Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 03:49 PM JST

PDB ID	:	5XNM
EMDB ID	:	EMD-6742
Title	:	Structure of unstacked C2S2M2-type PSII-LHCII supercomplex from Pisum sativum
Authors	:	Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on	:	2017-05-23
Resolution	:	3.20 Å(reported)

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 ⓘ 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 ⓘ) were used in the production of this report:

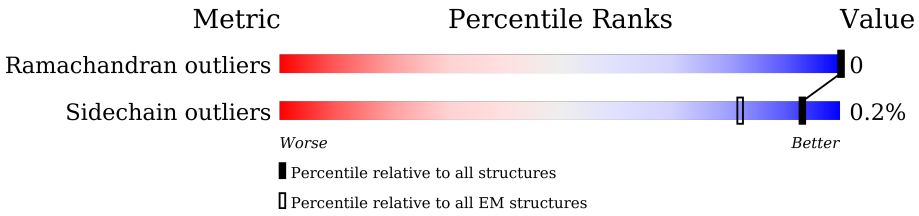
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	232	93% 94% 6%
1	2	232	94% 94% 6%
1	5	232	93% 94% 6%
1	6	232	94% 94% 6%
1	G	232	19% 94% 6%
1	N	232	12% 94% 6%
1	Y	232	5% 94% 6%
1	g	232	19% 94% 6%
1	n	232	12% 94% 6%

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Mol	Chain	Length	Quality of chain
1	y	232	5% 94% 6%
2	3	243	90% 90% 9%
2	7	243	90% 90% 9%
3	4	210	92% 94% 6%
3	8	210	93% 94% 6%
4	A	344	8% 97%
4	a	344	7% 97%
5	B	507	11% 99%
5	b	507	10% 99%
6	C	473	11% 95% 5%
6	c	473	12% 95% 5%
7	D	353	7% 96%
7	d	353	7% 96%
8	E	83	30% 90% 10%
8	e	83	34% 90% 10%
9	F	39	13% 77% 23%
9	f	39	13% 77% 23%
10	H	73	14% 81% 18%
10	h	73	12% 81% 18%
11	I	36	94% 6%
11	i	36	94% 6%
12	J	40	85% 85% 15%
12	j	40	82% 85% 15%
13	K	61	8% 61% 39%
13	k	61	7% 61% 39%

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Mol	Chain	Length	Quality of chain
14	L	38	13% 97%
14	l	38	13% 97%
15	M	34	29% 97%
15	m	34	29% 97%
16	O	248	38% 86% 14%
16	o	248	37% 86% 14%
17	R	246	23% 95% 5%
17	r	246	23% 95% 5%
18	S	244	41% 89% 11%
18	s	244	40% 89% 11%
19	T	35	14% 91% 9%
19	t	35	14% 91% 9%
20	U	99	14% 25% 75%
20	u	99	13% 25% 75%
21	W	54	22% 100%
21	w	54	20% 100%
22	X	86	15% 45% 55%
22	x	86	14% 45% 55%
23	Z	62	48% 100%
23	z	62	55% 100%

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
24	CHL	1	601	X	-	-	-
24	CHL	1	605	X	-	-	-
24	CHL	1	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	1	607	X	-	-	-
24	CHL	1	608	X	-	-	-
24	CHL	1	609	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	605	X	-	-	-
24	CHL	2	606	X	-	-	-
24	CHL	2	607	X	-	-	-
24	CHL	2	608	X	-	-	-
24	CHL	2	609	X	-	-	-
24	CHL	3	601	X	-	-	-
24	CHL	3	605	X	-	-	-
24	CHL	3	606	X	-	-	-
24	CHL	3	607	X	-	-	-
24	CHL	3	608	X	-	-	-
24	CHL	3	609	X	-	-	-
24	CHL	4	601	X	-	-	-
24	CHL	4	606	X	-	-	-
24	CHL	4	607	X	-	-	-
24	CHL	4	608	X	-	-	-
24	CHL	4	609	X	-	-	-
24	CHL	5	601	X	-	-	-
24	CHL	5	605	X	-	-	-
24	CHL	5	606	X	-	-	-
24	CHL	5	607	X	-	-	-
24	CHL	5	608	X	-	-	-
24	CHL	5	609	X	-	-	-
24	CHL	6	601	X	-	-	-
24	CHL	6	605	X	-	-	-
24	CHL	6	606	X	-	-	-
24	CHL	6	607	X	-	-	-
24	CHL	6	608	X	-	-	-
24	CHL	6	609	X	-	-	-
24	CHL	7	601	X	-	-	-
24	CHL	7	605	X	-	-	-
24	CHL	7	606	X	-	-	-
24	CHL	7	607	X	-	-	-
24	CHL	7	608	X	-	-	-
24	CHL	7	609	X	-	-	-
24	CHL	8	601	X	-	-	-
24	CHL	8	606	X	-	-	-
24	CHL	8	607	X	-	-	-
24	CHL	8	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	8	609	X	-	-	-
24	CHL	G	601	X	-	-	-
24	CHL	G	605	X	-	-	-
24	CHL	G	606	X	-	-	-
24	CHL	G	607	X	-	-	-
24	CHL	G	608	X	-	-	-
24	CHL	G	609	X	-	-	-
24	CHL	N	601	X	-	-	-
24	CHL	N	605	X	-	-	-
24	CHL	N	606	X	-	-	-
24	CHL	N	607	X	-	-	-
24	CHL	N	608	X	-	-	-
24	CHL	N	609	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	608	X	-	-	-
24	CHL	R	614	X	-	-	-
24	CHL	S	601	X	-	-	-
24	CHL	S	606	X	-	-	-
24	CHL	S	607	X	-	-	-
24	CHL	S	608	X	-	-	-
24	CHL	Y	601	X	-	-	-
24	CHL	Y	605	X	-	-	-
24	CHL	Y	606	X	-	-	-
24	CHL	Y	607	X	-	-	-
24	CHL	Y	608	X	-	-	-
24	CHL	Y	609	X	-	-	-
24	CHL	g	601	X	-	-	-
24	CHL	g	605	X	-	-	-
24	CHL	g	606	X	-	-	-
24	CHL	g	607	X	-	-	-
24	CHL	g	608	X	-	-	-
24	CHL	g	609	X	-	-	-
24	CHL	n	601	X	-	-	-
24	CHL	n	605	X	-	-	-
24	CHL	n	606	X	-	-	-
24	CHL	n	607	X	-	-	-
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-
24	CHL	r	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	r	614	X	-	-	-
24	CHL	s	601	X	-	-	-
24	CHL	s	606	X	-	-	-
24	CHL	s	607	X	-	-	-
24	CHL	s	608	X	-	-	-
24	CHL	y	601	X	-	-	-
24	CHL	y	605	X	-	-	-
24	CHL	y	606	X	-	-	-
24	CHL	y	607	X	-	-	-
24	CHL	y	608	X	-	-	-
24	CHL	y	609	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	604	X	-	-	-
25	CLA	1	610	X	-	-	-
25	CLA	1	611	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	614	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	603	X	-	-	-
25	CLA	3	604	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	611	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	614	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	5	611	X	-	-	-
25	CLA	5	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	5	614	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	7	602	X	-	-	-
25	CLA	7	603	X	-	-	-
25	CLA	7	604	X	-	-	-
25	CLA	7	610	X	-	-	-
25	CLA	7	611	X	-	-	-
25	CLA	7	612	X	-	-	-
25	CLA	7	613	X	-	-	-
25	CLA	7	614	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	603	X	-	-	-
25	CLA	8	610	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	407	X	-	-	-
25	CLA	A	410	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	B	617	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	602	X	-	-	-
25	CLA	N	603	X	-	-	-
25	CLA	N	604	X	-	-	-
25	CLA	N	610	X	-	-	-
25	CLA	N	611	X	-	-	-
25	CLA	N	612	X	-	-	-
25	CLA	N	613	X	-	-	-
25	CLA	N	614	X	-	-	-
25	CLA	R	601	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	R	613	X	-	-	-
25	CLA	S	602	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	613	X	-	-	-
25	CLA	S	614	X	-	-	-
25	CLA	Y	602	X	-	-	-
25	CLA	Y	603	X	-	-	-
25	CLA	Y	604	X	-	-	-
25	CLA	Y	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	Y	611	X	-	-	-
25	CLA	Y	612	X	-	-	-
25	CLA	Y	613	X	-	-	-
25	CLA	Y	614	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	a	407	X	-	-	-
25	CLA	a	410	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	610	X	-	-	-
25	CLA	g	611	X	-	-	-
25	CLA	g	612	X	-	-	-
25	CLA	g	614	X	-	-	-
25	CLA	n	602	X	-	-	-
25	CLA	n	603	X	-	-	-
25	CLA	n	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	n	610	X	-	-	-
25	CLA	n	611	X	-	-	-
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	-	-
25	CLA	n	614	X	-	-	-
25	CLA	r	601	X	-	-	-
25	CLA	r	602	X	-	-	-
25	CLA	r	603	X	-	-	-
25	CLA	r	604	X	-	-	-
25	CLA	r	609	X	-	-	-
25	CLA	r	610	X	-	-	-
25	CLA	r	611	X	-	-	-
25	CLA	r	612	X	-	-	-
25	CLA	r	613	X	-	-	-
25	CLA	s	602	X	-	-	-
25	CLA	s	603	X	-	-	-
25	CLA	s	604	X	-	-	-
25	CLA	s	609	X	-	-	-
25	CLA	s	610	X	-	-	-
25	CLA	s	611	X	-	-	-
25	CLA	s	612	X	-	-	-
25	CLA	s	613	X	-	-	-
25	CLA	s	614	X	-	-	-
25	CLA	y	602	X	-	-	-
25	CLA	y	603	X	-	-	-
25	CLA	y	604	X	-	-	-
25	CLA	y	610	X	-	-	-
25	CLA	y	611	X	-	-	-
25	CLA	y	612	X	-	-	-
25	CLA	y	613	X	-	-	-
25	CLA	y	614	X	-	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 92842 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 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	5	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	6	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		
2	7	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		
4	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		
5	b	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
6	c	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	340	Total	C	N	O	S	0	0
			2703	1784	443	464	12		
7	d	340	Total	C	N	O	S	0	0
			2703	1784	443	464	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	75	Total	C	N	O	0	0
			612	400	100	112		
8	e	75	Total	C	N	O	0	0
			612	400	100	112		

- Molecule 9 is a protein called Cytochrome b559 subunit beta, PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
9	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

- Molecule 10 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
10	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

- Molecule 11 is a protein called Photosystem II reaction center protein I, PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
11	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	34	Total	C	N	O	0	0
			247	168	38	41		
12	j	34	Total	C	N	O	0	0
			247	168	38	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
13	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	37	Total 311	C 205	N 49	O 57	0	0
14	l	37	Total 311	C 205	N 49	O 57	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	33	Total 256	C 176	N 36	O 43	S 1	0	0
15	m	33	Total 256	C 176	N 36	O 43	S 1	0	0

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	214	Total 1631	C 1039	N 260	O 329	S 3	0	0
16	o	214	Total 1631	C 1039	N 260	O 329	S 3	0	0

- Molecule 17 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	234	Total 1835	C 1194	N 297	O 341	S 3	0	0
17	r	234	Total 1835	C 1194	N 297	O 341	S 3	0	0

- Molecule 18 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	218	Total 1689	C 1107	N 273	O 305	S 4	0	0
18	s	218	Total 1689	C 1107	N 273	O 305	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	32	Total 261	C 182	N 37	O 41	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	32	Total 261	C 182	N 37	O 41	S 1	0	0

- Molecule 20 is a protein called Photosystem II luminal extrinsic protein Tn, PsbTn.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total 193	C 123	N 35	O 32	S 3	0	0
20	u	25	Total 193	C 123	N 35	O 32	S 3	0	0

- Molecule 21 is a protein called Photosystem II reaction center protein W, PSBW.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total 419	C 275	N 61	O 82	S 1	0	0
21	w	54	Total 419	C 275	N 61	O 82	S 1	0	0

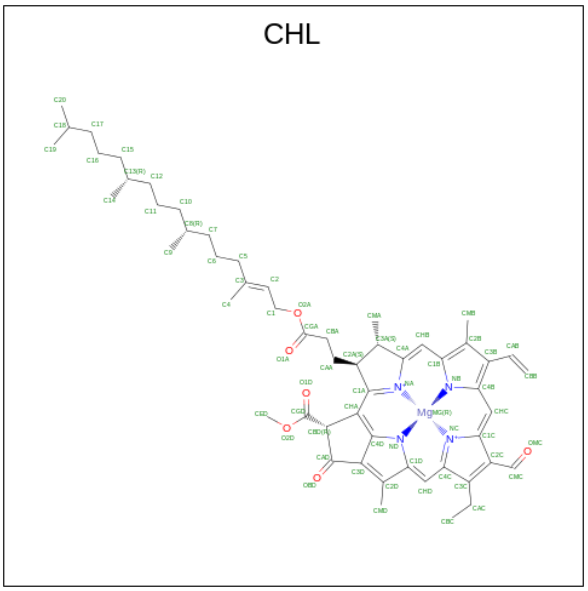
- Molecule 22 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	39	Total 276	C 180	N 46	O 50	0	0
22	x	39	Total 276	C 180	N 46	O 50	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	62	Total 464	C 312	N 69	O 82	S 1	0	0
23	z	62	Total 464	C 312	N 69	O 82	S 1	0	0

- Molecule 24 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	G	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	G	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	G	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	G	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	G	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	G	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	N	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	N	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	N	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	N	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	N	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	N	1	Total	C	Mg	N	O	0
			362	296	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	7	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	7	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	7	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	7	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	7	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	7	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
24	8	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	8	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	8	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	8	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	8	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
24	g	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	g	1	Total	C	Mg	N	O	0
			355	289	6	24	36	

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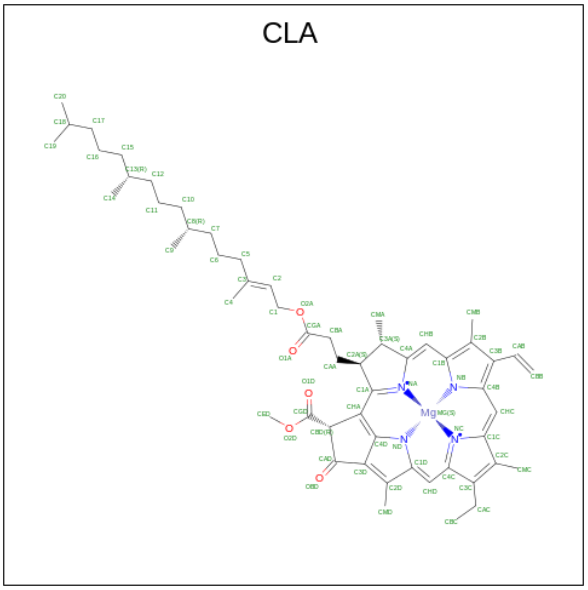
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total	C	Mg	N	O	0
			355	289	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	n	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	r	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	r	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	r	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	r	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	s	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	s	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	s	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	s	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	R	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	

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Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	S	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	Y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	Y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	

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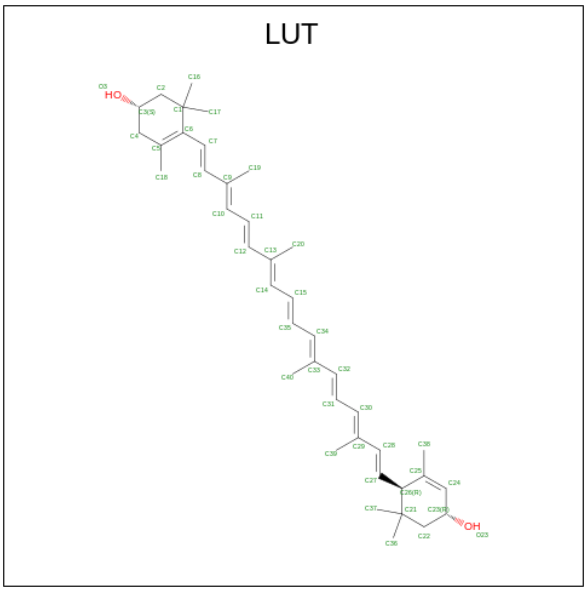
Mol	Chain	Residues	Atoms					AltConf
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
25	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
26	1	1	Total C O 84 80 4	0
26	1	1	Total C O 84 80 4	0
26	2	1	Total C O 84 80 4	0
26	2	1	Total C O 84 80 4	0
26	3	1	Total C O 84 80 4	0
26	3	1	Total C O 84 80 4	0
26	4	1	Total C O 42 40 2	0
26	G	1	Total C O 84 80 4	0
26	G	1	Total C O 84 80 4	0
26	N	1	Total C O 84 80 4	0
26	N	1	Total C O 84 80 4	0
26	R	1	Total C O 42 40 2	0
26	S	1	Total C O 84 80 4	0
26	S	1	Total C O 84 80 4	0

