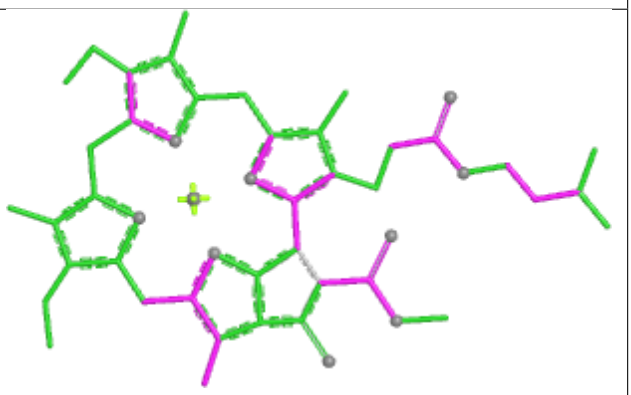
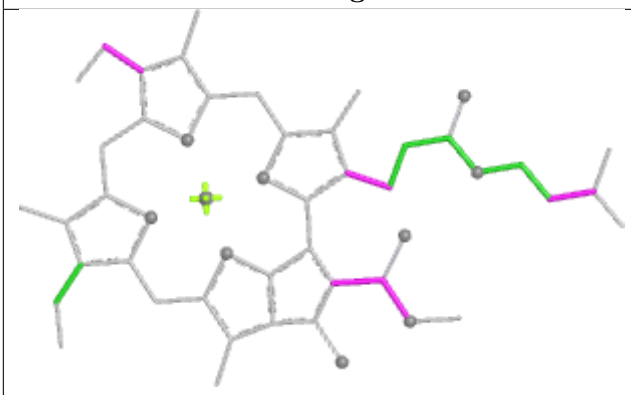


Bond angles



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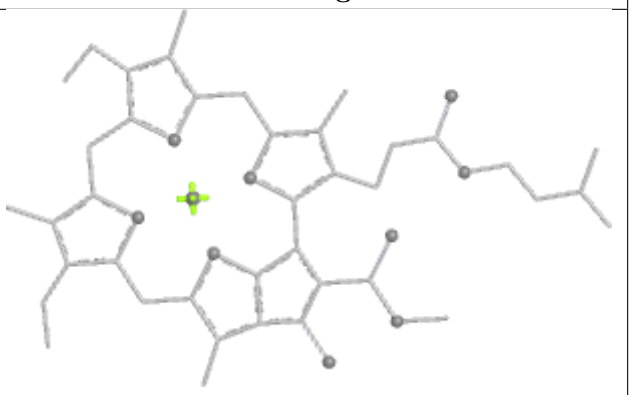
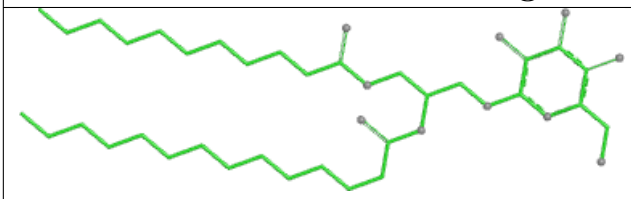


Rings

Ligand LMG D 410



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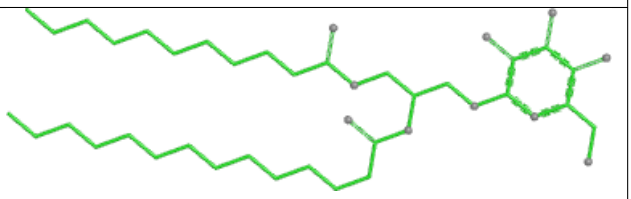
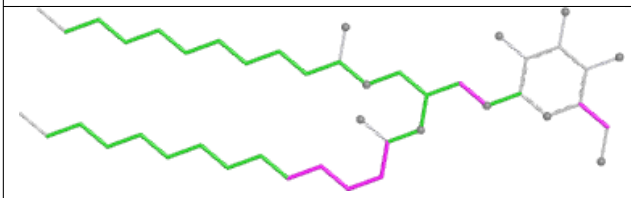


Bond angles



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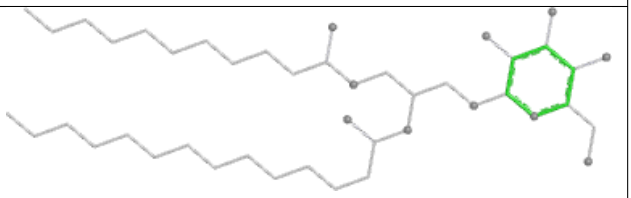
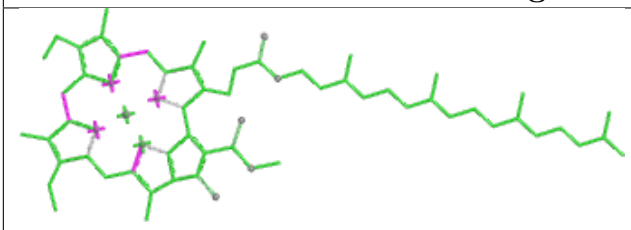
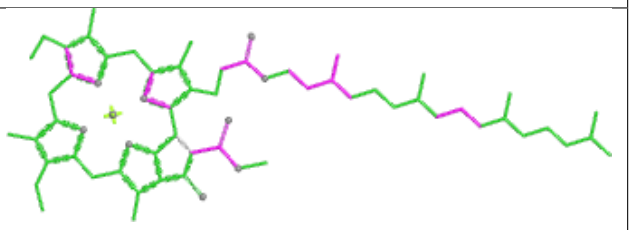
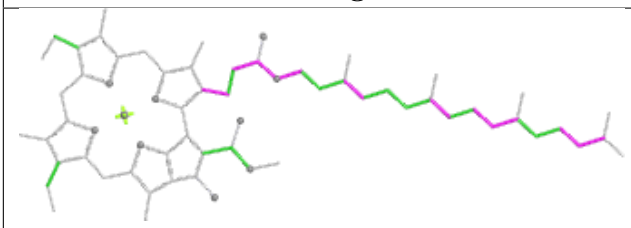
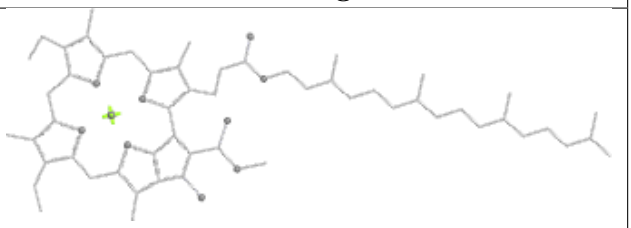


Rings

Ligand CLA 3 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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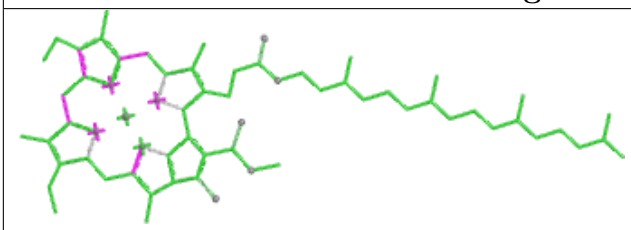
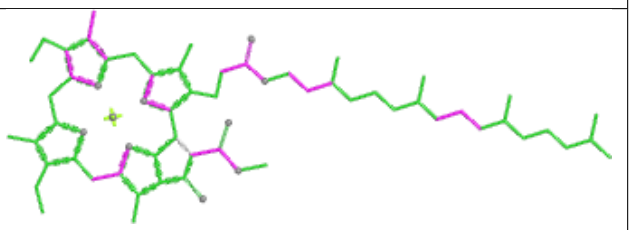
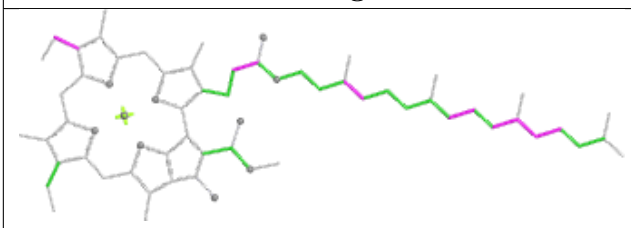
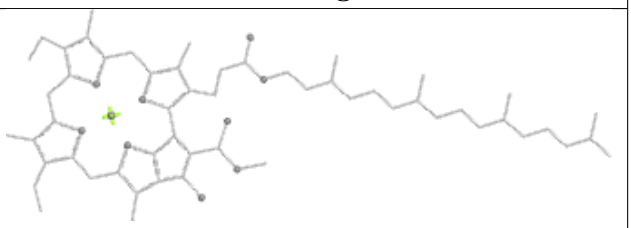
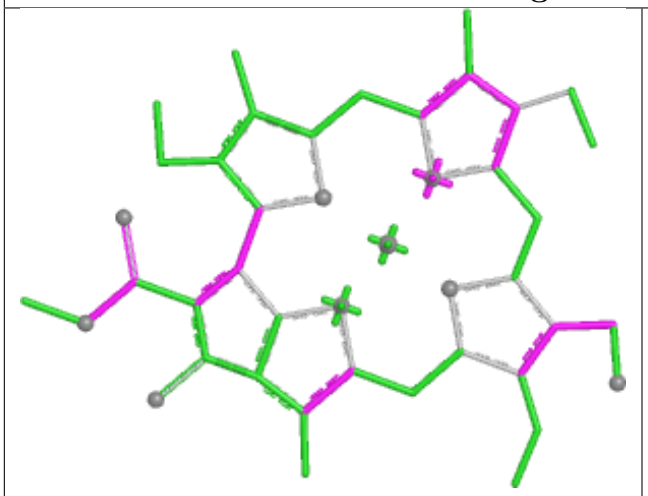
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL s 607



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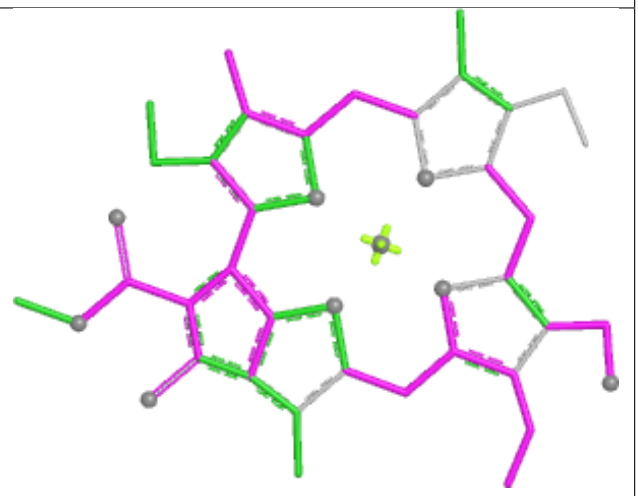
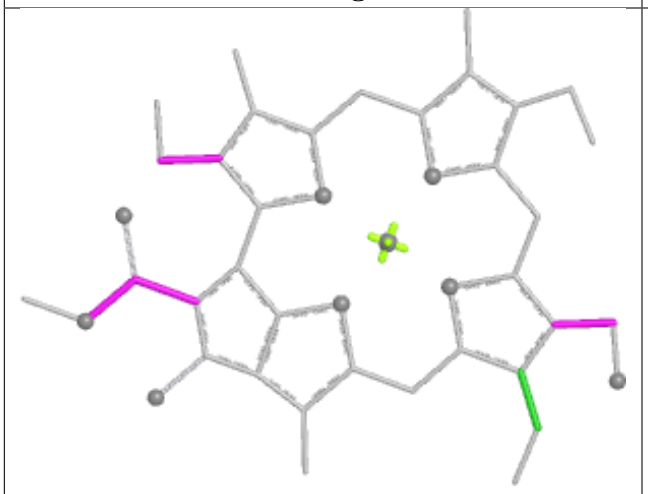


Bond angles



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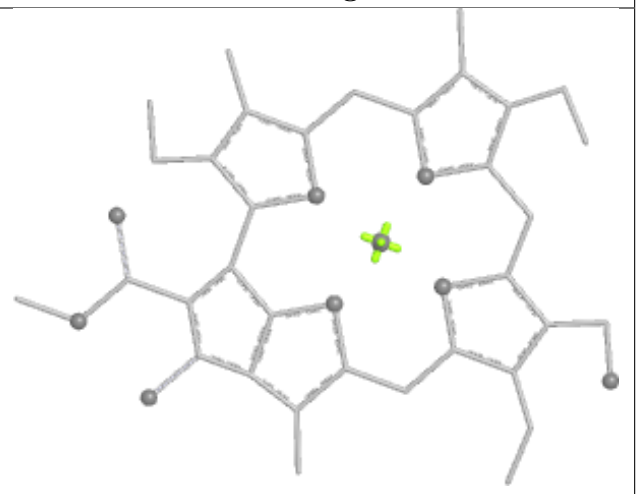
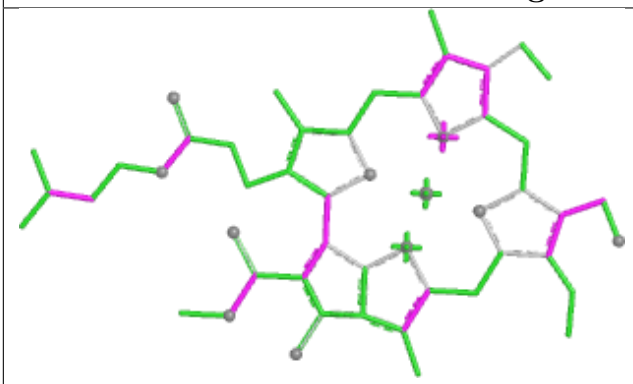


Rings

Ligand CHL 1 607



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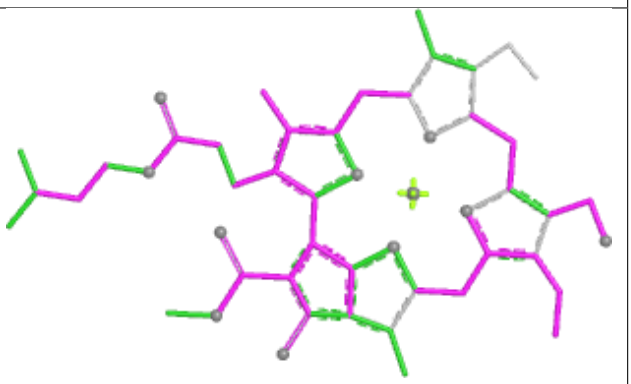
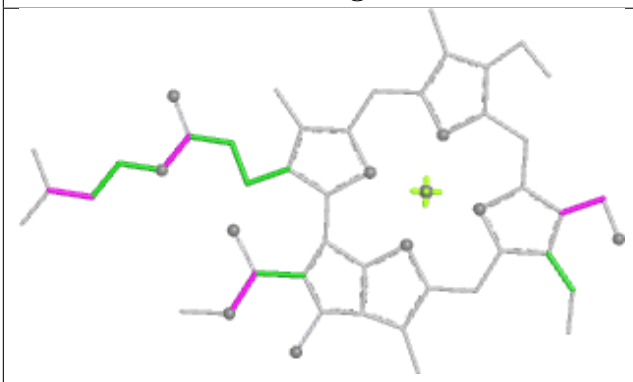


Bond angles



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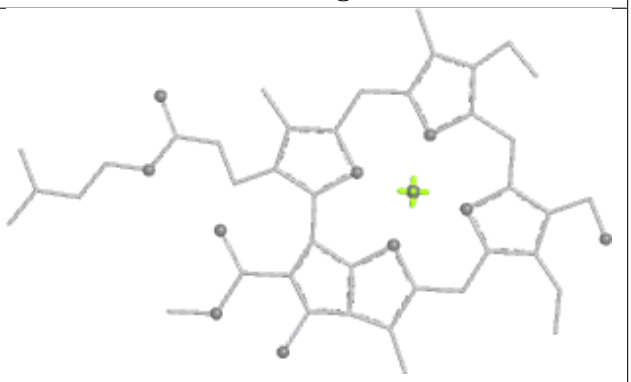
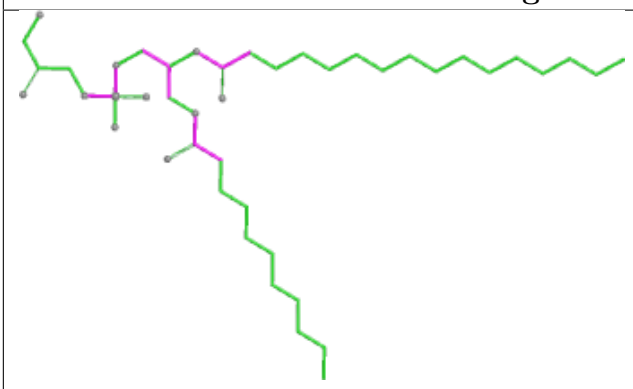
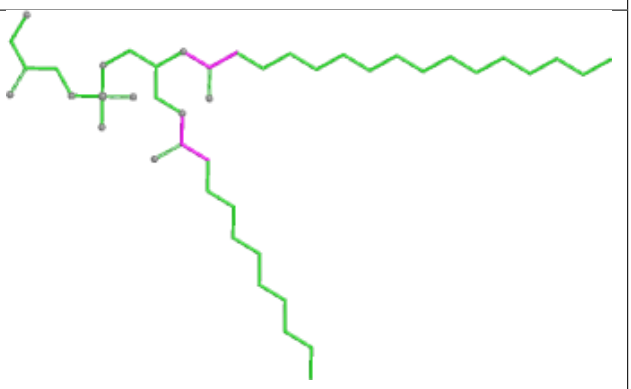


Rings

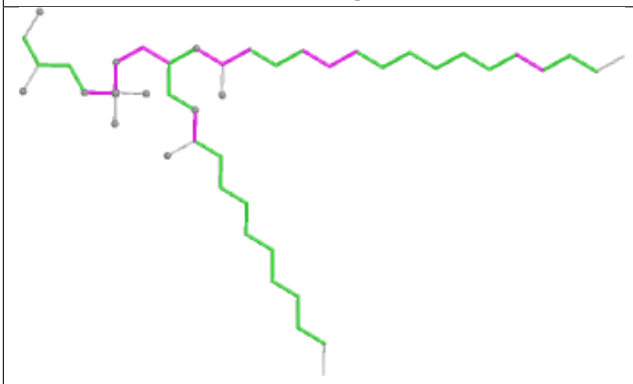
Ligand LHG R 621



Bond lengths



Bond angles



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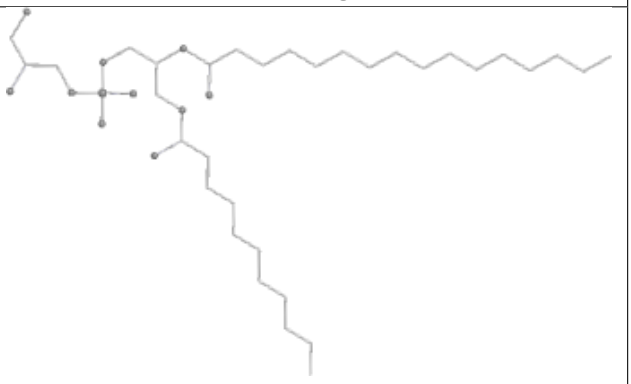
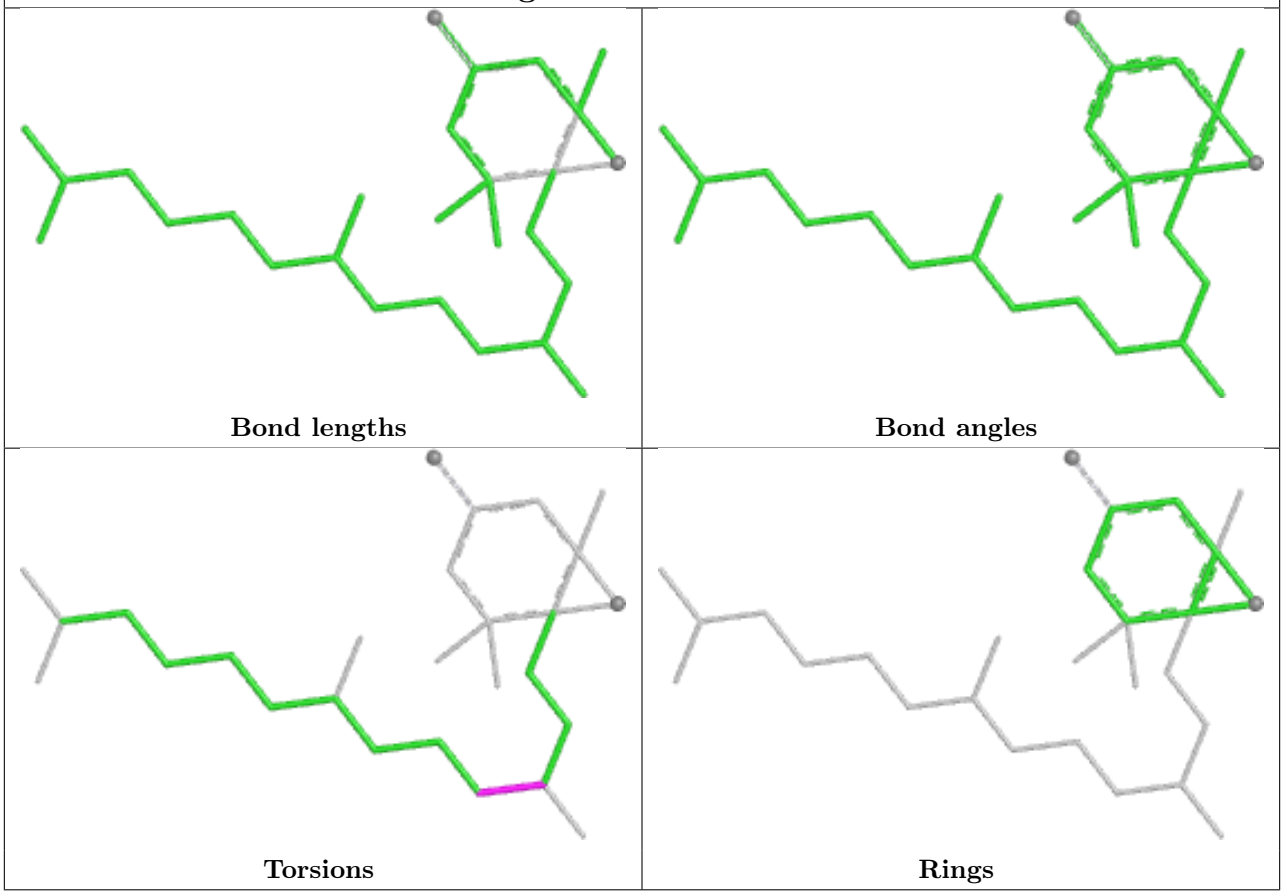
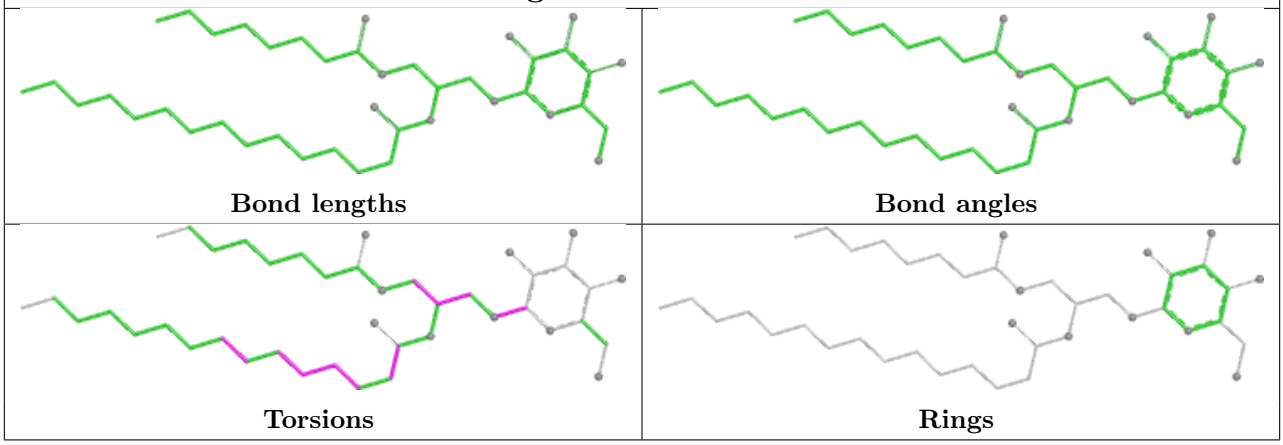


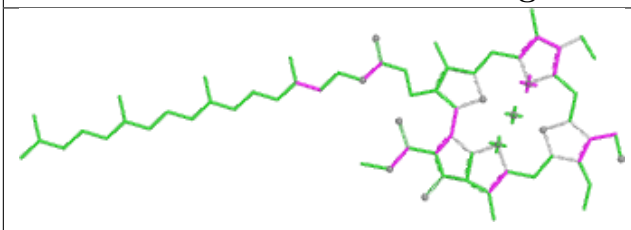
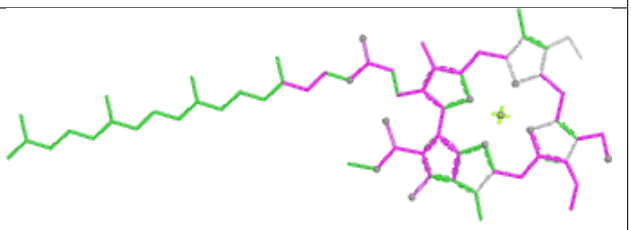
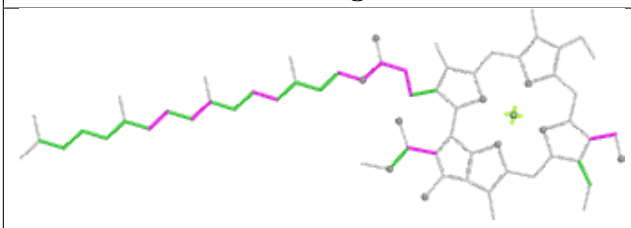
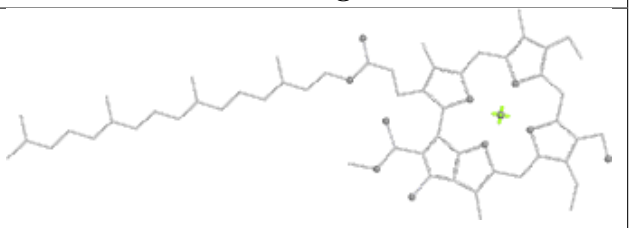
Rings

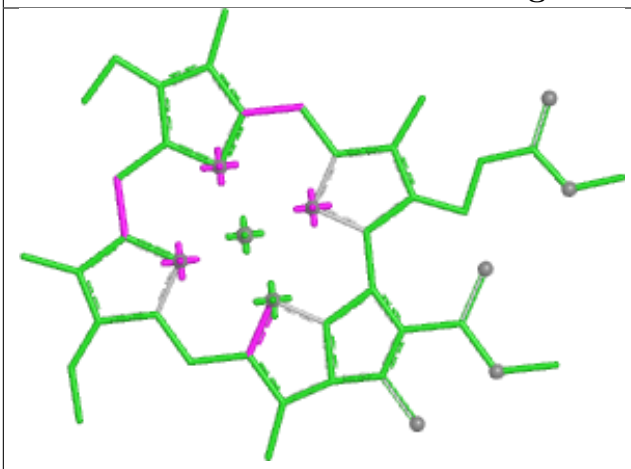
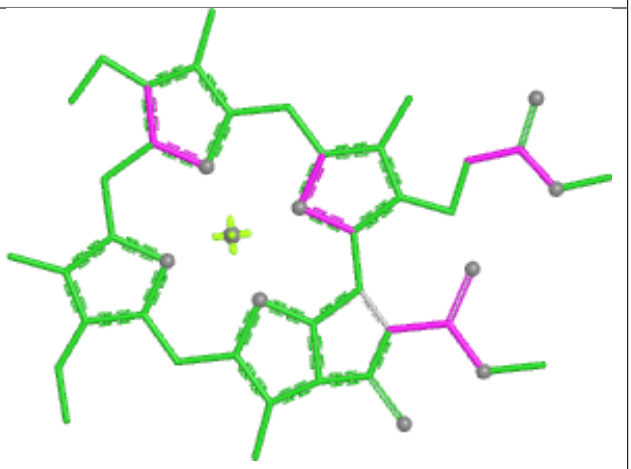
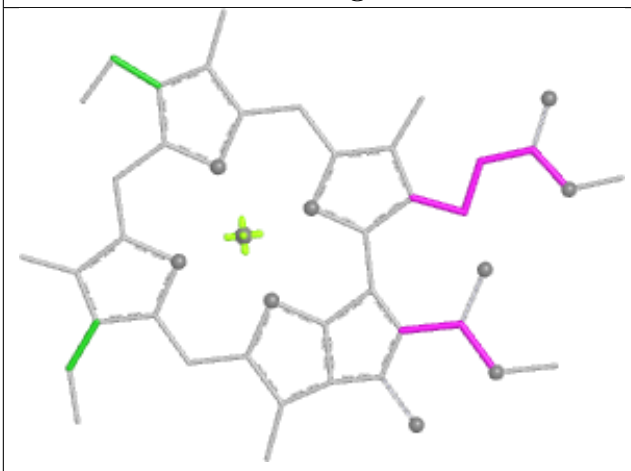
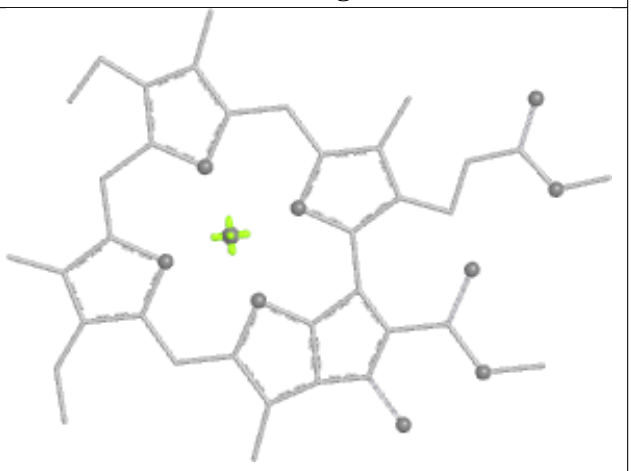
Ligand NEX 12 616

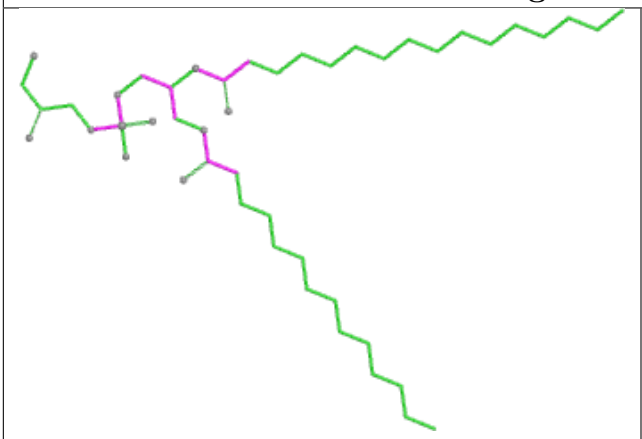
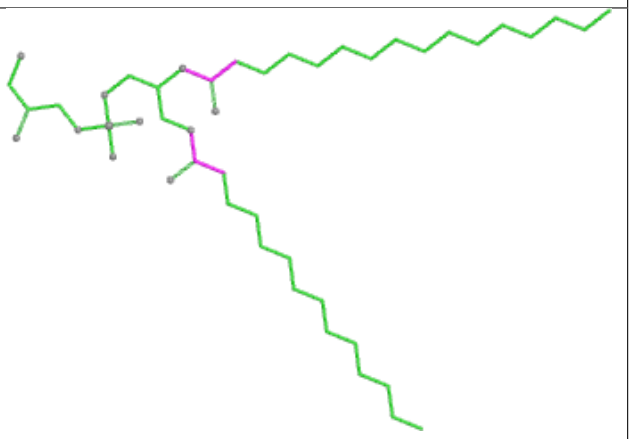
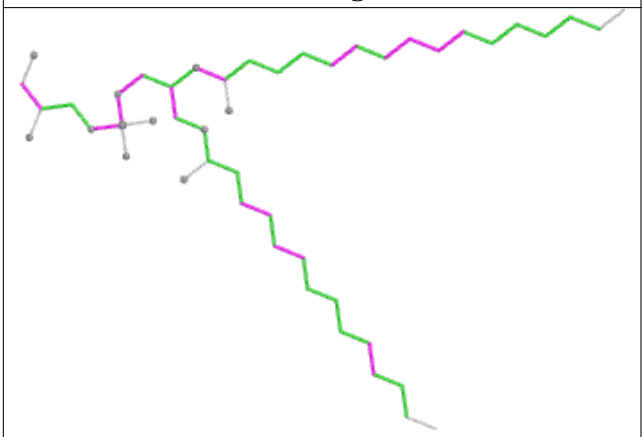
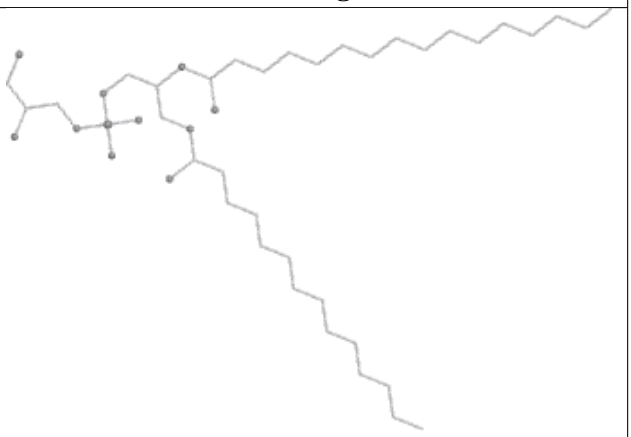


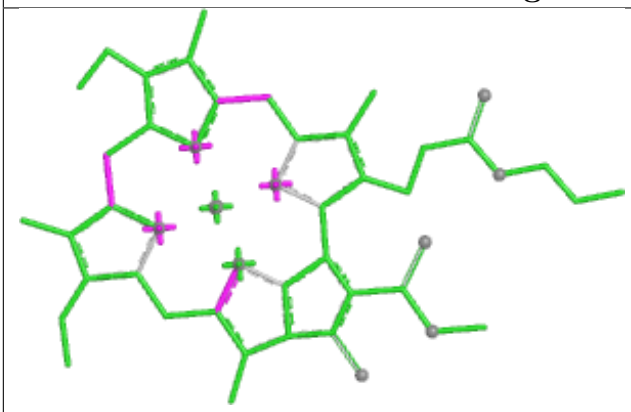
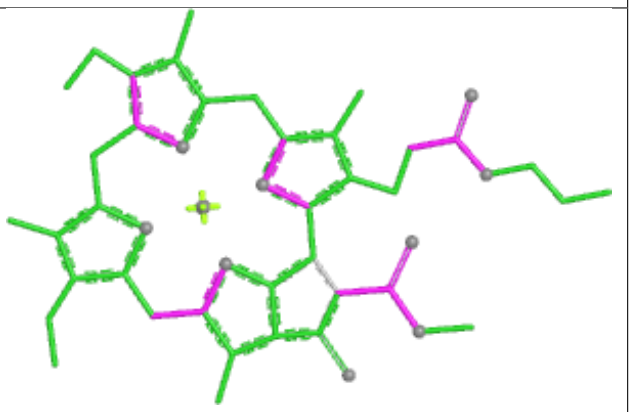
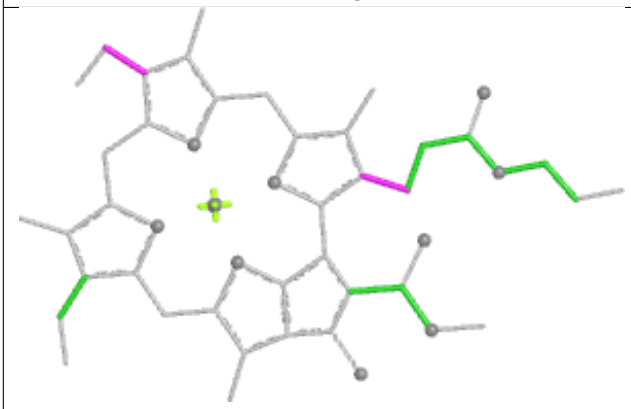
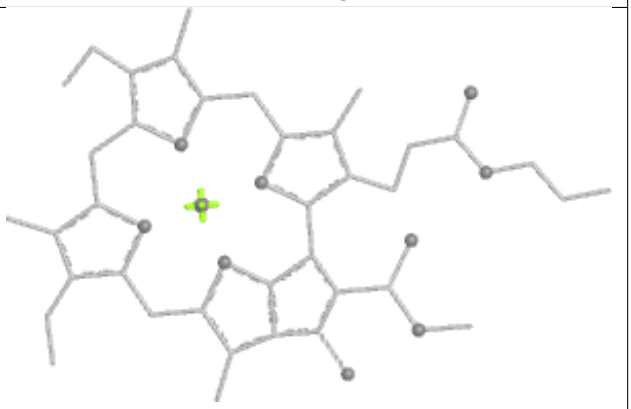
Ligand LMG s 616



Ligand CHL 11 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG r 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

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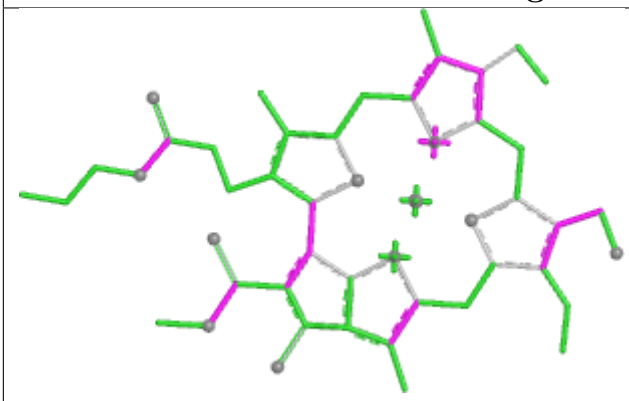
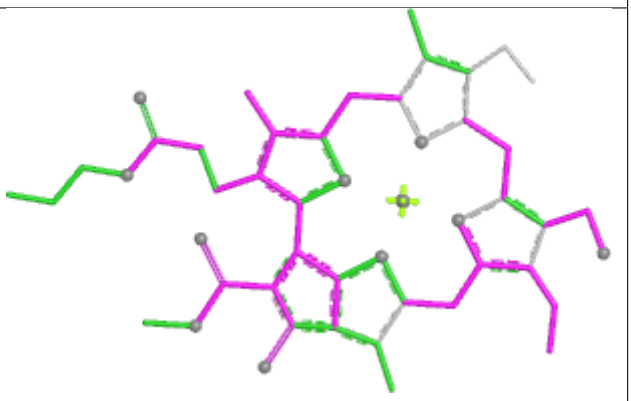
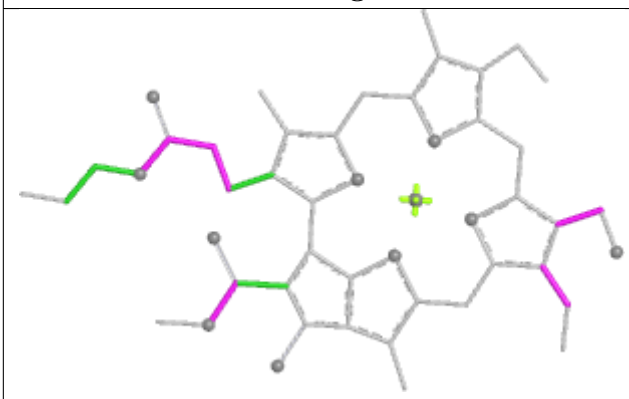
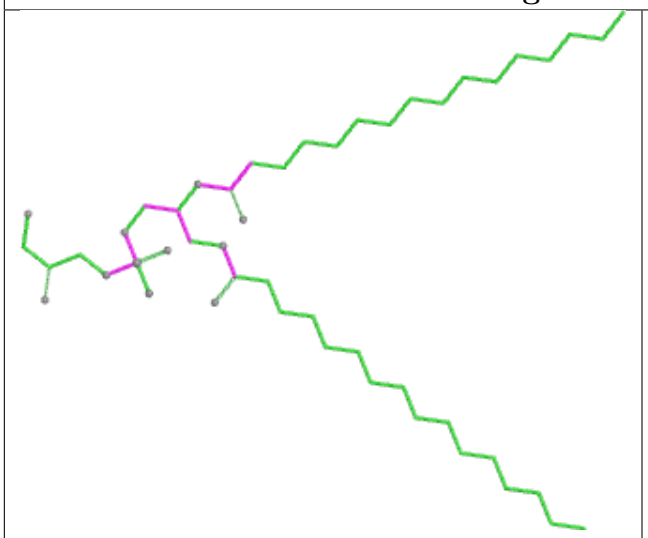
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LHG N 616



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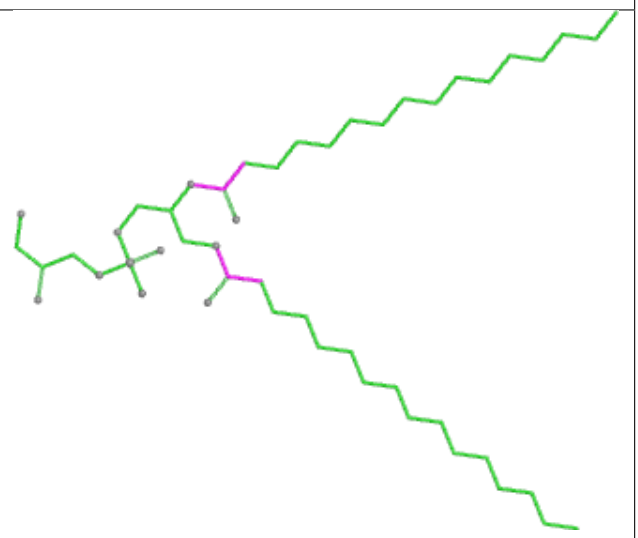

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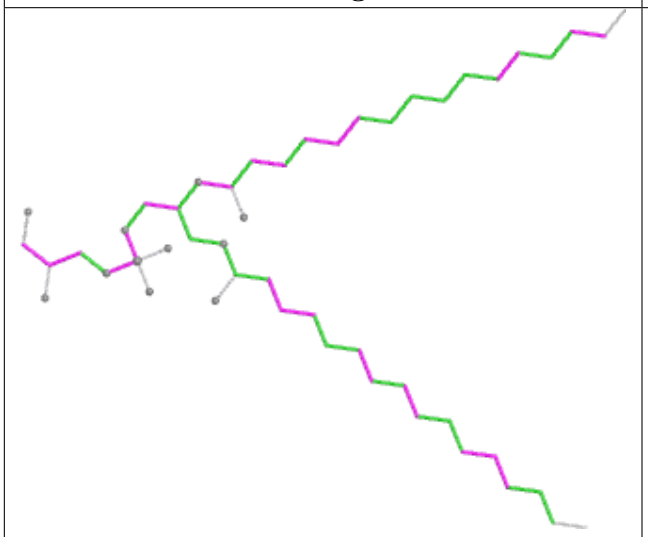

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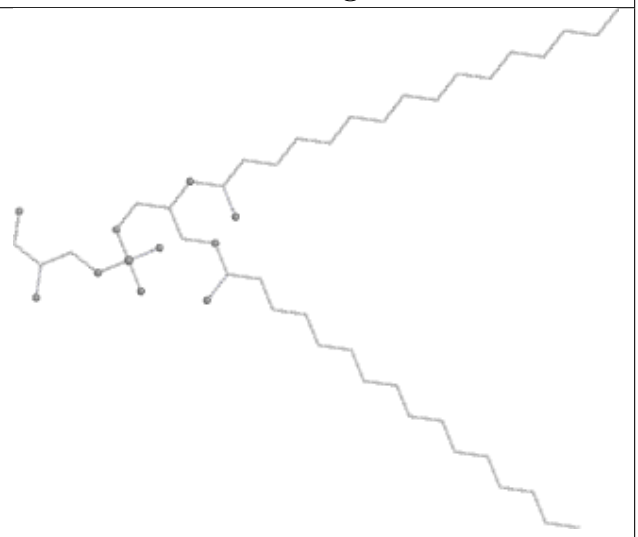
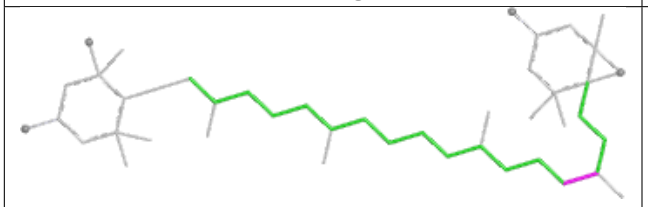


Rings

Ligand NEX s 620

Bond lengths

Bond angles



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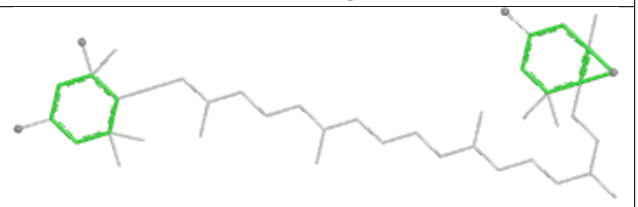

Rings

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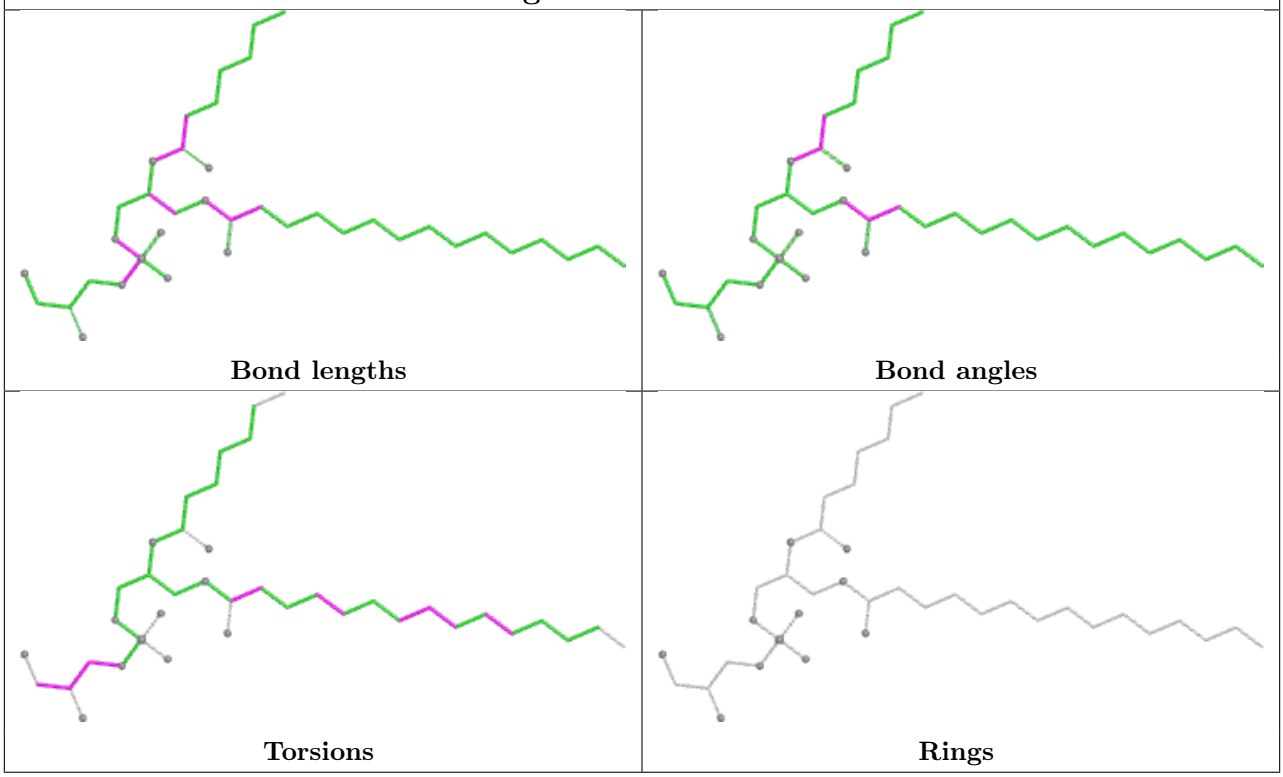

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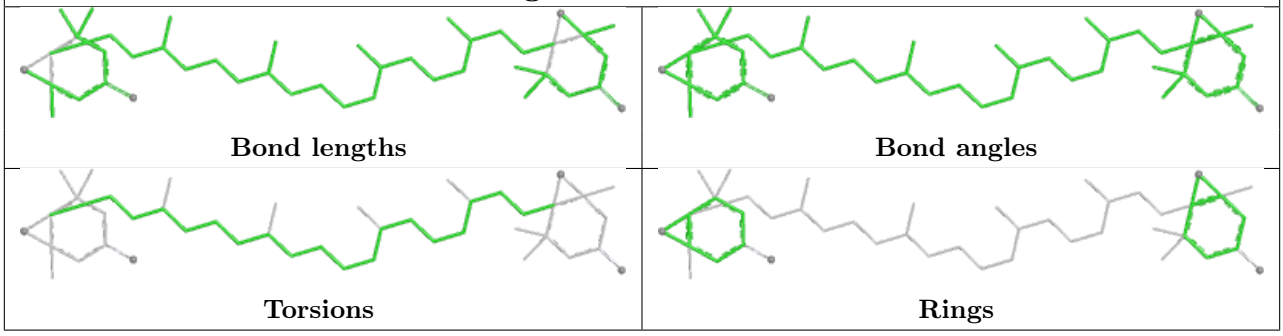

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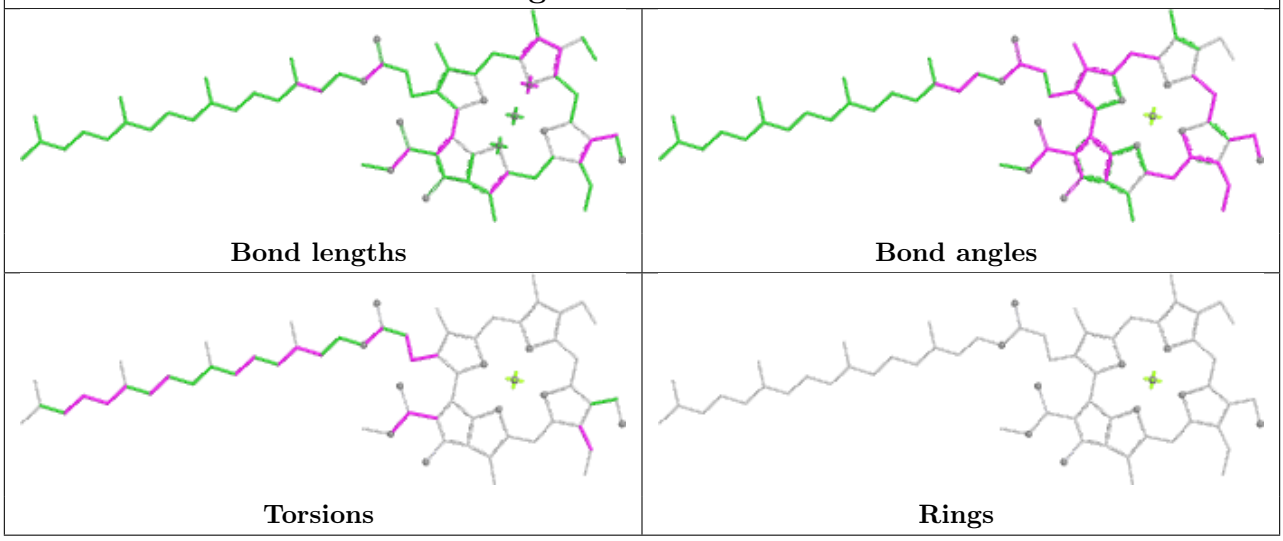

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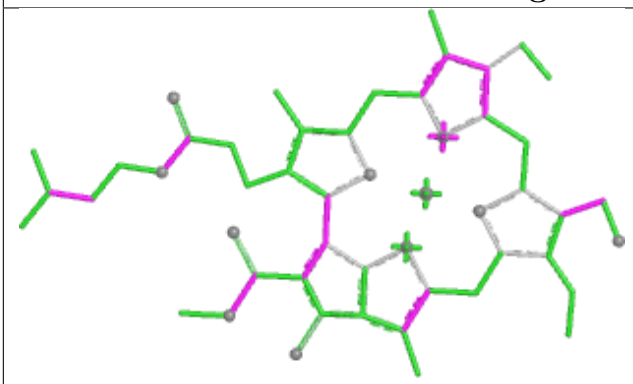

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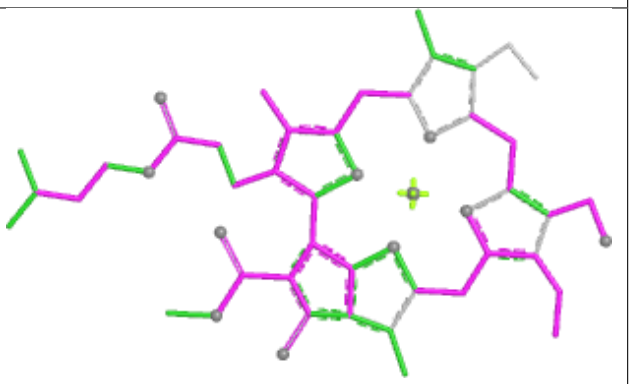

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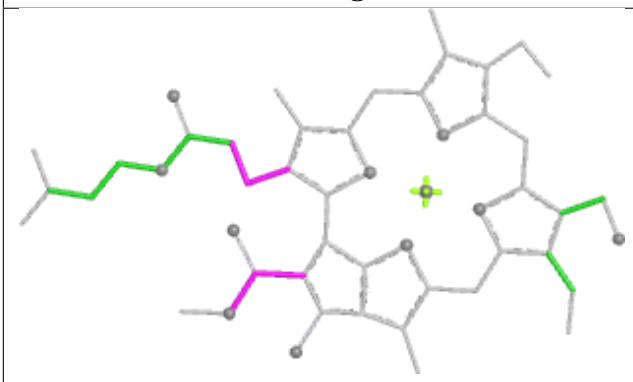

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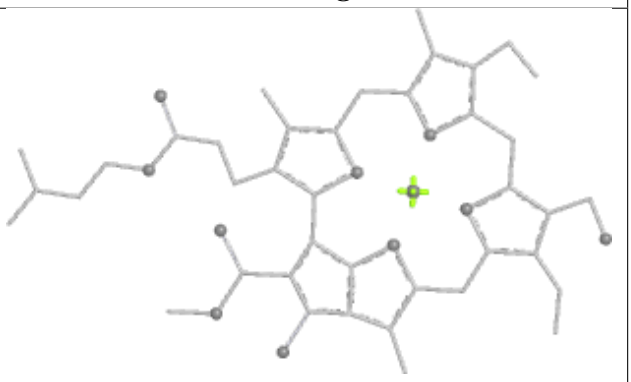
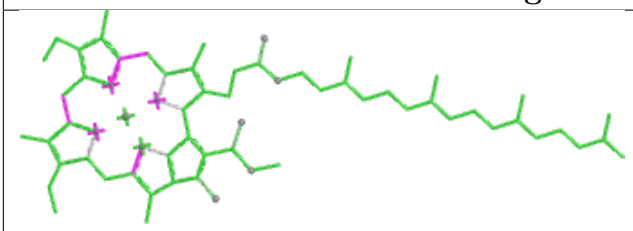


Rings

Ligand CLA B 610



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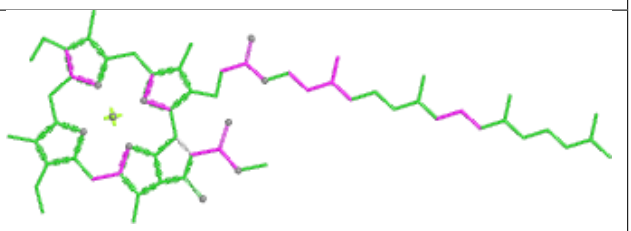

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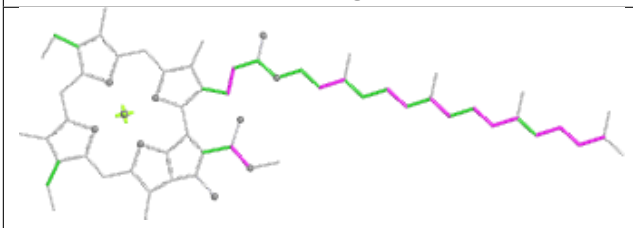

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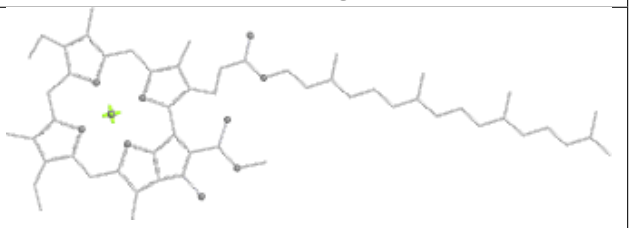

Rings

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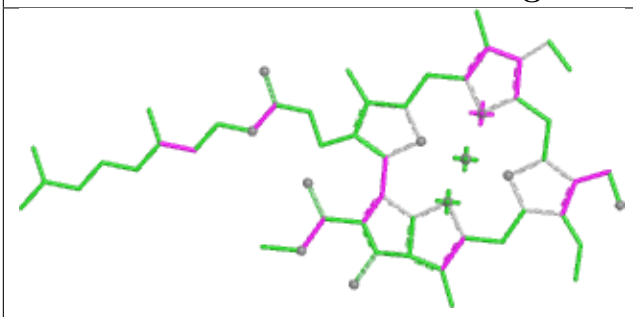

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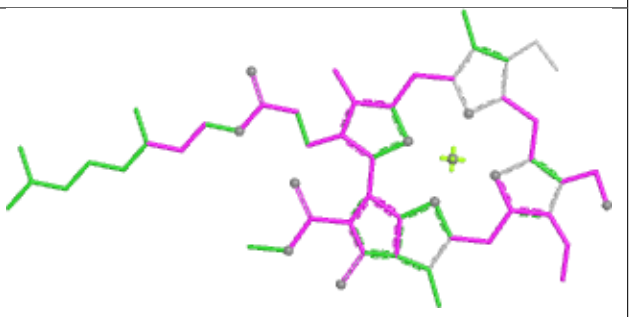

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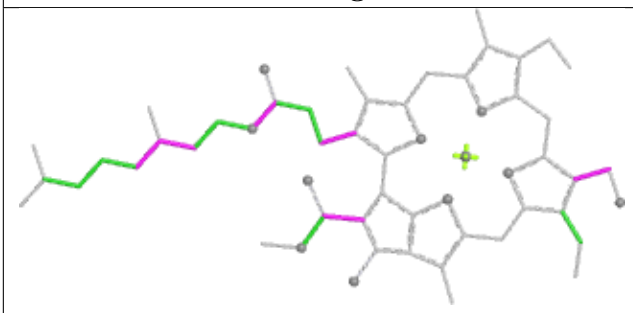

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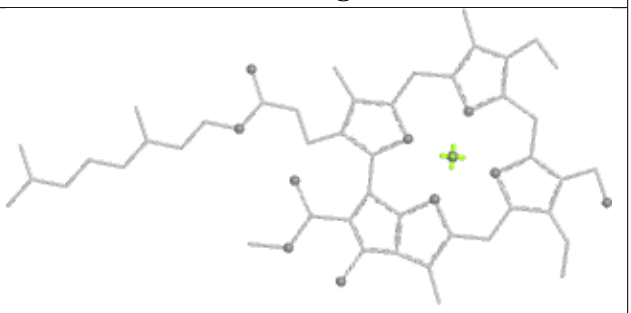

Rings

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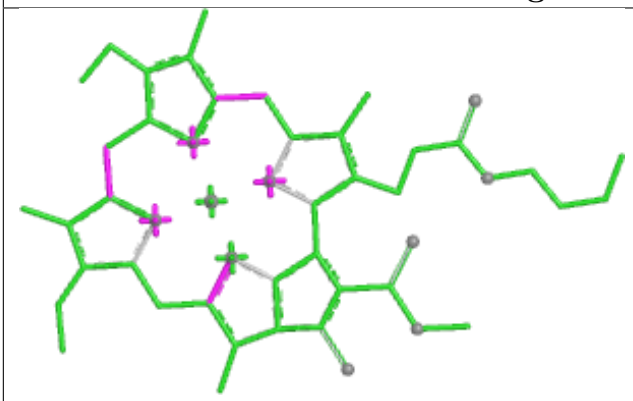

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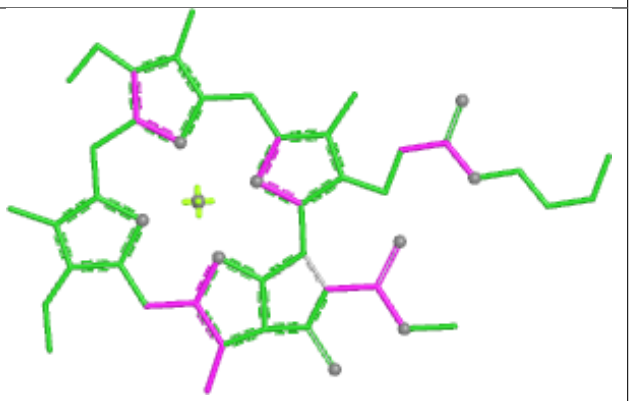

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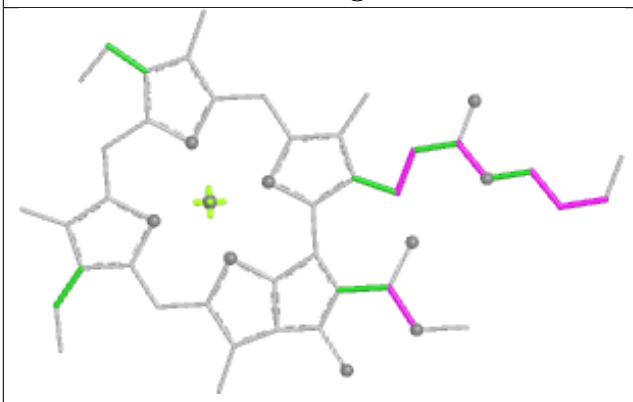

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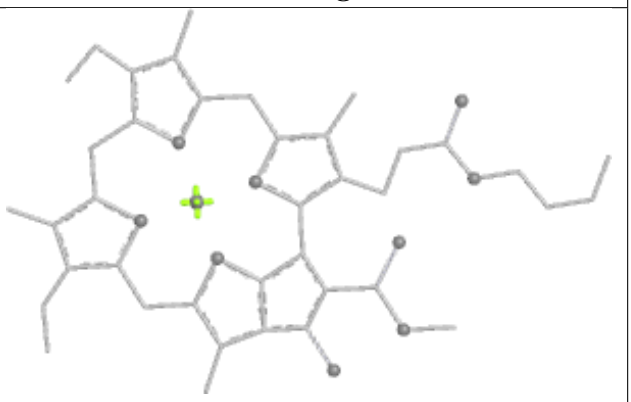
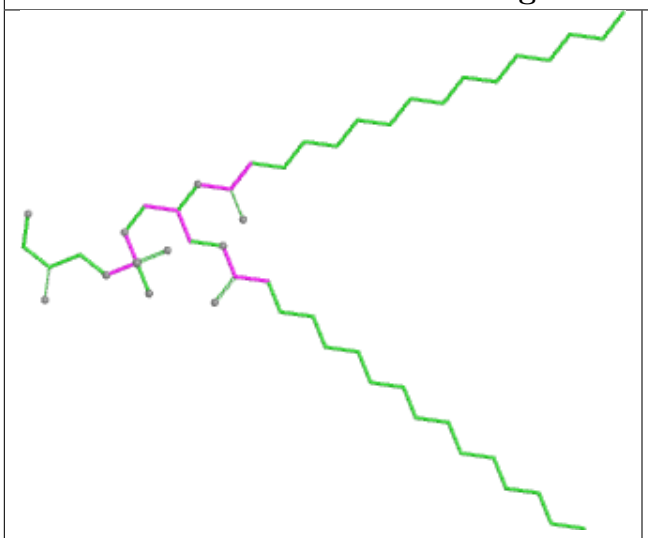


Rings

Ligand LHG 11 615



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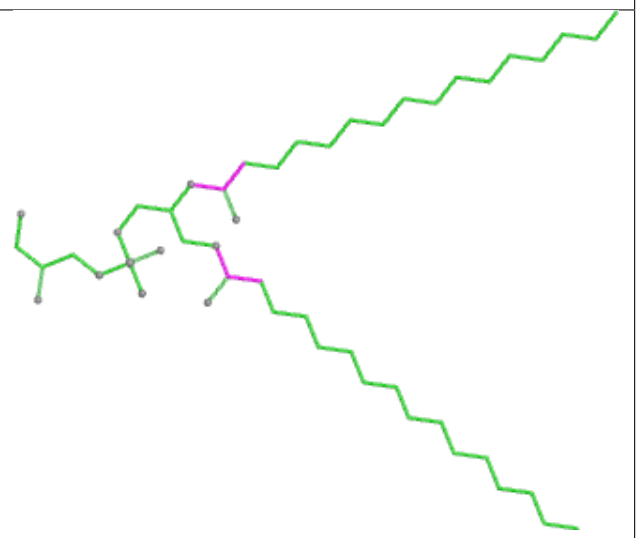

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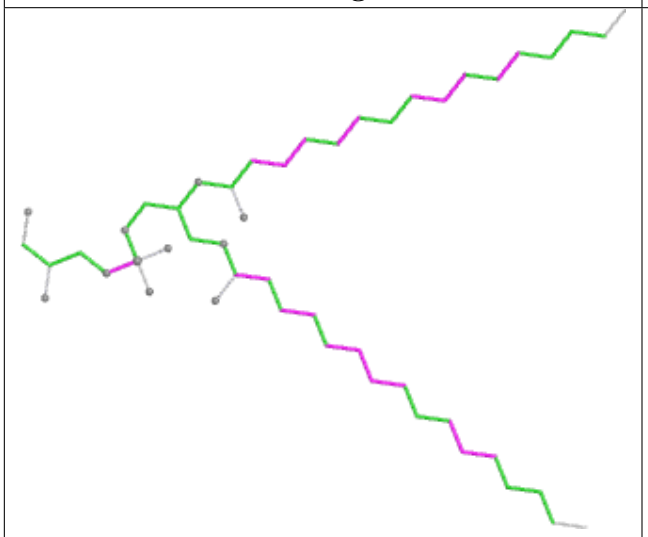

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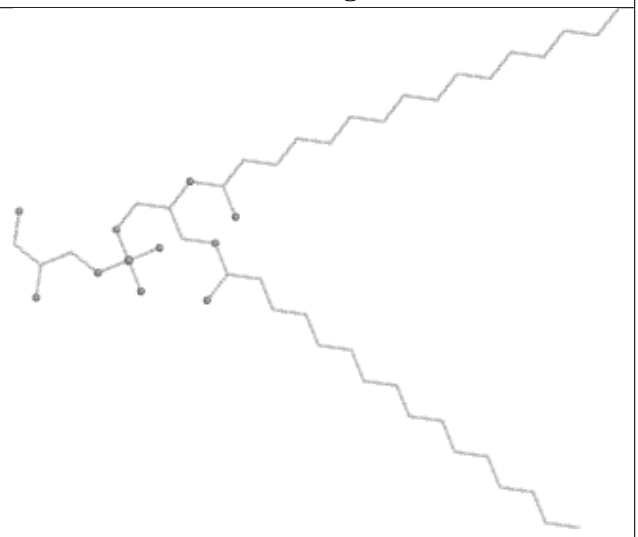


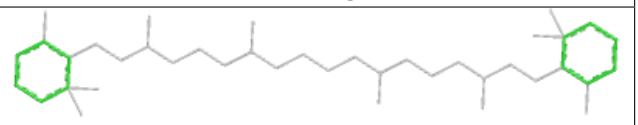
Rings

Ligand BCR J 101

Bond lengths

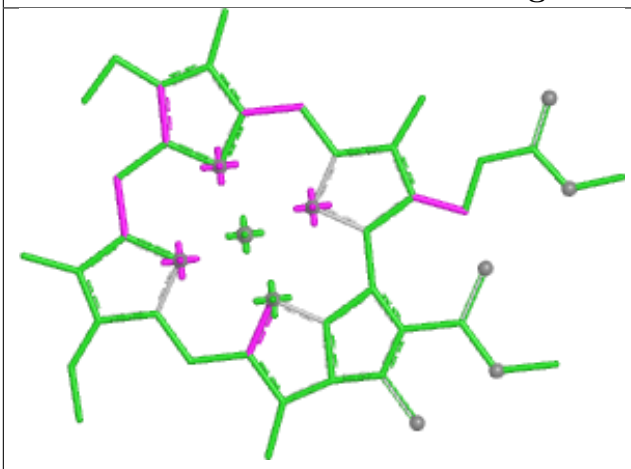
Bond angles

Torsions



Rings

Ligand CLA 2 611



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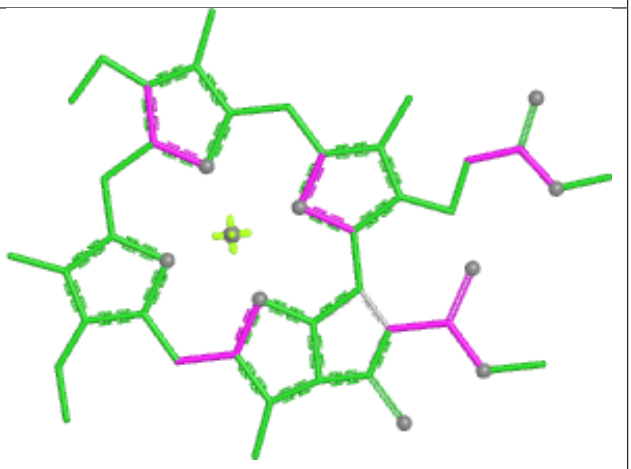

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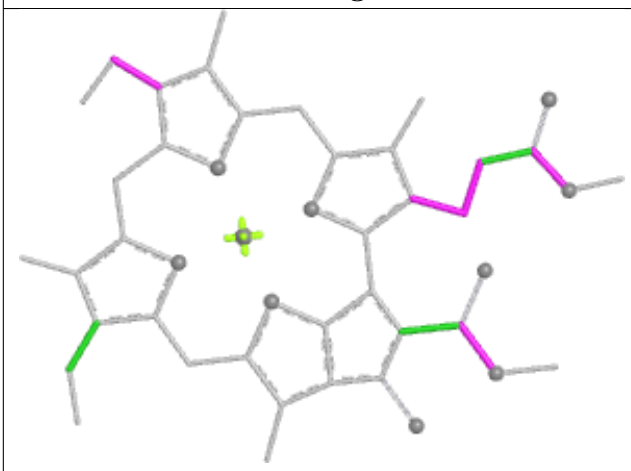

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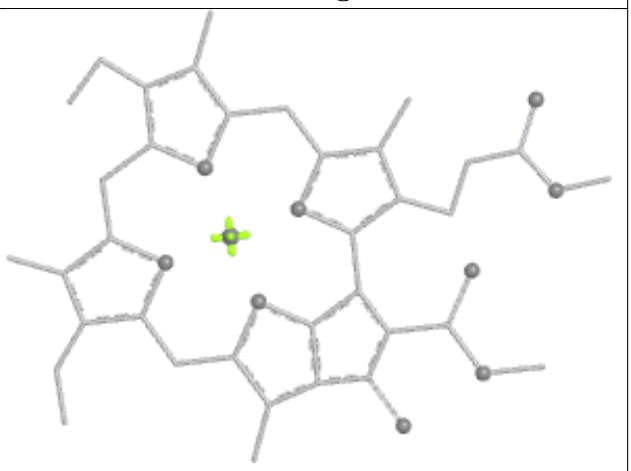

Rings

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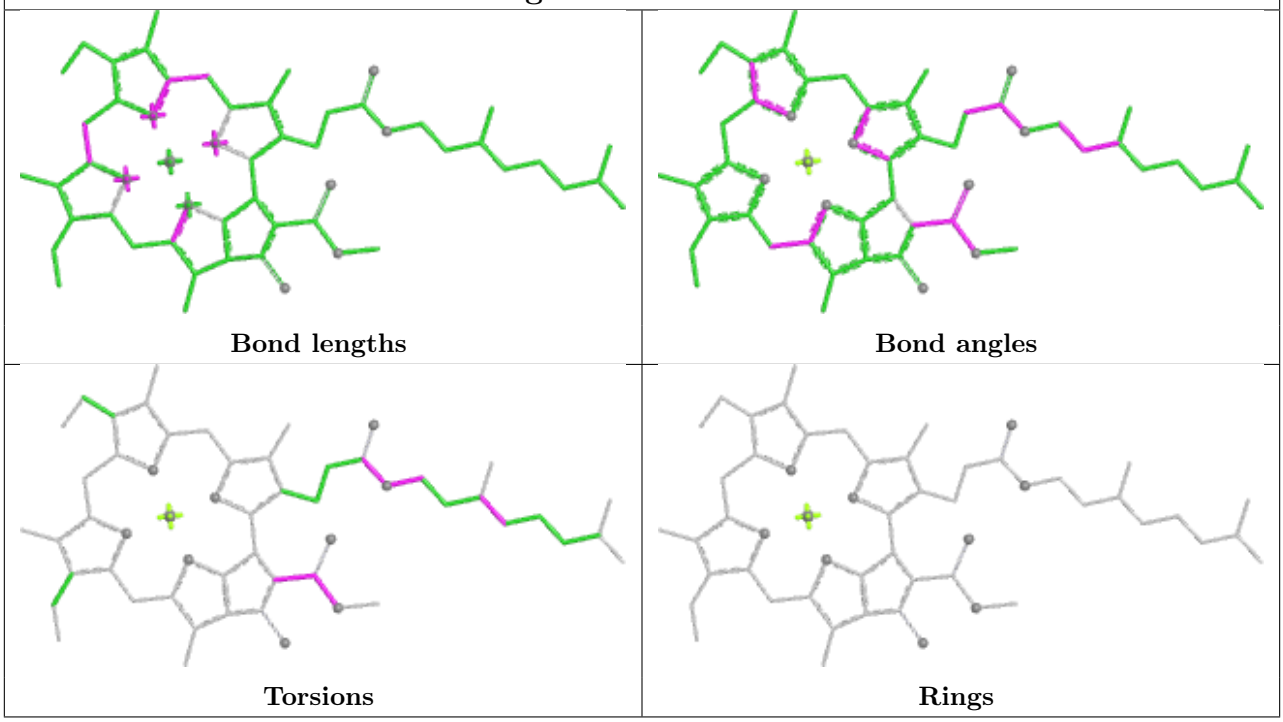

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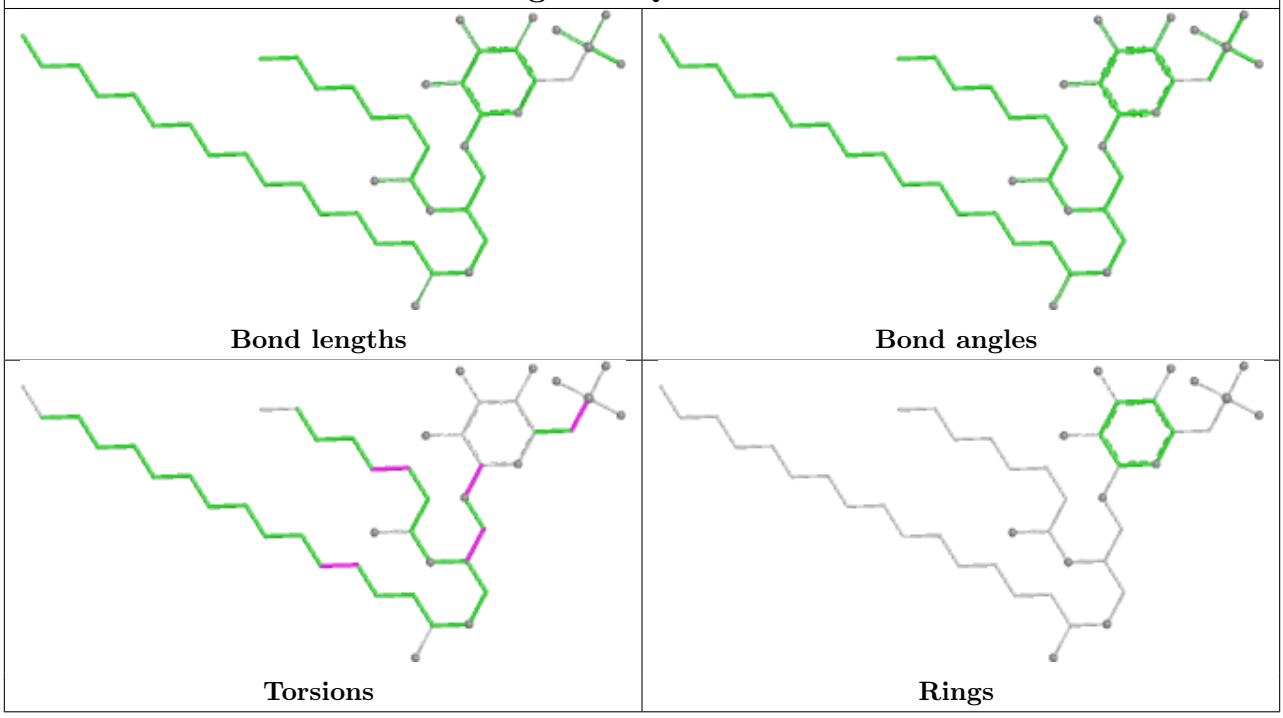

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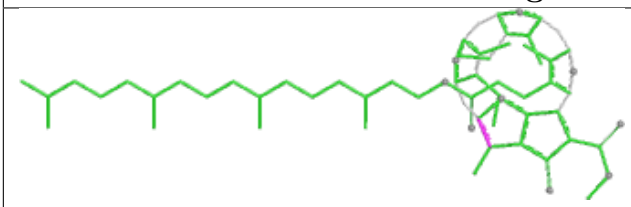

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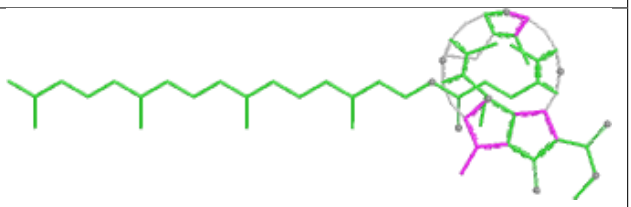
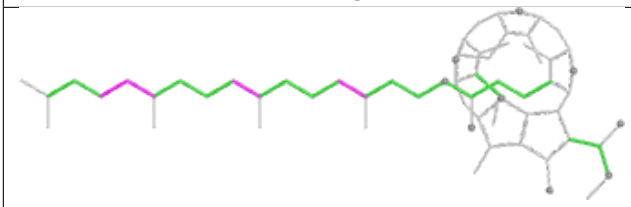


Bond angles



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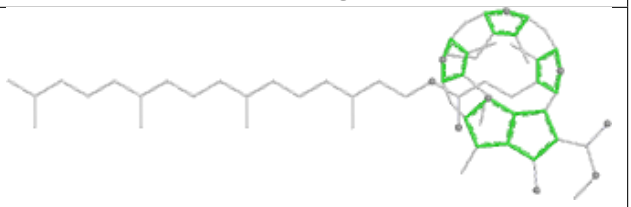

Rings

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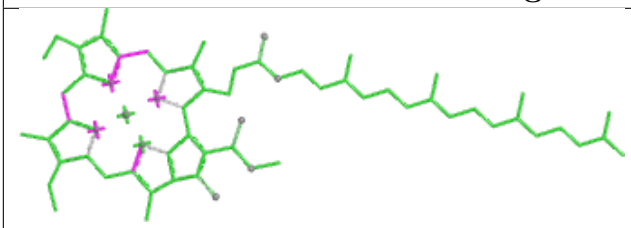

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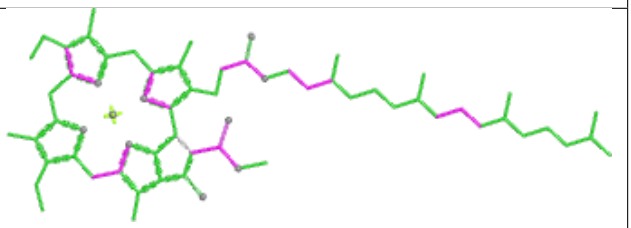
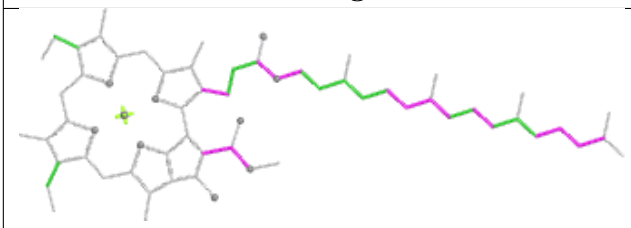


Bond angles



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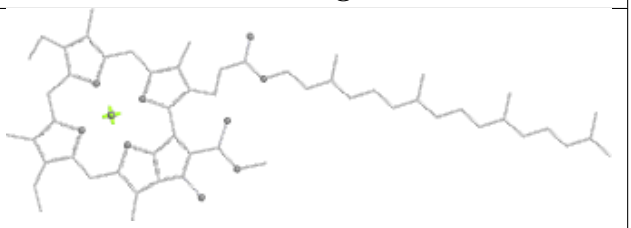

Rings

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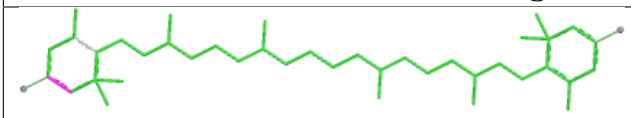
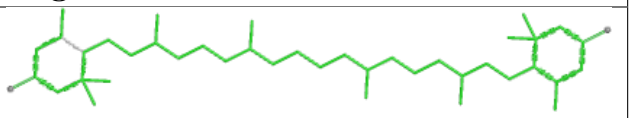
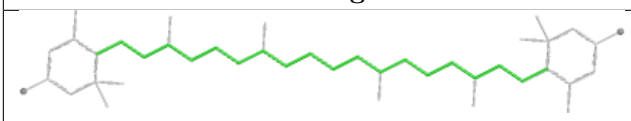


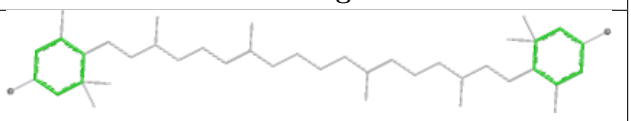
Bond lengths



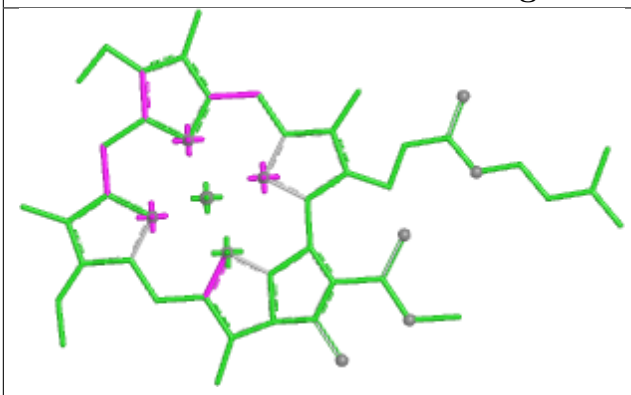
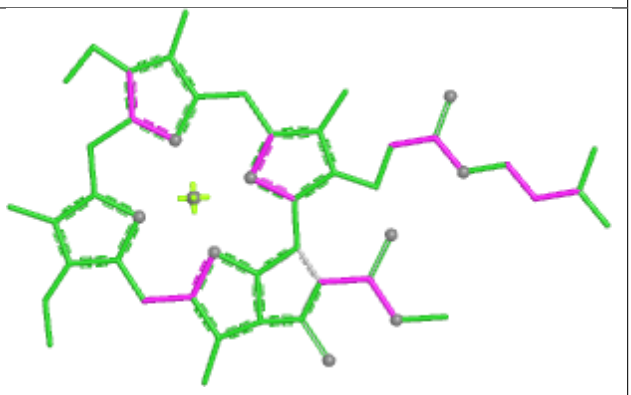
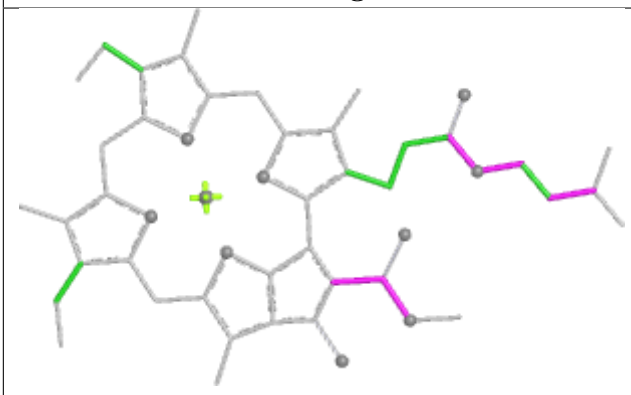
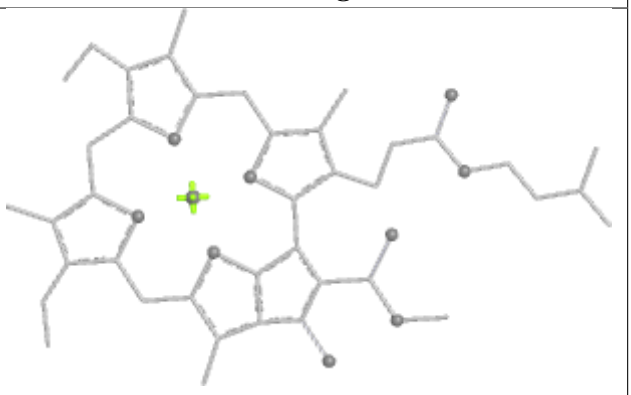
Bond angles



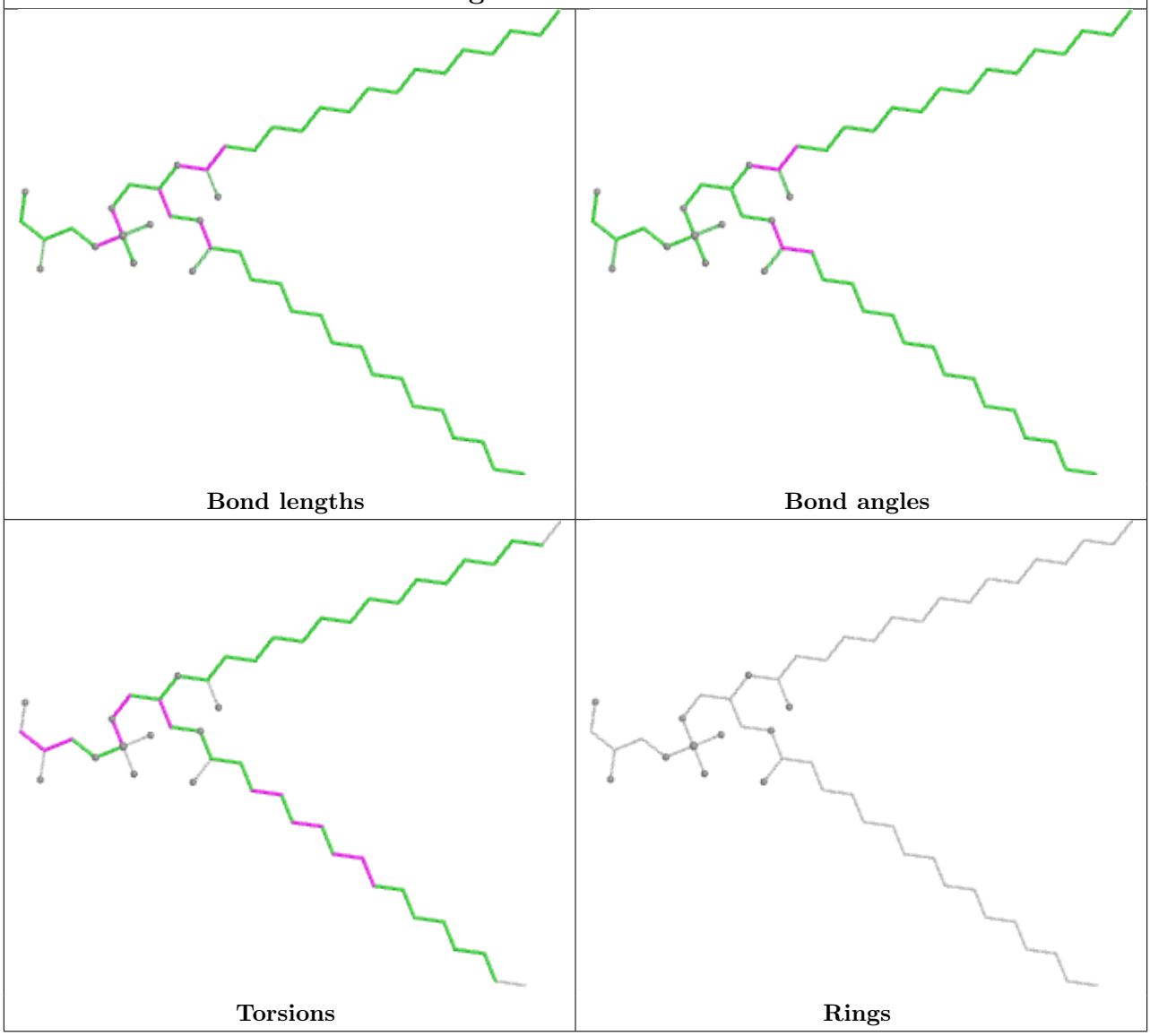
Torsions

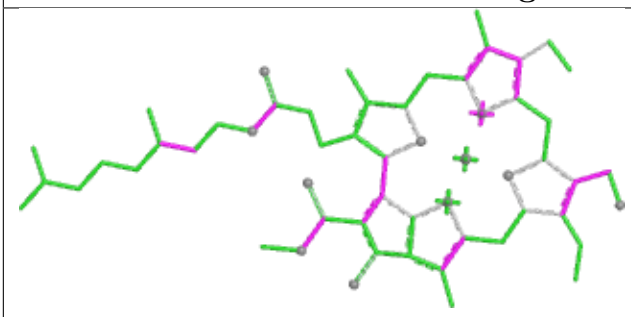
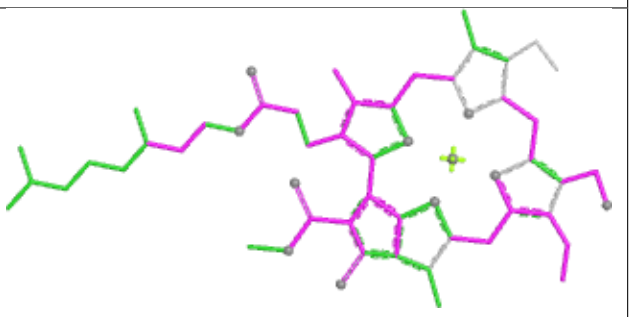
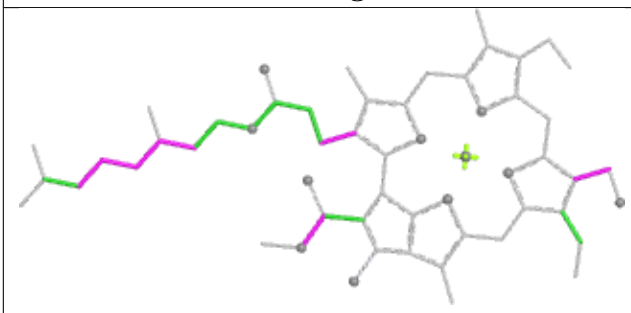
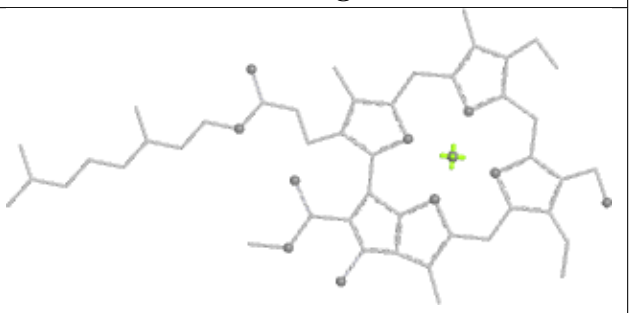


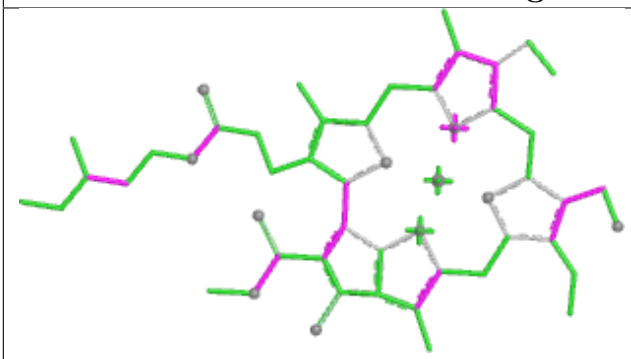
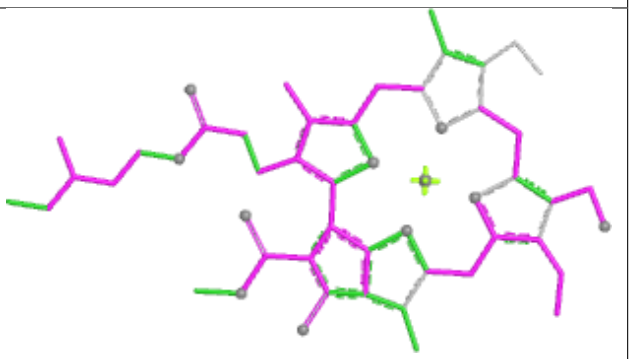
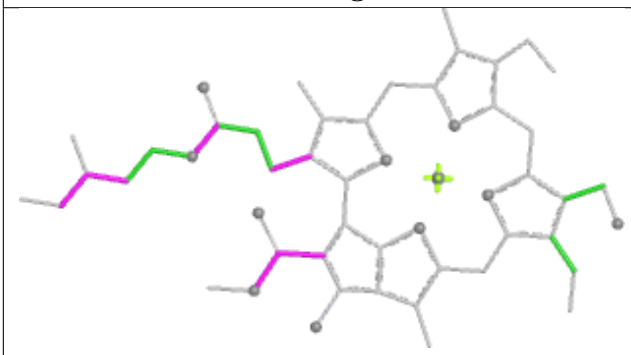
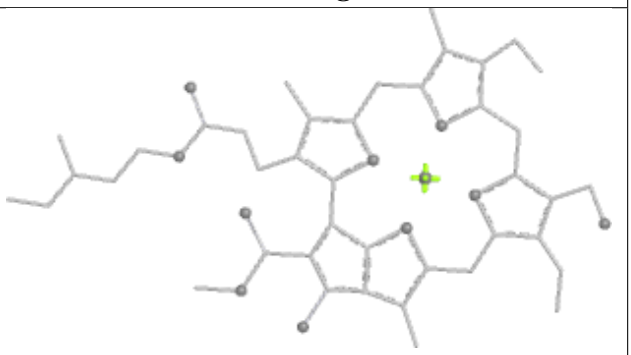
Rings

Ligand CLA 11 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

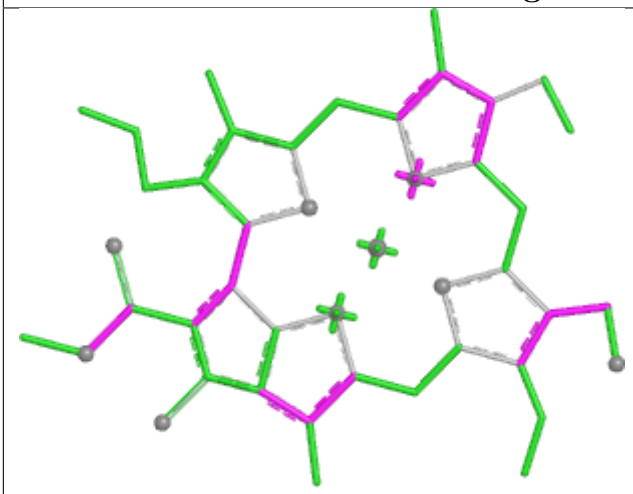
Ligand LHG Y 616



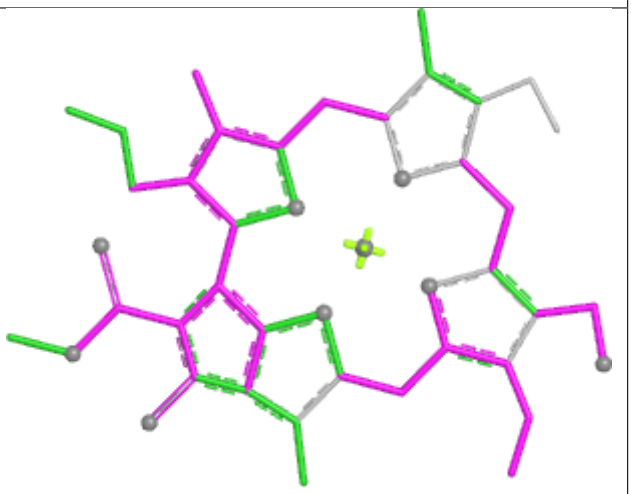
Ligand CHL 13 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL n 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

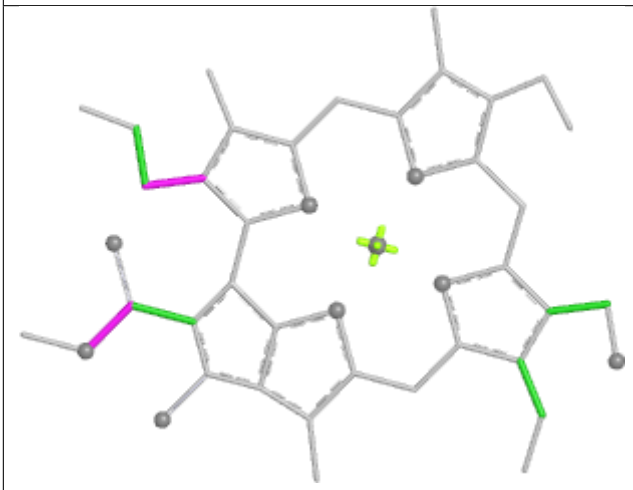
Ligand CHL Y 608



Bond lengths



Bond angles



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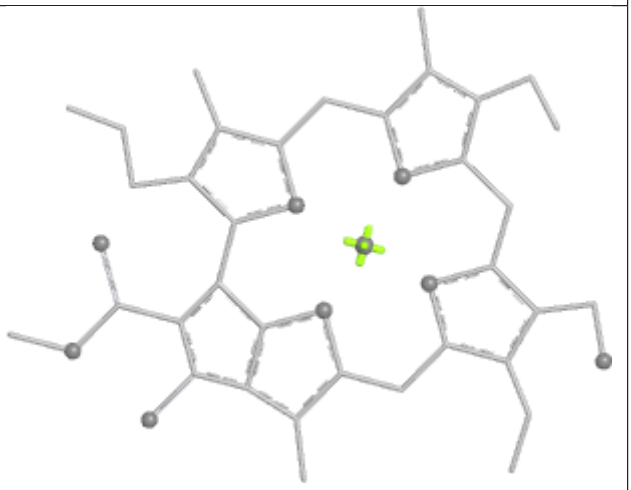
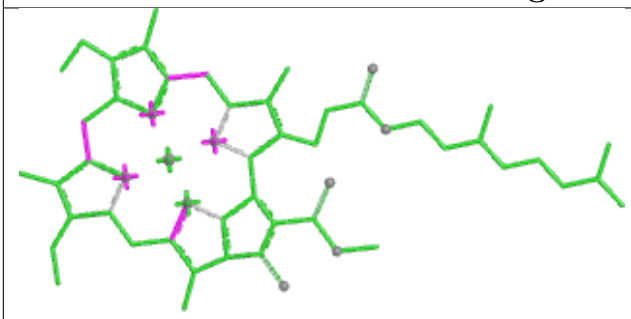


Rings

Ligand CLA 6 603



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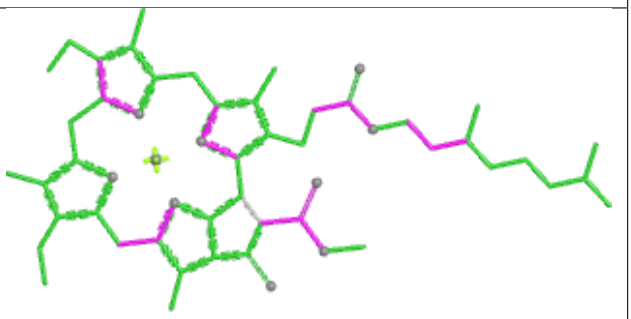

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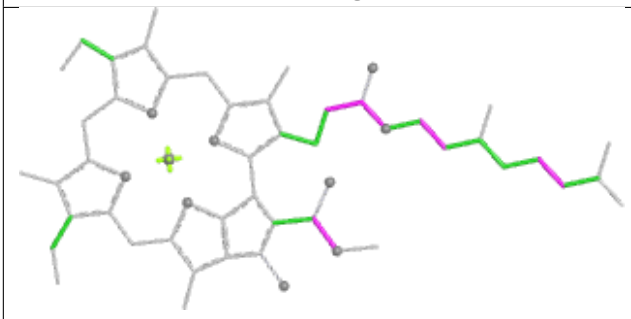

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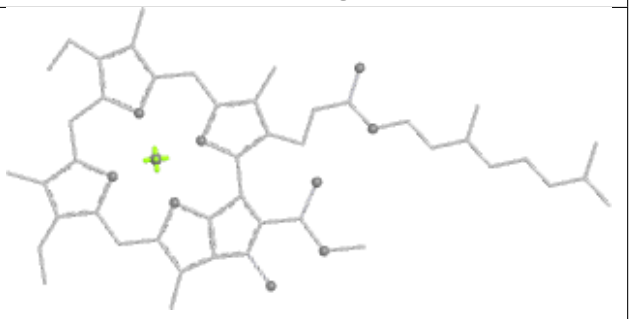
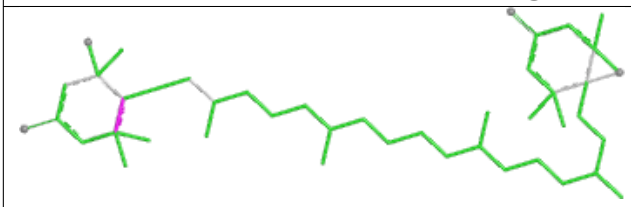


Rings

Ligand NEX n 619



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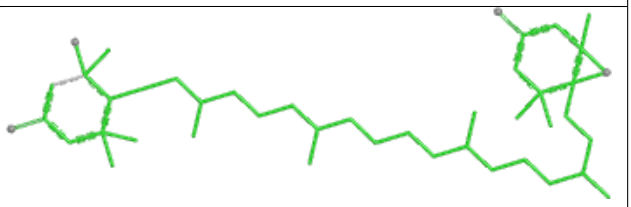
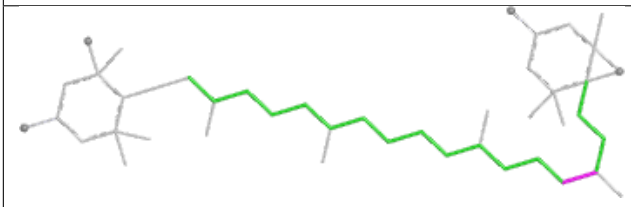


Bond angles



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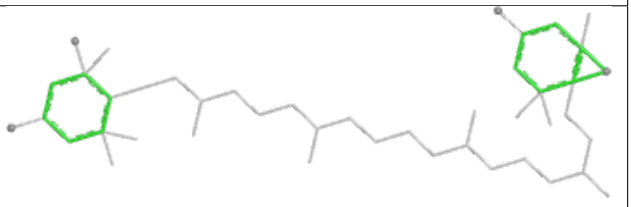
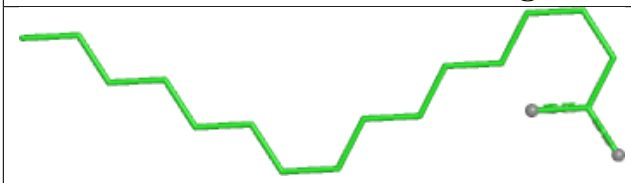


Rings

Ligand PAM N 621



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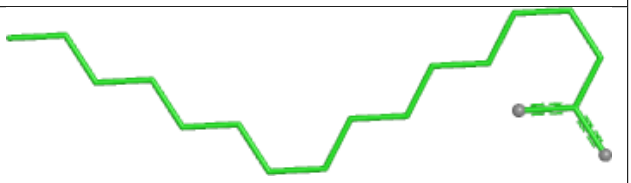
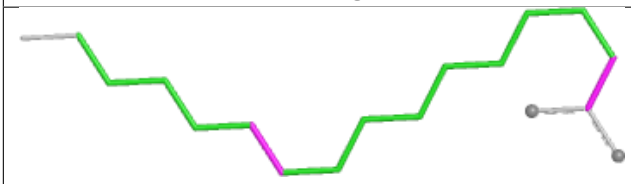


Bond angles



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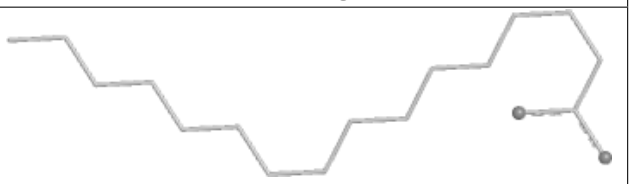
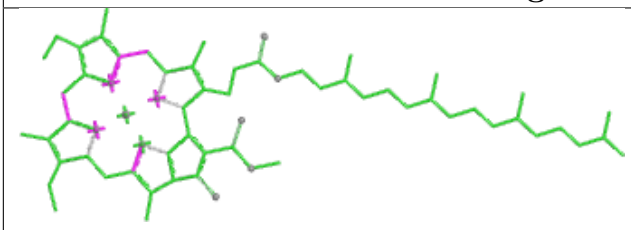
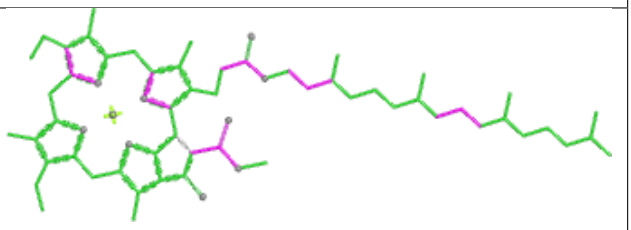


Rings

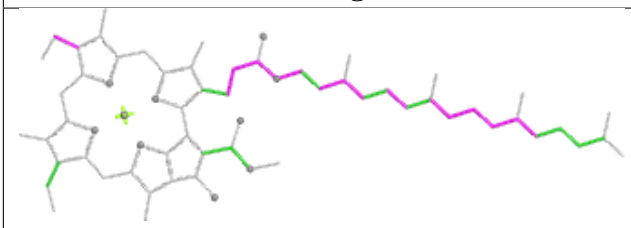
Ligand CLA b 613



Bond lengths



Bond angles



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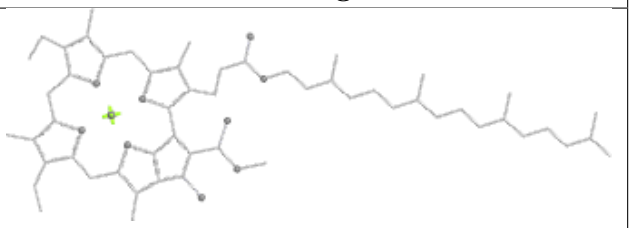
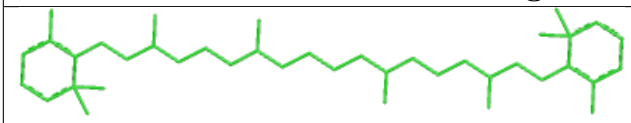


Rings

Ligand BCR b 617



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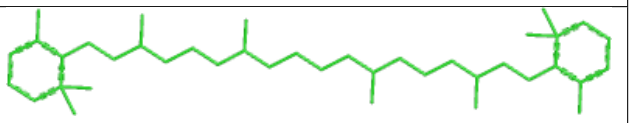
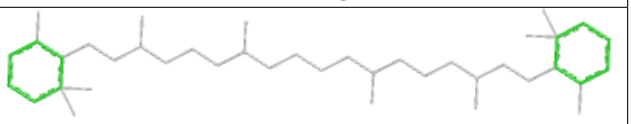


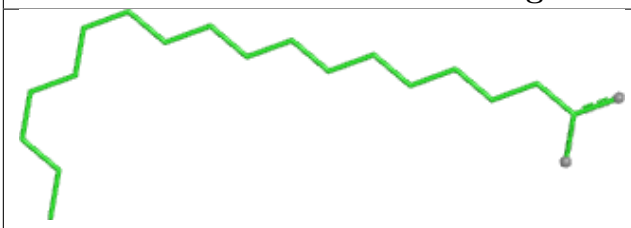
Bond angles

Torsions



Rings

Ligand LNL C 523



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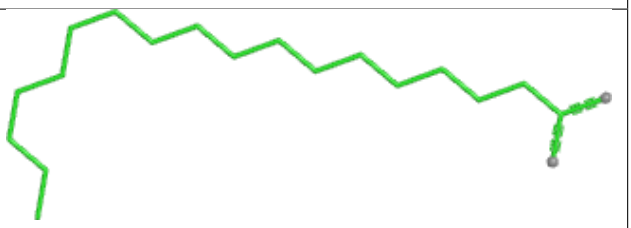

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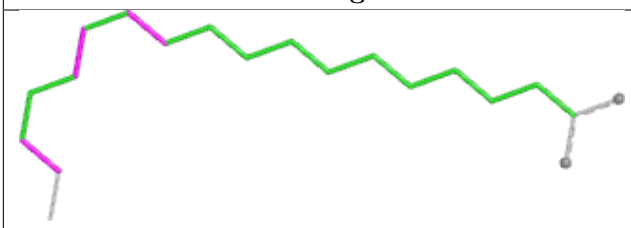

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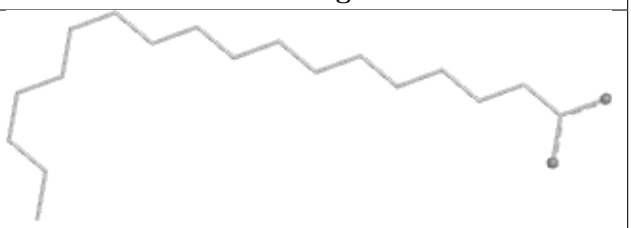
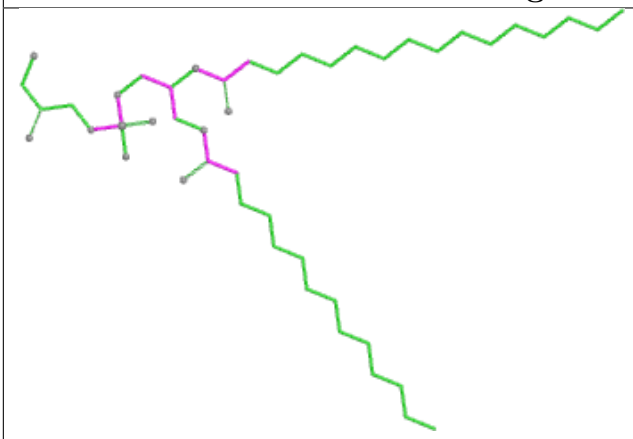


Rings

Ligand LHG 6 617



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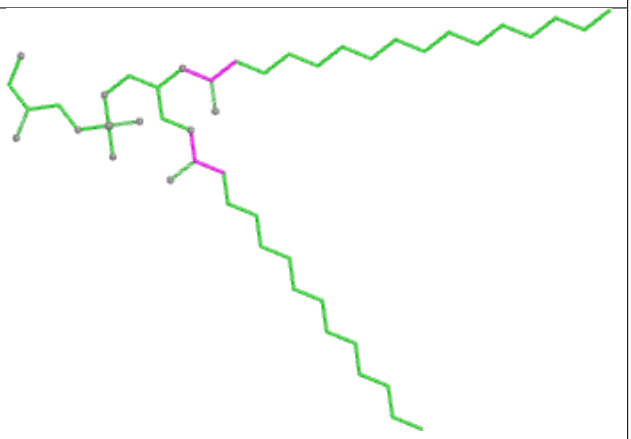

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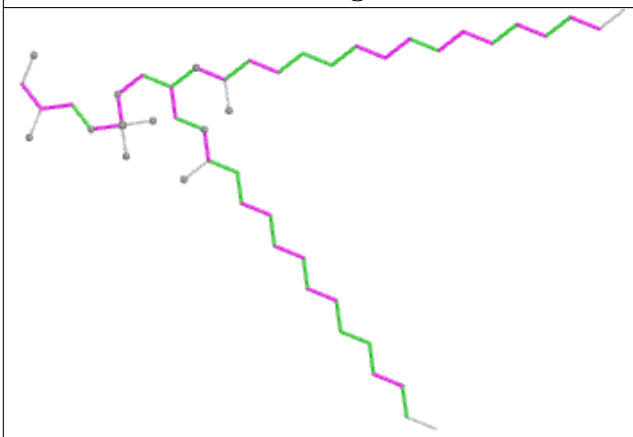

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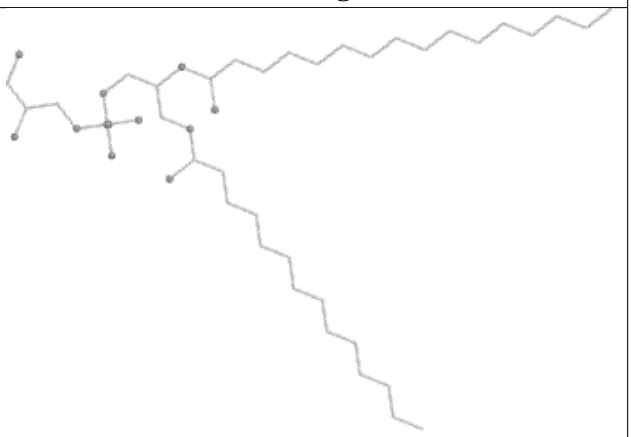
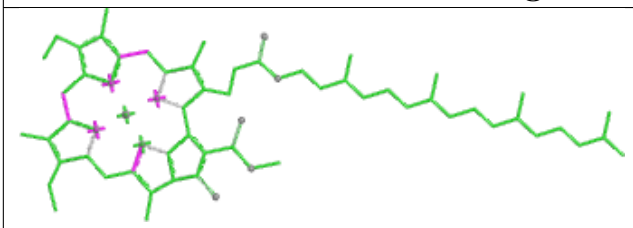


Rings

Ligand CLA B 603



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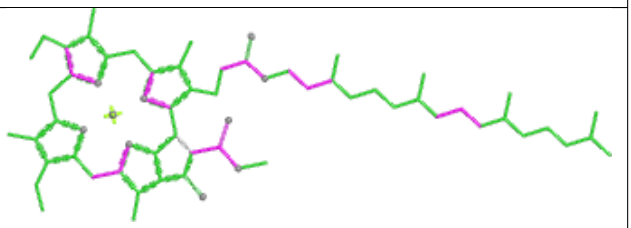
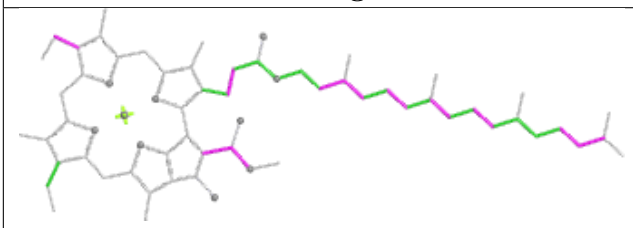


Bond angles



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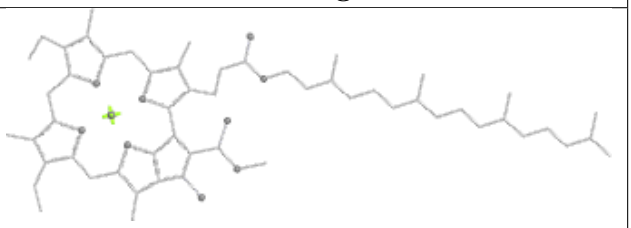
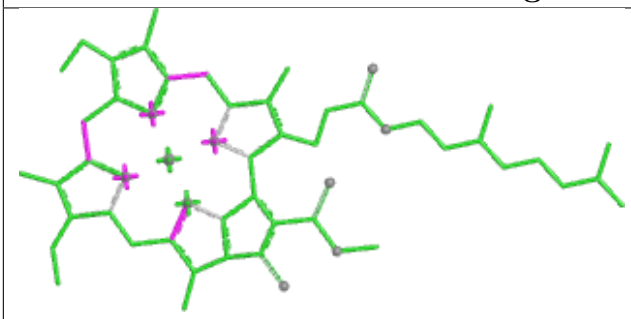
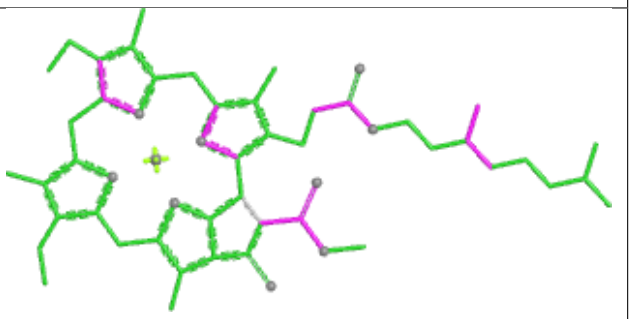


Rings

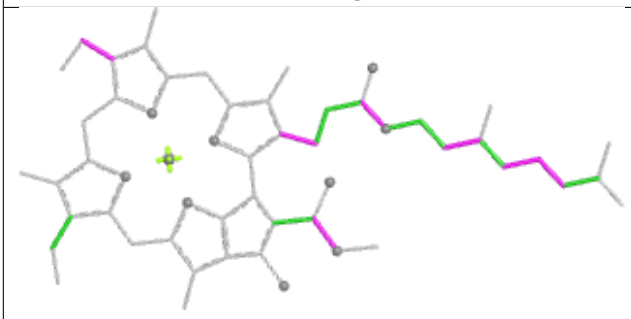
Ligand CLA A 406



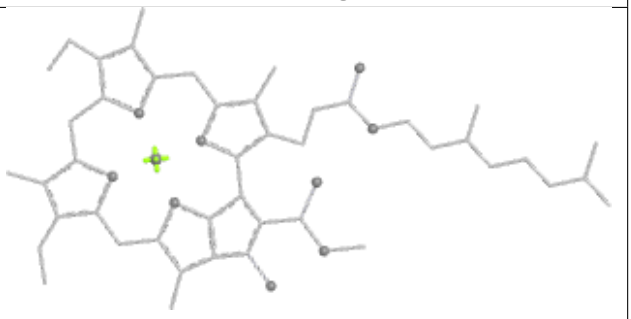
Bond lengths



Bond angles

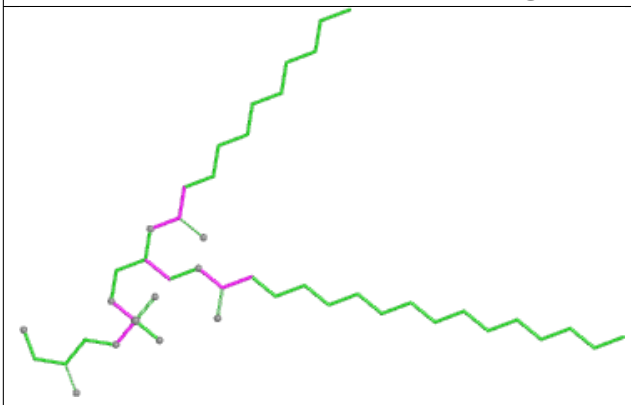


Torsions

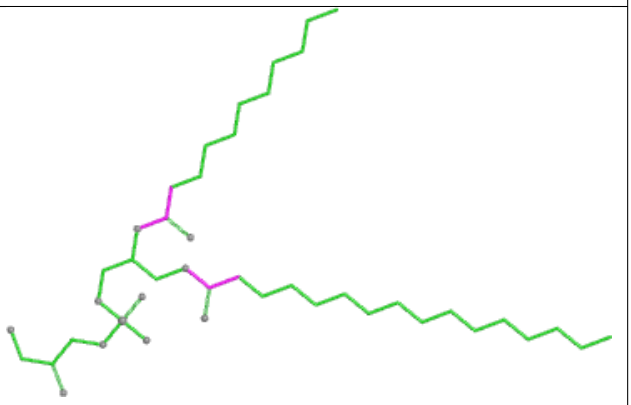


Rings

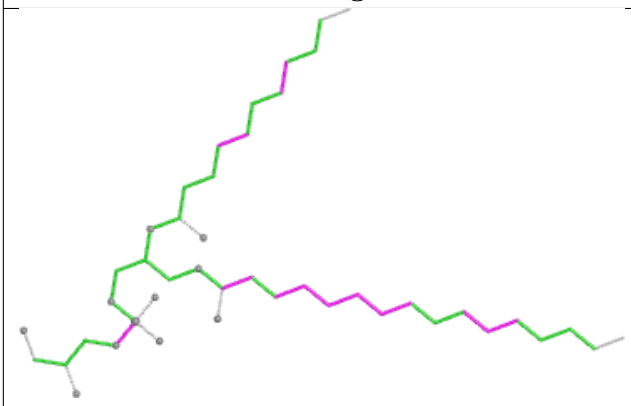
Ligand LHG A 413



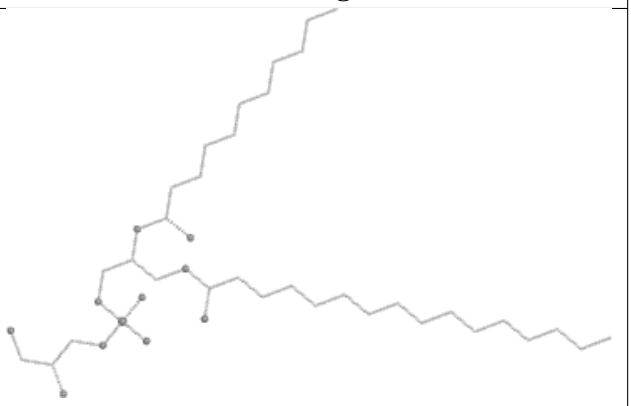
Bond lengths



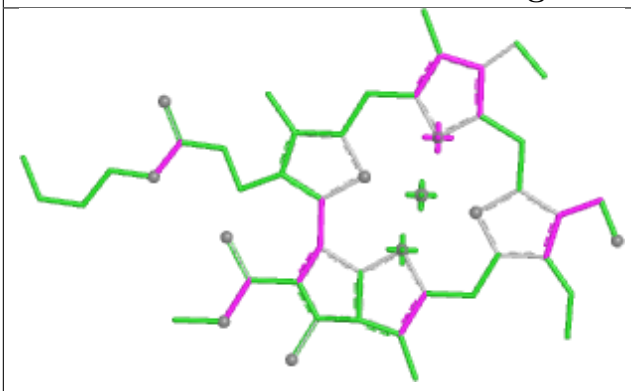
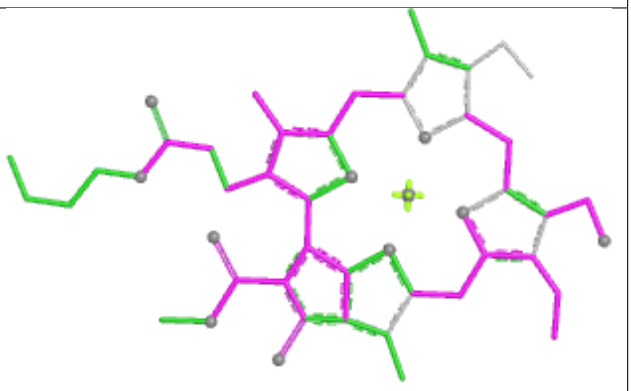
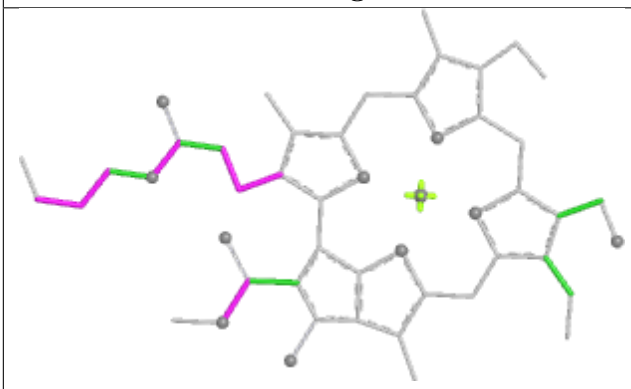
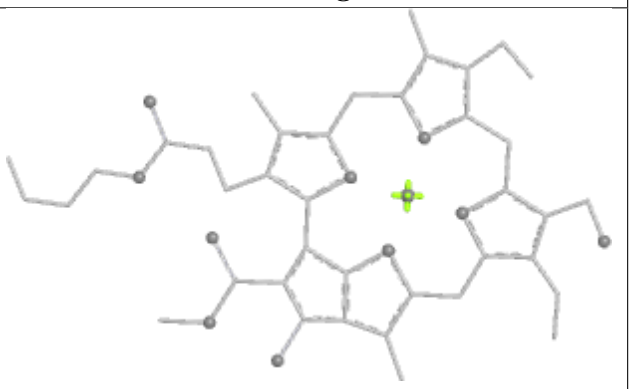
Bond angles

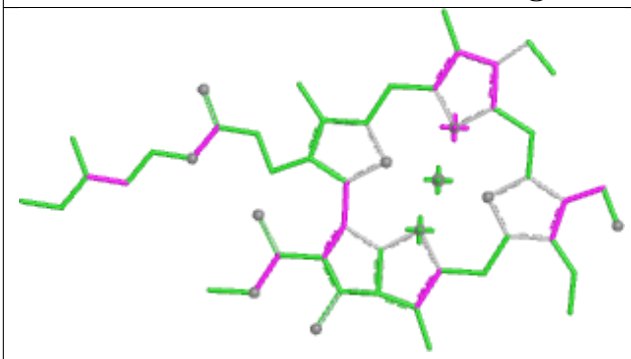
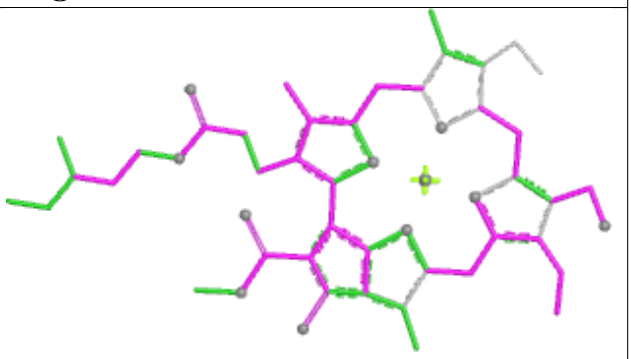
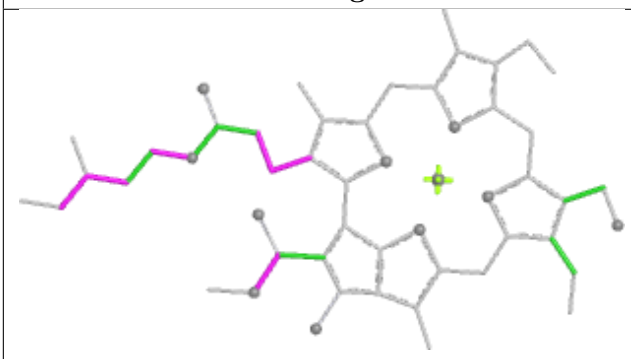
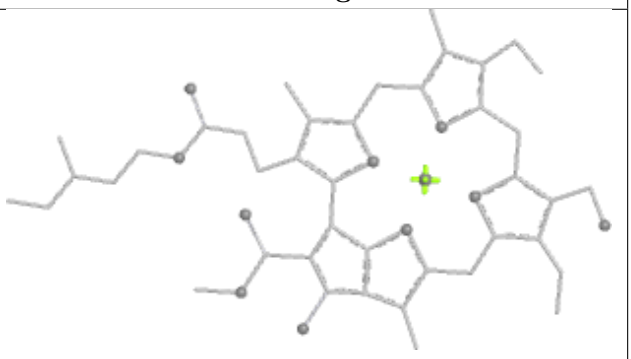


Torsions

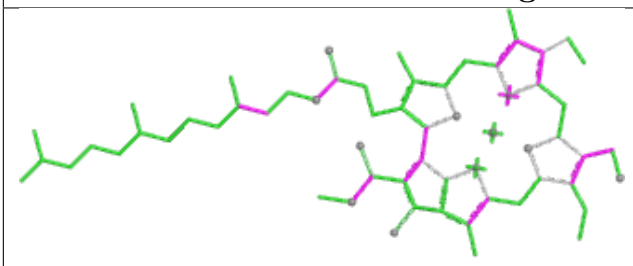


Rings

Ligand CHL 5 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL g 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 16 609



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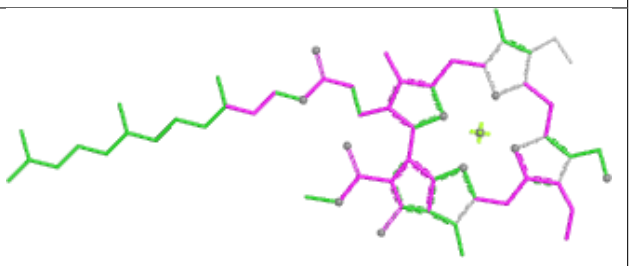
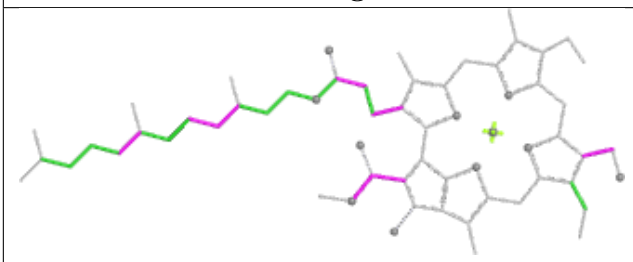
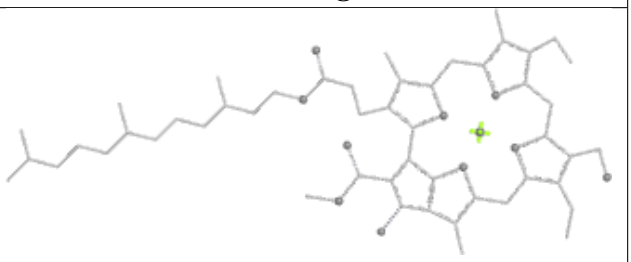


Bond angles

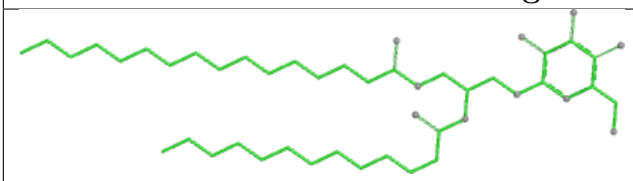


Torsions



Rings

Ligand LMG d 415



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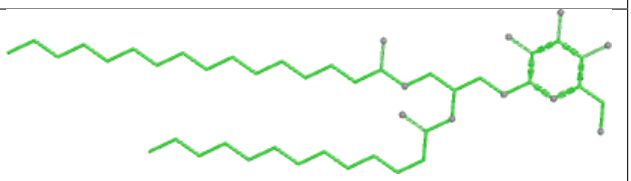
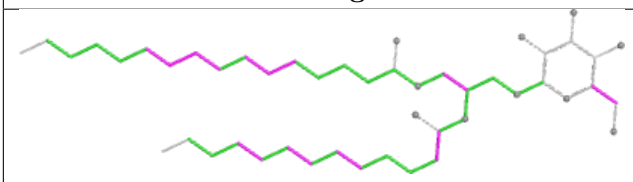


Bond angles



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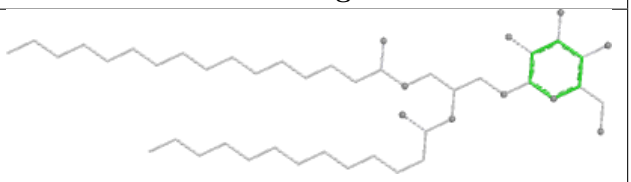
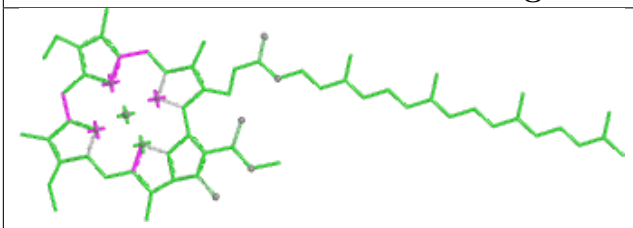


Rings

Ligand CLA B 612



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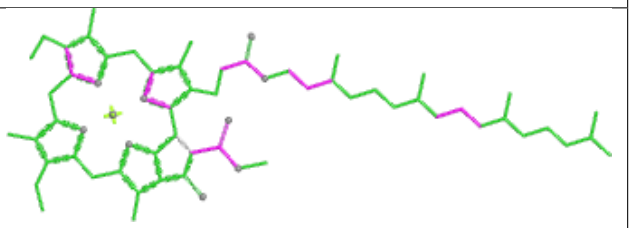
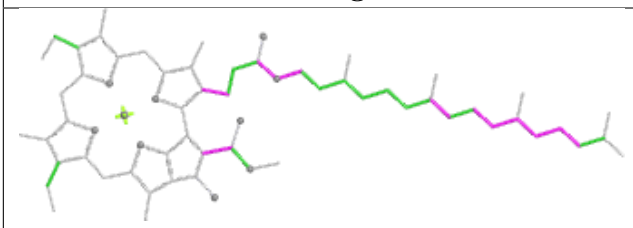


Bond angles



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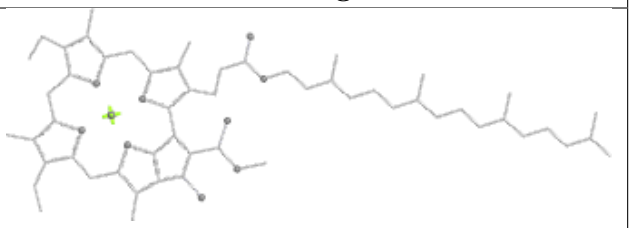
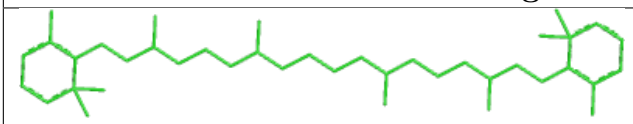


Rings

Ligand BCR A 407



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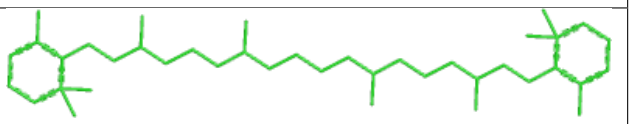
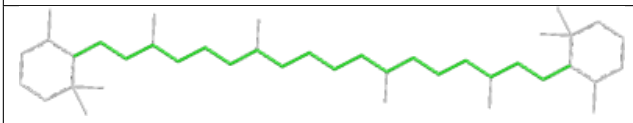


Bond angles



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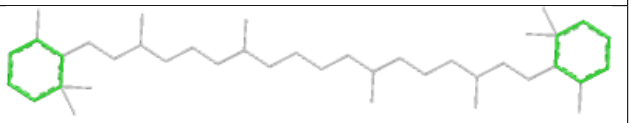
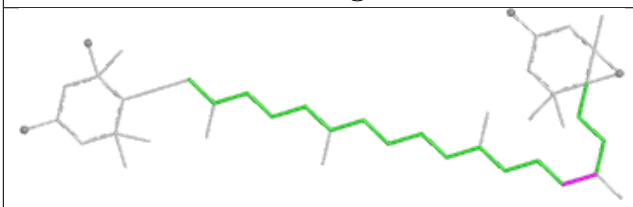


Rings

Ligand NEX 16 619

Bond lengths

Bond angles



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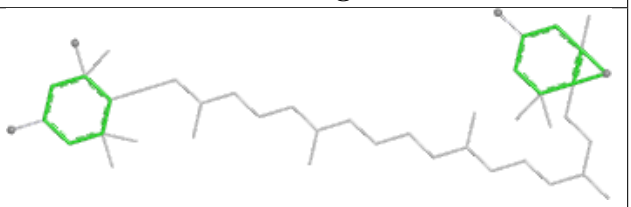
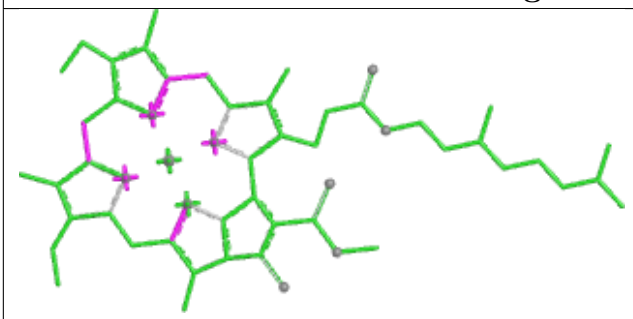
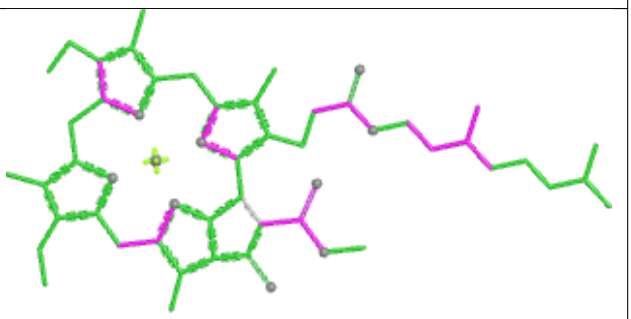


Rings

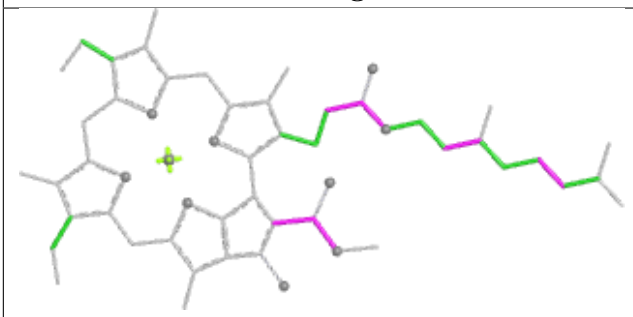
Ligand CLA R 614



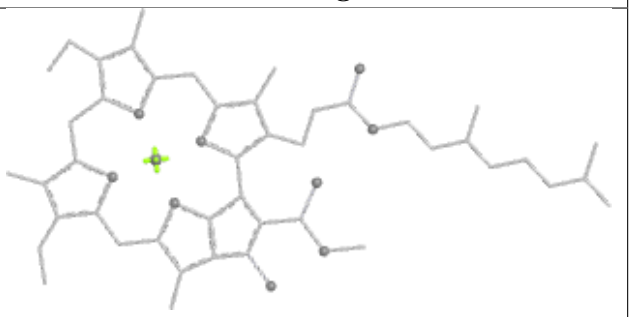
Bond lengths



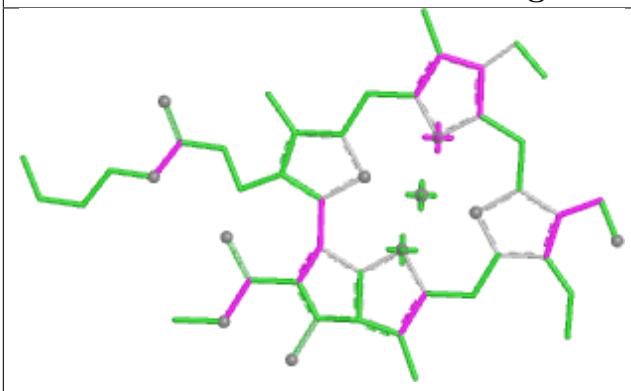
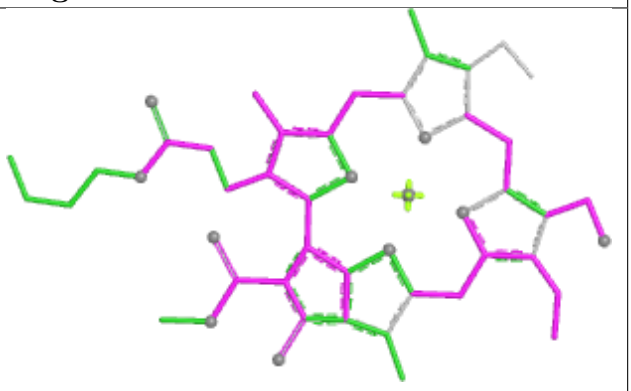
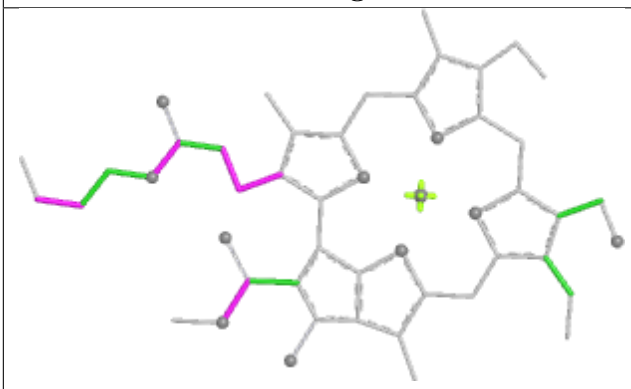
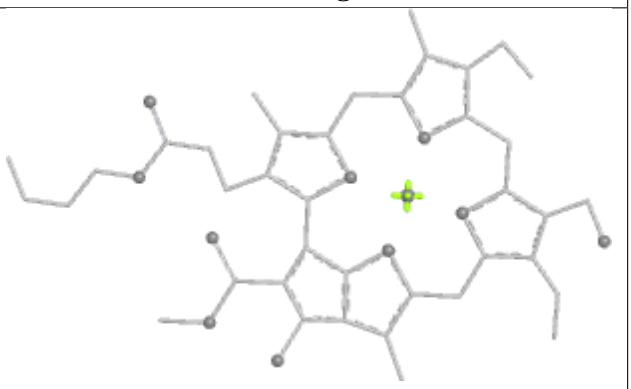
Bond angles

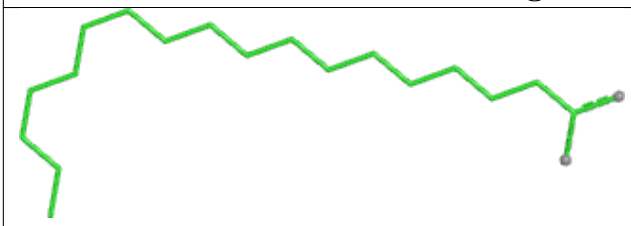
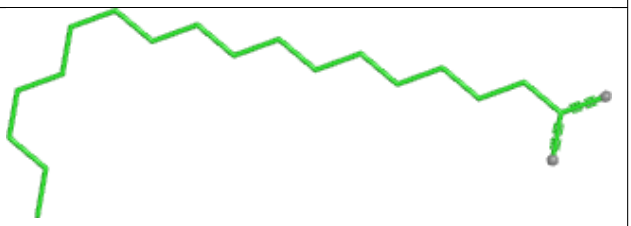
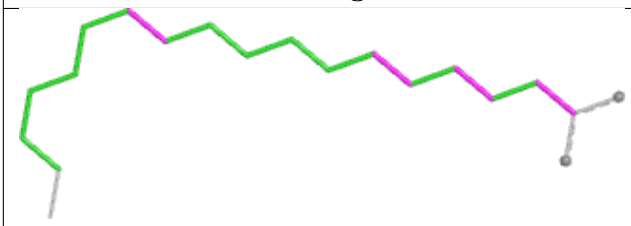
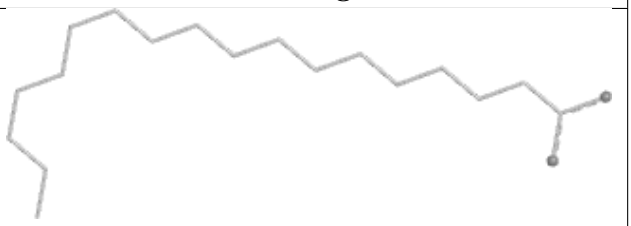


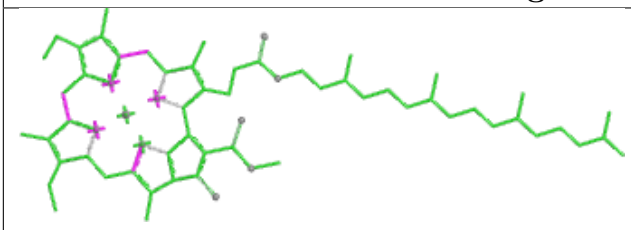
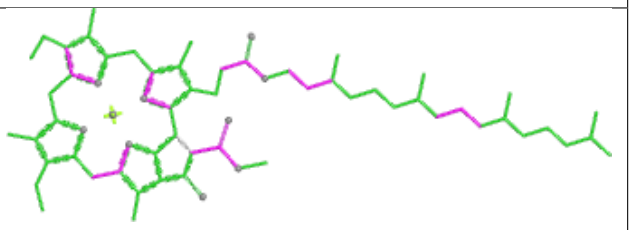
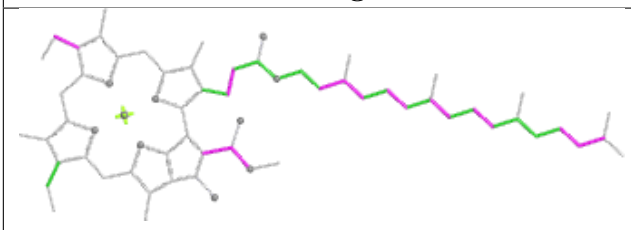
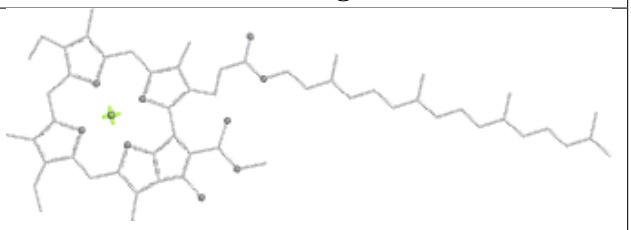
Torsions

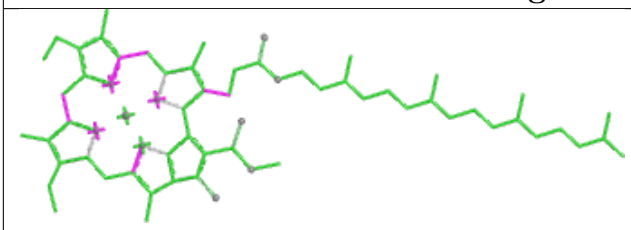
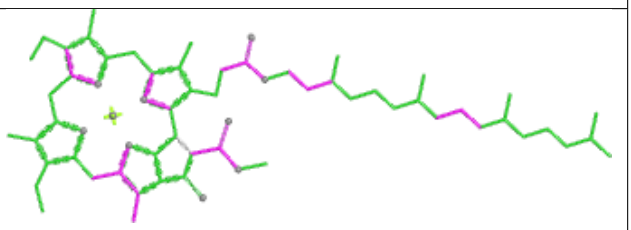
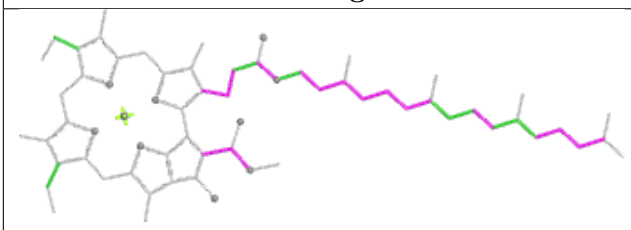
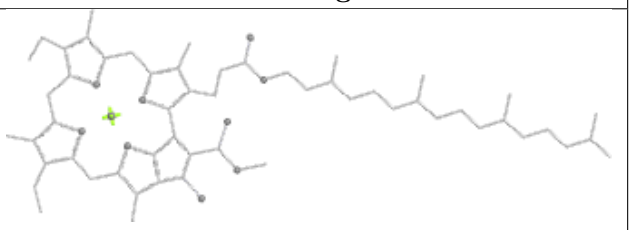


Rings

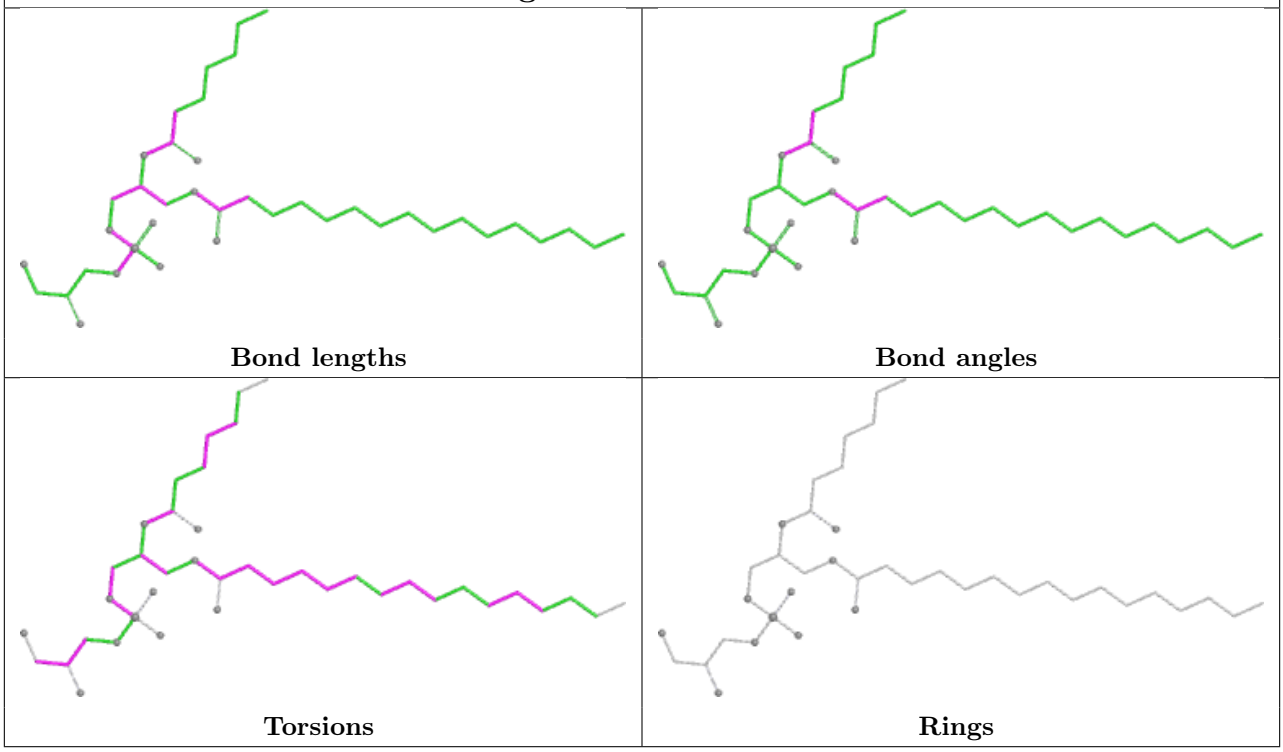
Ligand CHL g 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LNL C 524	
 Bond lengths	 Bond angles
 Torsions	 Rings

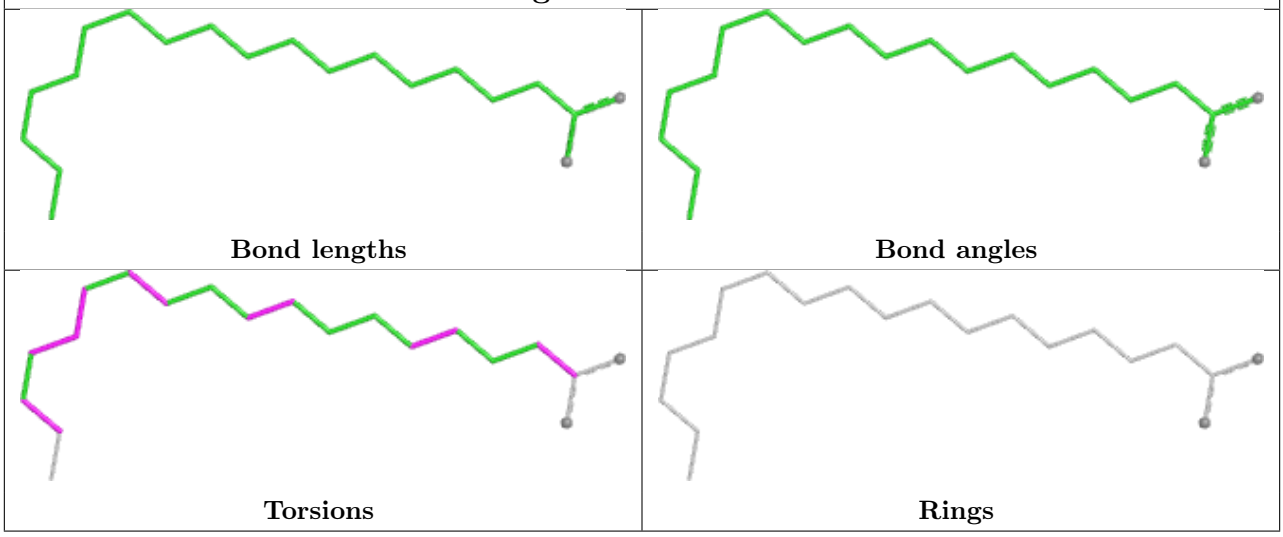
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 16 616



Ligand LNL r 620



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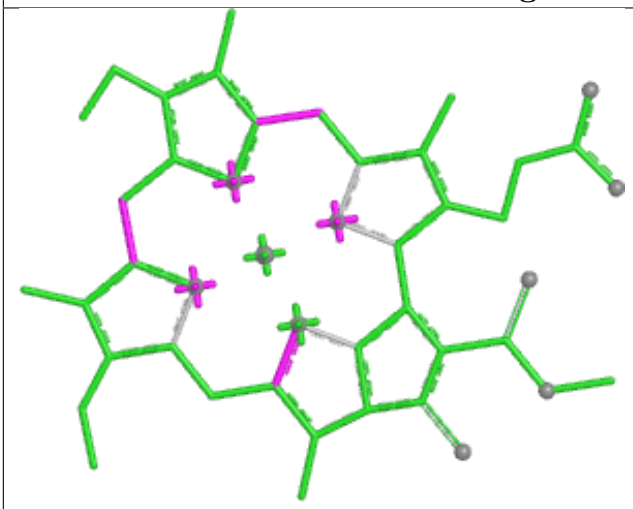
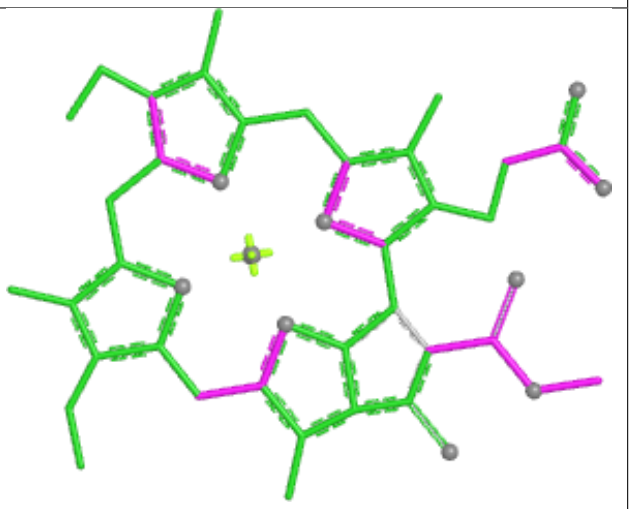
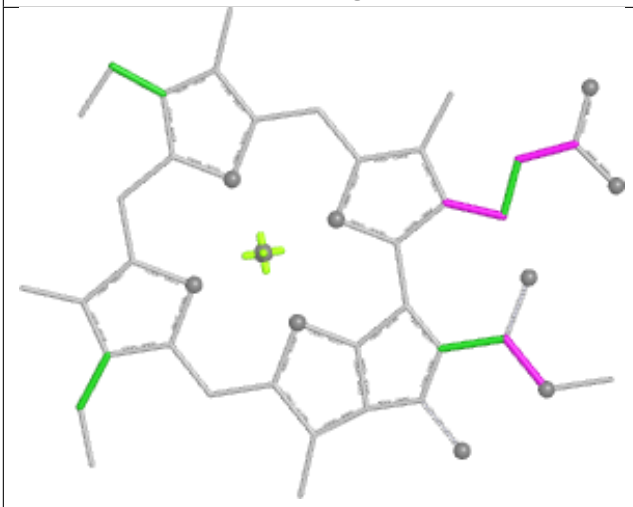


Bond lengths



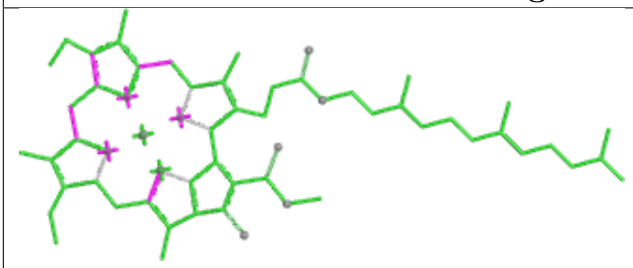
Bond angles



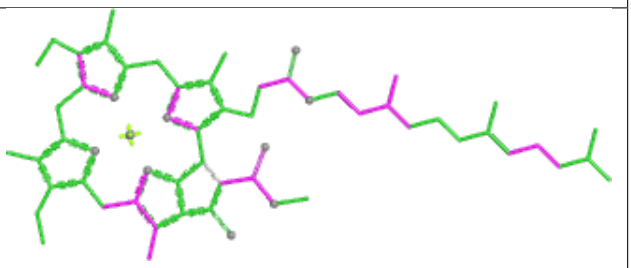
Torsions

Rings

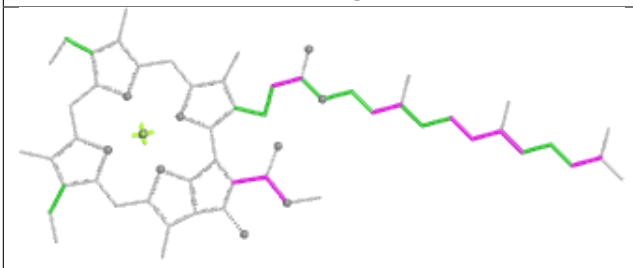
Ligand CLA 4 602



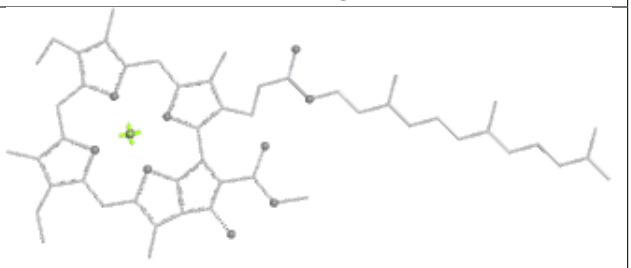
Bond lengths



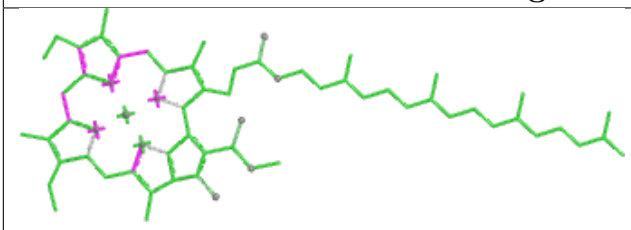
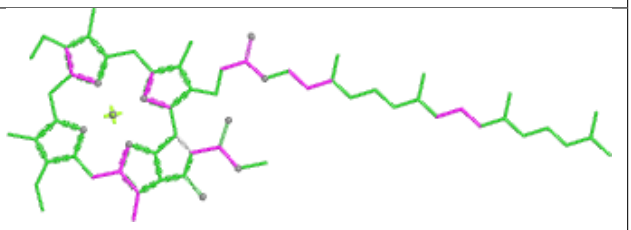
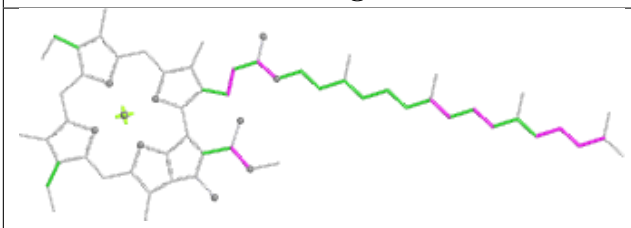
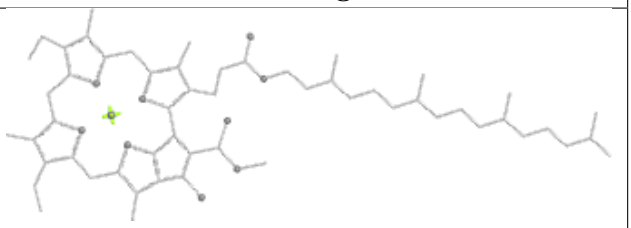
Bond angles

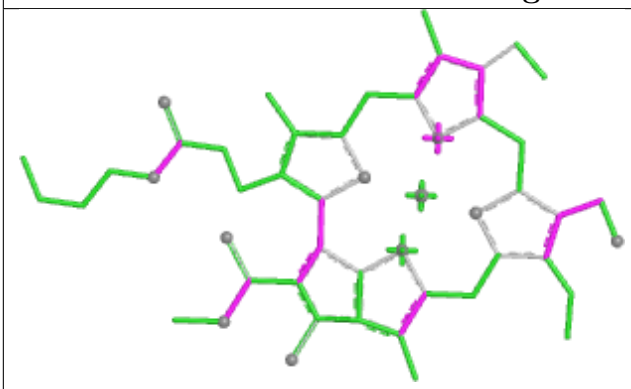
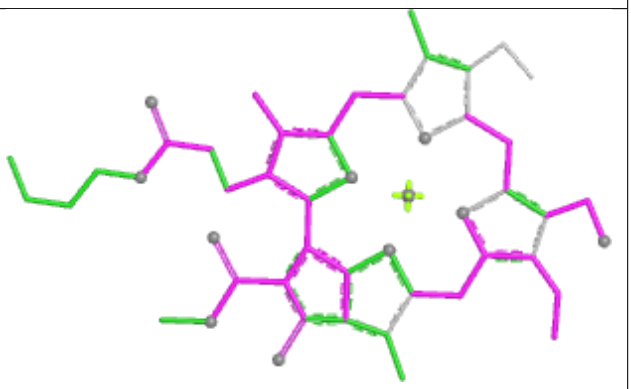
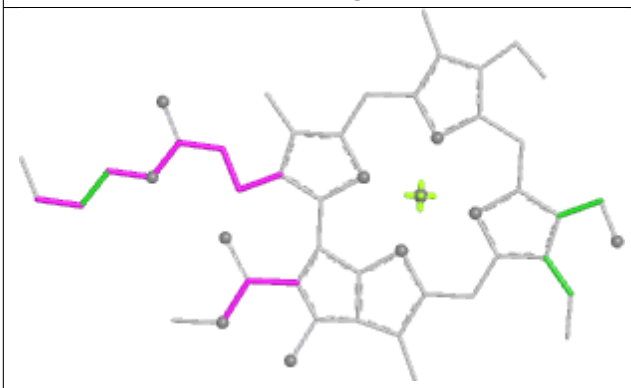
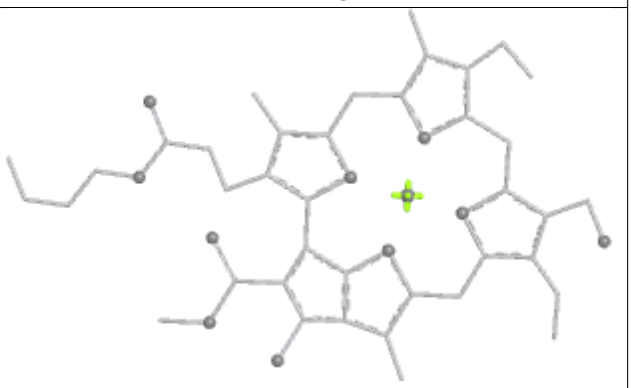


Torsions

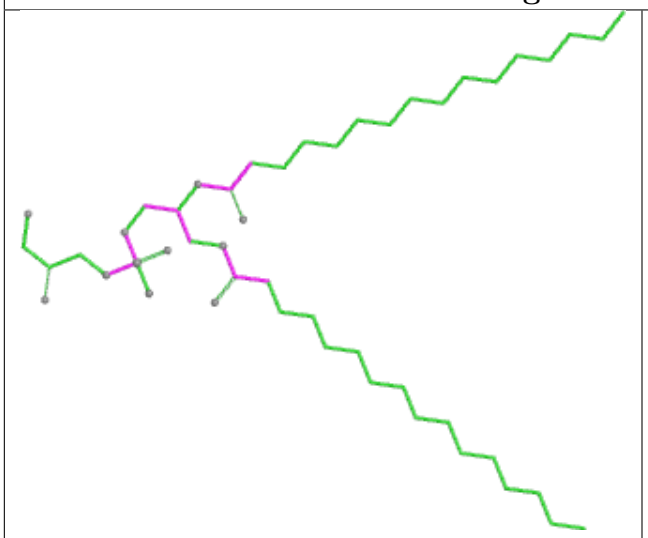


Rings

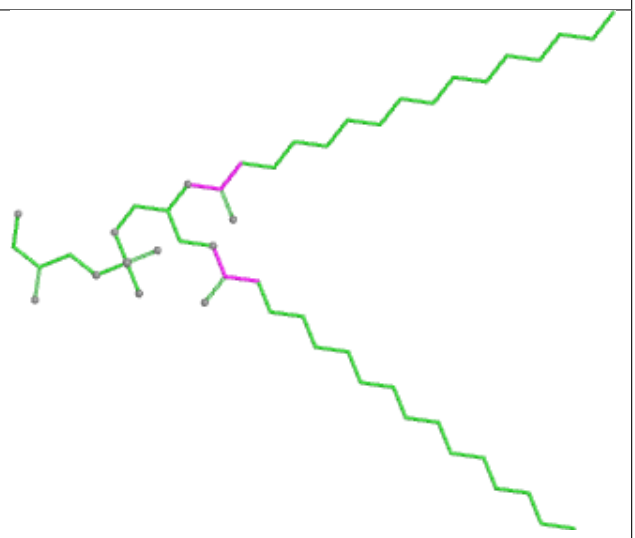
Ligand CLA a 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

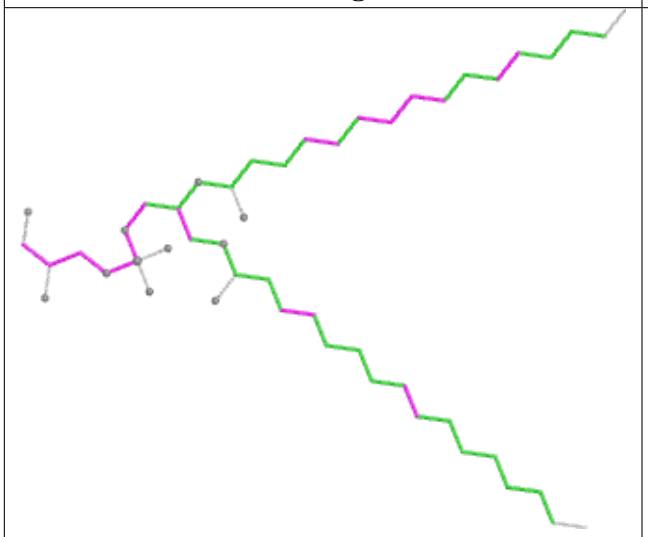
Ligand LHG D 412



Bond lengths



Bond angles



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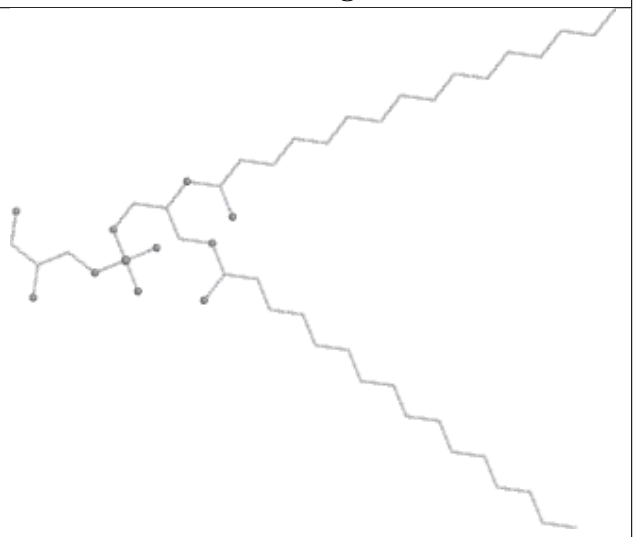
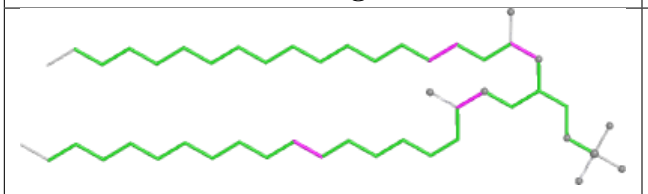


Rings

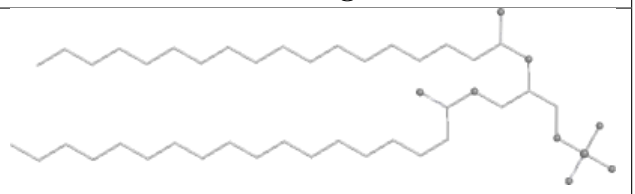
Ligand 3PH 8 201

Bond lengths

Bond angles

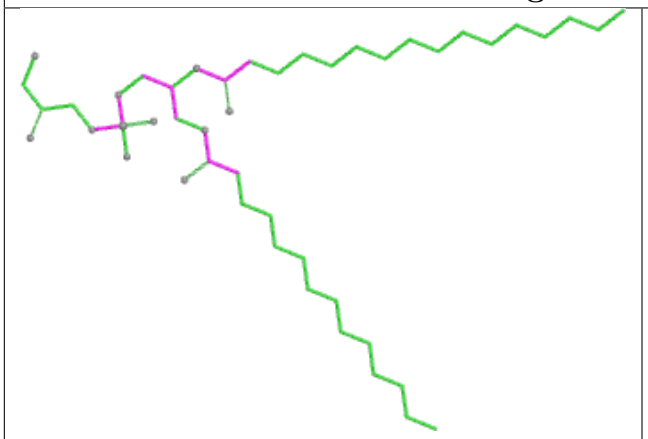


Torsions

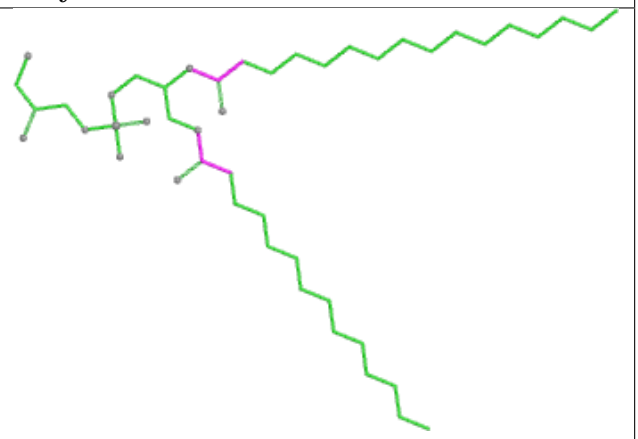


Rings

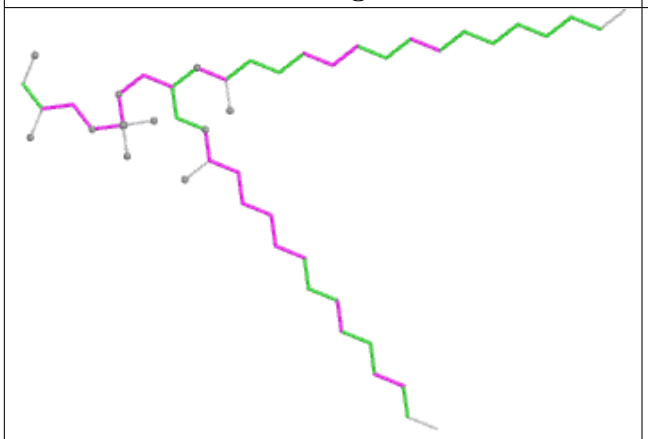
Ligand LHG y 617



Bond lengths



Bond angles



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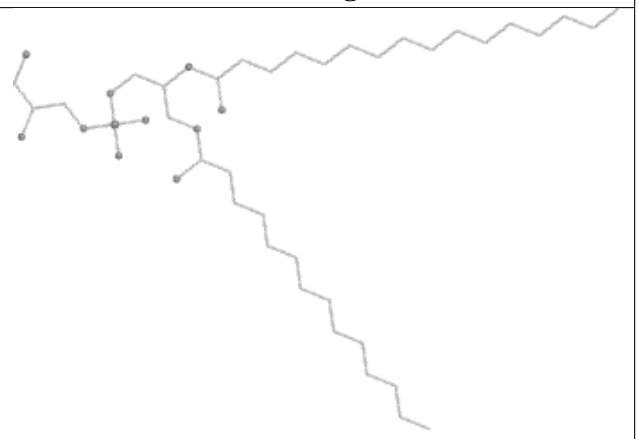
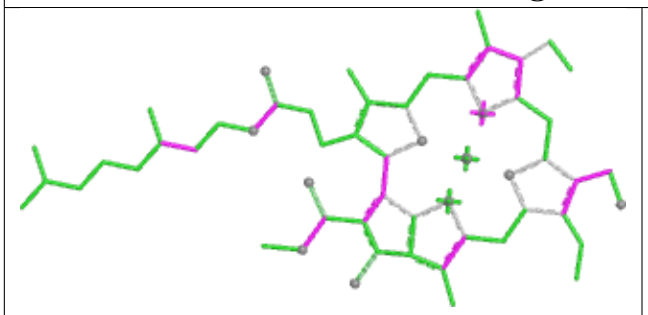


Rings

Ligand CHL 2 607



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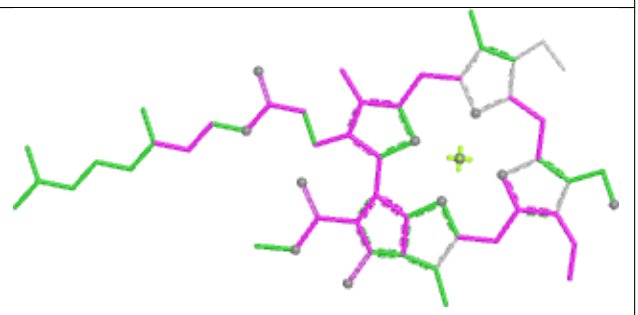
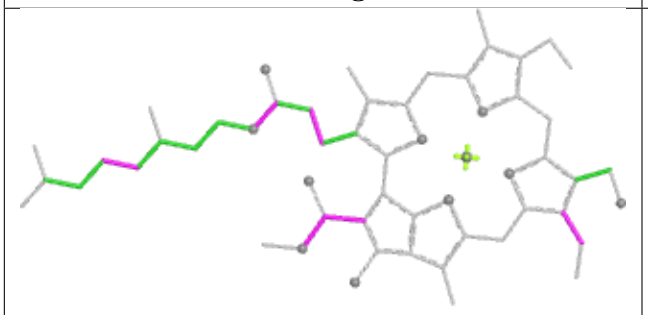


Bond angles



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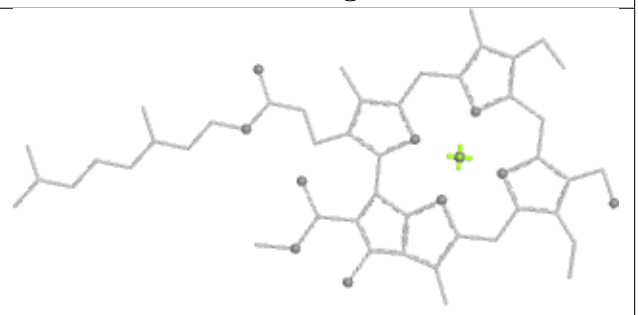
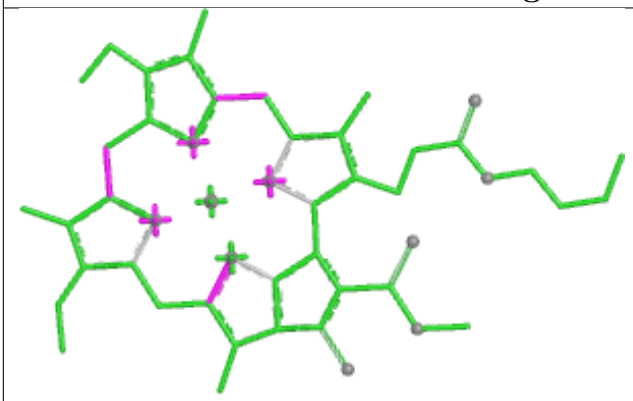


Rings

Ligand CLA G 614



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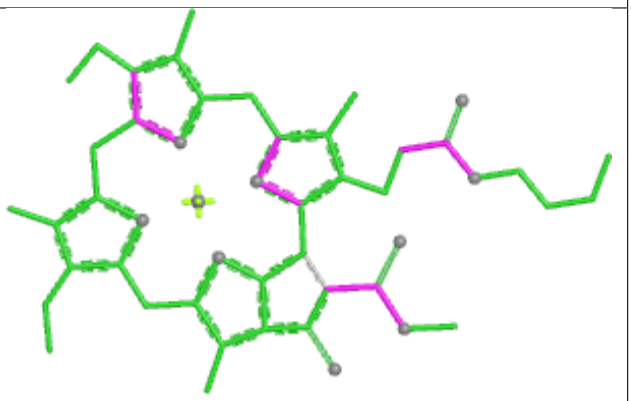
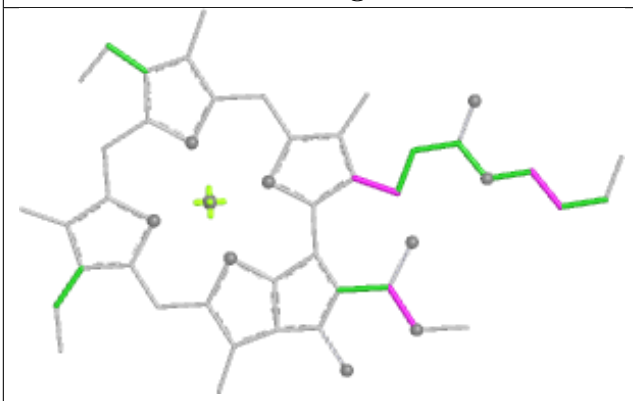


Bond angles



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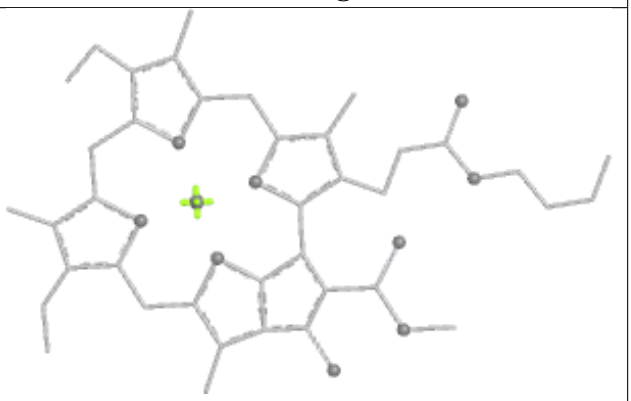
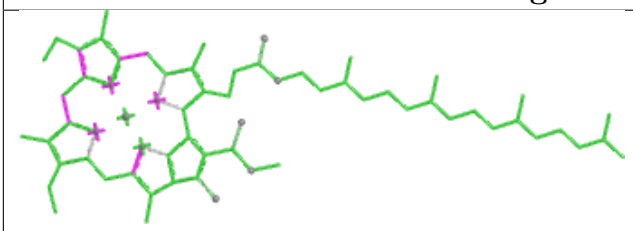
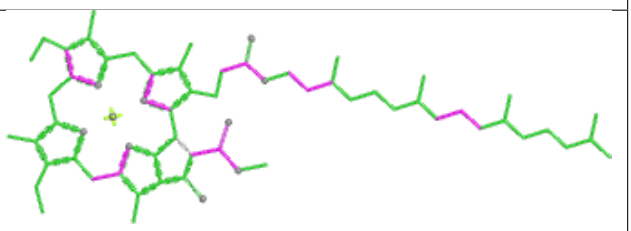


Rings

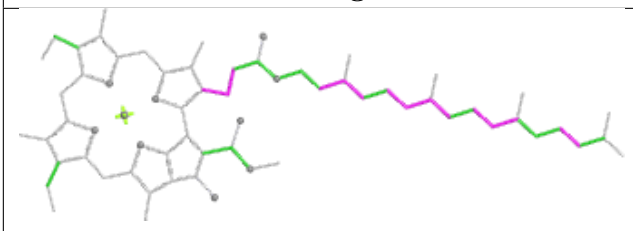
Ligand CLA s 610



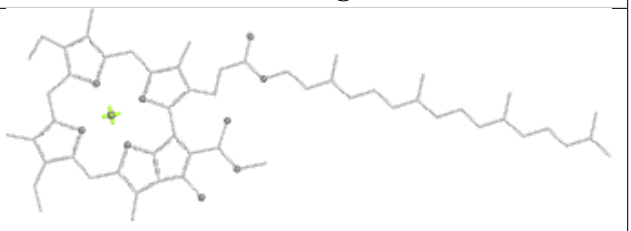
Bond lengths



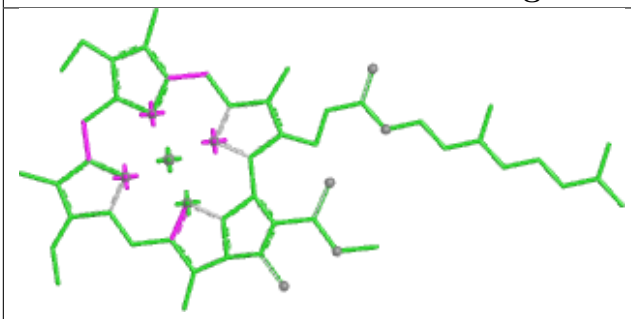
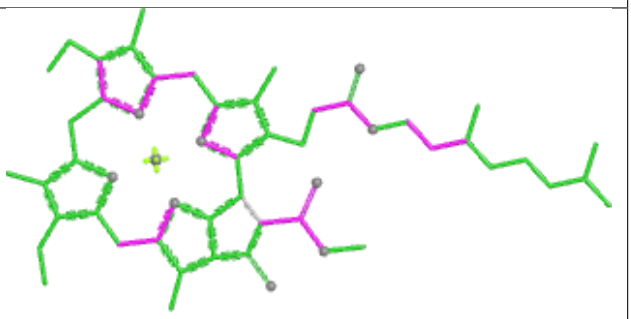
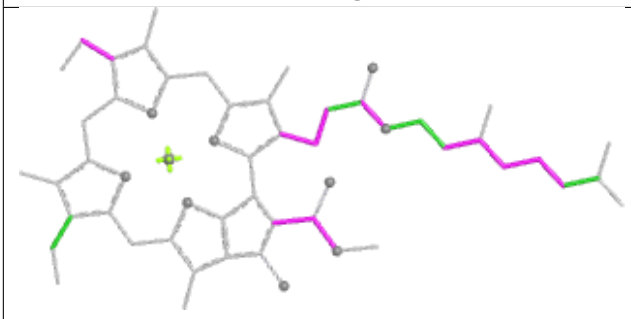
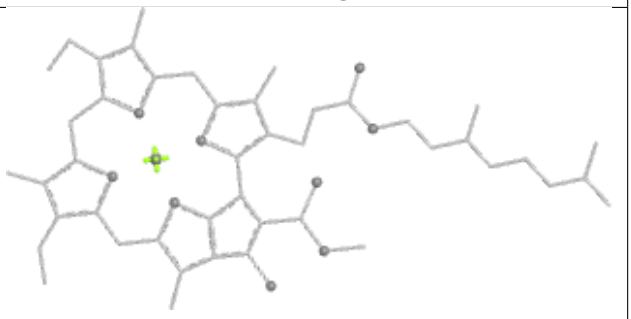
Bond angles



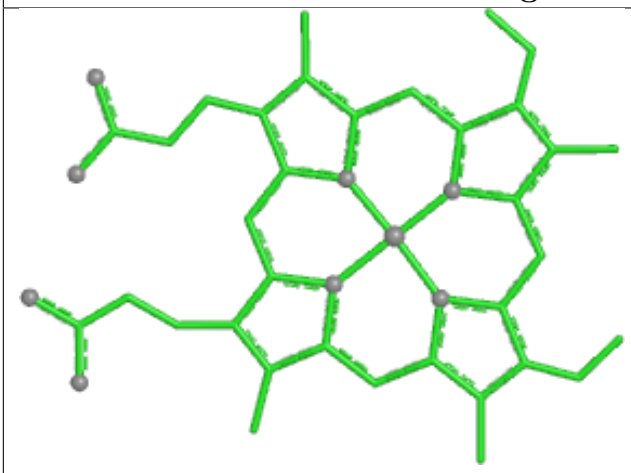
Torsions



Rings

Ligand CLA N 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM F 101



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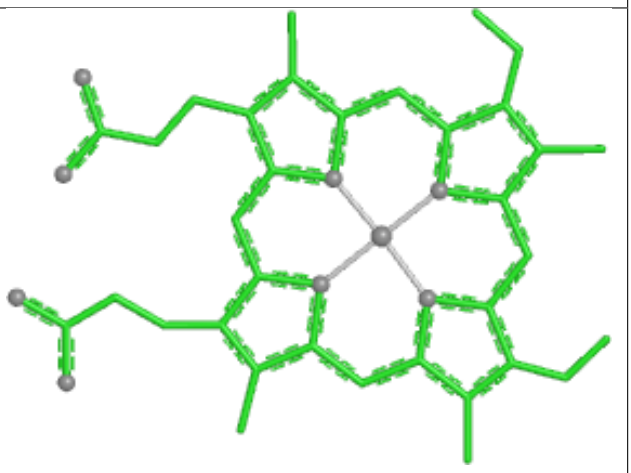
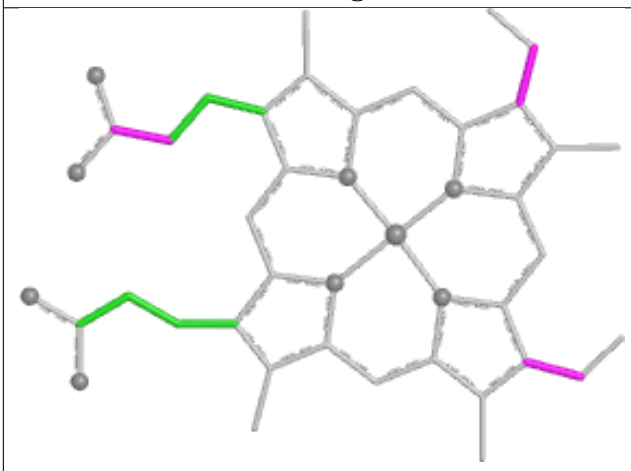
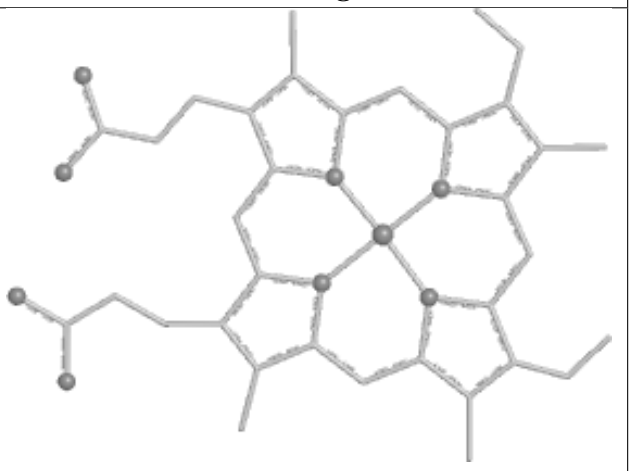