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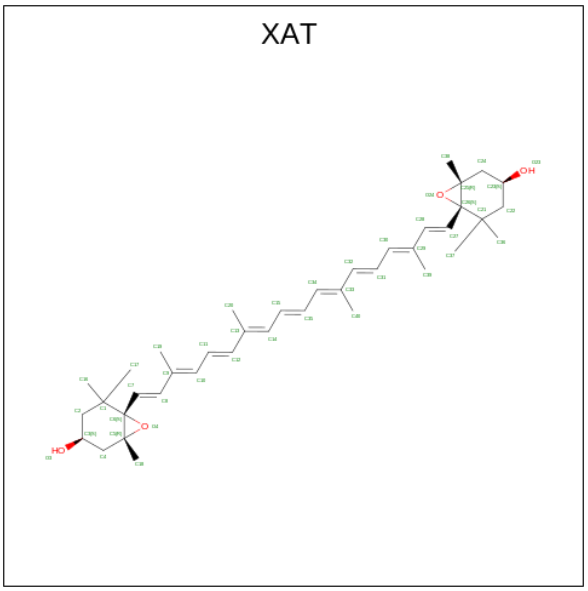
Mol	Chain	Residues	Atoms	AltConf
26	Y	1	Total C O 84 80 4	0
26	Y	1	Total C O 84 80 4	0
26	5	1	Total C O 84 80 4	0
26	5	1	Total C O 84 80 4	0
26	6	1	Total C O 84 80 4	0
26	6	1	Total C O 84 80 4	0
26	7	1	Total C O 84 80 4	0
26	7	1	Total C O 84 80 4	0
26	8	1	Total C O 42 40 2	0
26	g	1	Total C O 84 80 4	0
26	g	1	Total C O 84 80 4	0
26	n	1	Total C O 84 80 4	0
26	n	1	Total C O 84 80 4	0
26	r	1	Total C O 42 40 2	0
26	s	1	Total C O 84 80 4	0
26	s	1	Total C O 84 80 4	0
26	y	1	Total C O 84 80 4	0
26	y	1	Total C O 84 80 4	0

- Molecule 27 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 (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	G	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	Y	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	
27	g	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	

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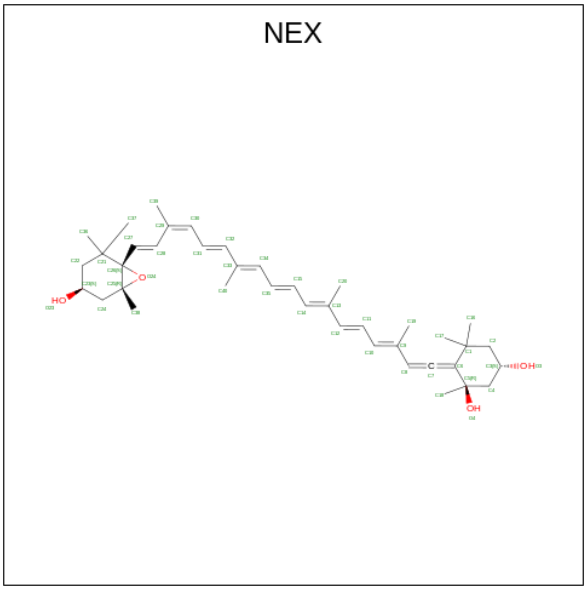
Mol	Chain	Residues	Atoms	AltConf
27	r	1	Total C O 44 40 4	0
27	y	1	Total C O 44 40 4	0

- Molecule 28 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 (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms	AltConf
28	1	1	Total C O 44 40 4	0
28	2	1	Total C O 44 40 4	0
28	3	1	Total C O 44 40 4	0
28	G	1	Total C O 44 40 4	0
28	N	1	Total C O 44 40 4	0
28	R	1	Total C O 44 40 4	0
28	S	1	Total C O 44 40 4	0
28	Y	1	Total C O 44 40 4	0

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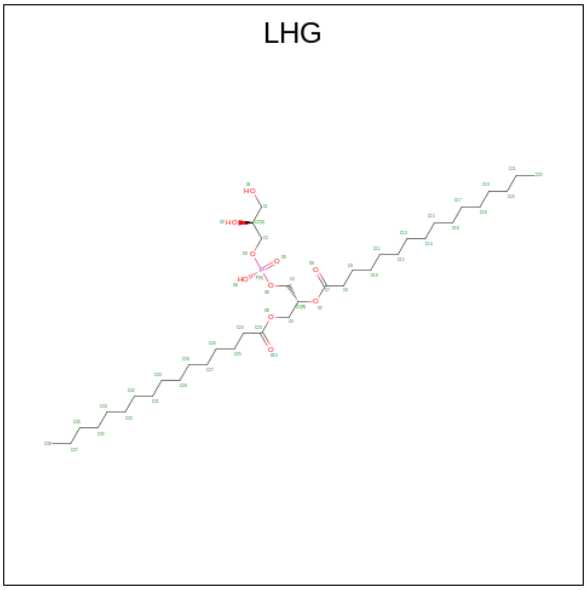
Mol	Chain	Residues	Atoms	AltConf
28	5	1	Total C O 44 40 4	0
28	6	1	Total C O 44 40 4	0
28	7	1	Total C O 44 40 4	0
28	g	1	Total C O 44 40 4	0
28	n	1	Total C O 44 40 4	0
28	r	1	Total C O 44 40 4	0
28	s	1	Total C O 44 40 4	0
28	y	1	Total C O 44 40 4	0

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C O P 41 30 10 1	0
29	2	1	Total C O P 37 26 10 1	0
29	3	1	Total C O P 47 36 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total	C	O	P	0
			21	10	10	1	
29	B	1	Total	C	O	P	0
			96	74	20	2	
29	B	1	Total	C	O	P	0
			96	74	20	2	
29	C	1	Total	C	O	P	0
			147	114	30	3	
29	C	1	Total	C	O	P	0
			147	114	30	3	
29	C	1	Total	C	O	P	0
			147	114	30	3	
29	D	1	Total	C	O	P	0
			138	105	30	3	
29	D	1	Total	C	O	P	0
			138	105	30	3	
29	D	1	Total	C	O	P	0
			138	105	30	3	
29	G	1	Total	C	O	P	0
			49	38	10	1	
29	L	1	Total	C	O	P	0
			49	38	10	1	
29	N	1	Total	C	O	P	0
			49	38	10	1	
29	R	1	Total	C	O	P	0
			42	31	10	1	
29	S	1	Total	C	O	P	0
			49	38	10	1	
29	Y	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			41	30	10	1	
29	6	1	Total	C	O	P	0
			37	26	10	1	
29	7	1	Total	C	O	P	0
			47	36	10	1	
29	8	1	Total	C	O	P	0
			21	10	10	1	
29	b	1	Total	C	O	P	0
			96	74	20	2	
29	b	1	Total	C	O	P	0
			96	74	20	2	

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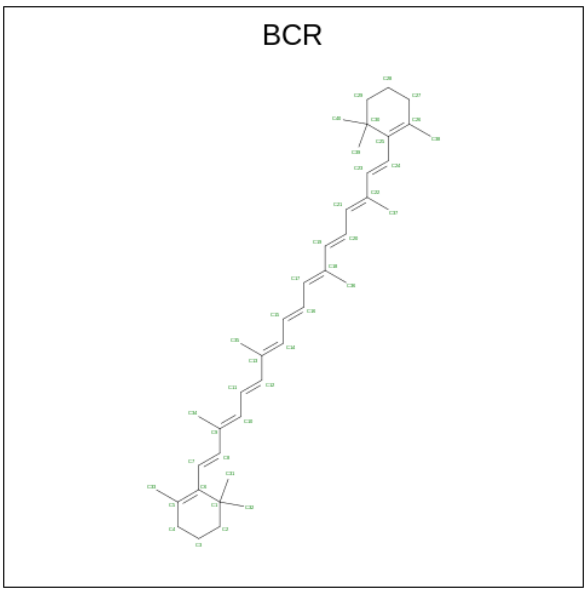
Mol	Chain	Residues	Atoms				AltConf
29	c	1	Total	C	O	P	0
			147	114	30	3	
29	c	1	Total	C	O	P	0
			147	114	30	3	
29	c	1	Total	C	O	P	0
			147	114	30	3	
29	d	1	Total	C	O	P	0
			138	105	30	3	
29	d	1	Total	C	O	P	0
			138	105	30	3	
29	d	1	Total	C	O	P	0
			138	105	30	3	
29	g	1	Total	C	O	P	0
			49	38	10	1	
29	l	1	Total	C	O	P	0
			49	38	10	1	
29	n	1	Total	C	O	P	0
			49	38	10	1	
29	r	1	Total	C	O	P	0
			42	31	10	1	
29	s	1	Total	C	O	P	0
			49	38	10	1	
29	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
30	4	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 120 120	0
30	B	1	Total C 120 120	0
30	B	1	Total C 120 120	0
30	C	1	Total C 160 160	0
30	C	1	Total C 160 160	0
30	C	1	Total C 160 160	0
30	C	1	Total C 160 160	0
30	D	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	T	1	Total C 40 40	0
30	8	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 120 120	0
30	b	1	Total C 120 120	0
30	b	1	Total C 120 120	0
30	c	1	Total C 160 160	0
30	c	1	Total C 160 160	0
30	c	1	Total C 160 160	0
30	c	1	Total C 160 160	0
30	d	1	Total C 40 40	0

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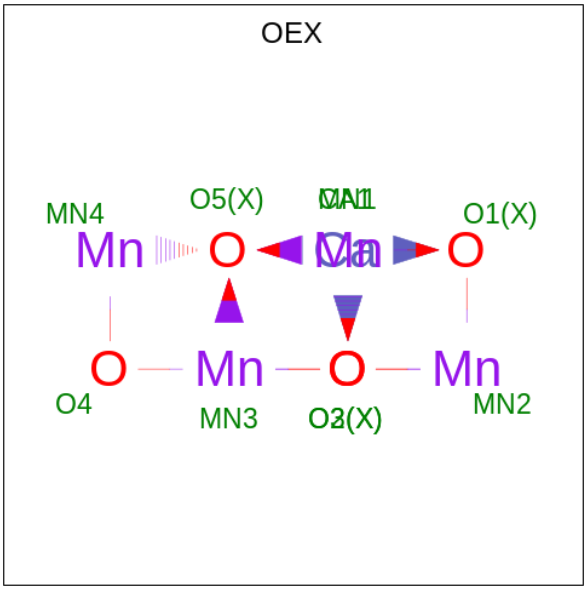
Mol	Chain	Residues	Atoms	AltConf
30	h	1	Total C 40 40	0
30	t	1	Total C 40 40	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).

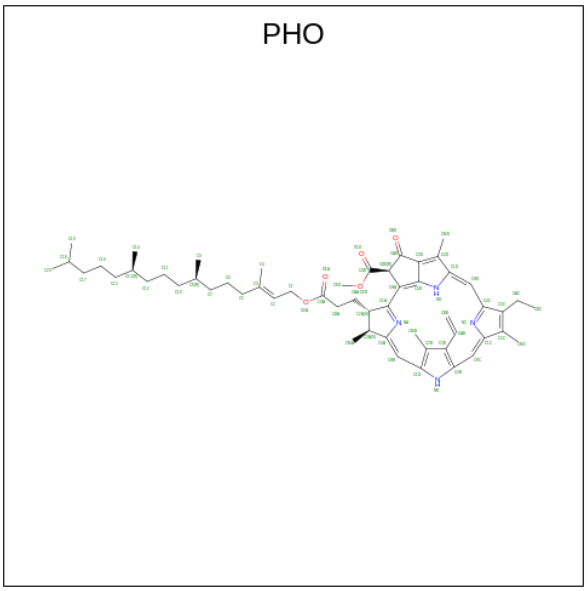


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Ca Mn O 10 1 4 5	0
31	a	1	Total Ca Mn O 10 1 4 5	0

- Molecule 32 is FE (II) ION (three-letter code: FE2) (formula: Fe).

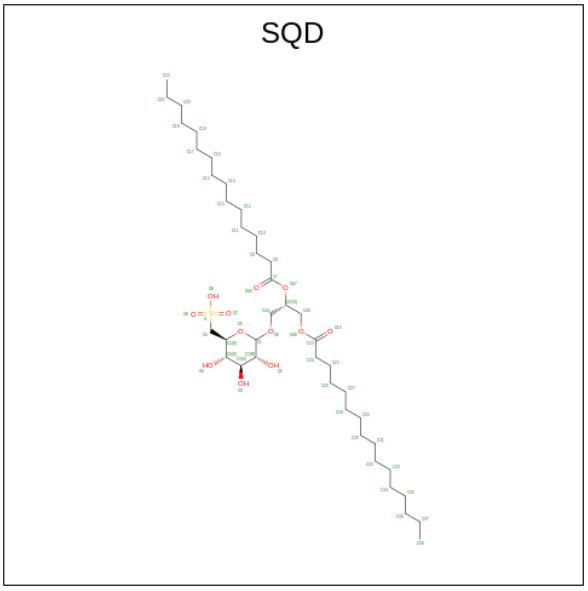
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Fe 1 1	0
32	a	1	Total Fe 1 1	0

- Molecule 33 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



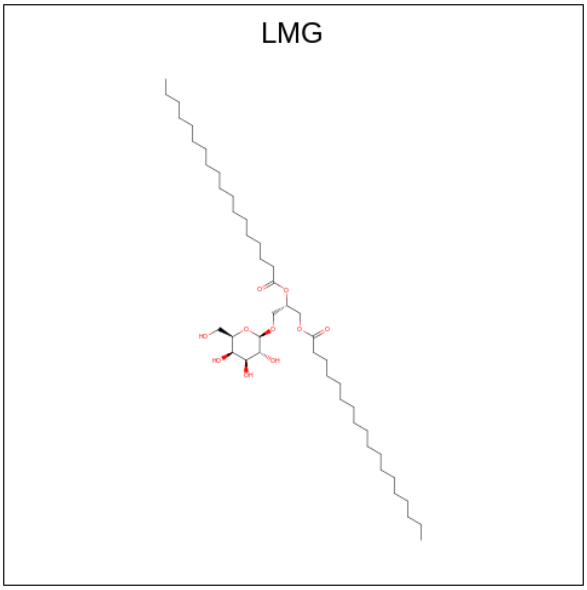
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			128	110	8	10	
33	A	1	Total	C	N	O	0
			128	110	8	10	
33	a	1	Total	C	N	O	0
			128	110	8	10	
33	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	S	0
			104	78	24	2	
34	A	1	Total	C	O	S	0
			104	78	24	2	
34	B	1	Total	C	O	S	0
			96	70	24	2	
34	B	1	Total	C	O	S	0
			96	70	24	2	
34	a	1	Total	C	O	S	0
			104	78	24	2	
34	a	1	Total	C	O	S	0
			104	78	24	2	
34	b	1	Total	C	O	S	0
			96	70	24	2	
34	b	1	Total	C	O	S	0
			96	70	24	2	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			88	68	20	
35	A	1	Total	C	O	0
			88	68	20	
35	B	1	Total	C	O	0
			106	86	20	

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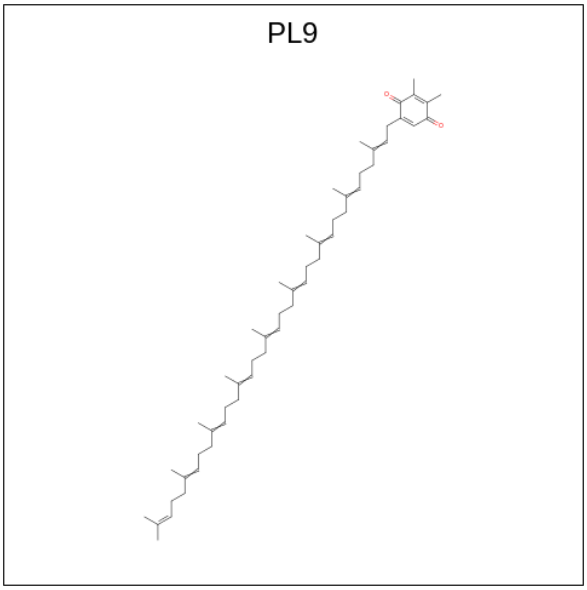
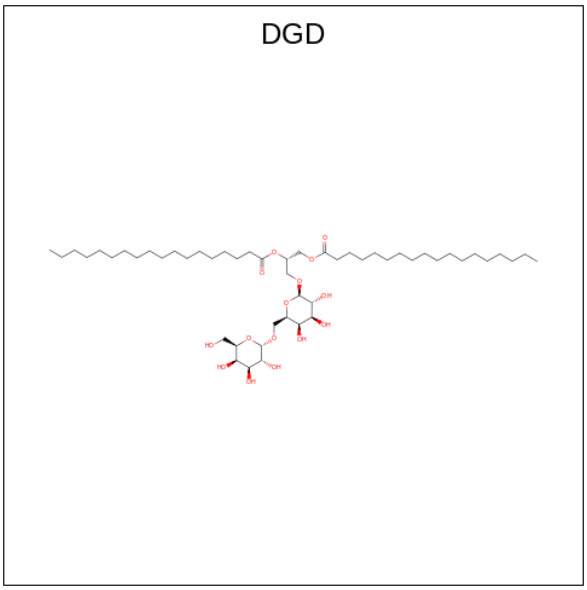
Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			106	86	20	
35	C	1	Total	C	O	0
			51	41	10	
35	D	1	Total	C	O	0
			46	36	10	
35	Z	1	Total	C	O	0
			51	41	10	
35	a	1	Total	C	O	0
			88	68	20	
35	a	1	Total	C	O	0
			88	68	20	
35	b	1	Total	C	O	0
			106	86	20	
35	b	1	Total	C	O	0
			106	86	20	
35	c	1	Total	C	O	0
			51	41	10	
35	d	1	Total	C	O	0
			46	36	10	
35	z	1	Total	C	O	0
			51	41	10	

- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total 13	C 11	O 2	0
36	D	1	Total 55	C 53	O 2	0
36	a	1	Total 13	C 11	O 2	0
36	d	1	Total 55	C 53	O 2	0

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



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total 59	C 44	O 15	0
37	C	1	Total 177	C 132	O 45	0
37	C	1	Total 177	C 132	O 45	0
37	C	1	Total 177	C 132	O 45	0
37	H	1	Total 62	C 47	O 15	0
37	b	1	Total 59	C 44	O 15	0
37	c	1	Total 177	C 132	O 45	0