Bond angles

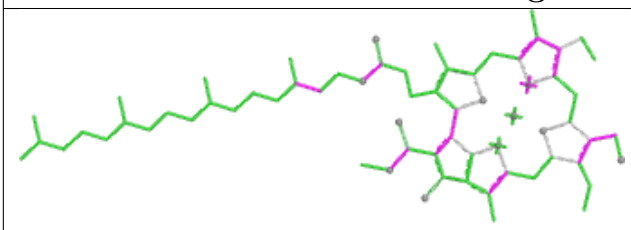


Torsions



Rings

Ligand CHL 4 609



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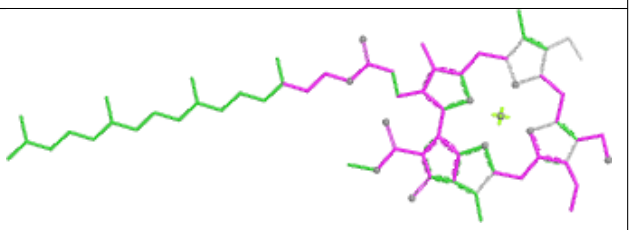
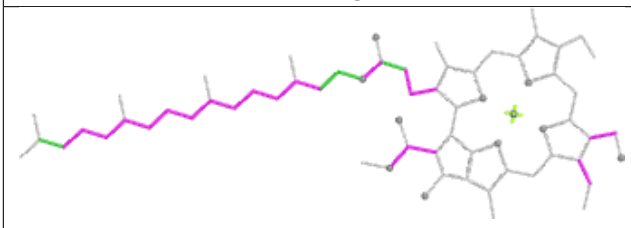
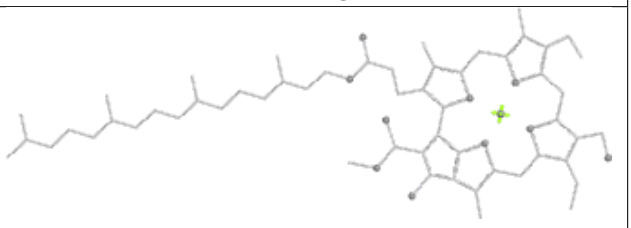


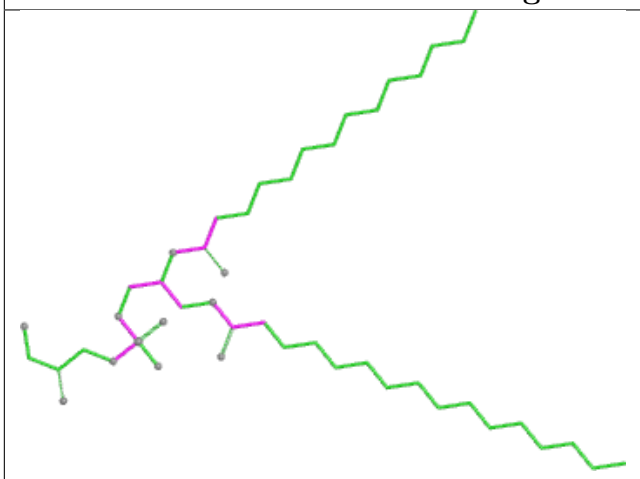
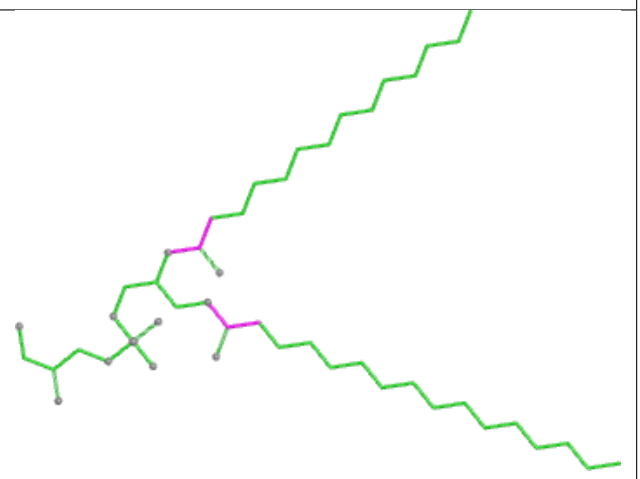
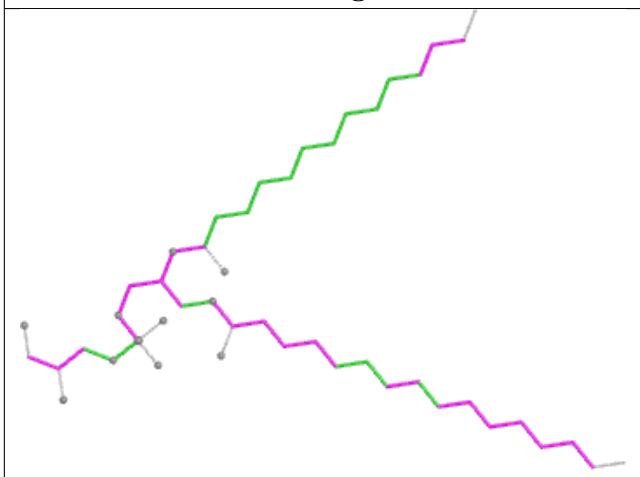
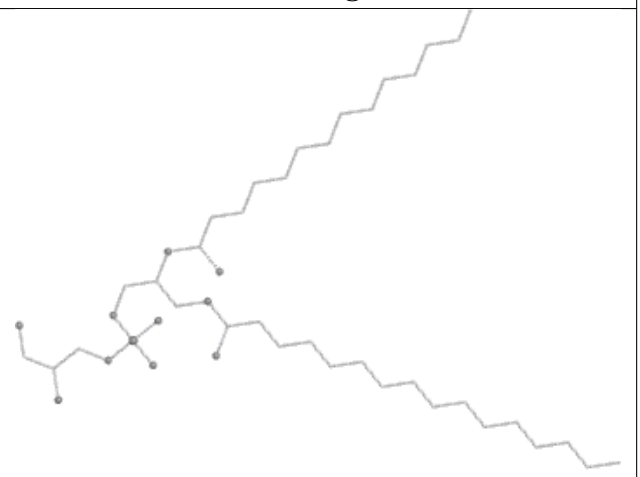
Bond angles



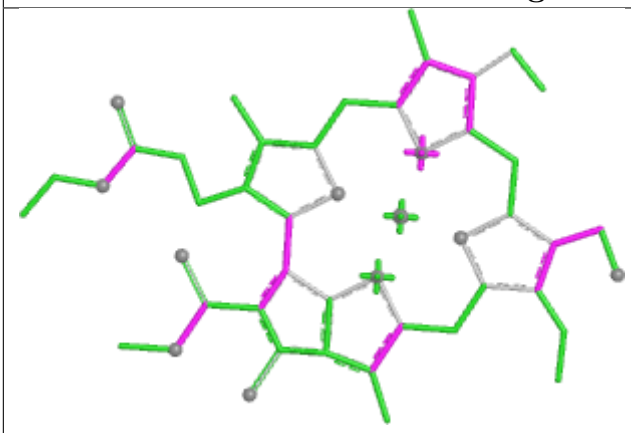
Torsions



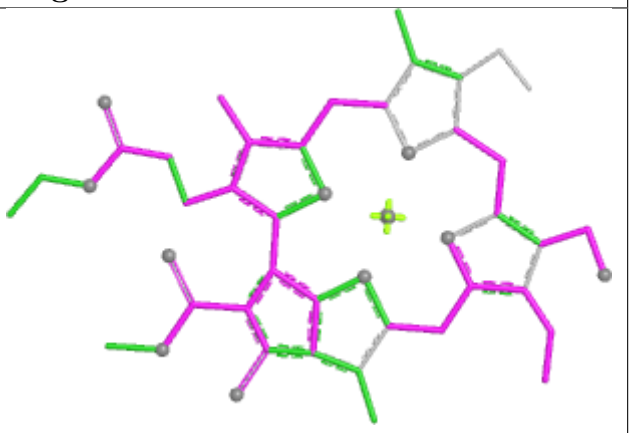
Rings

Ligand LHG Y 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

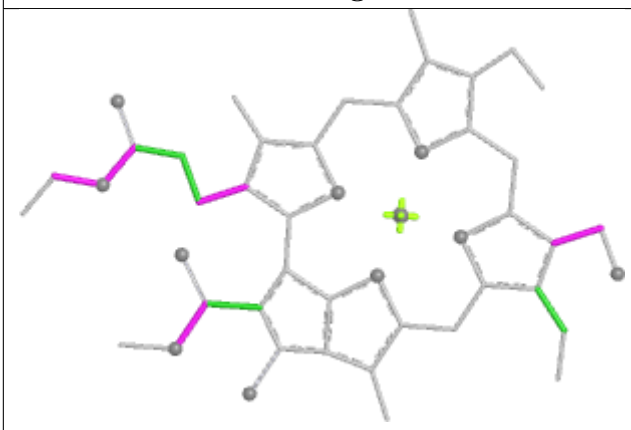
Ligand CHL g 605



Bond lengths



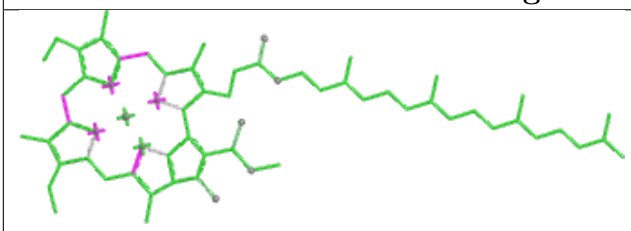
Bond angles



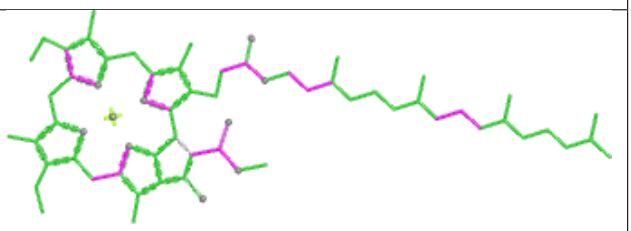
Torsions

Rings

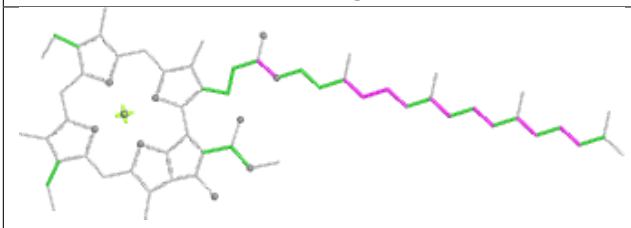
Ligand CLA G 611



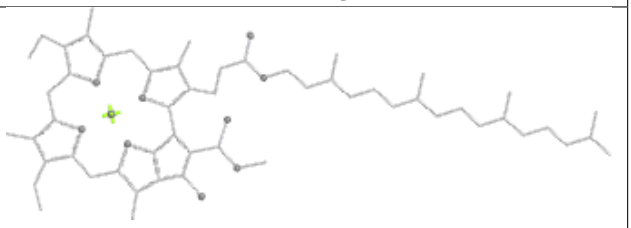
Bond lengths



Bond angles

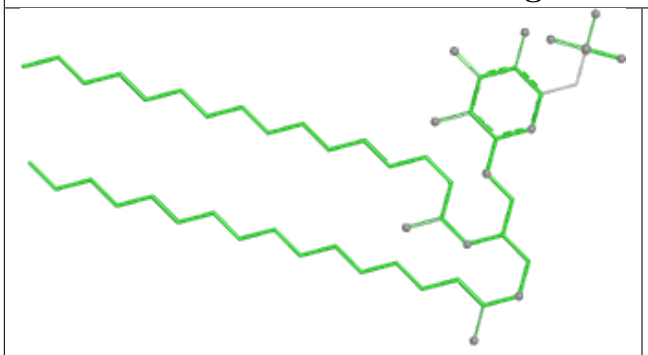


Torsions

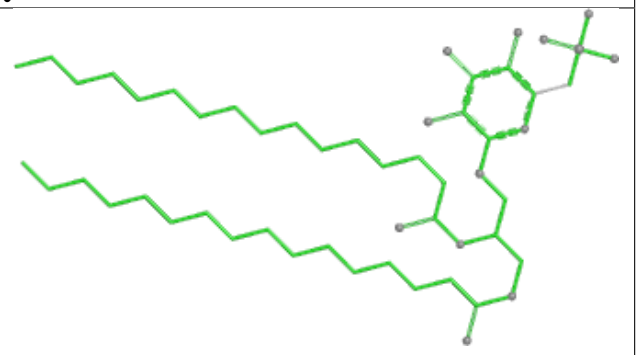


Rings

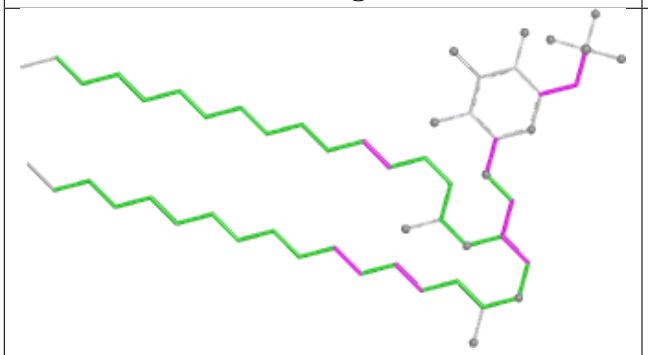
Ligand SQD D 411



Bond lengths



Bond angles



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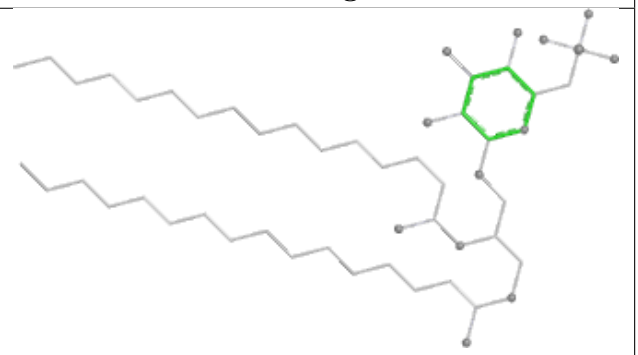
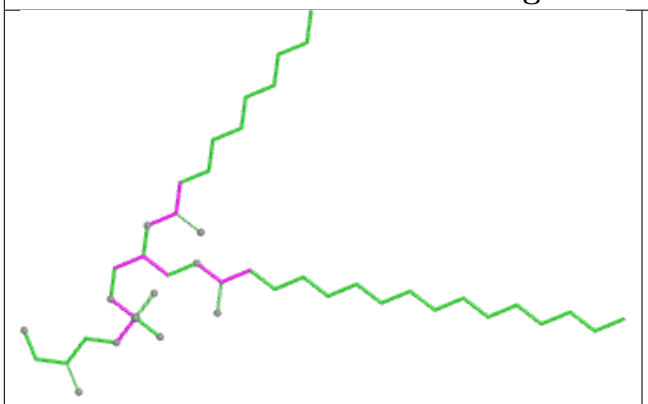


Rings

Ligand LHG A 414



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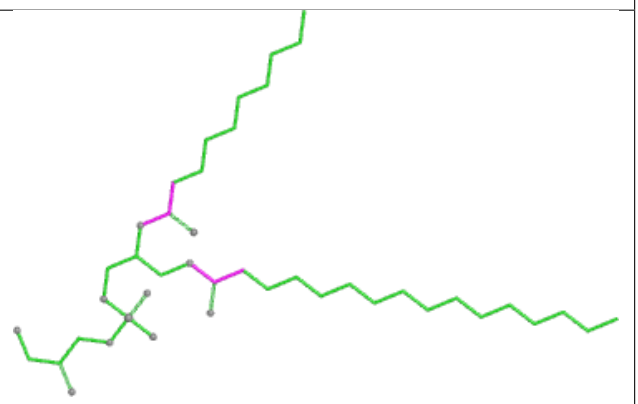
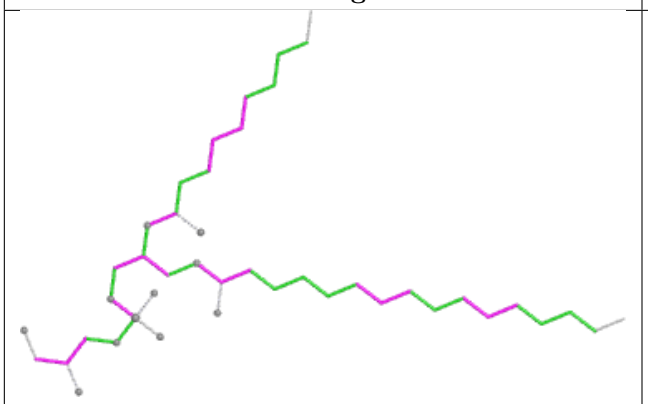


Bond angles



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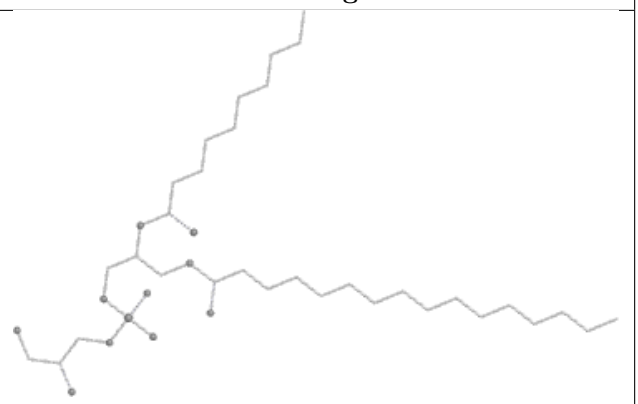
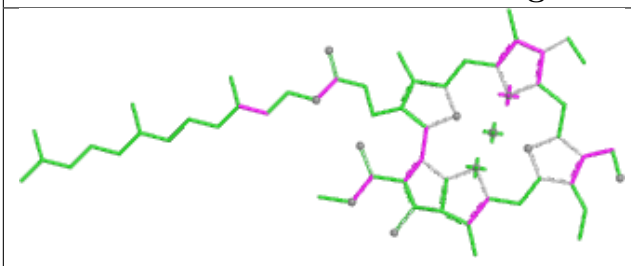


Rings

Ligand CHL 4 601



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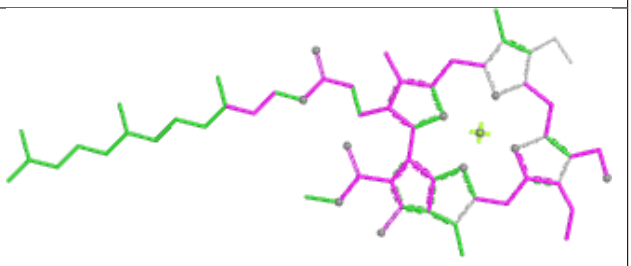
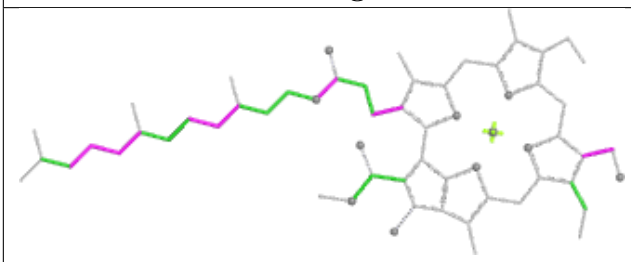


Bond angles



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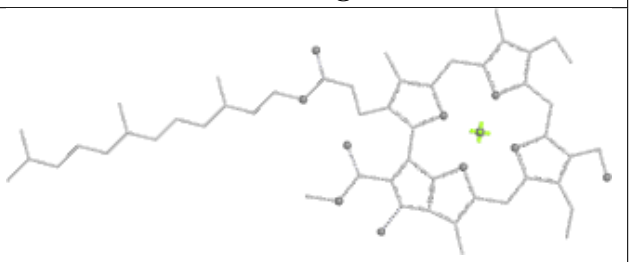
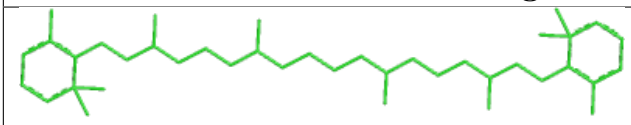


Rings

Ligand BCR H 103



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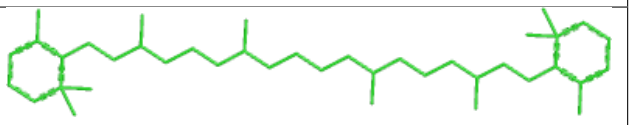
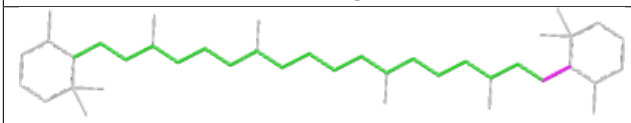


Bond angles



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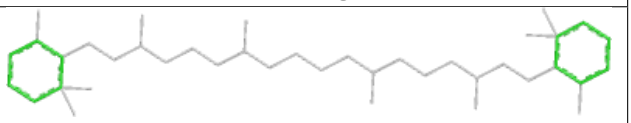
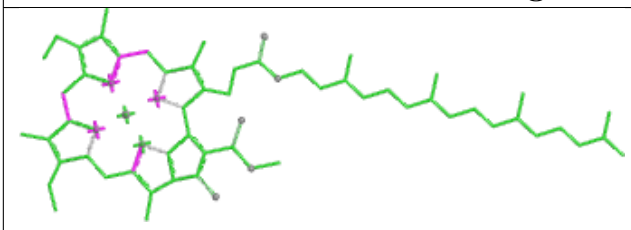


Rings

Ligand CLA b 608



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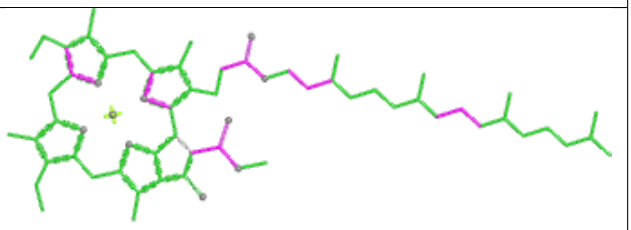
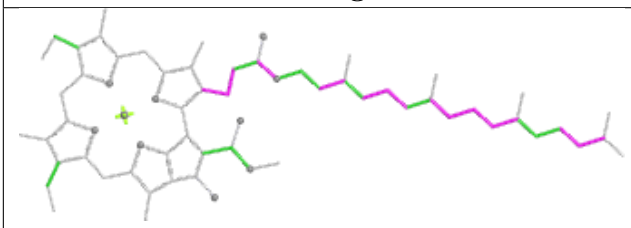


Bond angles



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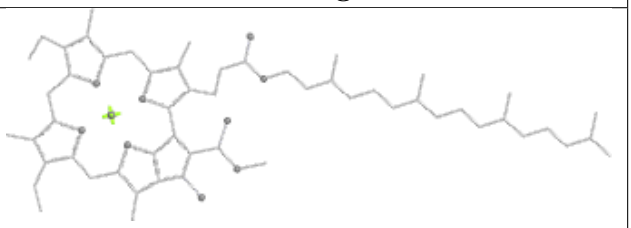
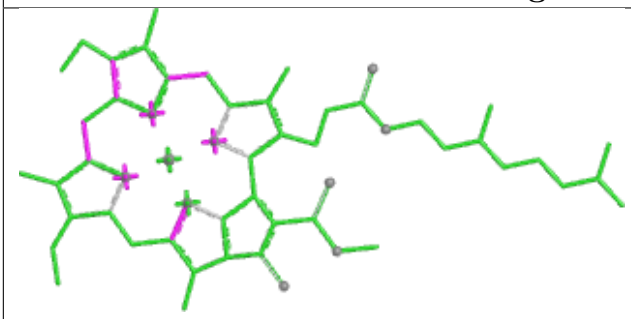
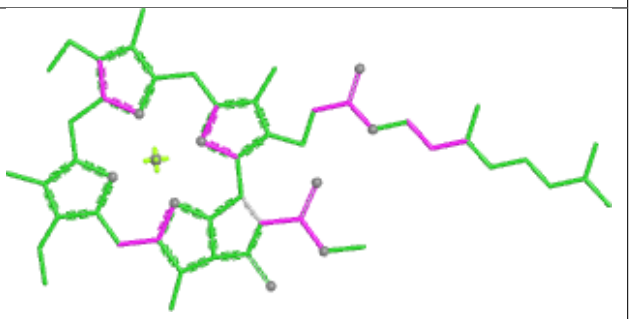
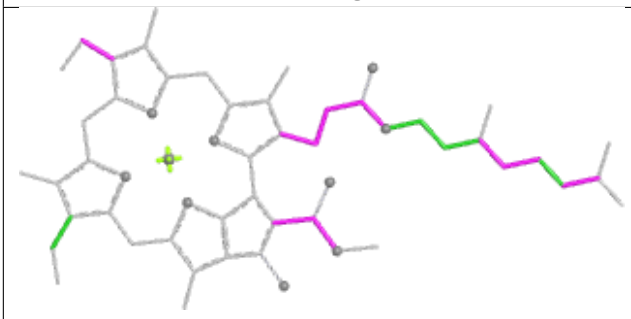
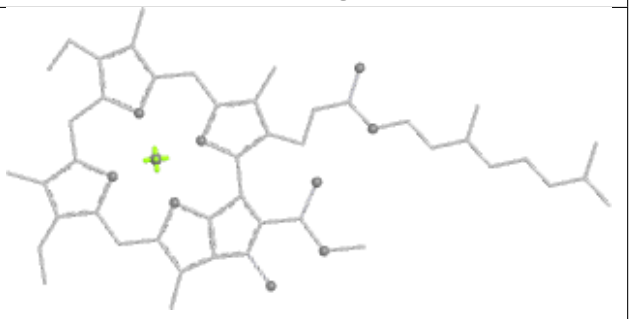
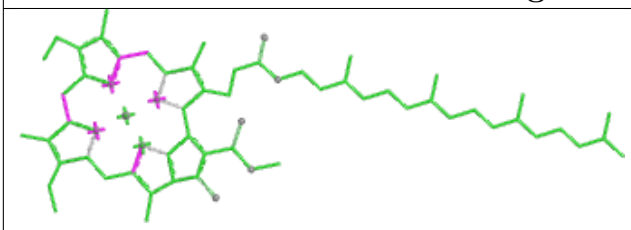
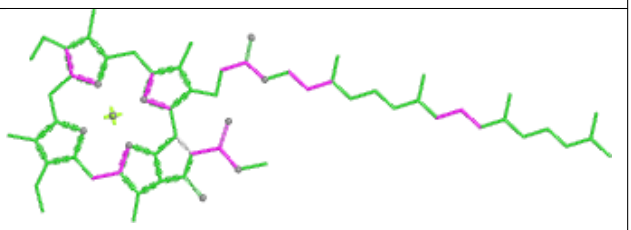
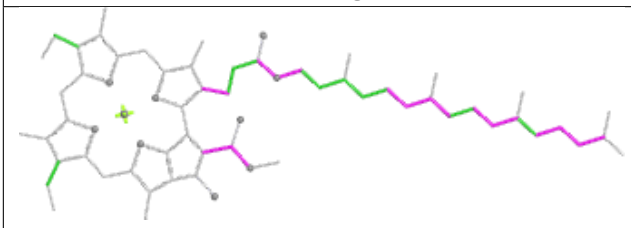
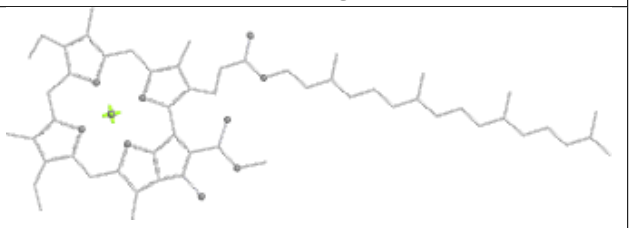
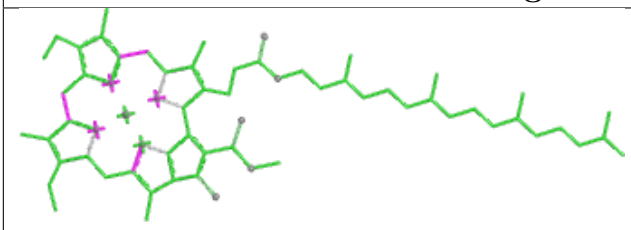


Rings

Ligand CLA 5 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 514



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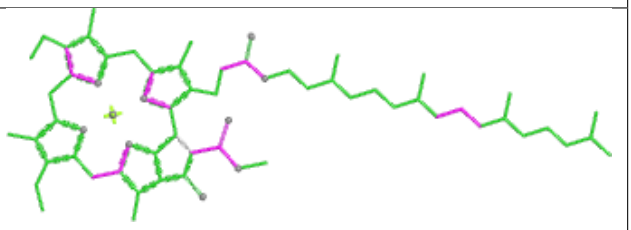
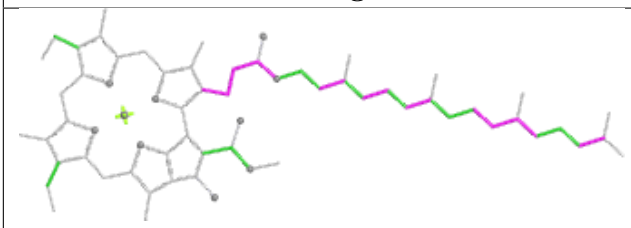


Bond angles



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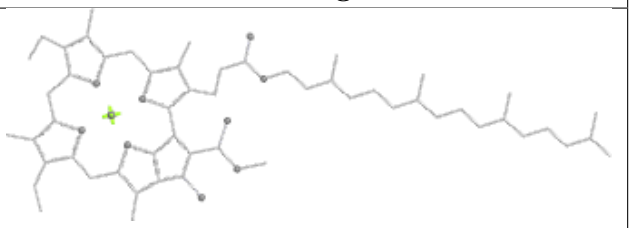
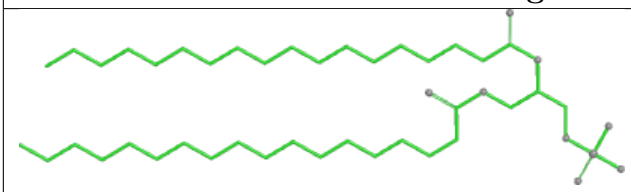


Rings

Ligand 3PH T 101



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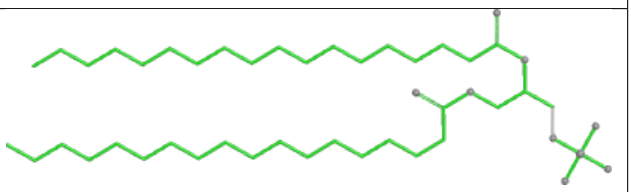

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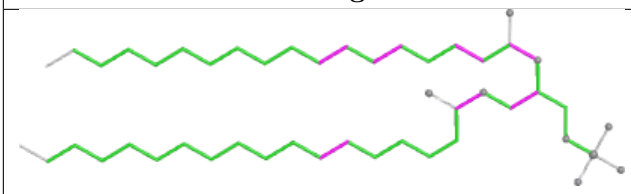

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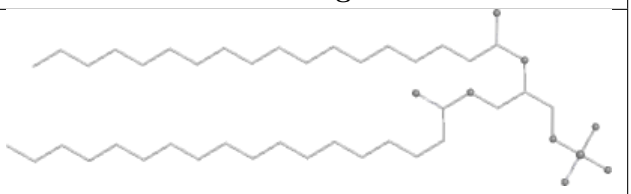
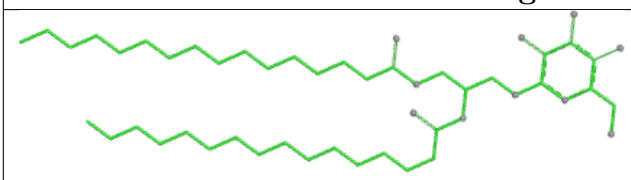


Rings

Ligand LMG K 102



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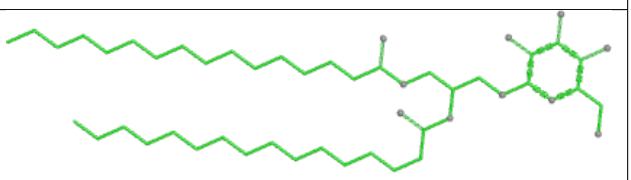
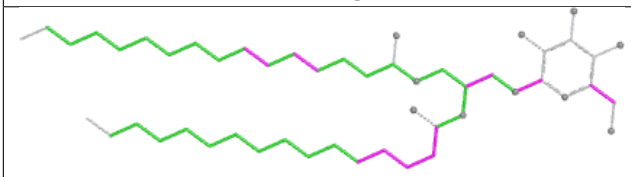


Bond angles



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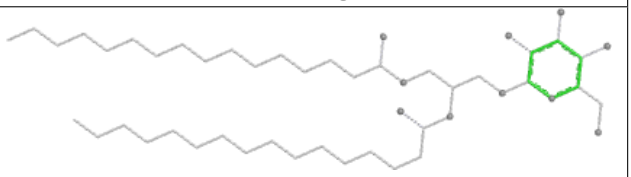
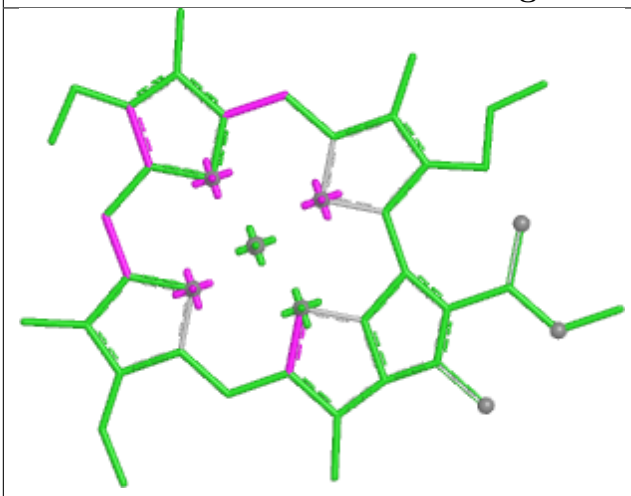
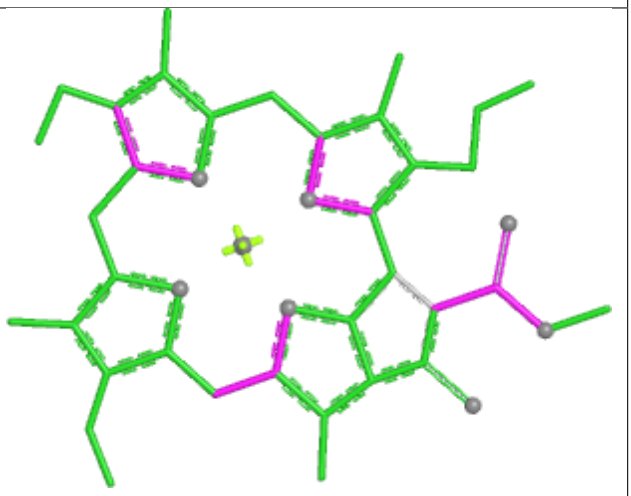
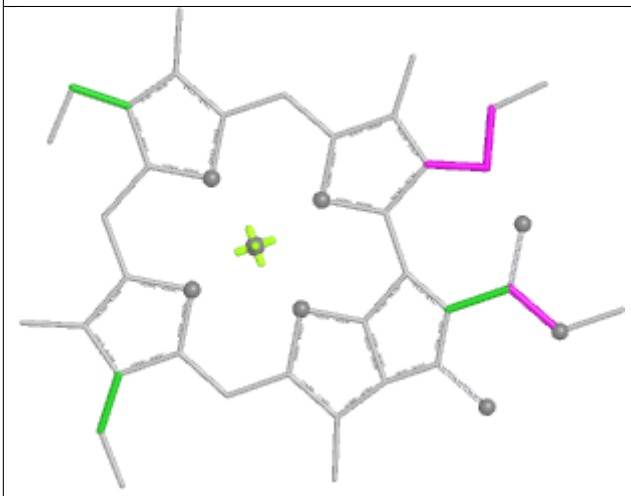
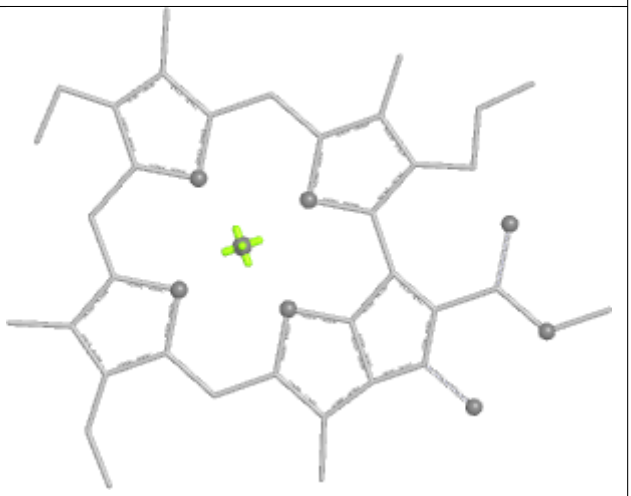
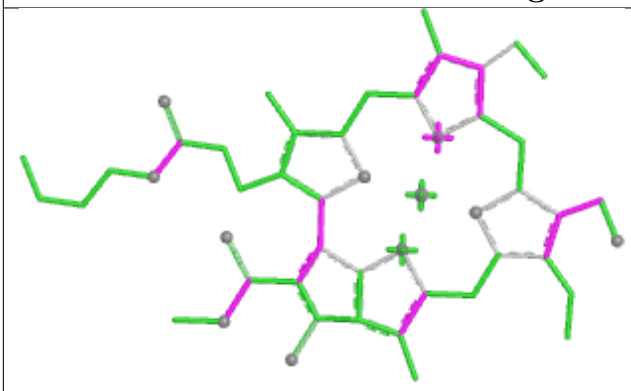
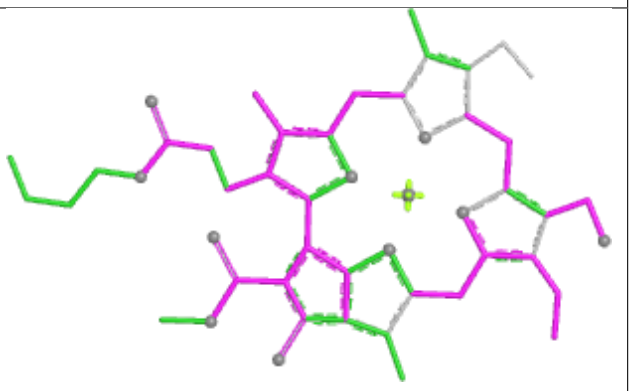
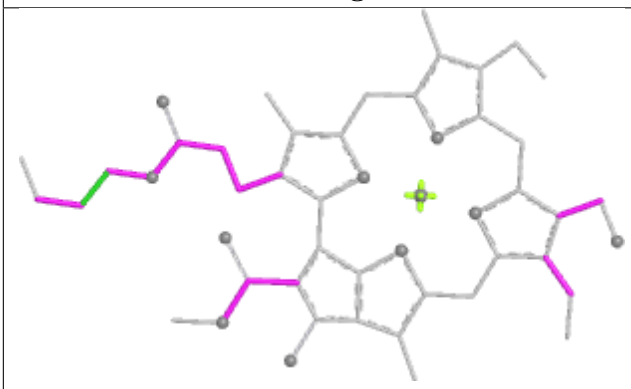
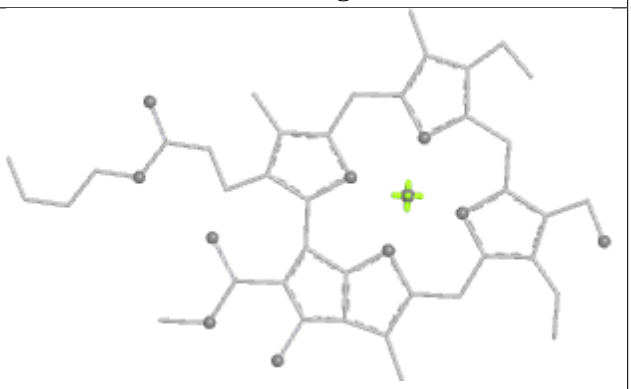
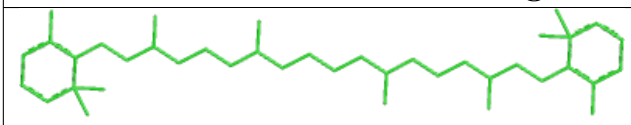
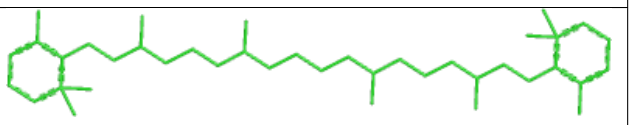
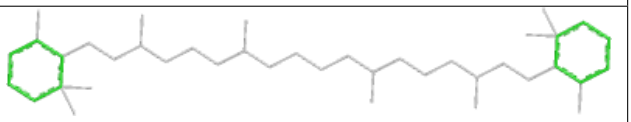
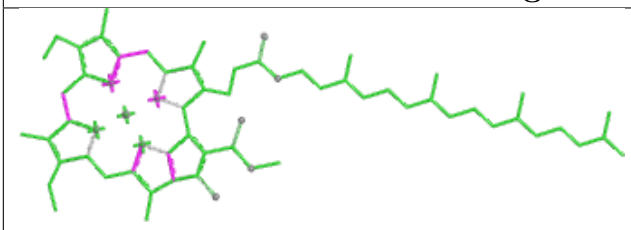
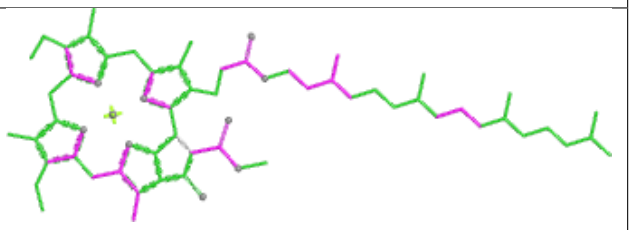
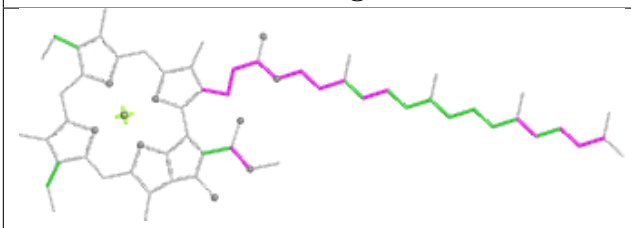
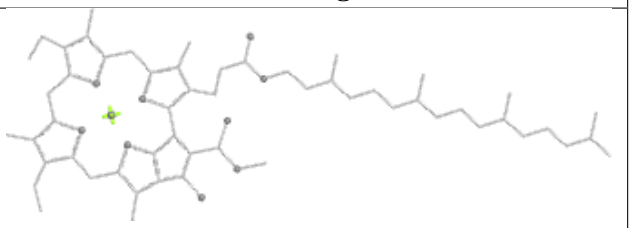


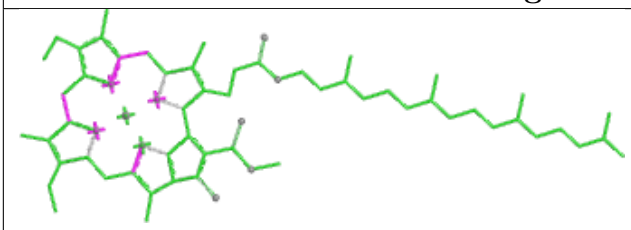
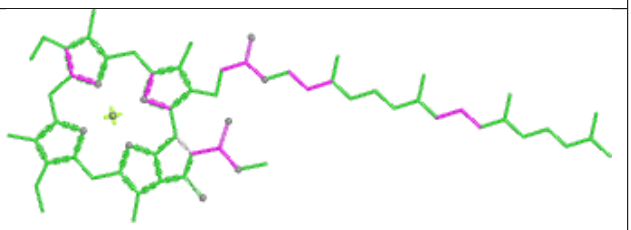
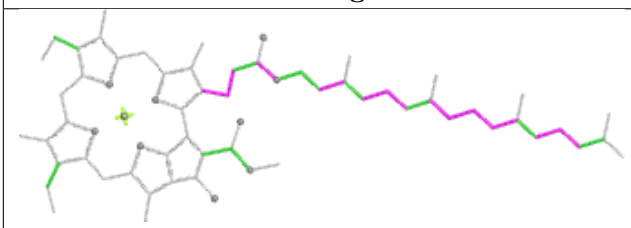
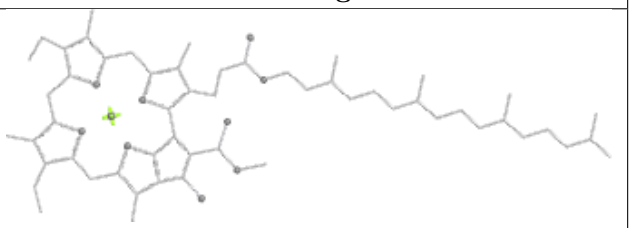
Rings

Ligand CLA 14 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

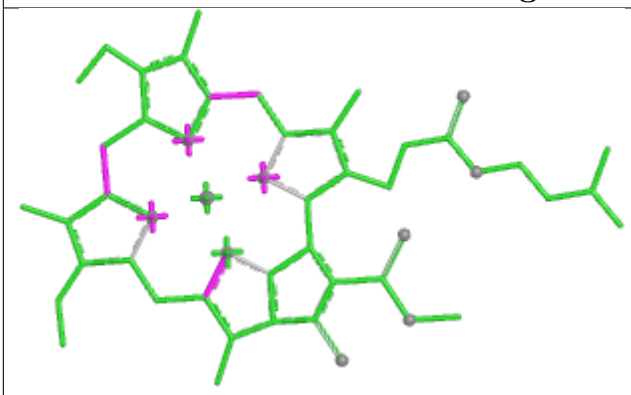
Ligand CHL 1 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR d 406	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA A 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 13 613



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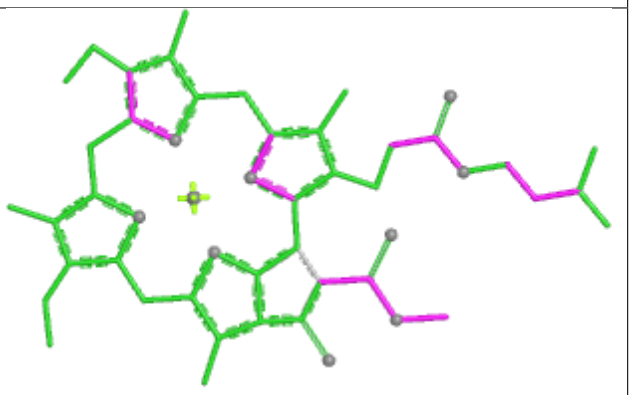
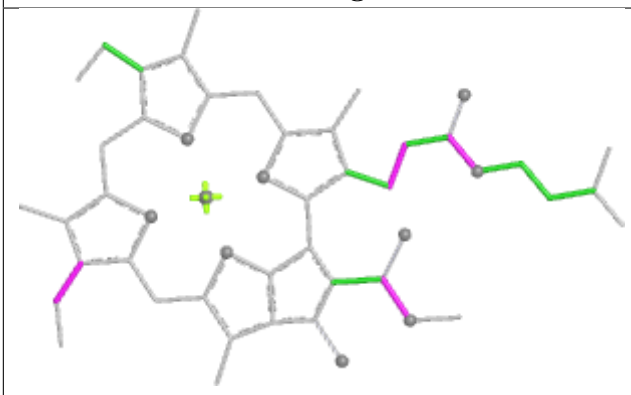


Bond angles



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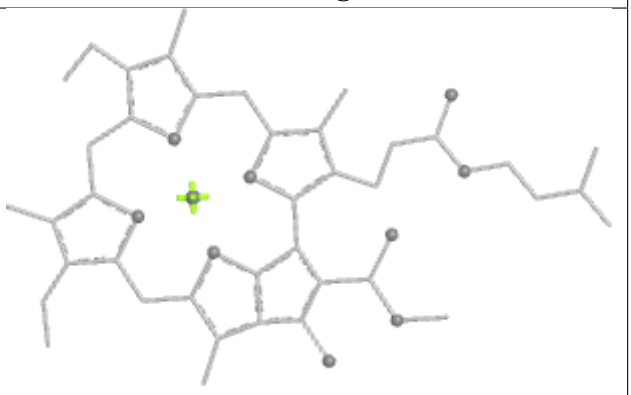
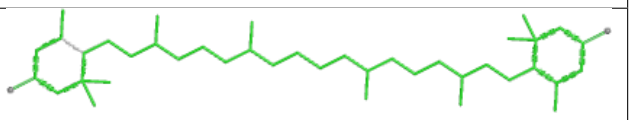


Rings

Ligand LUT 2 615

Bond lengths



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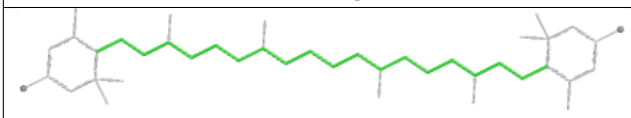

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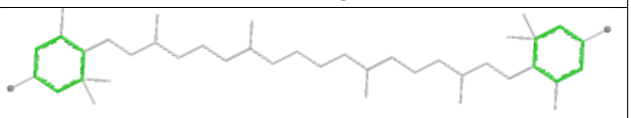
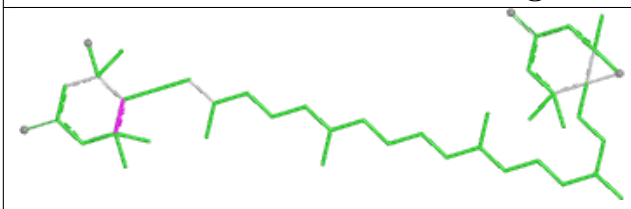


Rings

Ligand NEX 6 621



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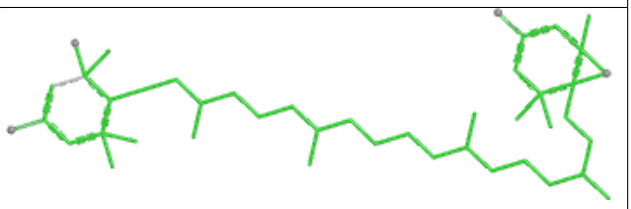
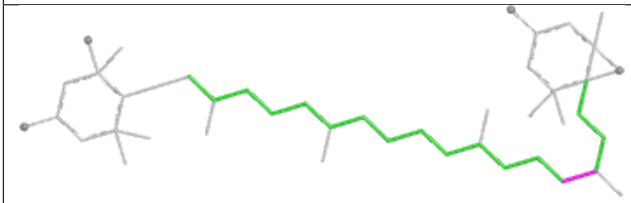


Bond angles



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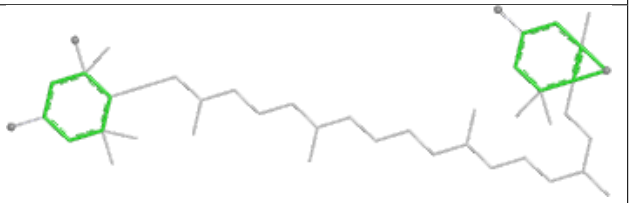
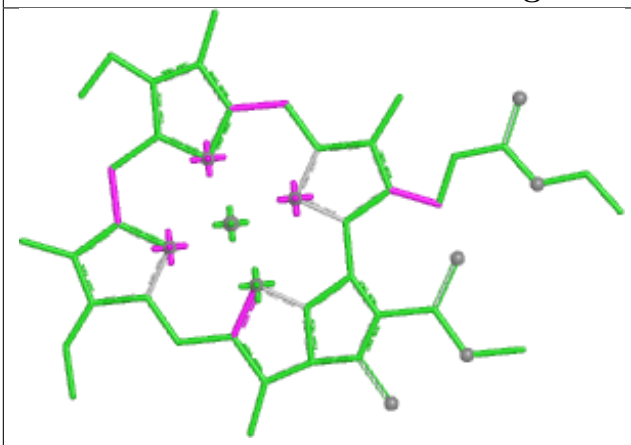


Rings

Ligand CLA N 615



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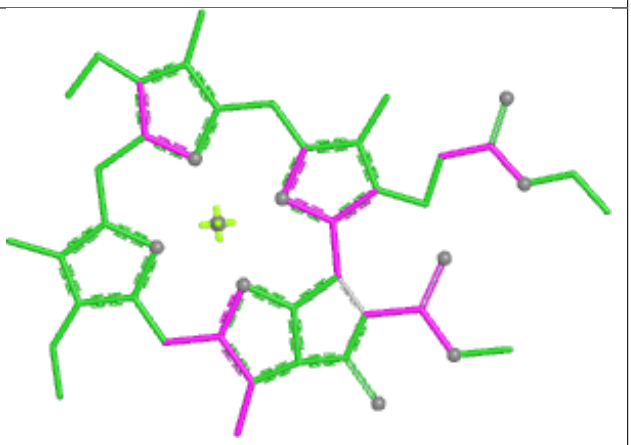
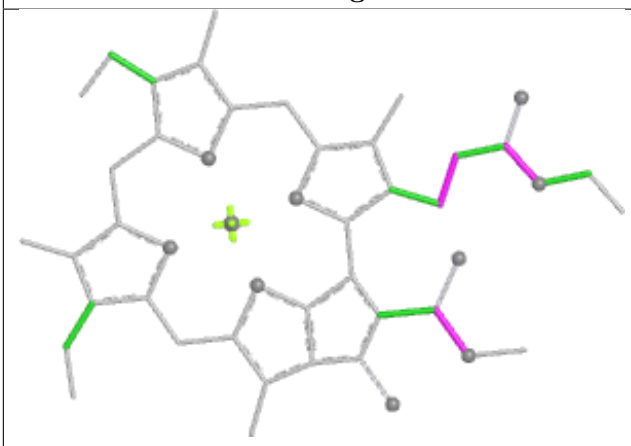


Bond angles



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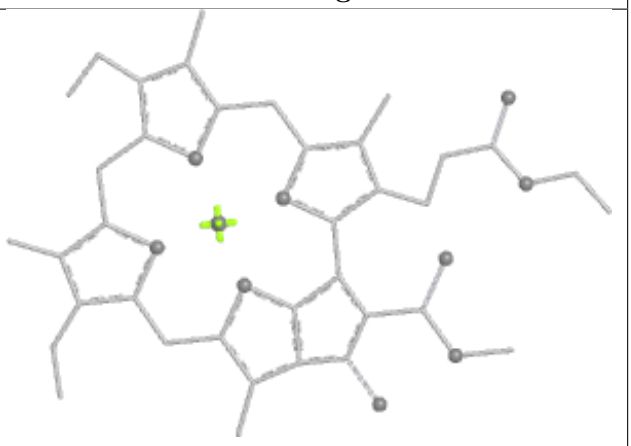
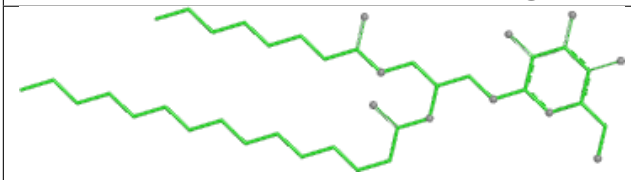


Rings

Ligand LMG S 616



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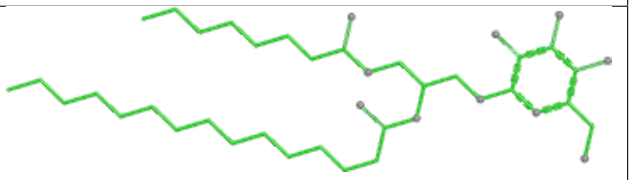
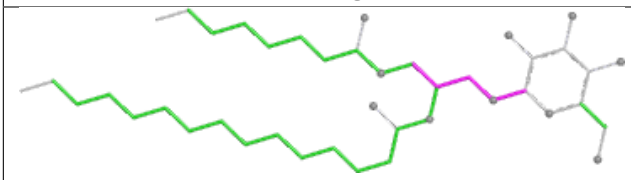


Bond angles



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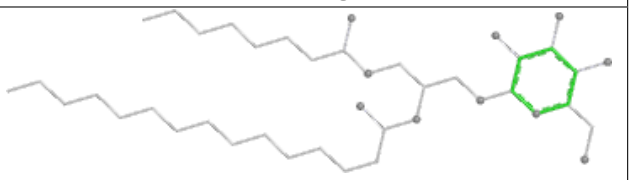
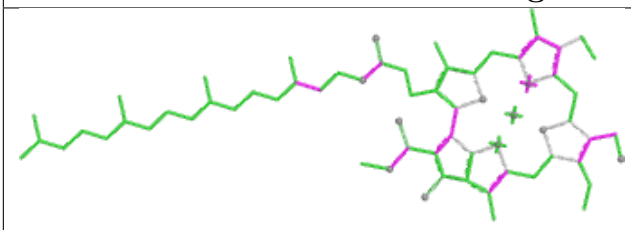
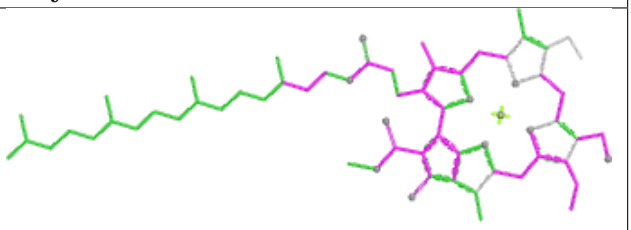
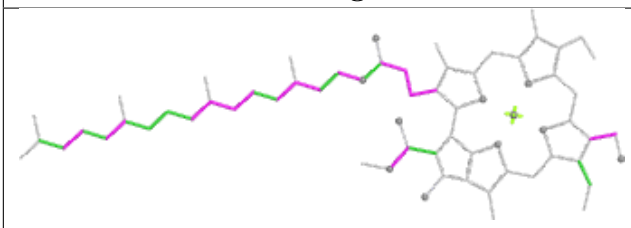
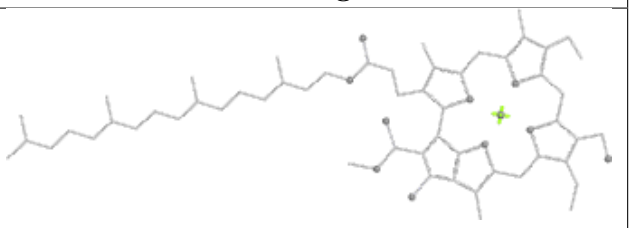


Rings

Ligand CHL y 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

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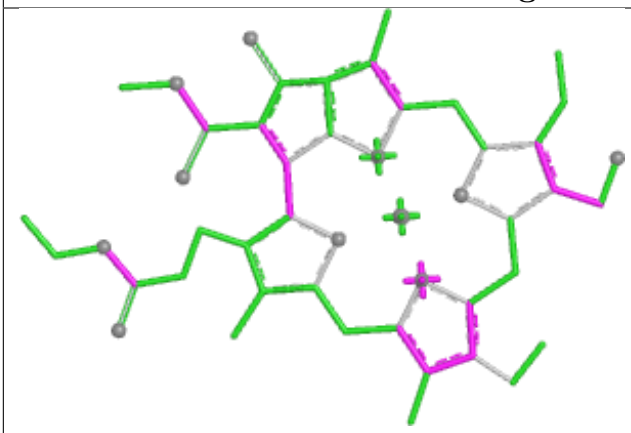
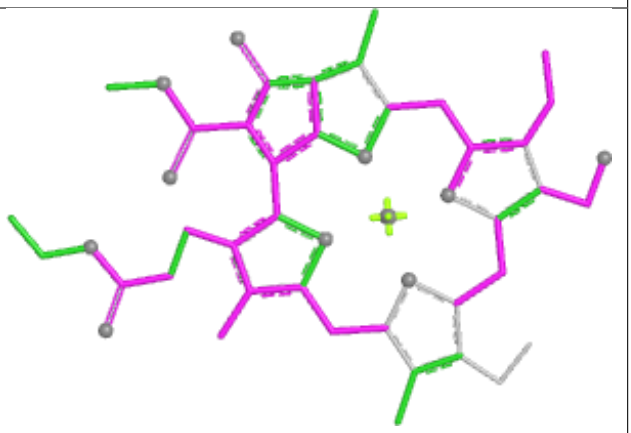
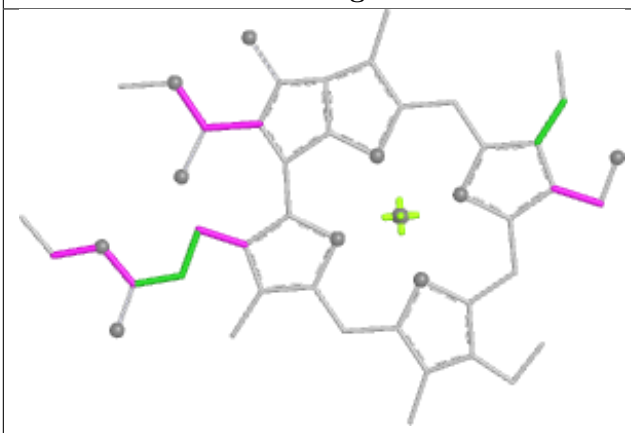
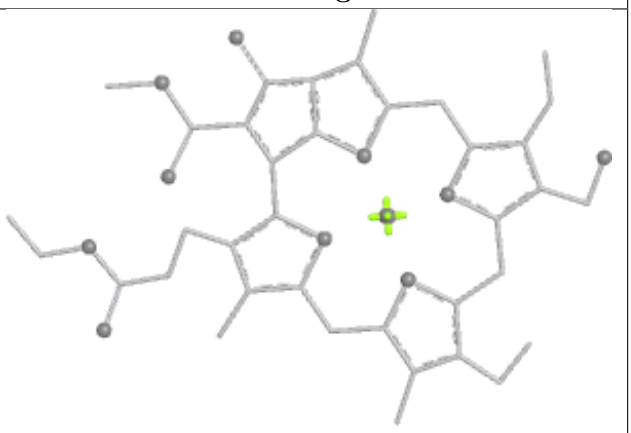
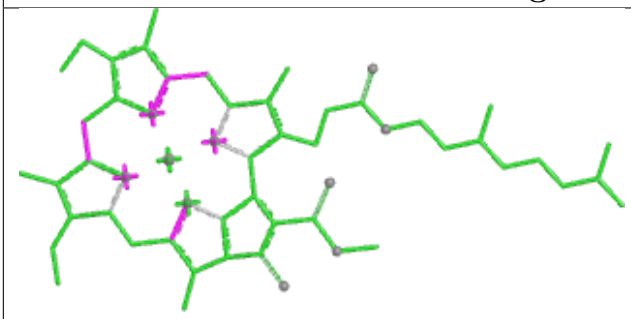
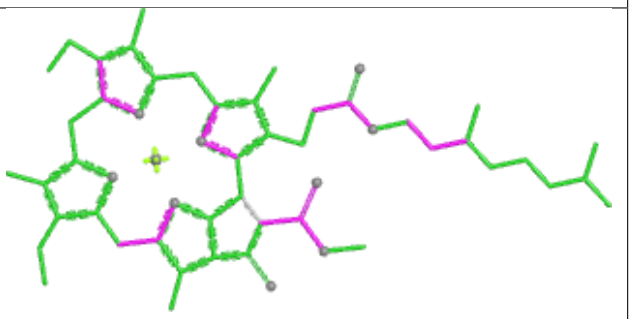
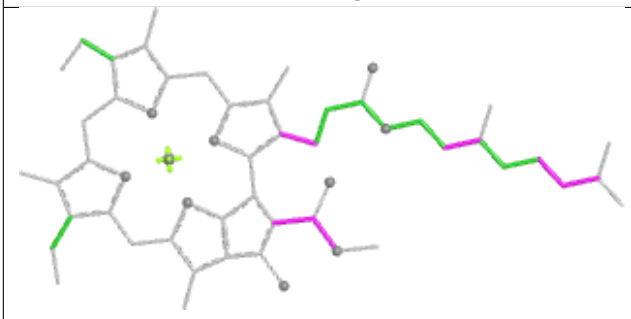
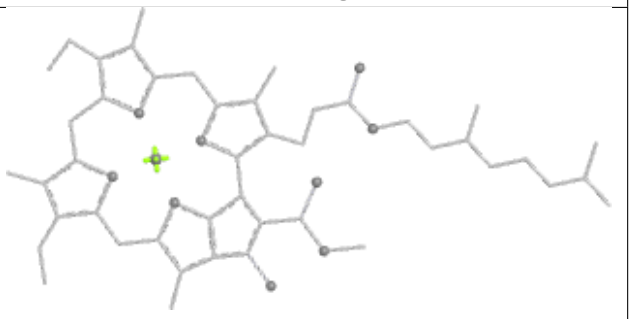
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

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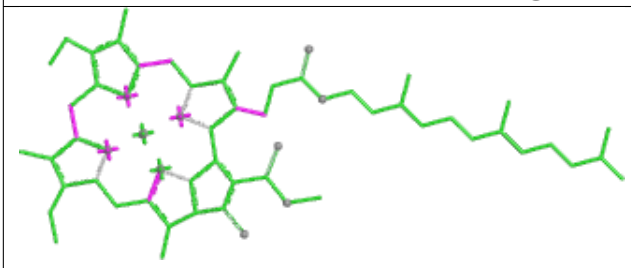
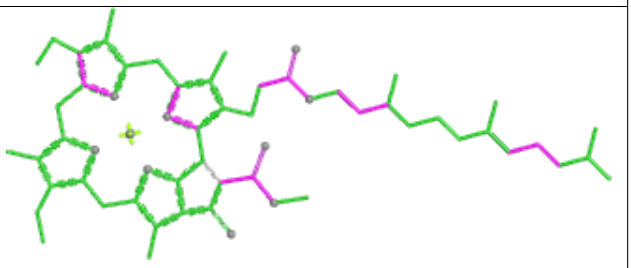
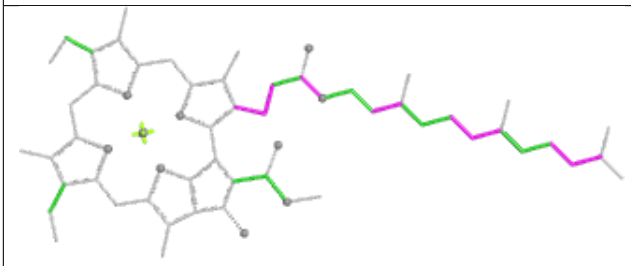
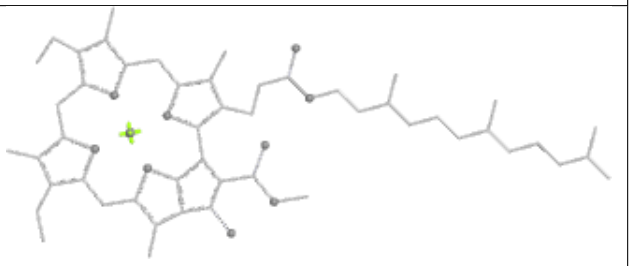
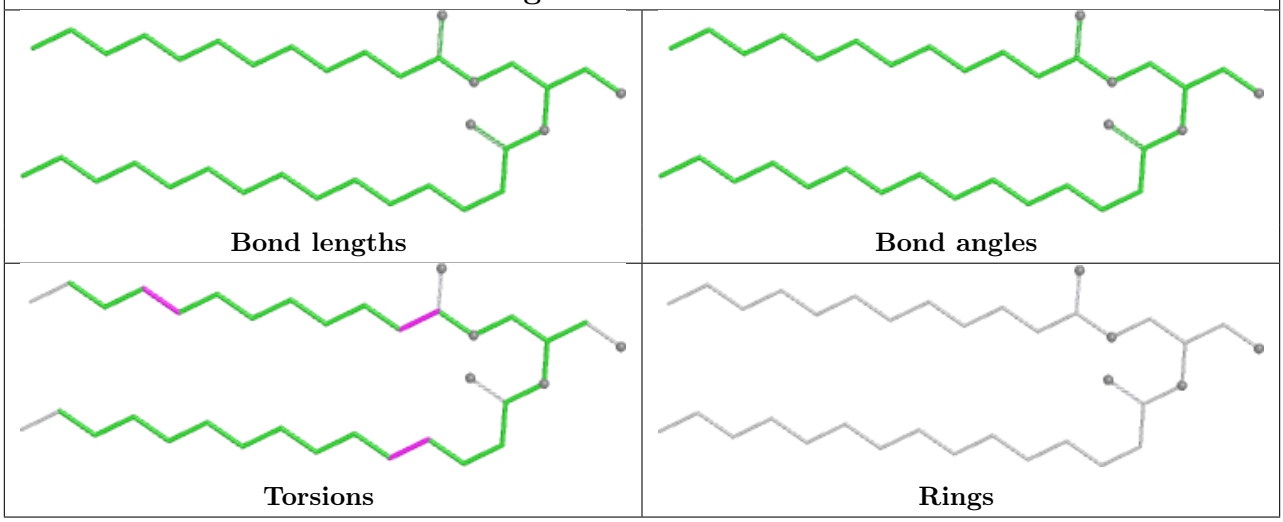
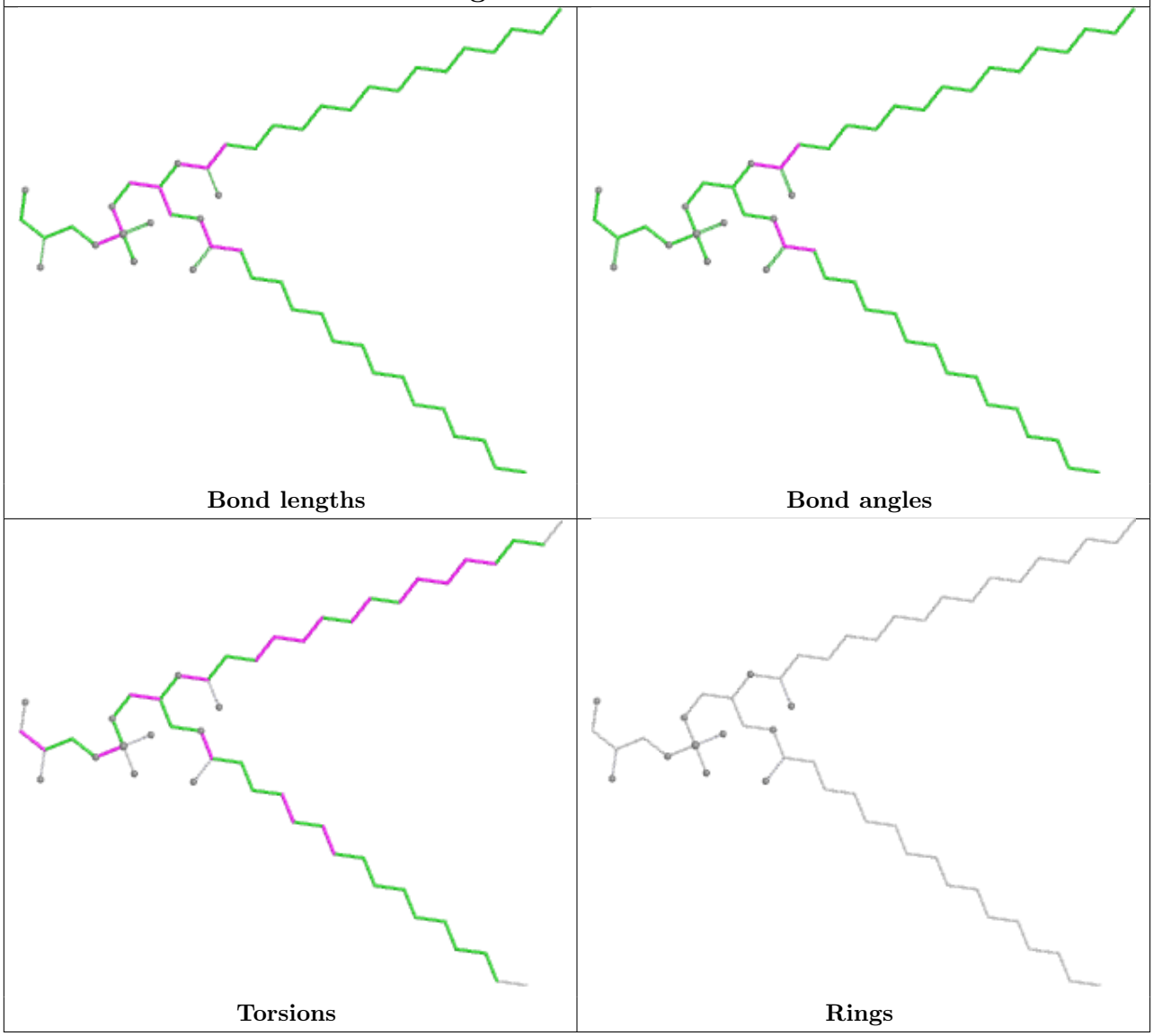
 Bond lengths	 Bond angles
 Torsions	 Rings

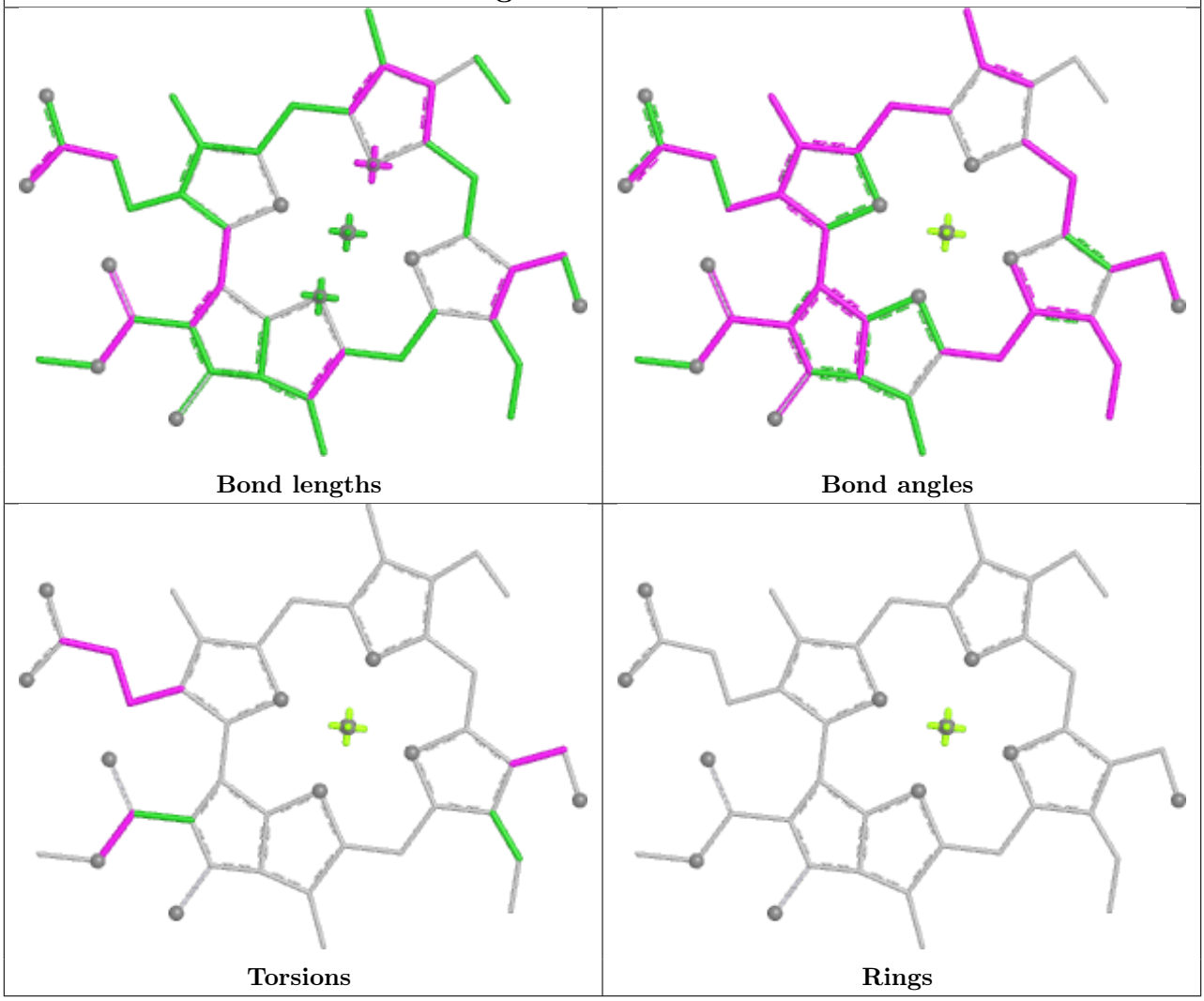
Ligand LMG d 411



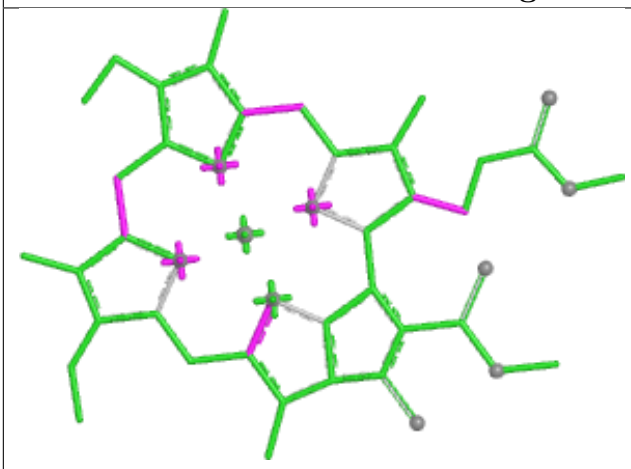
Ligand LHG A 411



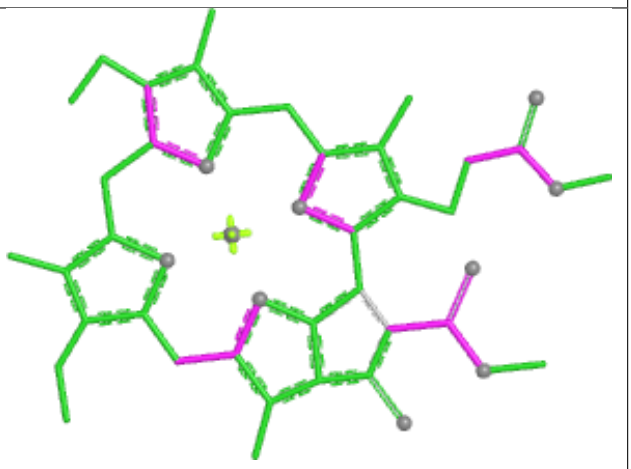
Ligand CHL 5 606



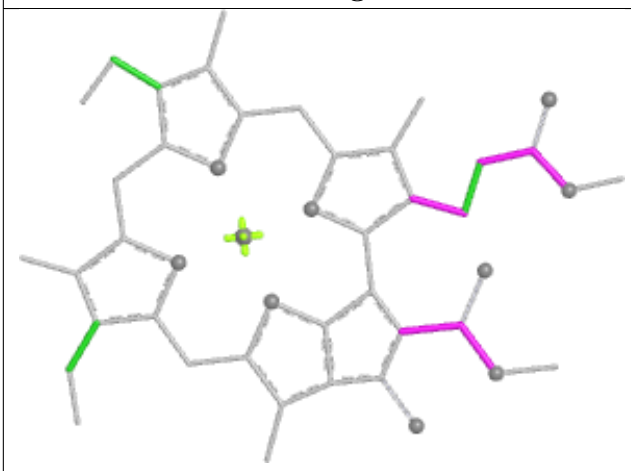
Ligand CLA 11 604



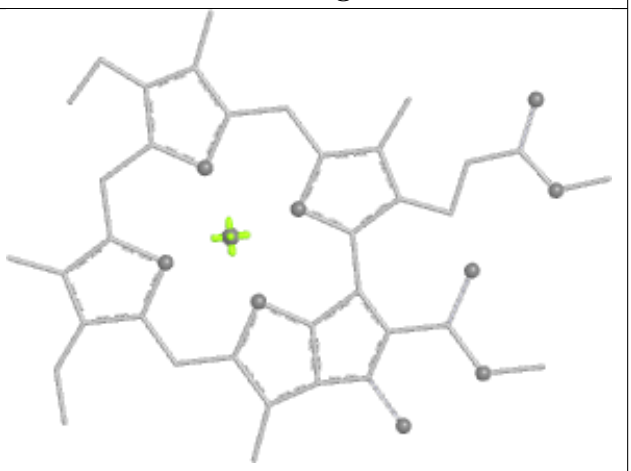
Bond lengths



Bond angles

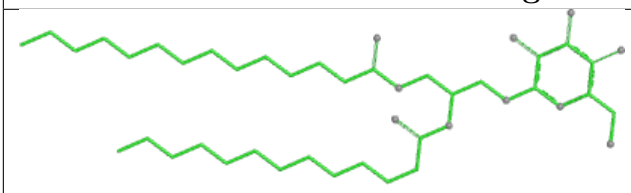


Torsions



Rings

Ligand LMG b 621



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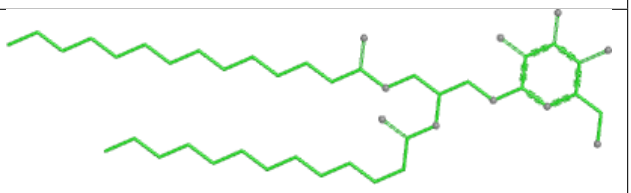
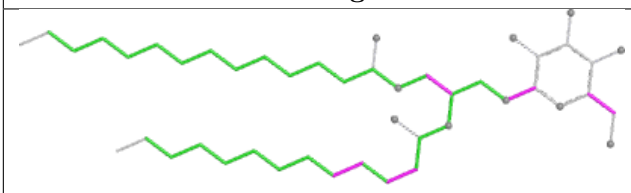


Bond angles



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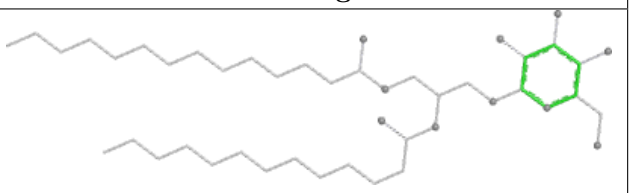
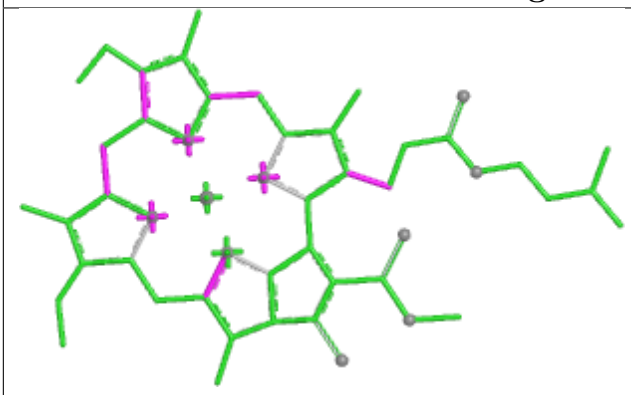
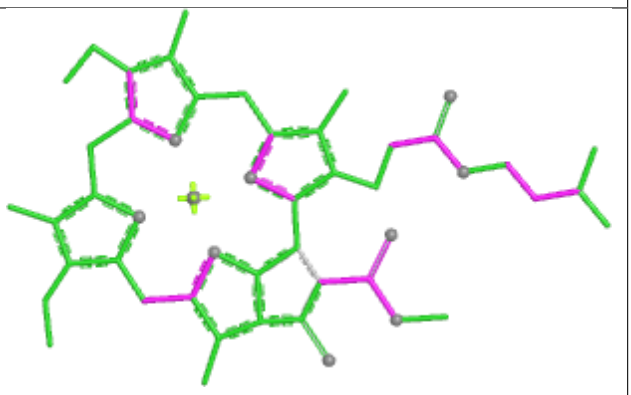
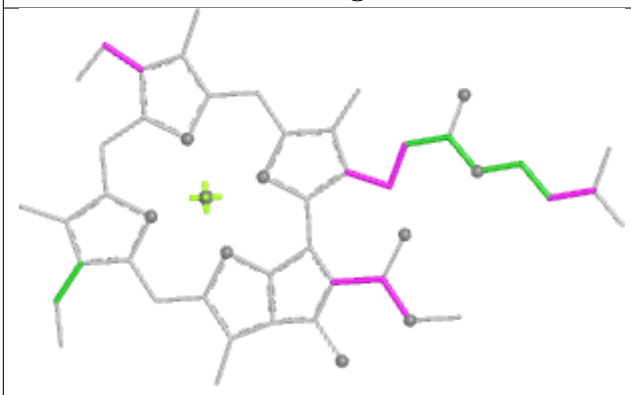
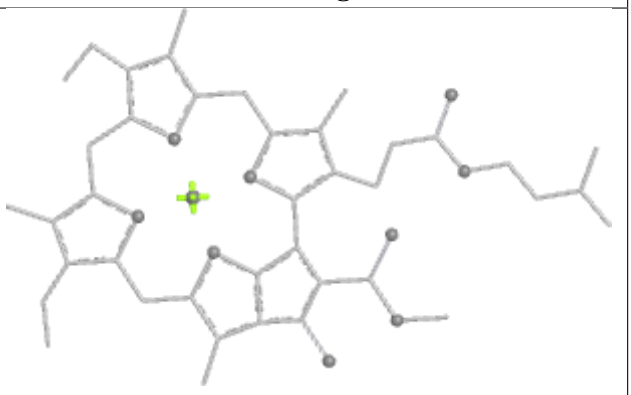
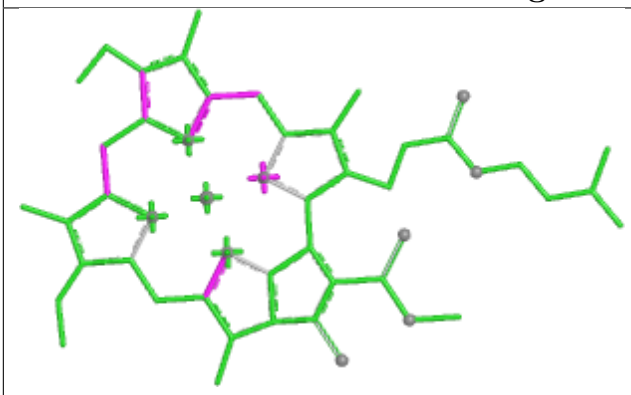
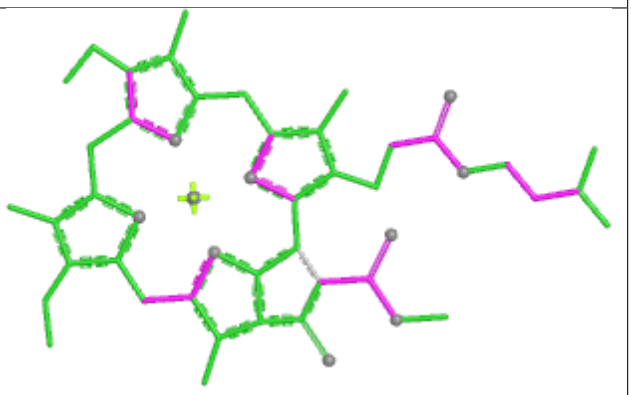
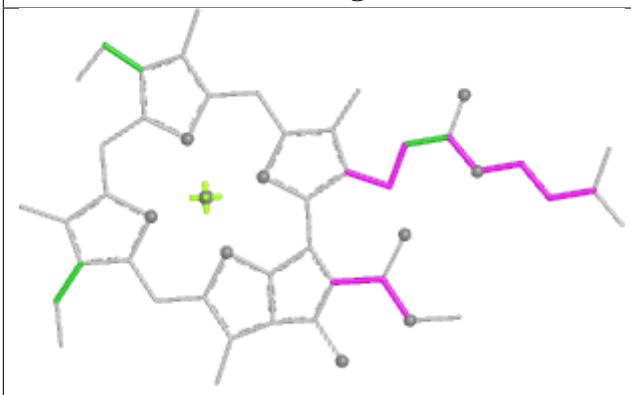
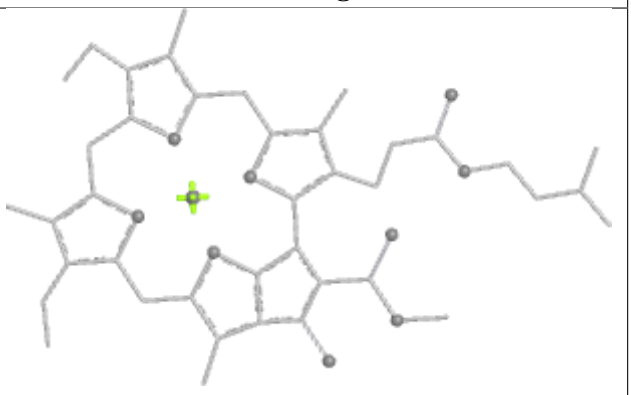
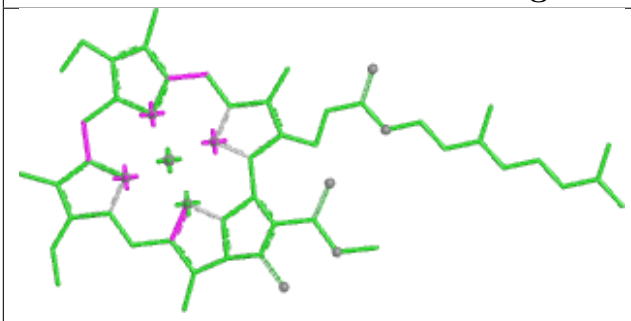
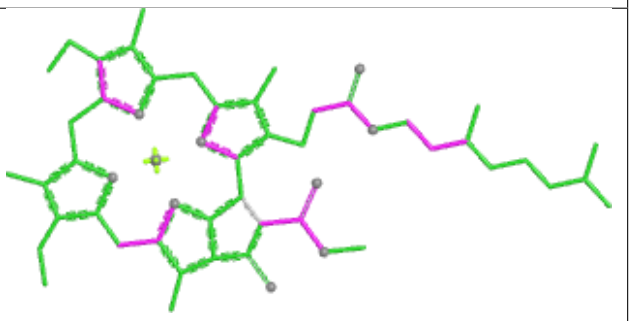
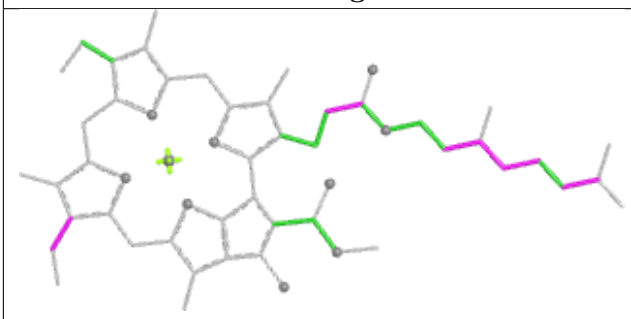
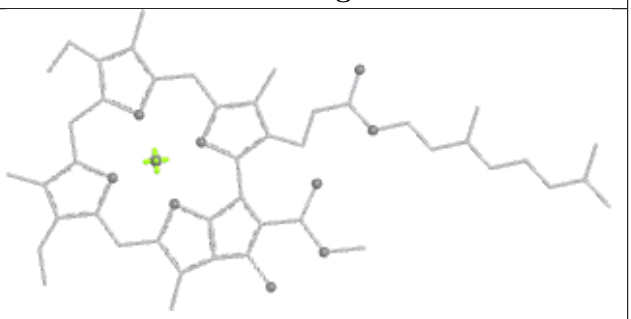
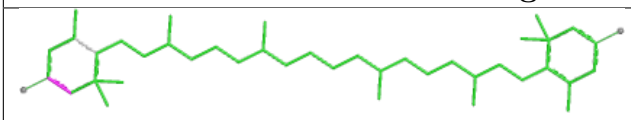
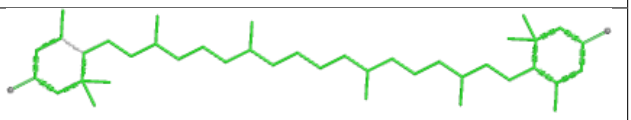
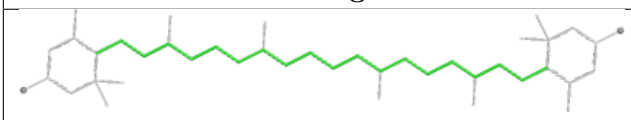
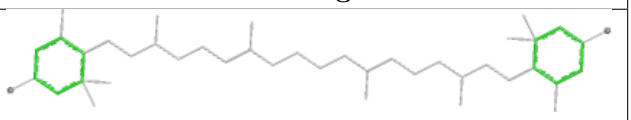


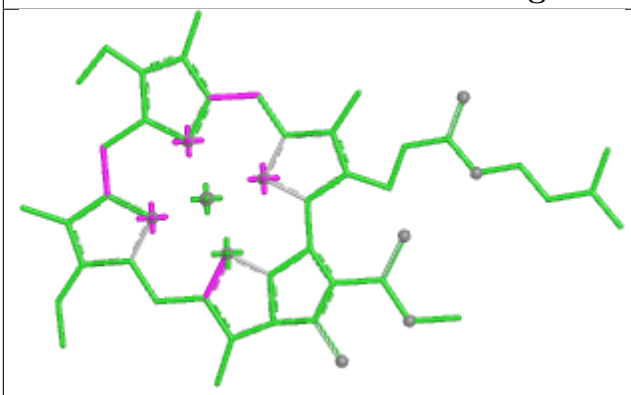
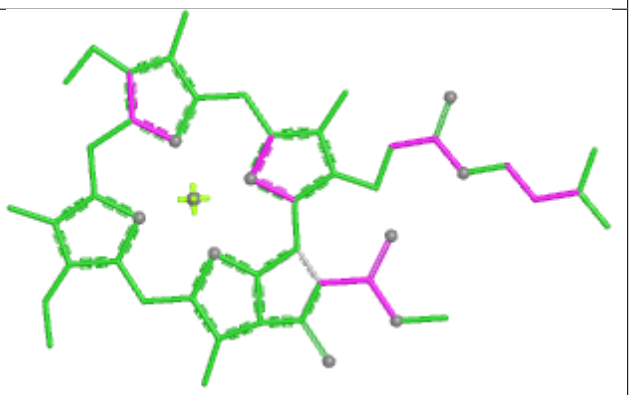
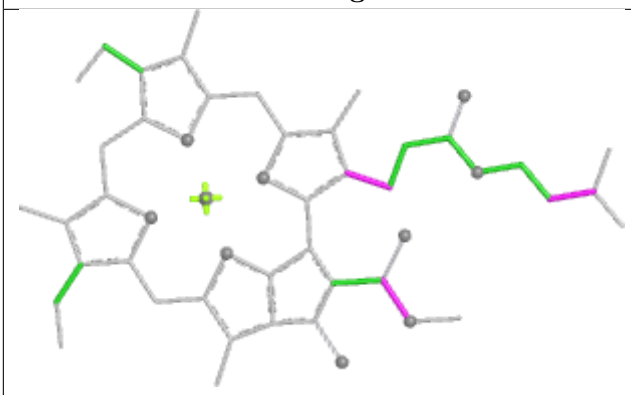
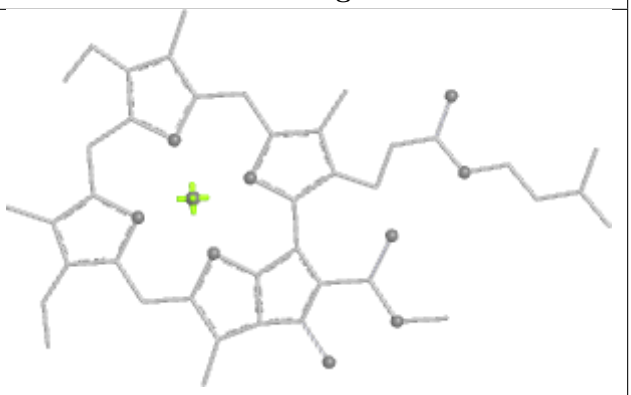
Rings