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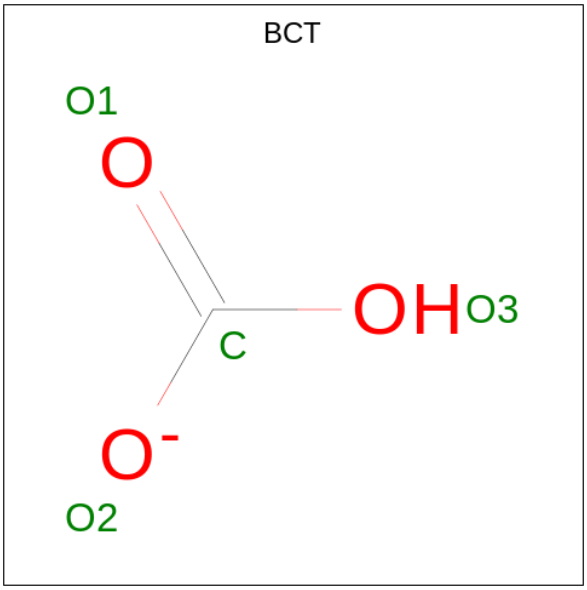
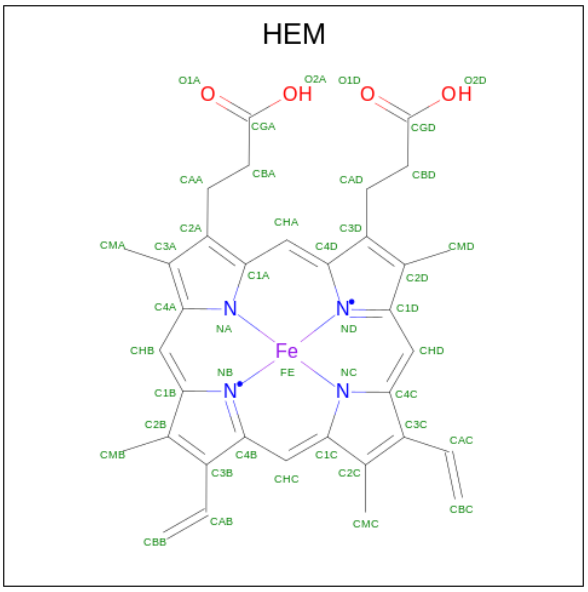
Mol	Chain	Residues	Atoms	AltConf
37	c	1	Total C O 177 132 45	0
37	c	1	Total C O 177 132 45	0
37	h	1	Total C O 62 47 15	0

- Molecule 38 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



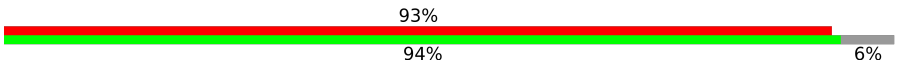
Mol	Chain	Residues	Atoms					AltConf
39	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
39	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

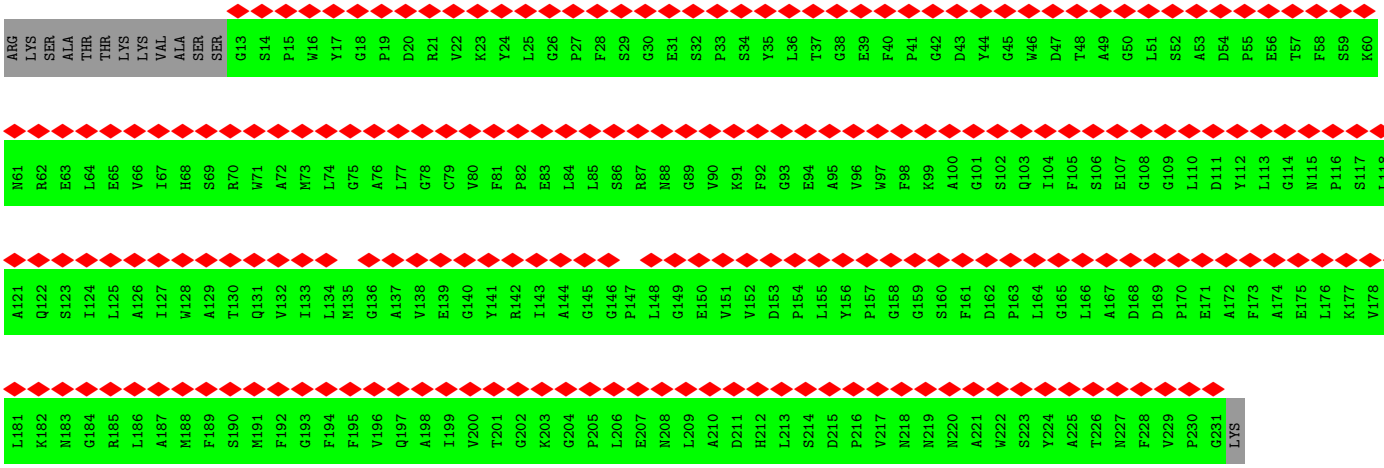
3 Residue-property plots (i)

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 8, chloroplastic

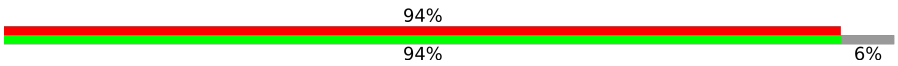
Chain 1:

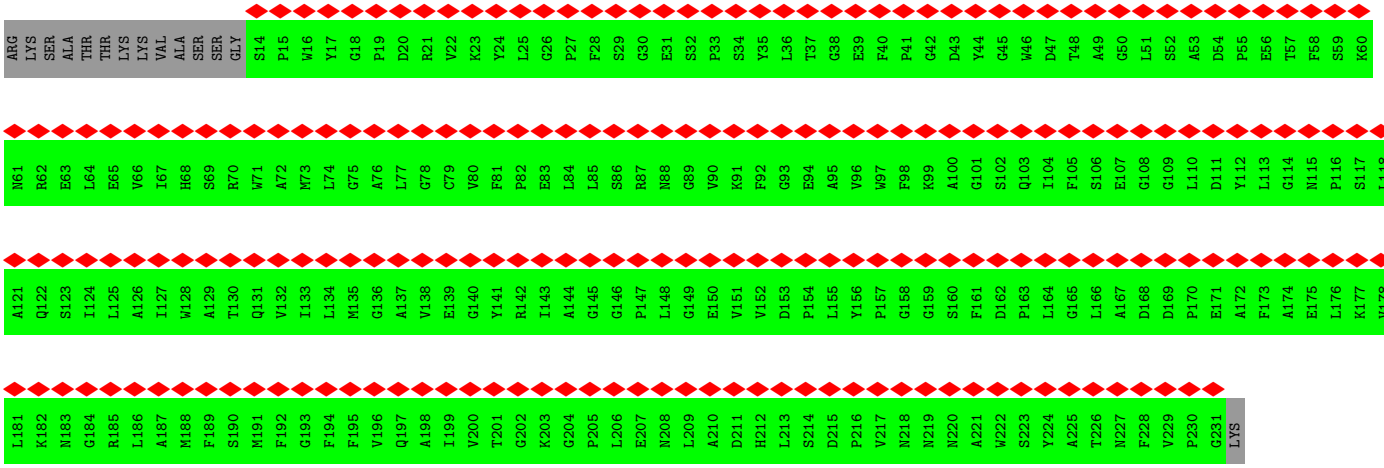




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

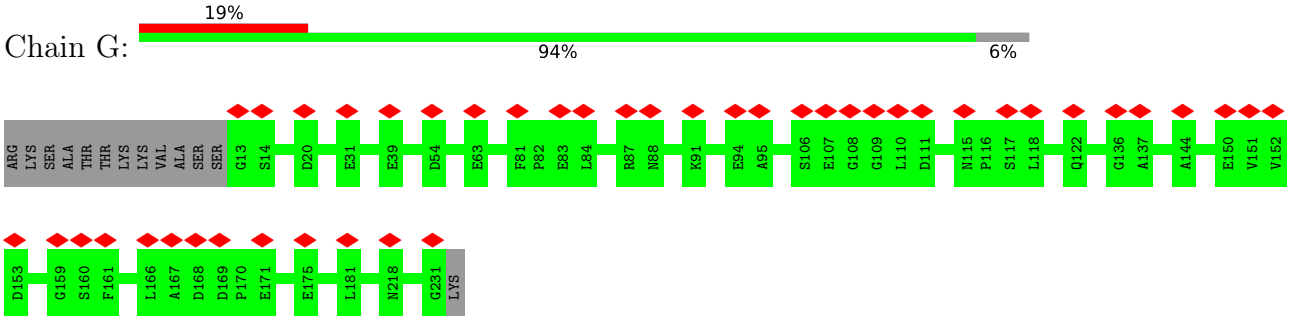
Chain 2:





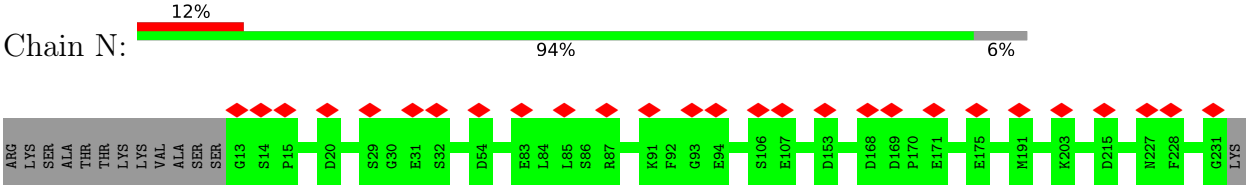
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain G:



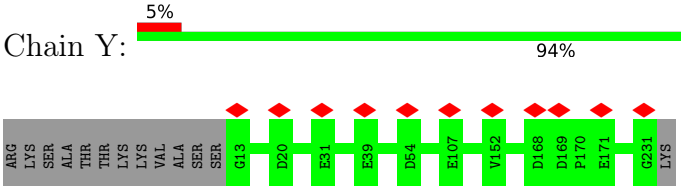
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain N:



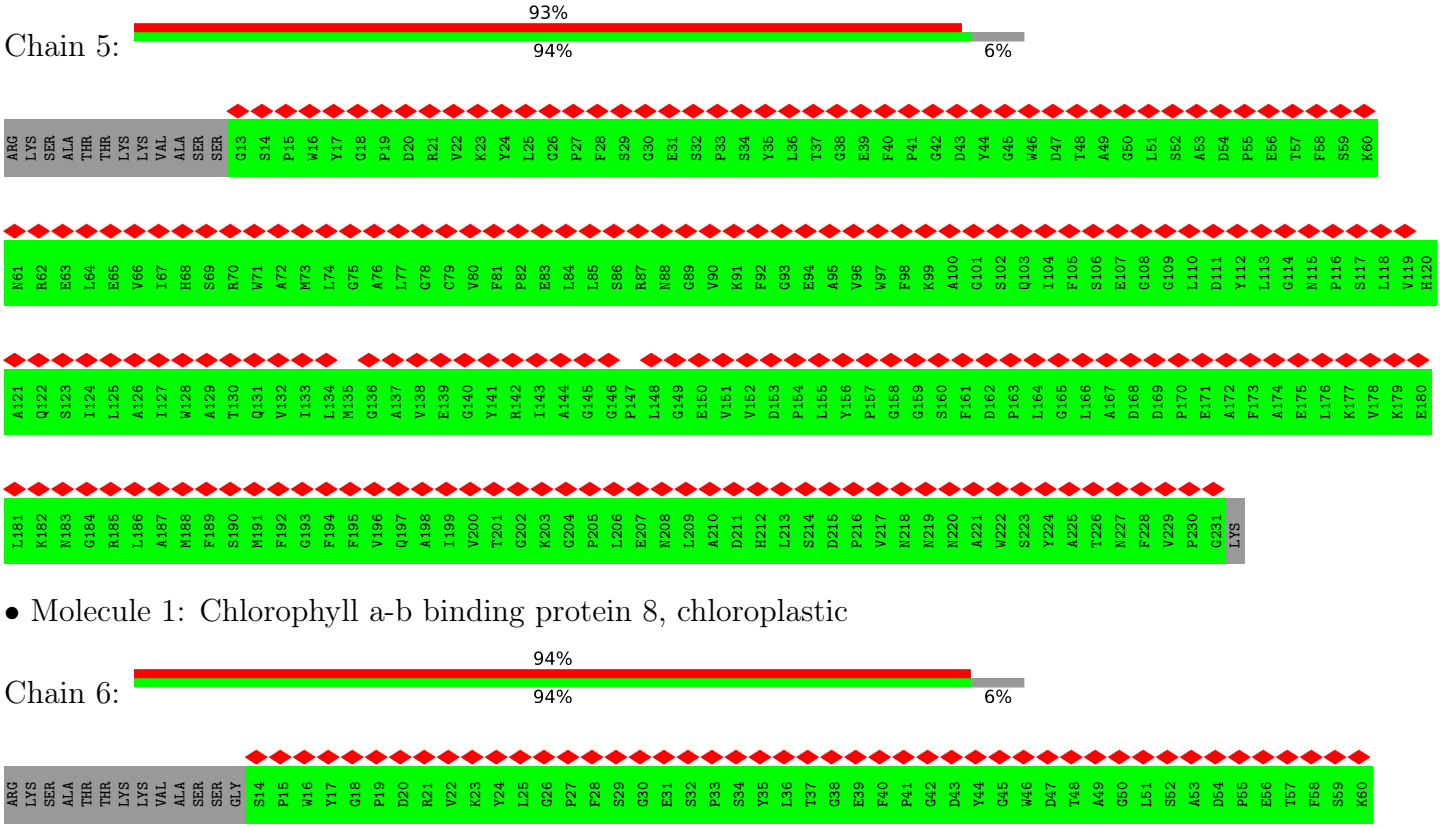
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain Y:



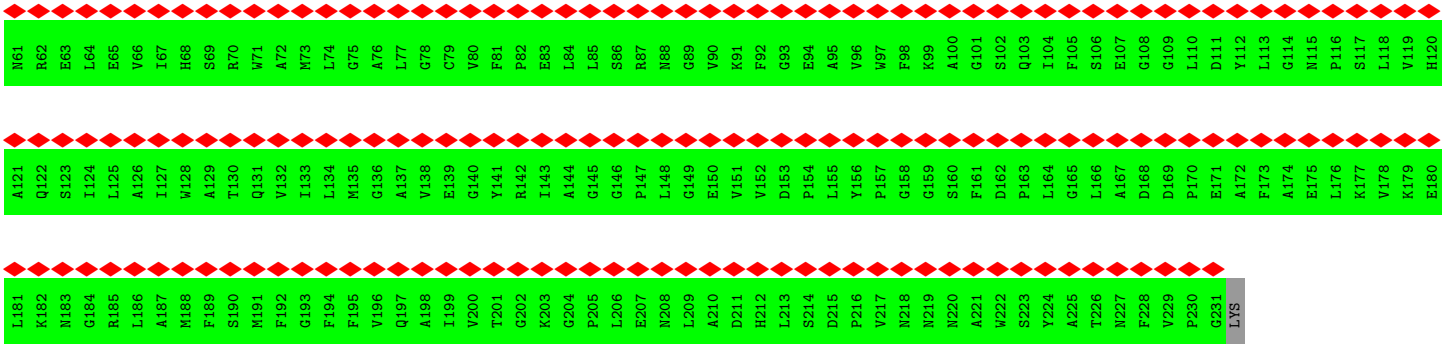
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain 5:



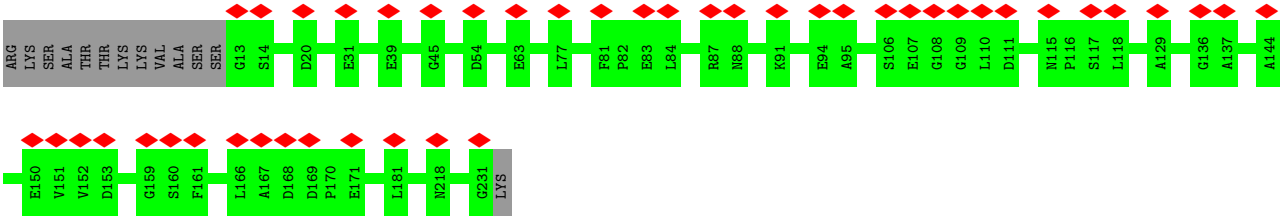
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain 6:



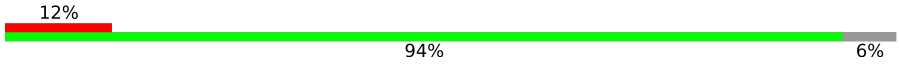
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

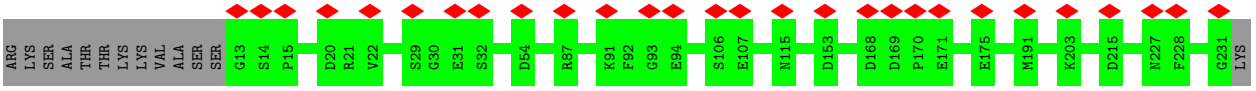
Chain g:



• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

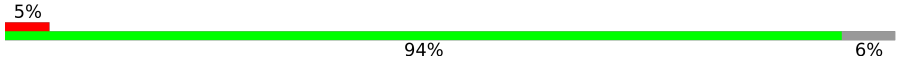
Chain n:

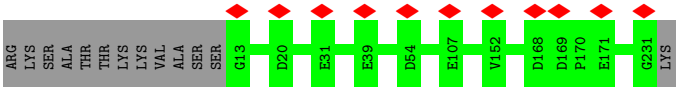




• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

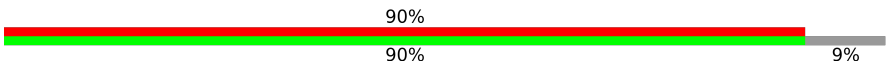
Chain y:

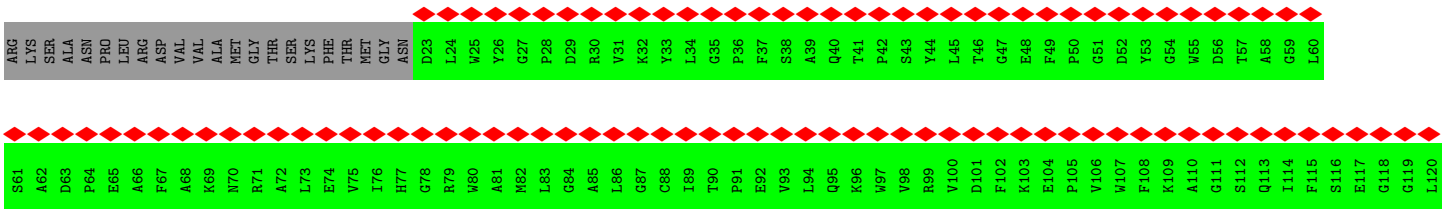


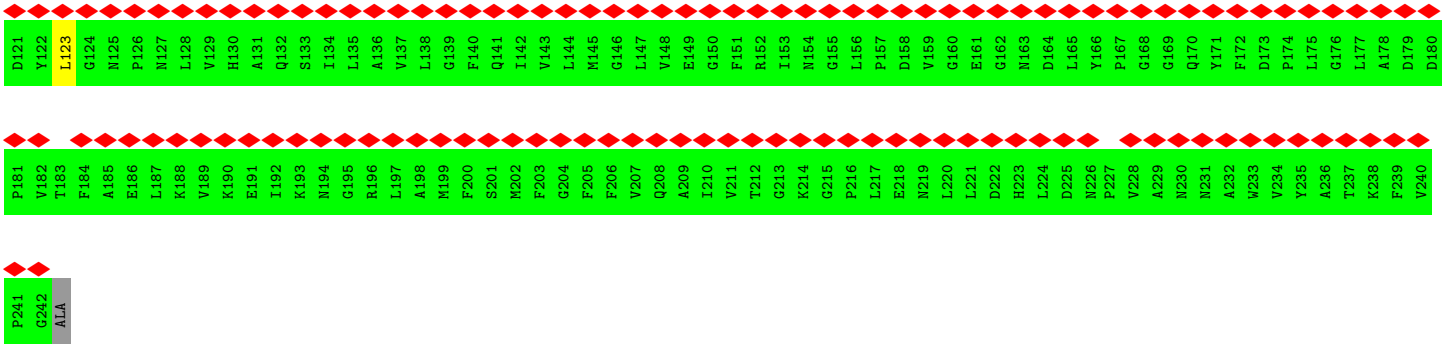


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

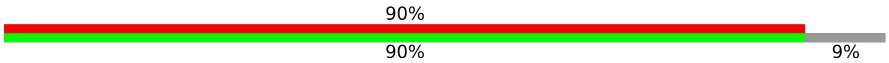


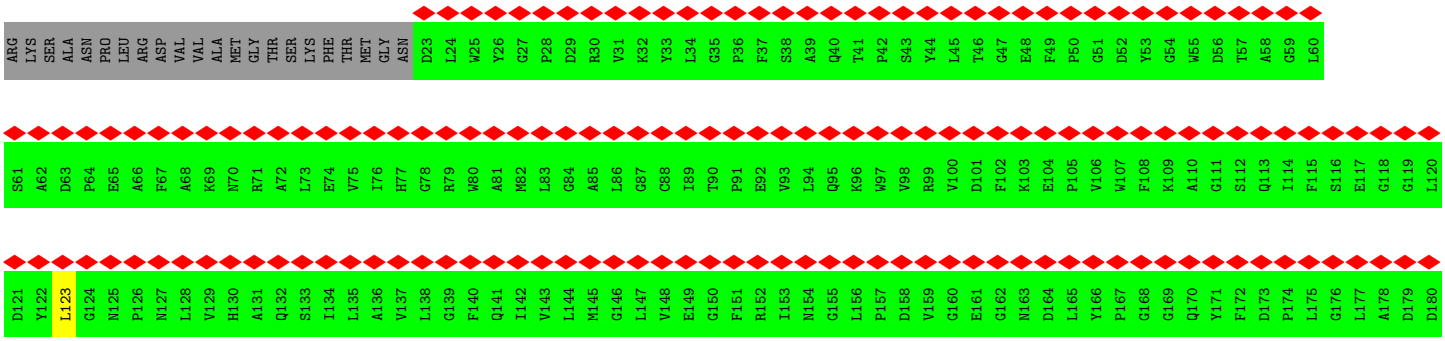




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

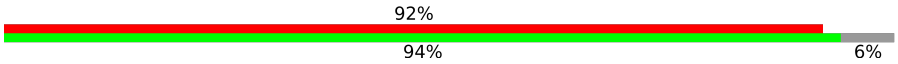
Chain 7:

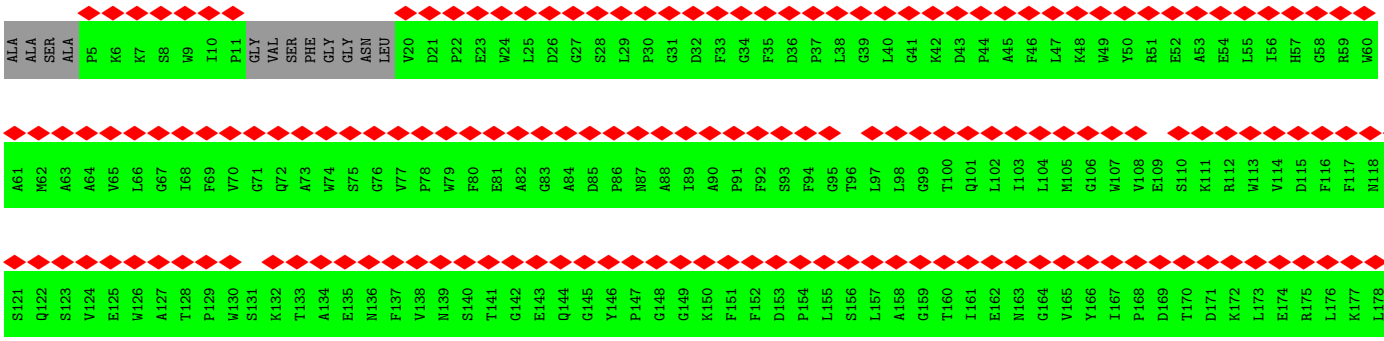




• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

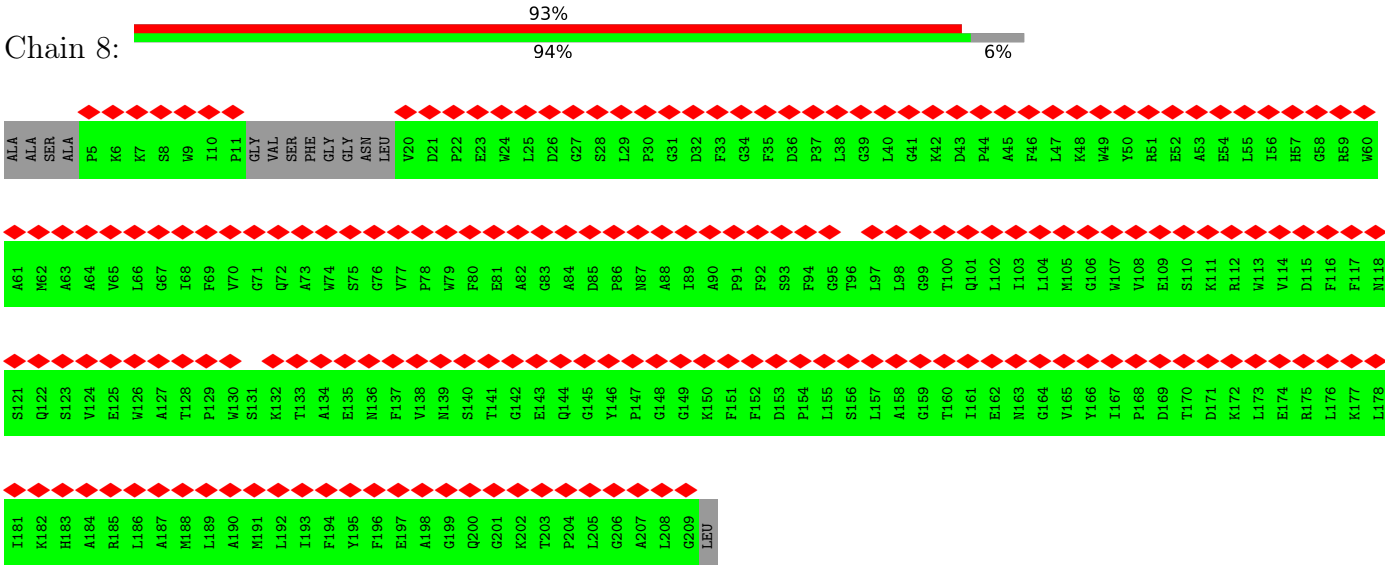
Chain 4:





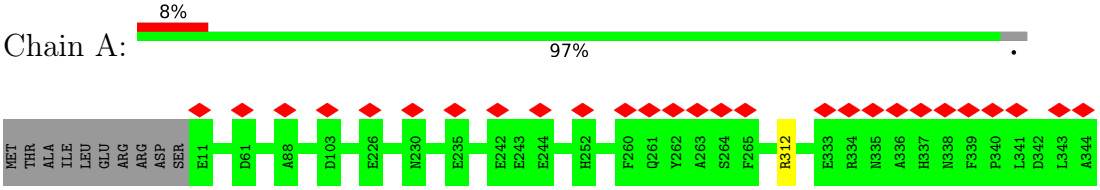
• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

Chain 8:



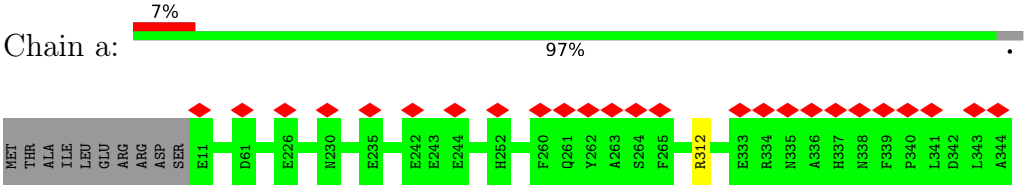
• Molecule 4: Photosystem II protein D1

Chain A:



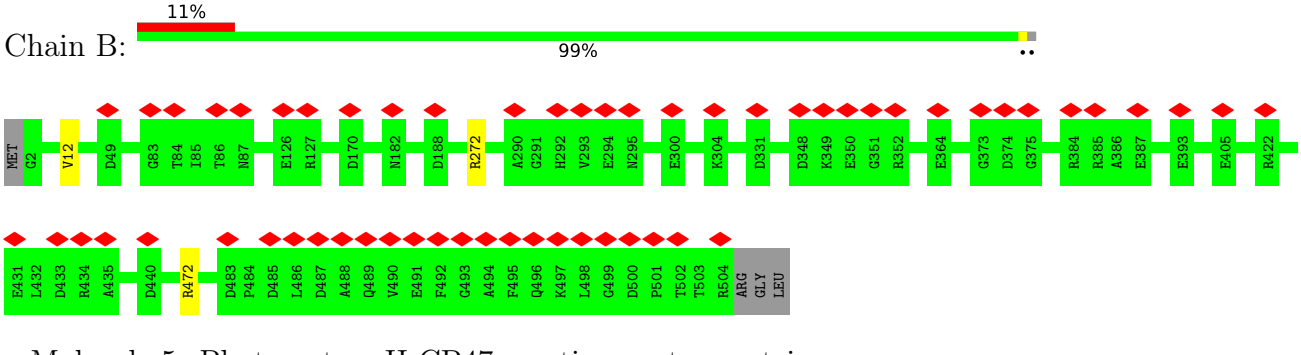
• Molecule 4: Photosystem II protein D1

Chain a:



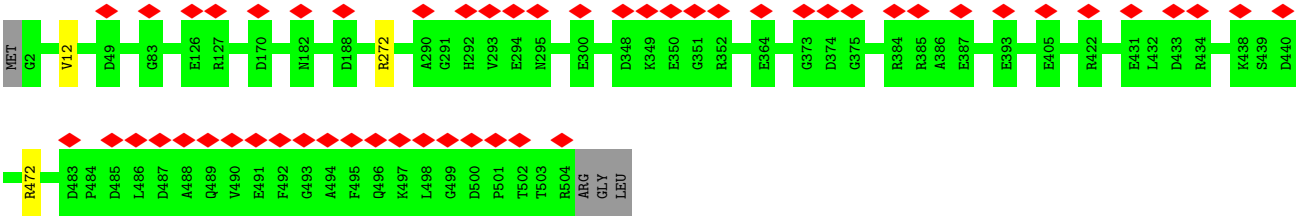
• Molecule 5: Photosystem II CP47 reaction center protein

Chain B:

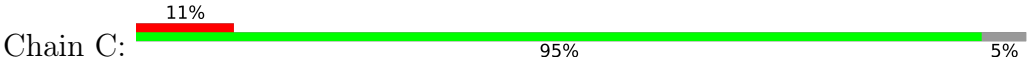


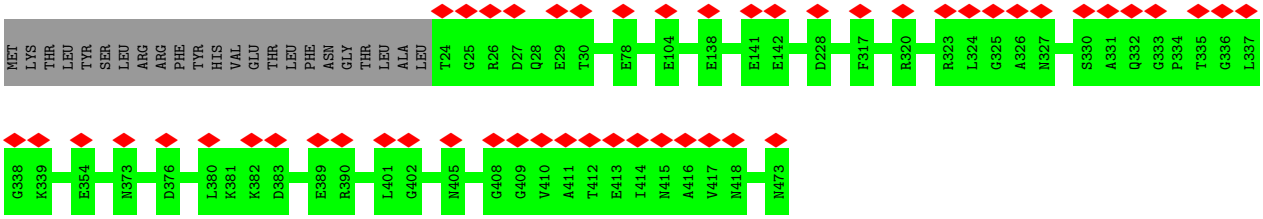
• Molecule 5: Photosystem II CP47 reaction center protein

Chain b:

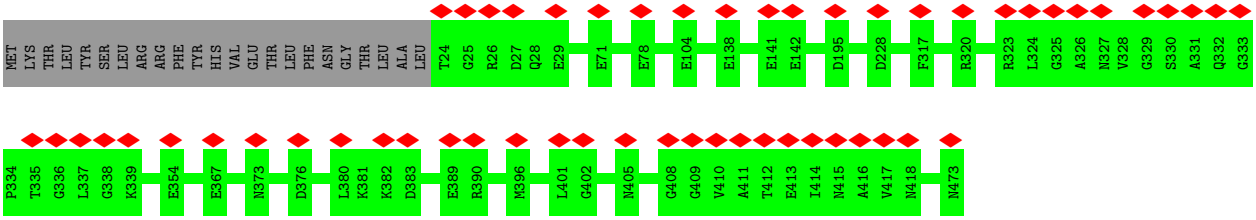


• Molecule 6: Photosystem II CP43 reaction center protein

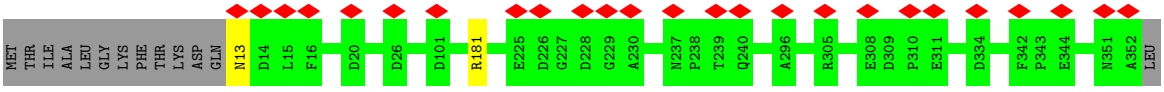




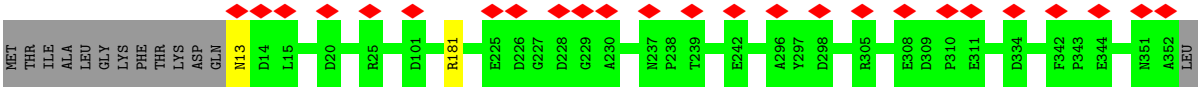
• Molecule 6: Photosystem II CP43 reaction center protein



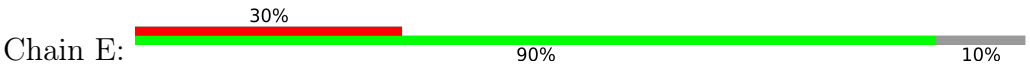
• Molecule 7: Photosystem II D2 protein

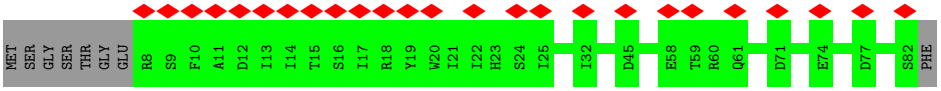


• Molecule 7: Photosystem II D2 protein

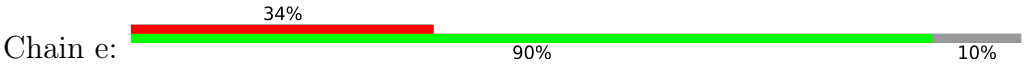


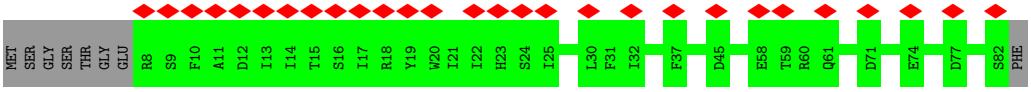
• Molecule 8: Cytochrome b559 subunit alpha