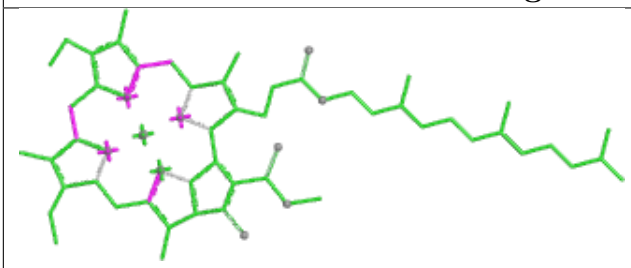
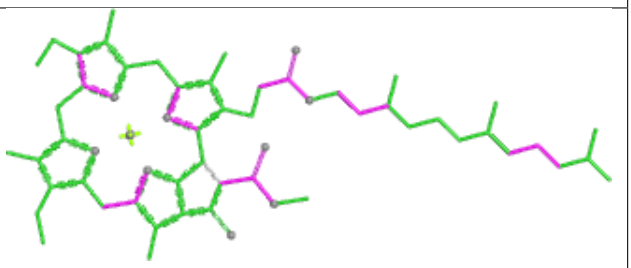
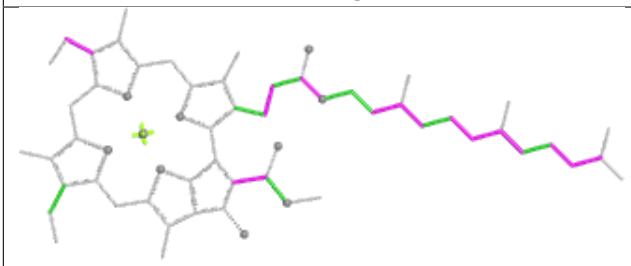
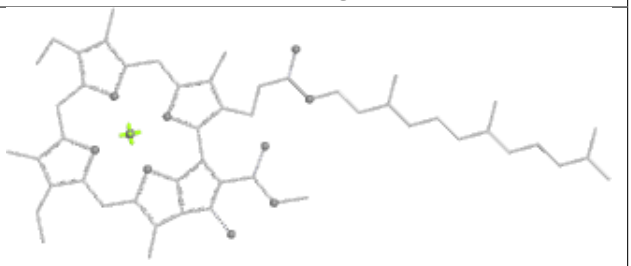
Ligand CLA 4 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 16 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

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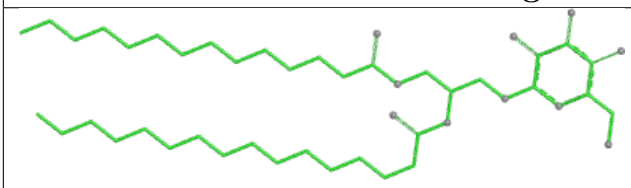
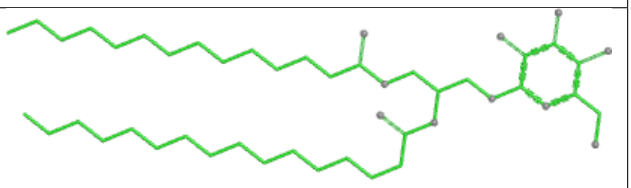
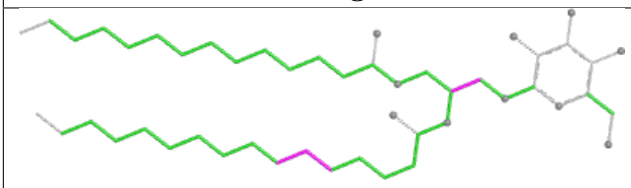
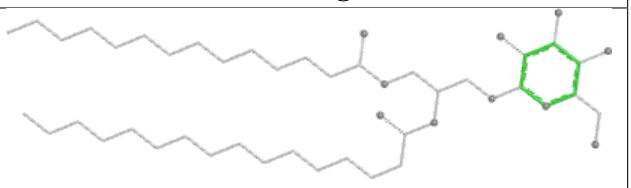
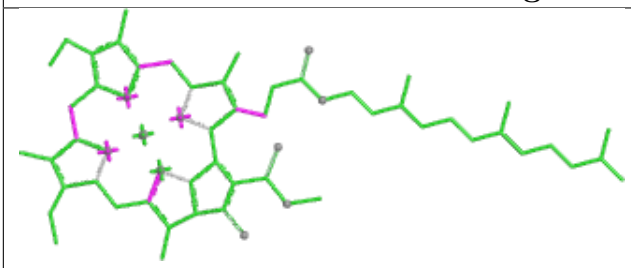
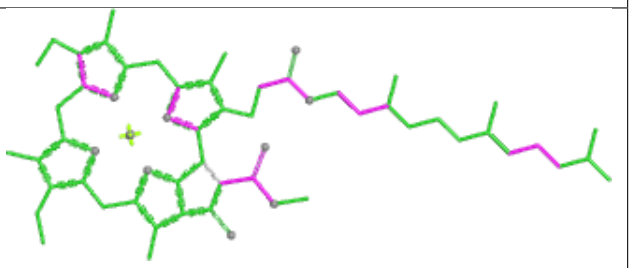
 Bond lengths	 Bond angles
 Torsions	 Rings

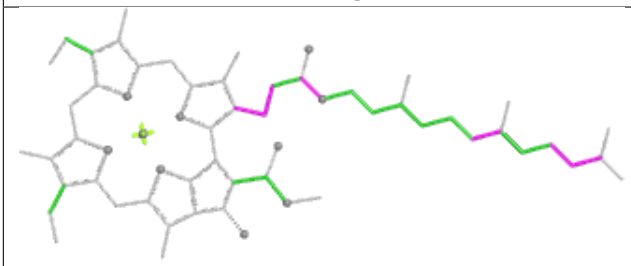
Ligand CLA N 611



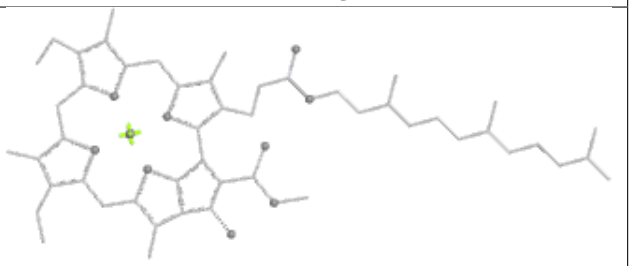
Bond lengths



Bond angles

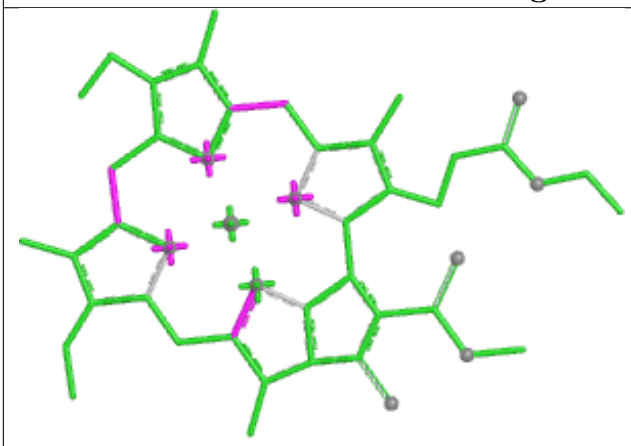


Torsions

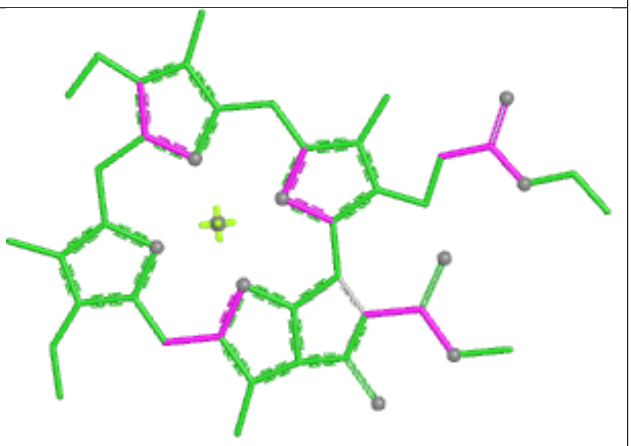


Rings

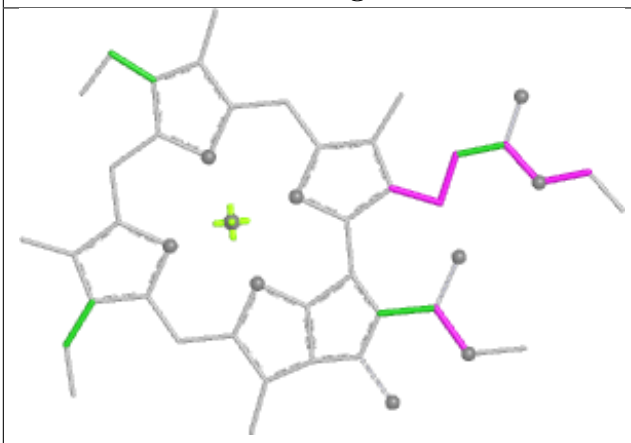
Ligand CLA s 615



Bond lengths



Bond angles



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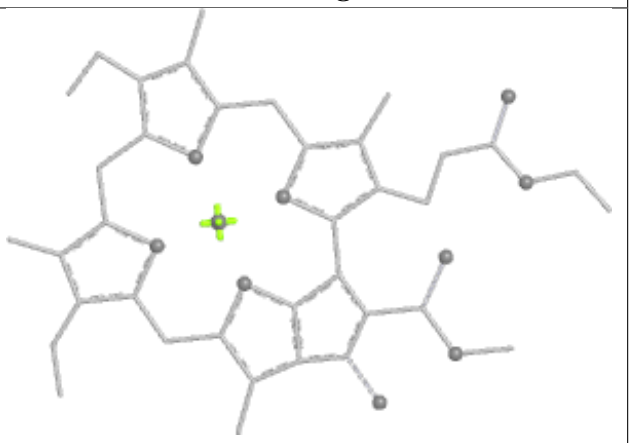
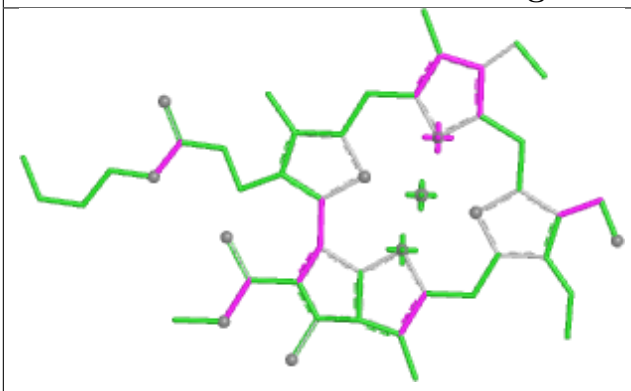
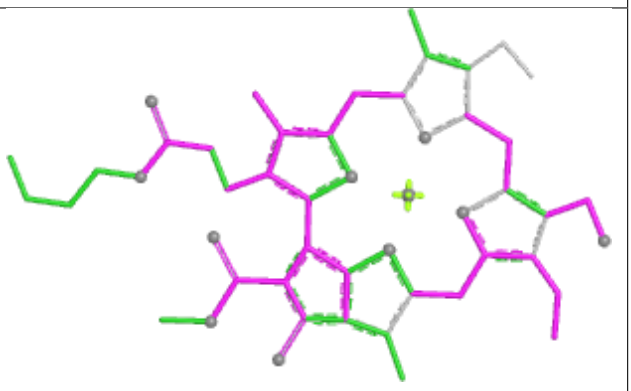
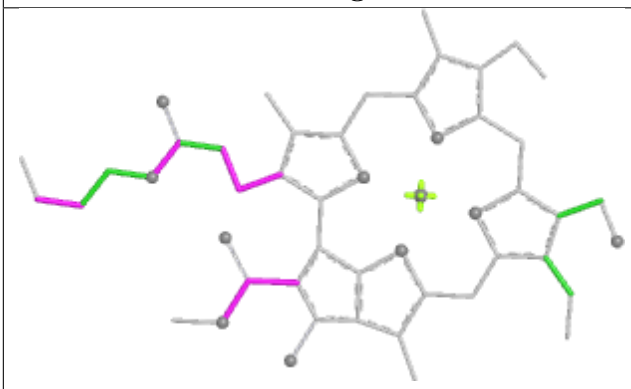
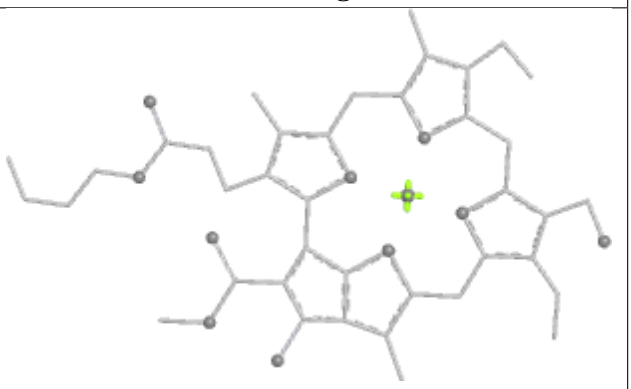
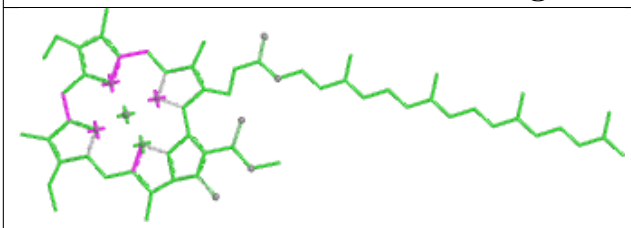
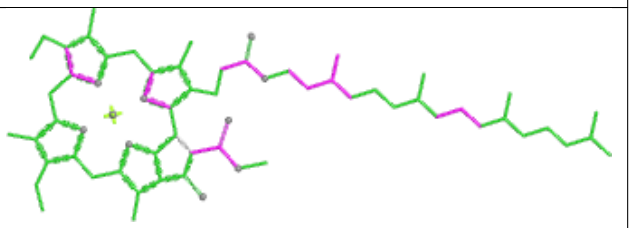
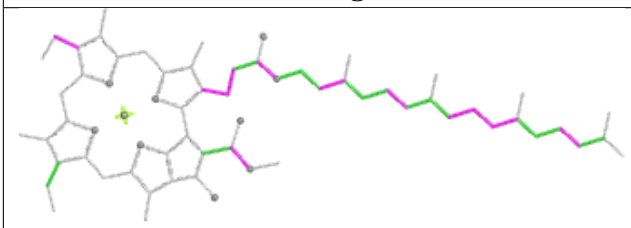
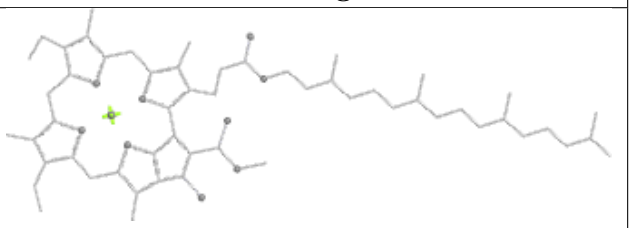
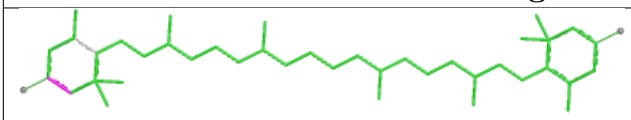
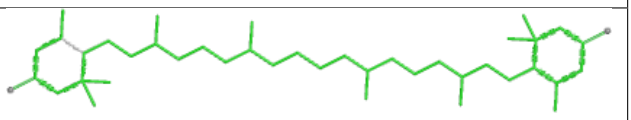
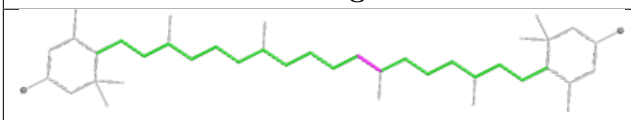
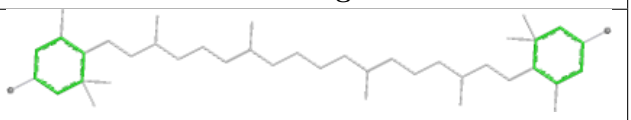


Rings

Ligand CHL 6 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 5 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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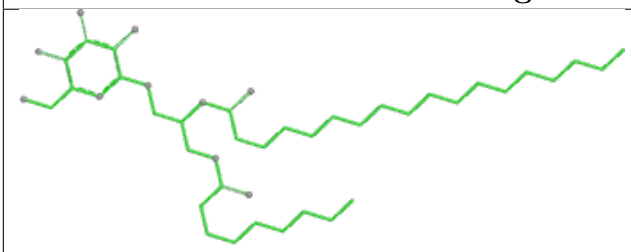
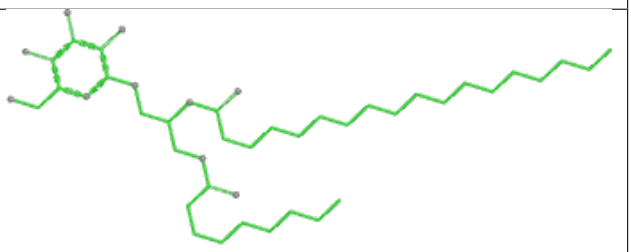
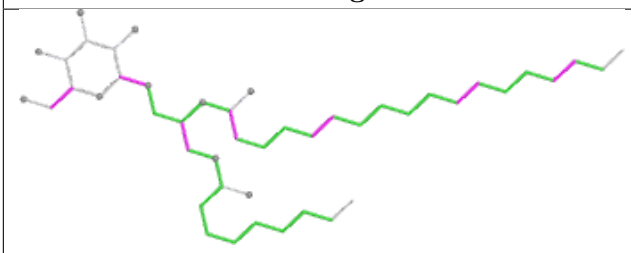
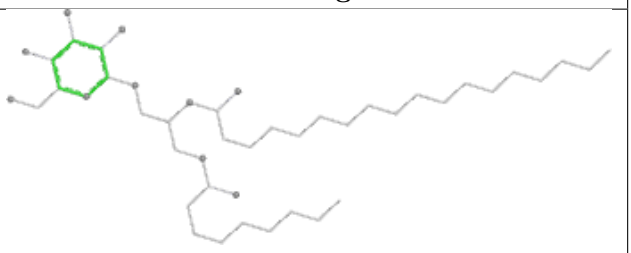
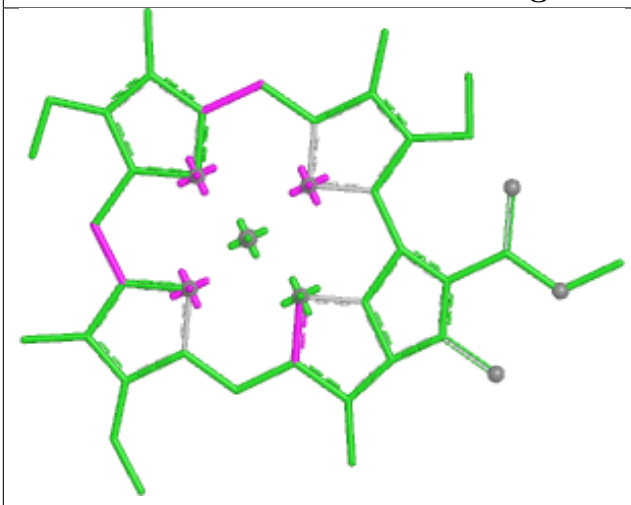
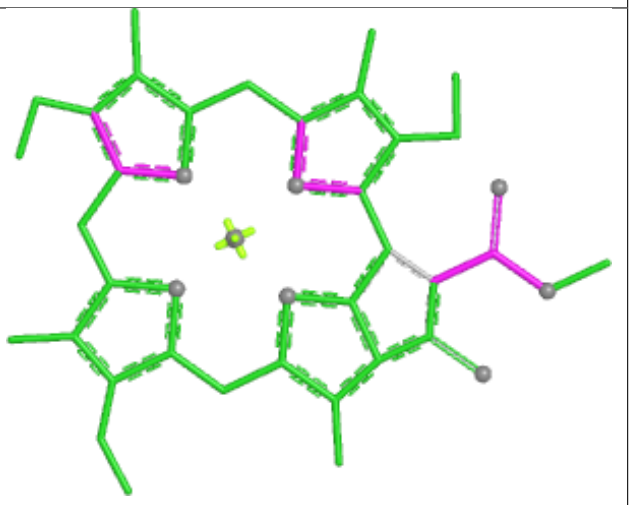
 Bond lengths	 Bond angles
 Torsions	 Rings

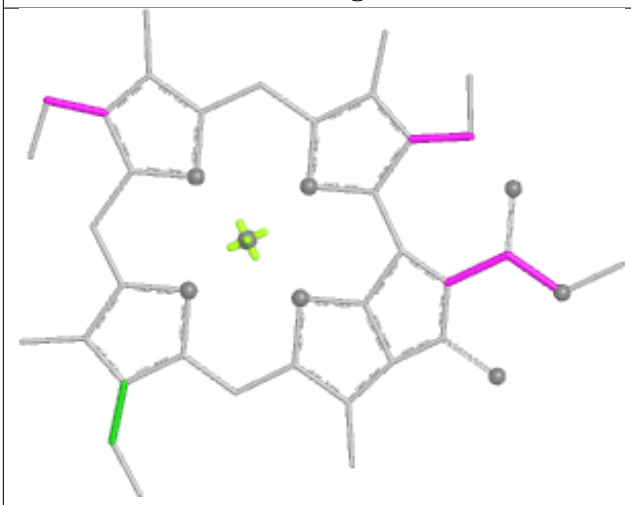
Ligand CLA s 603



Bond lengths



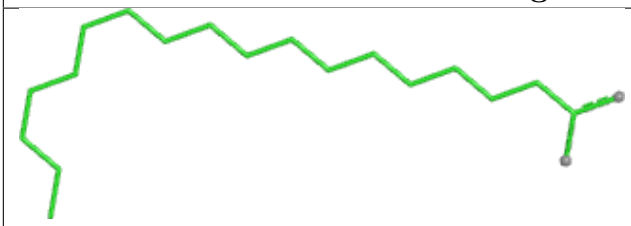
Bond angles



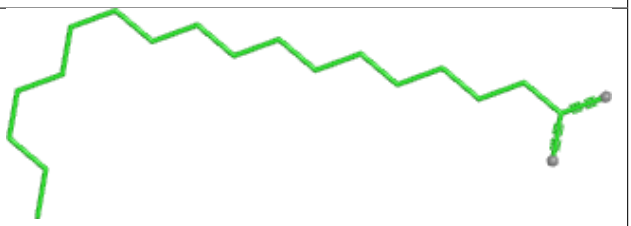
Torsions

Rings

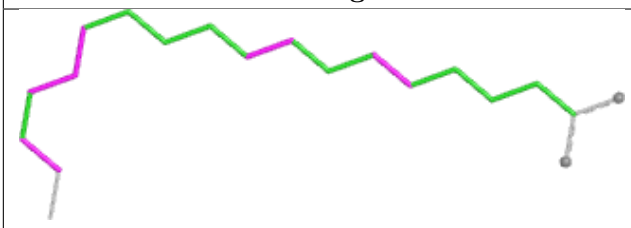
Ligand LNL a 412



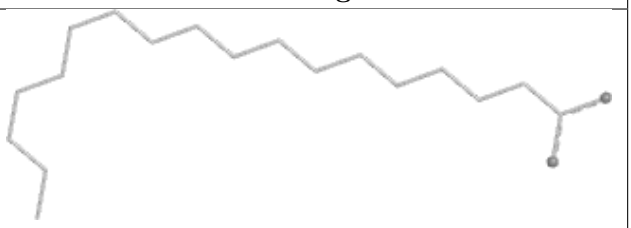
Bond lengths



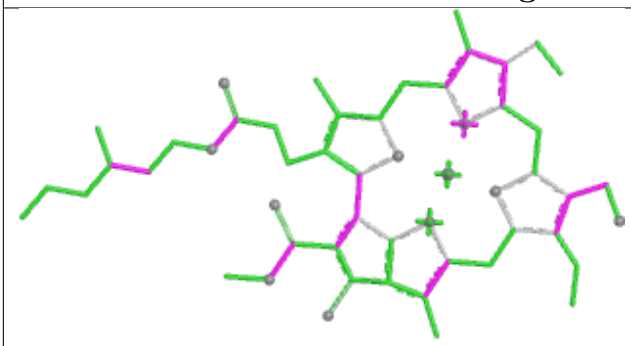
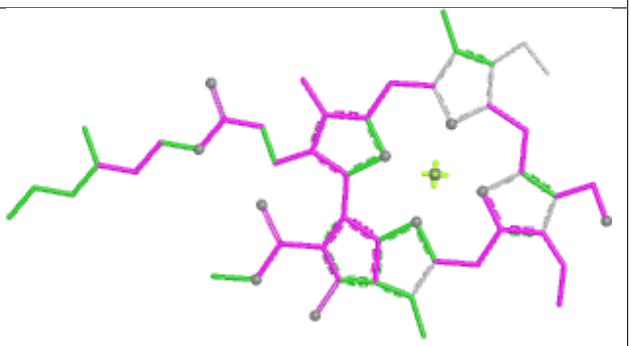
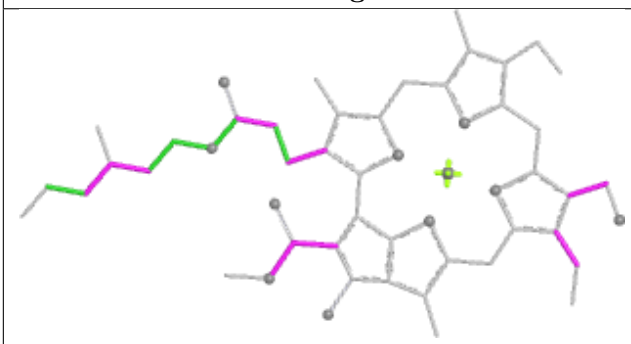
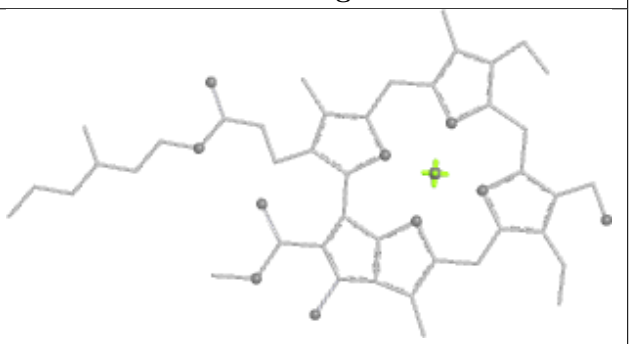
Bond angles

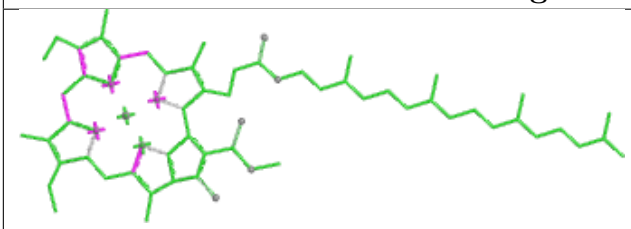
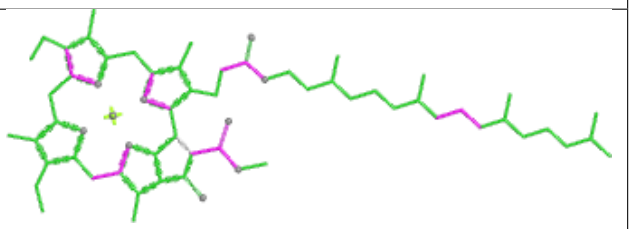
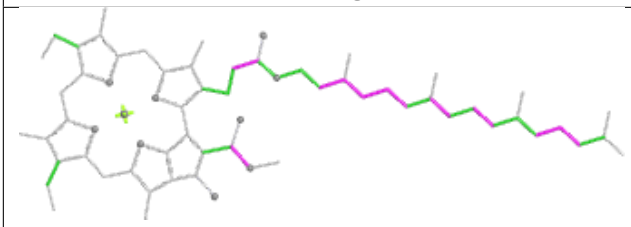
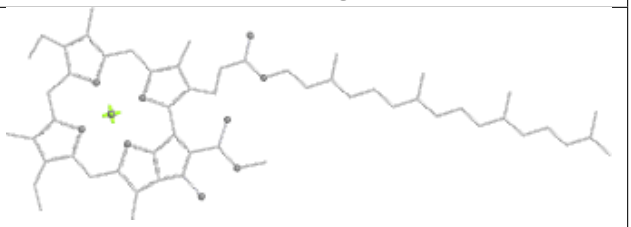


Torsions



Rings

Ligand CHL 12 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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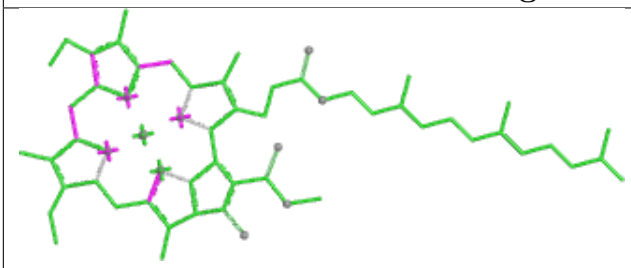
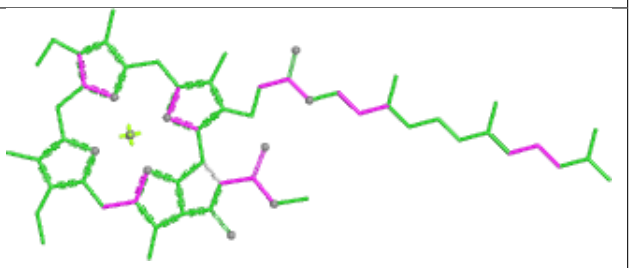
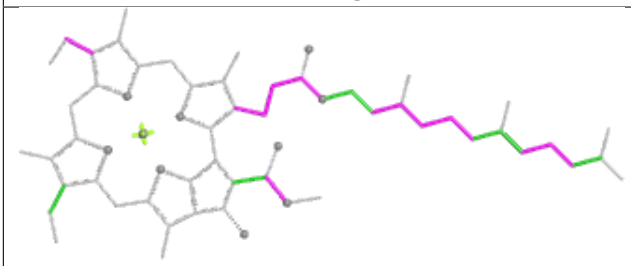
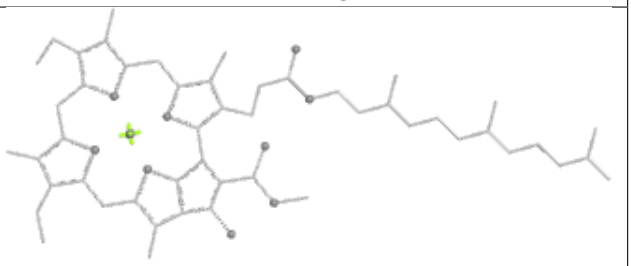
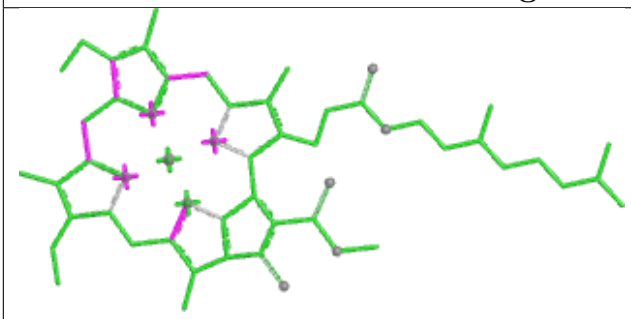
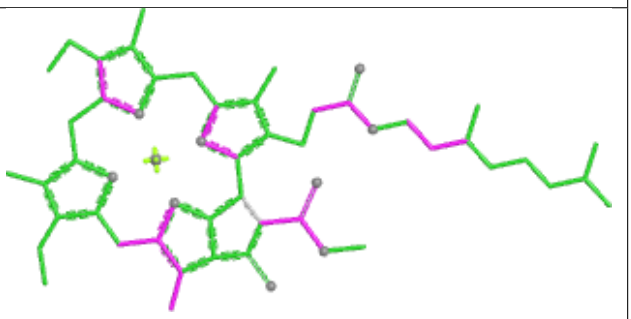
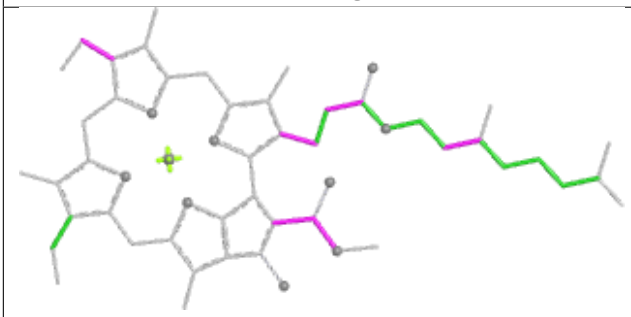
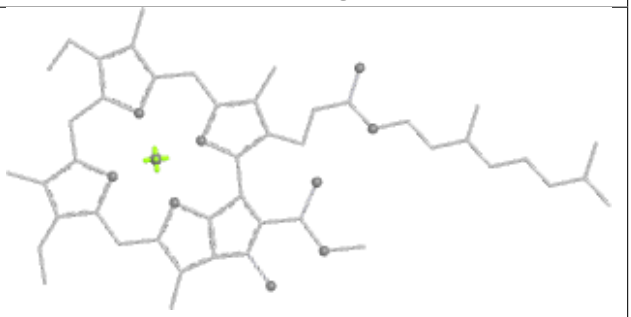
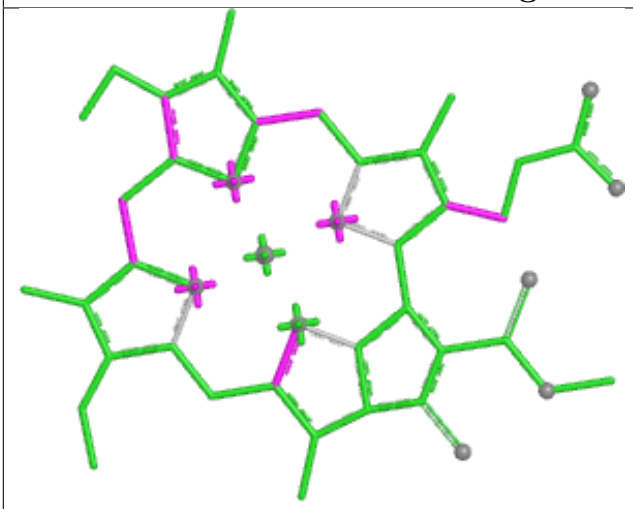
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 12 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 15 613



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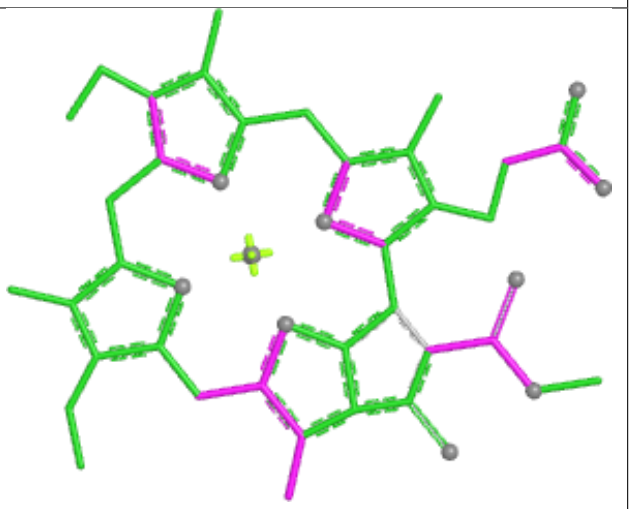

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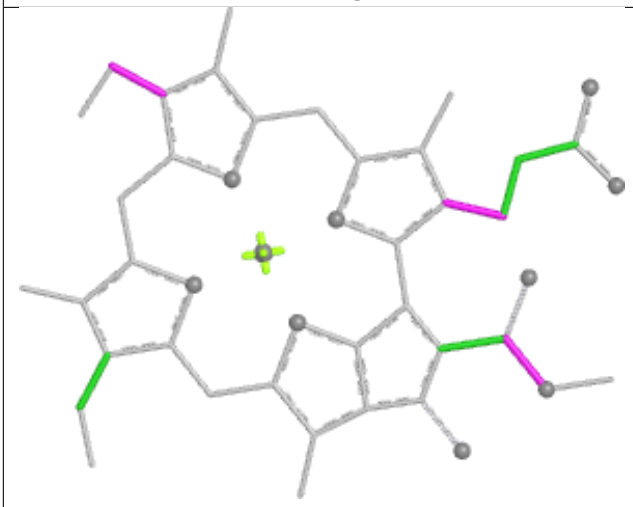
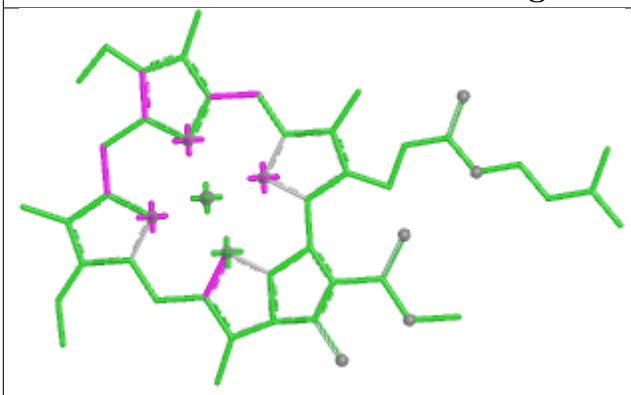


Torsions

Rings

Ligand CLA 5 604



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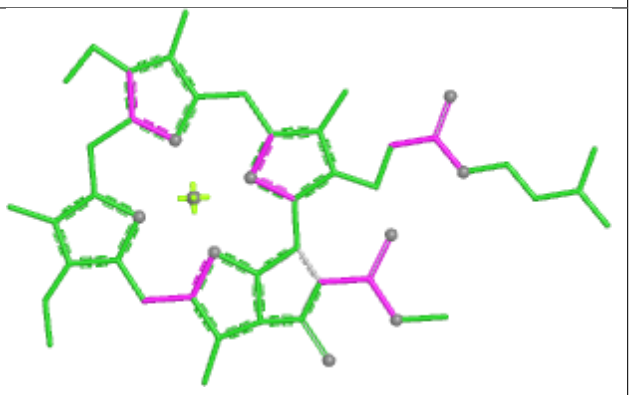

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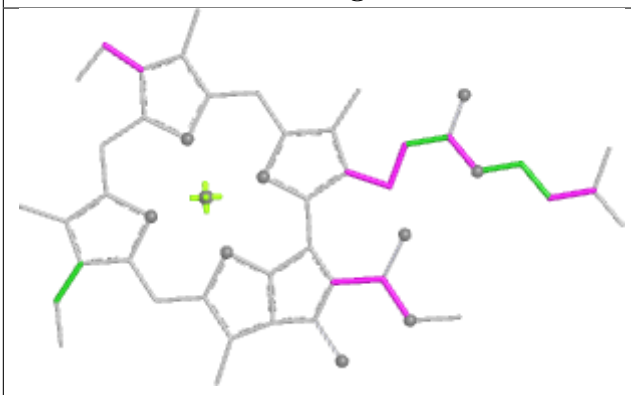

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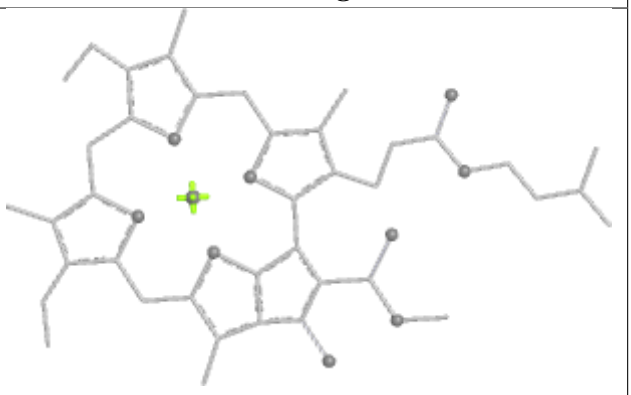
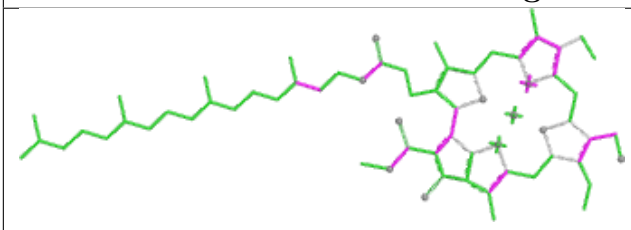


Rings

Ligand CHL Y 606



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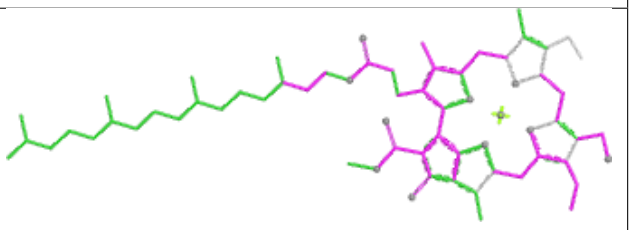

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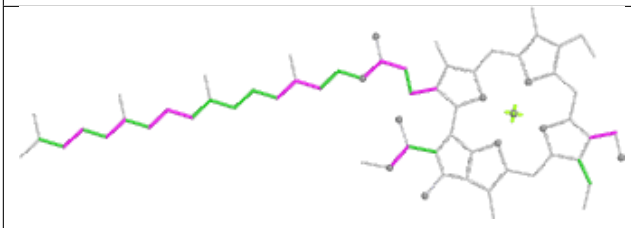

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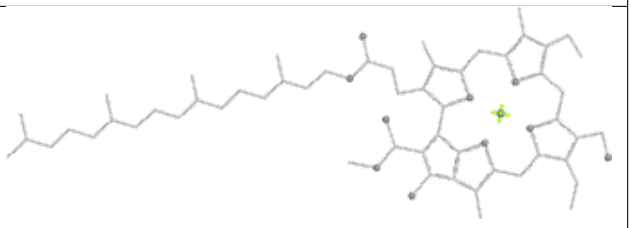

Rings

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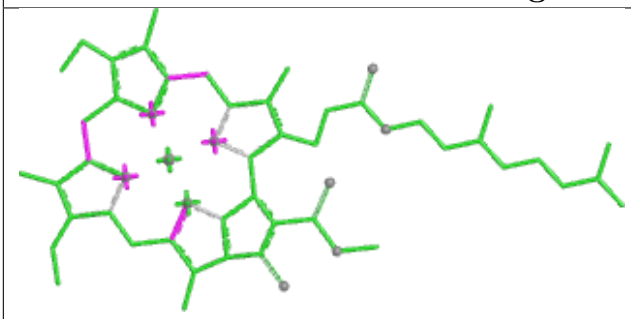

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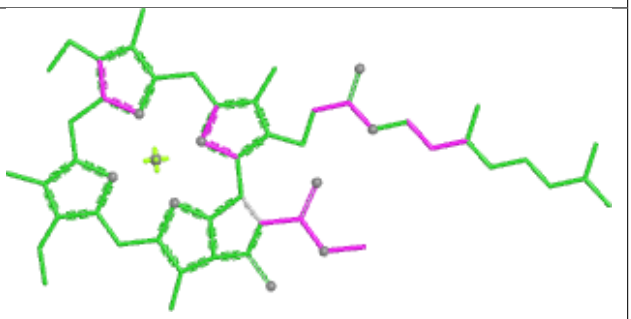

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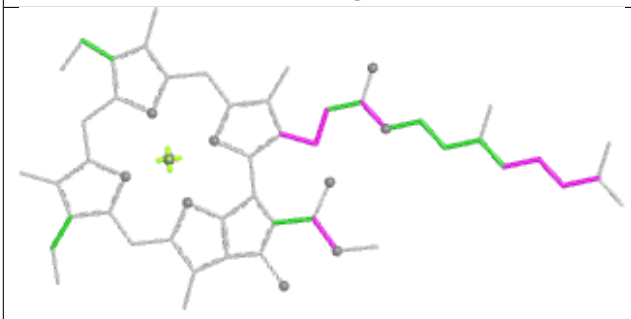

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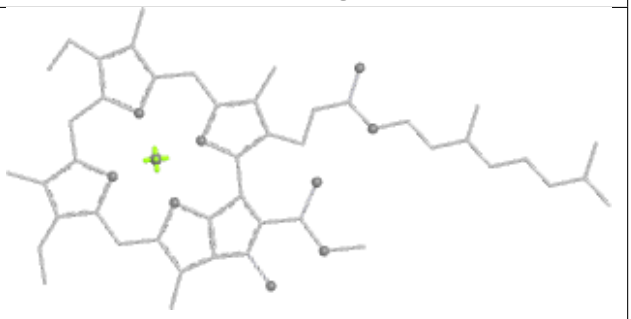

Rings

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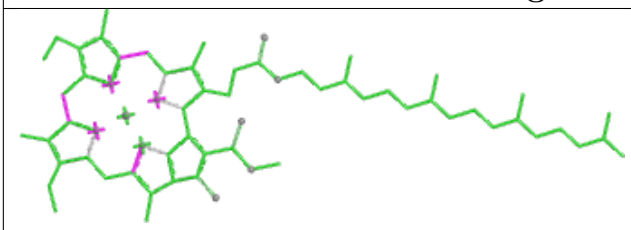

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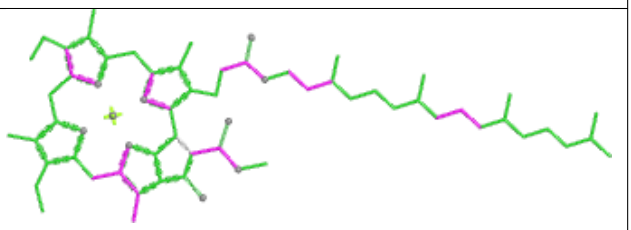

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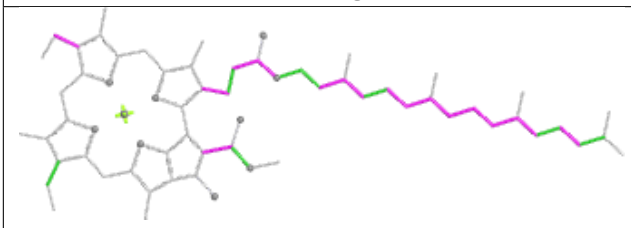

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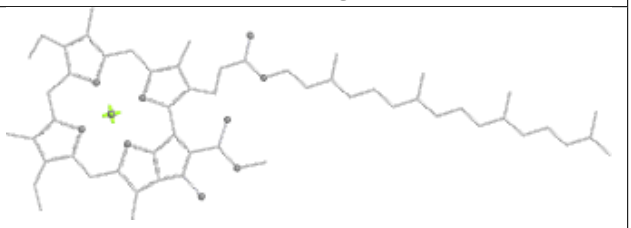

Rings

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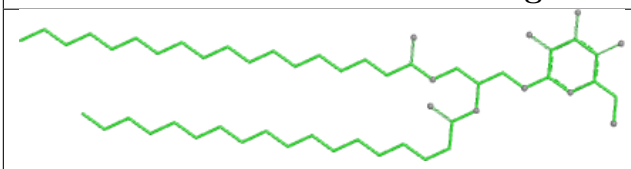

Bond lengths

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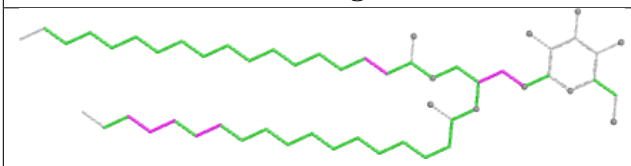

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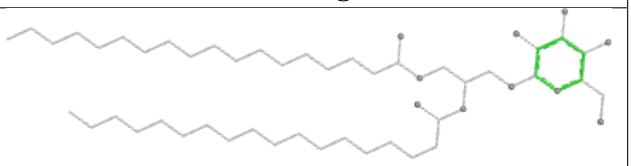
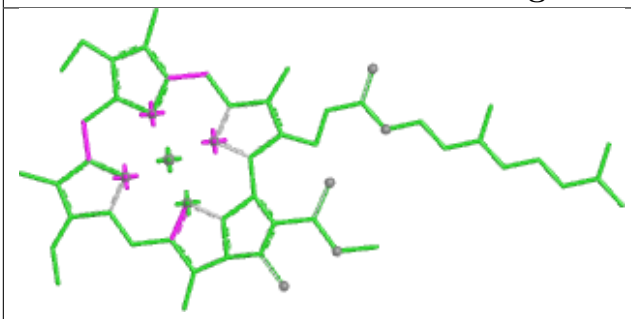
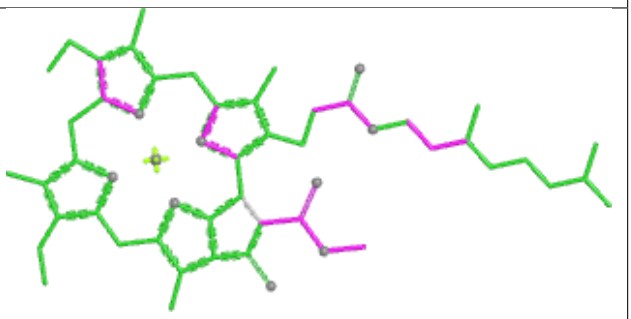
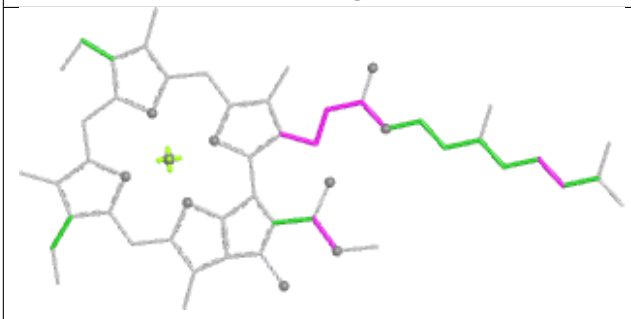
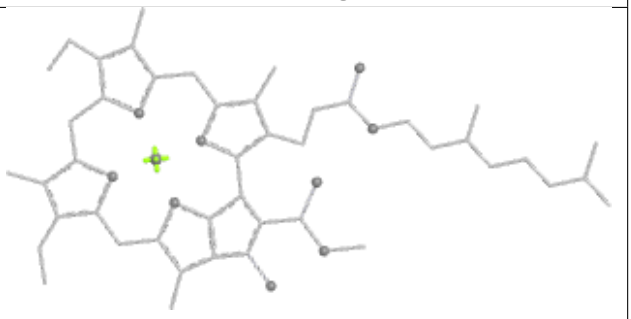


Rings

Ligand CLA 4 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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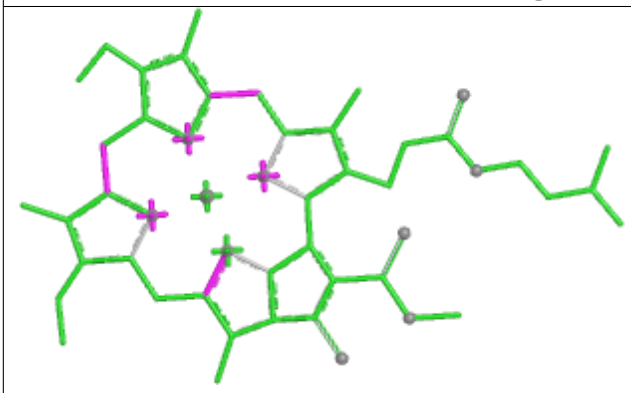
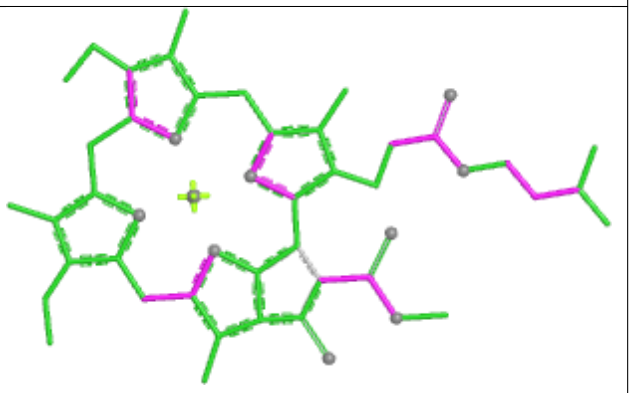
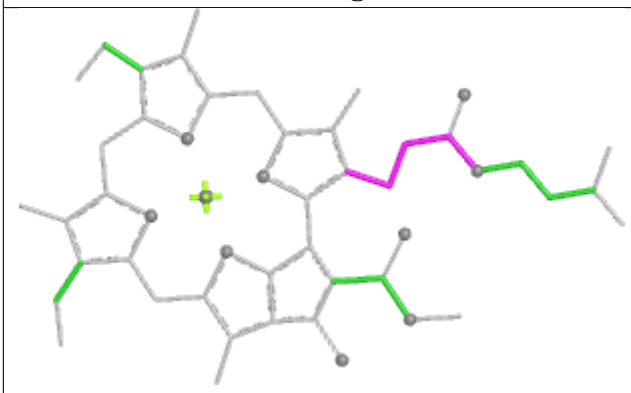
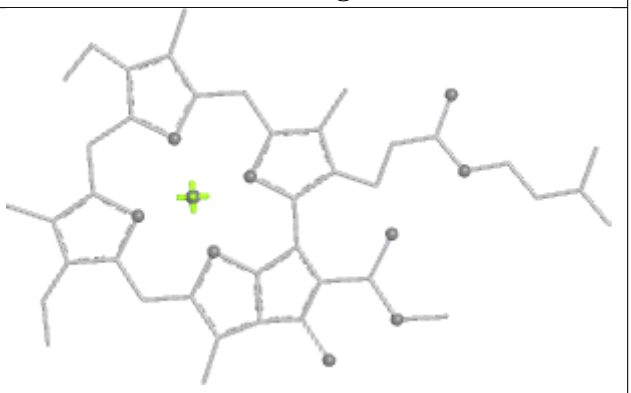
 Bond lengths	 Bond angles
 Torsions	 Rings

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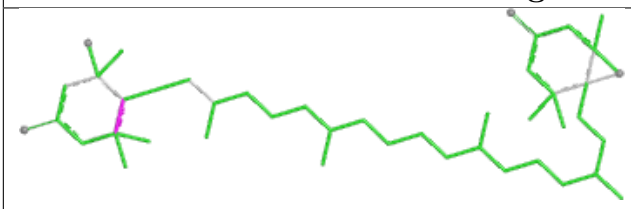
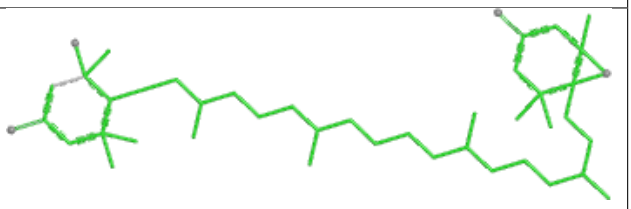
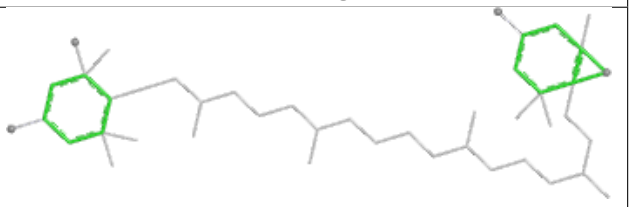
 Bond lengths	 Bond angles
Torsions	 Rings

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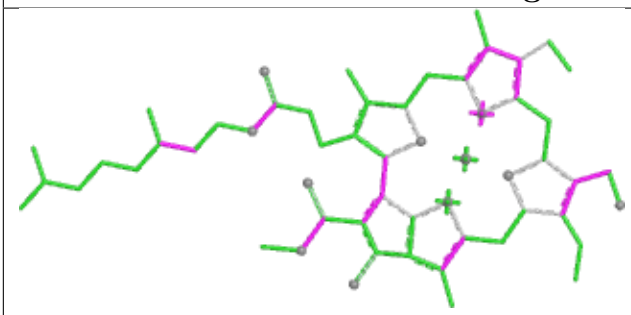
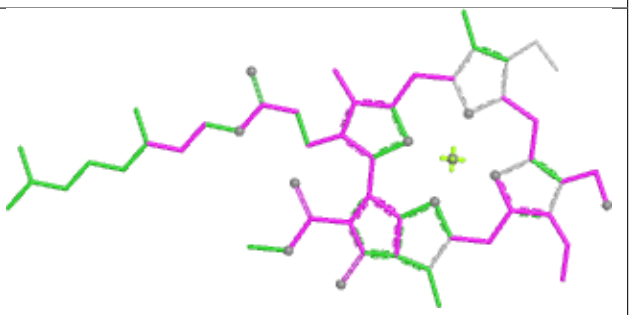
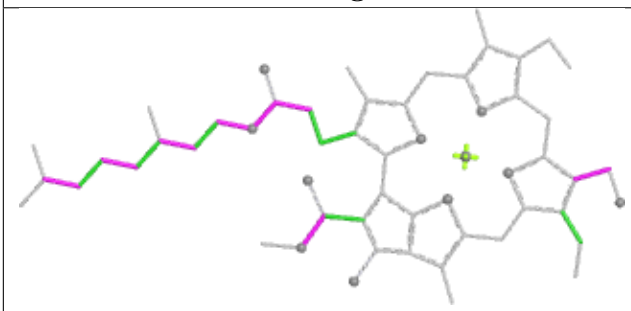
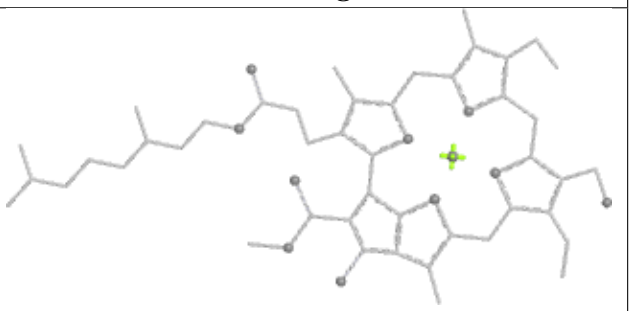
 Bond lengths	 Bond angles
 Torsions	 Rings

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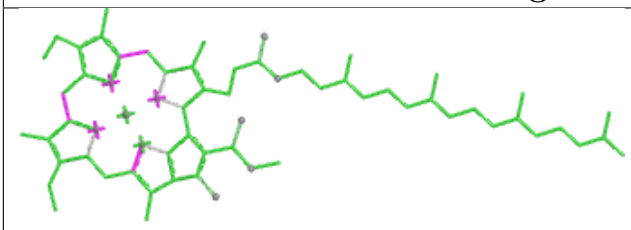
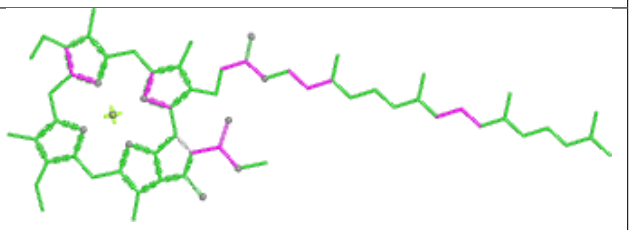
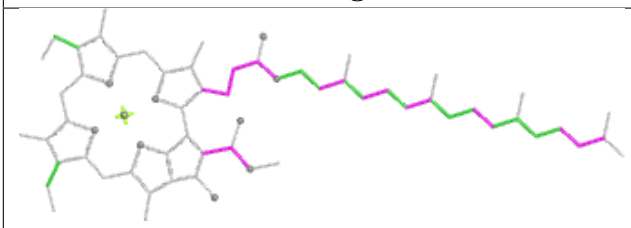
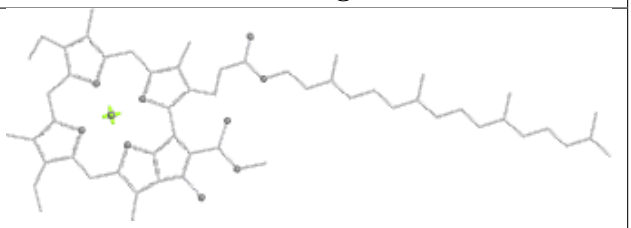
 Bond lengths	 Bond angles
 Torsions	 Rings

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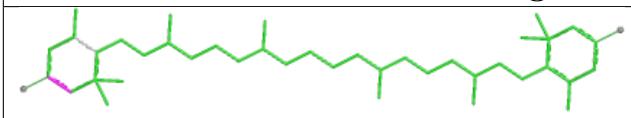
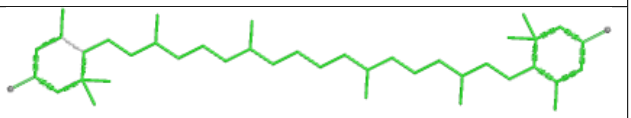
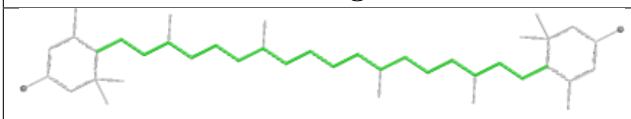
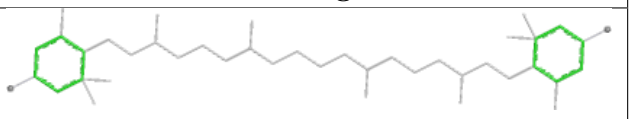
 Bond lengths	 Bond angles
 Torsions	 Rings

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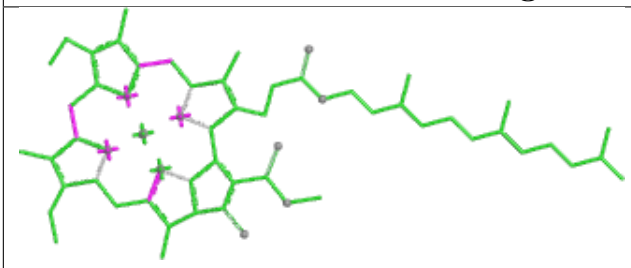
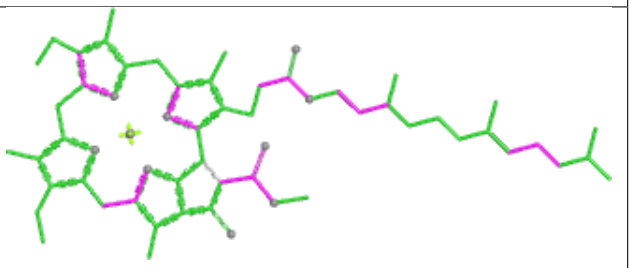
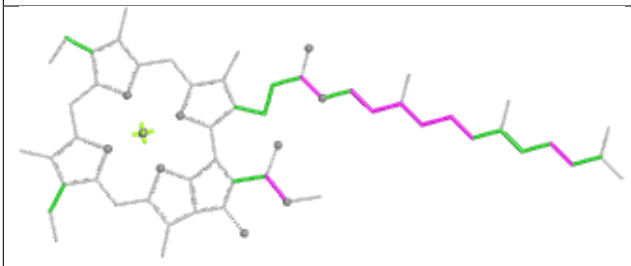
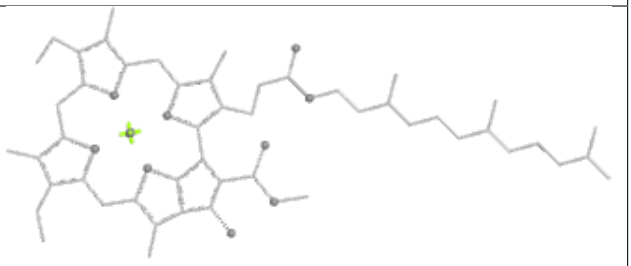
 Bond lengths	 Bond angles
 Torsions	 Rings

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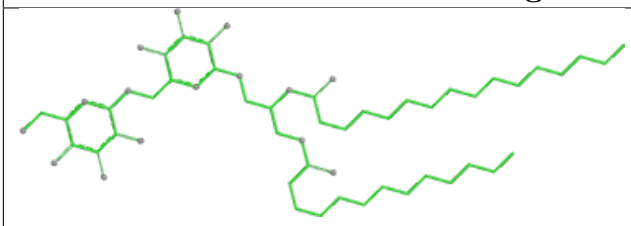
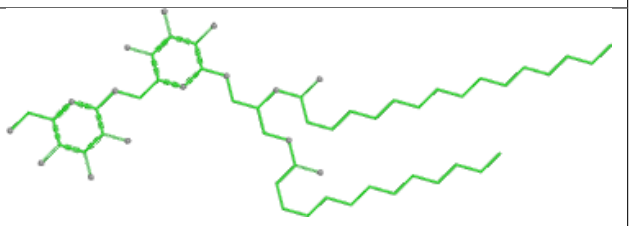
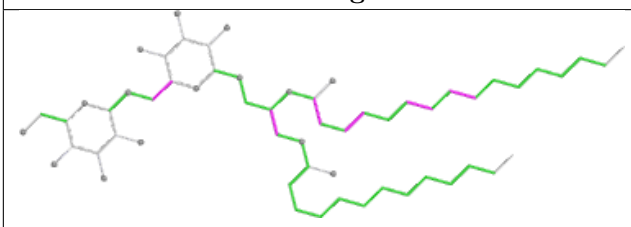
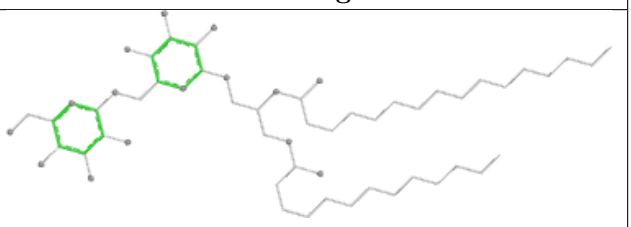
 Bond lengths	 Bond angles
 Torsions	 Rings

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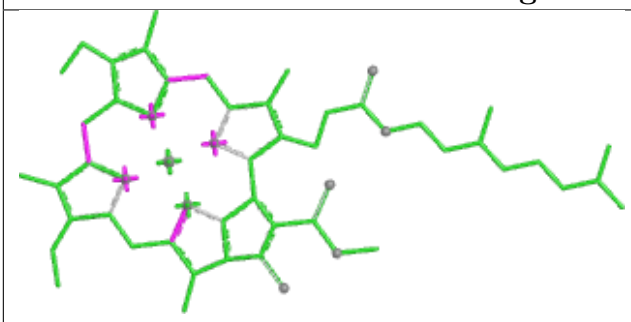
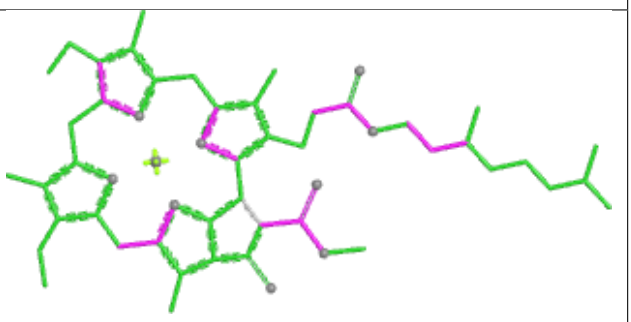
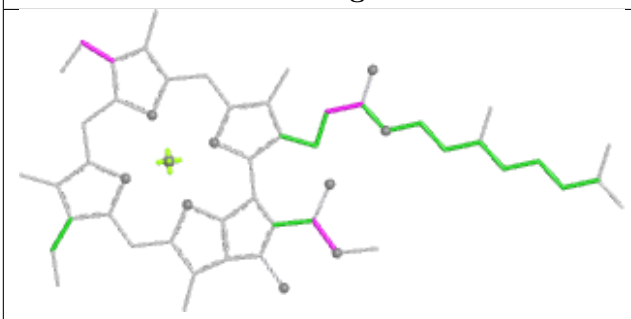
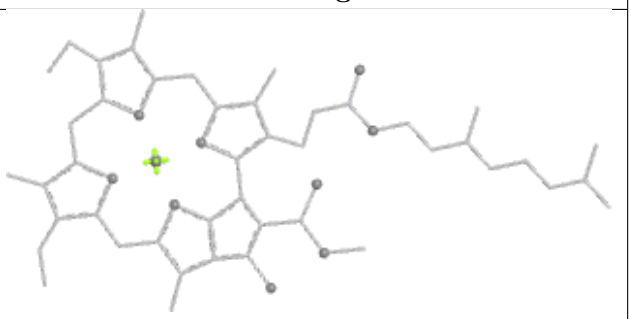
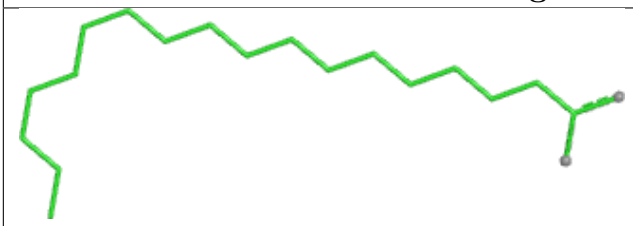
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LNL y 619



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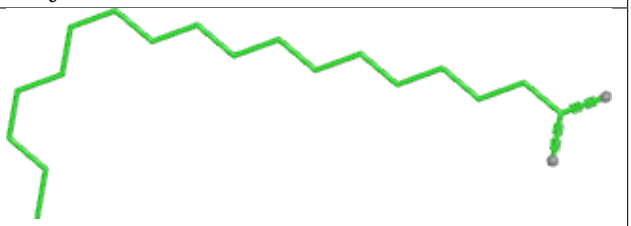
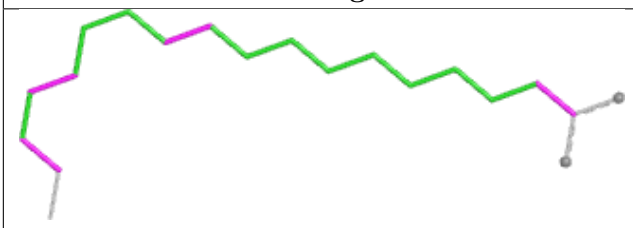


Bond angles



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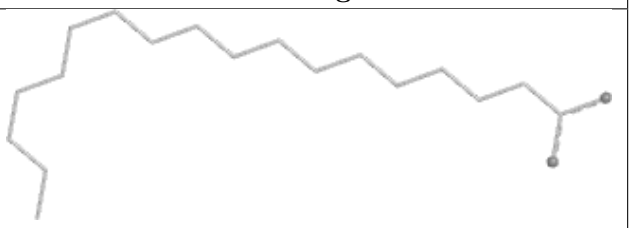
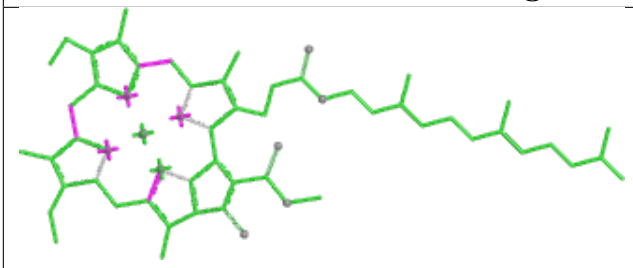


Rings

Ligand CLA R 610



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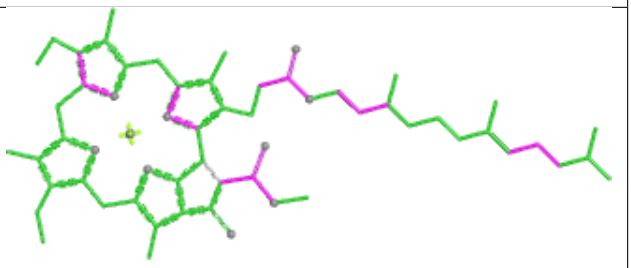
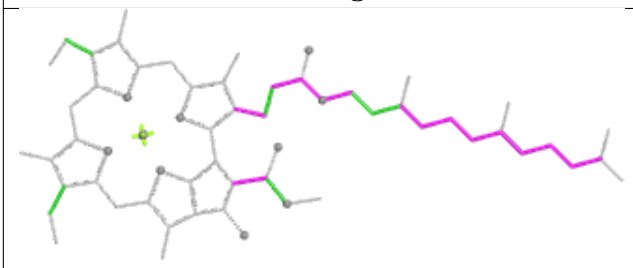


Bond angles



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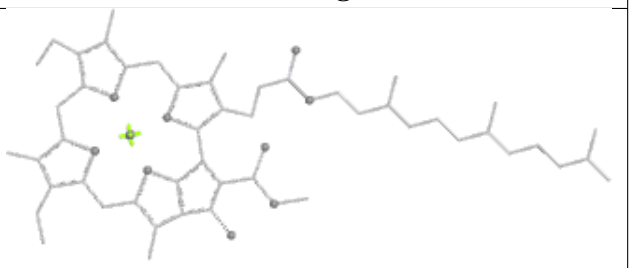

Rings

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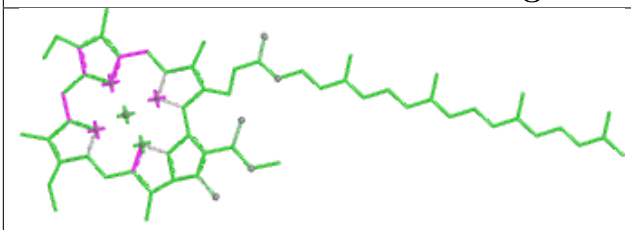
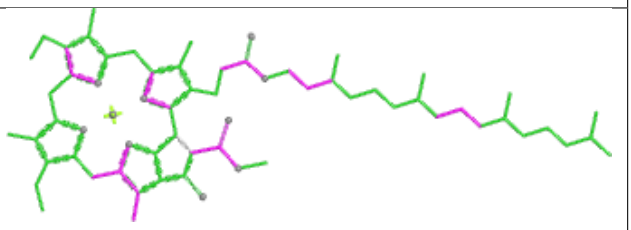
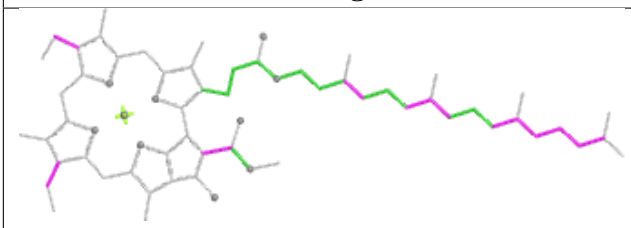
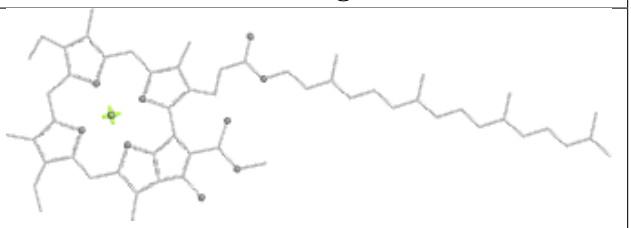
 Bond lengths	 Bond angles
 Torsions	 Rings

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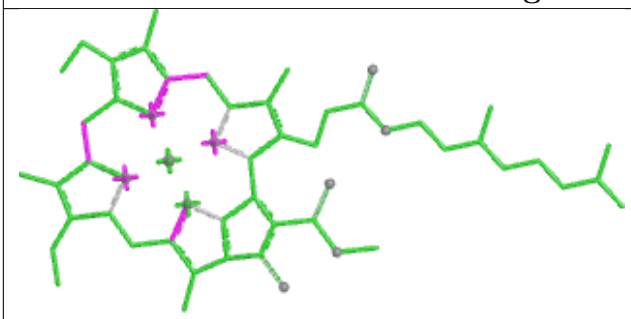
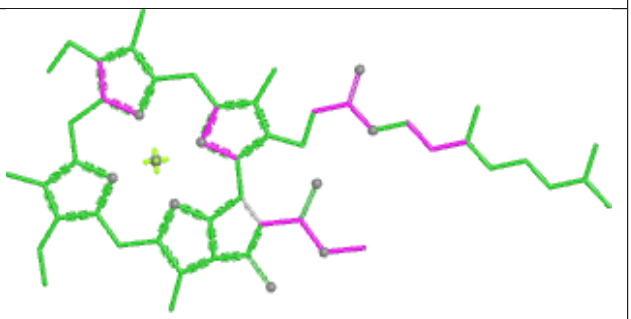
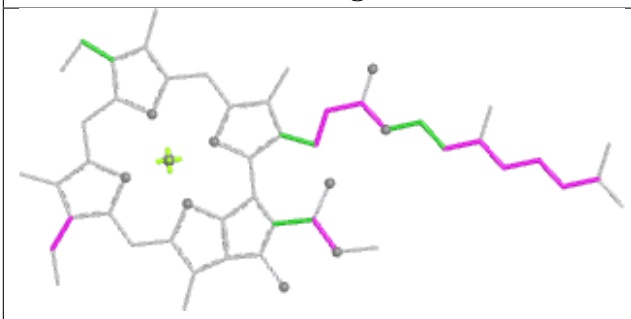
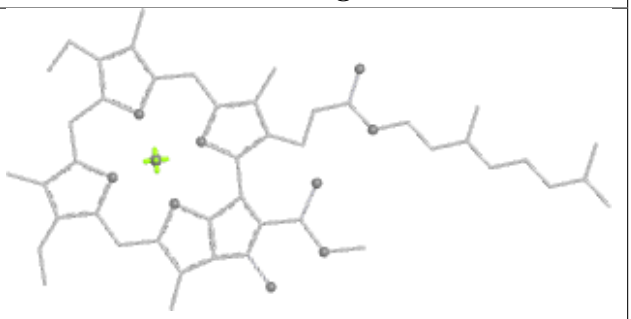
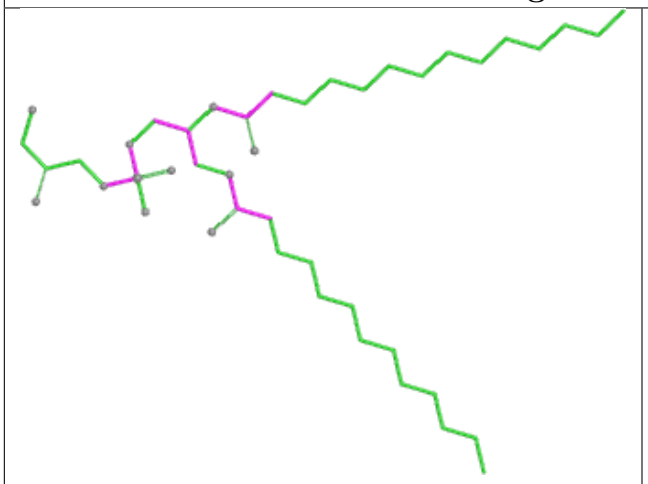
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 6 616



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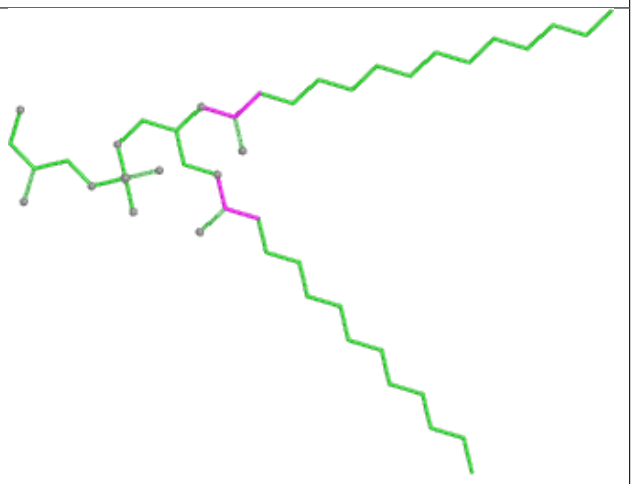

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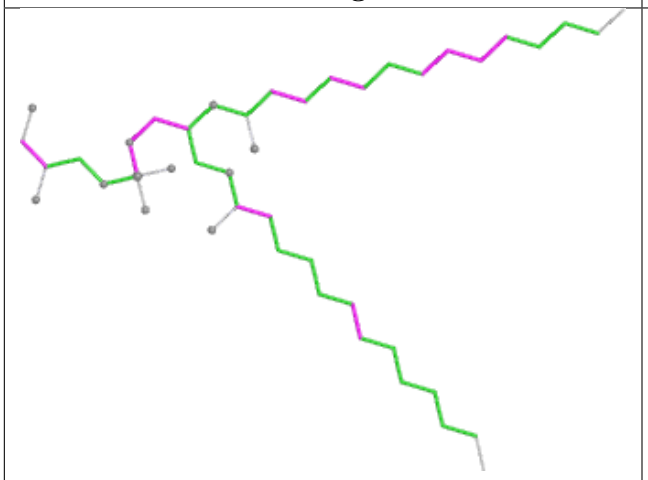

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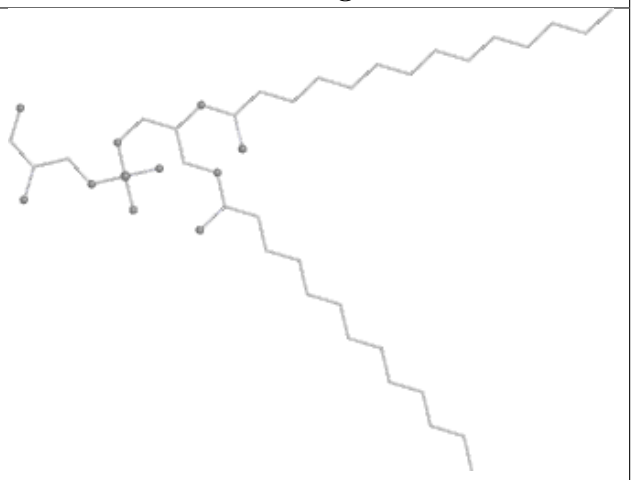
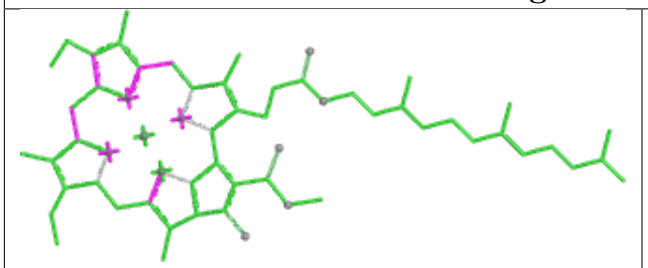


Rings

Ligand CLA 3 602



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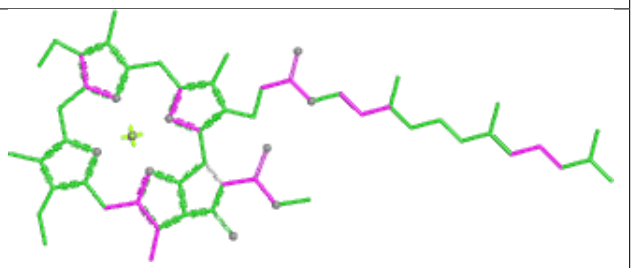
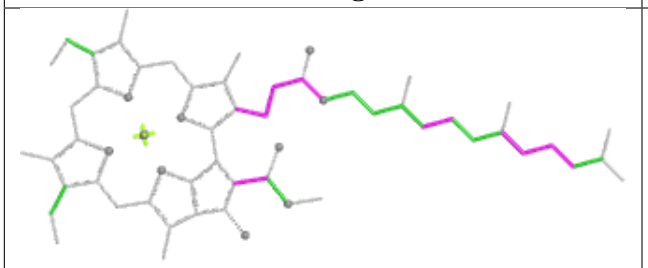


Bond angles



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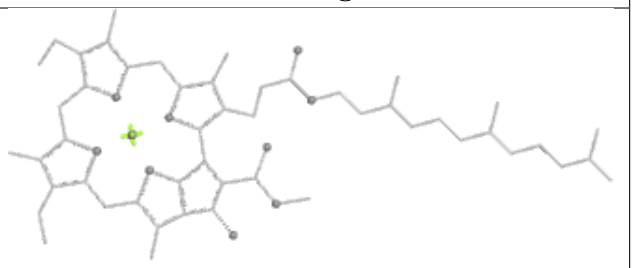

Rings

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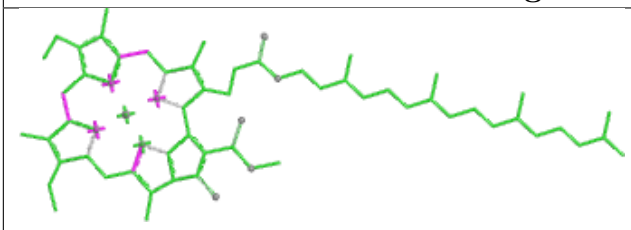

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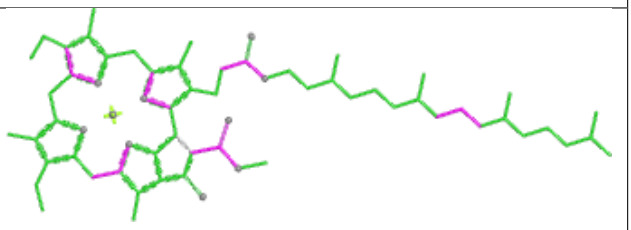
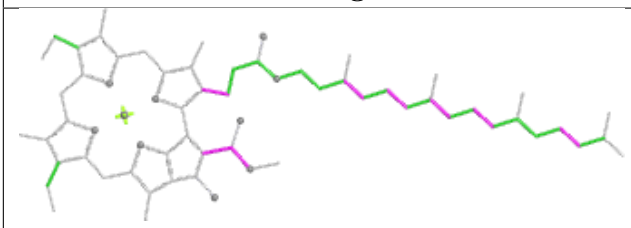


Bond angles



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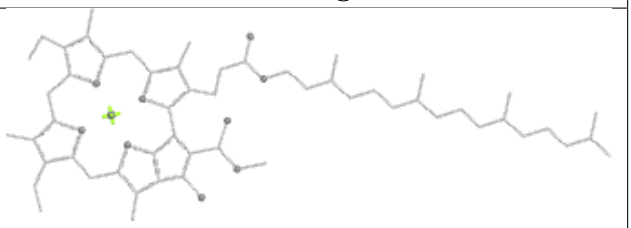
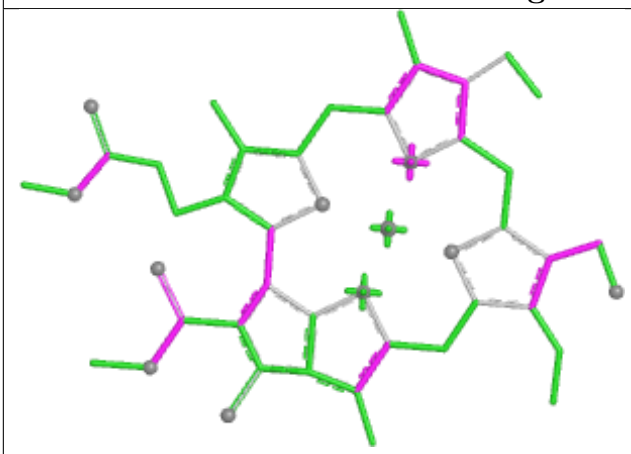


Rings

Ligand CHL 1 606



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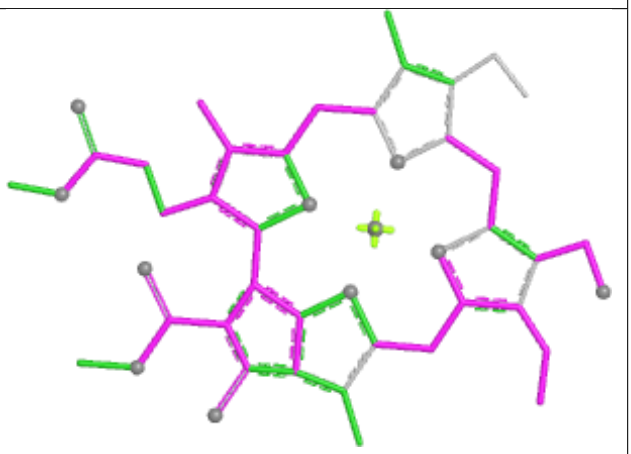
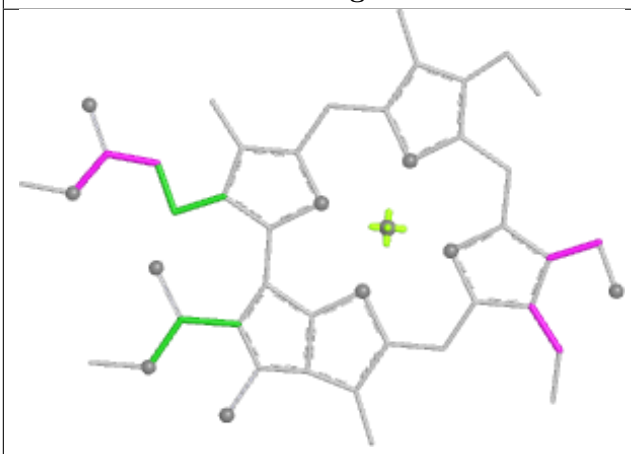


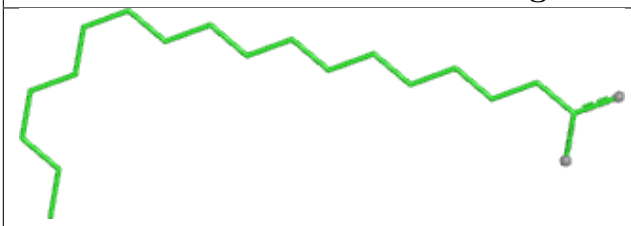
Bond angles



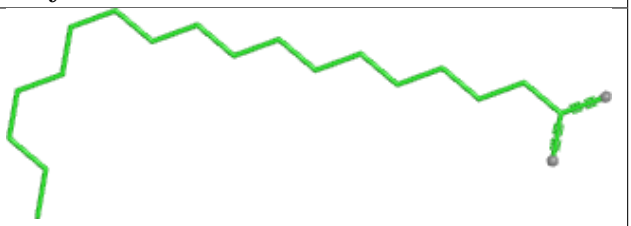
Torsions

Rings

Ligand LNL y 620



Bond lengths



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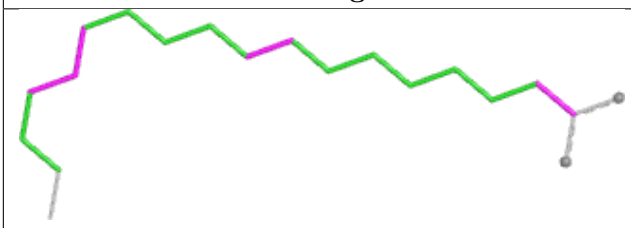
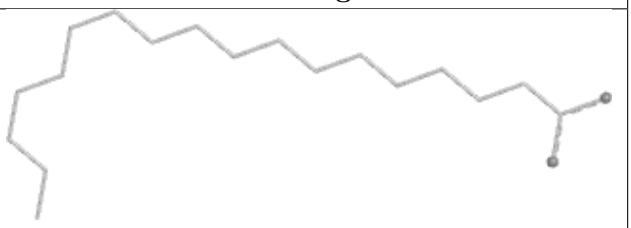
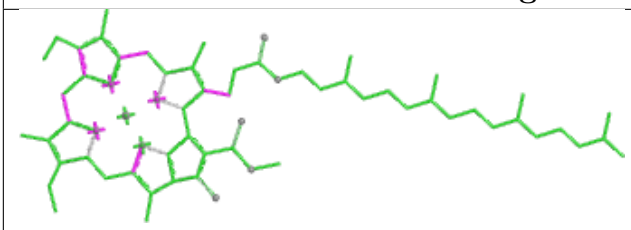


Torsions



Rings

Ligand CLA 16 602



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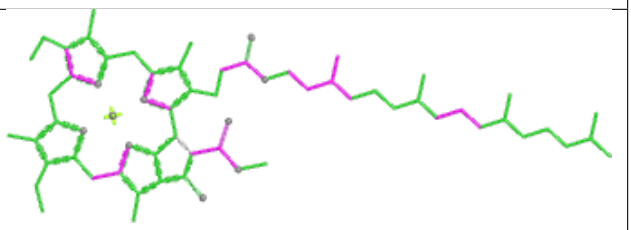

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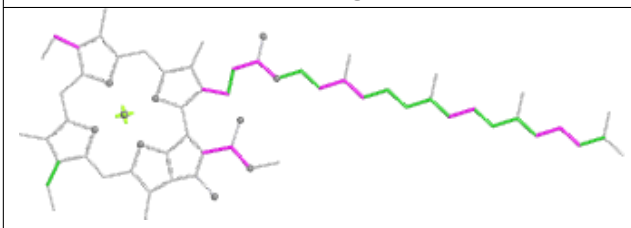