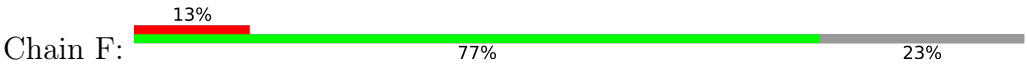


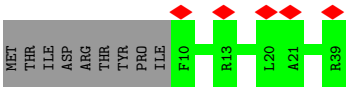
• Molecule 8: Cytochrome b559 subunit alpha



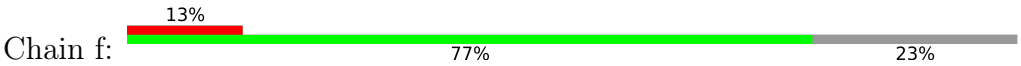


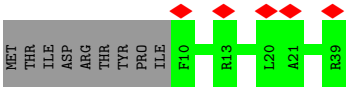
• Molecule 9: Cytochrome b559 subunit beta, PsbF



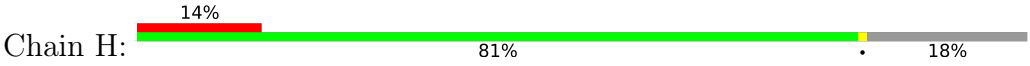


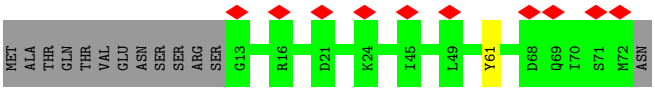
• Molecule 9: Cytochrome b559 subunit beta, PsbF



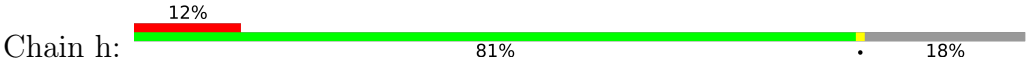


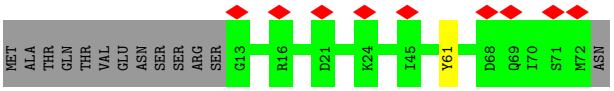
• Molecule 10: Photosystem II reaction center protein H



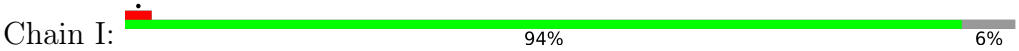


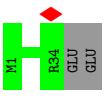
• Molecule 10: Photosystem II reaction center protein H





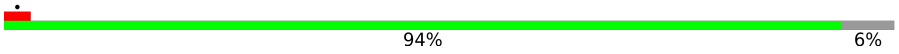
• Molecule 11: Photosystem II reaction center protein I, PsbI

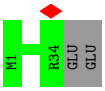




• Molecule 11: Photosystem II reaction center protein I, PsbI

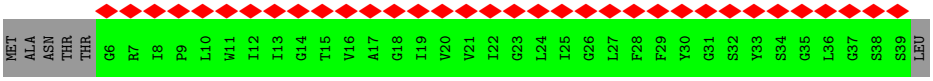
Chain i:





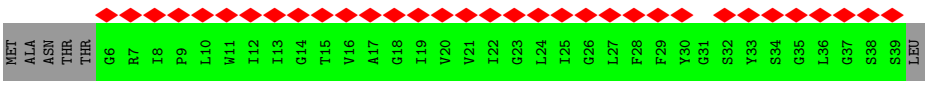
• Molecule 12: Photosystem II reaction center protein J

Chain J:



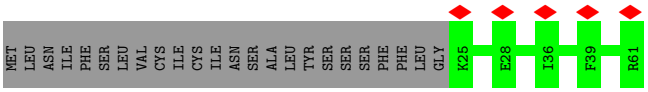
• Molecule 12: Photosystem II reaction center protein J

Chain j:



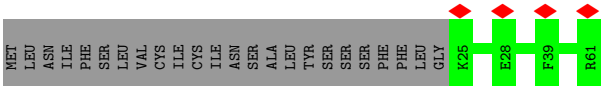
• Molecule 13: Photosystem II reaction center protein K

Chain K:



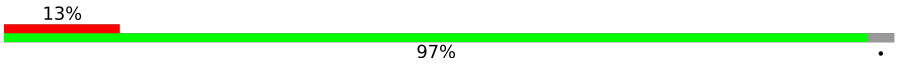
• Molecule 13: Photosystem II reaction center protein K

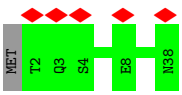
Chain k:



• Molecule 14: Photosystem II reaction center protein L

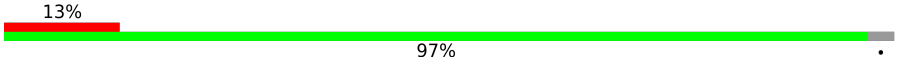
Chain L:

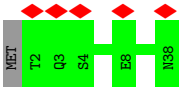




• Molecule 14: Photosystem II reaction center protein L

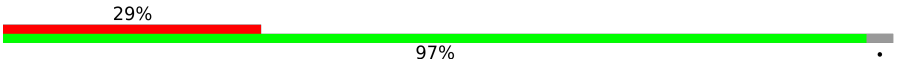
Chain l:

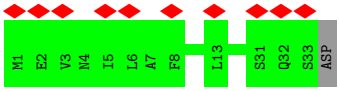




• Molecule 15: Photosystem II reaction center protein M

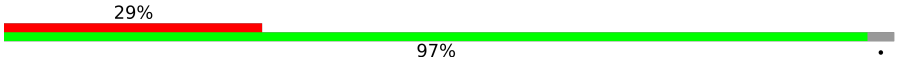
Chain M:

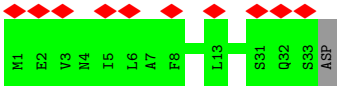




• Molecule 15: Photosystem II reaction center protein M

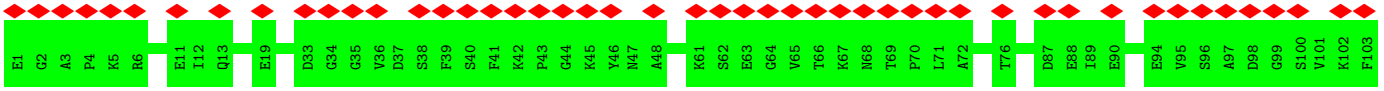
Chain m:

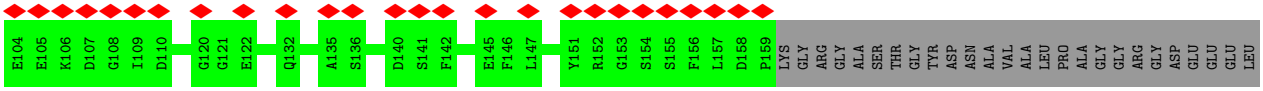


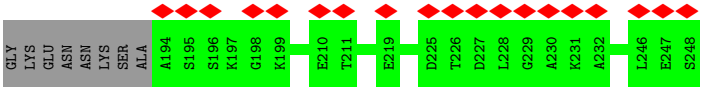


• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:

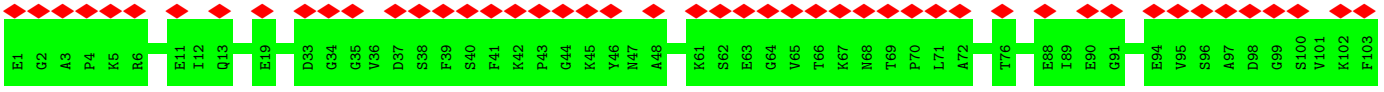


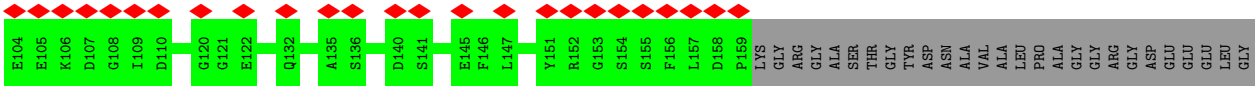


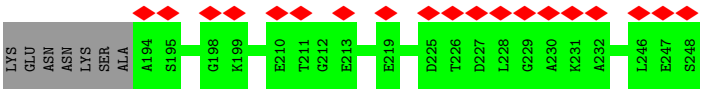


• Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:

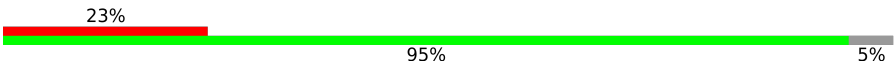


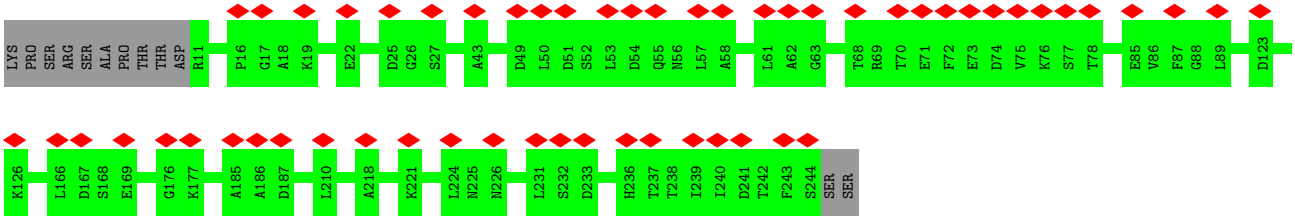




• Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

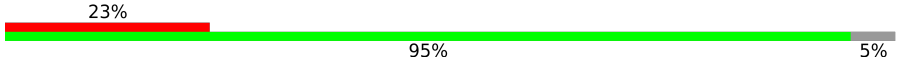
Chain R:

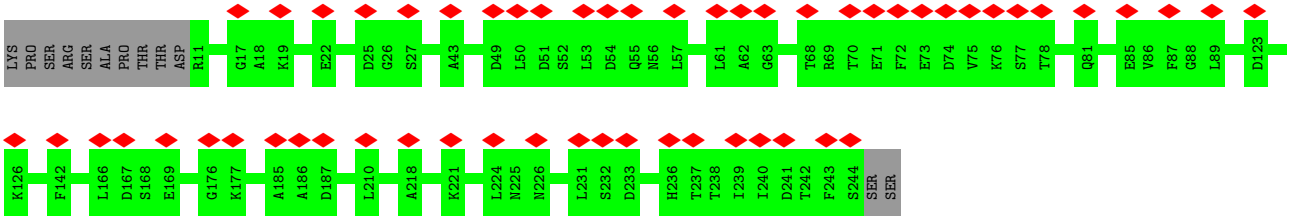




• Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

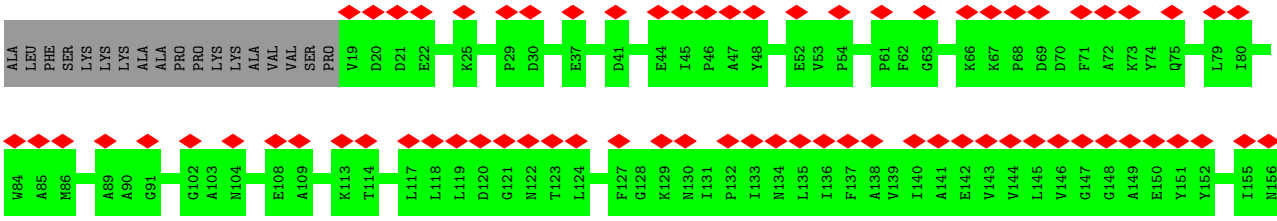
Chain r:

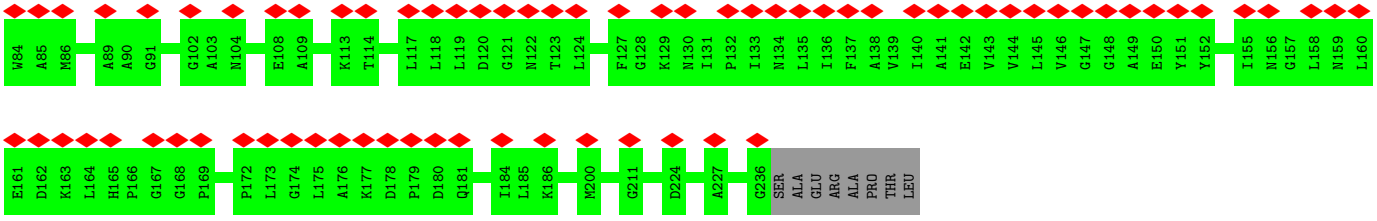




• Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

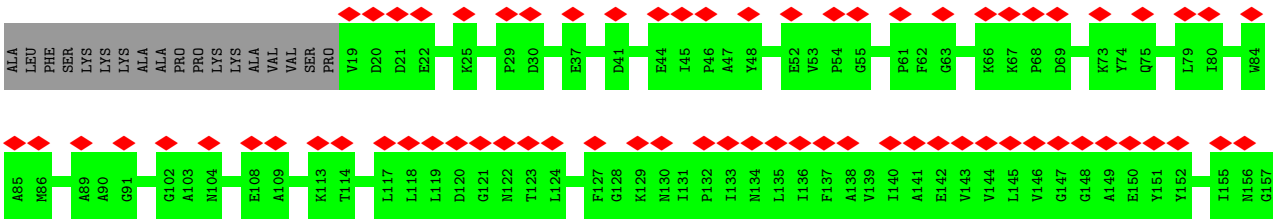
Chain S:

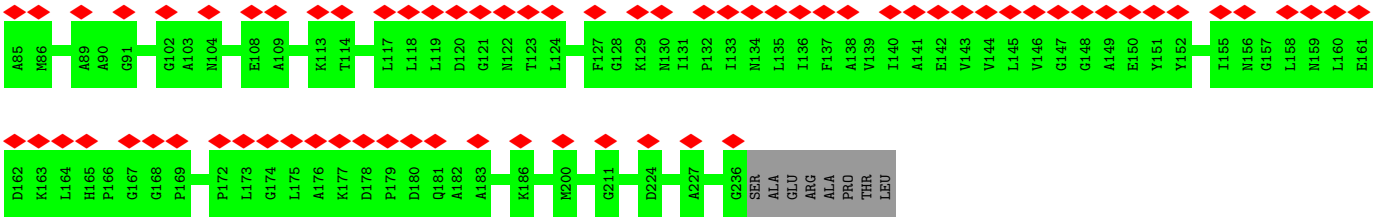




• Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

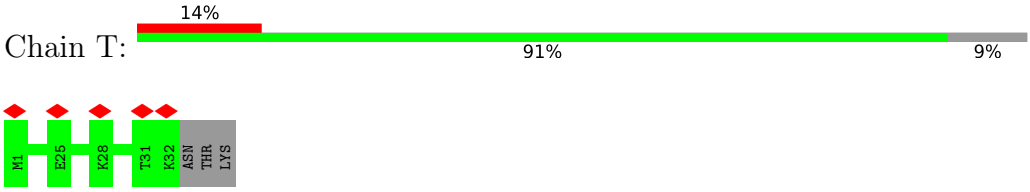
Chain s:





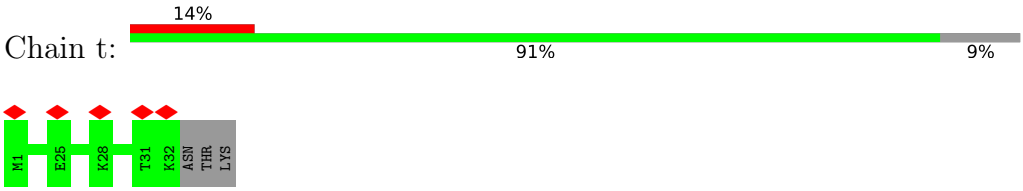
• Molecule 19: Photosystem II reaction center protein T

Chain T:



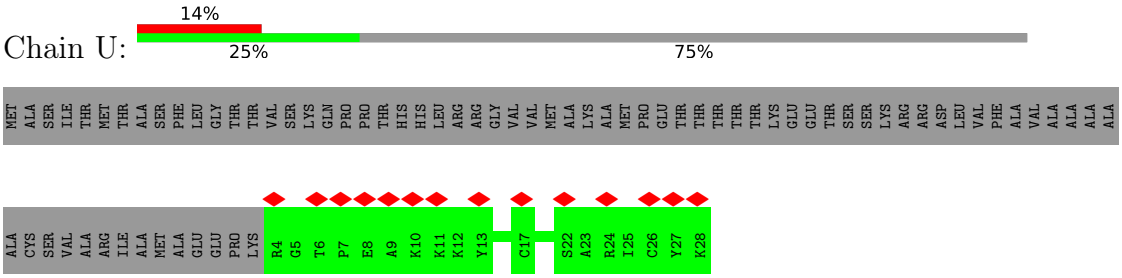
• Molecule 19: Photosystem II reaction center protein T

Chain t:



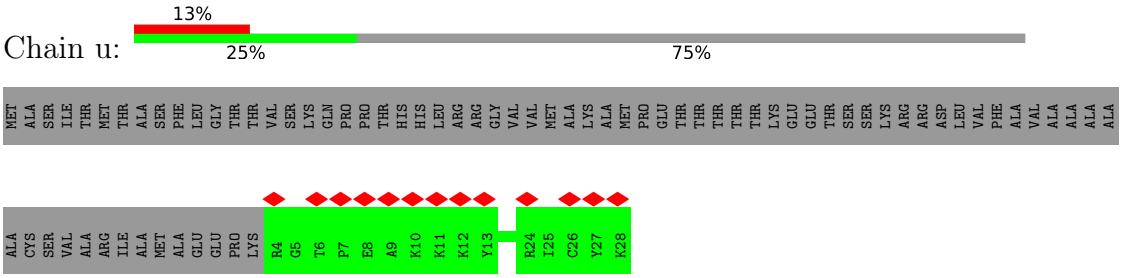
• Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn

Chain U:



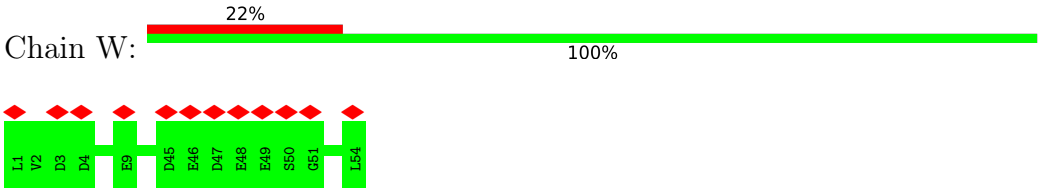
• Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn

Chain u:



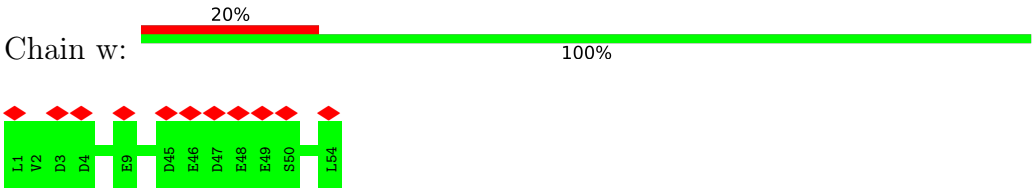
• Molecule 21: Photosystem II reaction center protein W, PSBW

Chain W:



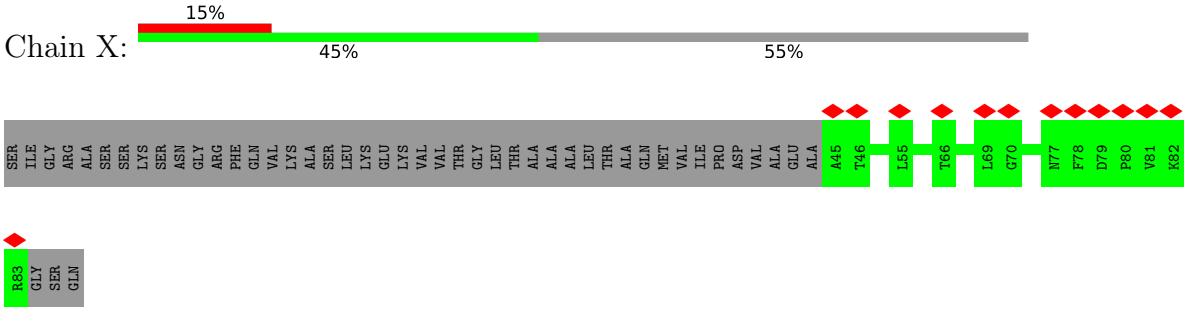
• Molecule 21: Photosystem II reaction center protein W, PSBW

Chain w:



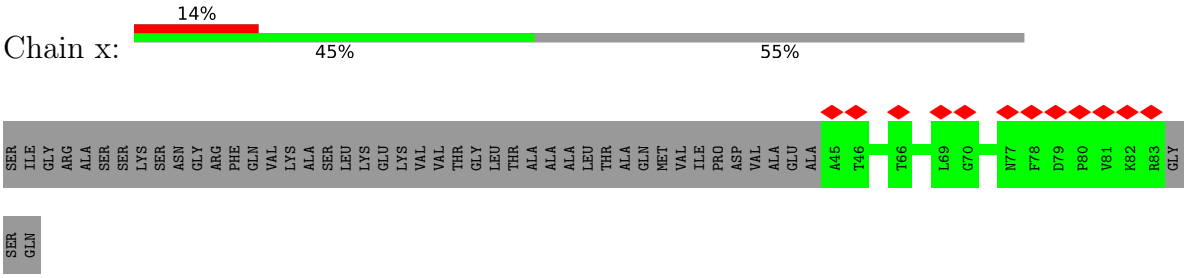
• Molecule 22: Photosystem II reaction center protein X

Chain X:



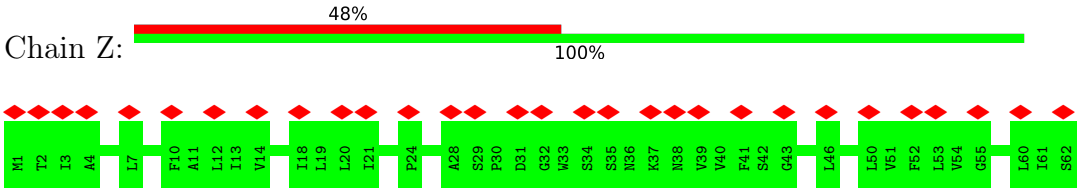
• Molecule 22: Photosystem II reaction center protein X

Chain x:



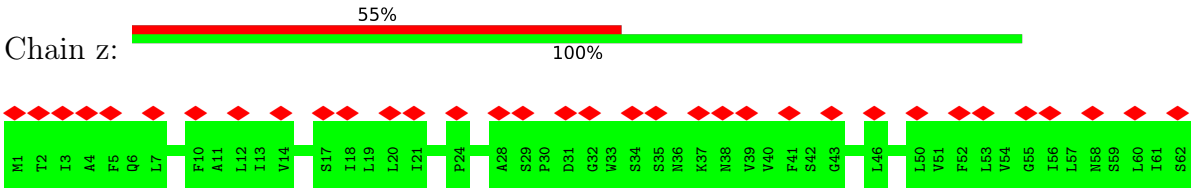
• Molecule 23: Photosystem II reaction center protein Z

Chain Z:



• Molecule 23: 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	50237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, CHL, DGD, LMG, XAT, BCR, FE2, LHG, HEM, CLA, OEX, BCT, PHO, LUT, NEX, PL9

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	0.48	0/1720	0.55	0/2342
1	2	0.43	0/1716	0.54	0/2337
1	5	0.48	0/1720	0.55	0/2342
1	6	0.43	0/1716	0.54	0/2337
1	G	0.44	0/1720	0.53	0/2342
1	N	0.45	0/1720	0.53	0/2342
1	Y	0.52	0/1720	0.55	0/2342
1	g	0.44	0/1720	0.53	0/2342
1	n	0.45	0/1720	0.53	0/2342
1	y	0.52	0/1720	0.55	0/2342
2	3	0.49	0/1759	0.59	1/2396 (0.0%)
2	7	0.49	0/1759	0.59	1/2396 (0.0%)
3	4	0.42	0/1586	0.59	0/2158
3	8	0.42	0/1586	0.59	0/2158
4	A	0.47	0/2697	0.57	0/3677
4	a	0.47	0/2697	0.57	0/3677
5	B	0.56	0/4081	0.59	0/5556
5	b	0.56	0/4081	0.59	0/5556
6	C	0.36	0/3614	0.54	0/4922
6	c	0.36	0/3614	0.54	0/4922
7	D	0.62	0/2795	0.65	0/3812
7	d	0.62	0/2795	0.65	0/3812
8	E	0.33	0/630	0.50	0/857
8	e	0.33	0/630	0.50	0/857
9	F	0.34	0/248	0.51	0/335
9	f	0.34	0/248	0.51	0/335
10	H	0.47	0/461	0.58	0/626
10	h	0.47	0/461	0.58	0/626
11	I	0.61	0/286	0.69	0/386
11	i	0.61	0/286	0.69	0/386
12	J	0.30	0/253	0.59	0/343
12	j	0.30	0/253	0.60	0/343

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	K	0.55	0/318	0.64	0/434
13	k	0.55	0/318	0.64	0/434
14	L	0.48	0/319	0.56	0/434
14	l	0.48	0/319	0.56	0/434
15	M	0.54	0/260	0.65	0/355
15	m	0.54	0/260	0.65	0/355
16	O	0.41	0/1664	0.56	0/2250
16	o	0.41	0/1664	0.56	0/2250
17	R	0.43	0/1886	0.57	0/2569
17	r	0.43	0/1886	0.57	0/2569
18	S	0.32	0/1736	0.54	0/2359
18	s	0.32	0/1736	0.54	0/2359
19	T	0.51	0/269	0.50	0/365
19	t	0.51	0/269	0.50	0/365
20	U	0.36	0/197	0.56	0/264
20	u	0.36	0/197	0.57	0/264
21	W	0.48	0/429	0.60	0/581
21	w	0.48	0/429	0.60	0/581
22	X	0.49	0/279	0.56	0/380
22	x	0.48	0/279	0.56	0/380
23	Z	0.42	0/474	0.53	0/648
23	z	0.42	0/474	0.53	0/648
All	All	0.47	0/69674	0.57	2/94824 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	123	LEU	CA-CB-CG	6.24	129.66	115.30
2	3	123	LEU	CA-CB-CG	6.24	129.64	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	2	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
1	5	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	6	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
1	G	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	N	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	Y	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	g	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	n	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	y	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
2	3	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
2	7	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
3	8	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
4	A	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
4	a	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
5	B	501/507 (99%)	488 (97%)	13 (3%)	0	100	100
5	b	501/507 (99%)	488 (97%)	13 (3%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
6	c	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
7	D	338/353 (96%)	332 (98%)	6 (2%)	0	100	100
7	d	338/353 (96%)	332 (98%)	6 (2%)	0	100	100
8	E	73/83 (88%)	73 (100%)	0	0	100	100
8	e	73/83 (88%)	73 (100%)	0	0	100	100
9	F	28/39 (72%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	f	28/39 (72%)	28 (100%)	0	0	100	100
10	H	58/73 (80%)	57 (98%)	1 (2%)	0	100	100
10	h	58/73 (80%)	57 (98%)	1 (2%)	0	100	100
11	I	32/36 (89%)	32 (100%)	0	0	100	100
11	i	32/36 (89%)	32 (100%)	0	0	100	100
12	J	32/40 (80%)	32 (100%)	0	0	100	100
12	j	32/40 (80%)	32 (100%)	0	0	100	100
13	K	35/61 (57%)	35 (100%)	0	0	100	100
13	k	35/61 (57%)	35 (100%)	0	0	100	100
14	L	35/38 (92%)	35 (100%)	0	0	100	100
14	l	35/38 (92%)	35 (100%)	0	0	100	100
15	M	31/34 (91%)	31 (100%)	0	0	100	100
15	m	31/34 (91%)	31 (100%)	0	0	100	100
16	O	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
16	o	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
17	R	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
17	r	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
18	S	216/244 (88%)	206 (95%)	10 (5%)	0	100	100
18	s	216/244 (88%)	206 (95%)	10 (5%)	0	100	100
19	T	30/35 (86%)	30 (100%)	0	0	100	100
19	t	30/35 (86%)	30 (100%)	0	0	100	100
20	U	23/99 (23%)	22 (96%)	1 (4%)	0	100	100
20	u	23/99 (23%)	22 (96%)	1 (4%)	0	100	100
21	W	52/54 (96%)	52 (100%)	0	0	100	100
21	w	52/54 (96%)	52 (100%)	0	0	100	100
22	X	37/86 (43%)	37 (100%)	0	0	100	100
22	x	37/86 (43%)	37 (100%)	0	0	100	100
23	Z	60/62 (97%)	60 (100%)	0	0	100	100
23	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	8596/9536 (90%)	8394 (98%)	202 (2%)	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	171/182 (94%)	171 (100%)	0	100 100
1	2	171/182 (94%)	171 (100%)	0	100 100
1	5	171/182 (94%)	171 (100%)	0	100 100
1	6	171/182 (94%)	171 (100%)	0	100 100
1	G	171/182 (94%)	171 (100%)	0	100 100
1	N	171/182 (94%)	171 (100%)	0	100 100
1	Y	171/182 (94%)	171 (100%)	0	100 100
1	g	171/182 (94%)	171 (100%)	0	100 100
1	n	171/182 (94%)	171 (100%)	0	100 100
1	y	171/182 (94%)	171 (100%)	0	100 100
2	3	175/193 (91%)	175 (100%)	0	100 100
2	7	175/193 (91%)	175 (100%)	0	100 100
3	4	154/162 (95%)	154 (100%)	0	100 100
3	8	154/162 (95%)	154 (100%)	0	100 100
4	A	270/279 (97%)	269 (100%)	1 (0%)	91 95
4	a	270/279 (97%)	269 (100%)	1 (0%)	91 95
5	B	400/403 (99%)	397 (99%)	3 (1%)	81 93
5	b	400/403 (99%)	397 (99%)	3 (1%)	81 93
6	C	352/373 (94%)	352 (100%)	0	100 100
6	c	352/373 (94%)	352 (100%)	0	100 100
7	D	274/285 (96%)	272 (99%)	2 (1%)	84 94
7	d	274/285 (96%)	272 (99%)	2 (1%)	84 94
8	E	67/73 (92%)	67 (100%)	0	100 100
8	e	67/73 (92%)	67 (100%)	0	100 100
9	F	25/34 (74%)	25 (100%)	0	100 100
9	f	25/34 (74%)	25 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	H	49/61 (80%)	48 (98%)	1 (2%)	55 80
10	h	49/61 (80%)	48 (98%)	1 (2%)	55 80
11	I	31/33 (94%)	31 (100%)	0	100 100
11	i	31/33 (94%)	31 (100%)	0	100 100
12	J	25/30 (83%)	25 (100%)	0	100 100
12	j	25/30 (83%)	25 (100%)	0	100 100
13	K	32/54 (59%)	32 (100%)	0	100 100
13	k	32/54 (59%)	32 (100%)	0	100 100
14	L	35/36 (97%)	35 (100%)	0	100 100
14	l	35/36 (97%)	35 (100%)	0	100 100
15	M	29/30 (97%)	29 (100%)	0	100 100
15	m	29/30 (97%)	29 (100%)	0	100 100
16	O	182/204 (89%)	182 (100%)	0	100 100
16	o	182/204 (89%)	182 (100%)	0	100 100
17	R	191/202 (95%)	191 (100%)	0	100 100
17	r	191/202 (95%)	191 (100%)	0	100 100
18	S	170/190 (90%)	170 (100%)	0	100 100
18	s	170/190 (90%)	170 (100%)	0	100 100
19	T	29/32 (91%)	29 (100%)	0	100 100
19	t	29/32 (91%)	29 (100%)	0	100 100
20	U	21/80 (26%)	21 (100%)	0	100 100
20	u	21/80 (26%)	21 (100%)	0	100 100
21	W	44/44 (100%)	44 (100%)	0	100 100
21	w	44/44 (100%)	44 (100%)	0	100 100
22	X	32/67 (48%)	32 (100%)	0	100 100
22	x	32/67 (48%)	32 (100%)	0	100 100
23	Z	54/54 (100%)	54 (100%)	0	100 100
23	z	54/54 (100%)	54 (100%)	0	100 100
All	All	6992/7658 (91%)	6978 (100%)	14 (0%)	93 98

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	312	ARG
5	B	12	VAL
5	B	272	ARG
5	B	472	ARG
7	D	13	ASN
7	D	181	ARG
10	H	61	TYR
4	a	312	ARG
5	b	12	VAL
5	b	272	ARG
5	b	472	ARG
7	d	13	ASN
7	d	181	ARG
10	h	61	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	2	61	ASN
1	2	88	ASN
2	3	95	GLN
2	3	219	ASN
3	4	72	GLN
4	A	234	ASN
4	A	301	ASN
4	A	303	ASN
4	A	335	ASN
5	B	216	HIS
6	C	28	GLN
6	C	322	GLN
6	C	415	ASN
7	D	13	ASN
7	D	84	ASN
7	D	351	ASN
1	G	122	GLN
14	L	5	ASN
14	L	10	ASN
16	O	74	GLN
16	O	222	GLN
17	R	47	GLN
17	R	55	GLN
1	Y	88	ASN