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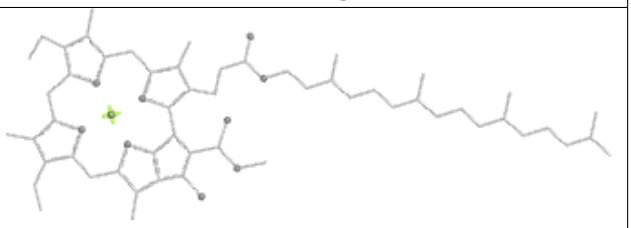
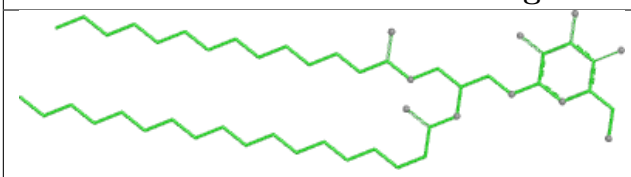


Rings

Ligand LMG J 102



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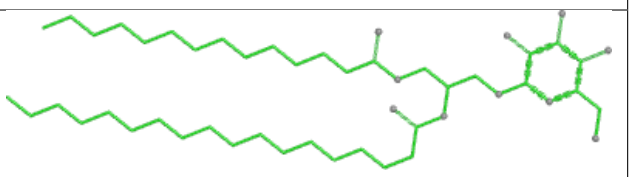

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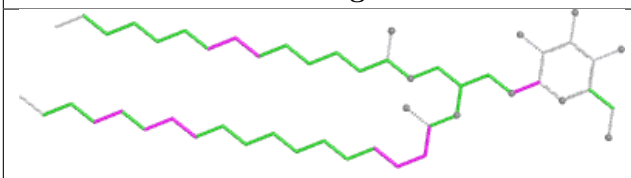

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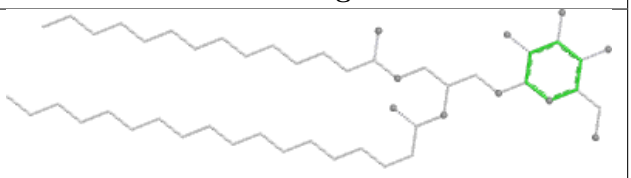
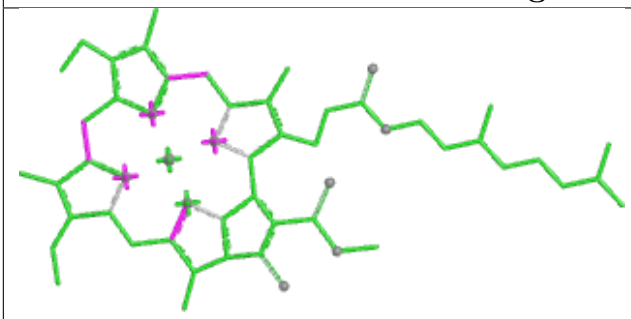
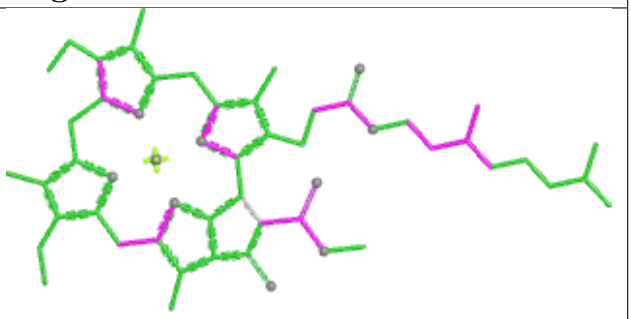
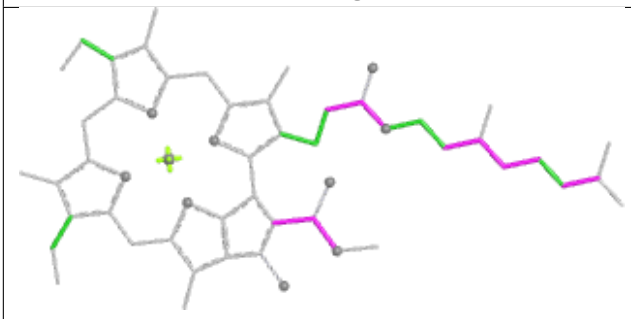
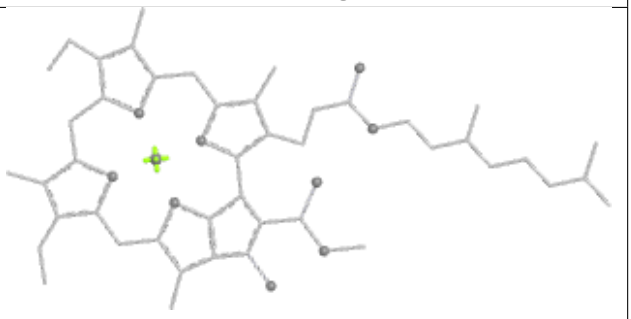
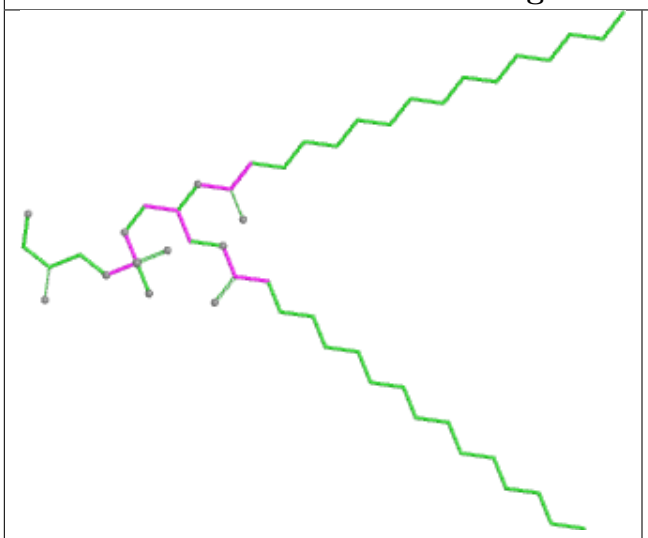


Rings

Ligand CLA g 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG d 413



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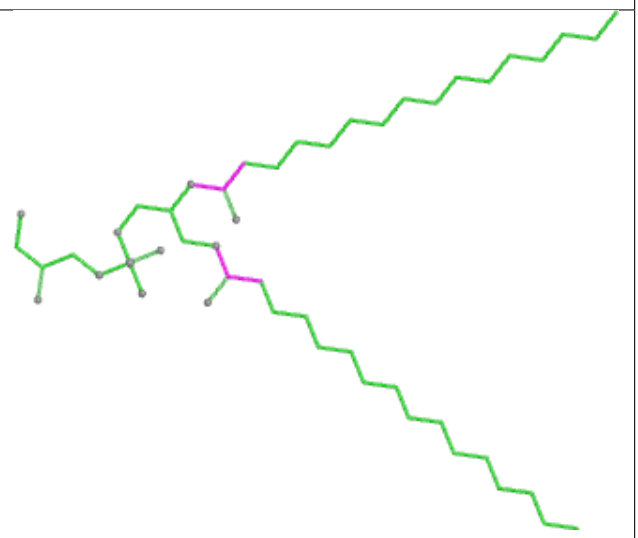
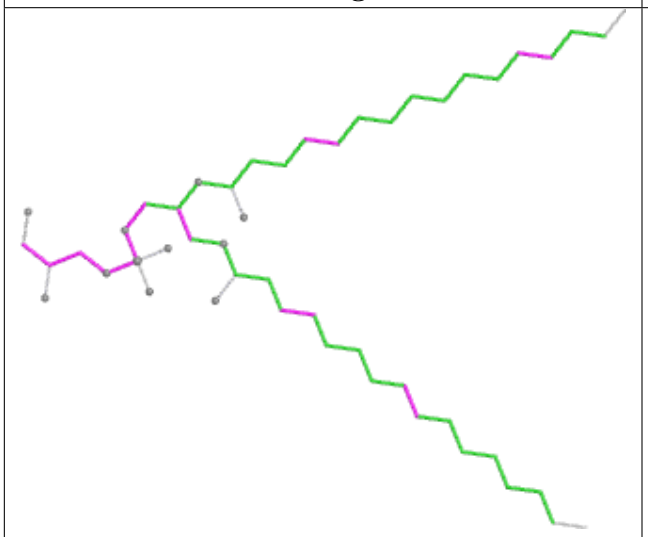


Bond angles



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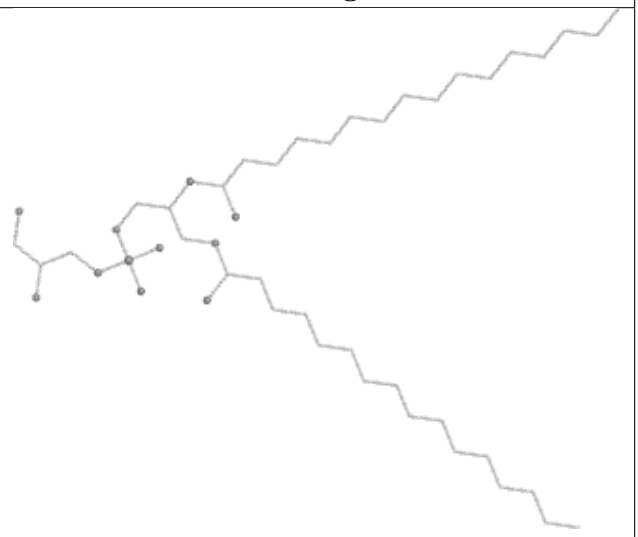
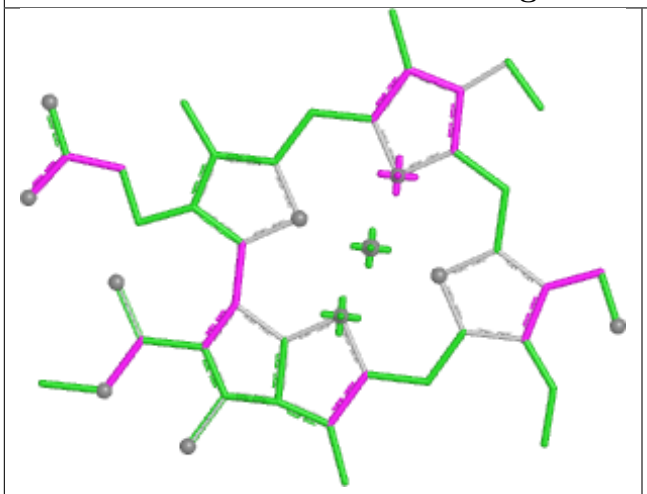


Rings

Ligand CHL 15 605



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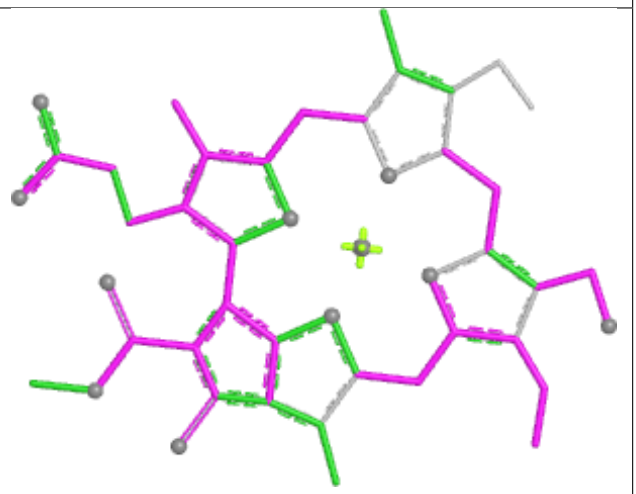

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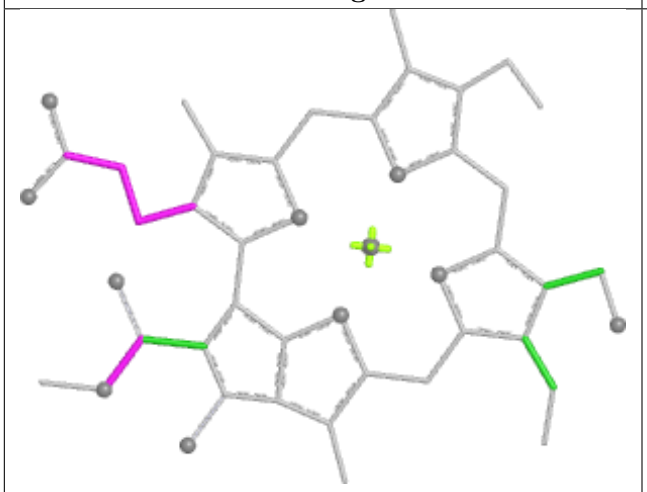

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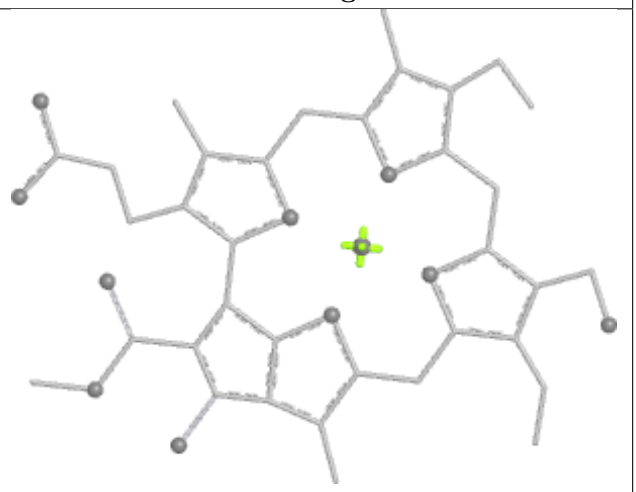
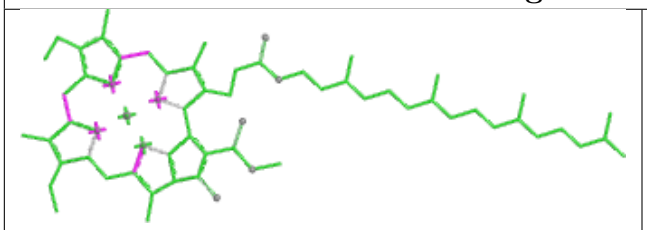


Rings

Ligand CLA B 606



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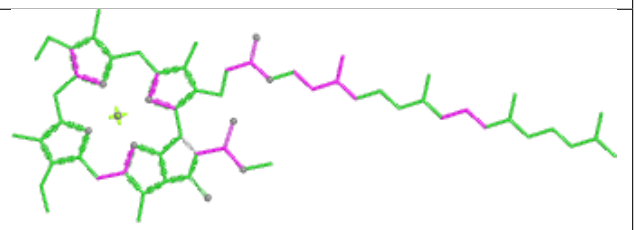

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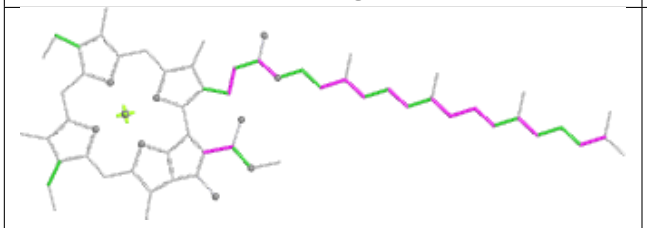

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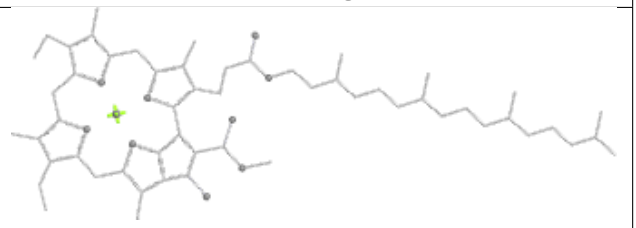
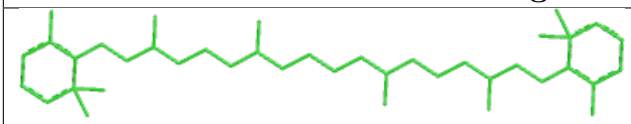


Rings

Ligand BCR j 101



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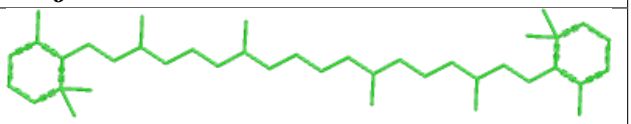

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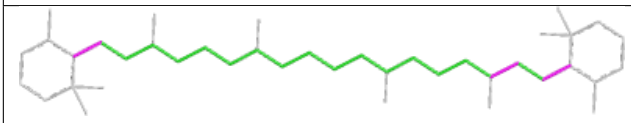

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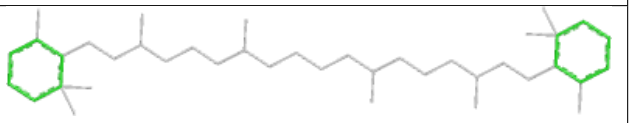
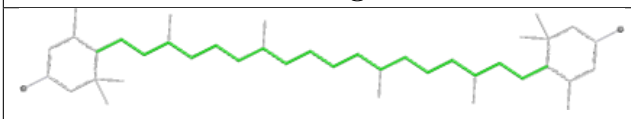


Rings

Ligand LUT 11 616

Bond lengths

Bond angles



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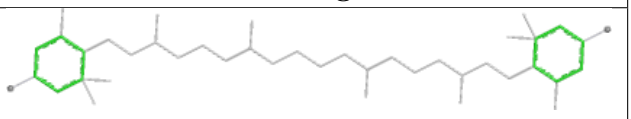
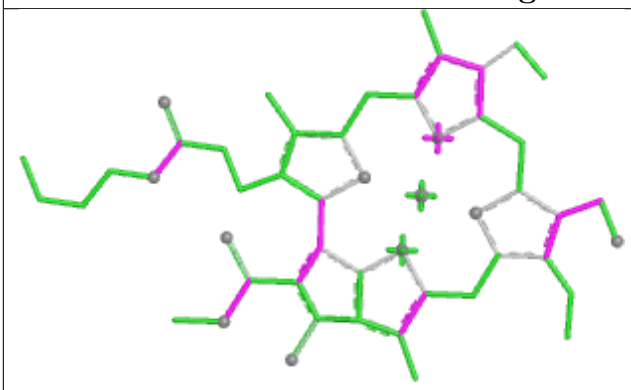


Rings

Ligand CHL 16 608



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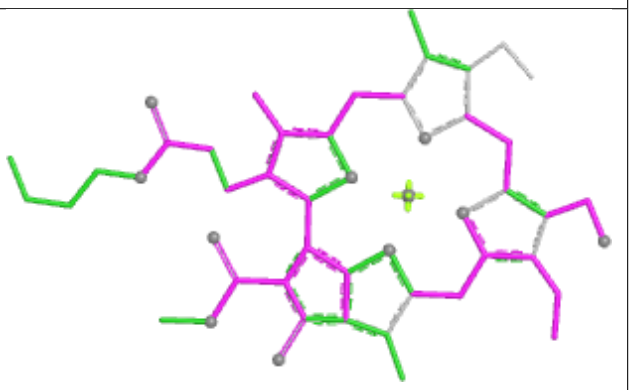
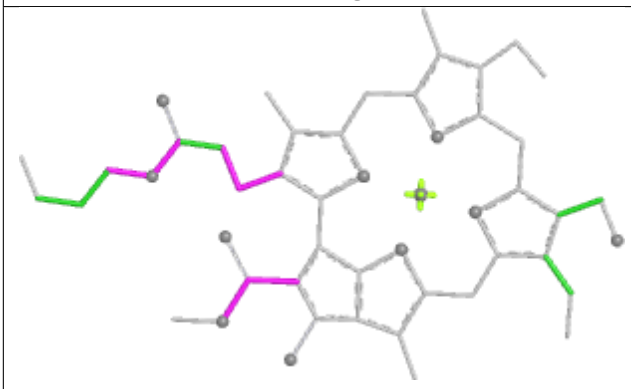


Bond angles



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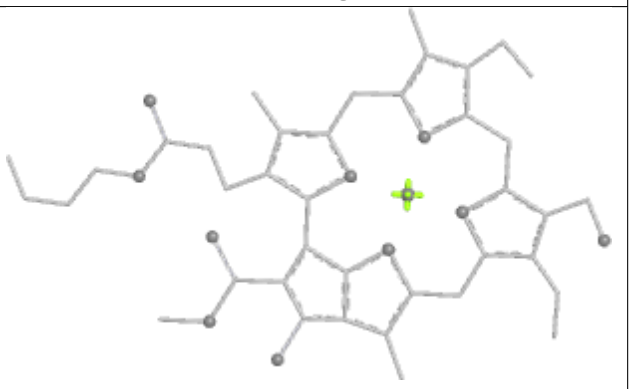
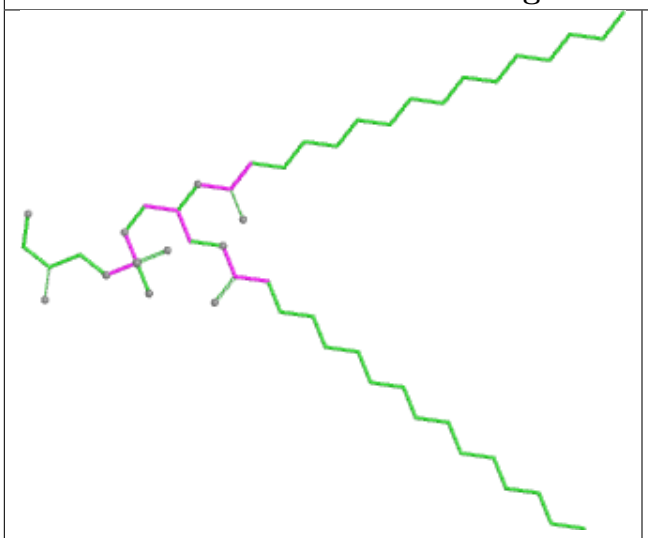


Rings

Ligand LHG A 415



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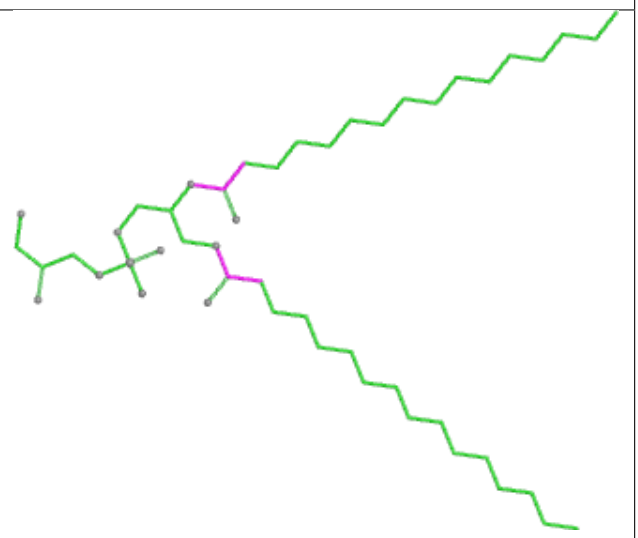

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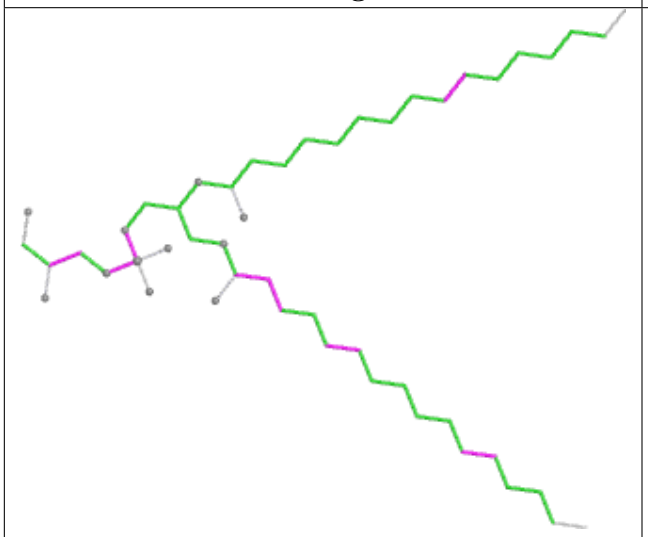

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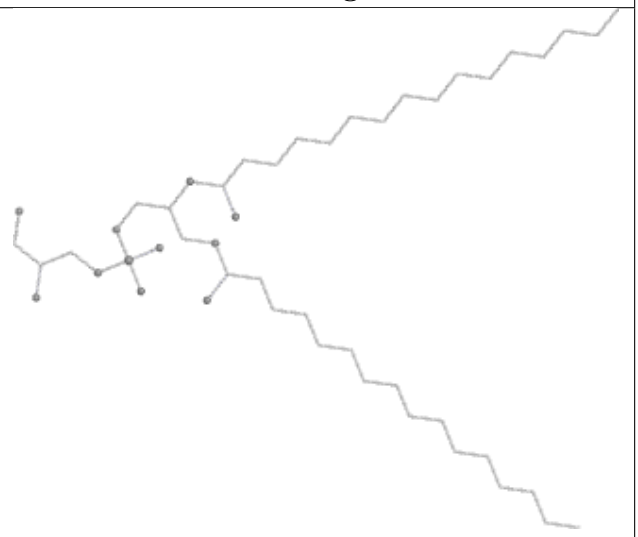
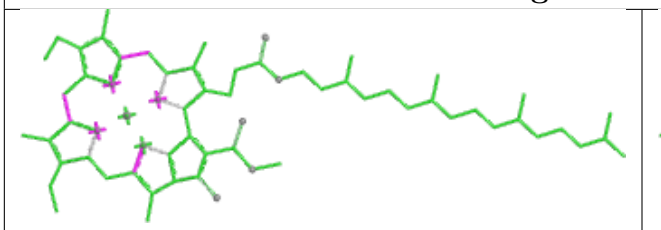


Rings

Ligand CLA s 614



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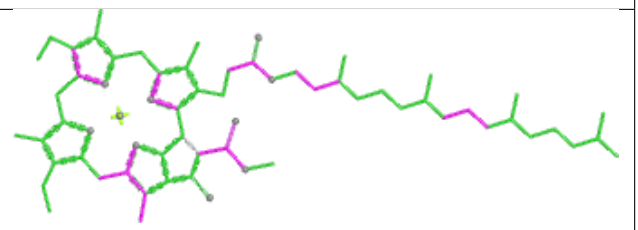
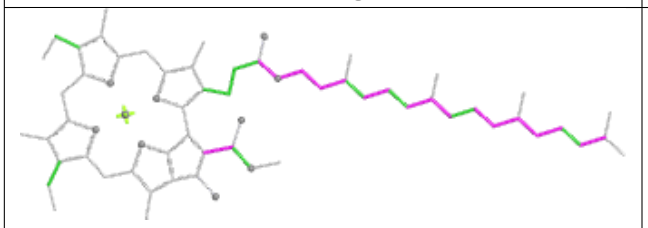


Bond angles



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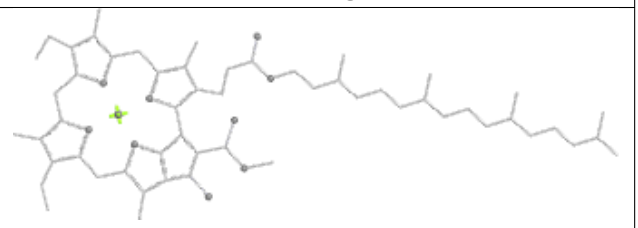
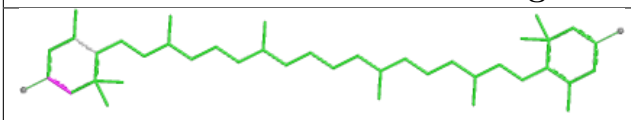


Rings

Ligand LUT 4 616



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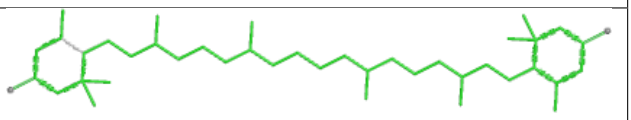
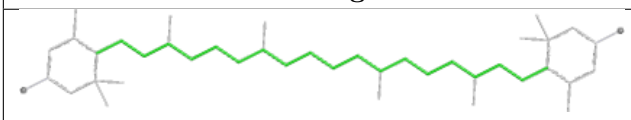


Bond angles



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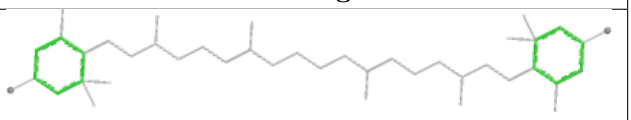
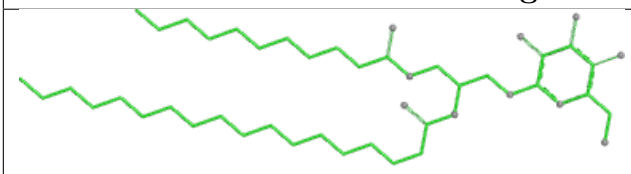


Rings

Ligand LMG B 622



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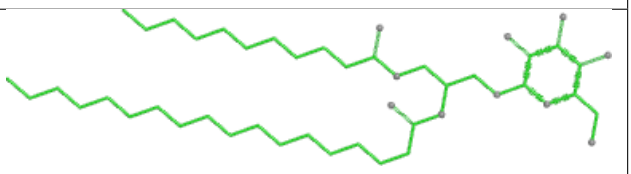
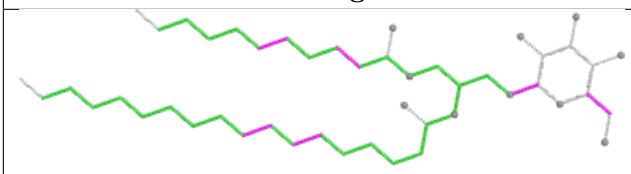


Bond angles



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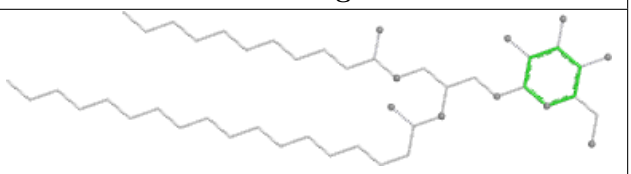
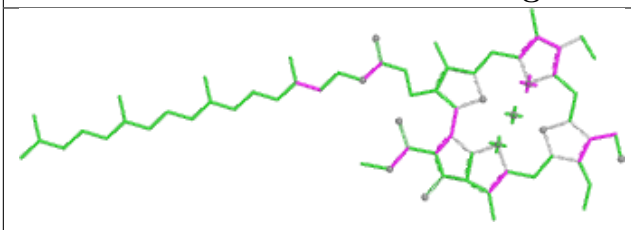
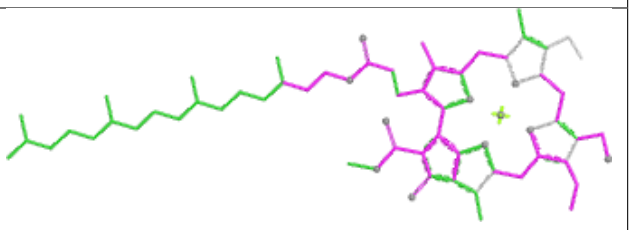


Rings

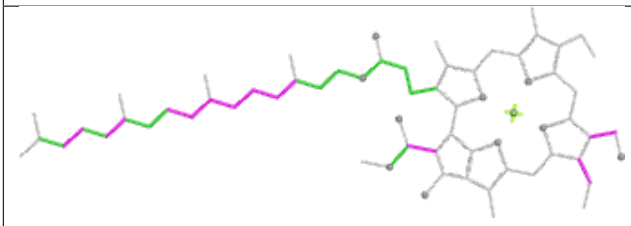
Ligand CHL G 609



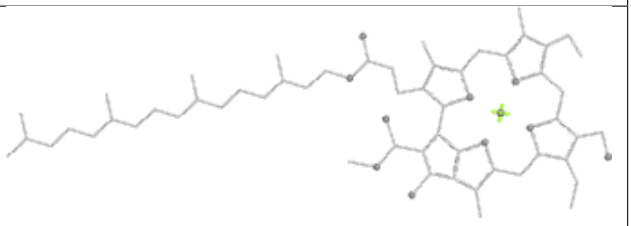
Bond lengths



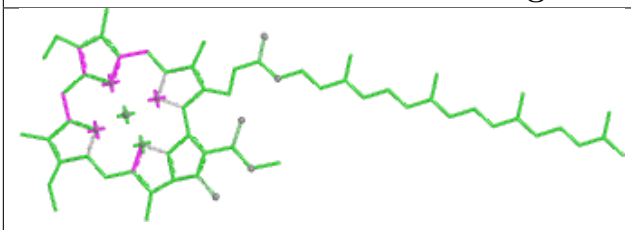
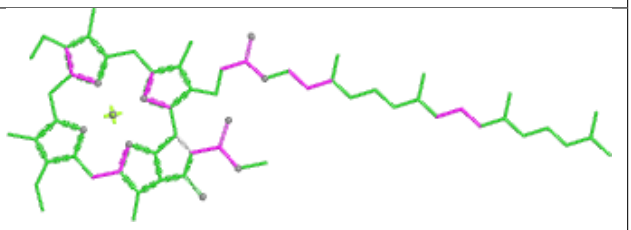
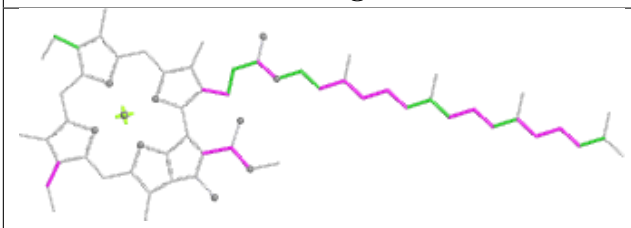
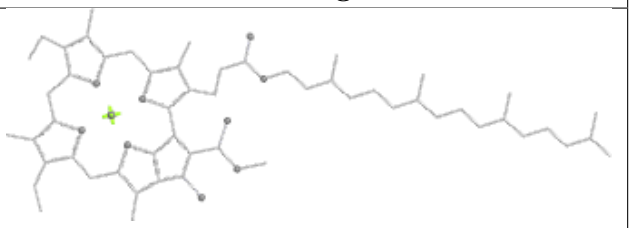
Bond angles

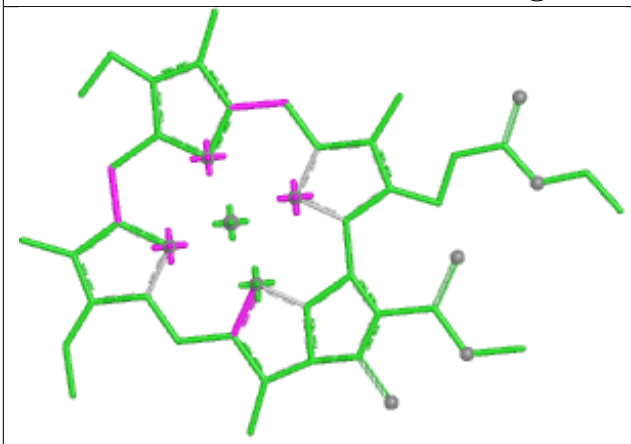
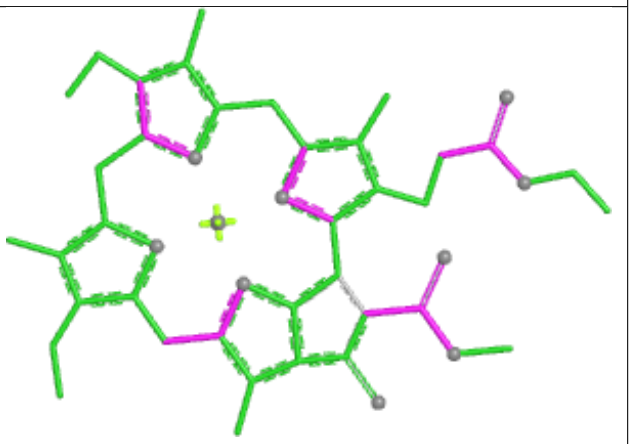
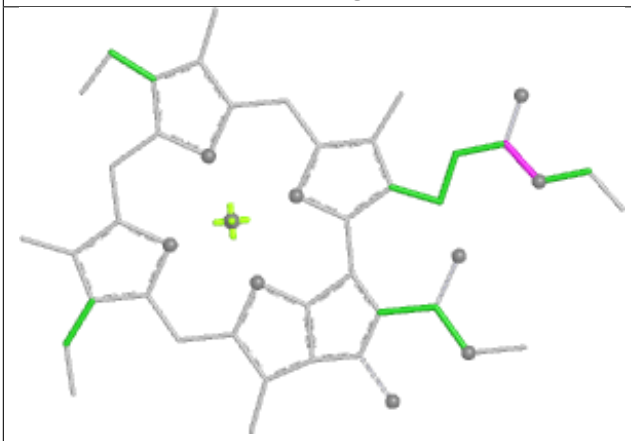
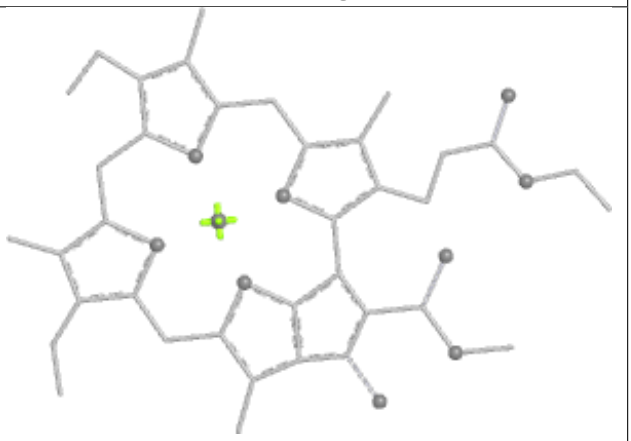


Torsions

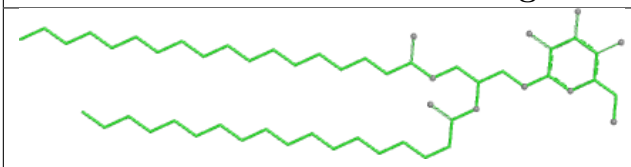


Rings

Ligand CLA n 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG A 409



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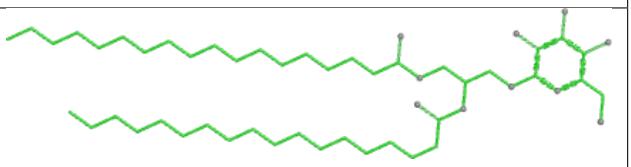
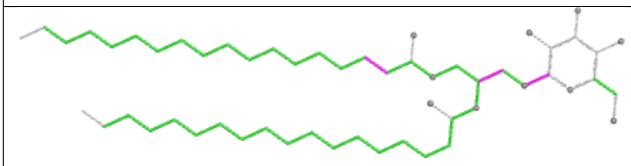


Bond angles



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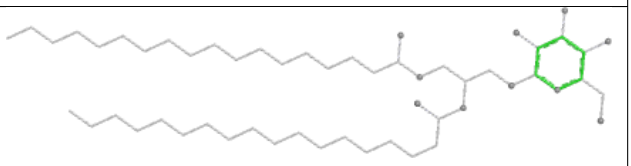
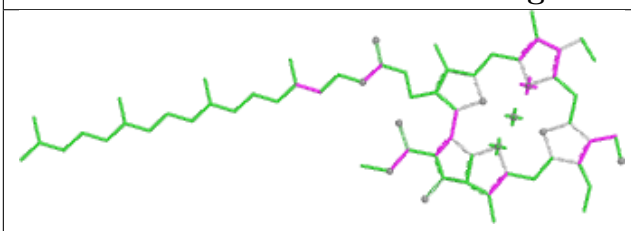


Rings

Ligand CHL y 609



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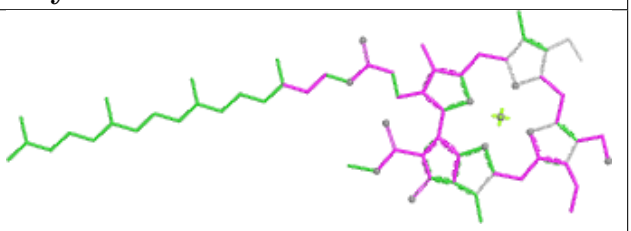
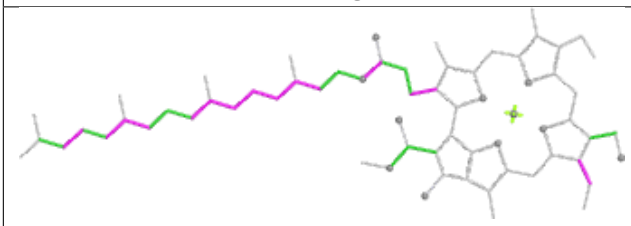


Bond angles



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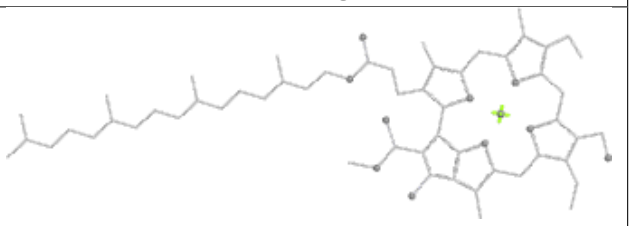
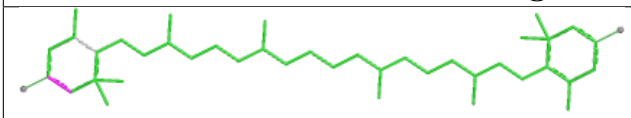


Rings

Ligand LUT 1 617



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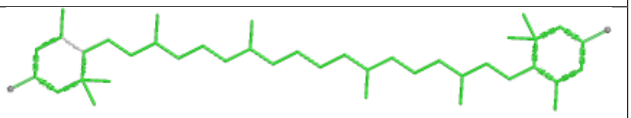
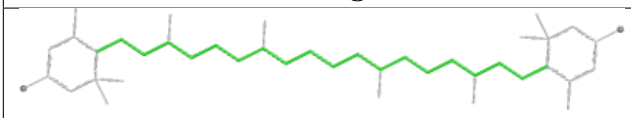


Bond angles



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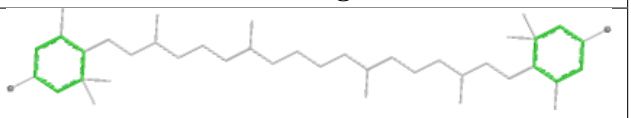
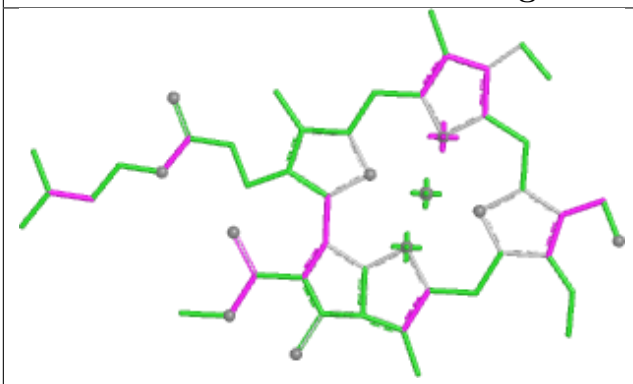


Rings

Ligand CHL 11 608



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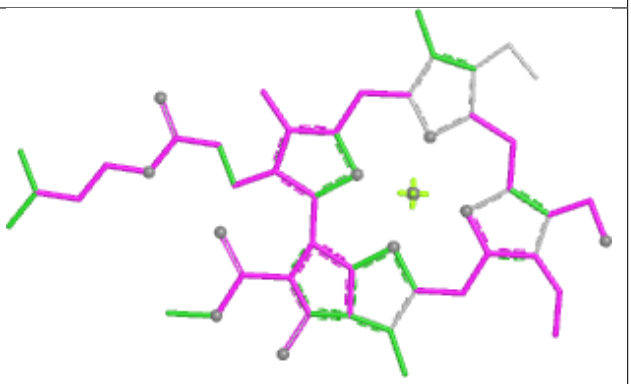
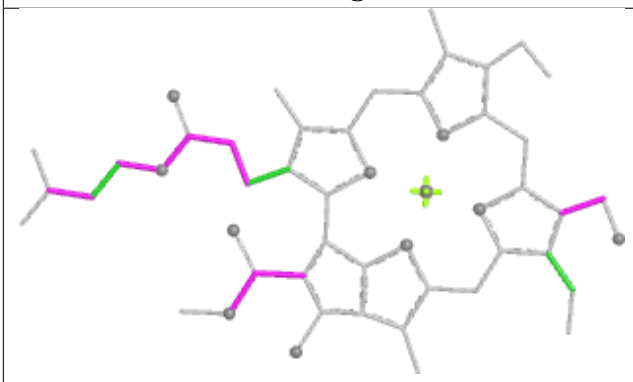


Bond angles



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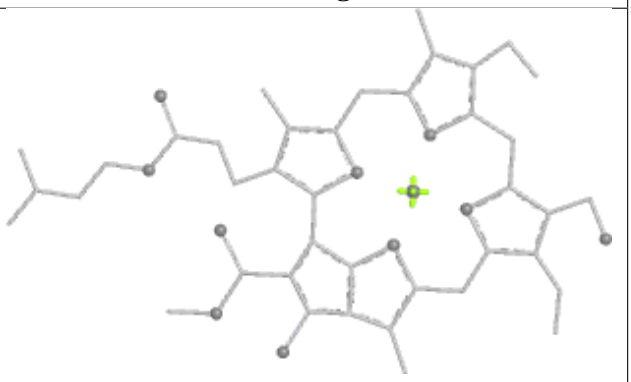
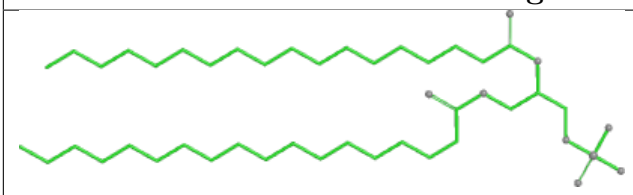


Rings

Ligand 3PH B 620



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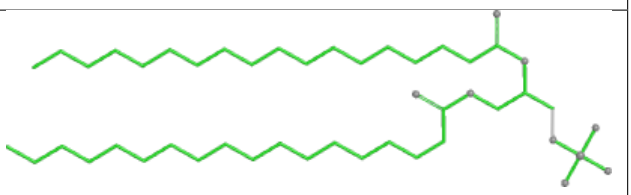
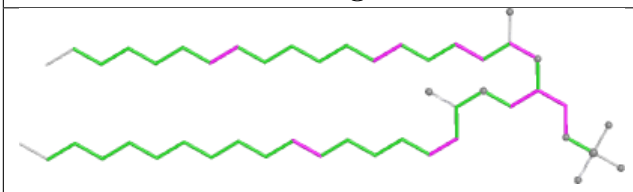


Bond angles



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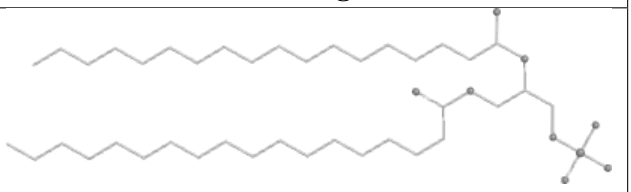
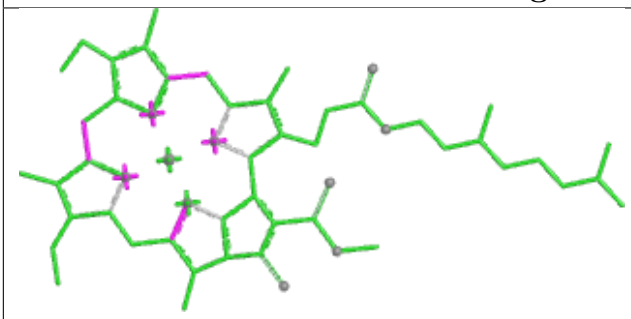


Rings

Ligand CLA r 614



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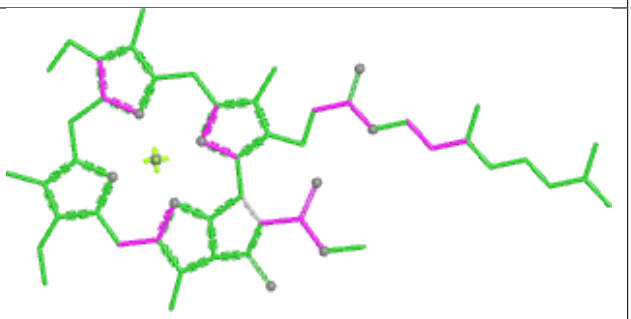
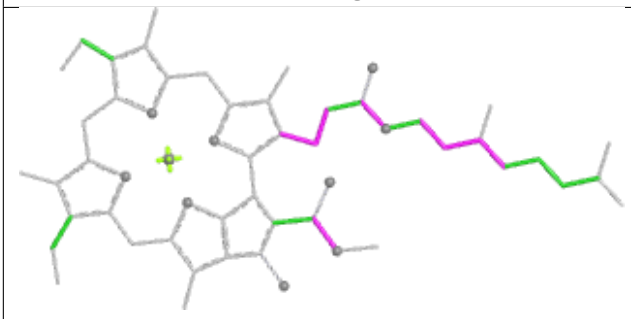


Bond angles



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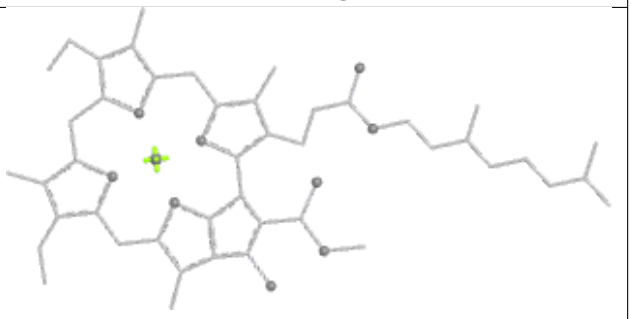
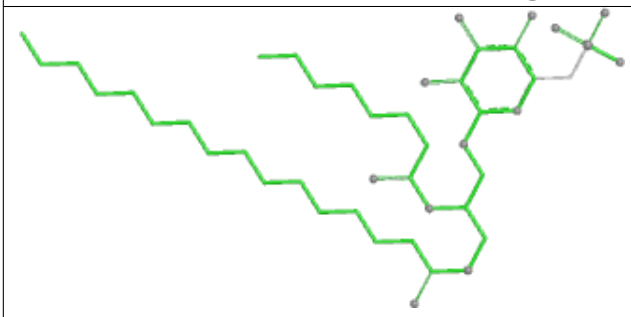


Rings

Ligand SQD D 413



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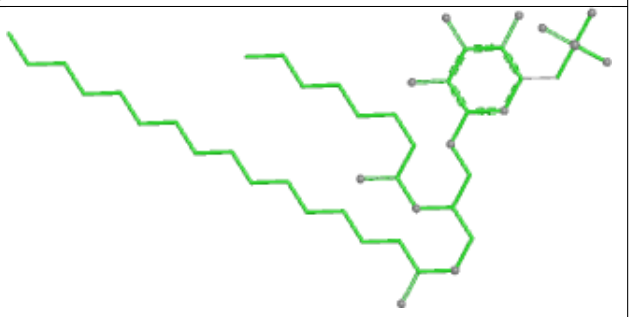

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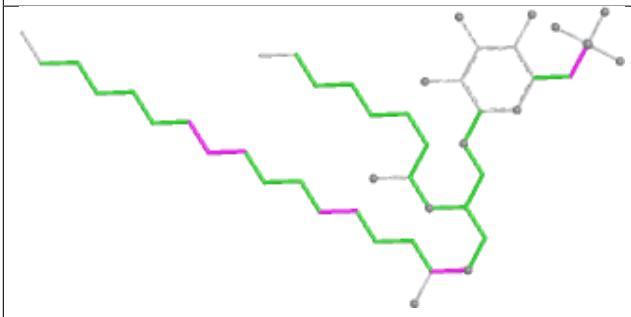

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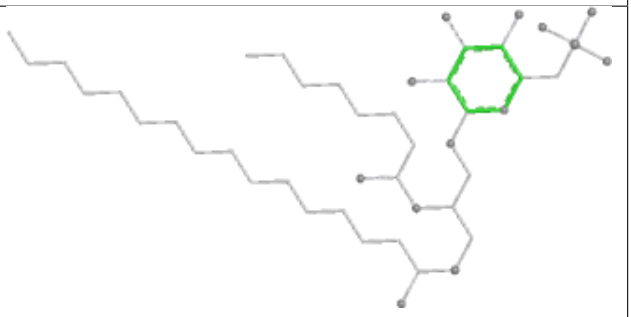
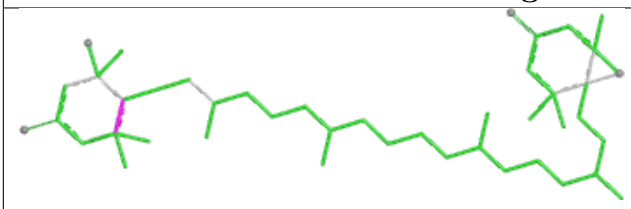
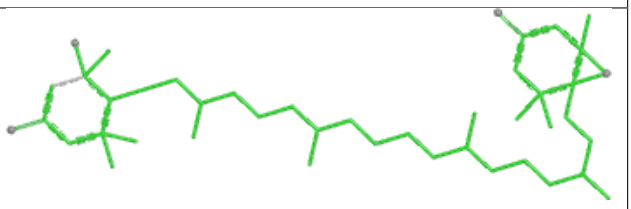
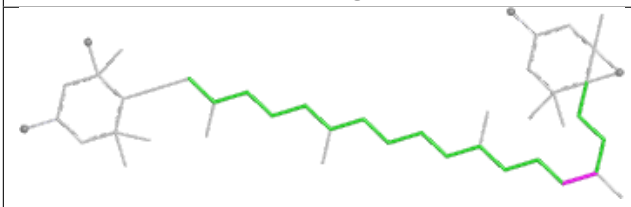
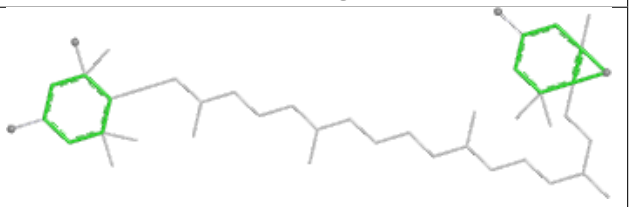
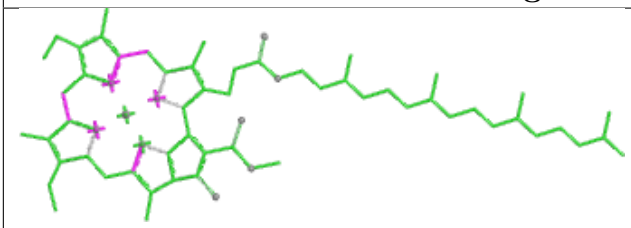
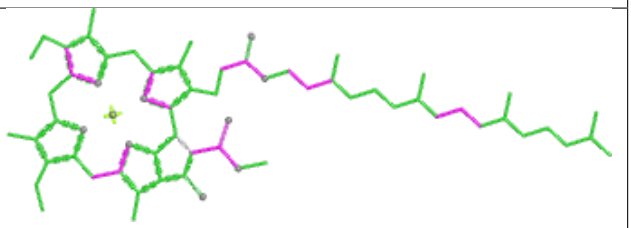
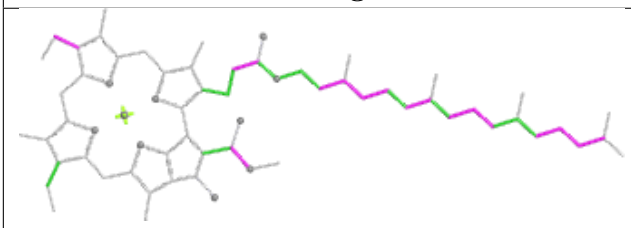
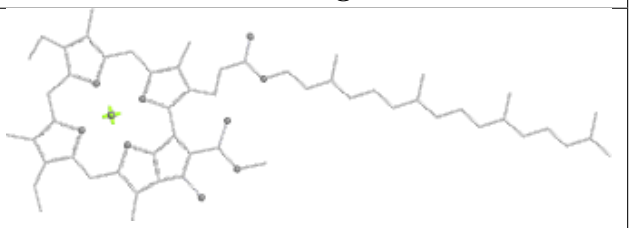
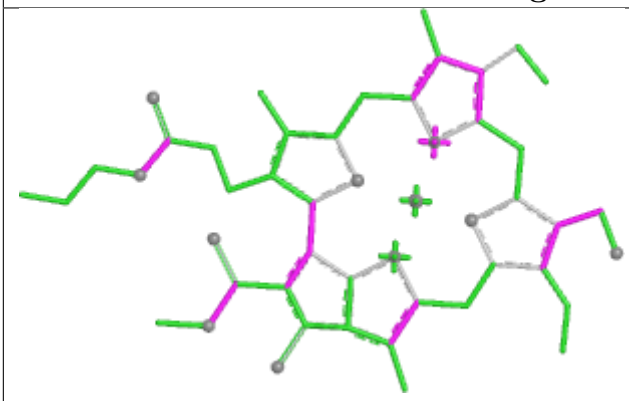
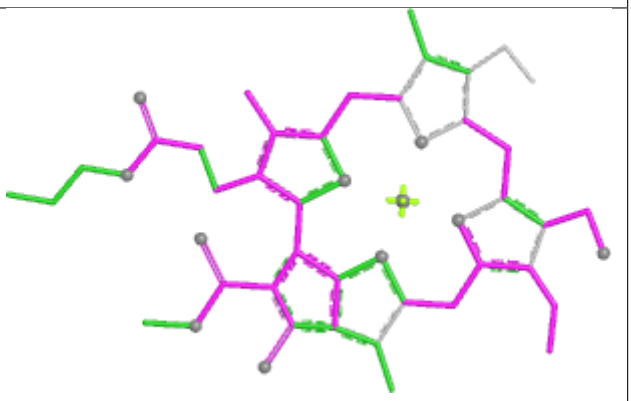
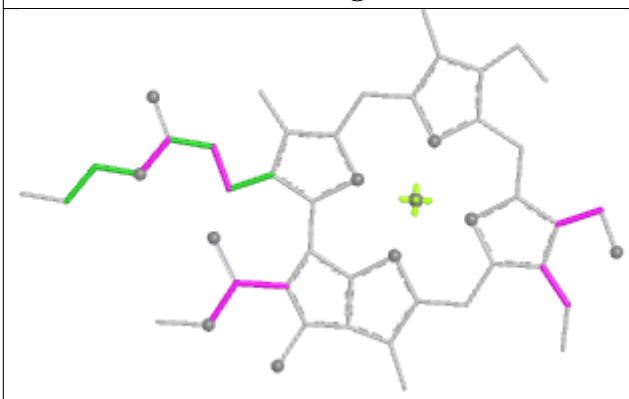


Rings

Ligand NEX N 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL s 608	
 Bond lengths	 Bond angles
 Torsions	Rings

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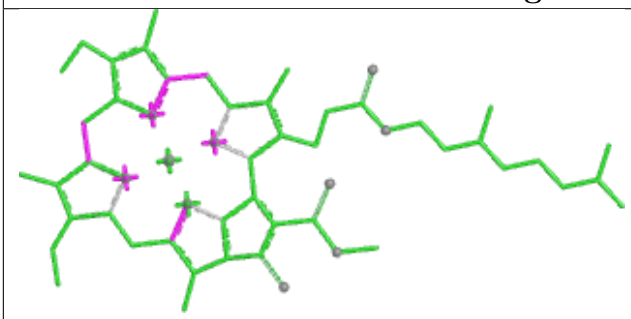
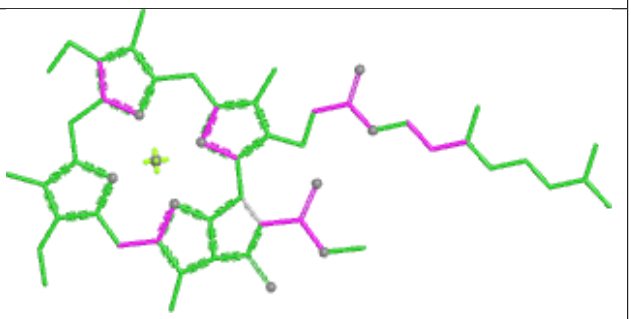
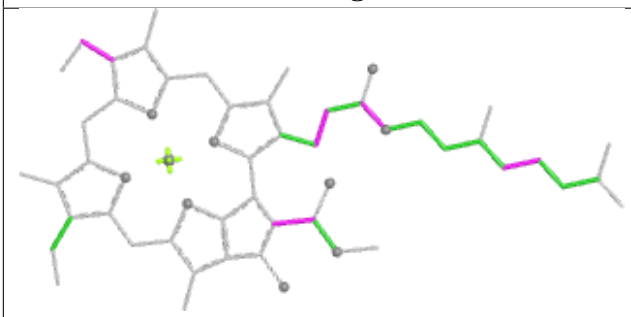
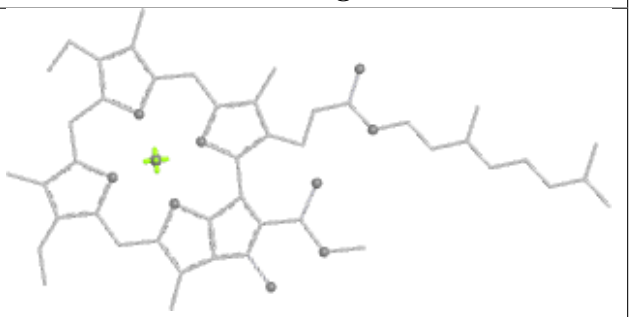
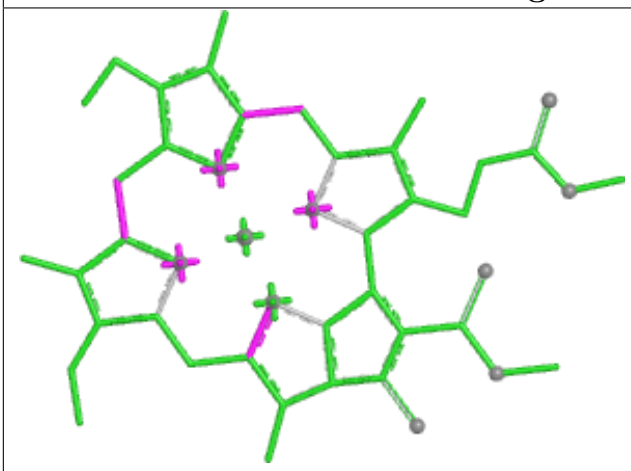
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 612



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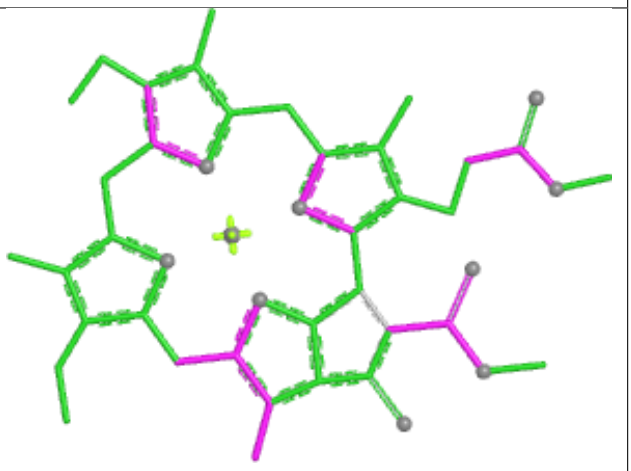

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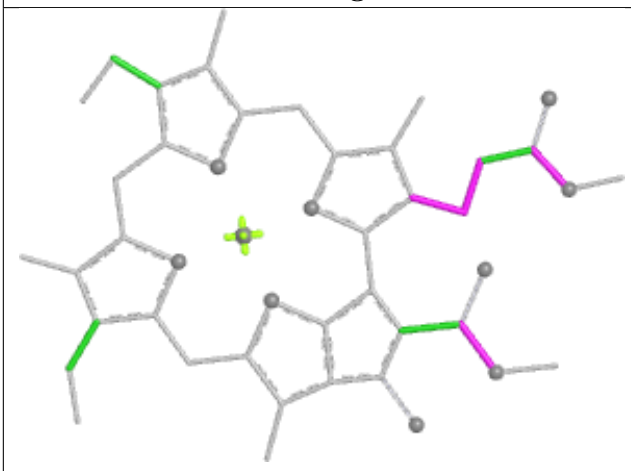

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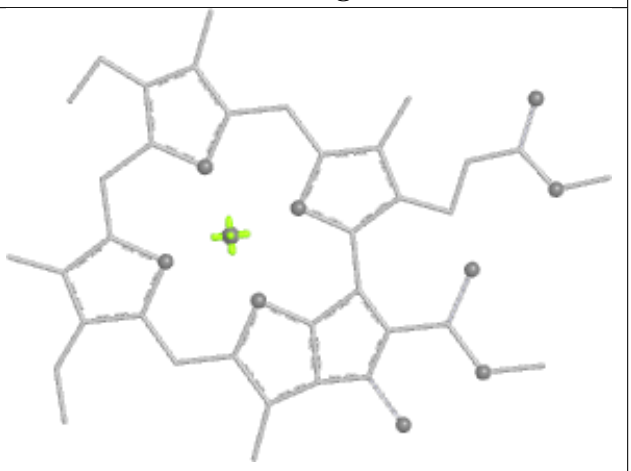
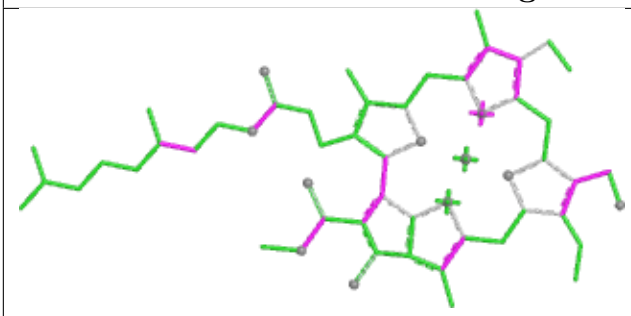


Rings

Ligand CHL 16 605



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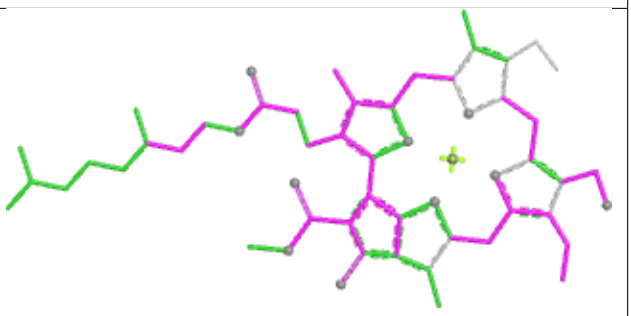

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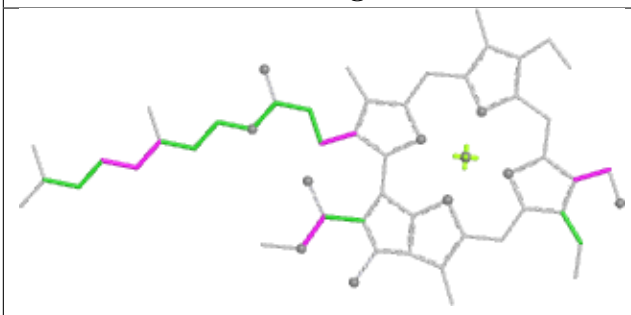

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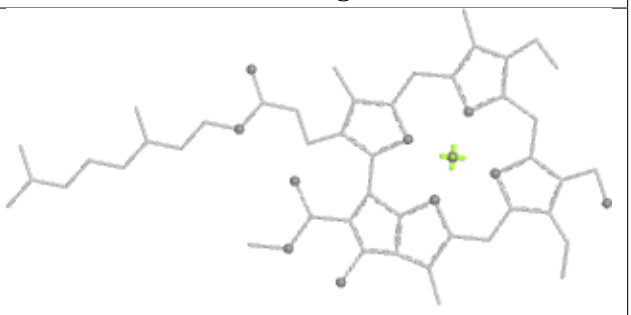

Rings

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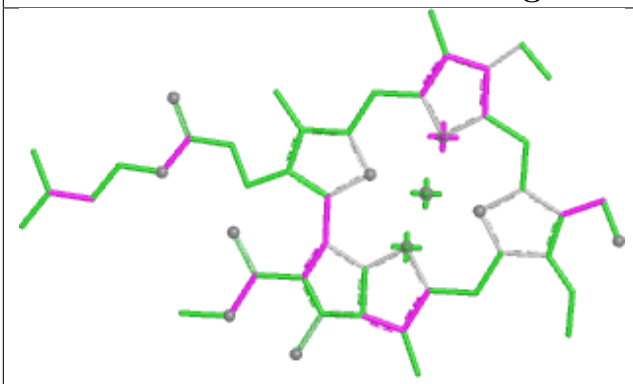

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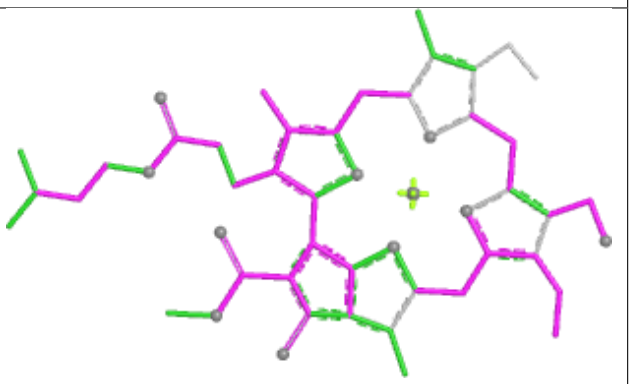

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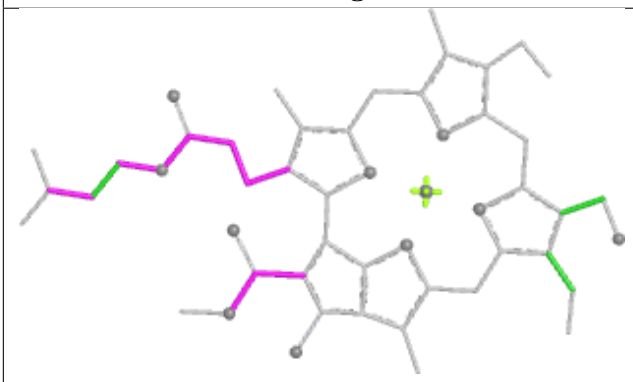

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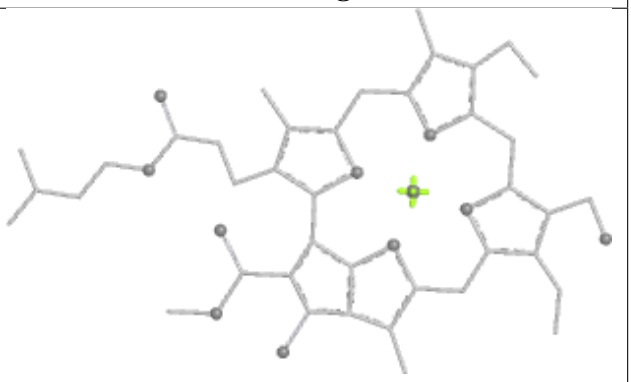
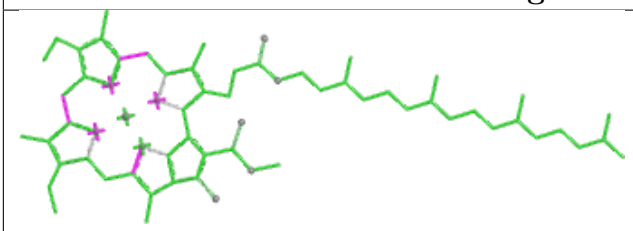


Rings

Ligand CLA b 605



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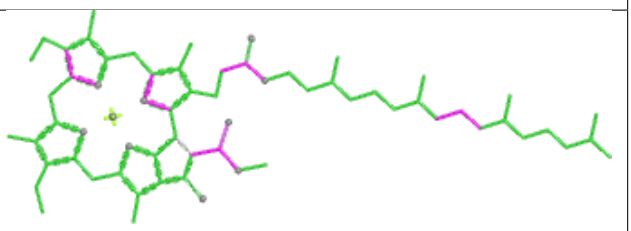

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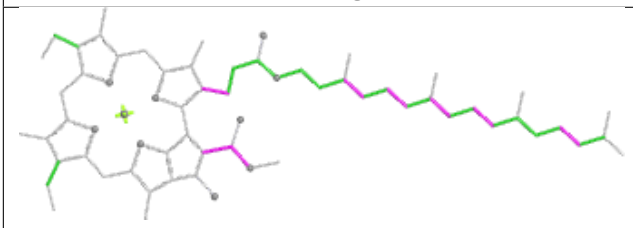

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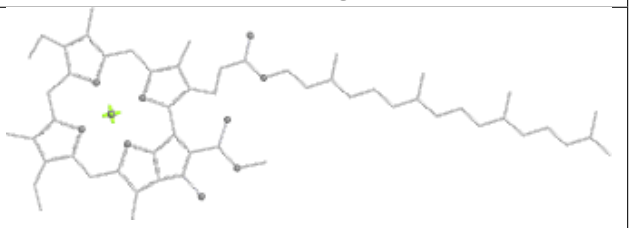

Rings

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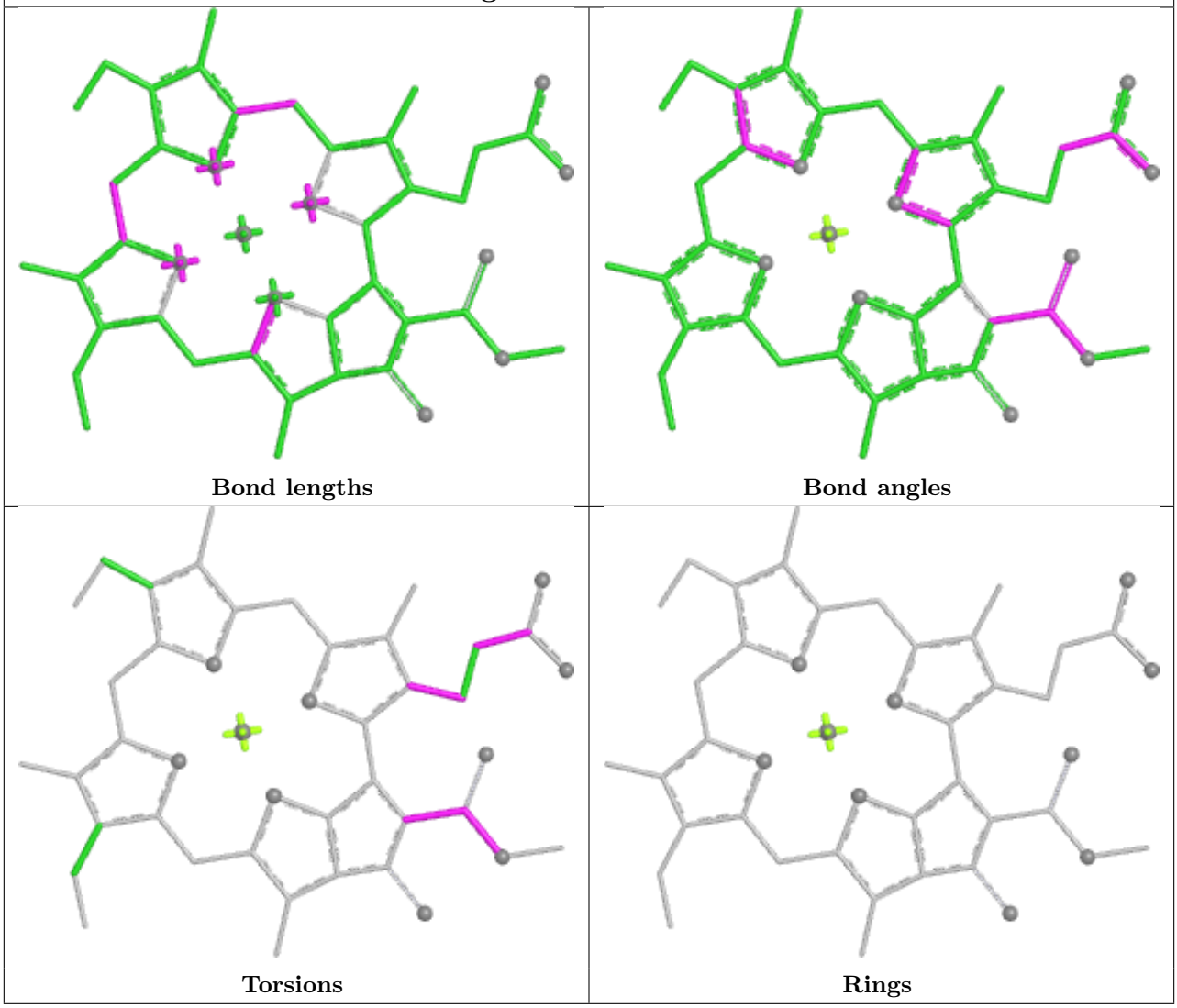

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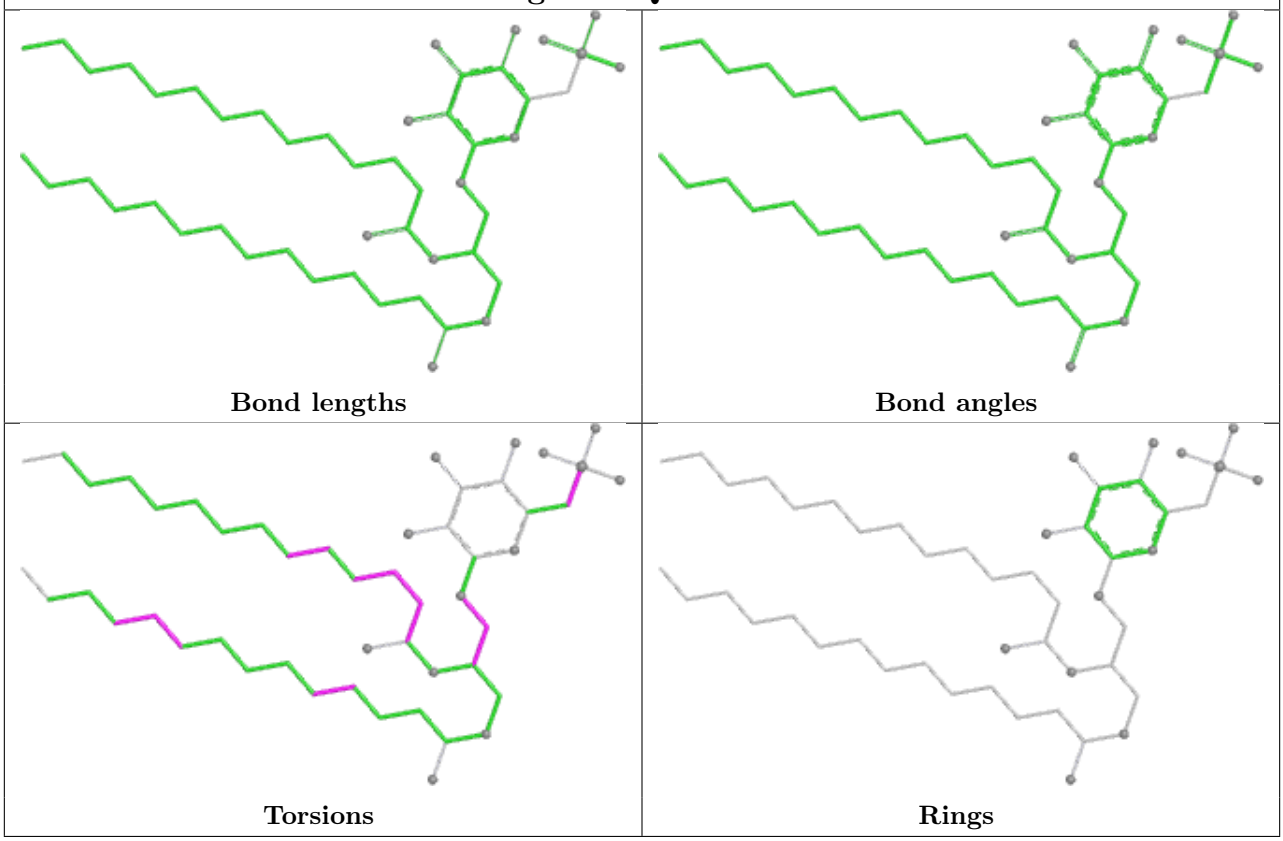

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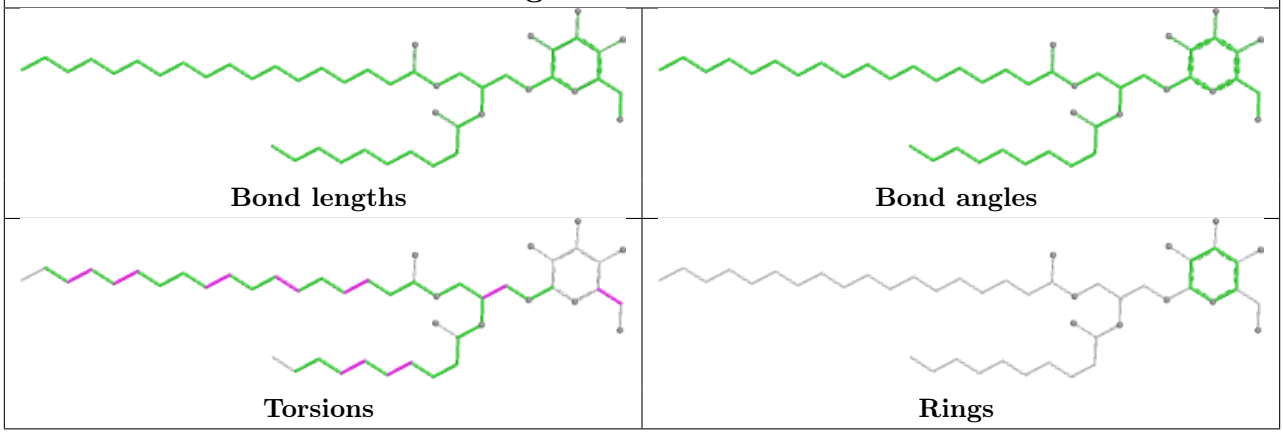

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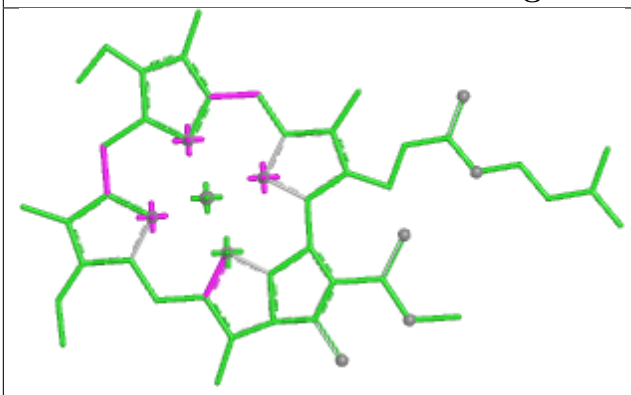

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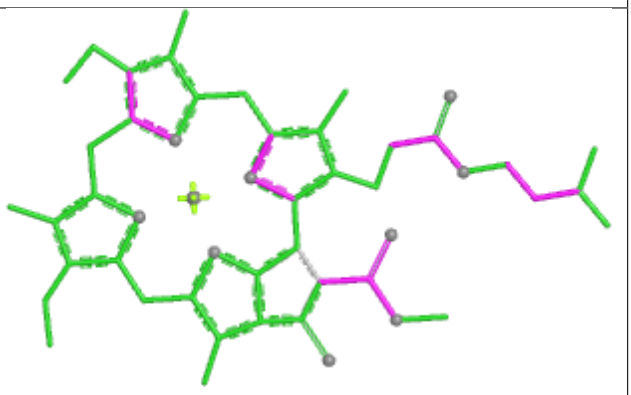

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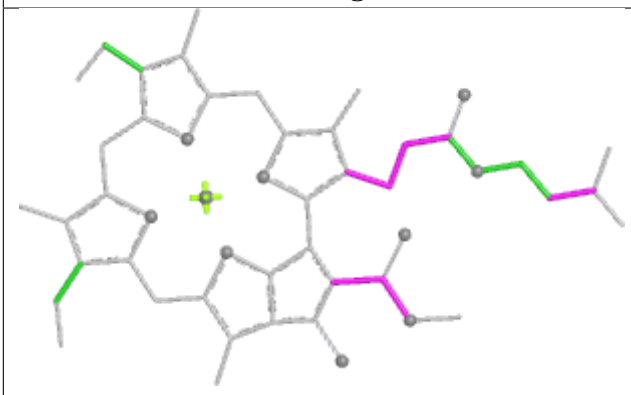

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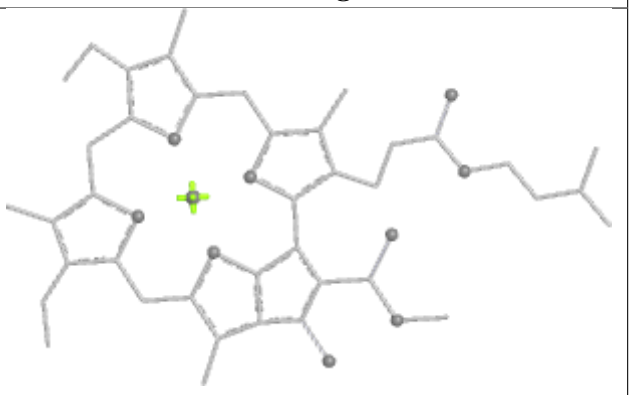
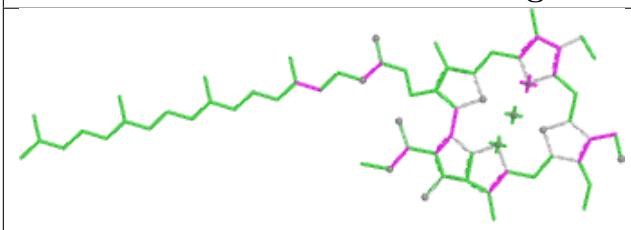


Rings

Ligand CHL n 607



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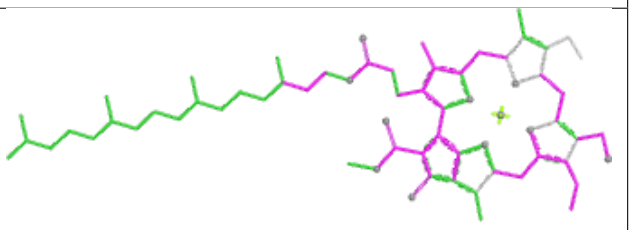

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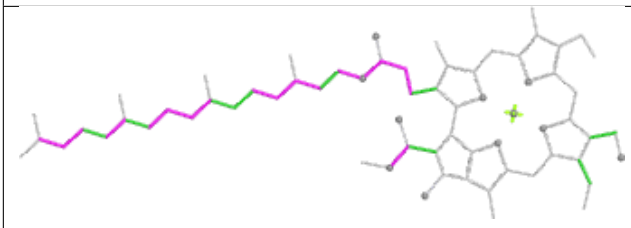

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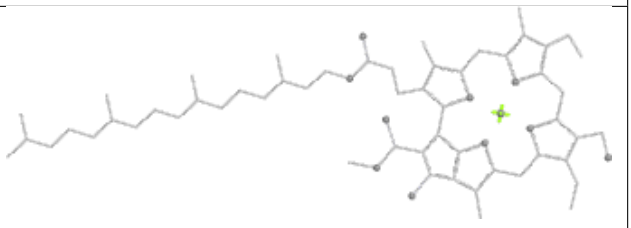

Rings

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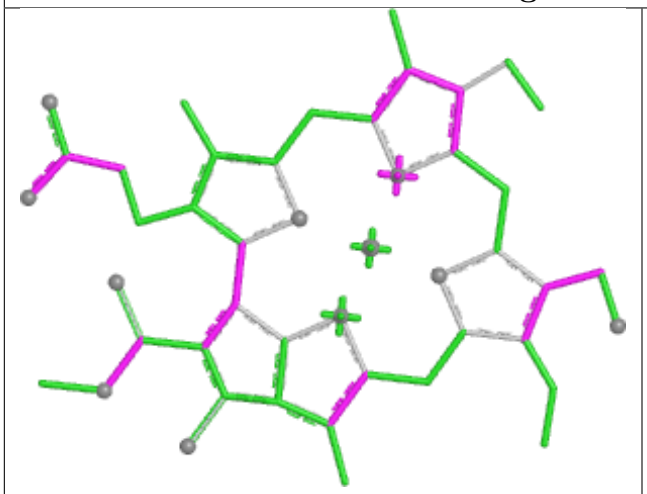

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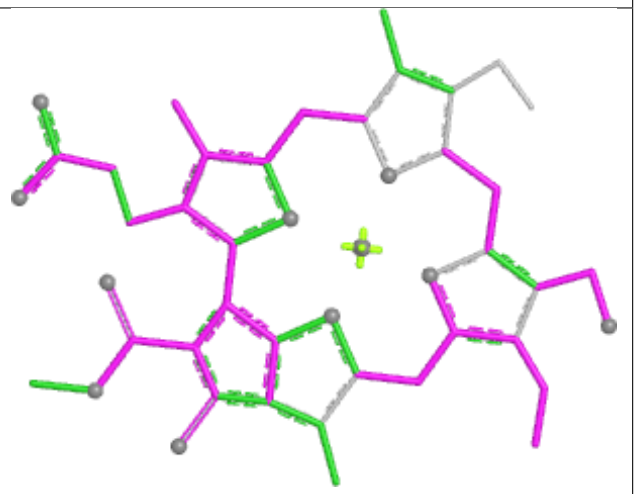

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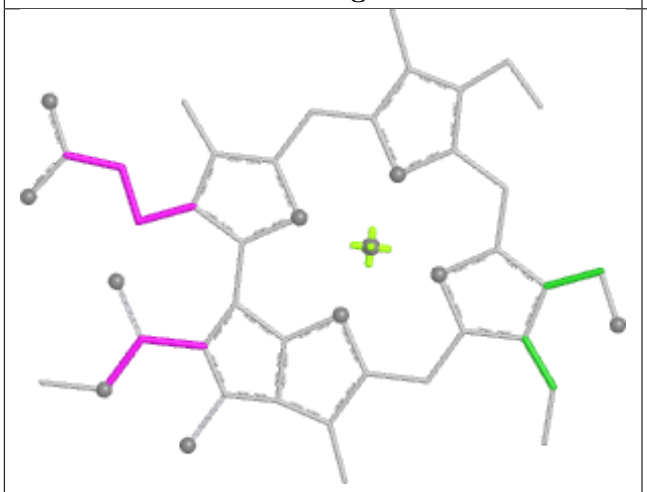

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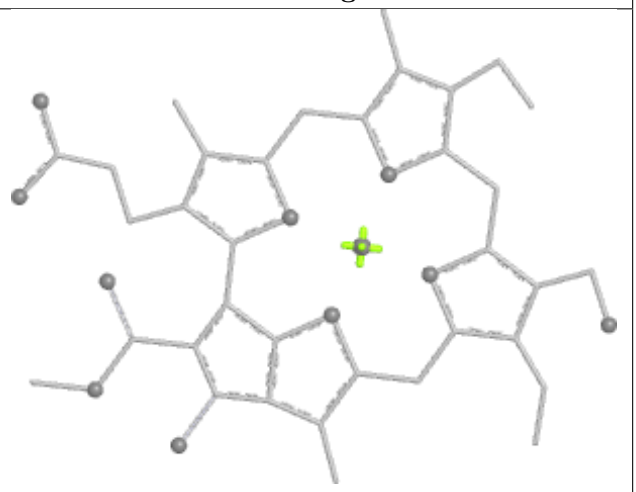

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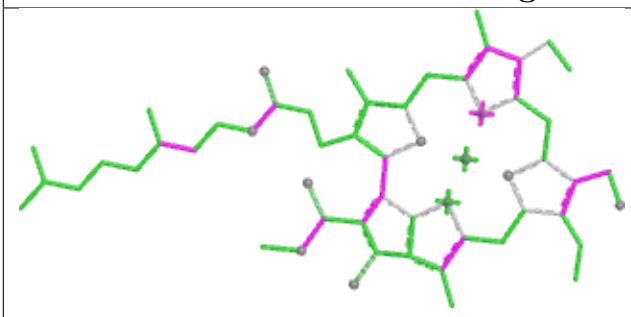
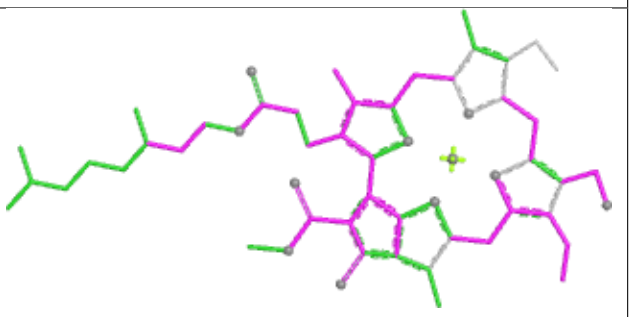
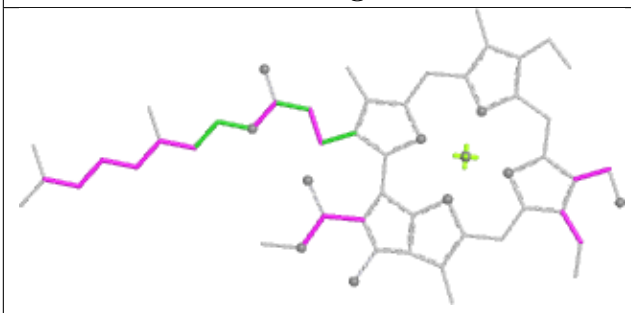
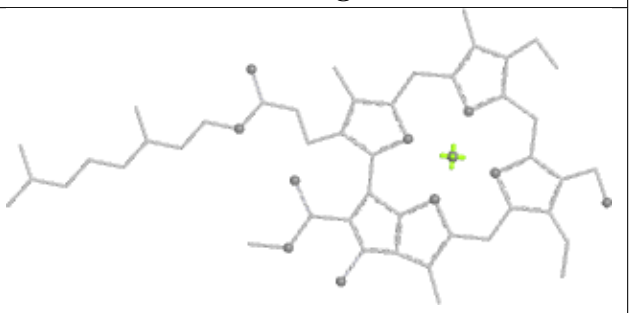
 Bond lengths	 Bond angles
 Torsions	 Rings