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Mol	Chain	Res	Type
1	5	61	ASN
1	6	61	ASN
1	6	88	ASN
2	7	95	GLN
2	7	219	ASN
3	8	72	GLN
4	a	234	ASN
4	a	301	ASN
4	a	303	ASN
4	a	335	ASN
5	b	216	HIS
6	c	28	GLN
6	c	322	GLN
6	c	415	ASN
7	d	13	ASN
7	d	84	ASN
7	d	351	ASN
1	g	122	GLN
14	l	5	ASN
14	l	10	ASN
16	o	74	GLN
16	o	222	GLN
17	r	47	GLN
17	r	55	GLN
1	y	88	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 486 ligands modelled in this entry, 2 are monoatomic - leaving 484 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	$\#\|Z\| > 2$
25	CLA	n	613	1	60,68,73	1.59	7 (11%)	70,107,113	1.69	7 (10%)
35	LMG	A	415	-	40,40,55	0.88	0	48,48,63	1.32	6 (12%)
25	CLA	d	402	7	65,73,73	1.51	12 (18%)	76,113,113	1.50	12 (15%)
24	CHL	y	607	-	66,74,74	1.81	12 (18%)	73,114,114	2.70	17 (23%)
29	LHG	D	410	-	42,42,48	0.66	1 (2%)	45,48,54	1.23	4 (8%)
25	CLA	c	510	6	65,73,73	1.46	7 (10%)	76,113,113	1.45	9 (11%)
25	CLA	r	603	17	60,68,73	1.52	10 (16%)	70,107,113	1.45	8 (11%)
25	CLA	g	604	-	50,58,73	1.75	11 (22%)	58,95,113	1.54	7 (12%)
25	CLA	1	612	1	45,53,73	1.81	11 (24%)	52,89,113	1.61	12 (23%)
29	LHG	n	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	7 (13%)
38	BCT	d	401	32	2,3,3	1.31	0	2,3,3	4.20	2 (100%)
25	CLA	4	611	29	45,53,73	1.77	9 (20%)	52,89,113	1.41	8 (15%)
25	CLA	A	406	-	65,73,73	1.49	10 (15%)	76,113,113	1.53	9 (11%)
25	CLA	C	509	6	65,73,73	1.45	8 (12%)	76,113,113	1.44	8 (10%)
25	CLA	6	612	1	45,53,73	1.83	9 (20%)	52,89,113	1.48	9 (17%)
25	CLA	b	606	5	65,73,73	1.52	12 (18%)	76,113,113	1.57	12 (15%)
25	CLA	c	502	6	65,73,73	1.44	6 (9%)	76,113,113	1.57	8 (10%)
24	CHL	N	601	1	66,74,74	1.89	14 (21%)	73,114,114	2.70	23 (31%)
26	LUT	1	1620	-	42,43,43	0.93	2 (4%)	51,60,60	1.87	14 (27%)
25	CLA	2	604	-	45,53,73	1.73	10 (22%)	52,89,113	1.64	10 (19%)
25	CLA	C	503	6	65,73,73	1.50	6 (9%)	76,113,113	1.34	6 (7%)
25	CLA	n	610	1	65,73,73	1.41	10 (15%)	76,113,113	1.40	8 (10%)
35	LMG	D	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.38	6 (11%)
24	CHL	r	614	17	42,50,74	2.39	15 (35%)	44,85,114	3.37	18 (40%)
25	CLA	8	604	-	45,53,73	1.77	11 (24%)	52,89,113	1.58	9 (17%)
24	CHL	5	601	1	46,54,74	2.26	13 (28%)	49,90,114	3.19	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	S	614	18	49,57,73	1.64	6 (12%)	55,93,113	1.60	8 (14%)
25	CLA	B	612	5	65,73,73	1.59	11 (16%)	76,113,113	1.70	13 (17%)
25	CLA	r	609	17	58,66,73	1.53	11 (18%)	67,104,113	1.40	7 (10%)
27	XAT	7	1622	-	39,47,47	1.20	5 (12%)	54,74,74	3.07	27 (50%)
24	CHL	g	607	-	66,74,74	1.83	12 (18%)	73,114,114	2.67	19 (26%)
28	NEX	g	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.53	17 (34%)
25	CLA	c	513	6	65,73,73	1.43	7 (10%)	76,113,113	1.47	10 (13%)
28	NEX	3	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.46	16 (32%)
25	CLA	r	610	17	65,73,73	1.46	9 (13%)	76,113,113	1.40	8 (10%)
27	XAT	n	1622	-	39,47,47	0.97	1 (2%)	54,74,74	3.01	23 (42%)
25	CLA	5	610	1	56,64,73	1.53	10 (17%)	65,102,113	1.36	6 (9%)
30	BCR	c	514	-	41,41,41	0.78	0	56,56,56	1.72	12 (21%)
25	CLA	b	613	5	65,73,73	1.49	11 (16%)	76,113,113	1.68	11 (14%)
30	BCR	B	618	-	41,41,41	1.05	3 (7%)	56,56,56	1.97	13 (23%)
25	CLA	G	610	1	64,72,73	1.43	10 (15%)	74,111,113	1.39	9 (12%)
25	CLA	b	602	-	65,73,73	1.46	11 (16%)	76,113,113	1.38	9 (11%)
24	CHL	8	606	-	46,54,74	2.23	13 (28%)	49,90,114	3.16	20 (40%)
25	CLA	B	608	-	65,73,73	1.50	11 (16%)	76,113,113	1.46	7 (9%)
25	CLA	y	604	-	50,58,73	1.75	9 (18%)	58,95,113	1.61	8 (13%)
25	CLA	C	505	6	65,73,73	1.46	8 (12%)	76,113,113	1.51	8 (10%)
24	CHL	n	608	-	66,74,74	1.80	12 (18%)	73,114,114	2.73	23 (31%)
25	CLA	1	611	29	45,53,73	1.75	12 (26%)	52,89,113	1.61	7 (13%)
25	CLA	B	616	5	65,73,73	1.49	10 (15%)	76,113,113	1.42	11 (14%)
25	CLA	B	604	5	65,73,73	1.54	11 (16%)	76,113,113	1.37	8 (10%)
24	CHL	y	606	-	50,58,74	2.06	15 (30%)	52,94,114	3.04	19 (36%)
25	CLA	D	402	7	65,73,73	1.51	12 (18%)	76,113,113	1.50	12 (15%)
25	CLA	5	612	1	45,53,73	1.81	11 (24%)	52,89,113	1.62	12 (23%)
33	PHO	a	409	-	51,69,69	1.02	5 (9%)	47,99,99	1.30	5 (10%)
25	CLA	1	614	1	45,53,73	1.77	9 (20%)	52,89,113	1.54	8 (15%)
24	CHL	7	606	-	46,54,74	2.31	14 (30%)	49,90,114	3.20	22 (44%)
25	CLA	G	611	29	60,68,73	1.52	10 (16%)	70,107,113	1.38	6 (8%)
24	CHL	7	609	2	61,69,74	2.03	16 (26%)	67,108,114	2.69	21 (31%)
24	CHL	6	601	1	46,54,74	2.25	14 (30%)	49,90,114	3.23	21 (42%)
25	CLA	s	612	18	49,57,73	1.68	7 (14%)	55,93,113	1.52	7 (12%)
25	CLA	3	602	2	60,68,73	1.49	9 (15%)	70,107,113	1.40	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	BCR	b	620	-	41,41,41	0.90	1 (2%)	56,56,56	2.02	15 (26%)
30	BCR	a	411	-	41,41,41	0.81	0	56,56,56	1.84	12 (21%)
26	LUT	Y	1621	-	42,43,43	1.07	4 (9%)	51,60,60	1.87	17 (33%)
24	CHL	4	608	-	46,54,74	2.16	13 (28%)	49,90,114	3.24	24 (48%)
35	LMG	A	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.30	4 (7%)
36	PL9	a	414	-	13,13,55	0.74	0	17,17,69	2.09	4 (23%)
26	LUT	5	1620	-	42,43,43	0.94	2 (4%)	51,60,60	1.87	14 (27%)
25	CLA	g	611	29	60,68,73	1.51	10 (16%)	70,107,113	1.38	6 (8%)
25	CLA	s	614	18	49,57,73	1.64	6 (12%)	55,93,113	1.59	8 (14%)
25	CLA	2	612	1	45,53,73	1.82	10 (22%)	52,89,113	1.48	9 (17%)
25	CLA	b	617	5	65,73,73	1.42	9 (13%)	76,113,113	1.47	9 (11%)
25	CLA	s	602	18	61,69,73	1.58	7 (11%)	71,108,113	1.39	8 (11%)
25	CLA	c	507	-	65,73,73	1.44	8 (12%)	76,113,113	1.54	10 (13%)
31	OEX	a	401	4,6	0,15,15	-	-	-		
26	LUT	y	1620	-	42,43,43	1.09	5 (11%)	51,60,60	1.91	20 (39%)
24	CHL	n	606	-	50,58,74	2.10	14 (28%)	52,94,114	3.10	18 (34%)
27	XAT	1	1622	-	39,47,47	0.95	2 (5%)	54,74,74	2.85	22 (40%)
29	LHG	c	522	-	48,48,48	0.66	1 (2%)	51,54,54	1.27	6 (11%)
25	CLA	C	501	6	65,73,73	1.55	8 (12%)	76,113,113	1.22	7 (9%)
25	CLA	b	603	5	65,73,73	1.46	10 (15%)	76,113,113	1.26	6 (7%)
24	CHL	Y	607	-	66,74,74	1.81	12 (18%)	73,114,114	2.70	17 (23%)
24	CHL	N	606	-	50,58,74	2.10	14 (28%)	52,94,114	3.10	18 (34%)
24	CHL	4	609	3	46,54,74	2.19	14 (30%)	49,90,114	3.29	20 (40%)
25	CLA	4	602	3	45,53,73	1.71	9 (20%)	52,89,113	1.68	8 (15%)
25	CLA	B	610	5	65,73,73	1.42	10 (15%)	76,113,113	1.48	10 (13%)
24	CHL	7	605	2	46,54,74	2.23	13 (28%)	49,90,114	3.18	22 (44%)
37	DGD	C	520	-	61,61,67	0.98	3 (4%)	75,75,81	1.44	10 (13%)
24	CHL	r	607	-	56,64,74	2.04	12 (21%)	61,102,114	2.93	25 (40%)
26	LUT	S	1621	-	42,43,43	0.80	0	51,60,60	1.74	15 (29%)
24	CHL	g	609	1	61,69,74	1.92	15 (24%)	67,108,114	2.71	22 (32%)
25	CLA	C	508	6	65,73,73	1.46	8 (12%)	76,113,113	1.54	8 (10%)
25	CLA	S	613	18	55,63,73	1.61	7 (12%)	64,101,113	1.41	6 (9%)
29	LHG	N	2630	25	48,48,48	0.75	1 (2%)	51,54,54	1.32	7 (13%)
25	CLA	5	611	29	45,53,73	1.74	12 (26%)	52,89,113	1.62	7 (13%)
25	CLA	a	405	4	65,73,73	1.46	9 (13%)	76,113,113	1.43	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	NEX	Y	1623	-	38,46,46	1.12	2 (5%)	50,70,70	2.70	22 (44%)
25	CLA	5	614	1	45,53,73	1.77	9 (20%)	52,89,113	1.53	8 (15%)
25	CLA	B	611	-	65,73,73	1.50	10 (15%)	76,113,113	1.48	12 (15%)
24	CHL	S	608	-	46,54,74	2.30	15 (32%)	49,90,114	3.06	17 (34%)
25	CLA	C	511	6	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
25	CLA	8	610	3	45,53,73	1.75	10 (22%)	52,89,113	1.44	7 (13%)
33	PHO	A	408	-	51,69,69	1.09	8 (15%)	47,99,99	1.19	6 (12%)
24	CHL	Y	605	1	48,56,74	2.14	12 (25%)	51,92,114	3.03	18 (35%)
24	CHL	1	607	-	63,71,74	1.90	14 (22%)	69,110,114	2.88	23 (33%)
25	CLA	G	602	1	65,73,73	1.46	8 (12%)	76,113,113	1.56	11 (14%)
25	CLA	c	508	6	65,73,73	1.46	8 (12%)	76,113,113	1.54	8 (10%)
39	HEM	f	101	8,9	41,50,50	1.44	4 (9%)	45,82,82	1.26	4 (8%)
35	LMG	b	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.41	6 (10%)
25	CLA	2	611	29	45,53,73	1.73	9 (20%)	52,89,113	1.58	7 (13%)
34	SQD	a	418	-	53,54,54	0.91	4 (7%)	62,65,65	1.66	13 (20%)
29	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
37	DGD	c	519	-	63,63,67	0.99	3 (4%)	77,77,81	1.39	9 (11%)
25	CLA	y	610	1	60,68,73	1.54	9 (15%)	70,107,113	1.34	8 (11%)
25	CLA	s	610	18	55,63,73	1.65	8 (14%)	64,101,113	1.42	8 (12%)
28	NEX	G	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.53	17 (34%)
34	SQD	b	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.72	11 (22%)
25	CLA	b	610	5	65,73,73	1.41	10 (15%)	76,113,113	1.48	10 (13%)
25	CLA	R	610	17	65,73,73	1.46	9 (13%)	76,113,113	1.40	8 (10%)
25	CLA	2	614	1	45,53,73	1.75	9 (20%)	52,89,113	1.50	7 (13%)
34	SQD	a	412	-	49,50,54	0.97	6 (12%)	58,61,65	1.67	9 (15%)
24	CHL	2	601	1	46,54,74	2.26	14 (30%)	49,90,114	3.23	21 (42%)
29	LHG	1	2630	25	40,40,48	0.75	1 (2%)	43,46,54	1.33	6 (13%)
25	CLA	8	611	29	45,53,73	1.76	8 (17%)	52,89,113	1.40	8 (15%)
25	CLA	Y	602	1	65,73,73	1.47	11 (16%)	76,113,113	1.42	11 (14%)
24	CHL	3	608	-	46,54,74	2.22	14 (30%)	49,90,114	3.29	19 (38%)
25	CLA	G	603	1	65,73,73	1.56	10 (15%)	76,113,113	1.43	10 (13%)
25	CLA	g	613	1	65,73,73	1.53	11 (16%)	76,113,113	1.45	5 (6%)
30	BCR	b	619	-	41,41,41	0.87	2 (4%)	56,56,56	1.86	17 (30%)
25	CLA	N	612	1	60,68,73	1.52	10 (16%)	70,107,113	1.42	8 (11%)
28	NEX	1	1623	-	38,46,46	1.13	4 (10%)	50,70,70	2.62	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	611	-	65,73,73	1.50	10 (15%)	76,113,113	1.48	12 (15%)
24	CHL	Y	606	-	50,58,74	2.06	15 (30%)	52,94,114	3.04	19 (36%)
24	CHL	s	601	18	46,54,74	2.23	13 (28%)	49,90,114	3.21	22 (44%)
29	LHG	B	2631	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	5 (9%)
30	BCR	4	623	-	41,41,41	0.78	0	56,56,56	2.18	15 (26%)
28	NEX	6	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.42	14 (28%)
25	CLA	7	603	2	55,63,73	1.59	12 (21%)	64,101,113	1.57	10 (15%)
25	CLA	y	614	1	48,56,73	1.73	10 (20%)	55,92,113	1.43	7 (12%)
31	OEX	A	401	4,6	0,15,15	-	-	-		
39	HEM	F	101	8,9	41,50,50	1.44	4 (9%)	45,82,82	1.26	4 (8%)
24	CHL	2	609	1	61,69,74	1.95	13 (21%)	67,108,114	2.78	22 (32%)
33	PHO	a	408	-	51,69,69	1.09	8 (15%)	47,99,99	1.19	7 (14%)
24	CHL	6	607	-	61,69,74	2.05	15 (24%)	67,108,114	2.59	22 (32%)
24	CHL	y	601	1	66,74,74	1.81	11 (16%)	73,114,114	2.83	23 (31%)
25	CLA	R	602	17	60,68,73	1.48	10 (16%)	70,107,113	1.52	10 (14%)
29	LHG	G	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	6 (11%)
25	CLA	2	603	1	55,63,73	1.62	11 (20%)	64,101,113	1.53	10 (15%)
26	LUT	N	1621	-	42,43,43	1.01	2 (4%)	51,60,60	1.85	15 (29%)
35	LMG	Z	101	-	51,51,55	0.90	3 (5%)	59,59,63	1.29	5 (8%)
25	CLA	N	613	1	60,68,73	1.59	7 (11%)	70,107,113	1.68	7 (10%)
29	LHG	C	522	-	48,48,48	0.66	1 (2%)	51,54,54	1.27	6 (11%)
25	CLA	S	602	18	61,69,73	1.58	7 (11%)	71,108,113	1.39	8 (11%)
34	SQD	B	621	-	53,54,54	0.92	4 (7%)	62,65,65	1.72	11 (17%)
33	PHO	A	409	-	51,69,69	1.02	5 (9%)	47,99,99	1.30	5 (10%)
25	CLA	b	612	5	65,73,73	1.59	11 (16%)	76,113,113	1.69	12 (15%)
25	CLA	n	602	1	65,73,73	1.46	10 (15%)	76,113,113	1.43	10 (13%)
25	CLA	g	610	1	64,72,73	1.44	10 (15%)	74,111,113	1.39	9 (12%)
36	PL9	d	405	-	55,55,55	2.29	18 (32%)	68,69,69	1.64	17 (25%)
24	CHL	1	606	-	46,54,74	2.21	15 (32%)	49,90,114	3.06	18 (36%)
25	CLA	A	405	4	65,73,73	1.46	9 (13%)	76,113,113	1.44	6 (7%)
34	SQD	B	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.72	11 (22%)
24	CHL	6	606	-	46,54,74	2.23	14 (30%)	49,90,114	3.10	20 (40%)
24	CHL	8	607	-	46,54,74	2.27	15 (32%)	49,90,114	3.11	19 (38%)
25	CLA	y	603	1	65,73,73	1.53	11 (16%)	76,113,113	1.42	12 (15%)
28	NEX	5	1623	-	38,46,46	1.13	3 (7%)	50,70,70	2.62	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	R	607	-	56,64,74	2.04	12 (21%)	61,102,114	2.93	25 (40%)