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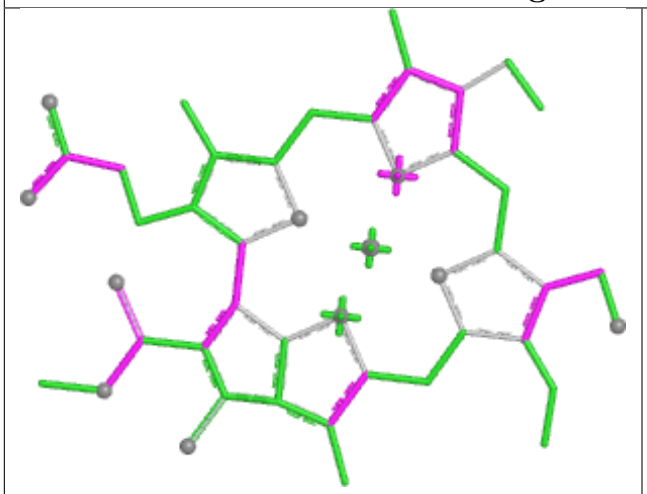

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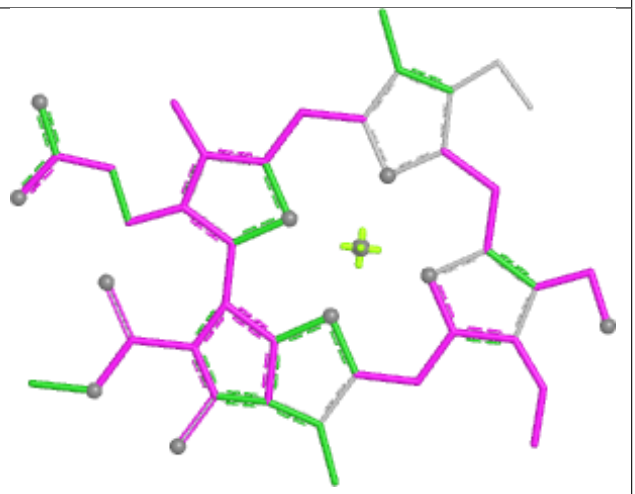

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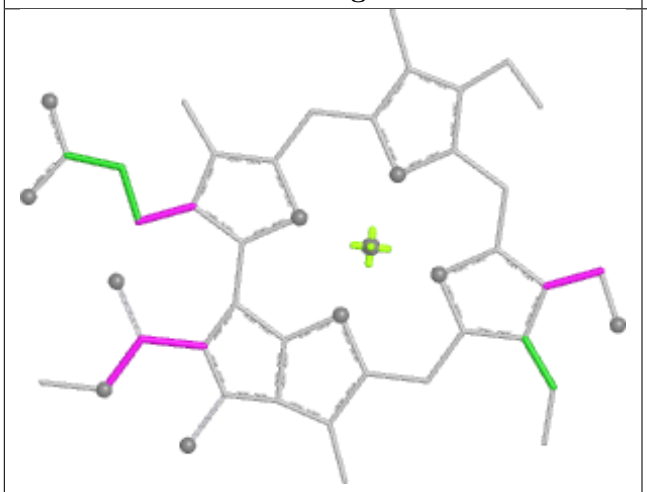

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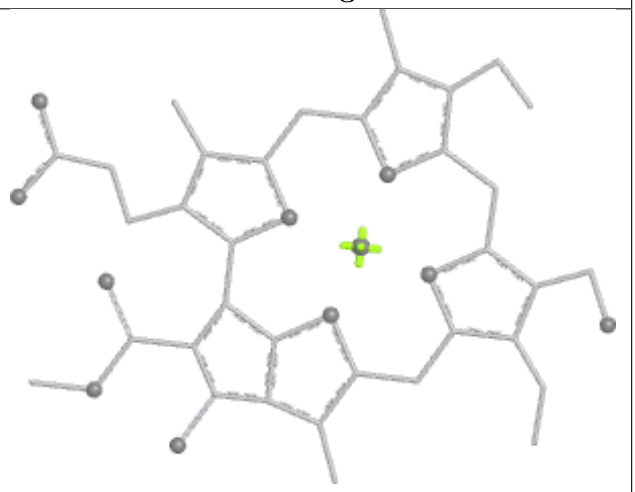

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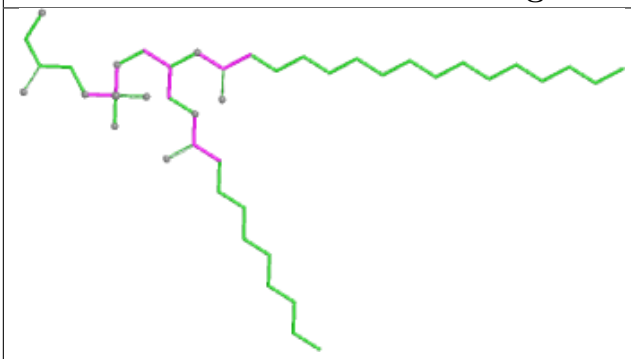
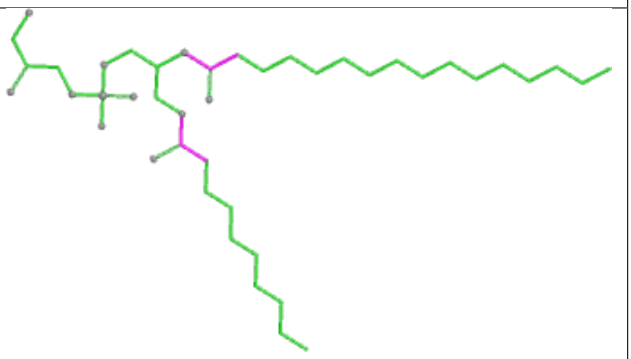
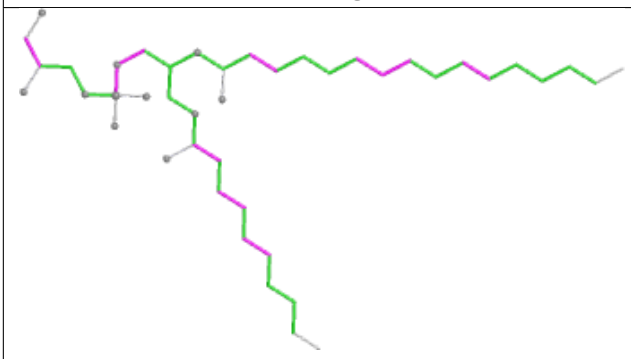
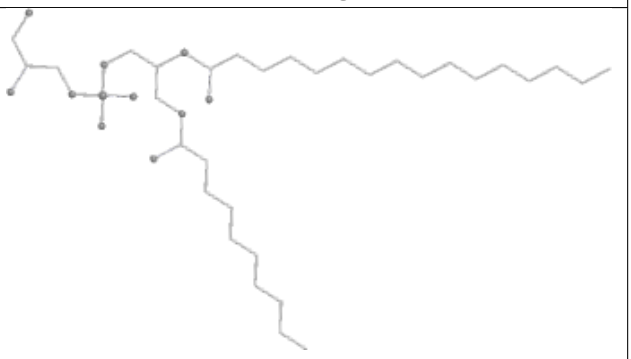
 Bond lengths	 Bond angles
 Torsions	 Rings

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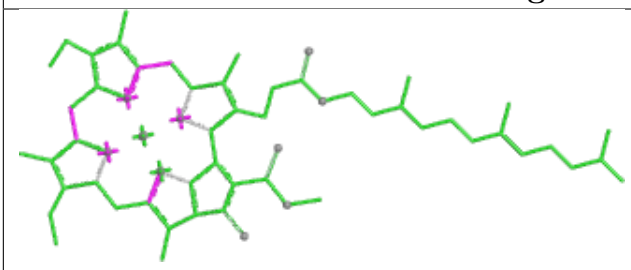
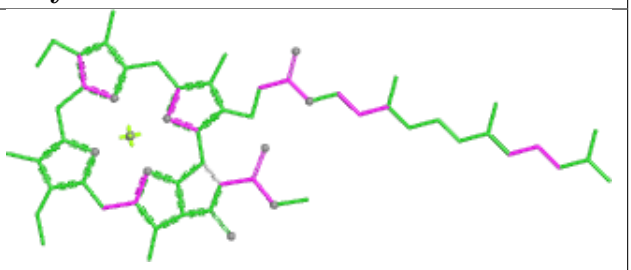
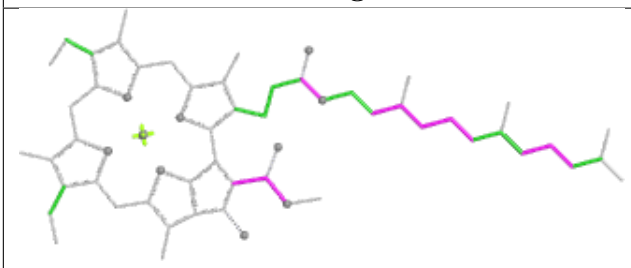
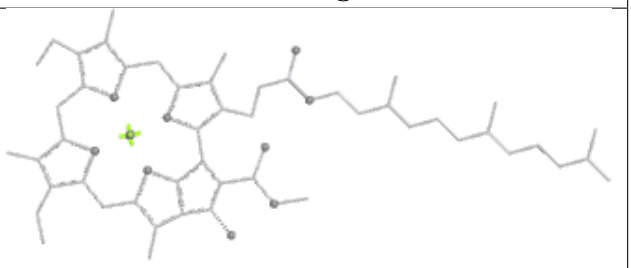
 Bond lengths	 Bond angles
 Torsions	 Rings

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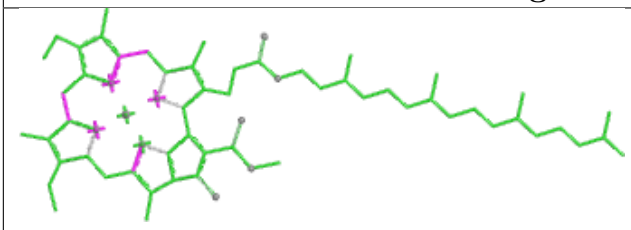
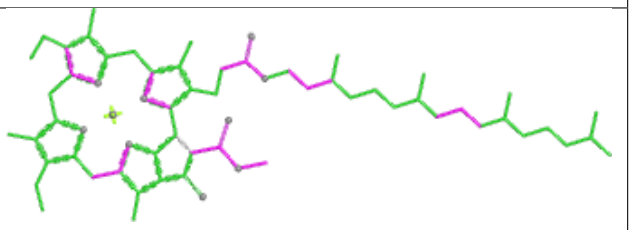
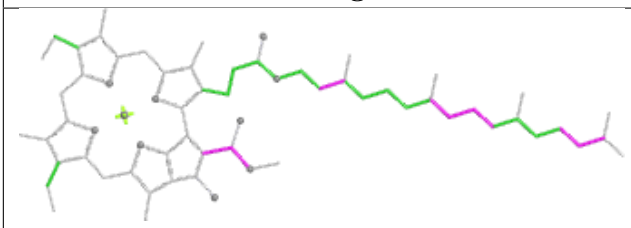
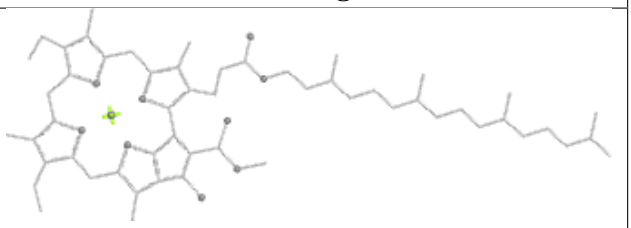
 Bond lengths	 Bond angles
 Torsions	 Rings

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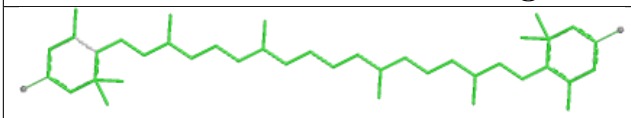
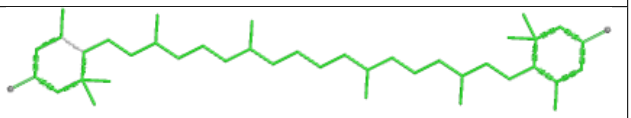
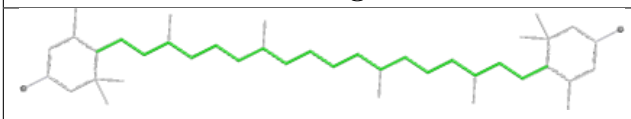
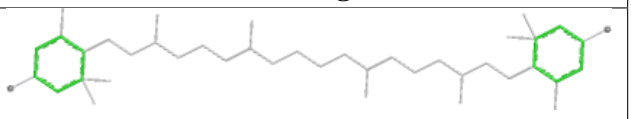
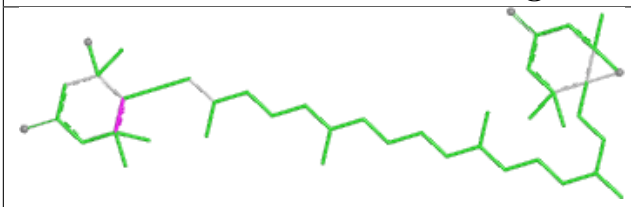
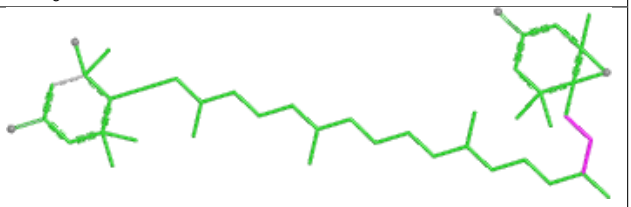
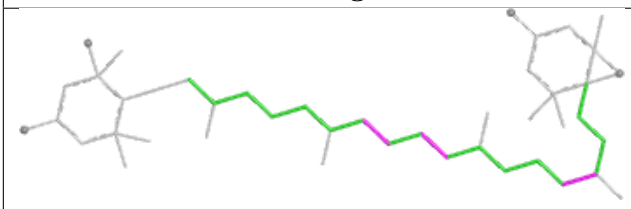
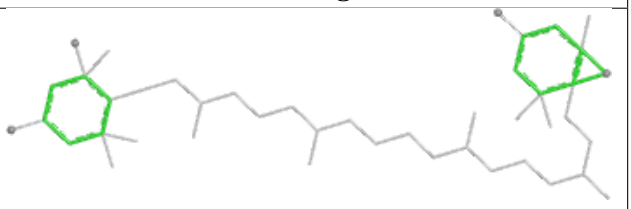
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX y 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

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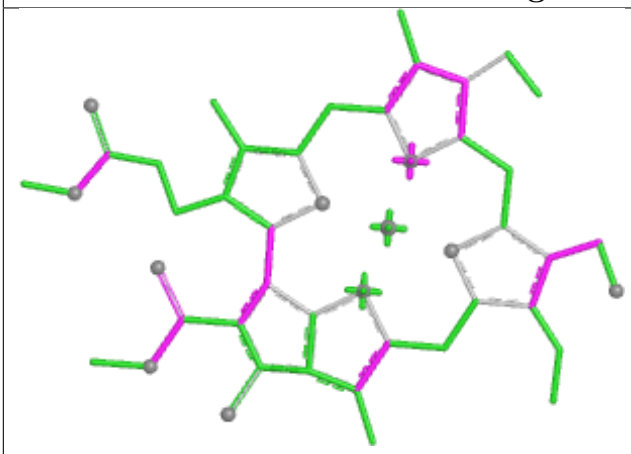
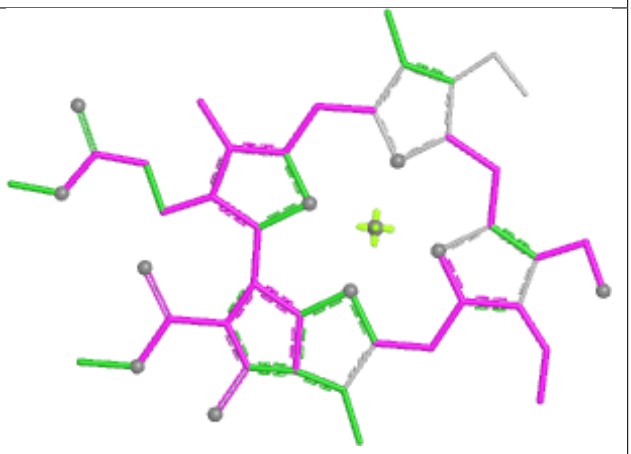
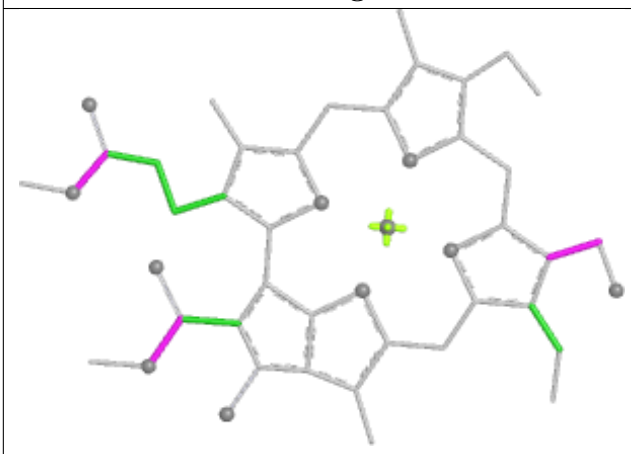
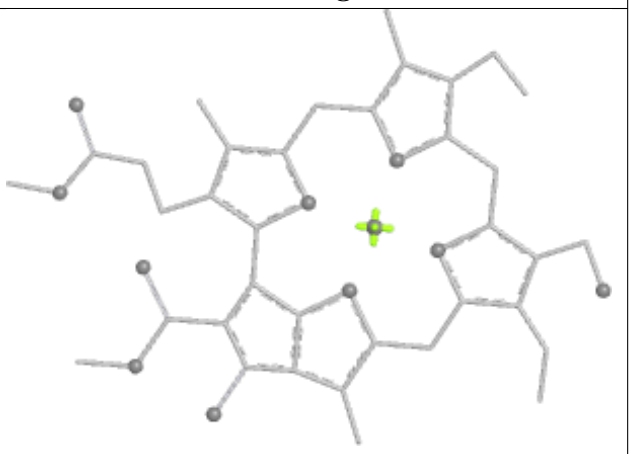
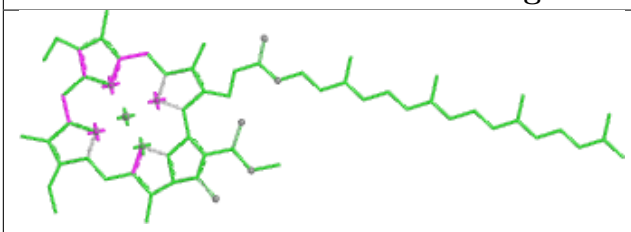
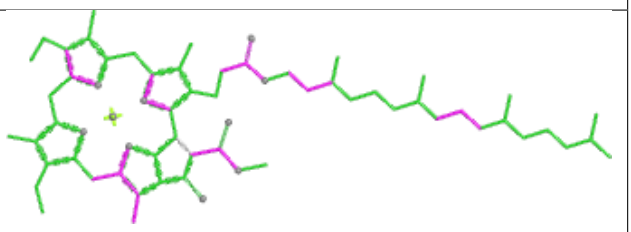
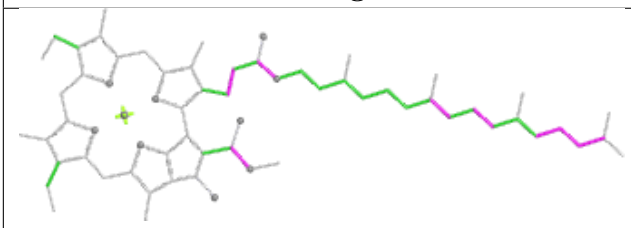
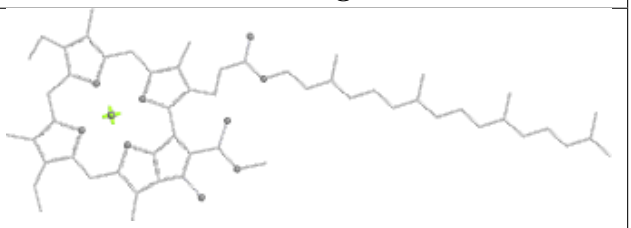
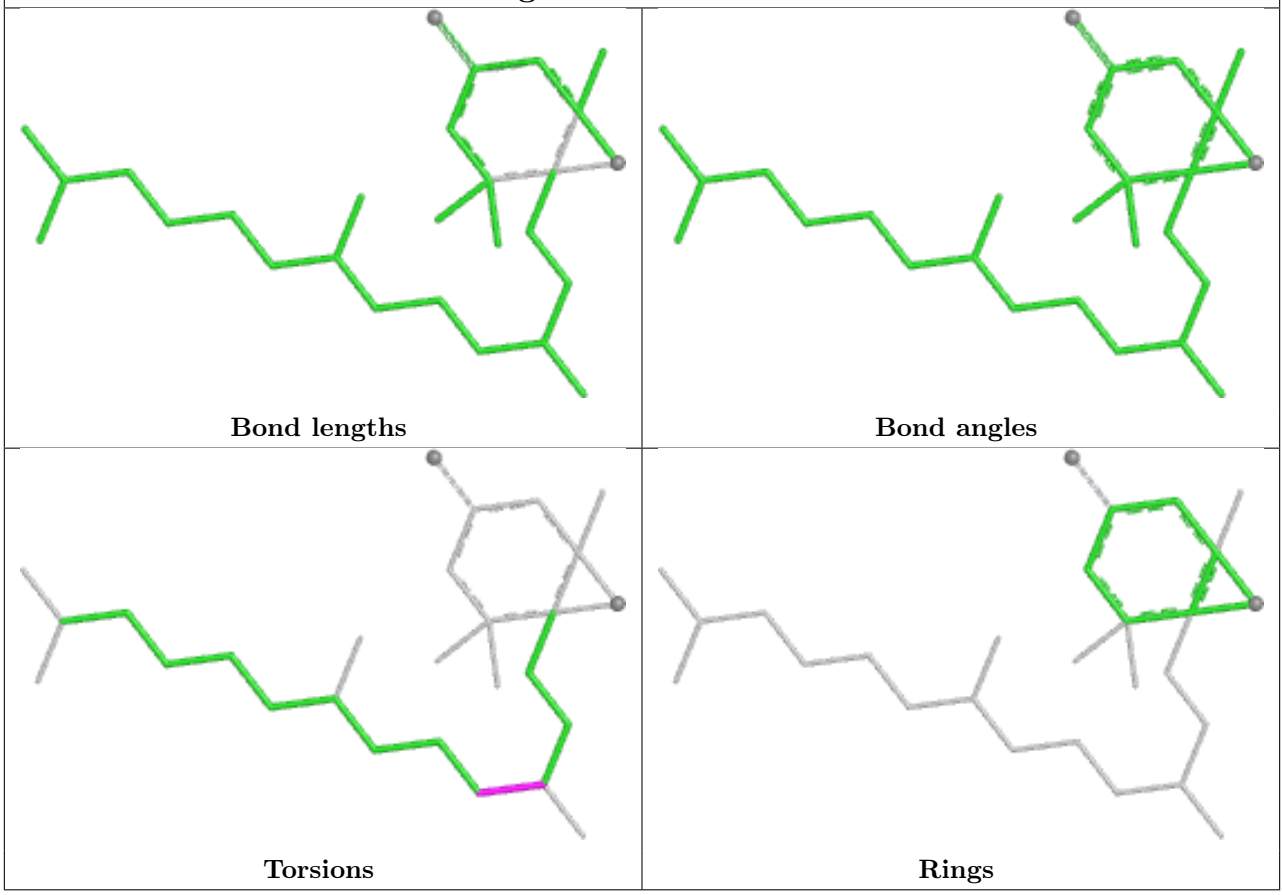
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX 15 616



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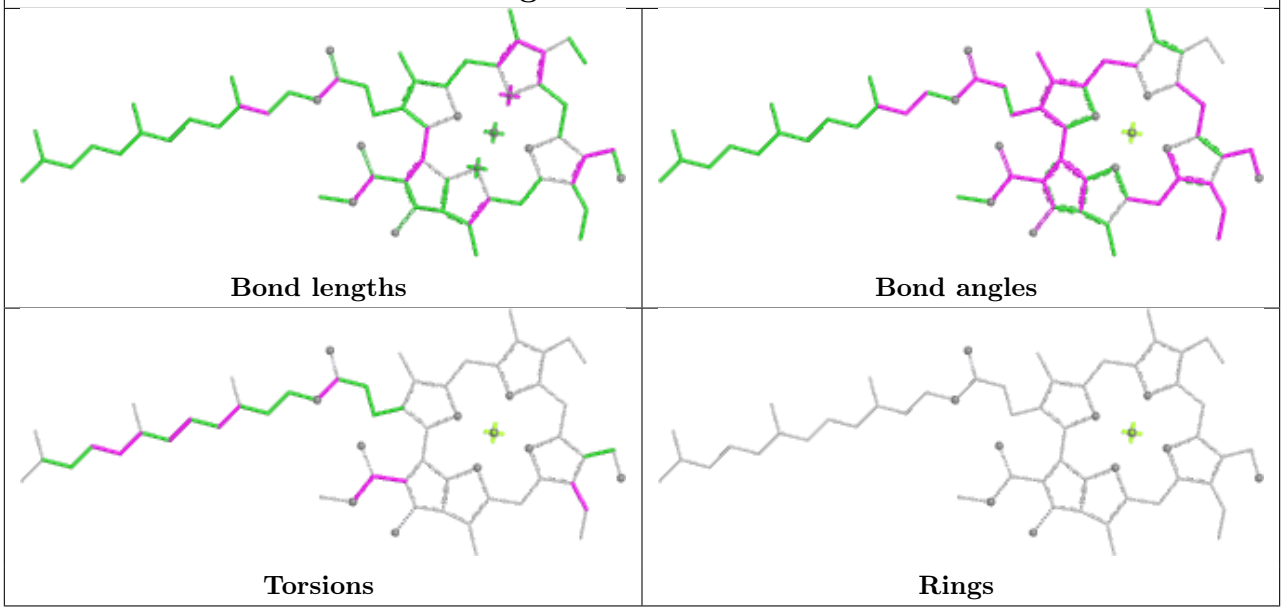
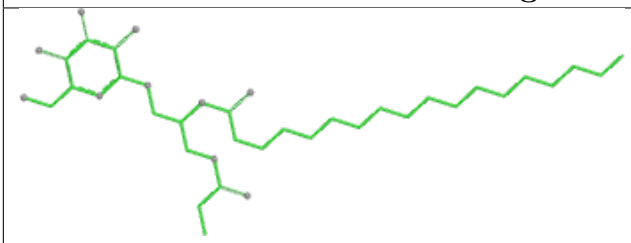
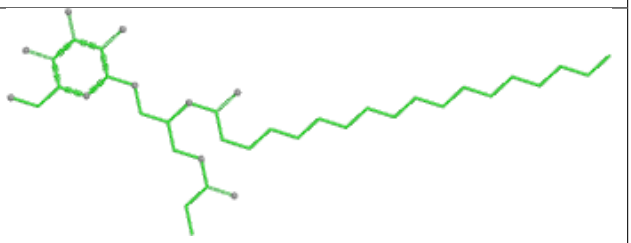


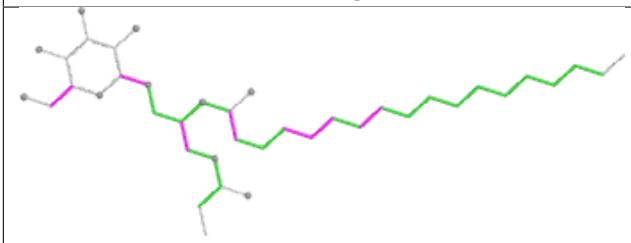
Ligand DGD w 502



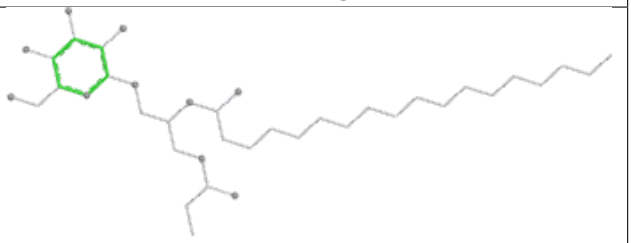
Bond lengths



Bond angles



Torsions

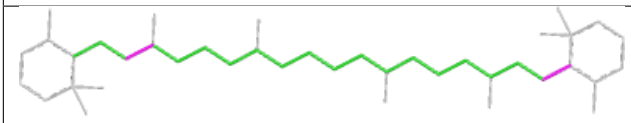


Rings

Ligand BCR D 406

Bond lengths

Bond angles



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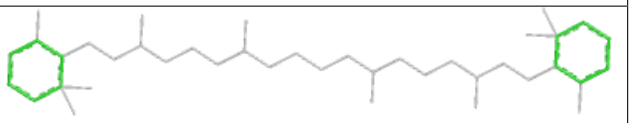
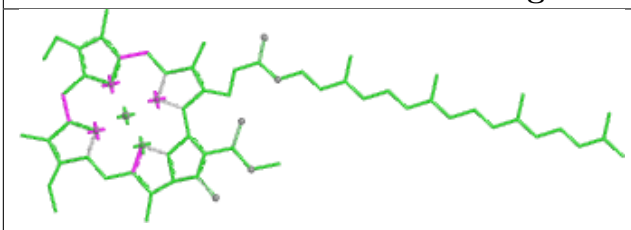
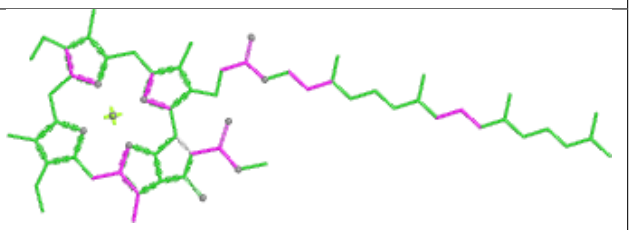


Rings

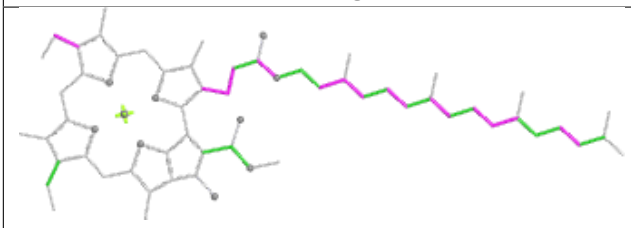
Ligand CLA S 610



Bond lengths



Bond angles



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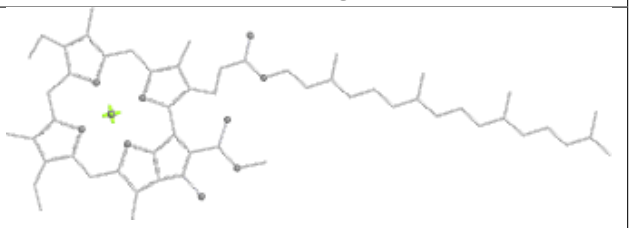
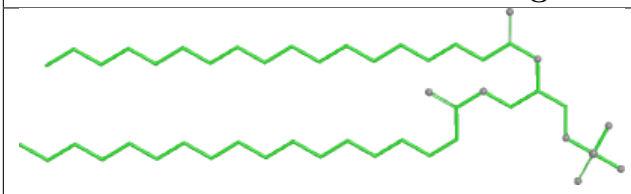
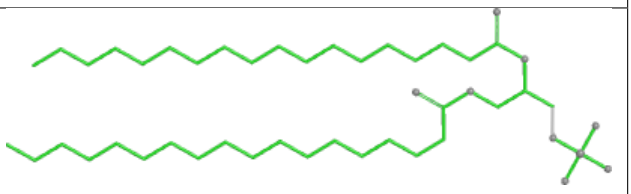
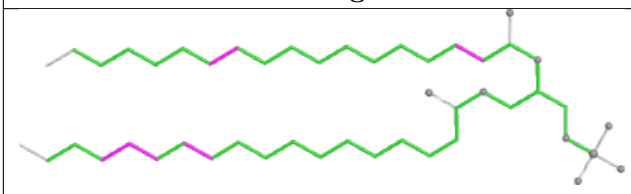
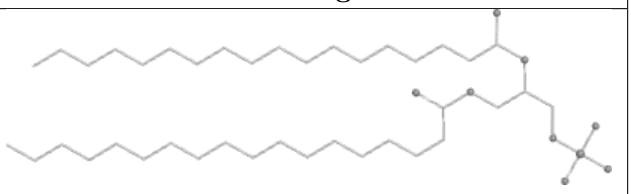
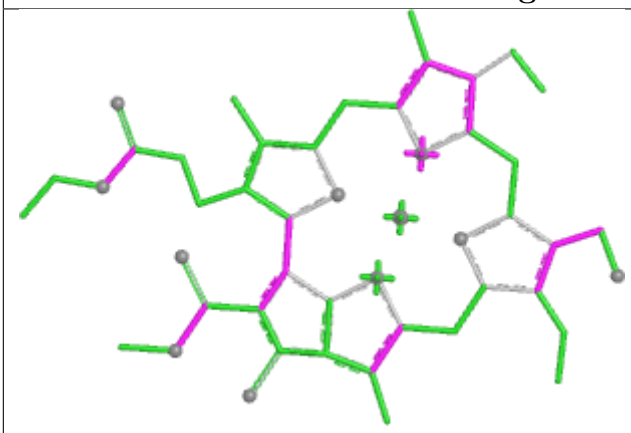
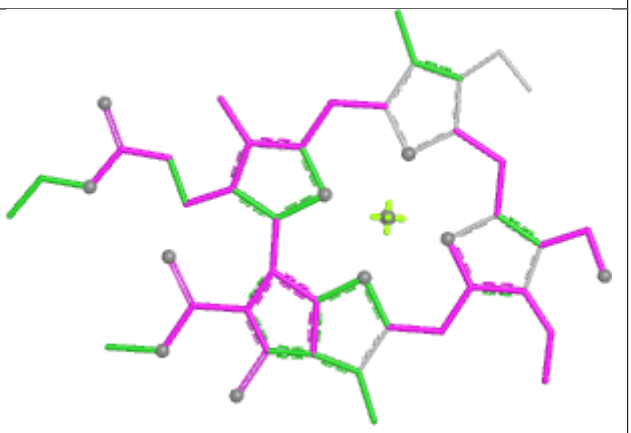
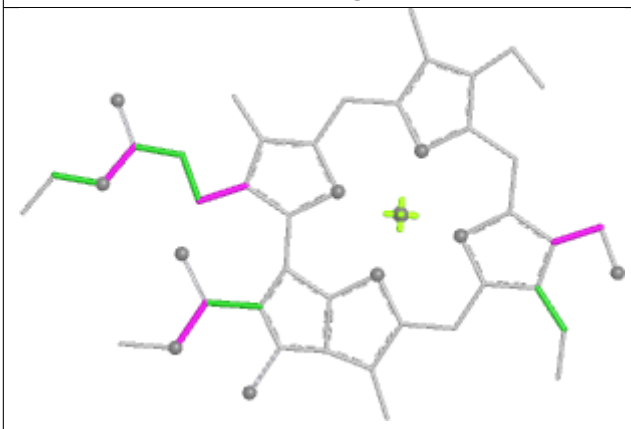
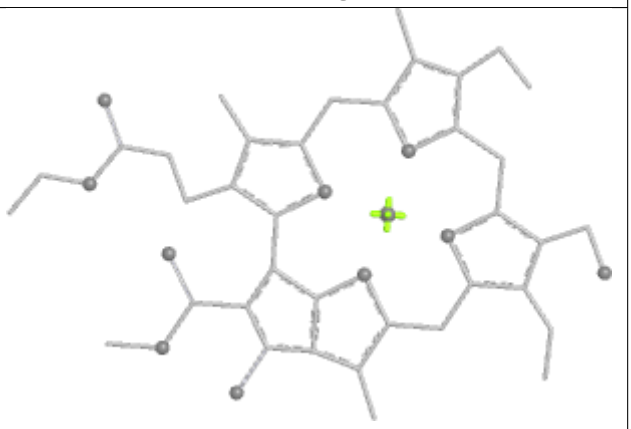
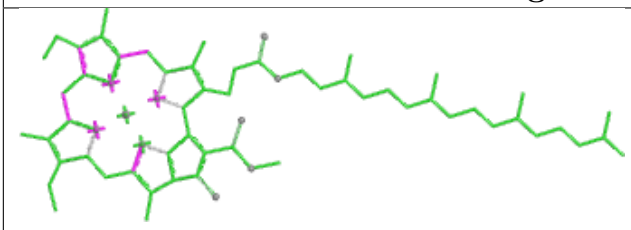
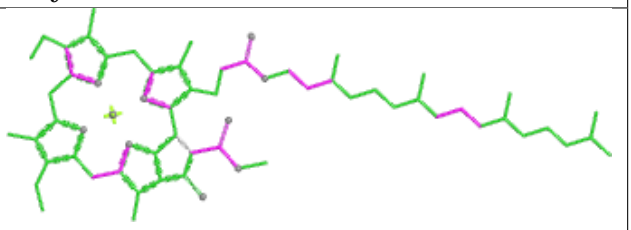
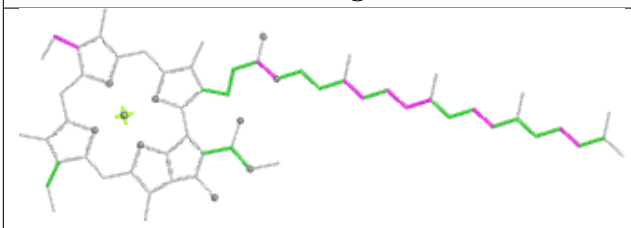
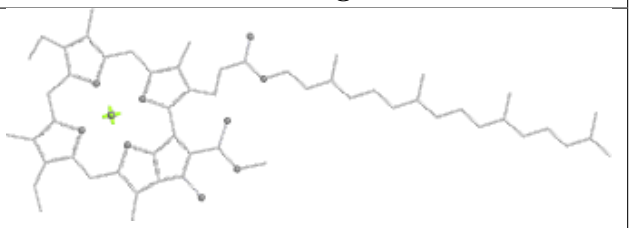
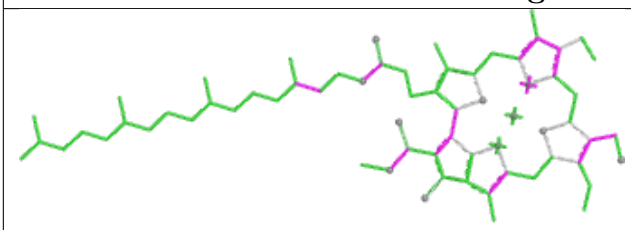
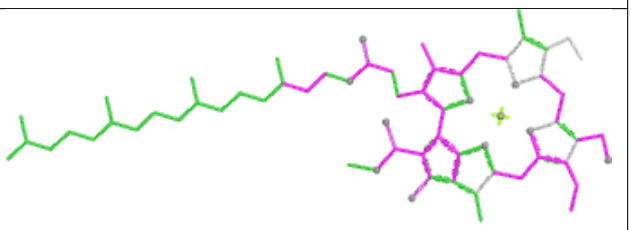
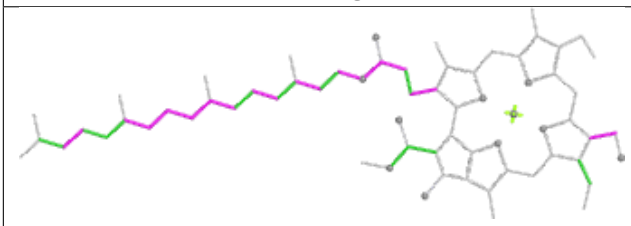
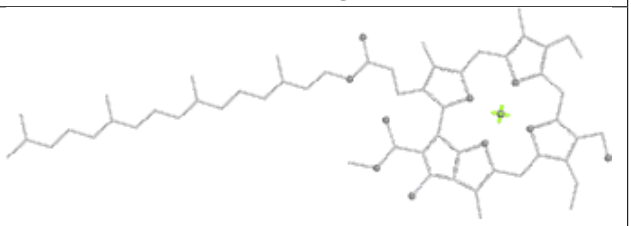


Rings

Ligand 3PH 7 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 11 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA y 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 3 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

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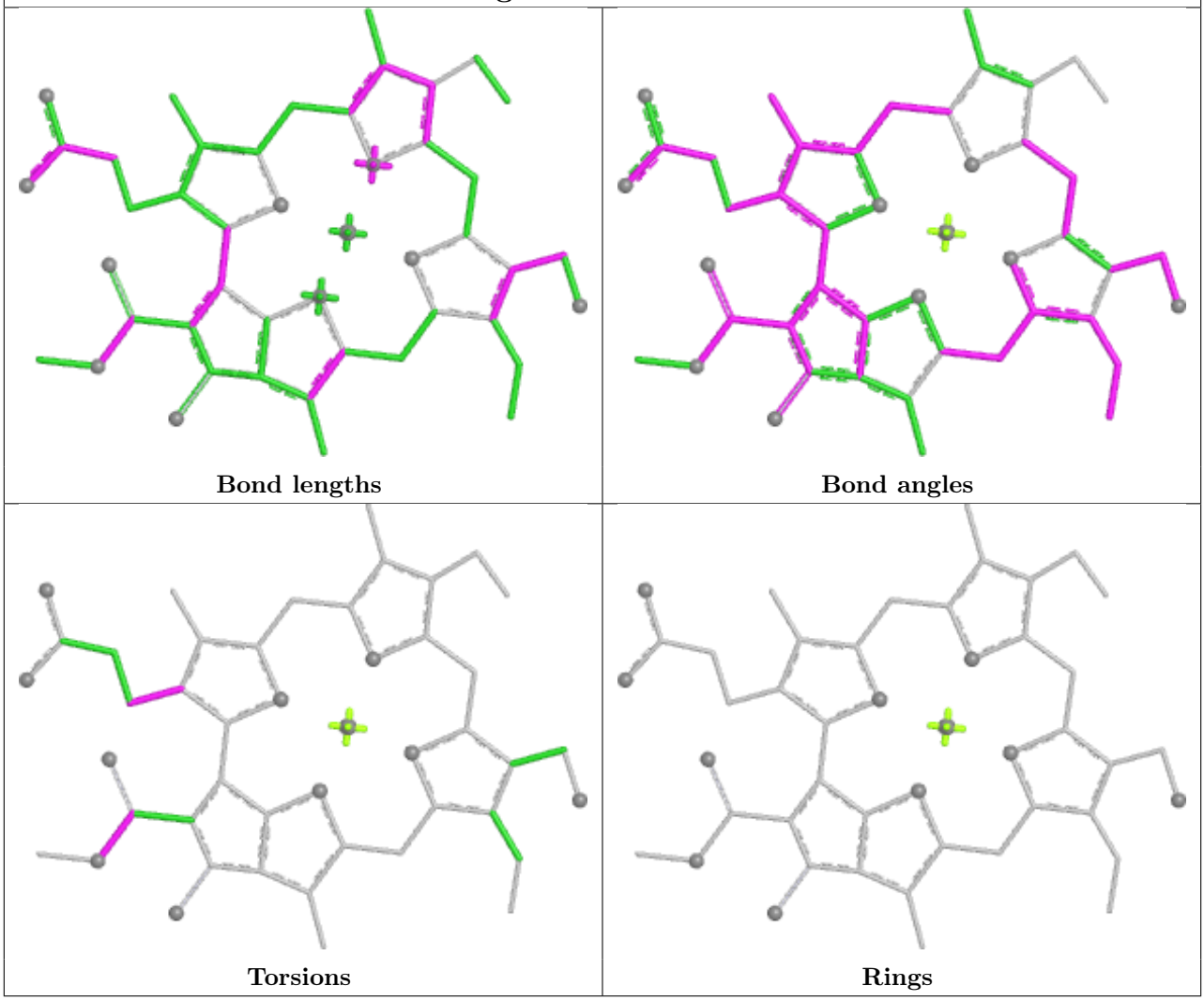
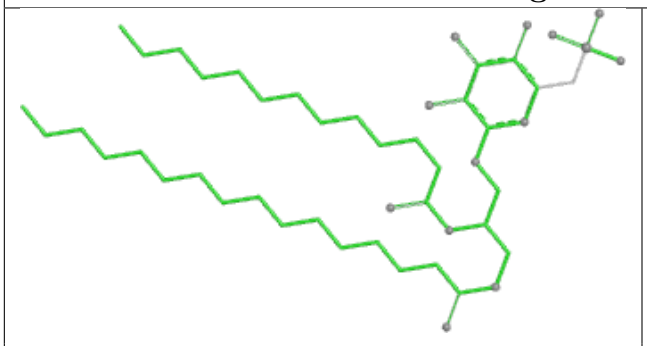
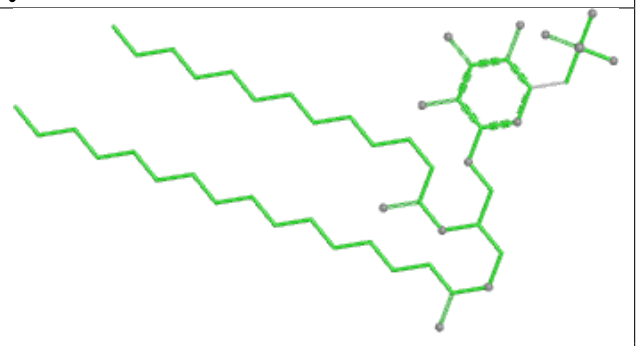


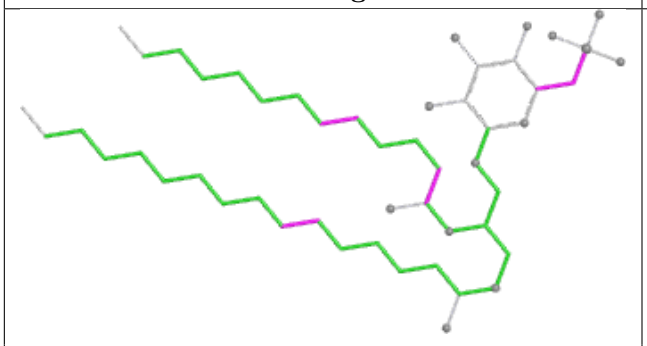
Ligand SQD a 409



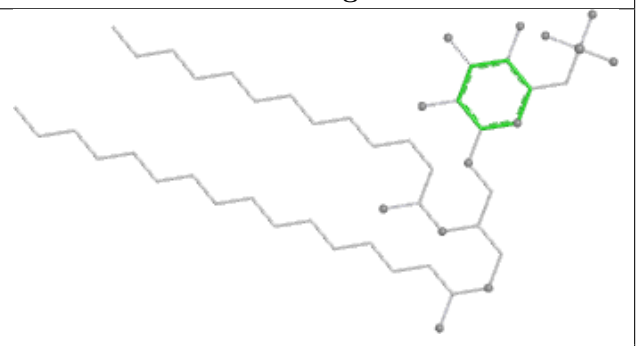
Bond lengths



Bond angles



Torsions

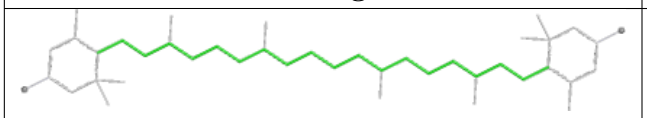


Rings

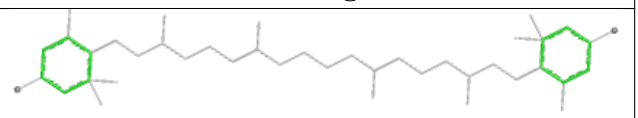
Ligand LUT R 615

Bond lengths

Bond angles

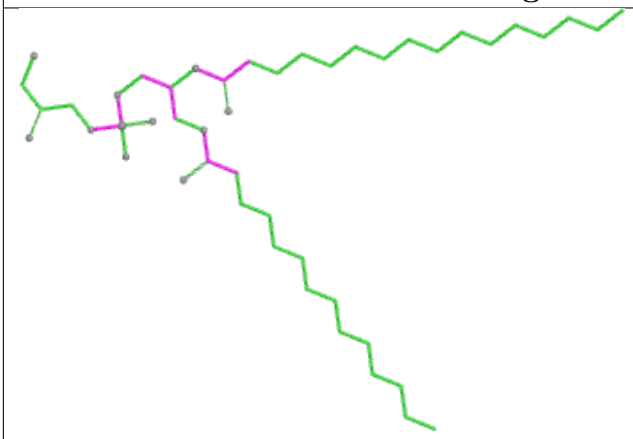


Torsions

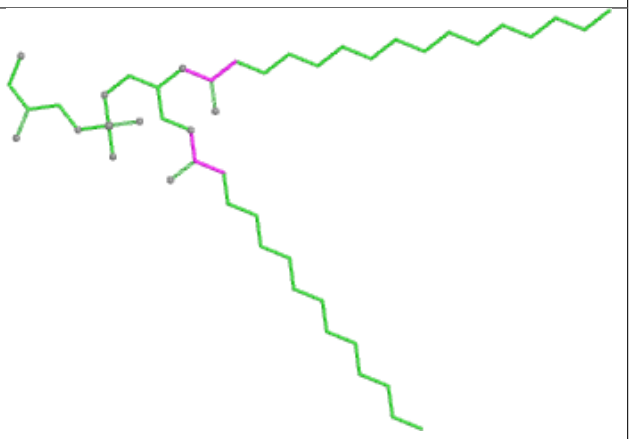


Rings

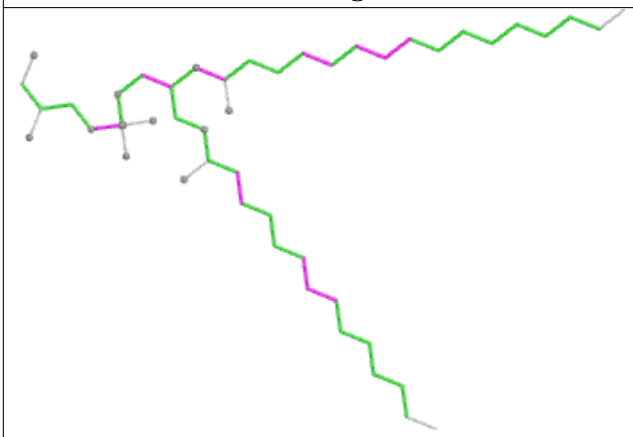
Ligand LHG R 619



Bond lengths



Bond angles



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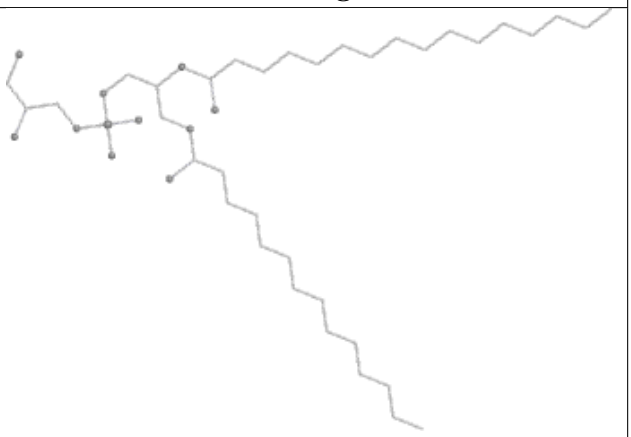
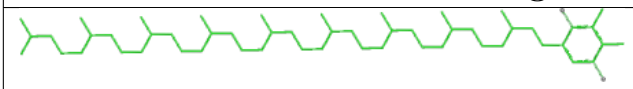
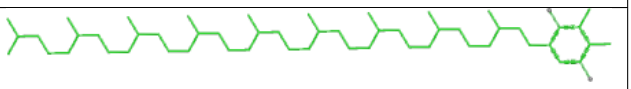


Rings

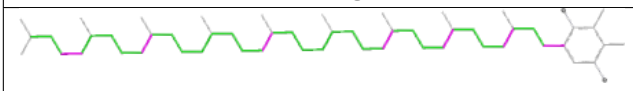
Ligand PL9 D 407



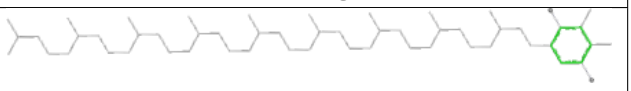
Bond lengths



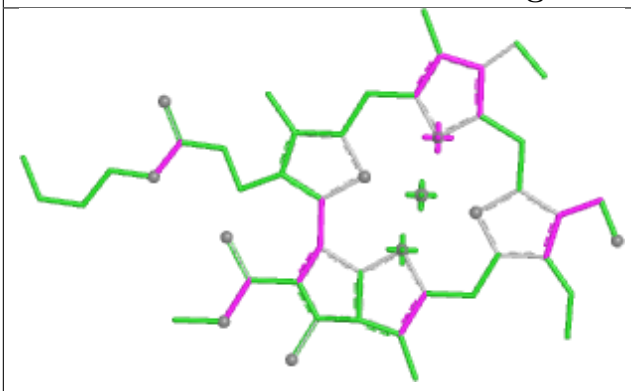
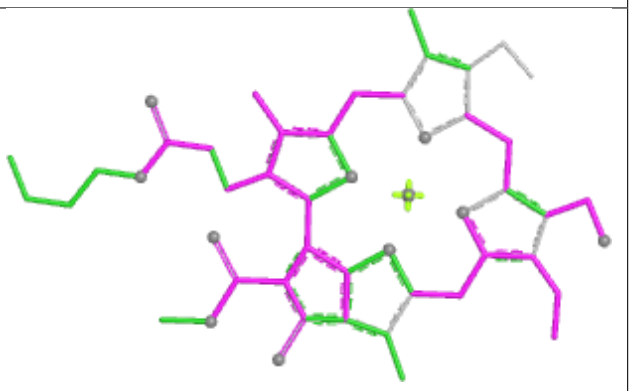
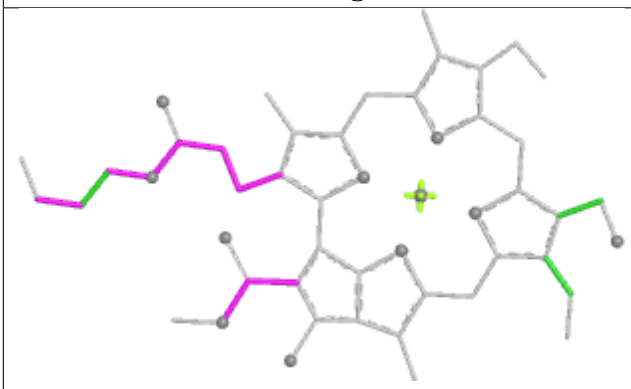
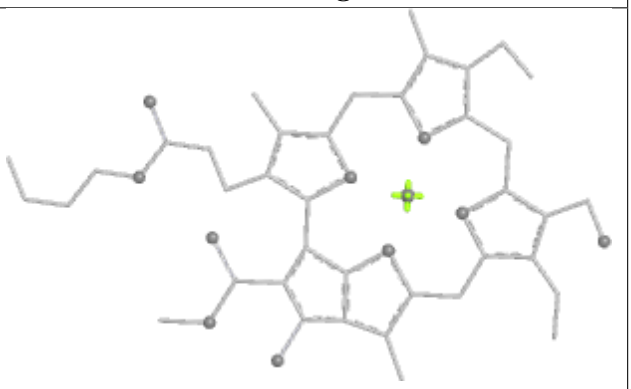
Bond angles



Torsions



Rings

Ligand CHL n 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

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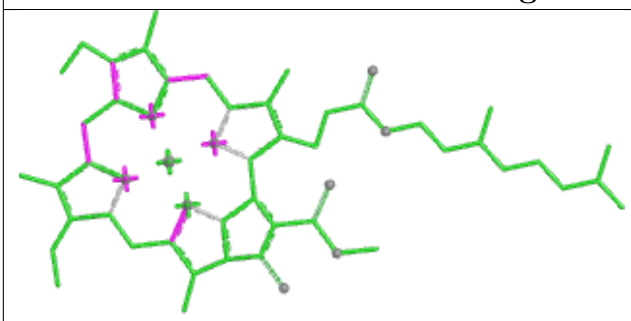
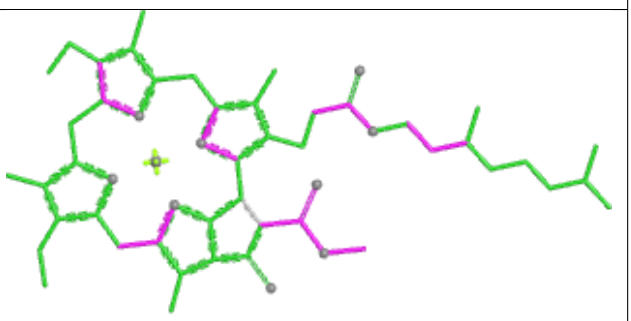
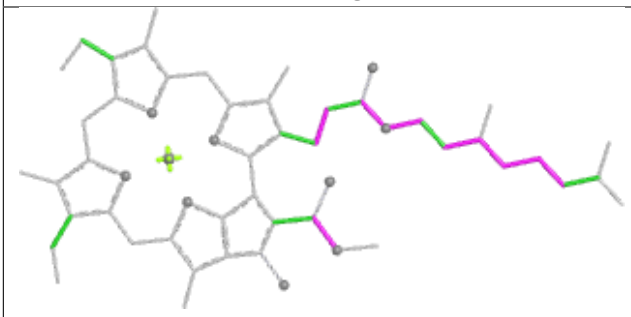
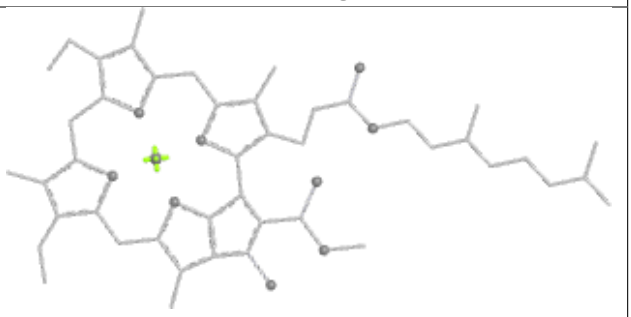
 Bond lengths	 Bond angles
 Torsions	 Rings

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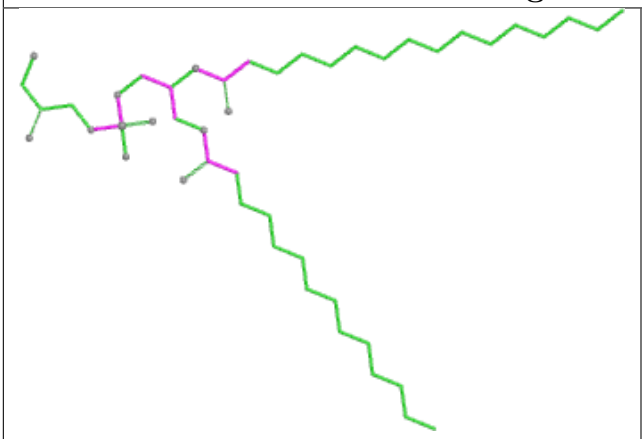
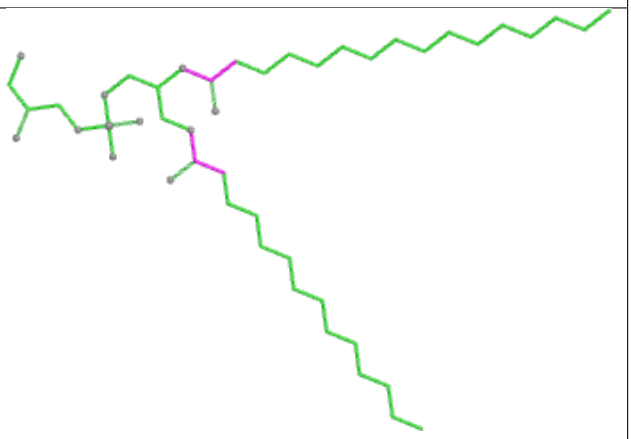
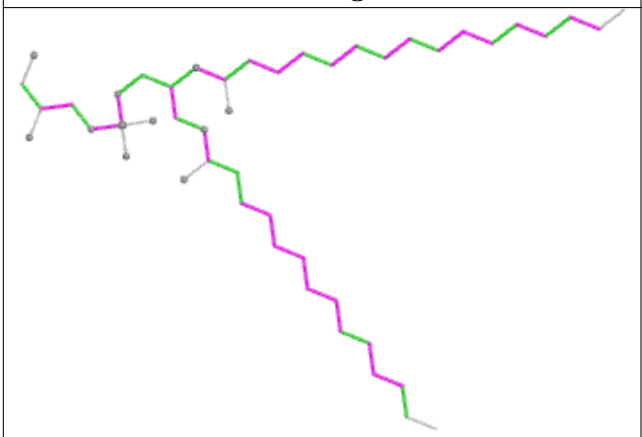
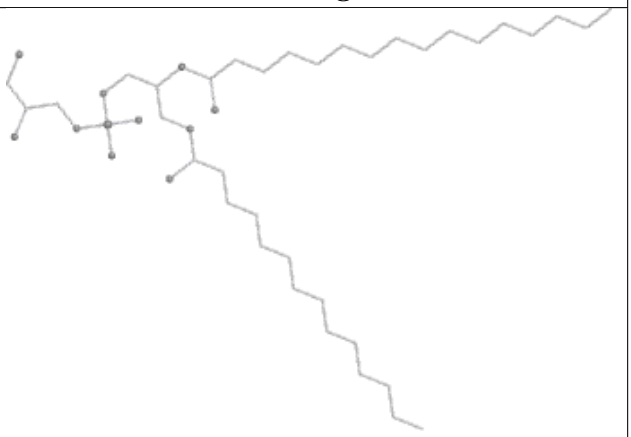
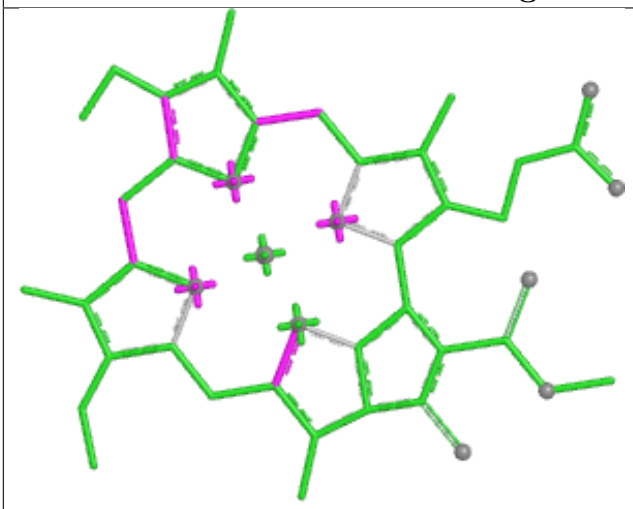
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 12 613



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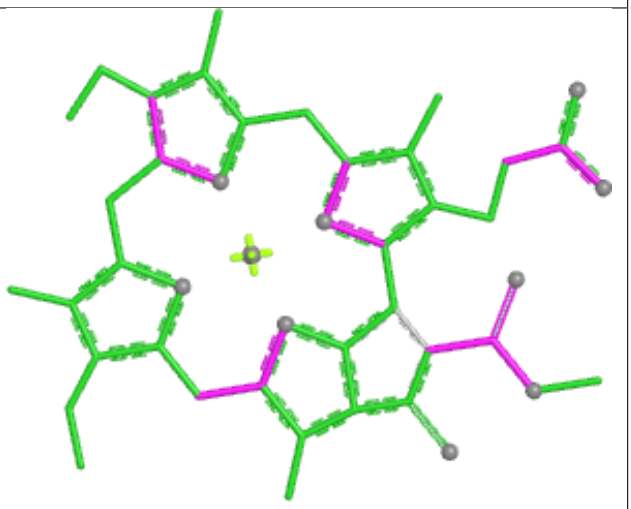

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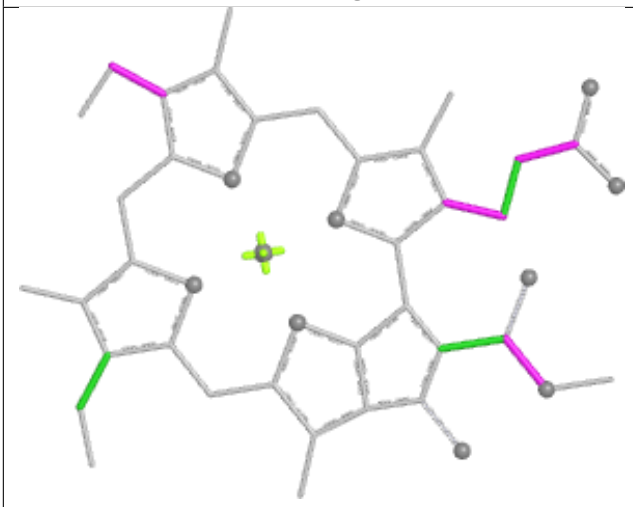
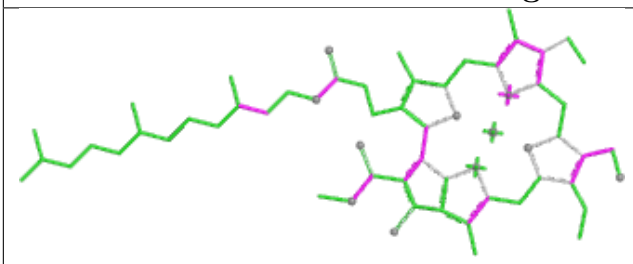


Torsions

Rings

Ligand CHL N 605



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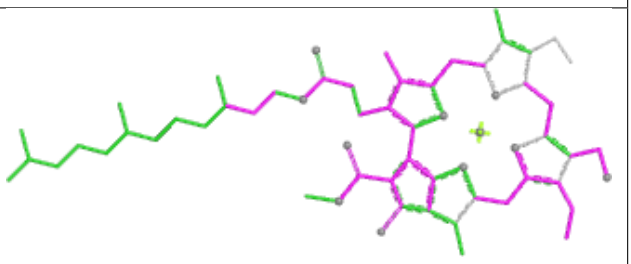

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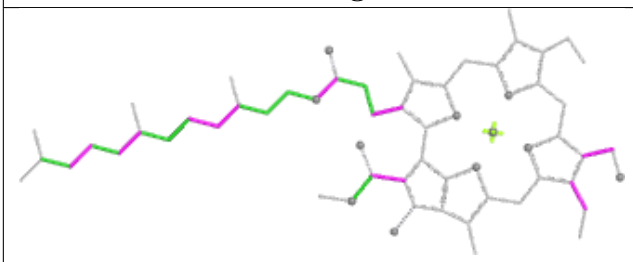

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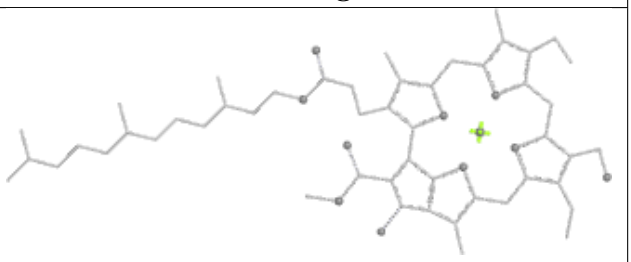
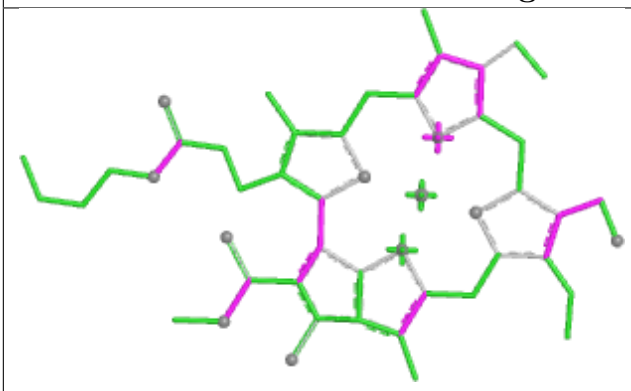
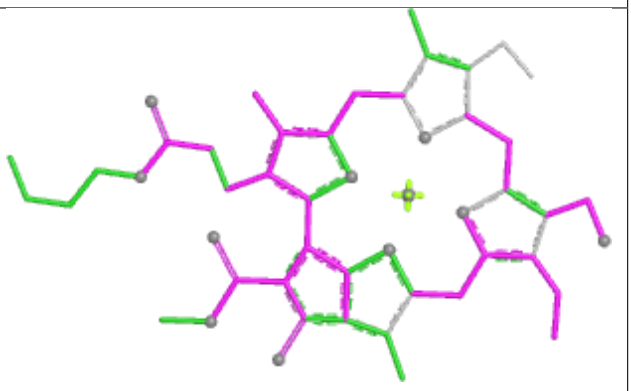
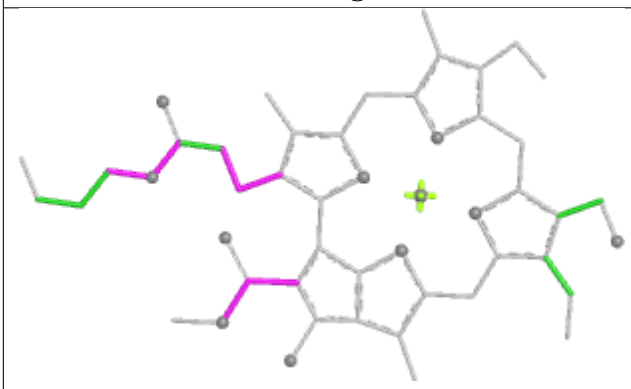
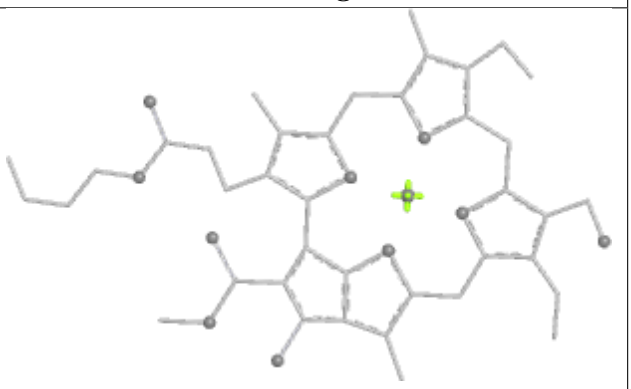
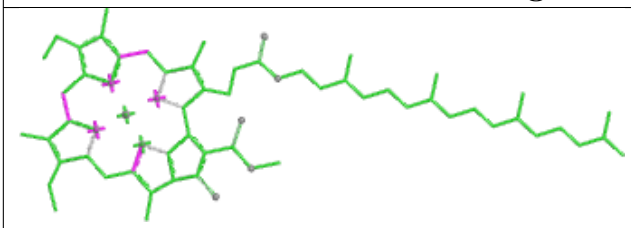
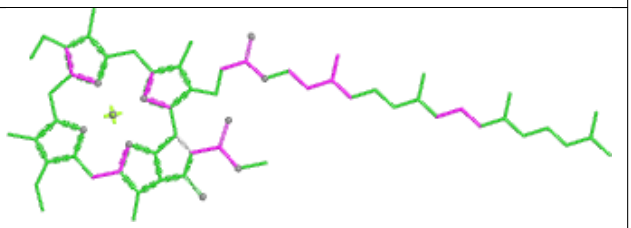
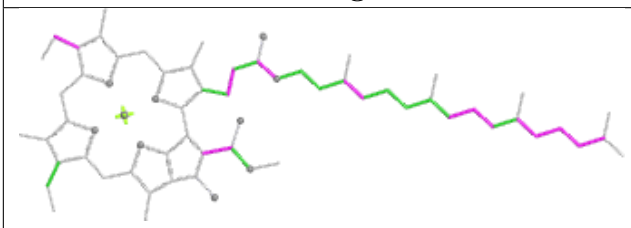
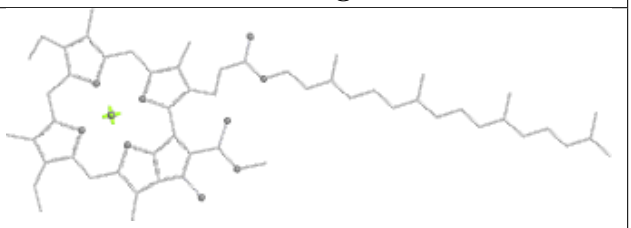


Rings

Ligand CHL 13 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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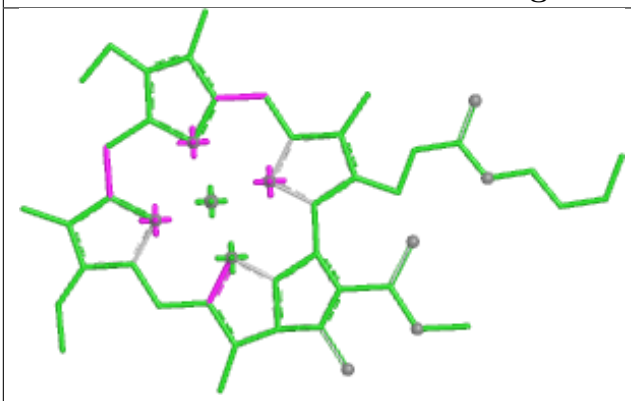
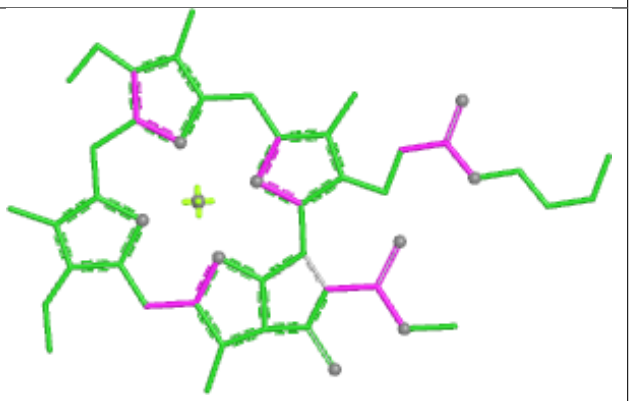
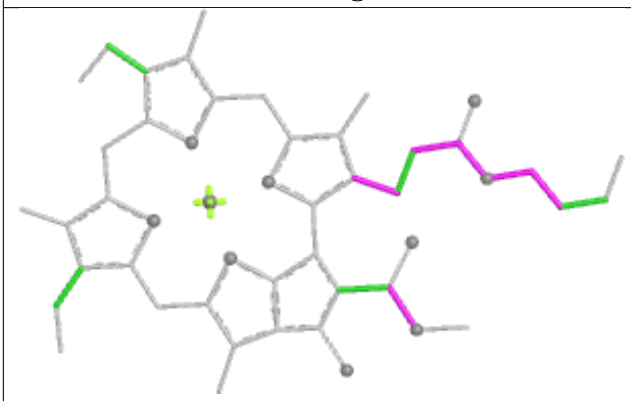
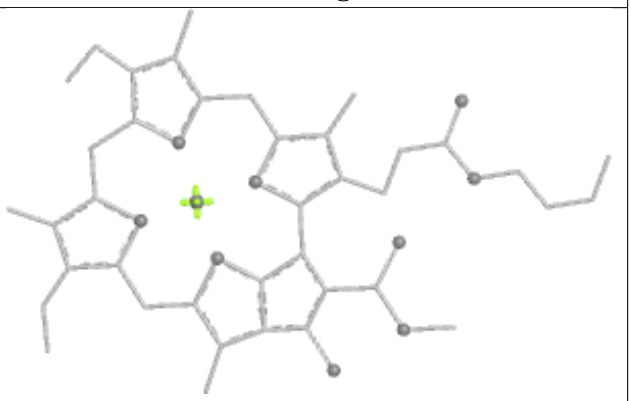
 Bond lengths	 Bond angles
 Torsions	 Rings

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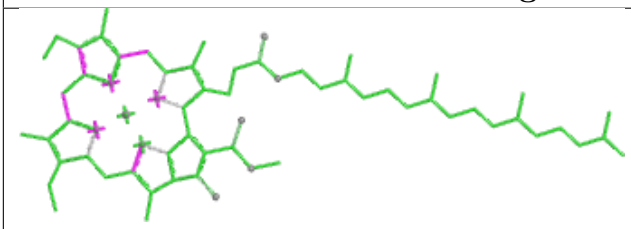
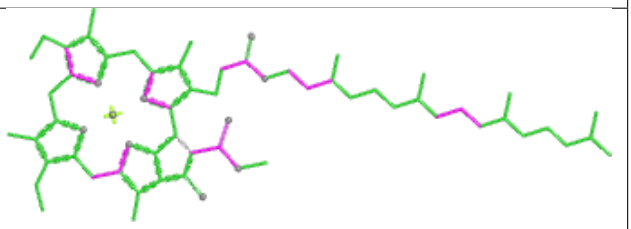
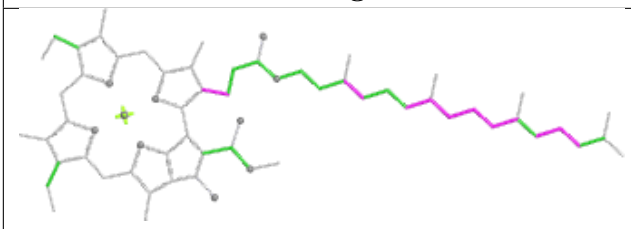
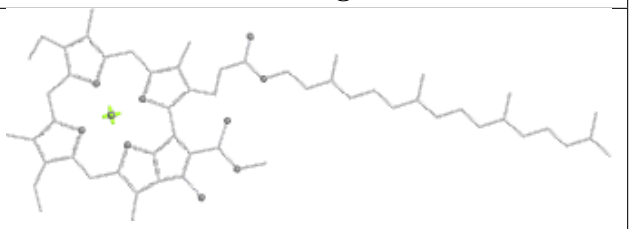
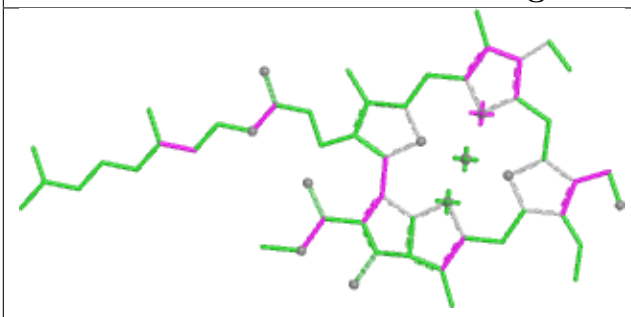
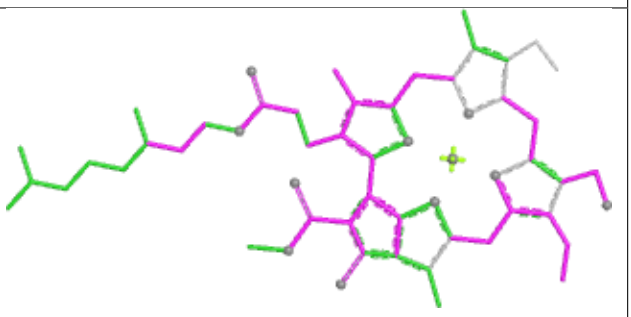
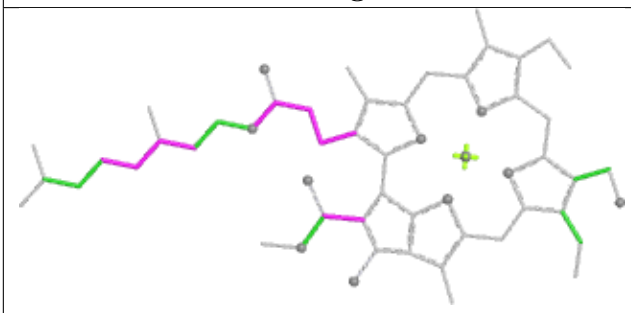
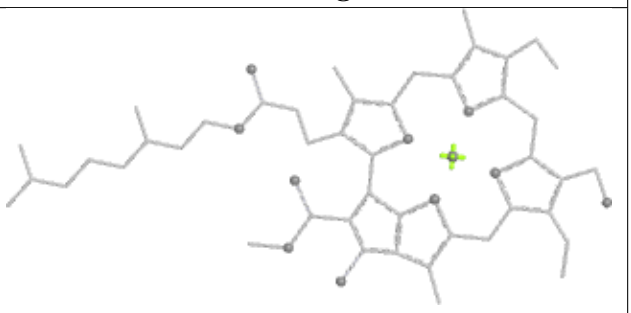
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 6 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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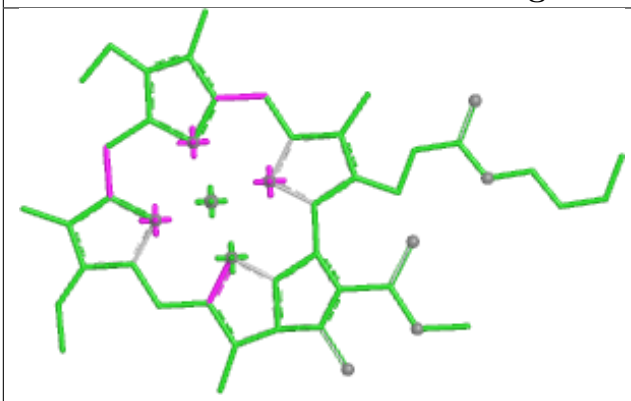
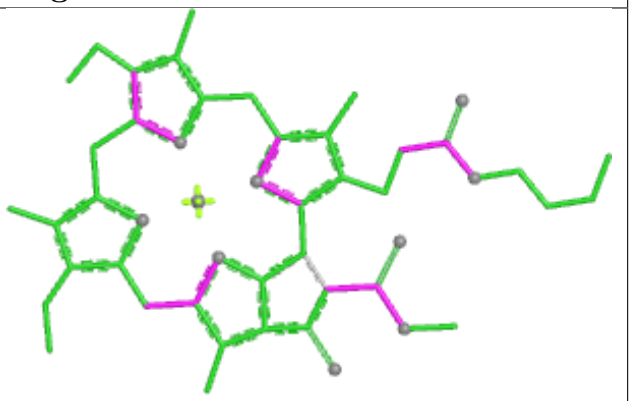
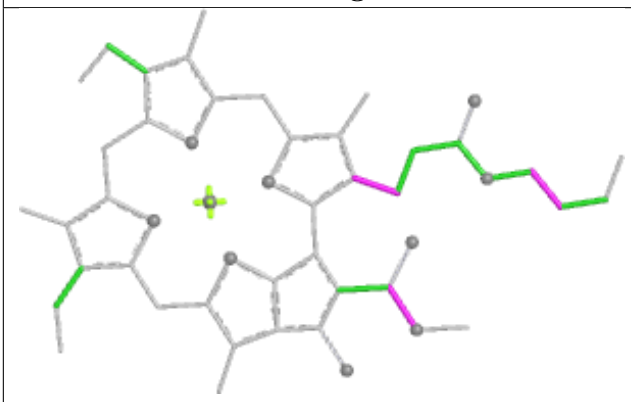
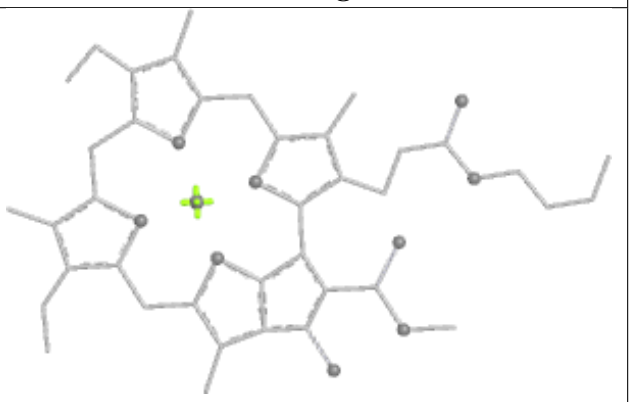
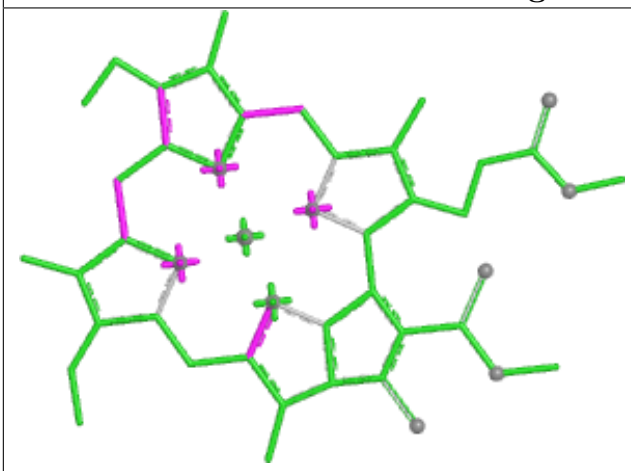
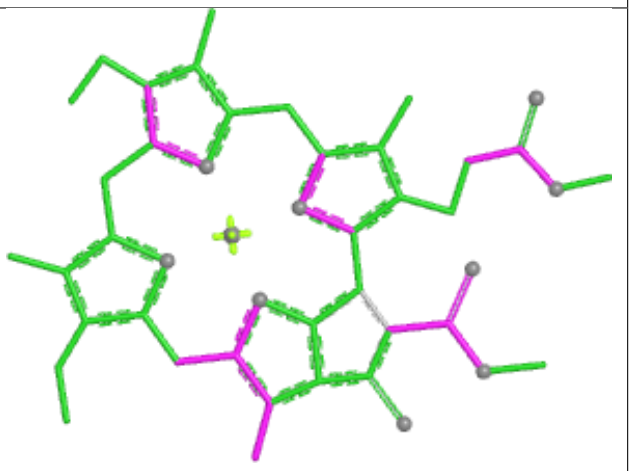
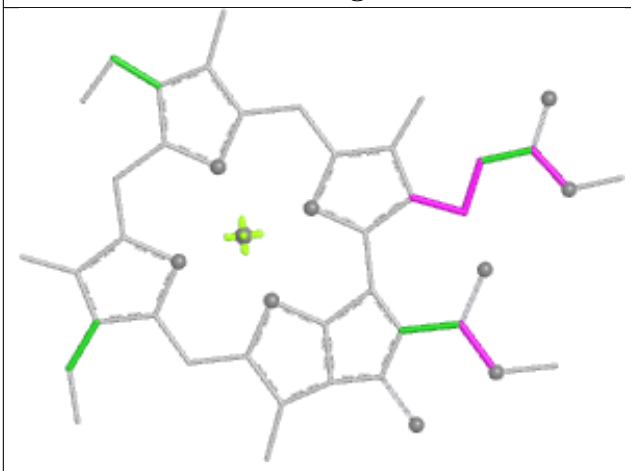
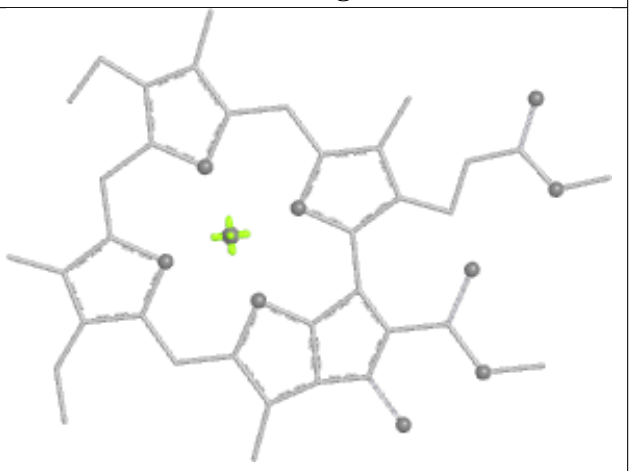
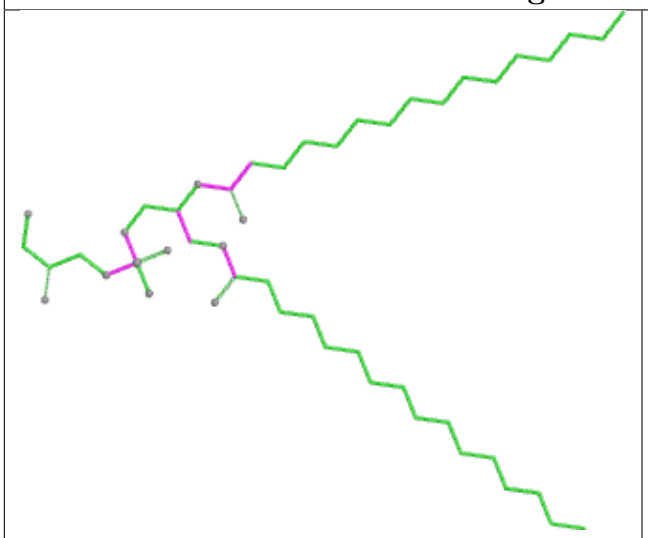
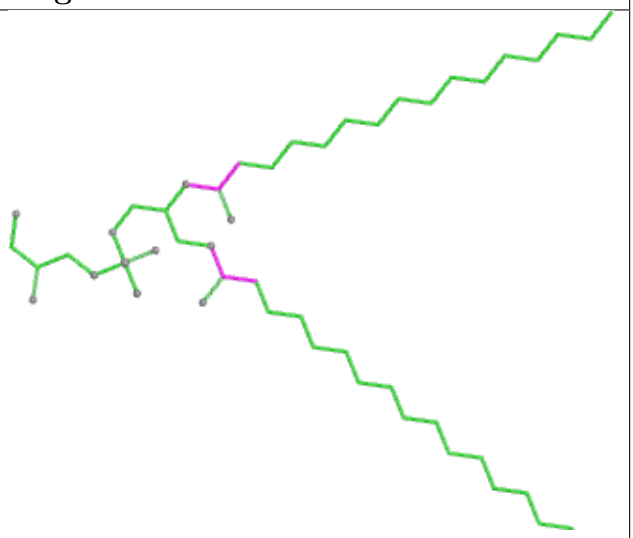
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

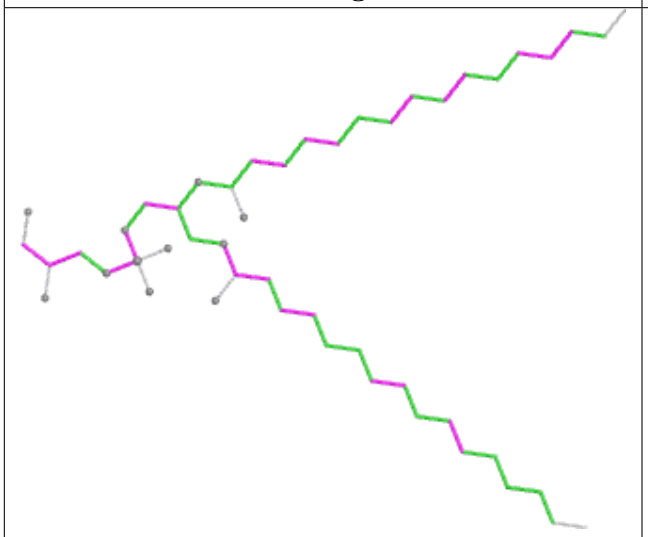
Ligand LHG g 615



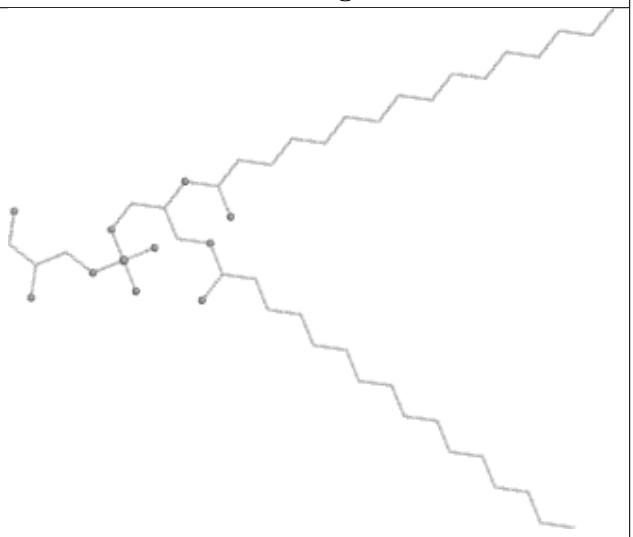
Bond lengths



Bond angles

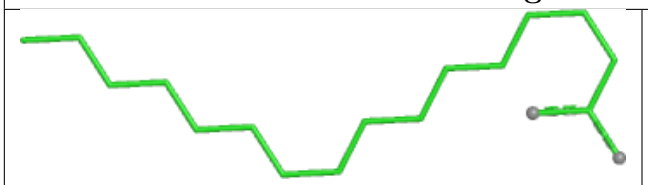


Torsions



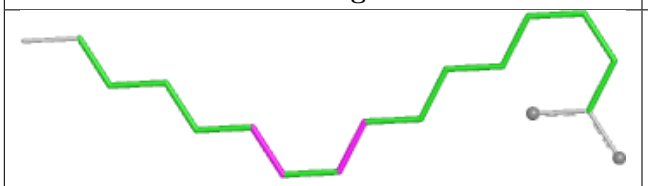
Rings

Ligand PAM n 620

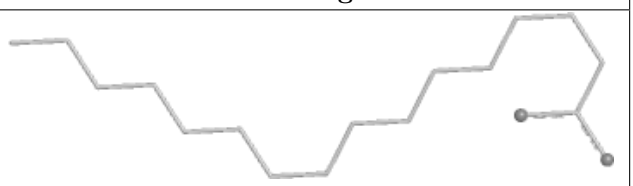


Bond lengths

Bond angles

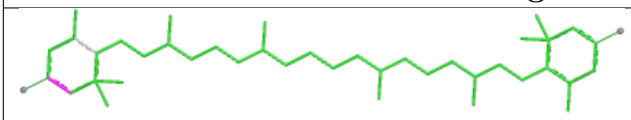


Torsions

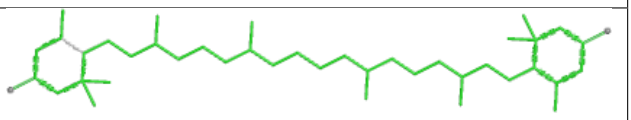


Rings

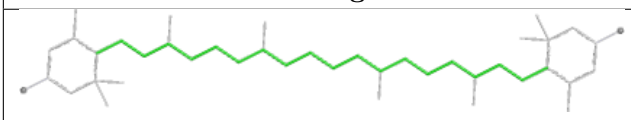
Ligand LUT S 619



Bond lengths



Bond angles



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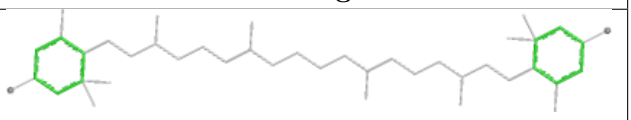
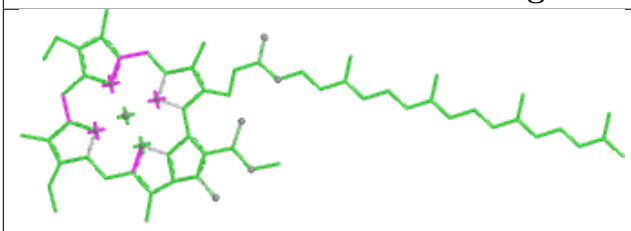


Rings

Ligand CLA b 607



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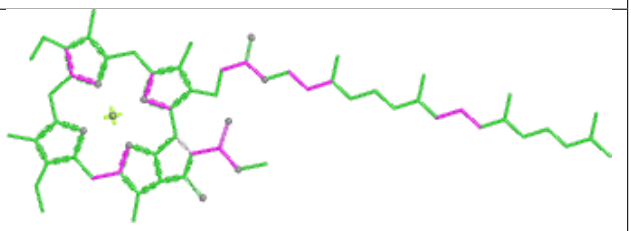
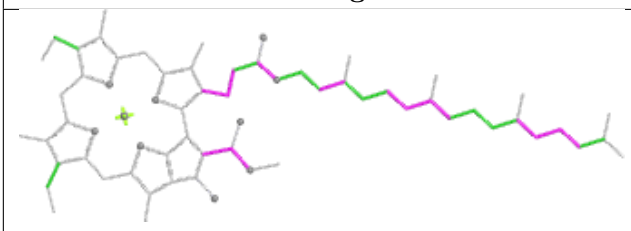


Bond angles



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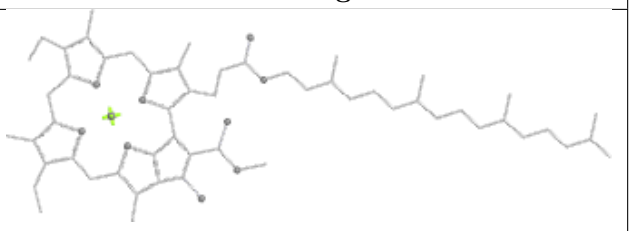
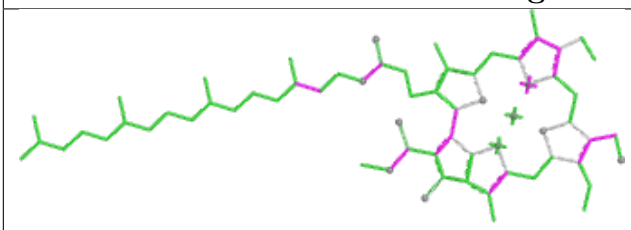
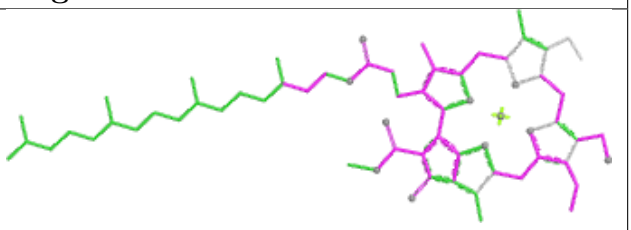


Rings

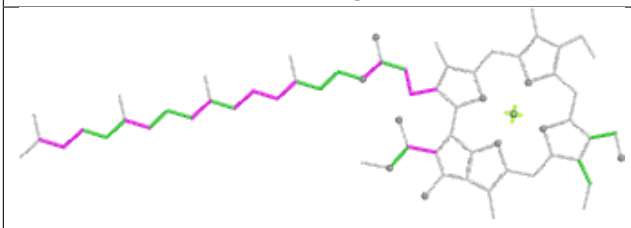
Ligand CHL g 601



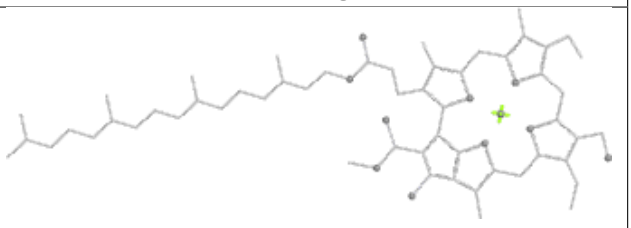
Bond lengths



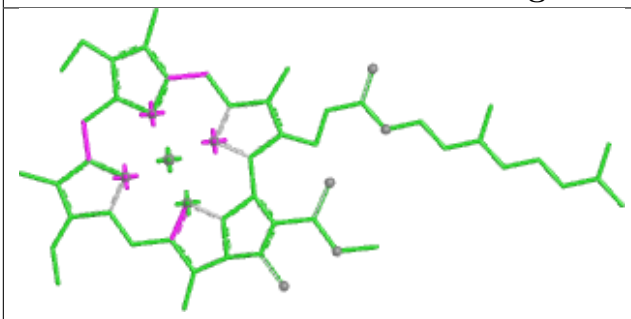
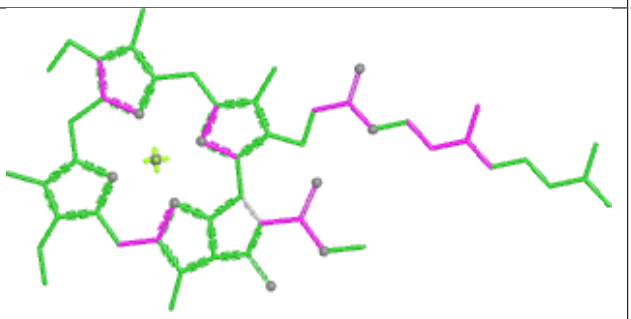
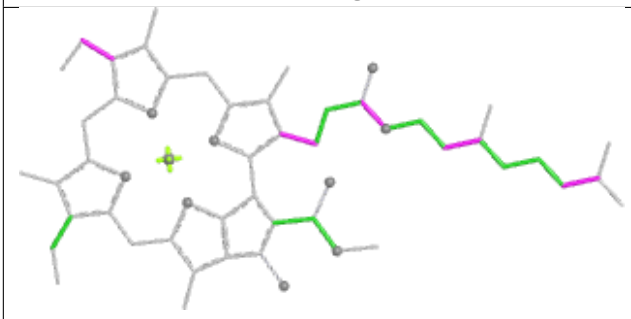
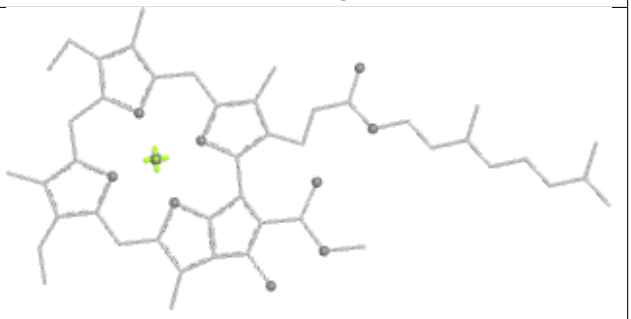
Bond angles

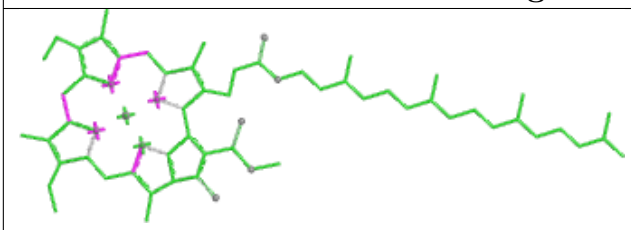
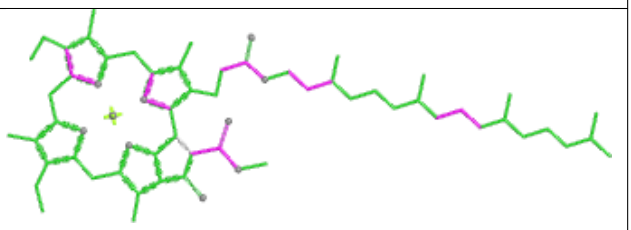
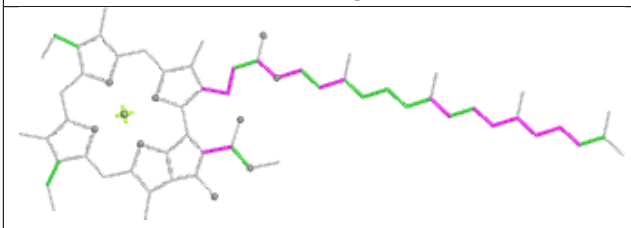
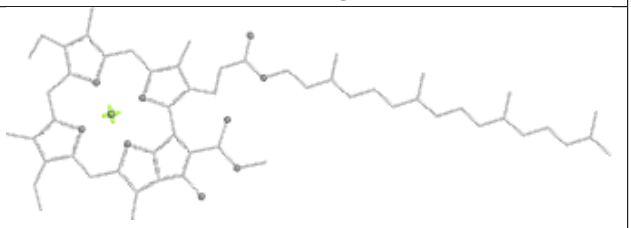


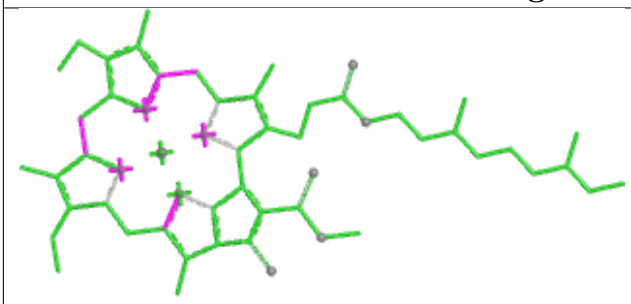
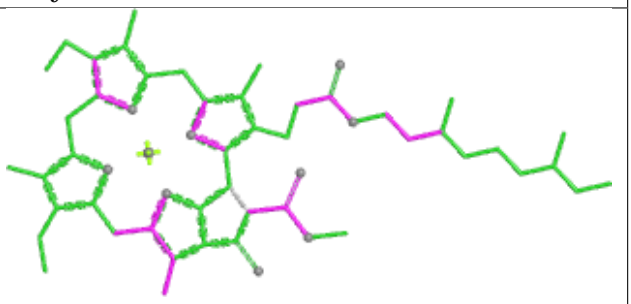
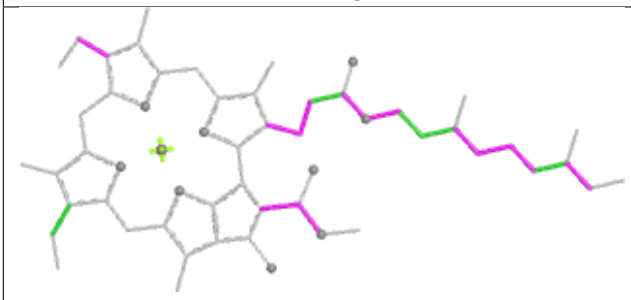
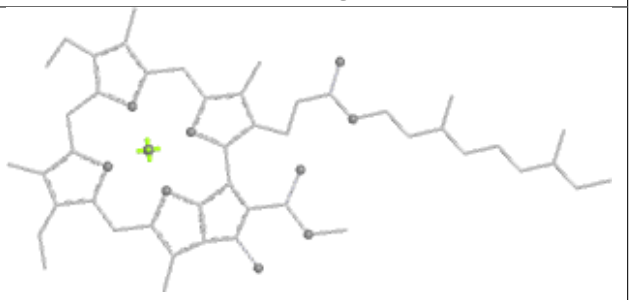
Torsions

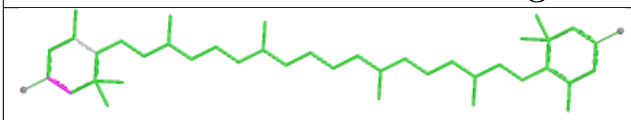
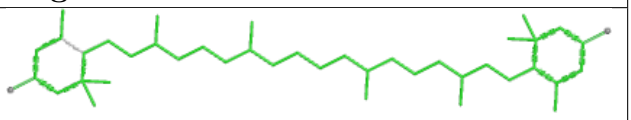
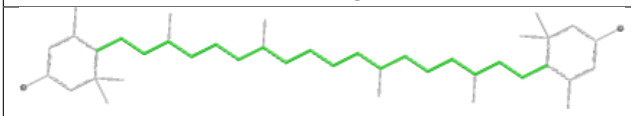
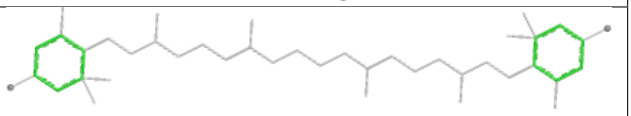


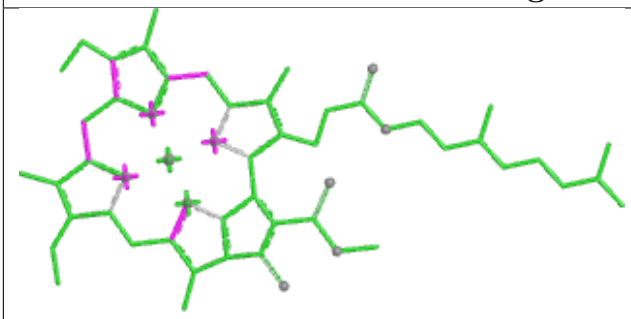
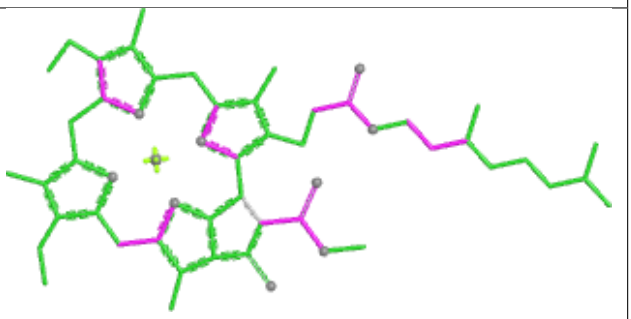
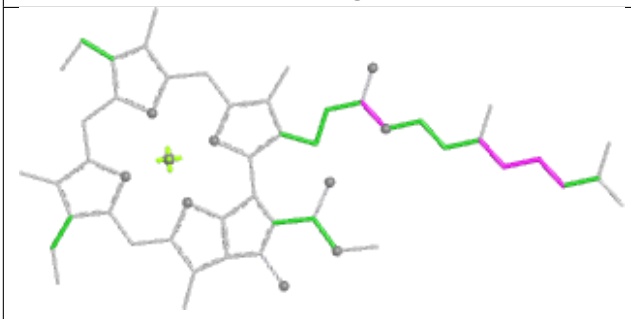
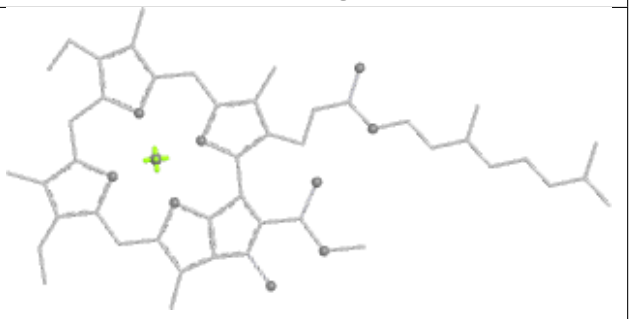
Rings

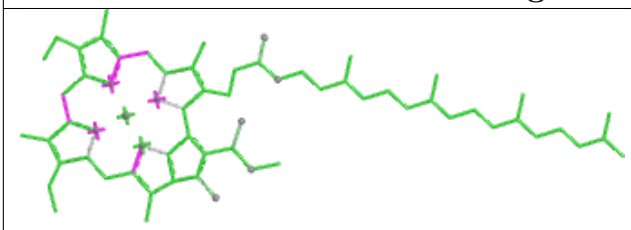
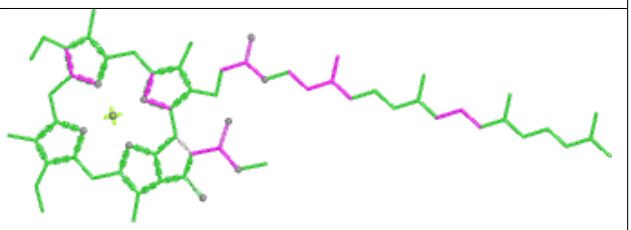
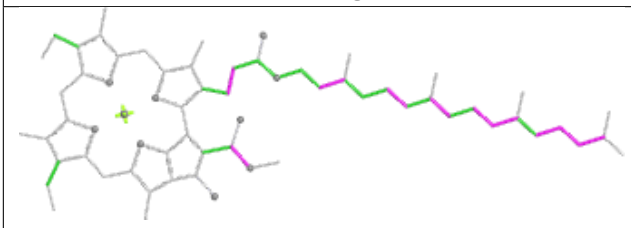
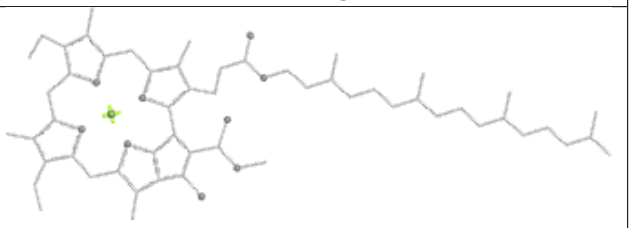
Ligand CLA 1 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

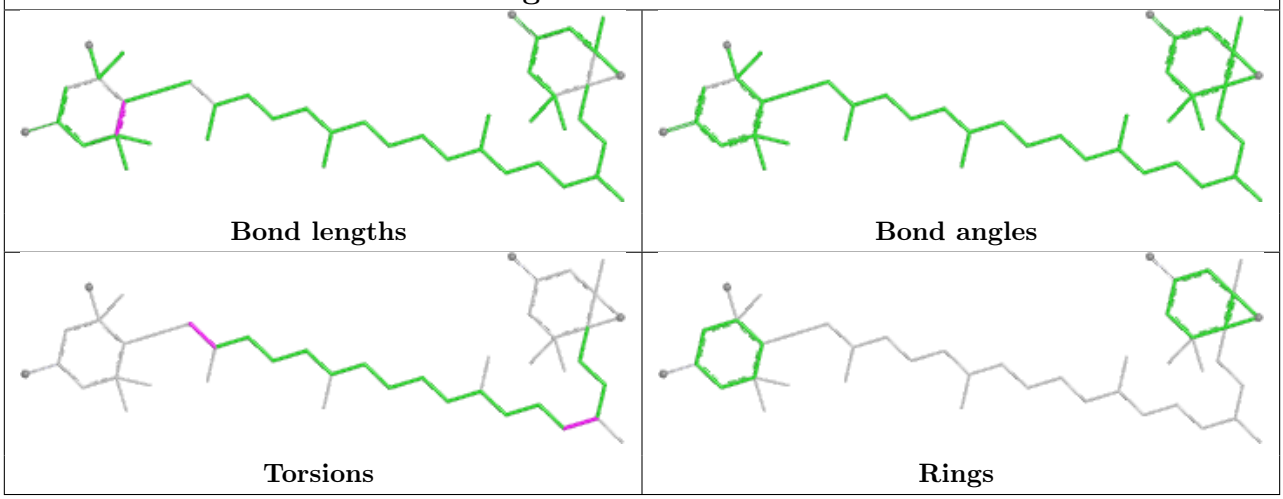
Ligand CLA y 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT g 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

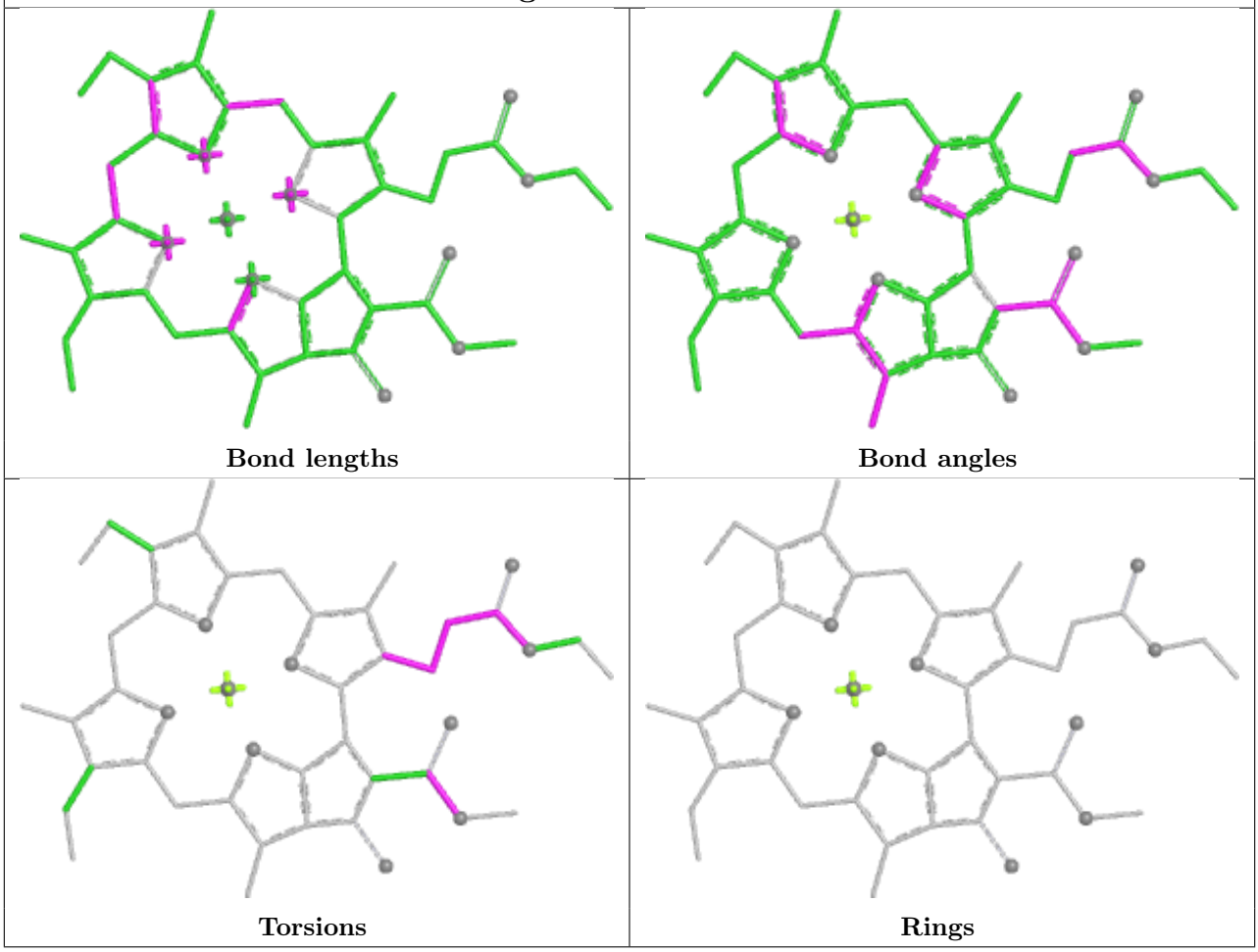
Ligand CLA S 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

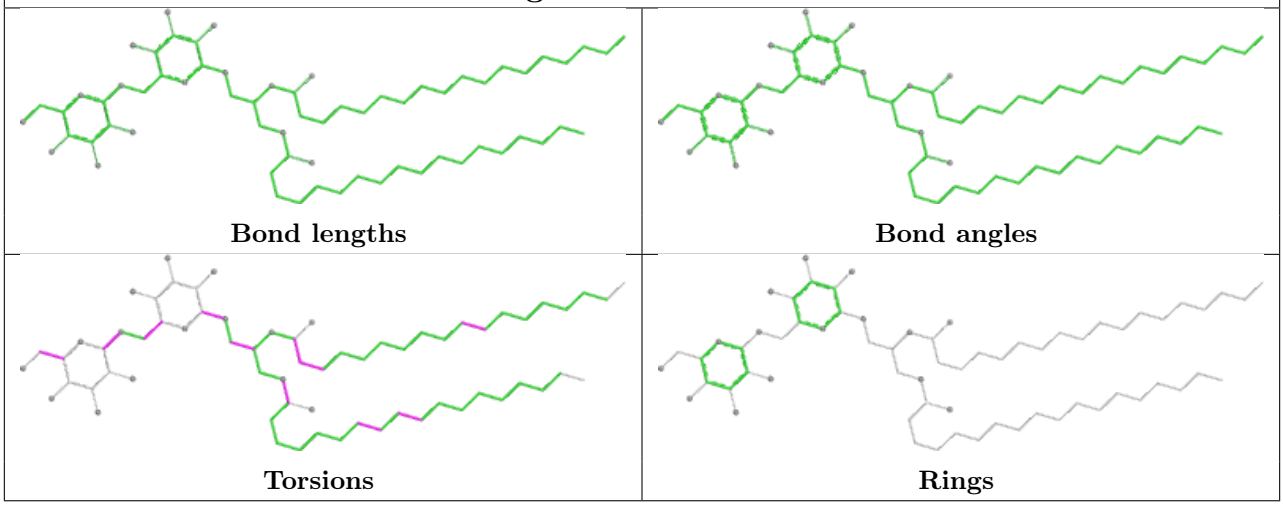
Ligand NEX R 617



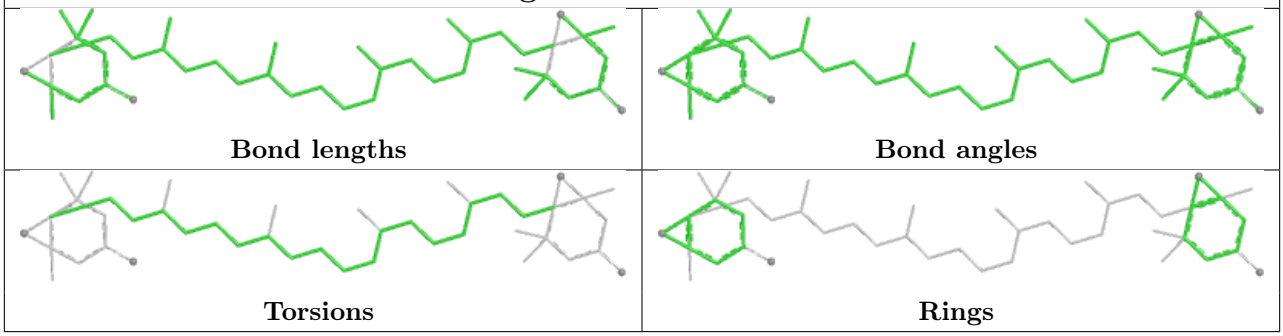
Ligand CLA 2 613



Ligand DGD c 517



Ligand XAT 11 619



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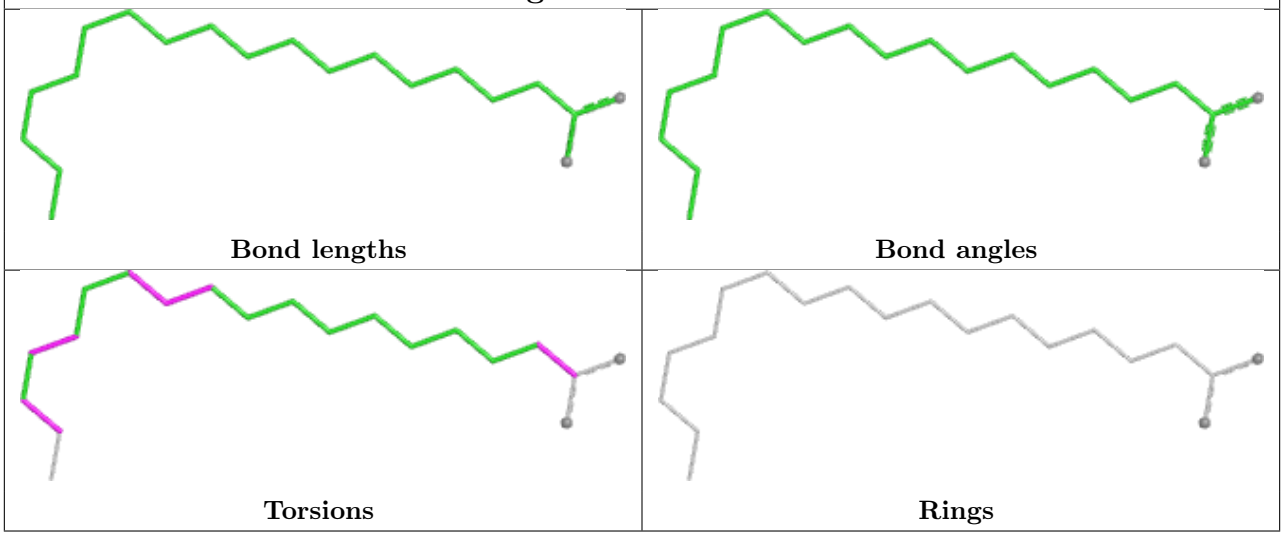
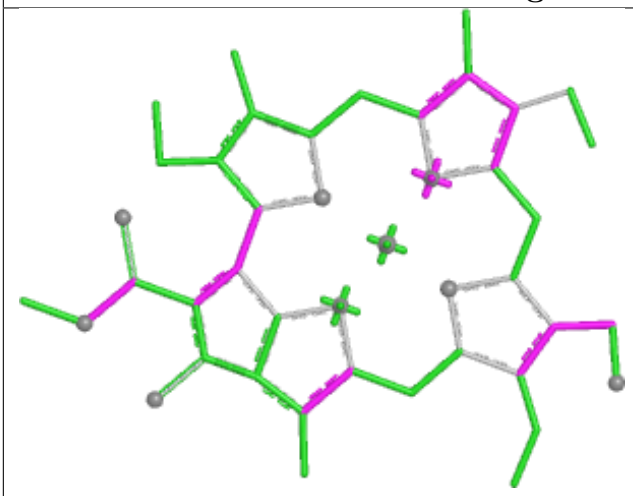
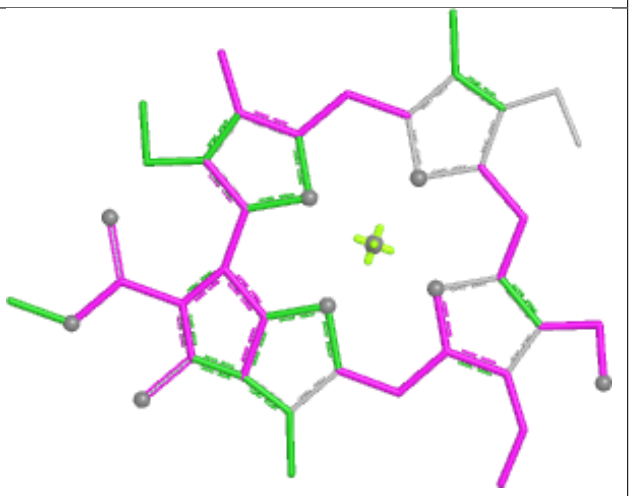


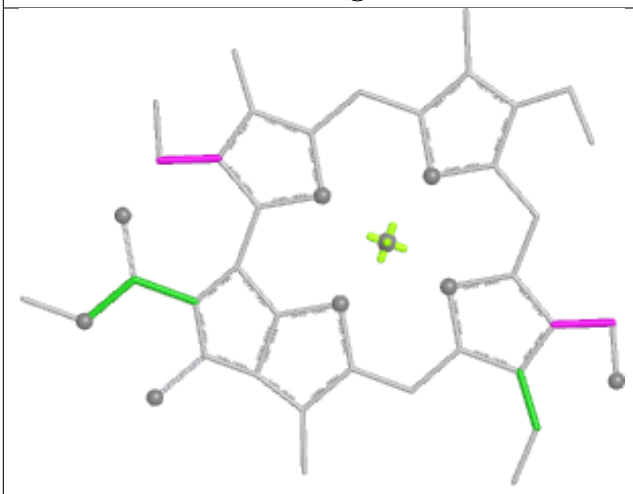
Ligand CHL S 607



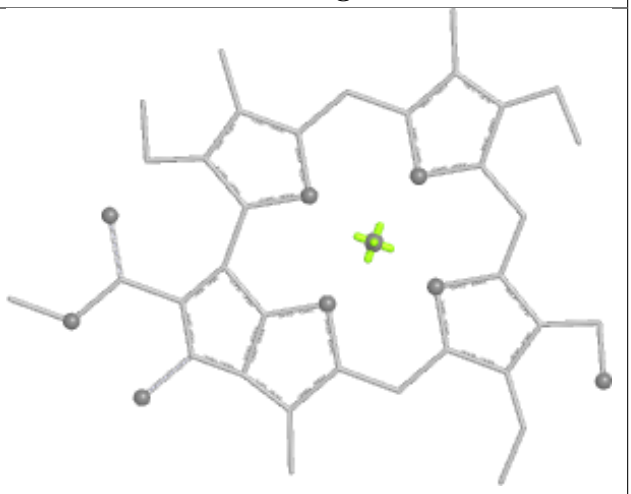
Bond lengths



Bond angles

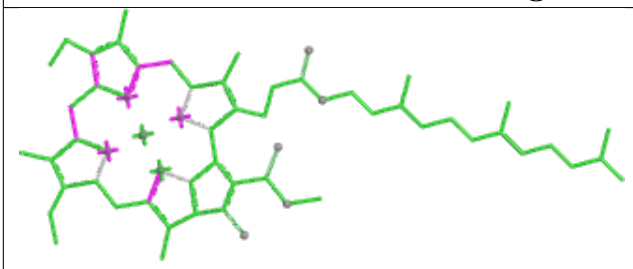


Torsions

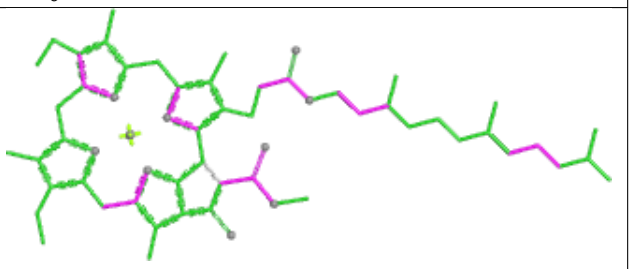


Rings

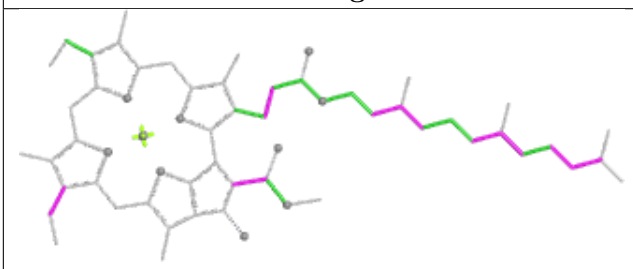
Ligand CLA y 602



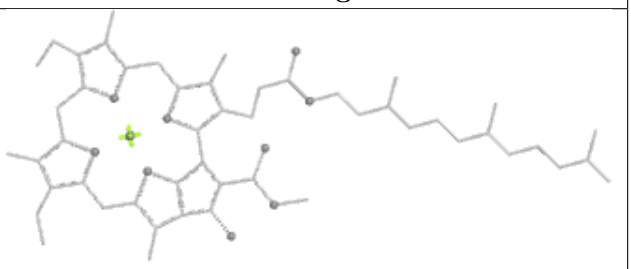
Bond lengths



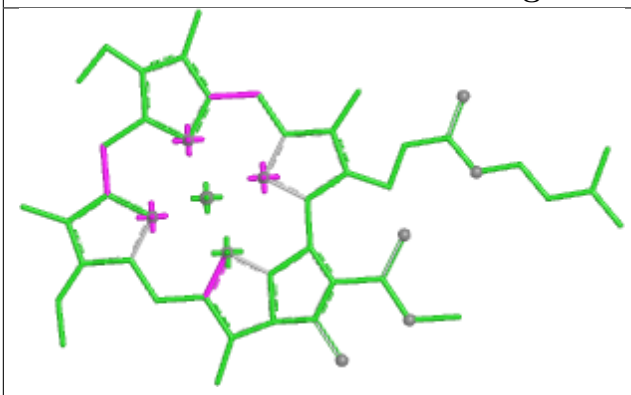
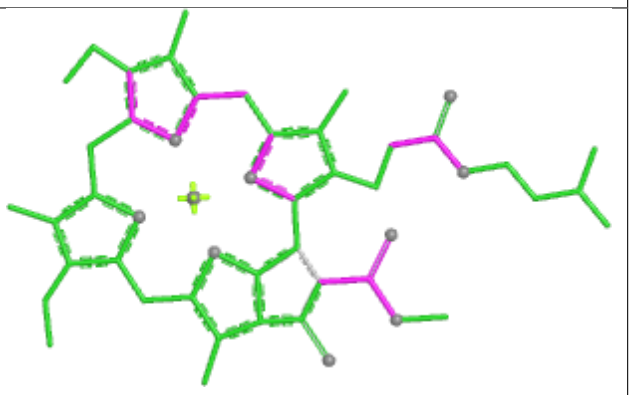
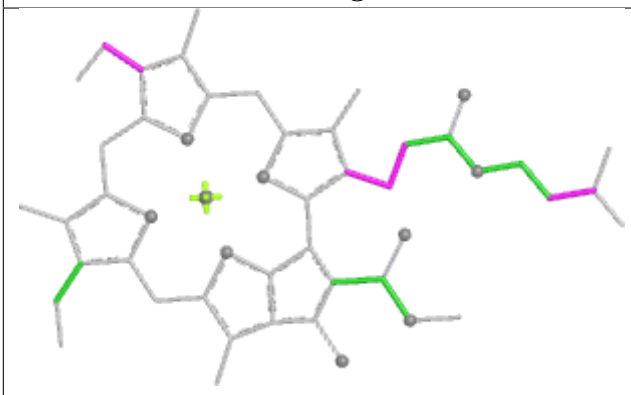
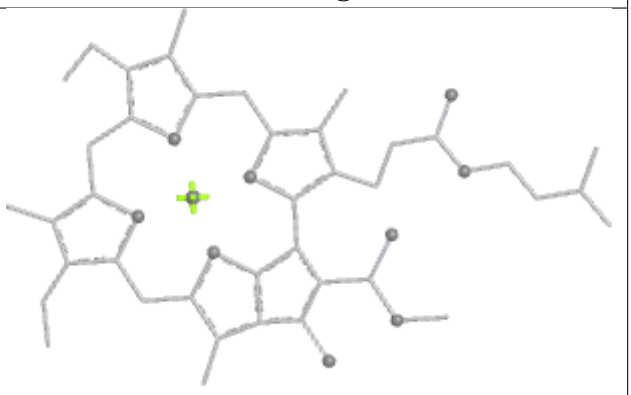
Bond angles

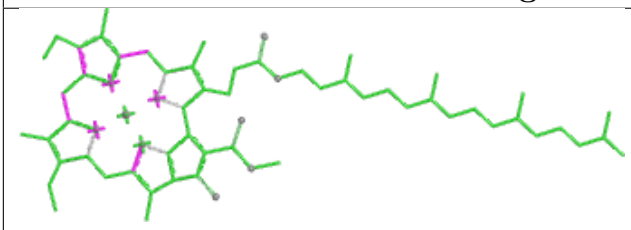
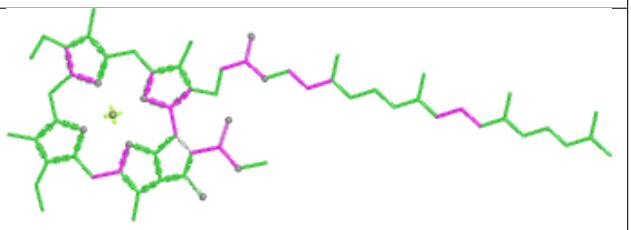
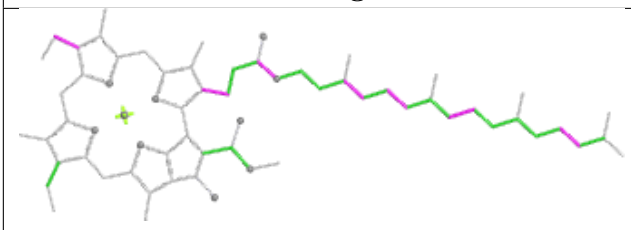
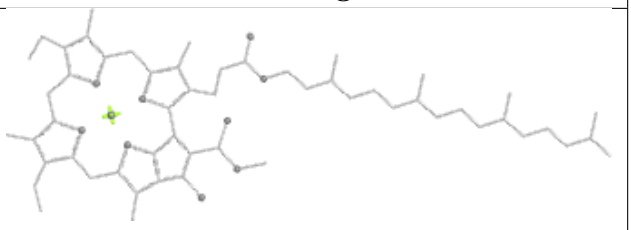


Torsions



Rings

Ligand CLA G 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 16 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

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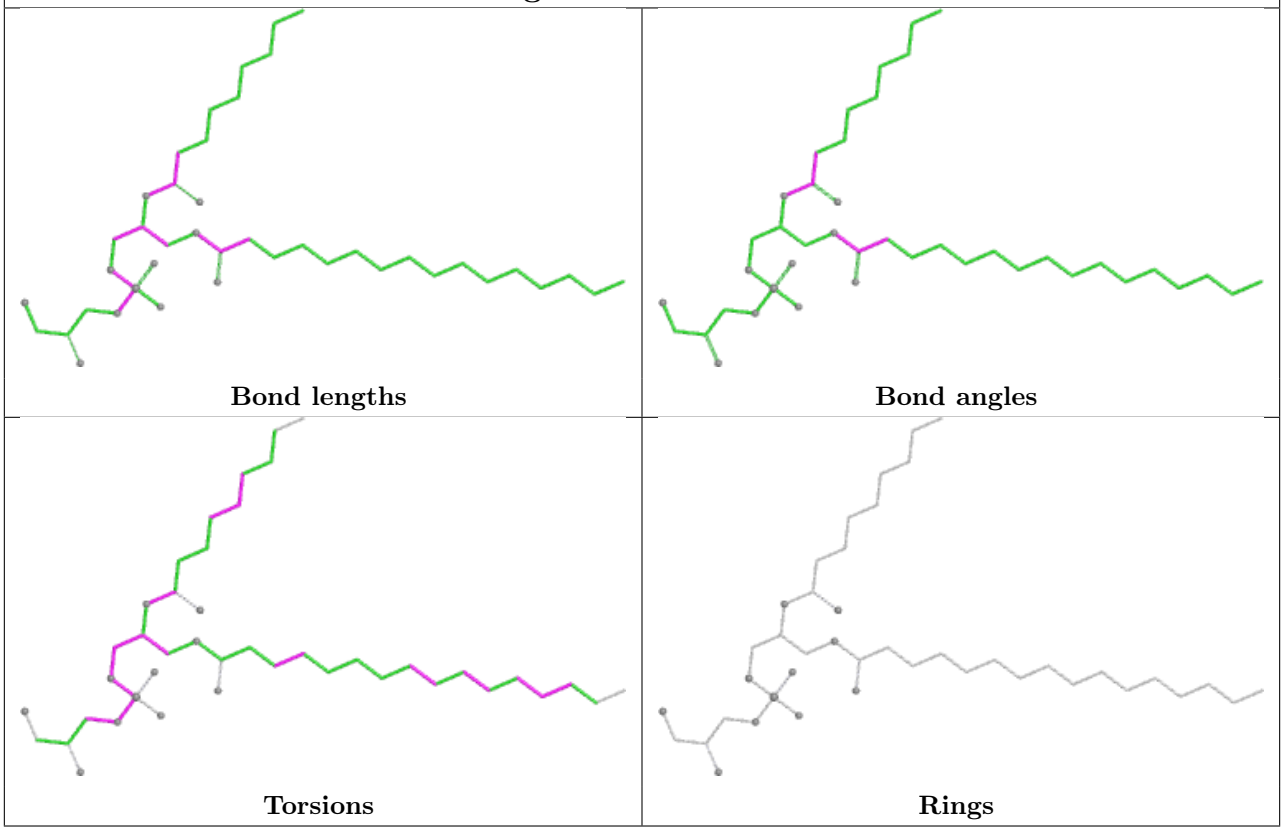

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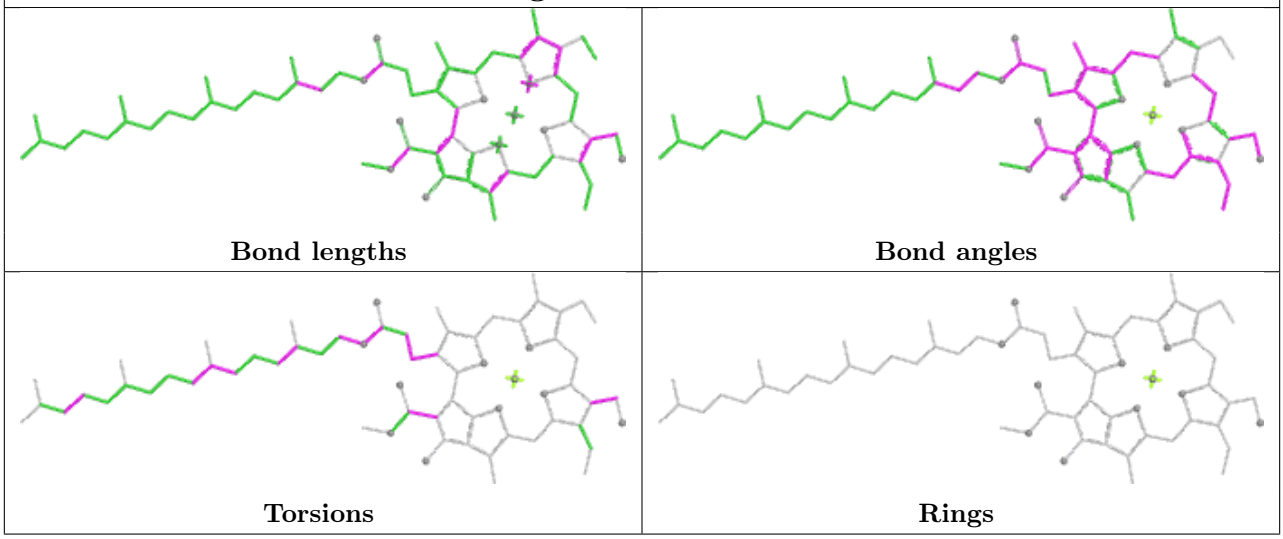
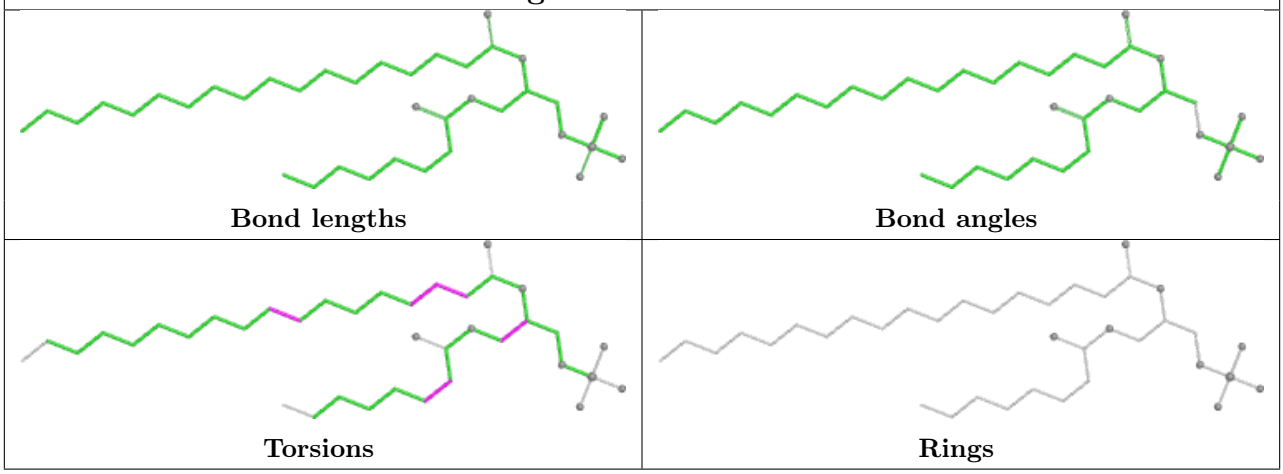
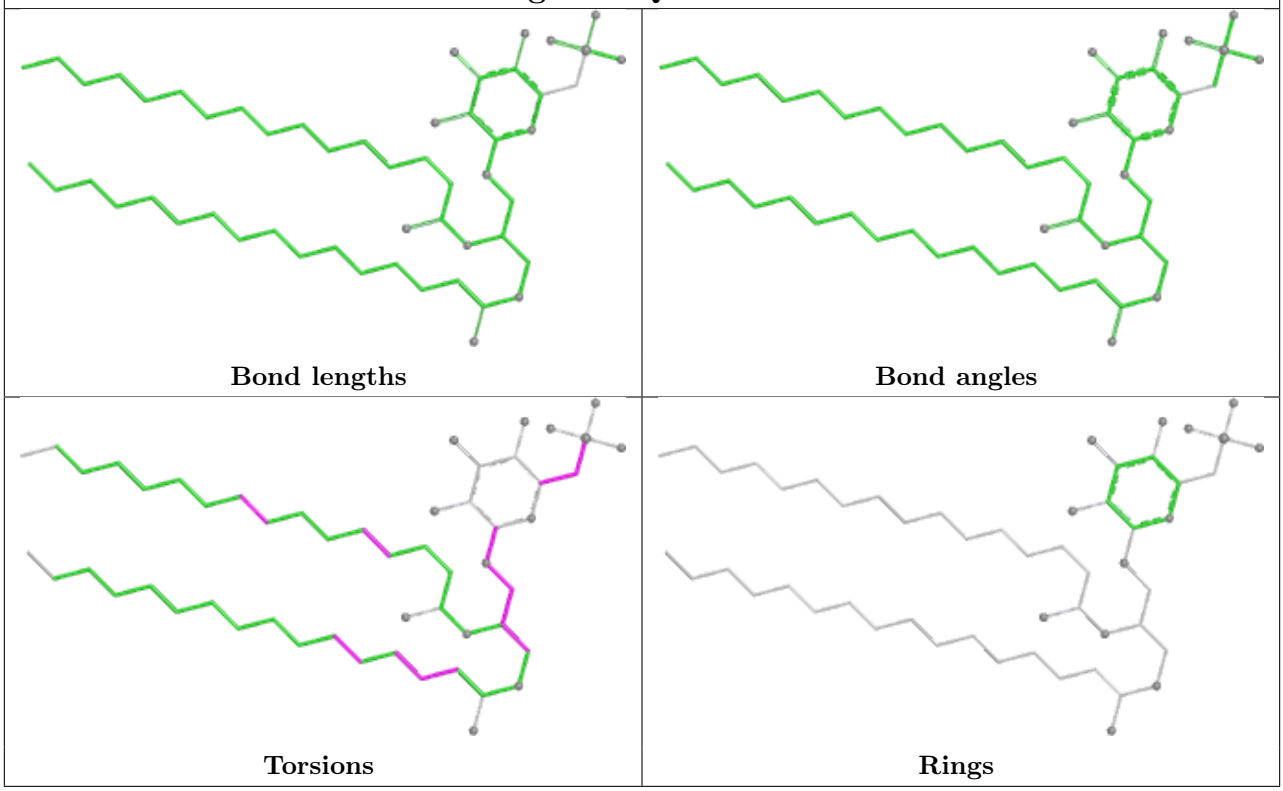


Ligand 3PH B 624



Ligand SQD d 412



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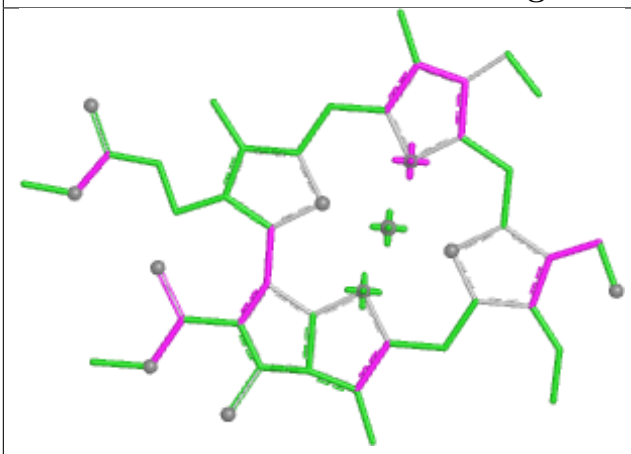
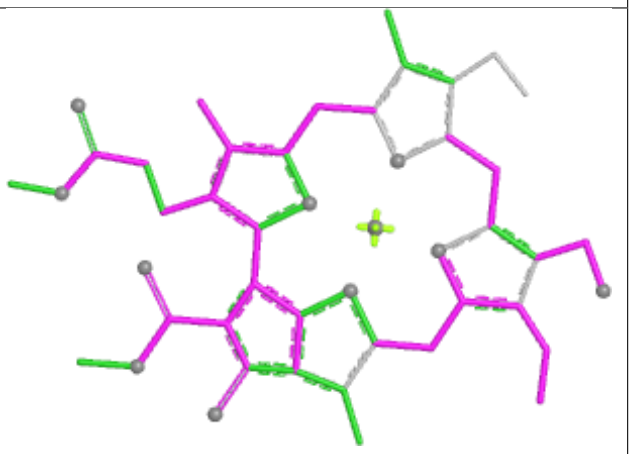
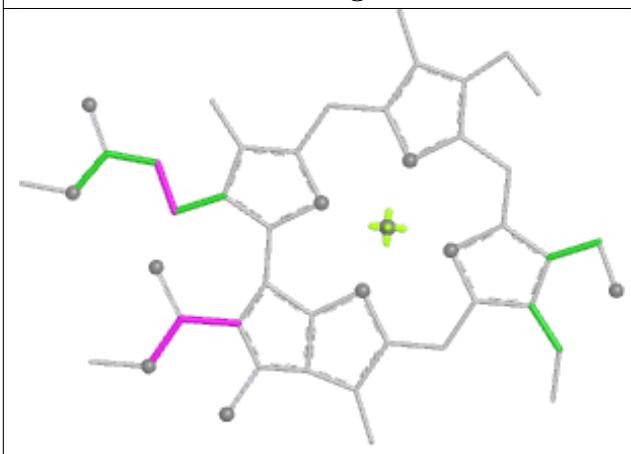
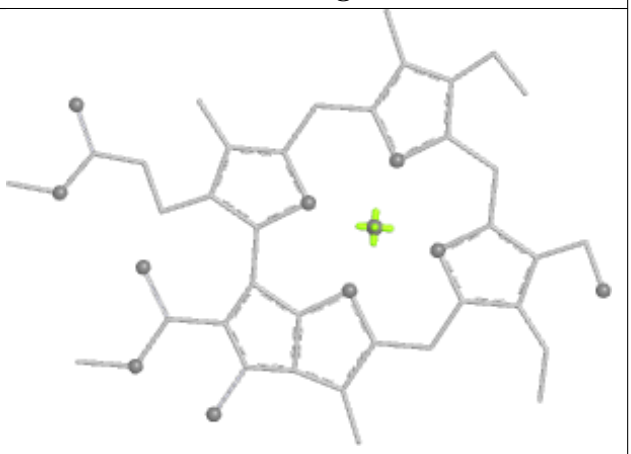
 Bond lengths	 Bond angles
 Torsions	 Rings

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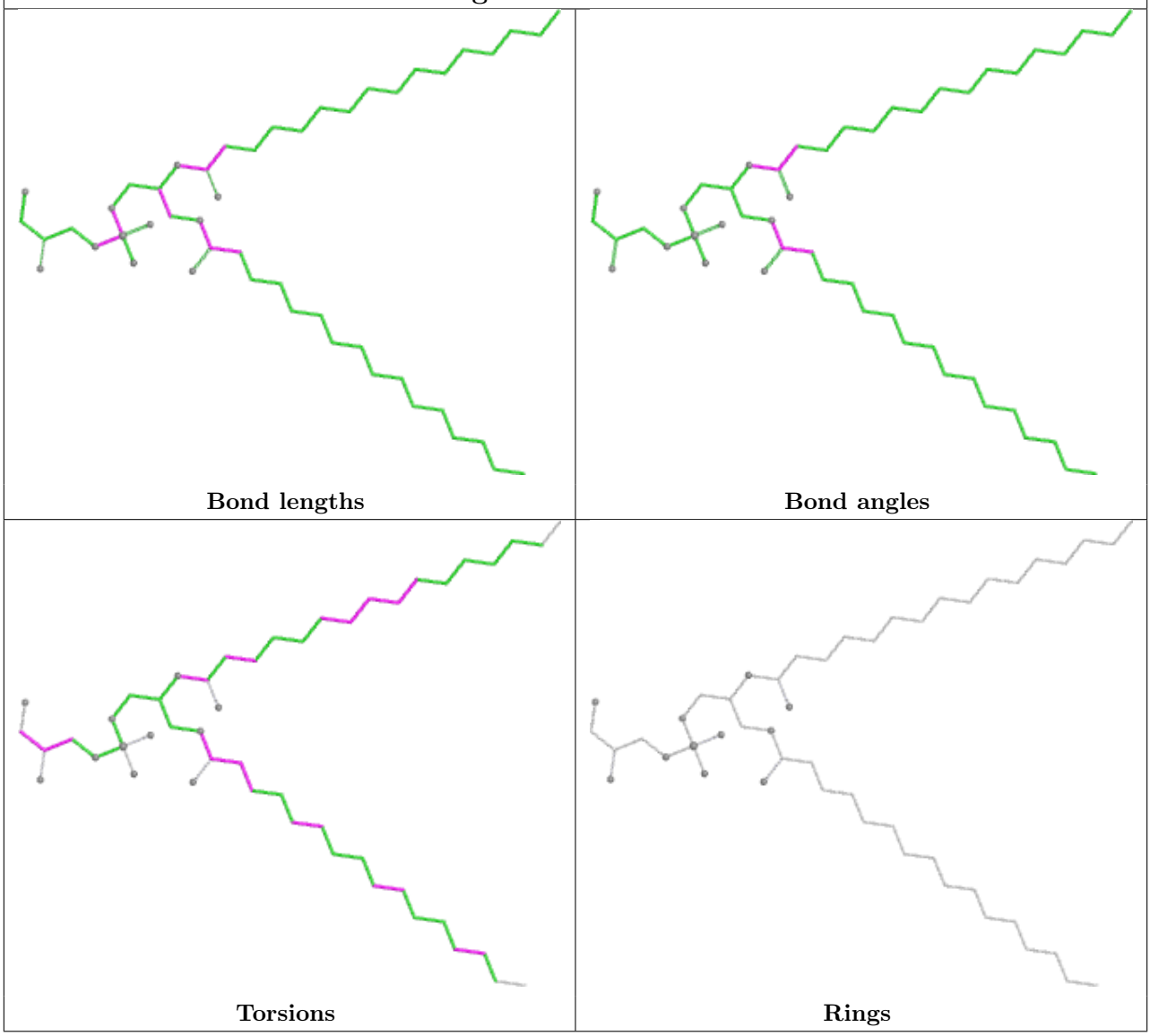
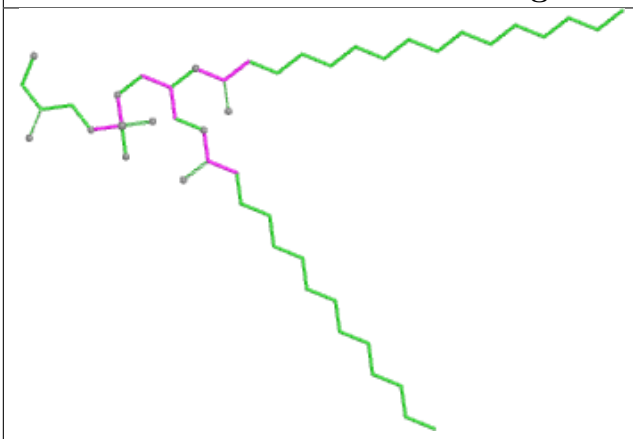
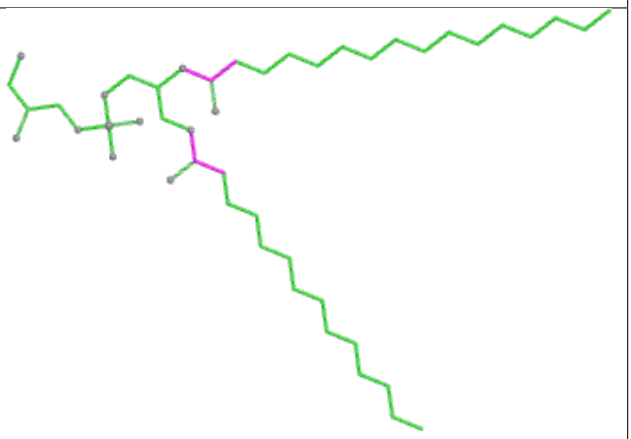


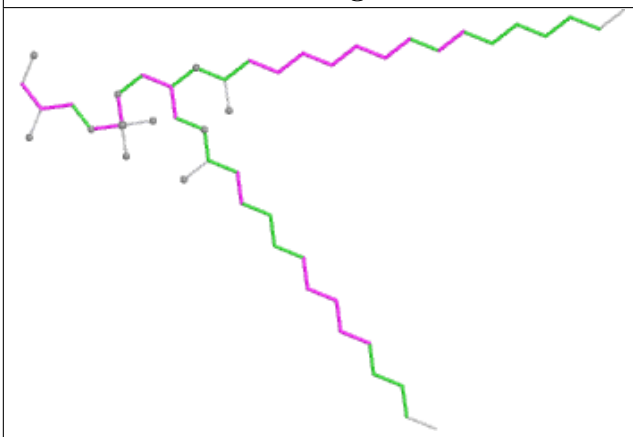
Ligand LHG l 102



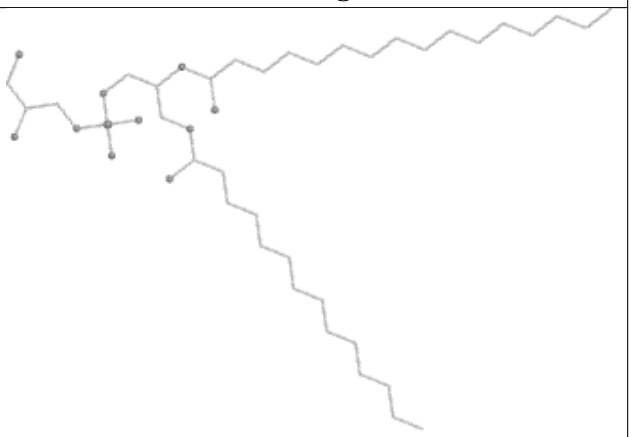
Bond lengths



Bond angles

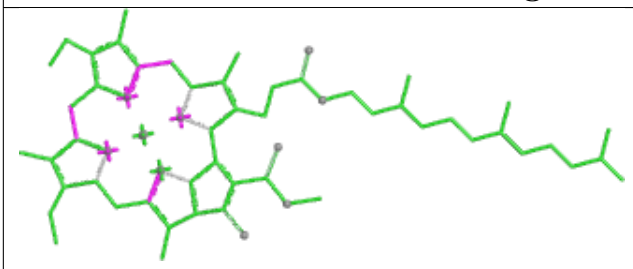


Torsions



Rings

Ligand CLA Y 603



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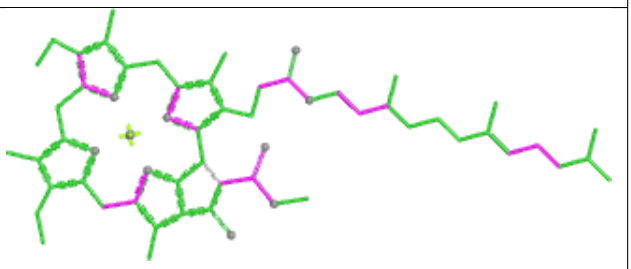

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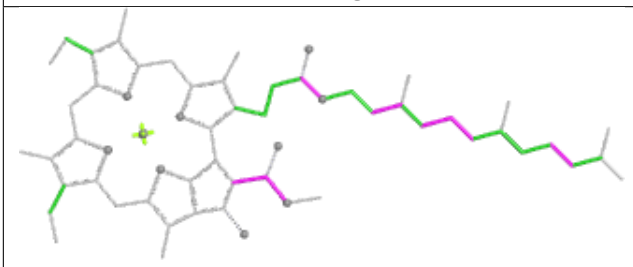

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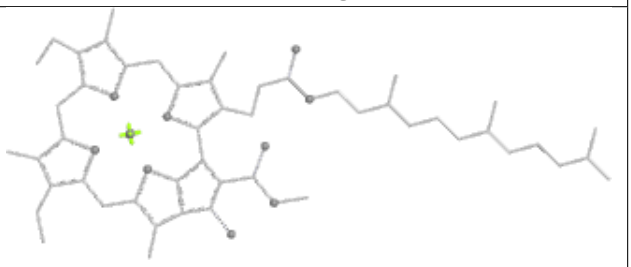
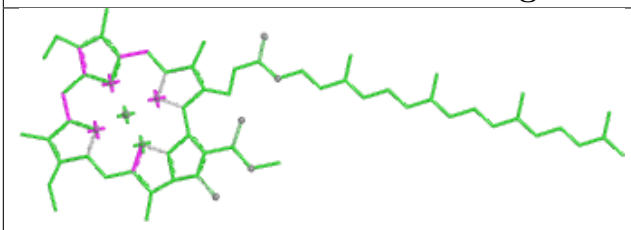
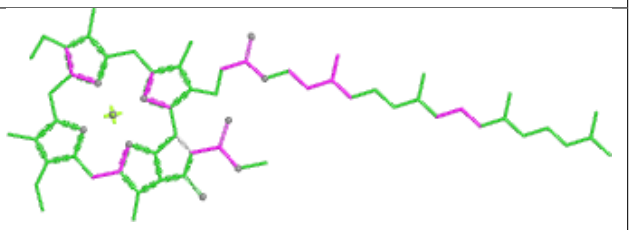
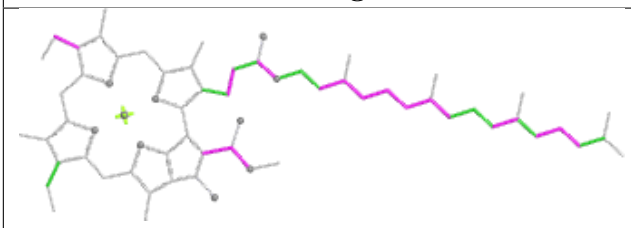
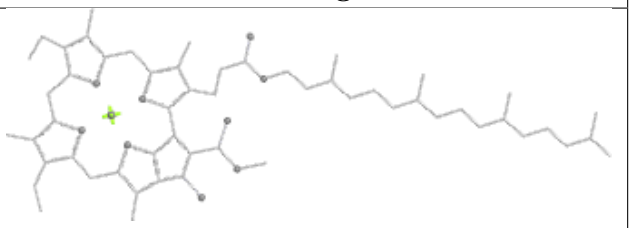


Rings

Ligand CLA 13 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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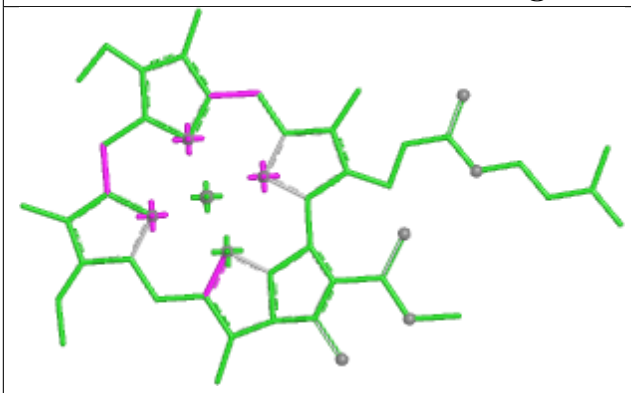
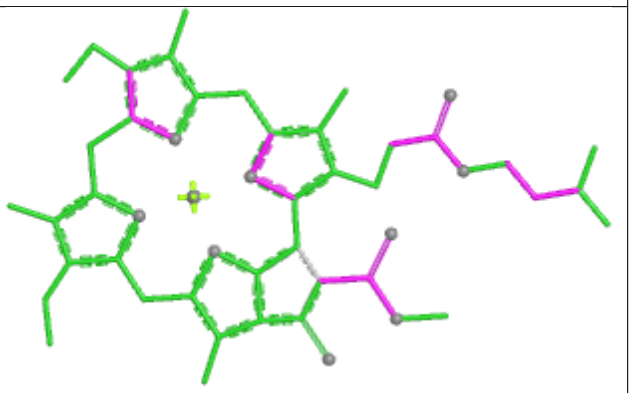
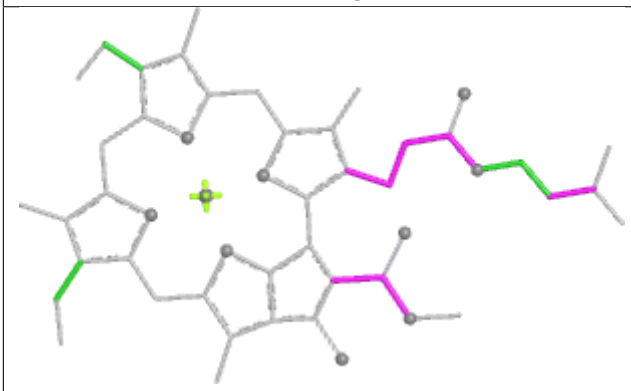
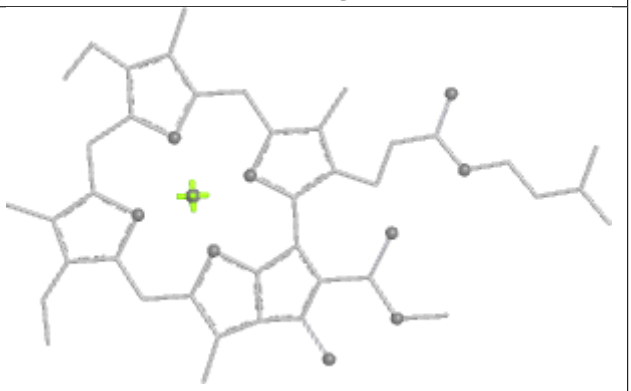
 Bond lengths	 Bond angles
 Torsions	 Rings

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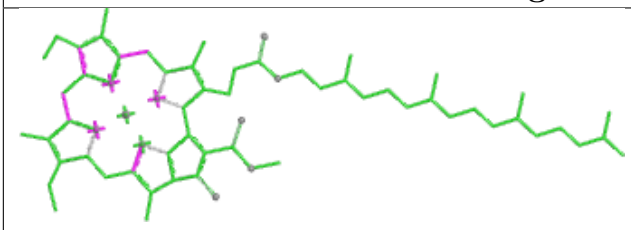
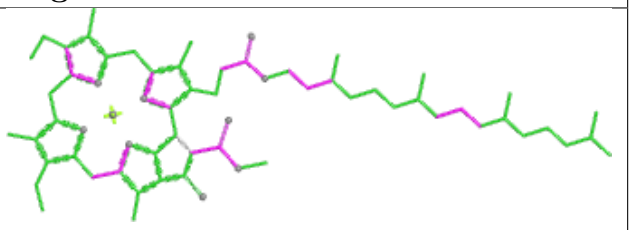
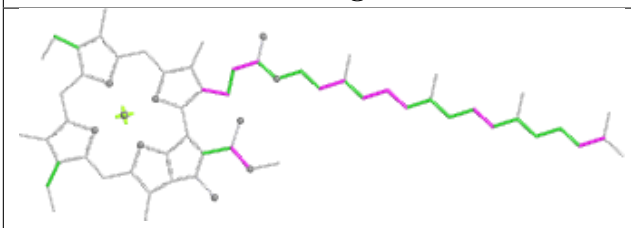
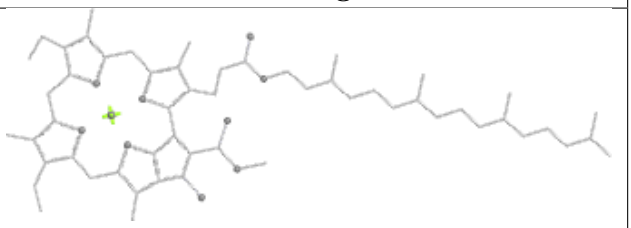
 Bond lengths	 Bond angles
 Torsions	 Rings

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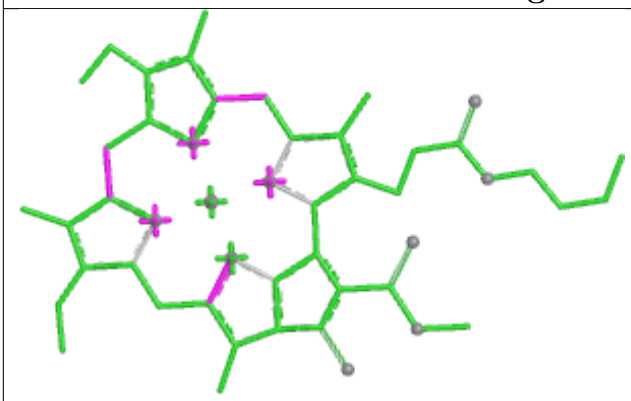
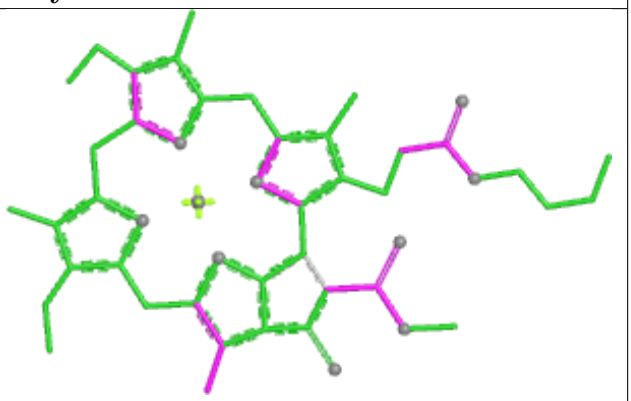
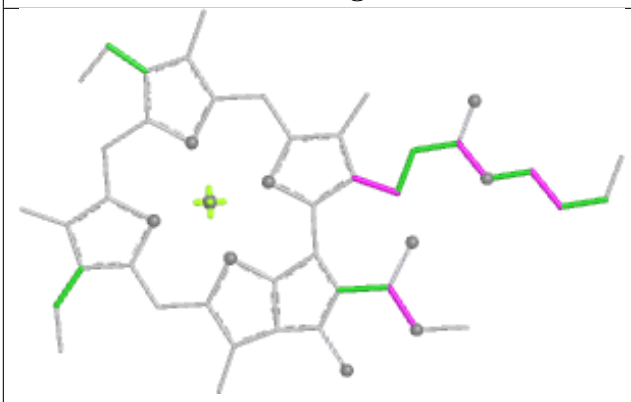
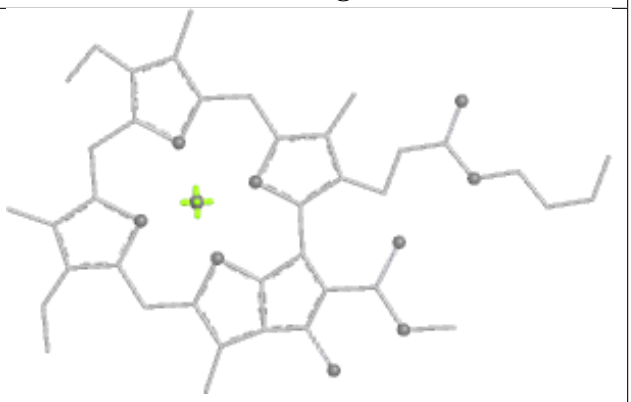
 Bond lengths	 Bond angles
 Torsions	 Rings

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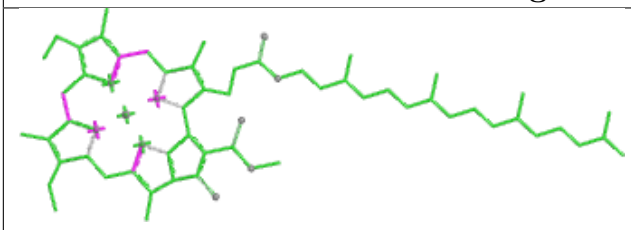
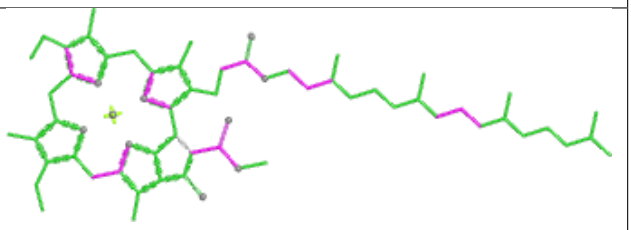
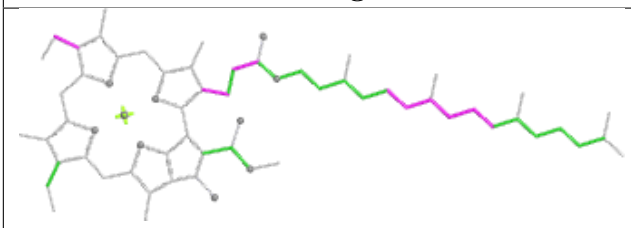
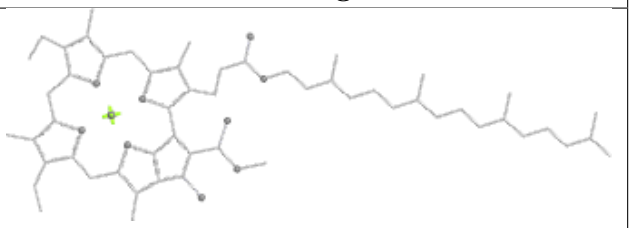
 Bond lengths	 Bond angles
 Torsions	 Rings

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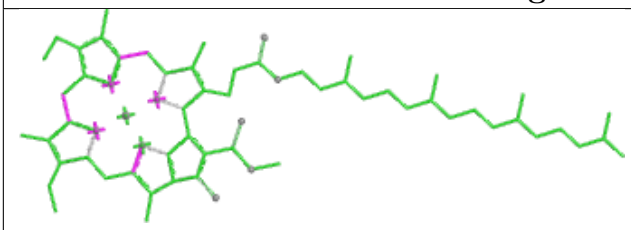
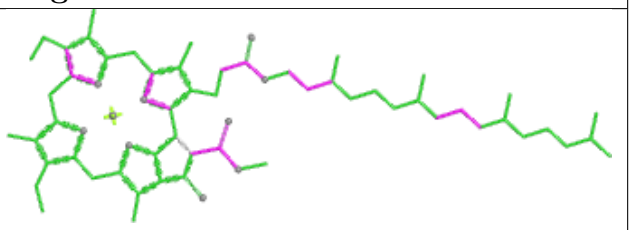
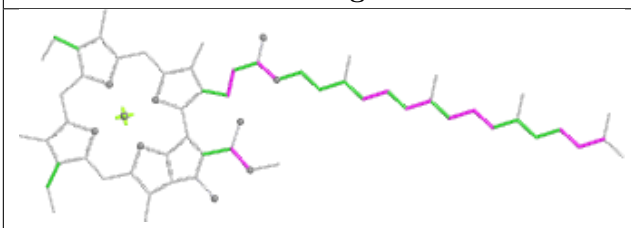
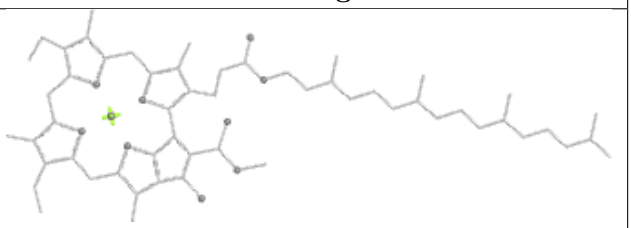
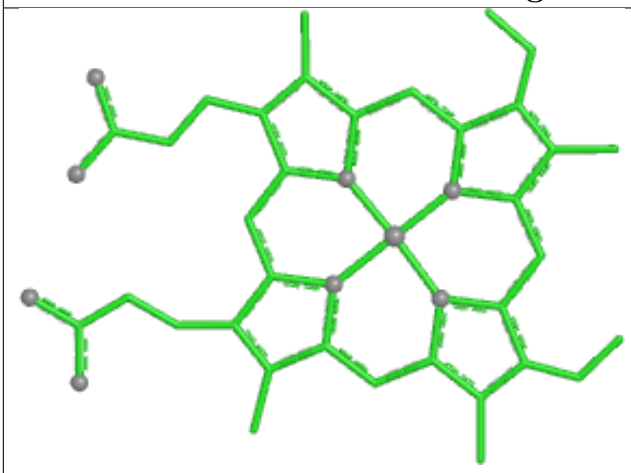
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM f 101



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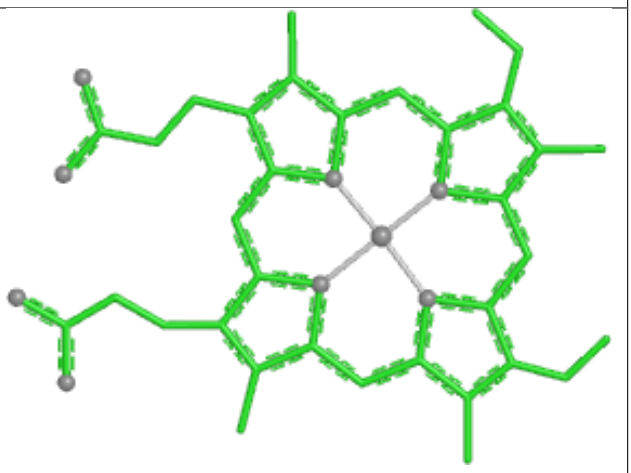
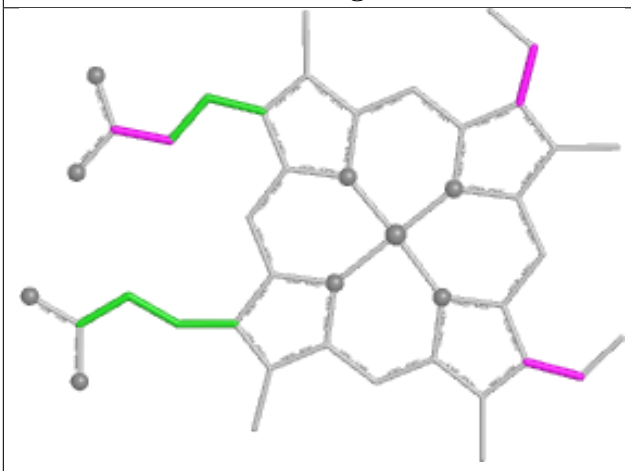
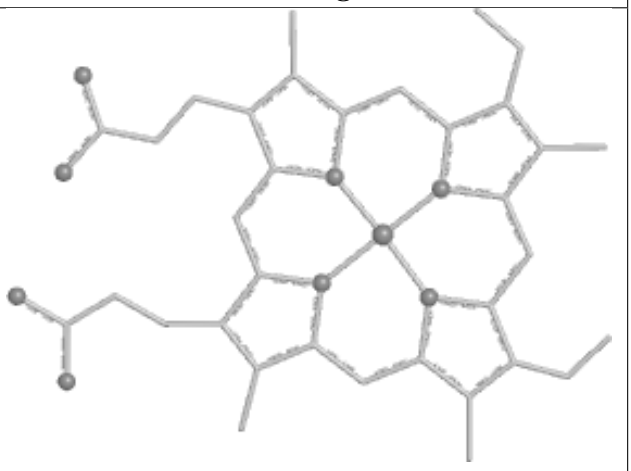


Bond angles

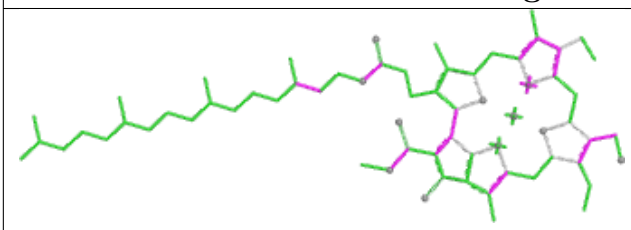


Torsions

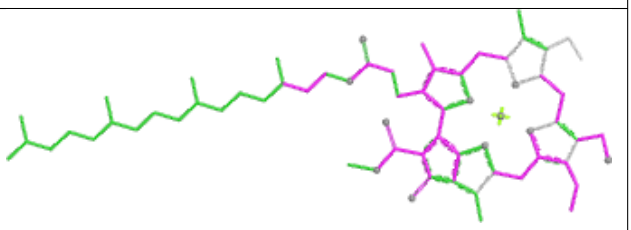


Rings

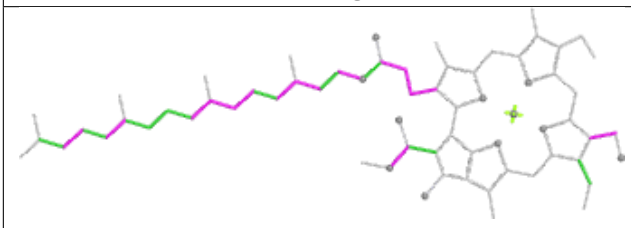
Ligand CHL Y 607



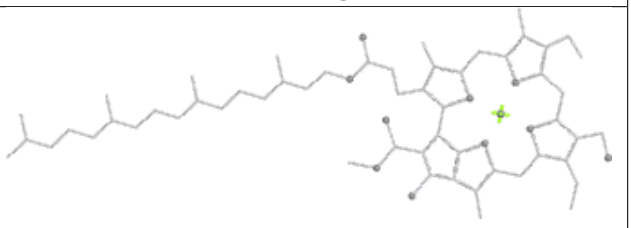
Bond lengths



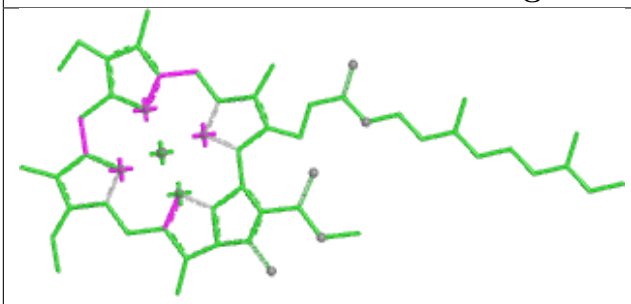
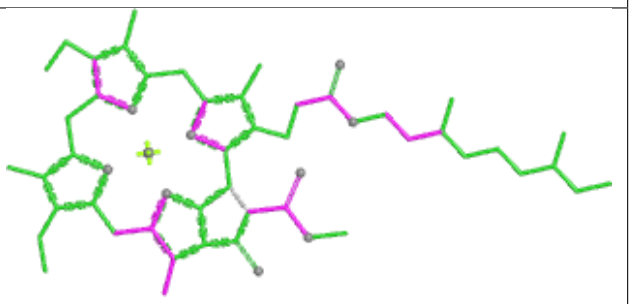
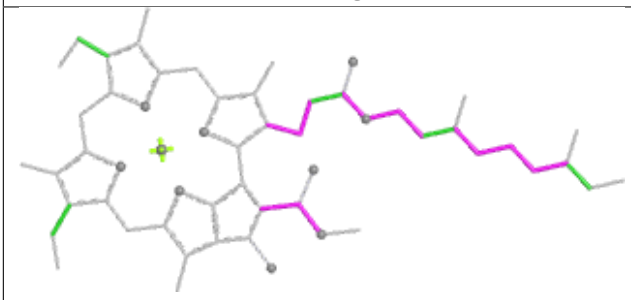
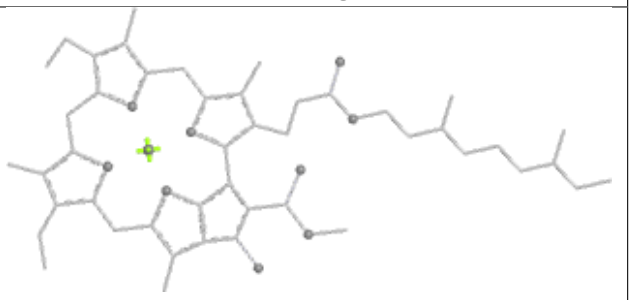
Bond angles

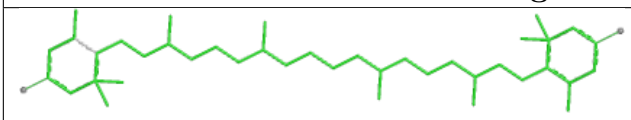
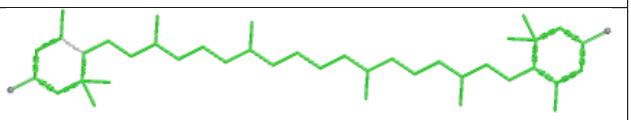
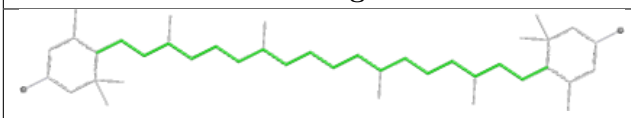
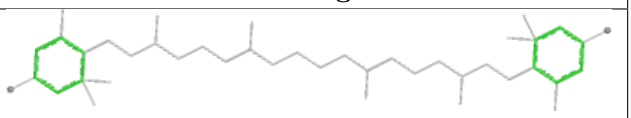


Torsions



Rings

Ligand CLA Y 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT s 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

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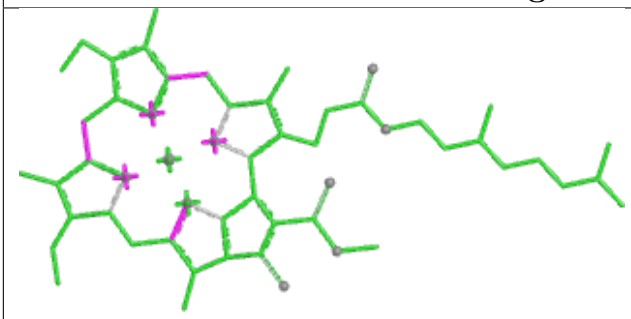
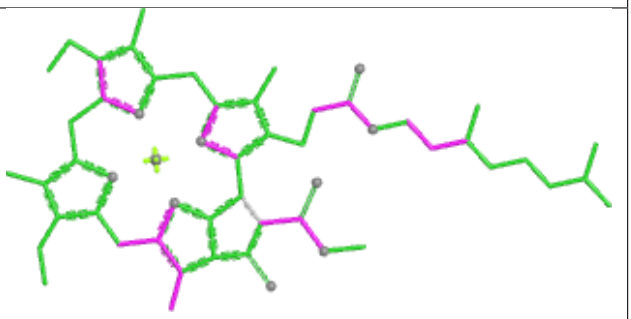
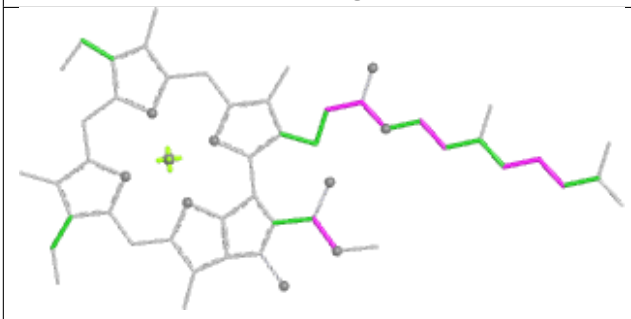
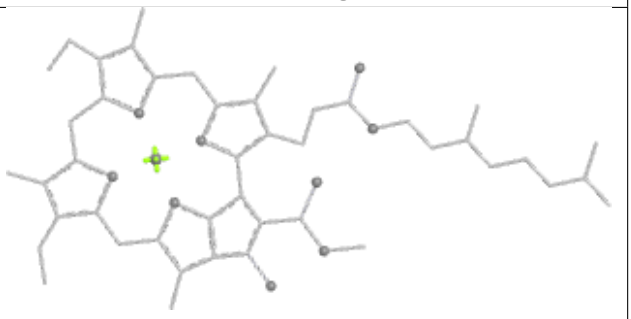
 Bond lengths	 Bond angles
 Torsions	 Rings

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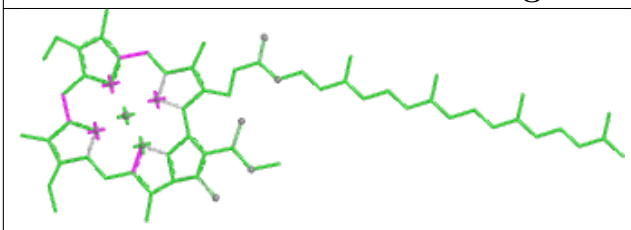
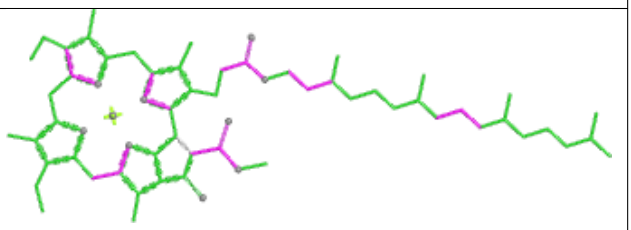
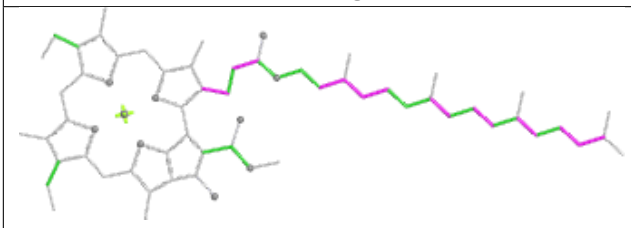
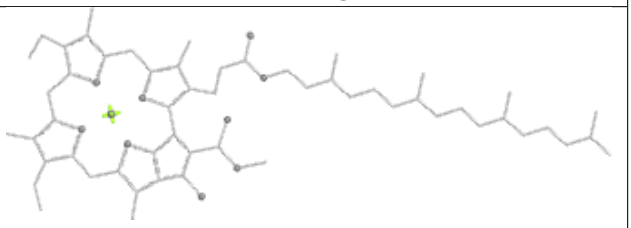
 Bond lengths	 Bond angles
 Torsions	 Rings

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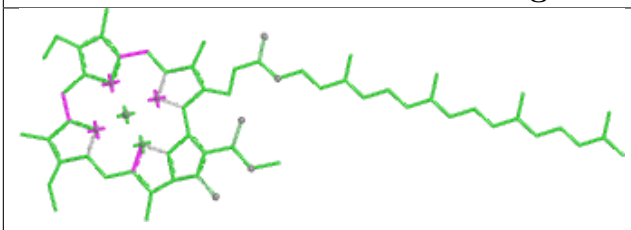
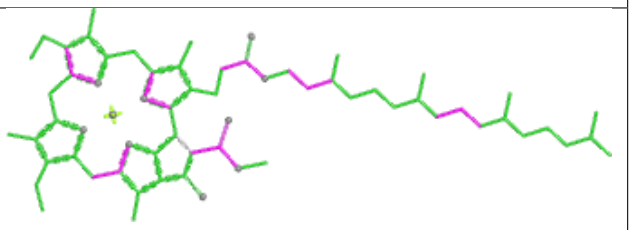
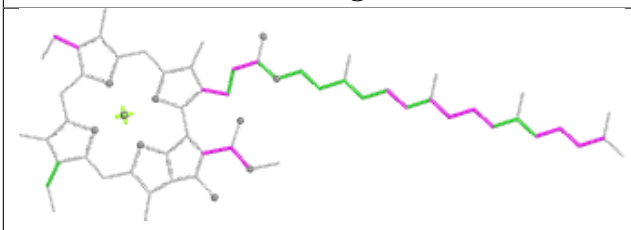
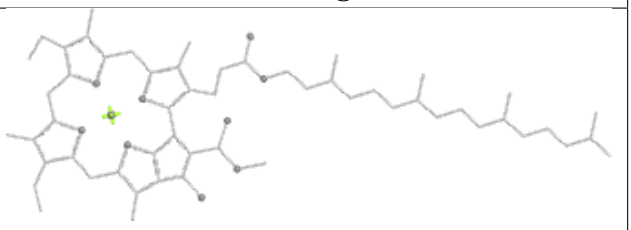
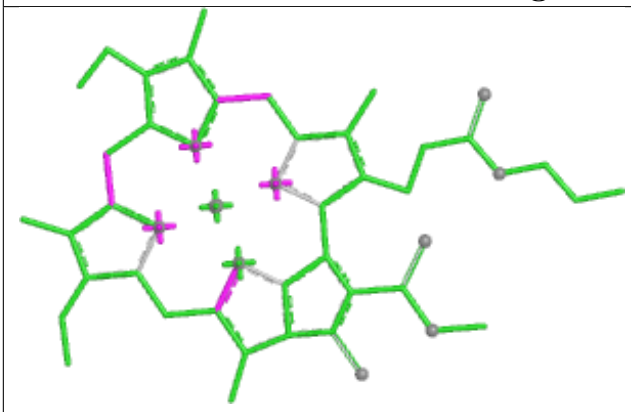
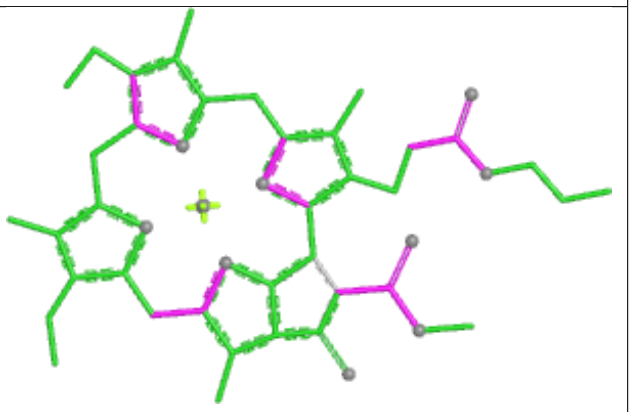
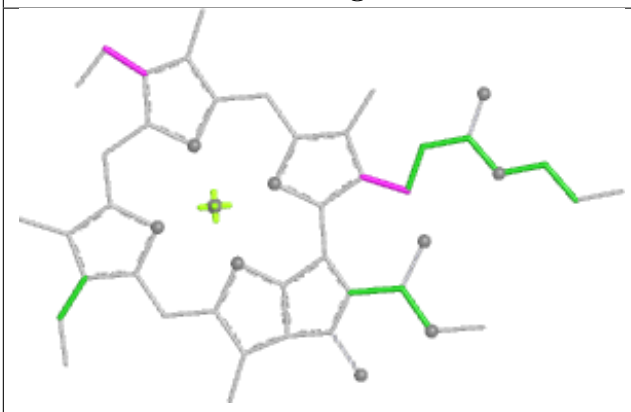
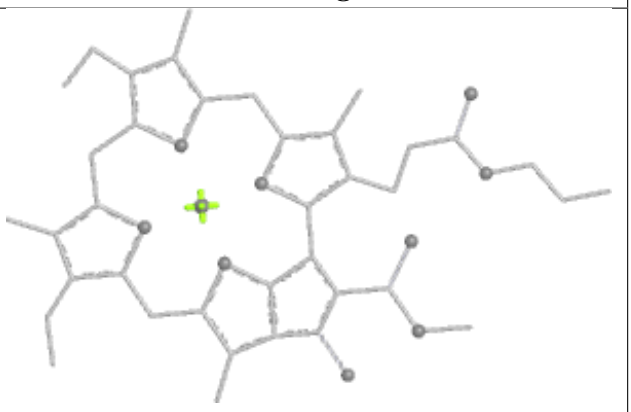
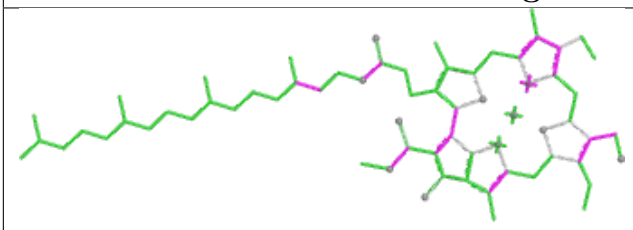
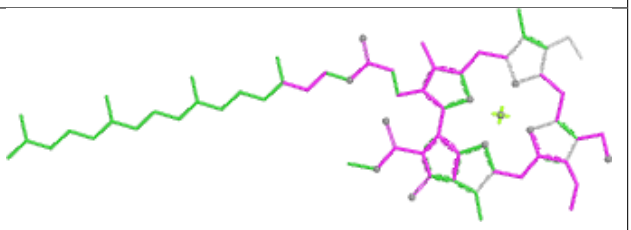
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

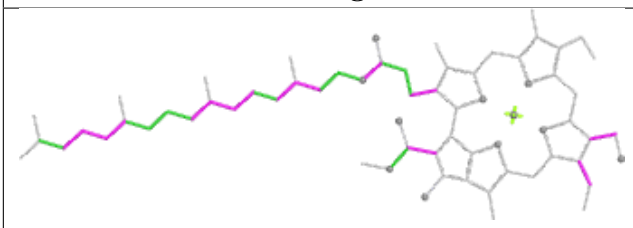
Ligand CHL N 609



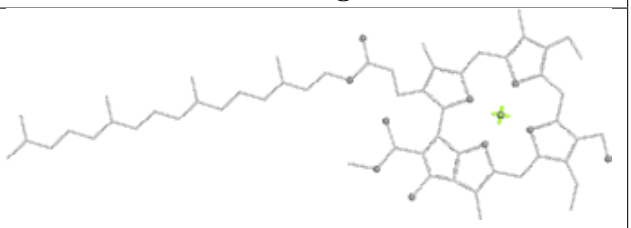
Bond lengths



Bond angles

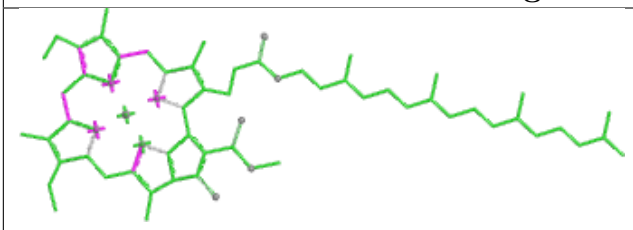


Torsions



Rings

Ligand CLA R 602



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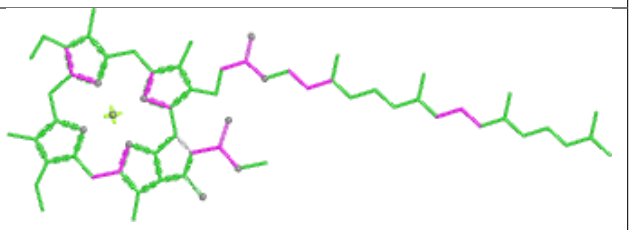
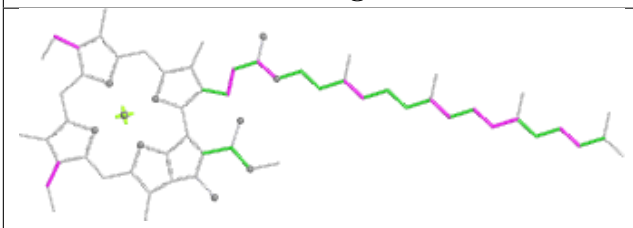


Bond angles



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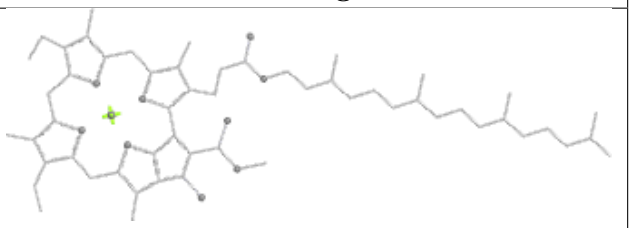
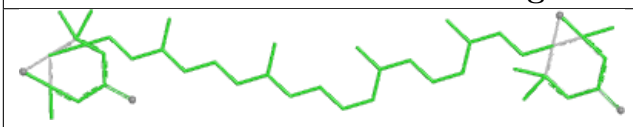


Rings

Ligand XAT 3 620



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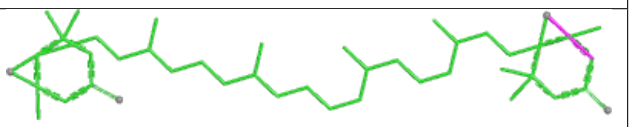
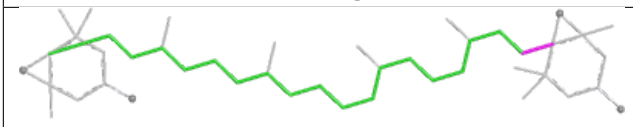


Bond angles



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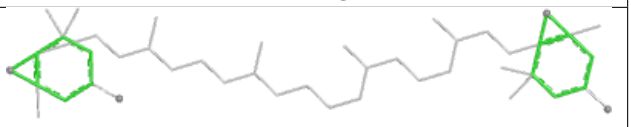
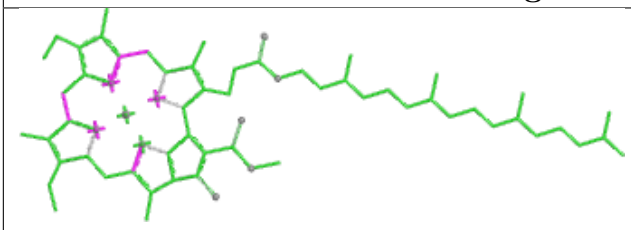
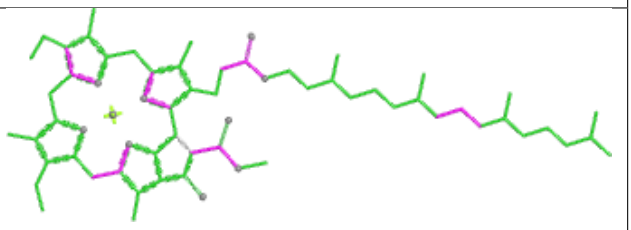
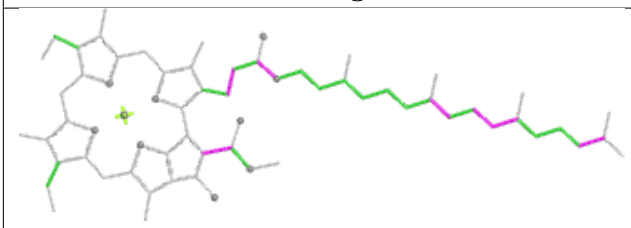
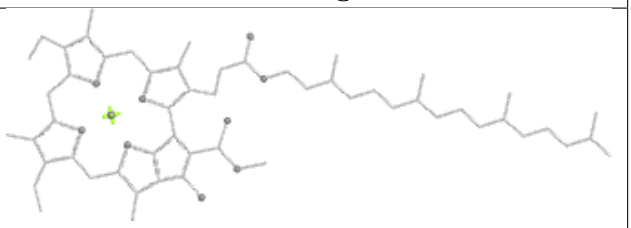
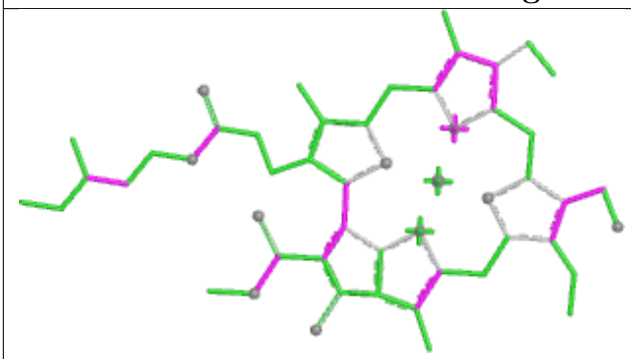
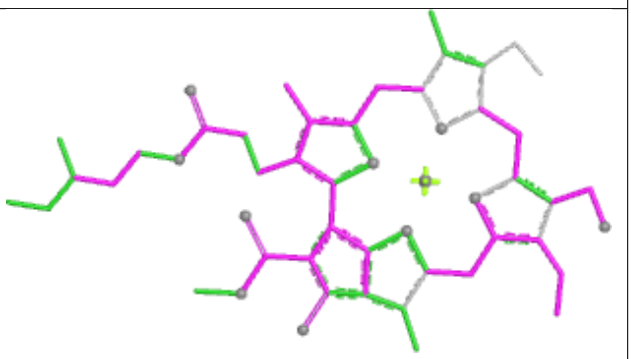
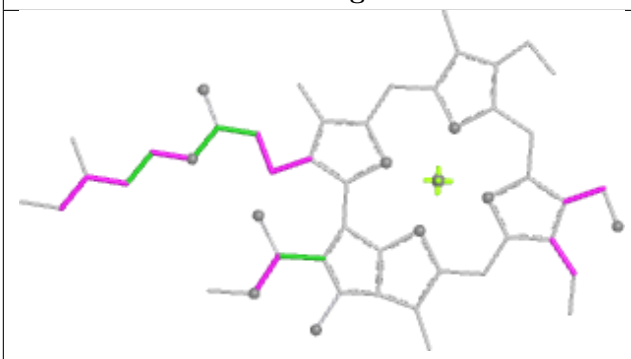
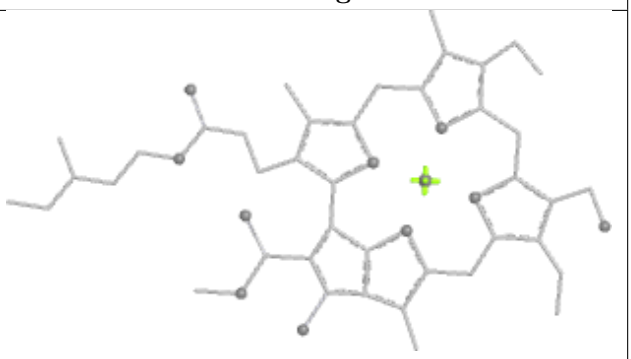
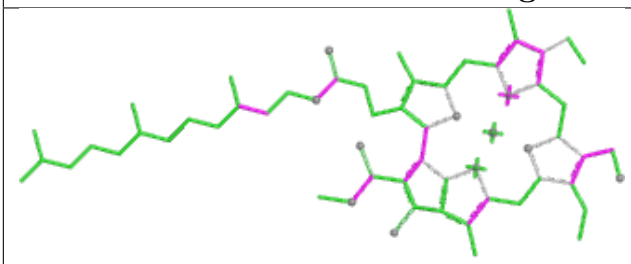


Rings

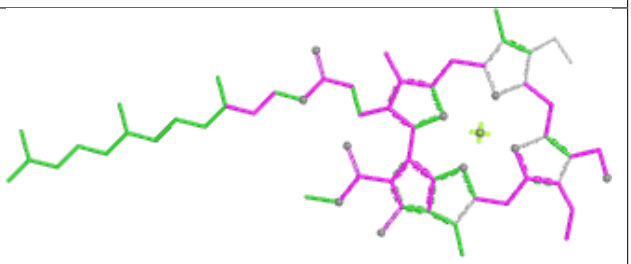
Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

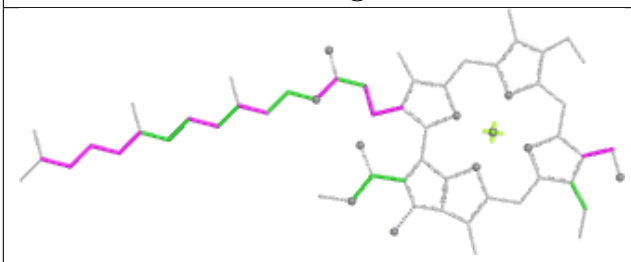
Ligand CHL 13 606



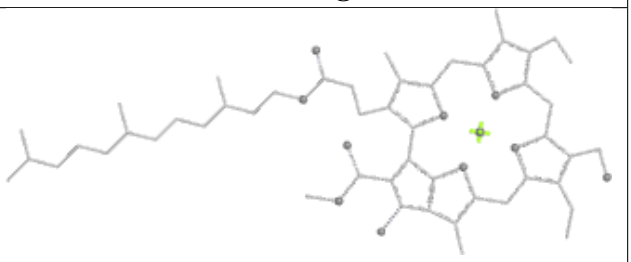
Bond lengths



Bond angles

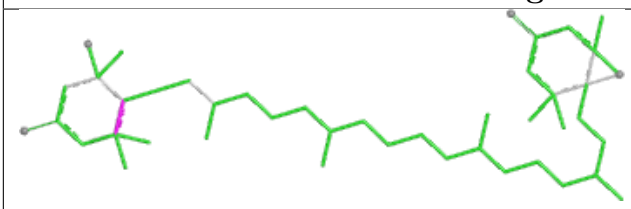


Torsions



Rings

Ligand NEX g 618



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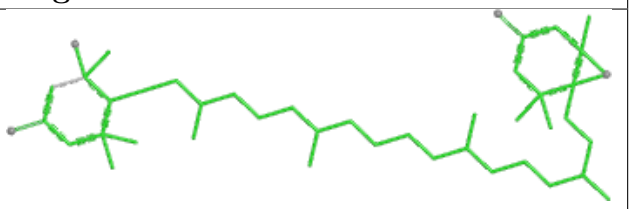
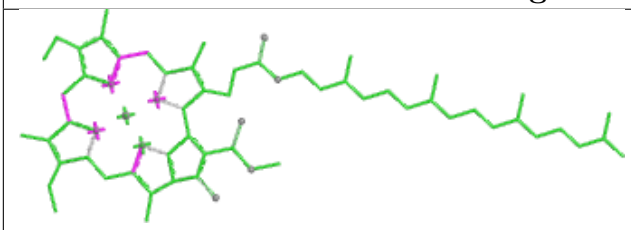


Bond angles

Torsions

Rings

Ligand CLA c 511



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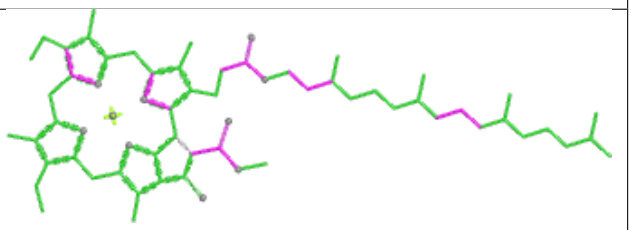
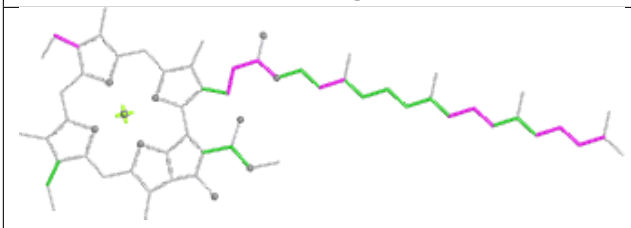


Bond angles



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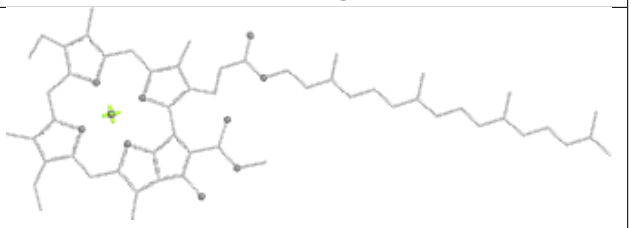
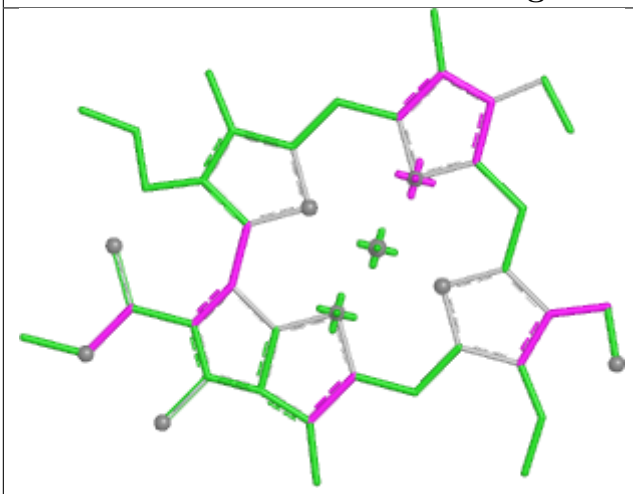
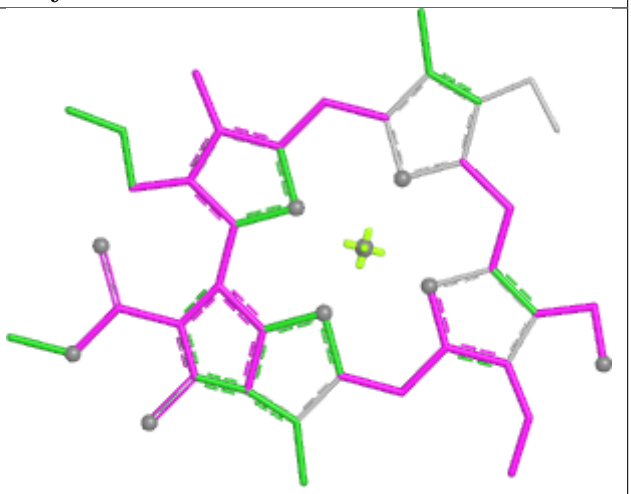
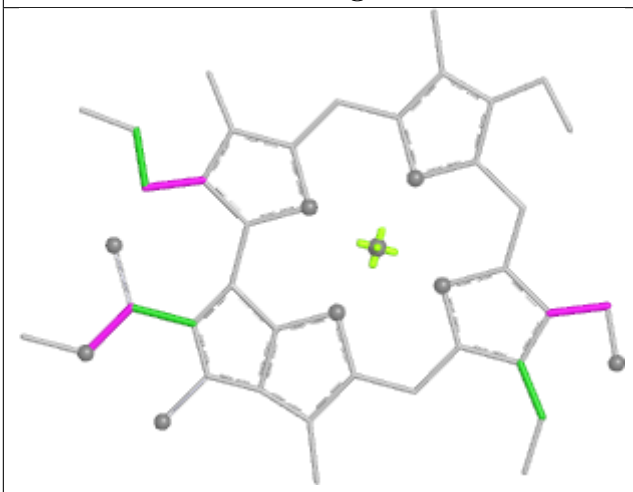
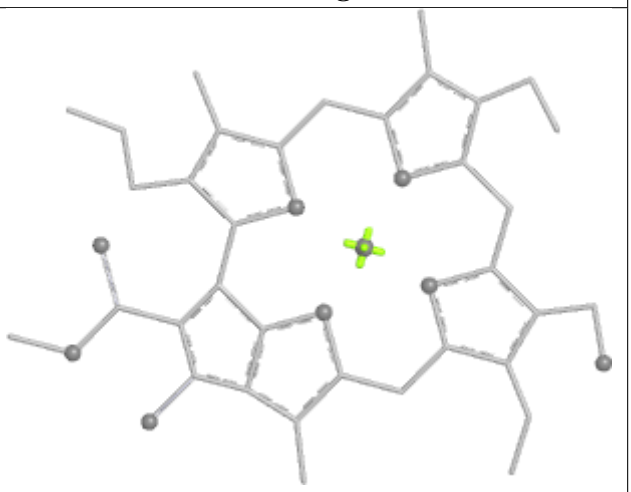
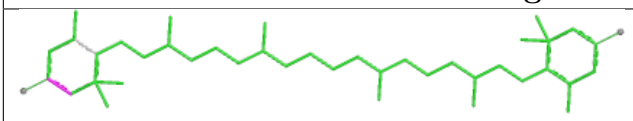
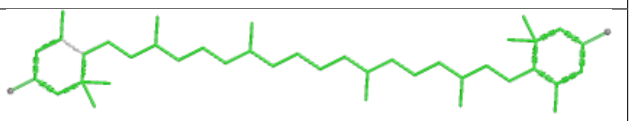
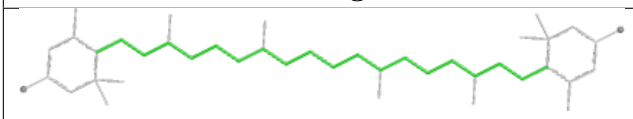
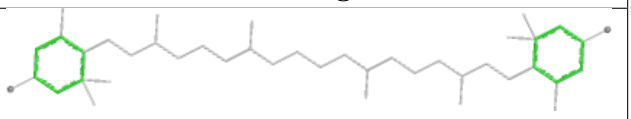
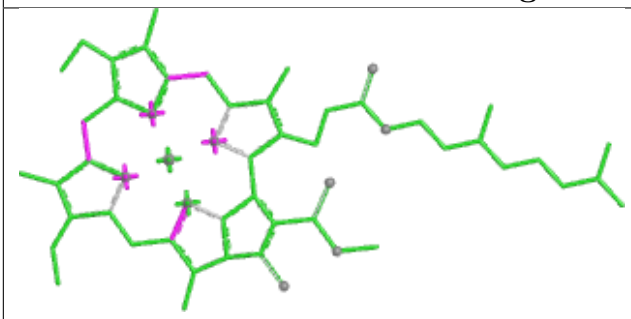


Rings

Ligand CHL y 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT Y 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 11 603



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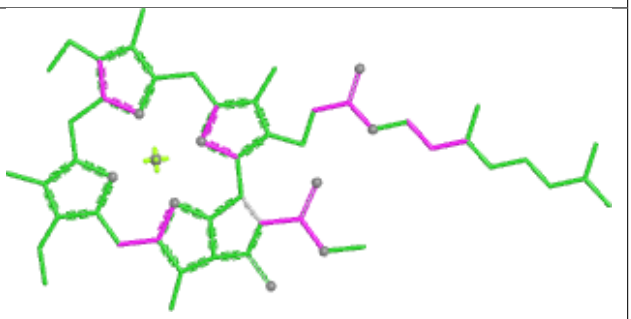

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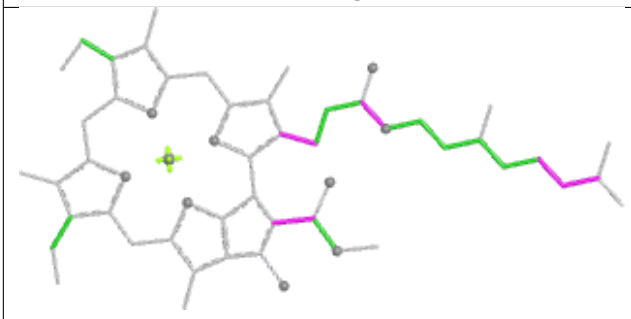

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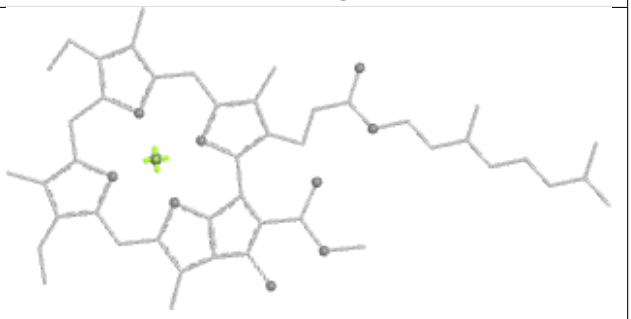
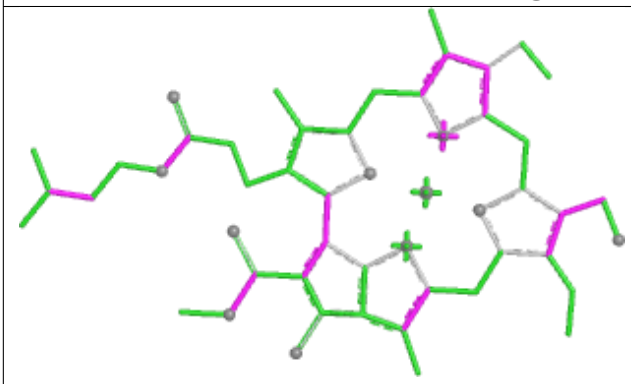


Rings

Ligand CHL 4 607



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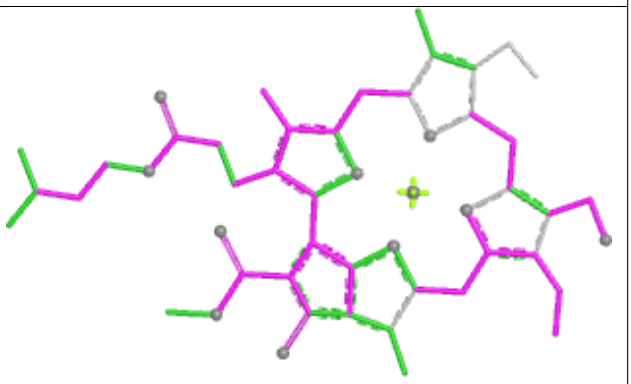

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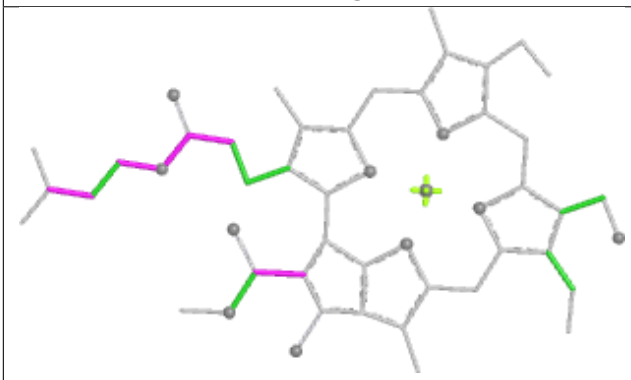

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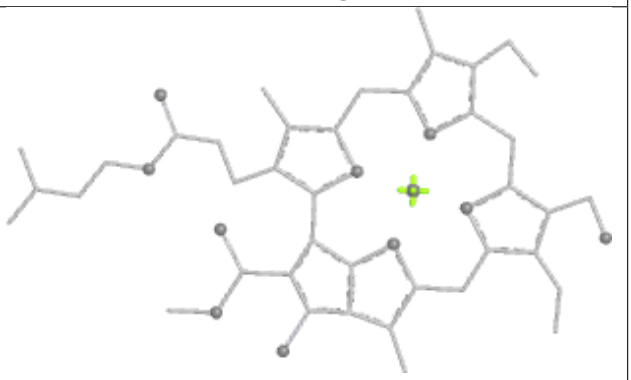
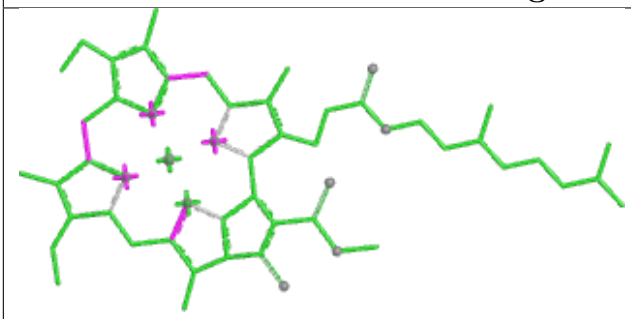


Rings

Ligand CLA 4 603



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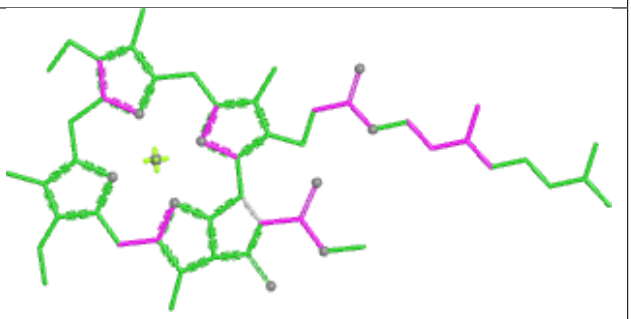
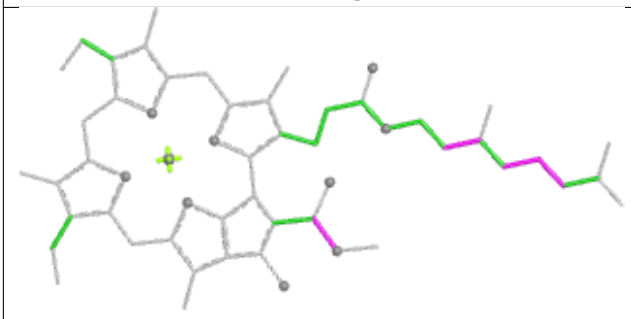


Bond angles



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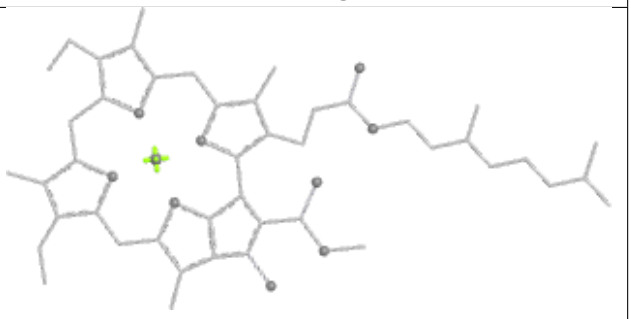
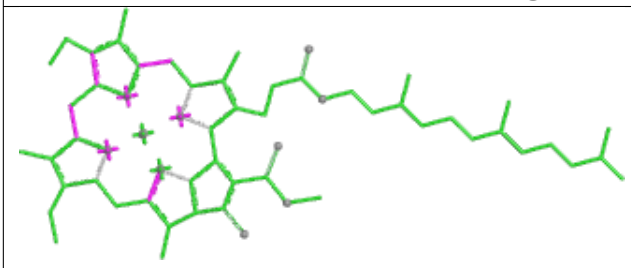


Rings

Ligand CLA C 509



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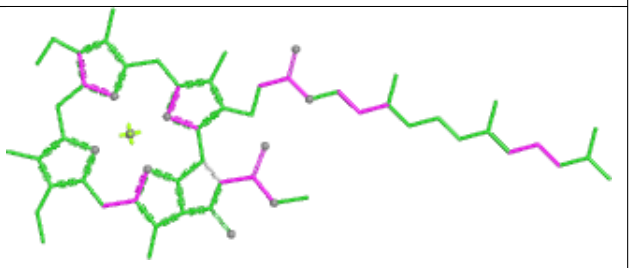

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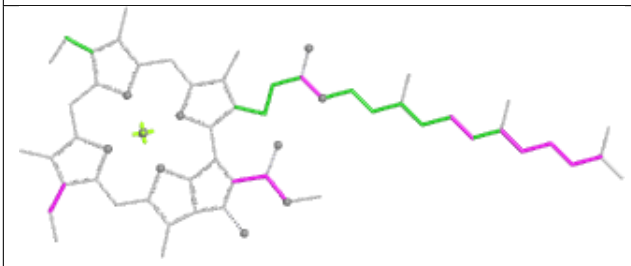

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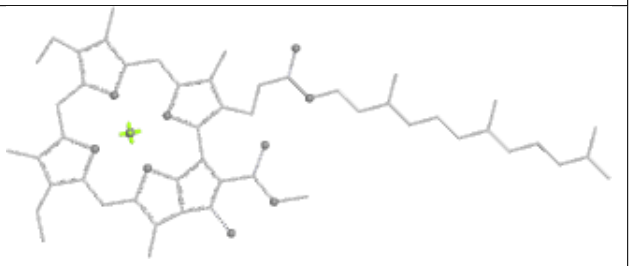
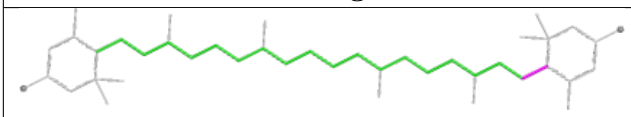


Rings

Ligand LUT y 622

Bond lengths

Bond angles



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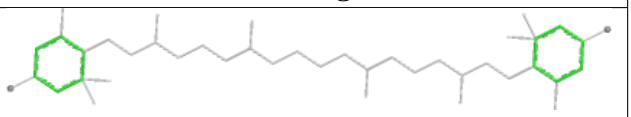
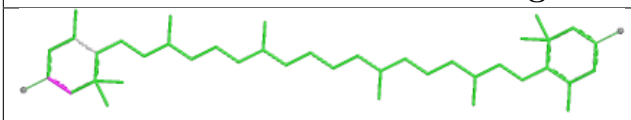


Rings

Ligand LUT 4 617



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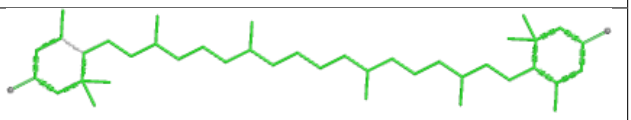
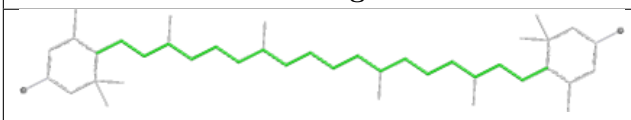


Bond angles



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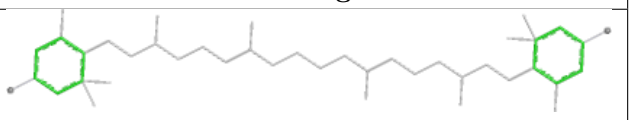
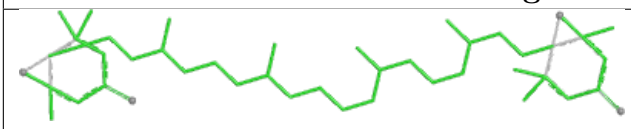


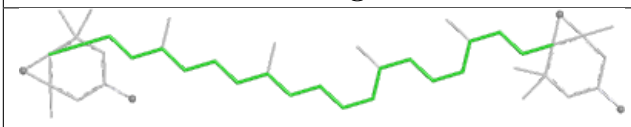
Rings

Ligand XAT R 616



Bond lengths

Bond angles



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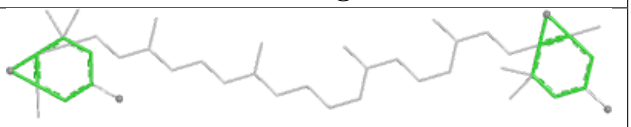
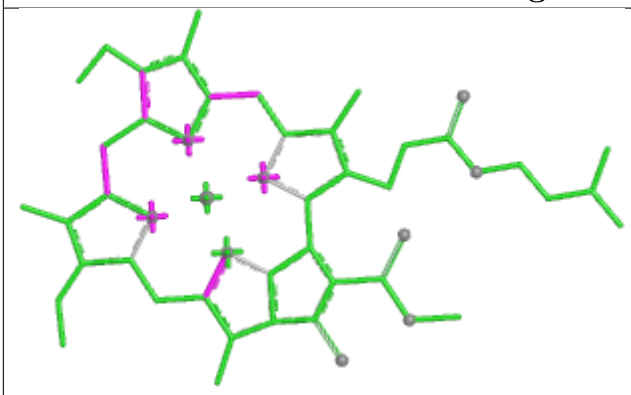
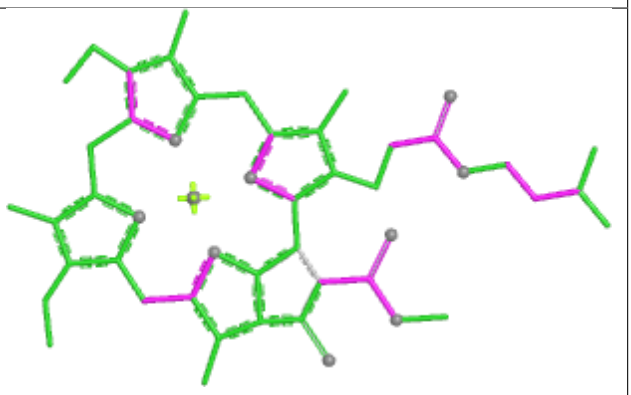


Rings

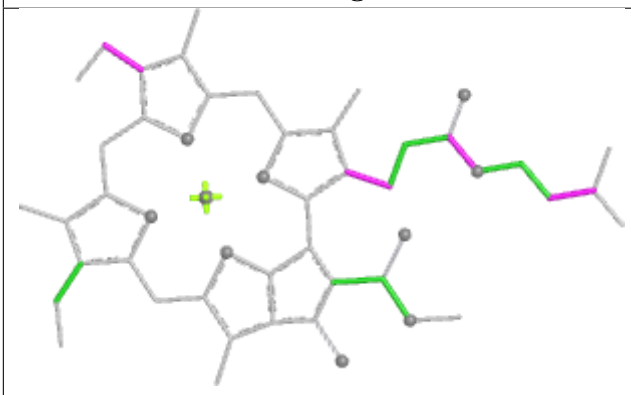
Ligand CLA 2 610



Bond lengths



Bond angles



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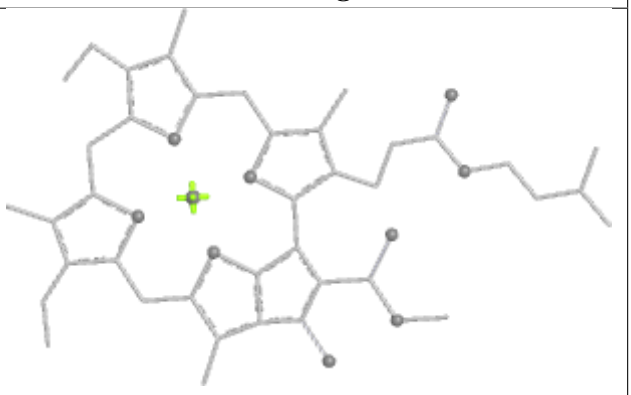
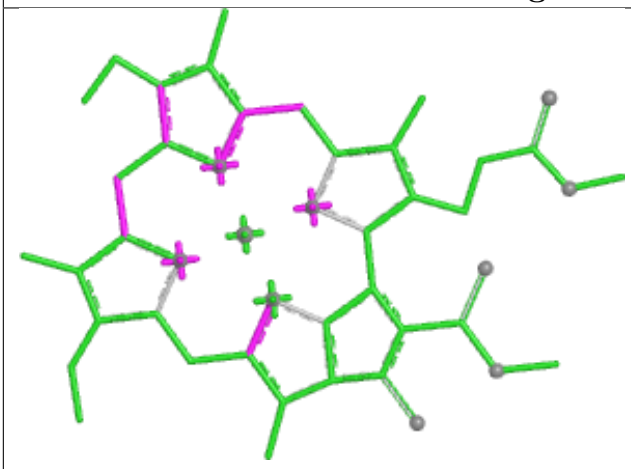
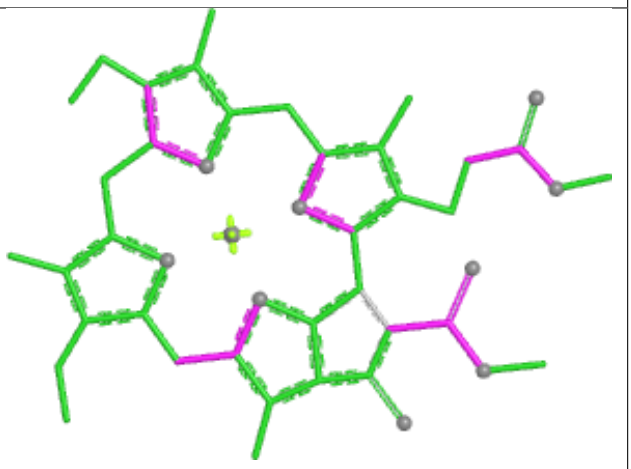


Rings

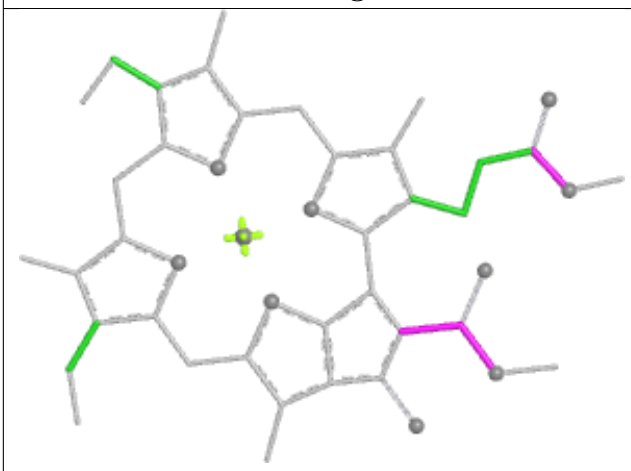
Ligand CLA 3 615



Bond lengths



Bond angles



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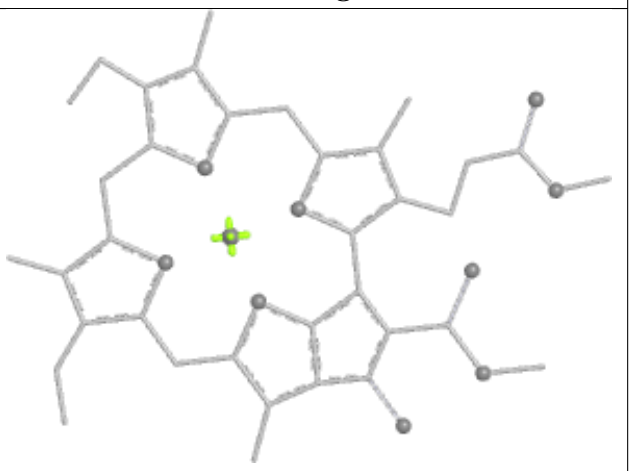
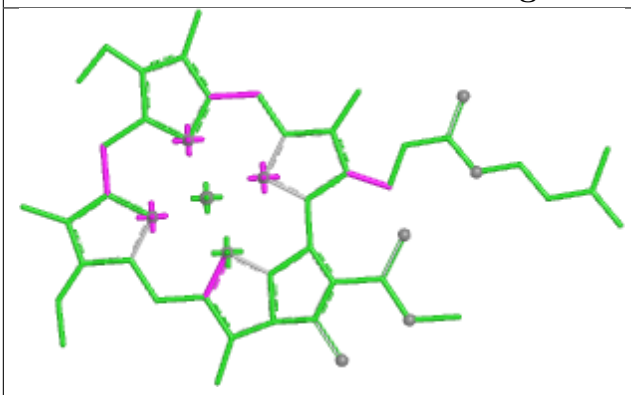
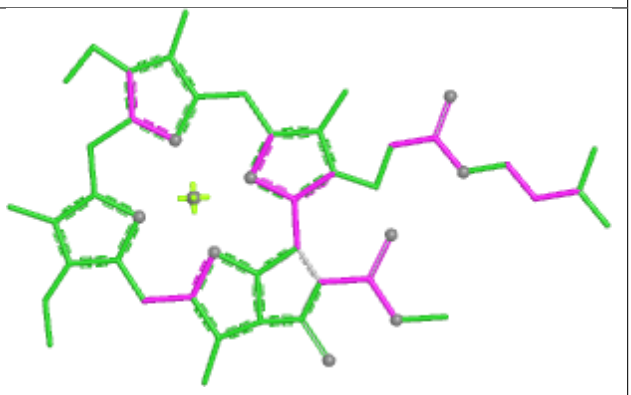
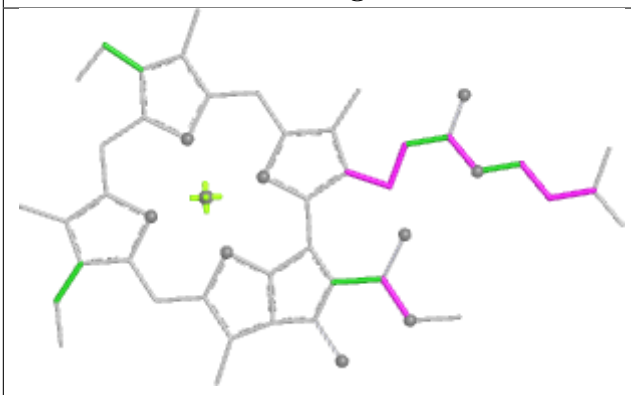
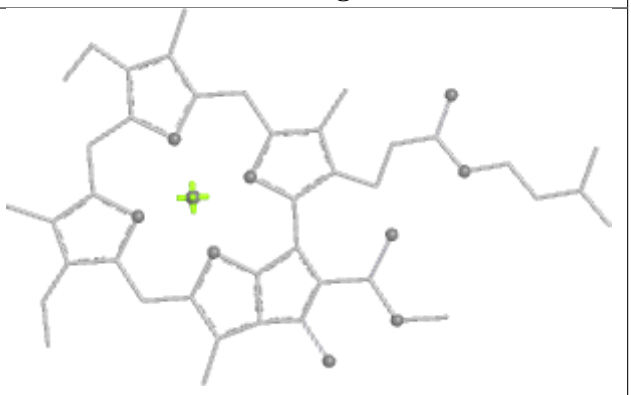
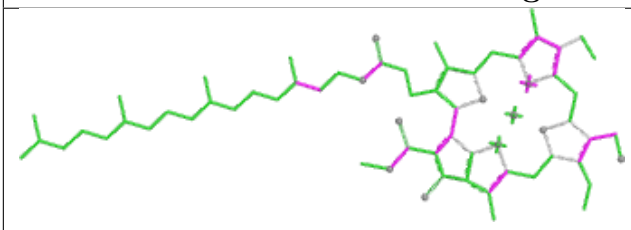
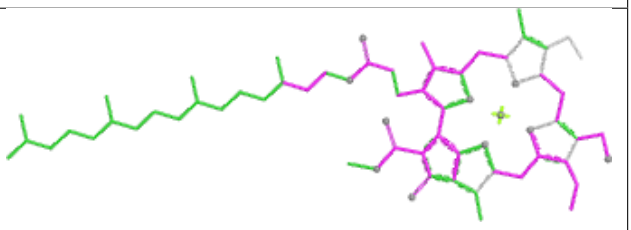
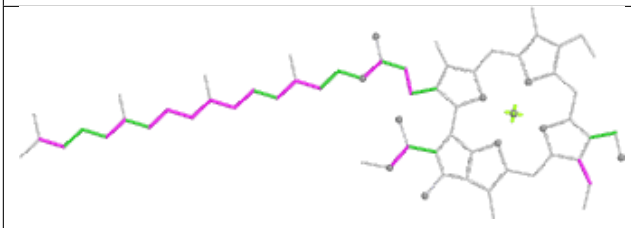
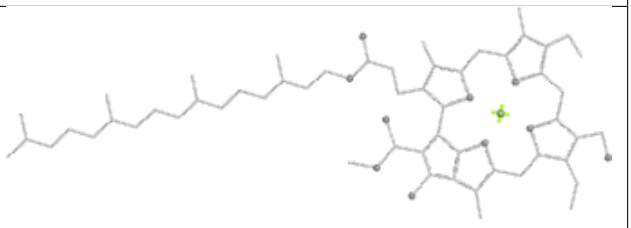
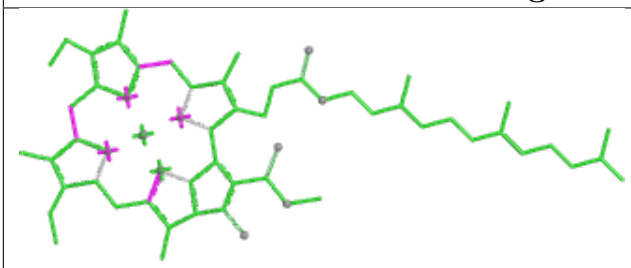
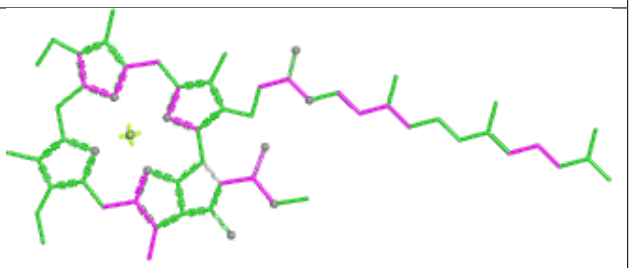
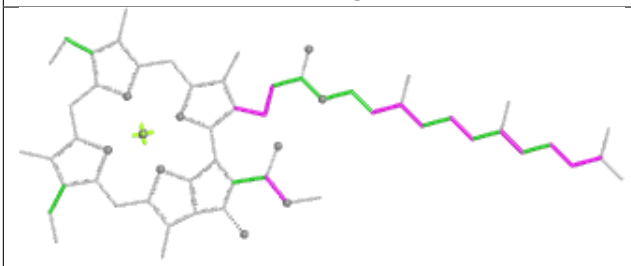
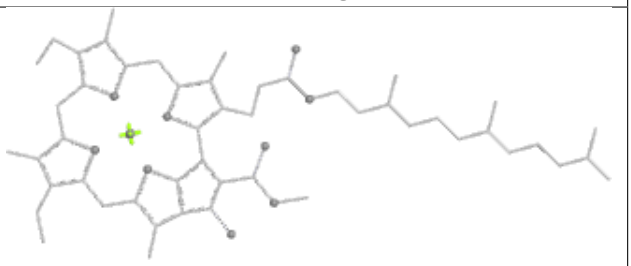


Rings

Ligand CLA 15 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

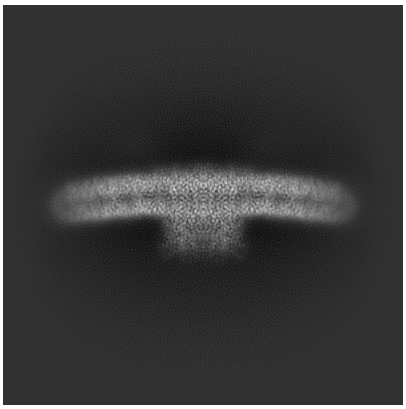
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-52056. These allow visual inspection of the internal detail of the map and identification of artifacts.

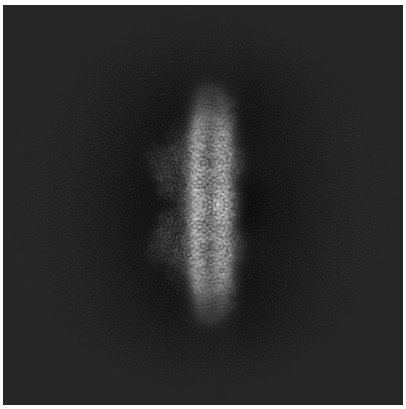
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

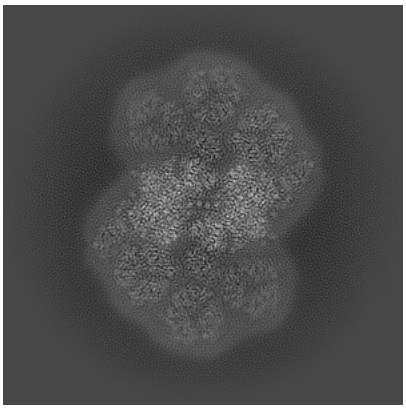
6.1.1 Primary map



X

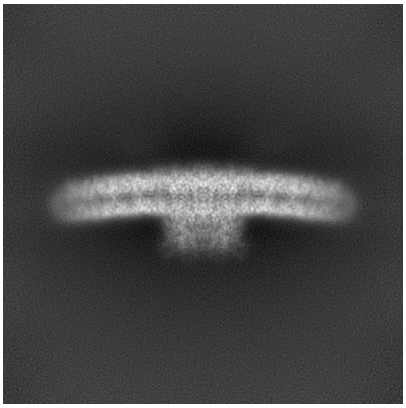


Y

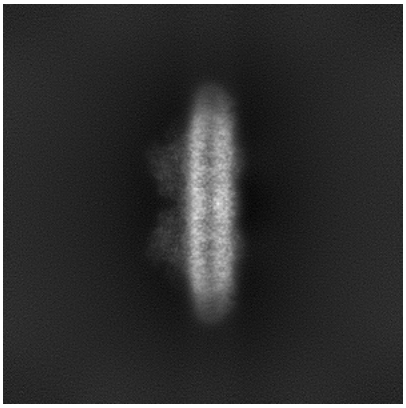


Z

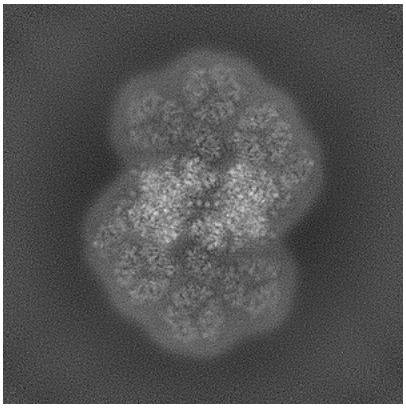
6.1.2 Raw map



X



Y

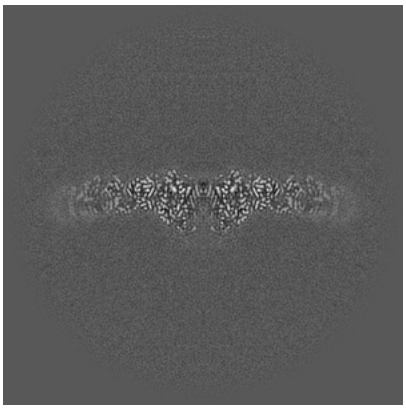


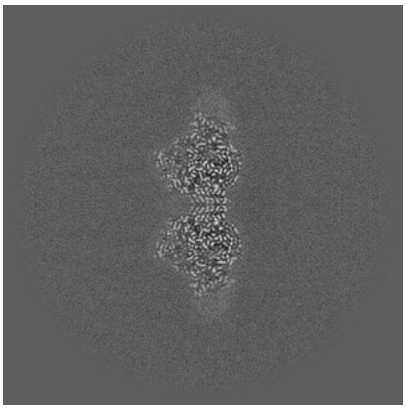
Z

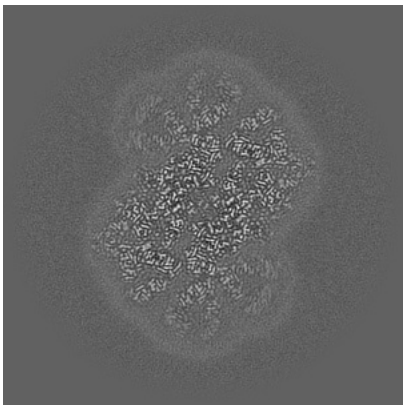
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

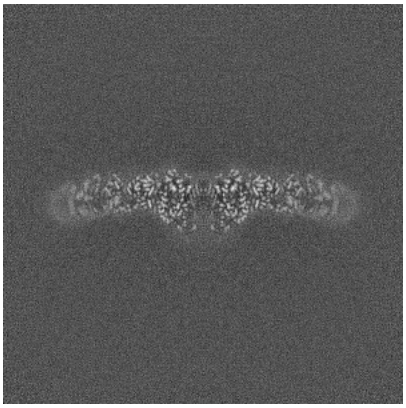
6.2.1 Primary map

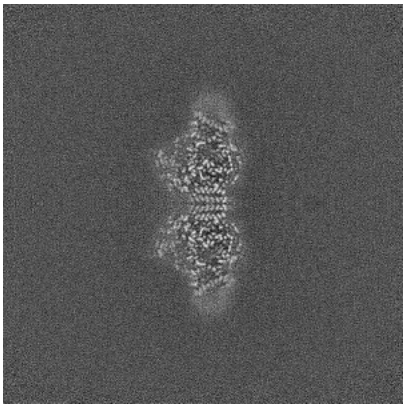

X Index: 240

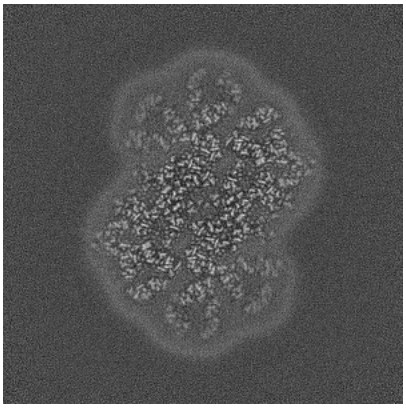

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

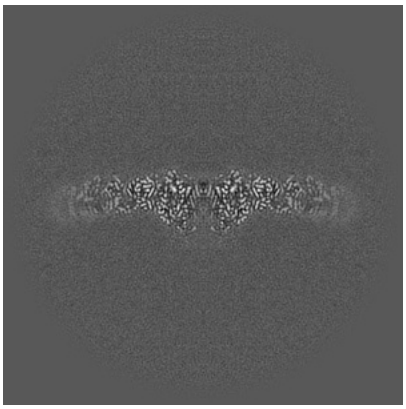

Y Index: 240

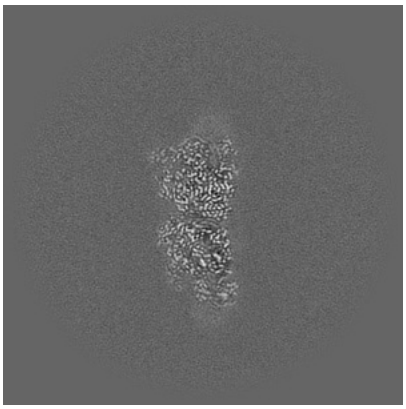

Z Index: 240

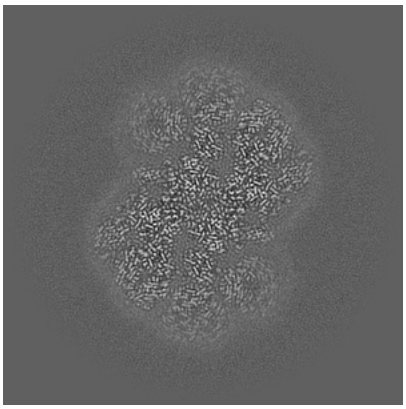
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

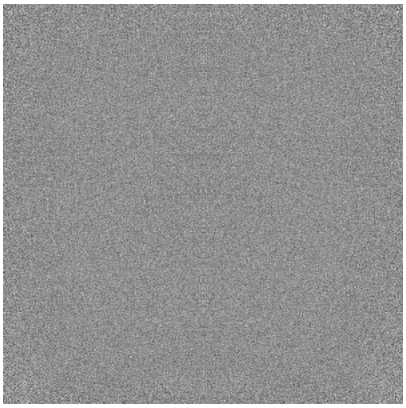
6.3.1 Primary map

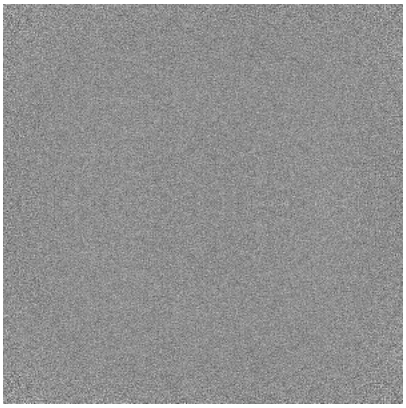

X Index: 240

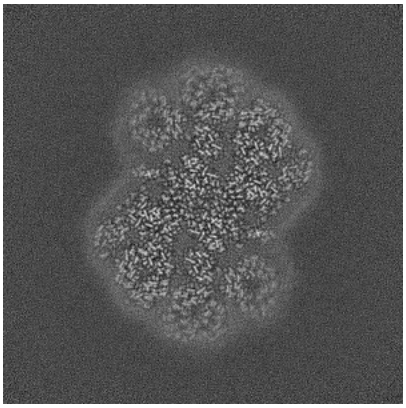

Y Index: 214


Z Index: 259

6.3.2 Raw map


X Index: 0

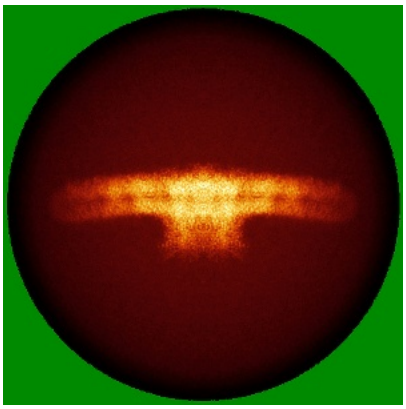

Y Index: 0

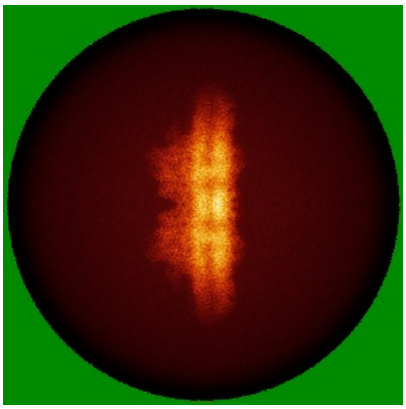

Z Index: 259

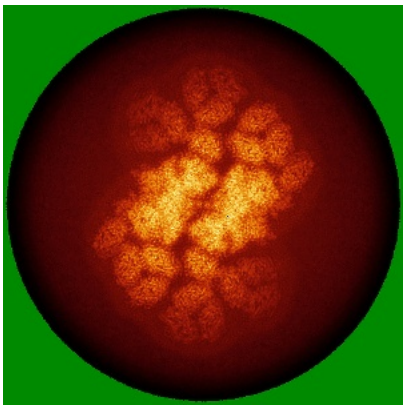
The images above show the largest variance slices of the map in three orthogonal directions.

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

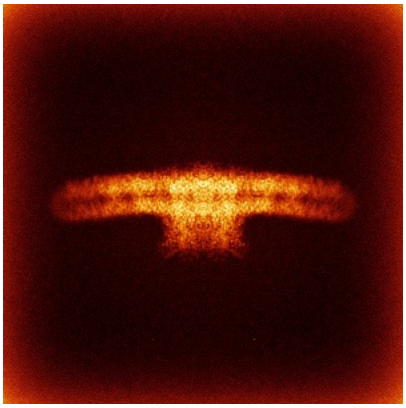
6.4.1 Primary map

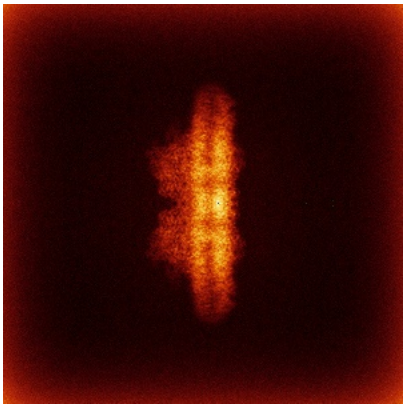

X

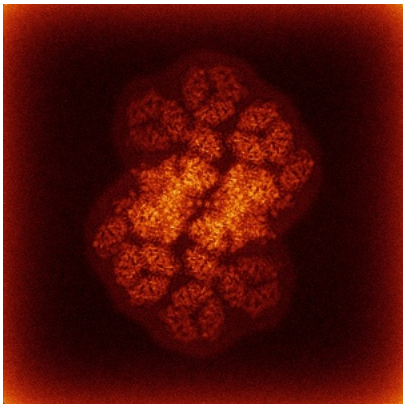

Y


Z

6.4.2 Raw map


X

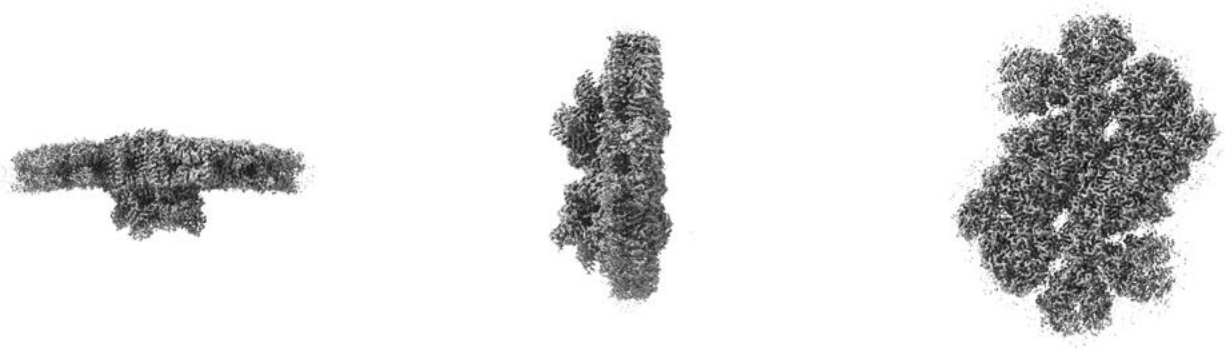

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

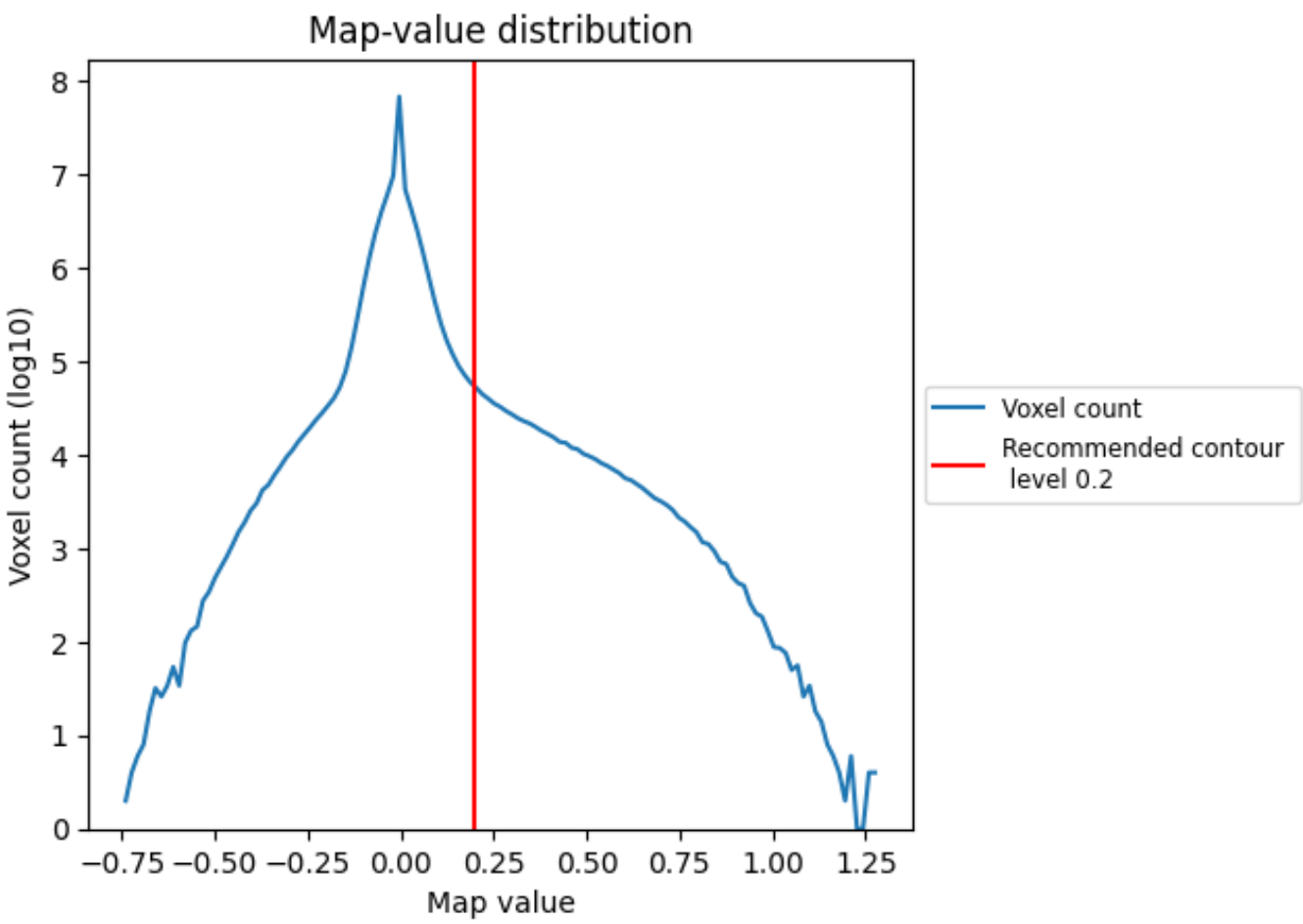
6.6 Mask visualisation (i)

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

7 Map analysis (i)

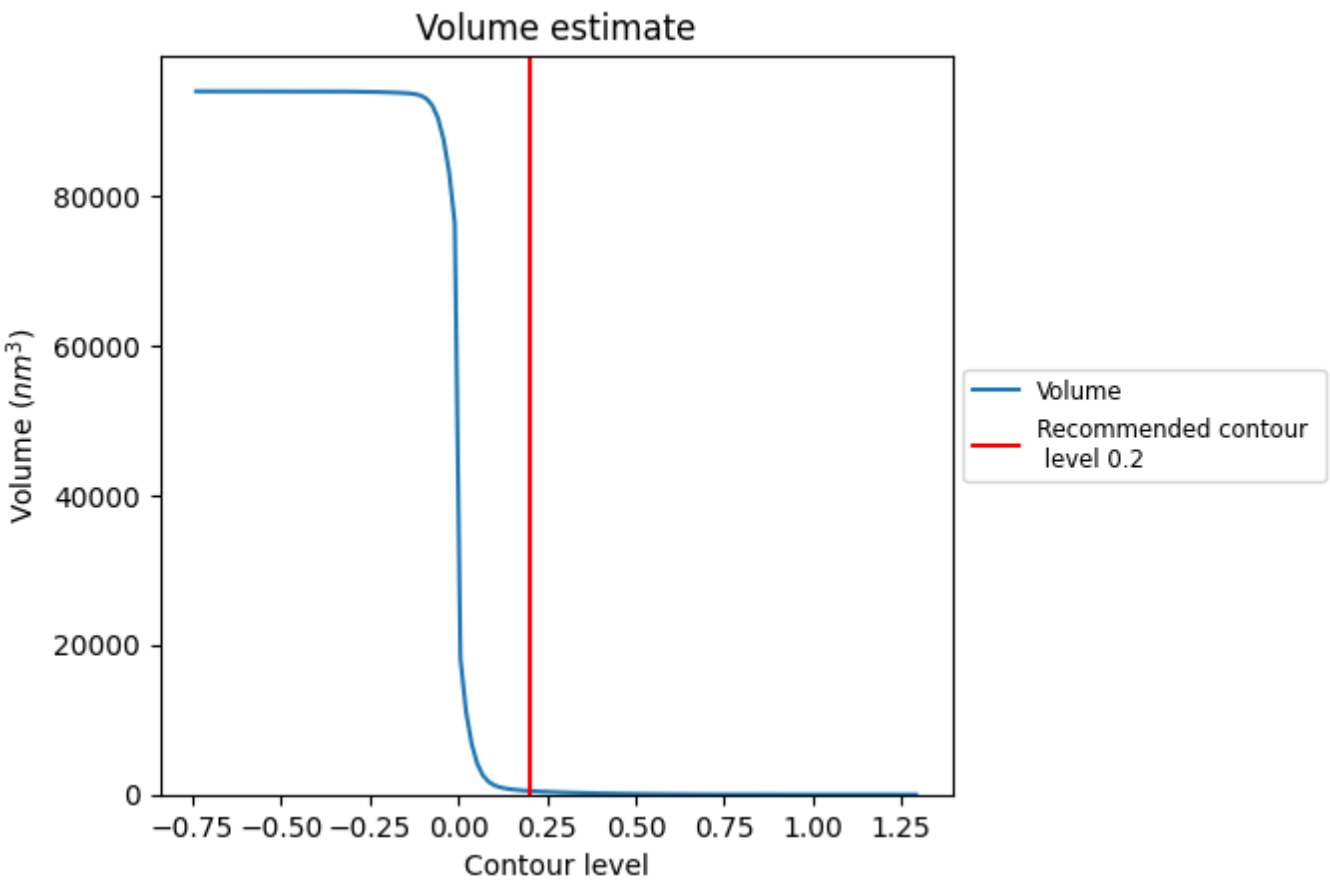
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

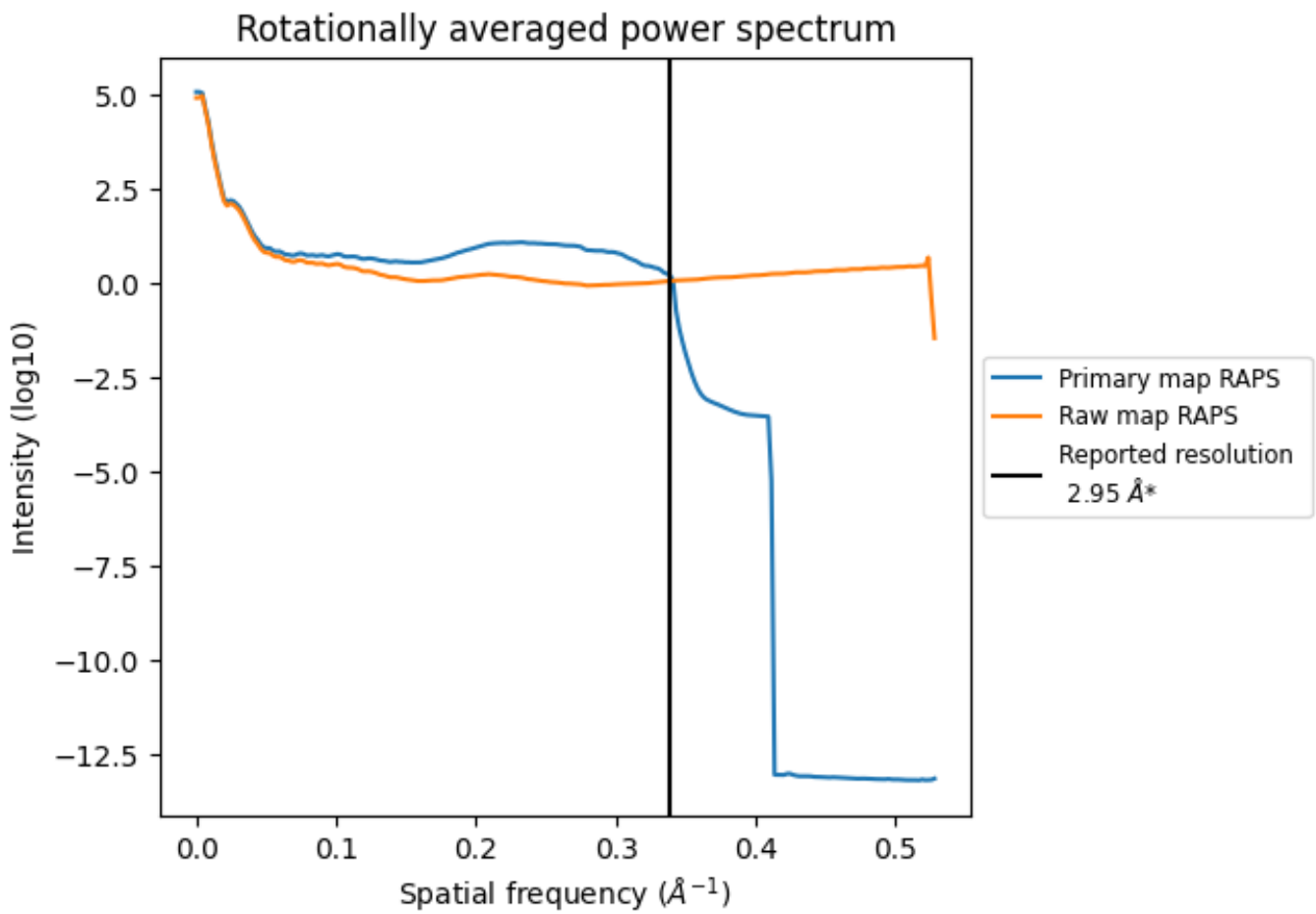
7.2 Volume estimate (i)



The volume at the recommended contour level is 486 nm^3; this corresponds to an approximate mass of 439 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)

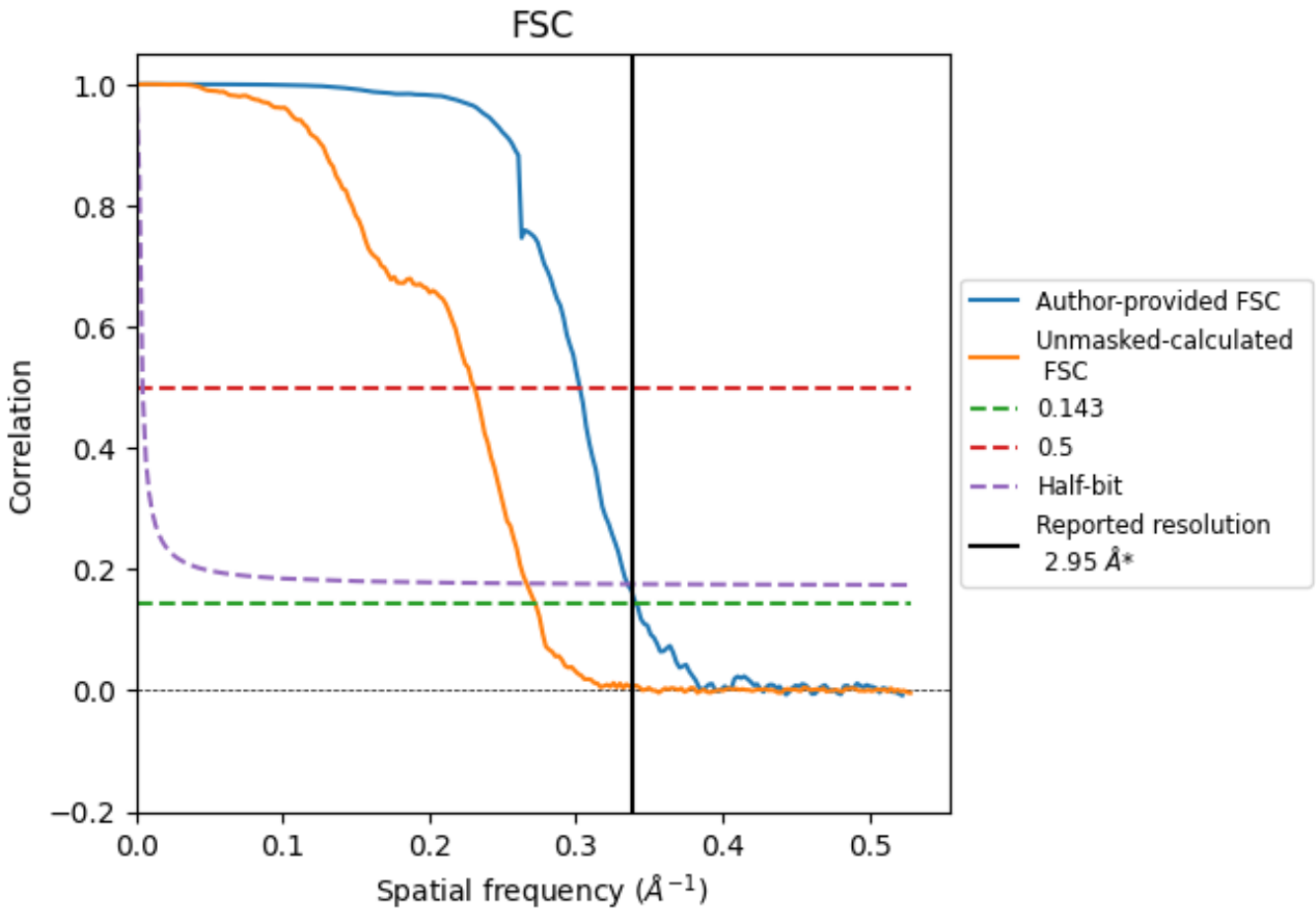


*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

8.2 Resolution estimates (i)

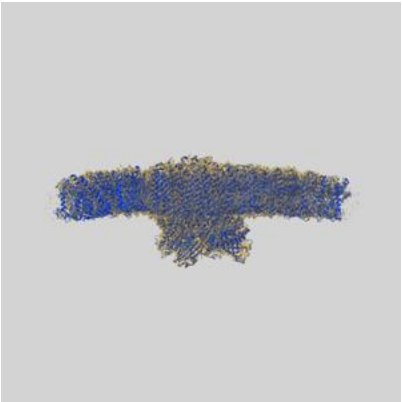
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.93	3.31	2.98
Unmasked-calculated*	3.67	4.33	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.95 by more than 10 %

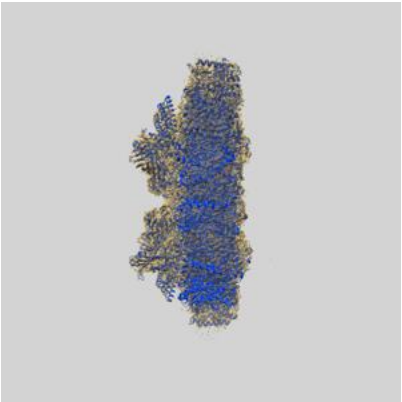
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-52056 and PDB model 9HD7. Per-residue inclusion information can be found in section 3 on page 60.

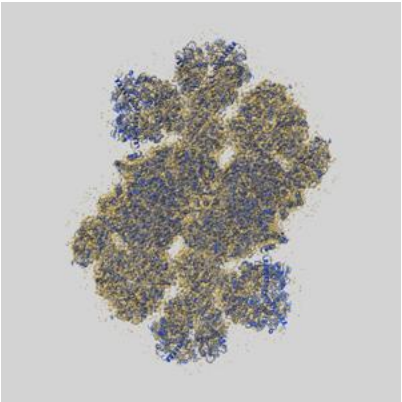
9.1 Map-model overlay (i)



X



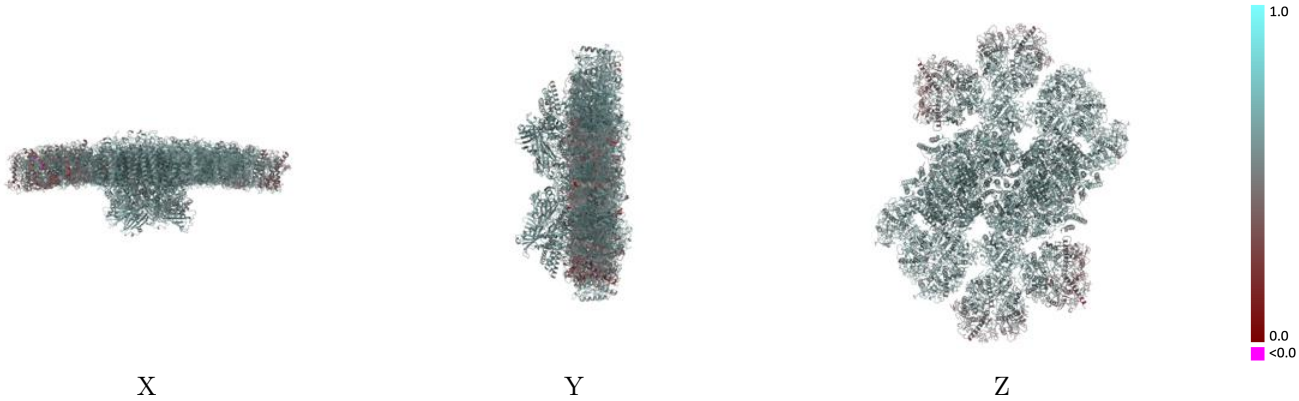
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

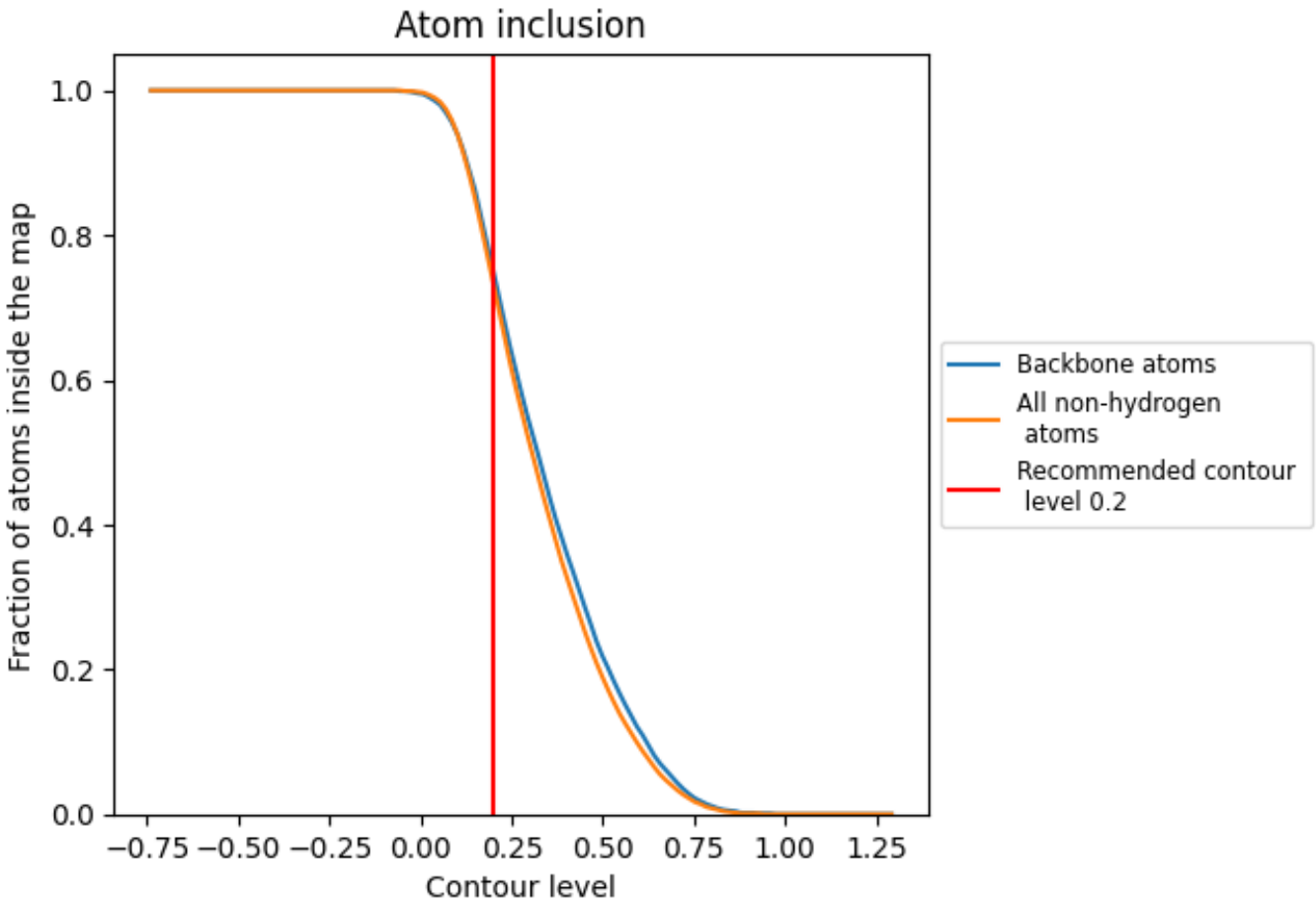


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.5760
1	0.4700	0.5130
11	0.4260	0.4850
12	0.2500	0.4300
13	0.6560	0.5560
14	0.4220	0.4860
15	0.2480	0.4320
16	0.6510	0.5550
2	0.3760	0.4700
3	0.7550	0.5810
4	0.4620	0.5080
5	0.3760	0.4760
6	0.7570	0.5790
7	0.6010	0.5670
8	0.6000	0.5670
A	0.8840	0.6170
B	0.8780	0.6130
C	0.8840	0.6110
D	0.8990	0.6200
E	0.8340	0.6050
F	0.8600	0.6090
G	0.7700	0.5830
H	0.8650	0.6040
I	0.8970	0.6150
J	0.7330	0.5830
K	0.7920	0.5790
L	0.8230	0.5940
M	0.7750	0.5830
N	0.7950	0.5870
O	0.7220	0.5880
P	0.6690	0.5880
Q	0.5370	0.5550
R	0.8390	0.6050
S	0.7130	0.5740
T	0.7730	0.5840

Continued on next page...

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Chain	Atom inclusion	Q-score
U	0.4520	0.5170
V	0.5520	0.5230
W	0.8050	0.6020
X	0.8100	0.6010
Y	0.8720	0.6150
Z	0.7120	0.5670
a	0.8900	0.6180
b	0.8820	0.6160
c	0.8820	0.6110
d	0.8970	0.6190
e	0.8380	0.6050
f	0.8510	0.6090
g	0.7660	0.5830
h	0.8700	0.6070
i	0.9000	0.6140
j	0.7420	0.5820
k	0.8320	0.5760
l	0.8230	0.5950
m	0.7800	0.5820
n	0.7960	0.5850
o	0.7230	0.5880
p	0.6770	0.5890
q	0.5380	0.5530
r	0.8360	0.6070
s	0.7150	0.5760
t	0.8090	0.5910
u	0.4570	0.5240
v	0.5660	0.5370
w	0.8060	0.6010
x	0.7990	0.6060
y	0.8730	0.6140
z	0.7040	0.5670