26	LUT	s	1620	-	42,43,43	0.78	0	51,60,60	1.78	14 (27%)
29	LHG	5	2630	25	40,40,48	0.75	1 (2%)	43,46,54	1.33	6 (13%)
25	CLA	7	611	29	55,63,73	1.67	11 (20%)	64,101,113	1.45	9 (14%)
25	CLA	b	608	-	65,73,73	1.49	11 (16%)	76,113,113	1.46	7 (9%)
25	CLA	c	506	6	65,73,73	1.52	10 (15%)	76,113,113	1.41	7 (9%)
25	CLA	b	616	5	65,73,73	1.49	10 (15%)	76,113,113	1.42	11 (14%)
25	CLA	C	502	6	65,73,73	1.43	6 (9%)	76,113,113	1.56	8 (10%)
25	CLA	G	614	1	48,56,73	1.70	10 (20%)	55,92,113	1.34	6 (10%)
25	CLA	b	604	5	65,73,73	1.54	11 (16%)	76,113,113	1.37	9 (11%)
26	LUT	g	1621	-	42,43,43	1.02	4 (9%)	51,60,60	1.94	18 (35%)
29	LHG	B	2630	-	46,46,48	0.69	2 (4%)	49,52,54	1.22	5 (10%)
27	XAT	g	1622	-	39,47,47	1.03	1 (2%)	54,74,74	2.86	22 (40%)
25	CLA	n	612	1	60,68,73	1.51	10 (16%)	70,107,113	1.41	8 (11%)
26	LUT	r	620	-	42,43,43	0.98	4 (9%)	51,60,60	1.95	18 (35%)
25	CLA	6	604	-	45,53,73	1.73	11 (24%)	52,89,113	1.64	10 (19%)
34	SQD	A	418	-	53,54,54	0.91	4 (7%)	62,65,65	1.67	13 (20%)
25	CLA	N	610	1	65,73,73	1.41	10 (15%)	76,113,113	1.39	8 (10%)
25	CLA	c	503	6	65,73,73	1.50	6 (9%)	76,113,113	1.34	6 (7%)
27	XAT	8	622	-	39,47,47	0.97	2 (5%)	54,74,74	2.70	21 (38%)
24	CHL	5	607	-	63,71,74	1.90	14 (22%)	69,110,114	2.88	23 (33%)
29	LHG	2	2630	25	36,36,48	0.74	1 (2%)	39,42,54	1.26	4 (10%)
24	CHL	Y	608	-	66,74,74	1.78	12 (18%)	73,114,114	2.80	18 (24%)
24	CHL	7	608	-	46,54,74	2.22	14 (30%)	49,90,114	3.27	19 (38%)
25	CLA	1	604	-	50,58,73	1.73	11 (22%)	58,95,113	1.51	9 (15%)
24	CHL	8	609	3	46,54,74	2.19	14 (30%)	49,90,114	3.28	20 (40%)
25	CLA	3	611	29	55,63,73	1.67	11 (20%)	64,101,113	1.45	9 (14%)
25	CLA	6	603	1	55,63,73	1.62	11 (20%)	64,101,113	1.53	10 (15%)
25	CLA	B	614	5	65,73,73	1.51	11 (16%)	76,113,113	1.51	9 (11%)
30	BCR	D	404	-	41,41,41	0.76	0	56,56,56	1.93	14 (25%)
30	BCR	c	516	-	41,41,41	0.68	0	56,56,56	1.94	14 (25%)
25	CLA	N	611	29	60,68,73	1.52	8 (13%)	70,107,113	1.44	8 (11%)
29	LHG	r	2630	25	41,41,48	0.73	1 (2%)	44,47,54	1.33	6 (13%)
25	CLA	s	611	29	56,64,73	1.60	6 (10%)	65,102,113	1.34	6 (9%)
26	LUT	4	620	-	42,43,43	0.95	2 (4%)	51,60,60	2.09	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	7	613	2	58,66,73	1.61	12 (20%)	67,104,113	1.42	7 (10%)
27	XAT	N	1622	-	39,47,47	0.96	1 (2%)	54,74,74	3.00	23 (42%)
25	CLA	G	612	1	60,68,73	1.53	9 (15%)	70,107,113	1.38	9 (12%)
26	LUT	N	1620	-	42,43,43	0.91	2 (4%)	51,60,60	1.85	16 (31%)
25	CLA	2	613	1	45,53,73	1.81	10 (22%)	52,89,113	1.46	8 (15%)
36	PL9	D	405	-	55,55,55	2.29	18 (32%)	68,69,69	1.64	17 (25%)
25	CLA	R	603	17	60,68,73	1.52	10 (16%)	70,107,113	1.45	8 (11%)
26	LUT	G	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.81	12 (23%)
25	CLA	b	607	5	65,73,73	1.52	11 (16%)	76,113,113	1.43	8 (10%)
35	LMG	B	2633	-	55,55,55	0.74	2 (3%)	63,63,63	1.36	6 (9%)
30	BCR	d	404	-	41,41,41	0.75	0	56,56,56	1.93	15 (26%)
25	CLA	R	612	17	49,57,73	1.70	9 (18%)	55,93,113	1.55	7 (12%)
29	LHG	g	2630	25	48,48,48	0.76	1 (2%)	51,54,54	1.32	6 (11%)
25	CLA	6	613	1	45,53,73	1.80	10 (22%)	52,89,113	1.46	8 (15%)
25	CLA	4	610	3	45,53,73	1.75	10 (22%)	52,89,113	1.44	7 (13%)
25	CLA	r	613	17	60,68,73	1.56	8 (13%)	70,107,113	1.50	9 (12%)
24	CHL	N	609	1	66,74,74	1.85	15 (22%)	73,114,114	2.62	23 (31%)
25	CLA	3	614	2	48,56,73	1.79	7 (14%)	55,92,113	1.48	7 (12%)
25	CLA	4	604	-	45,53,73	1.77	11 (24%)	52,89,113	1.57	8 (15%)
24	CHL	2	606	-	46,54,74	2.23	14 (30%)	49,90,114	3.10	20 (40%)
25	CLA	G	613	1	65,73,73	1.53	11 (16%)	76,113,113	1.45	5 (6%)
26	LUT	3	1620	-	42,43,43	0.96	3 (7%)	51,60,60	2.03	19 (37%)
24	CHL	3	601	2	64,72,74	1.88	13 (20%)	70,111,114	2.78	24 (34%)
25	CLA	6	610	1	50,58,73	1.67	9 (18%)	58,95,113	1.26	6 (10%)
24	CHL	6	608	-	46,54,74	2.21	14 (30%)	49,90,114	3.22	17 (34%)
29	LHG	c	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.24	6 (11%)
35	LMG	c	521	-	51,51,55	0.76	1 (1%)	59,59,63	1.31	6 (10%)
27	XAT	5	1622	-	39,47,47	0.96	2 (5%)	54,74,74	2.84	22 (40%)
25	CLA	5	604	-	50,58,73	1.73	11 (22%)	58,95,113	1.51	9 (15%)
38	BCT	D	401	32	2,3,3	1.30	0	2,3,3	4.21	2 (100%)
25	CLA	A	407	-	50,58,73	1.69	11 (22%)	58,95,113	1.48	8 (13%)
24	CHL	5	606	-	46,54,74	2.22	15 (32%)	49,90,114	3.06	18 (36%)
25	CLA	y	613	1	65,73,73	1.54	10 (15%)	76,113,113	1.67	7 (9%)
35	LMG	z	101	-	51,51,55	0.89	3 (5%)	59,59,63	1.29	5 (8%)
25	CLA	c	505	6	65,73,73	1.47	8 (12%)	76,113,113	1.51	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	NEX	s	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.36	15 (30%)
24	CHL	4	601	3	44,53,74	2.45	16 (36%)	46,89,114	3.07	17 (36%)
25	CLA	Y	613	1	65,73,73	1.54	10 (15%)	76,113,113	1.68	8 (10%)
25	CLA	N	614	1	48,56,73	1.64	9 (18%)	55,92,113	1.55	8 (14%)
25	CLA	s	603	18	45,53,73	1.83	7 (15%)	52,89,113	1.56	8 (15%)
25	CLA	g	614	1	48,56,73	1.70	10 (20%)	55,92,113	1.34	6 (10%)
25	CLA	Y	611	29	60,68,73	1.60	9 (15%)	70,107,113	1.33	9 (12%)
24	CHL	N	607	-	66,74,74	1.81	13 (19%)	73,114,114	2.77	19 (26%)
24	CHL	G	608	-	66,74,74	1.85	13 (19%)	73,114,114	2.74	21 (28%)
30	BCR	c	517	-	41,41,41	0.80	0	56,56,56	2.11	13 (23%)
26	LUT	R	620	-	42,43,43	0.99	4 (9%)	51,60,60	1.95	18 (35%)
28	NEX	n	1623	-	38,46,46	1.08	3 (7%)	50,70,70	2.42	17 (34%)
29	LHG	3	2630	25	46,46,48	0.79	1 (2%)	49,52,54	1.30	4 (8%)
25	CLA	3	603	2	55,63,73	1.59	12 (21%)	64,101,113	1.57	10 (15%)
26	LUT	1	1621	-	42,43,43	1.02	3 (7%)	51,60,60	1.91	17 (33%)
24	CHL	3	609	2	61,69,74	2.03	16 (26%)	67,108,114	2.69	21 (31%)
24	CHL	5	605	1	46,54,74	2.28	15 (32%)	49,90,114	3.15	17 (34%)
25	CLA	R	611	29	49,57,73	1.72	9 (18%)	55,93,113	1.37	8 (14%)
29	LHG	s	2630	25	48,48,48	0.65	1 (2%)	51,54,54	1.26	7 (13%)
25	CLA	C	504	-	65,73,73	1.49	8 (12%)	76,113,113	1.41	7 (9%)
29	LHG	b	2630	-	46,46,48	0.69	2 (4%)	49,52,54	1.22	5 (10%)
25	CLA	c	509	6	65,73,73	1.45	8 (12%)	76,113,113	1.44	8 (10%)
27	XAT	G	1622	-	39,47,47	1.03	1 (2%)	54,74,74	2.85	22 (40%)
29	LHG	d	408	-	45,45,48	0.83	1 (2%)	48,51,54	1.37	5 (10%)
24	CHL	1	608	-	46,54,74	2.19	13 (28%)	49,90,114	3.25	19 (38%)
24	CHL	3	607	-	53,61,74	2.09	15 (28%)	57,98,114	2.95	20 (35%)
25	CLA	c	501	6	65,73,73	1.54	8 (12%)	76,113,113	1.22	7 (9%)
25	CLA	S	611	29	56,64,73	1.60	7 (12%)	65,102,113	1.35	6 (9%)
24	CHL	n	605	1	48,56,74	2.18	13 (27%)	51,92,114	3.12	23 (45%)
25	CLA	R	604	-	48,56,73	1.68	10 (20%)	55,92,113	1.65	10 (18%)
24	CHL	S	606	-	46,54,74	2.29	16 (34%)	49,90,114	3.12	17 (34%)
25	CLA	B	609	5	65,73,73	1.38	9 (13%)	76,113,113	1.61	9 (11%)
24	CHL	1	601	1	46,54,74	2.26	14 (30%)	49,90,114	3.19	20 (40%)
26	LUT	6	1620	-	42,43,43	0.81	0	51,60,60	1.72	15 (29%)
29	LHG	Y	2630	25	48,48,48	0.81	2 (4%)	51,54,54	1.26	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	r	616	17	45,53,73	1.76	10 (22%)	52,89,113	1.52	7 (13%)
24	CHL	1	605	1	46,54,74	2.28	15 (32%)	49,90,114	3.15	17 (34%)
24	CHL	5	608	-	46,54,74	2.19	13 (28%)	49,90,114	3.25	19 (38%)
29	LHG	4	2630	25	20,20,48	0.87	0	23,26,54	1.32	1 (4%)
30	BCR	b	618	-	41,41,41	1.05	3 (7%)	56,56,56	1.97	13 (23%)
24	CHL	s	607	-	58,66,74	2.00	16 (27%)	63,104,114	2.77	21 (33%)
25	CLA	2	610	1	50,58,73	1.67	9 (18%)	58,95,113	1.26	6 (10%)
35	LMG	a	415	-	40,40,55	0.88	0	48,48,63	1.31	6 (12%)
25	CLA	g	602	1	65,73,73	1.46	9 (13%)	76,113,113	1.56	11 (14%)
26	LUT	g	1620	-	42,43,43	0.88	1 (2%)	51,60,60	1.81	12 (23%)
25	CLA	6	602	1	61,69,73	1.51	8 (13%)	71,108,113	1.37	8 (11%)
25	CLA	B	617	5	65,73,73	1.42	9 (13%)	76,113,113	1.47	8 (10%)
26	LUT	2	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.79	17 (33%)
26	LUT	n	1620	-	42,43,43	0.91	2 (4%)	51,60,60	1.85	16 (31%)
25	CLA	N	603	1	65,73,73	1.51	10 (15%)	76,113,113	1.44	11 (14%)
25	CLA	D	403	7	65,73,73	1.43	10 (15%)	76,113,113	1.43	9 (11%)
24	CHL	4	607	-	46,54,74	2.28	14 (30%)	49,90,114	3.11	19 (38%)
28	NEX	r	623	-	38,46,46	1.08	3 (7%)	50,70,70	2.52	21 (42%)
24	CHL	y	608	-	66,74,74	1.78	12 (18%)	73,114,114	2.80	18 (24%)
25	CLA	1	603	1	55,63,73	1.60	12 (21%)	64,101,113	1.57	11 (17%)
25	CLA	c	511	6	65,73,73	1.50	6 (9%)	76,113,113	1.36	8 (10%)
24	CHL	5	609	1	62,70,74	2.02	15 (24%)	68,109,114	2.73	20 (29%)
25	CLA	s	609	18	45,53,73	1.86	5 (11%)	52,89,113	1.45	9 (17%)
24	CHL	2	607	-	61,69,74	2.05	15 (24%)	67,108,114	2.60	22 (32%)
25	CLA	b	609	5	65,73,73	1.37	9 (13%)	76,113,113	1.61	9 (11%)
26	LUT	2	1620	-	42,43,43	0.81	0	51,60,60	1.72	15 (29%)
25	CLA	5	603	1	55,63,73	1.60	12 (21%)	64,101,113	1.57	11 (17%)
25	CLA	7	612	2	45,53,73	1.76	11 (24%)	52,89,113	1.52	9 (17%)
25	CLA	S	603	18	45,53,73	1.82	7 (15%)	52,89,113	1.56	8 (15%)
24	CHL	8	608	-	46,54,74	2.16	13 (28%)	49,90,114	3.24	23 (46%)
29	LHG	6	2630	25	36,36,48	0.74	1 (2%)	39,42,54	1.26	4 (10%)
24	CHL	1	609	1	62,70,74	2.02	15 (24%)	68,109,114	2.73	20 (29%)
28	NEX	7	1623	-	38,46,46	0.96	2 (5%)	50,70,70	2.46	16 (32%)
25	CLA	R	616	17	45,53,73	1.76	10 (22%)	52,89,113	1.53	7 (13%)
26	LUT	y	1621	-	42,43,43	1.07	4 (9%)	51,60,60	1.86	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	s	606	-	46,54,74	2.29	16 (34%)	49,90,114	3.12	17 (34%)
27	XAT	r	622	-	39,47,47	1.06	2 (5%)	54,74,74	2.72	19 (35%)
25	CLA	g	603	1	65,73,73	1.56	10 (15%)	76,113,113	1.43	10 (13%)
27	XAT	y	1622	-	39,47,47	1.14	4 (10%)	54,74,74	2.99	20 (37%)
24	CHL	g	608	-	66,74,74	1.86	14 (21%)	73,114,114	2.75	21 (28%)
25	CLA	c	504	-	65,73,73	1.49	7 (10%)	76,113,113	1.41	7 (9%)
25	CLA	n	603	1	65,73,73	1.51	10 (15%)	76,113,113	1.45	11 (14%)
27	XAT	4	622	-	39,47,47	0.97	2 (5%)	54,74,74	2.70	19 (35%)
28	NEX	2	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.41	14 (28%)
24	CHL	3	606	-	46,54,74	2.31	14 (30%)	49,90,114	3.19	22 (44%)
25	CLA	8	603	3	45,53,73	1.76	9 (20%)	52,89,113	1.60	7 (13%)
24	CHL	n	607	-	66,74,74	1.81	13 (19%)	73,114,114	2.77	19 (26%)
25	CLA	y	602	1	65,73,73	1.46	11 (16%)	76,113,113	1.42	11 (14%)
25	CLA	s	604	-	50,58,73	1.69	5 (10%)	58,95,113	1.62	8 (13%)
25	CLA	6	611	29	45,53,73	1.74	9 (20%)	52,89,113	1.58	7 (13%)
25	CLA	r	601	17	49,57,73	1.71	9 (18%)	55,93,113	1.73	10 (18%)
30	BCR	c	515	-	41,41,41	0.77	0	56,56,56	1.90	17 (30%)
25	CLA	C	506	6	65,73,73	1.52	10 (15%)	76,113,113	1.40	7 (9%)
25	CLA	7	602	2	60,68,73	1.50	10 (16%)	70,107,113	1.39	8 (11%)
25	CLA	Y	604	-	50,58,73	1.75	9 (18%)	58,95,113	1.61	8 (13%)
37	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.54	12 (17%)
25	CLA	6	614	1	45,53,73	1.75	9 (20%)	52,89,113	1.50	7 (13%)
25	CLA	7	610	2	60,68,73	1.54	10 (16%)	70,107,113	1.25	10 (14%)
24	CHL	4	606	-	46,54,74	2.24	13 (28%)	49,90,114	3.17	20 (40%)
25	CLA	8	602	3	45,53,73	1.71	9 (20%)	52,89,113	1.68	8 (15%)
25	CLA	4	603	3	45,53,73	1.77	9 (20%)	52,89,113	1.60	7 (13%)
24	CHL	y	609	1	66,74,74	1.87	14 (21%)	73,114,114	2.68	26 (35%)
24	CHL	N	608	-	66,74,74	1.80	13 (19%)	73,114,114	2.73	22 (30%)
26	LUT	s	1621	-	42,43,43	0.80	0	51,60,60	1.73	15 (29%)
35	LMG	C	521	-	51,51,55	0.76	0	59,59,63	1.31	6 (10%)
25	CLA	3	613	2	58,66,73	1.60	12 (20%)	67,104,113	1.42	7 (10%)
25	CLA	2	602	1	61,69,73	1.52	8 (13%)	71,108,113	1.37	8 (11%)
25	CLA	y	612	1	60,68,73	1.59	11 (18%)	70,107,113	1.38	9 (12%)
25	CLA	r	604	-	48,56,73	1.69	10 (20%)	55,92,113	1.65	9 (16%)
24	CHL	g	606	-	50,58,74	2.13	13 (26%)	52,94,114	3.14	20 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	Y	612	1	60,68,73	1.59	11 (18%)	70,107,113	1.38	9 (12%)
25	CLA	G	604	-	50,58,73	1.75	11 (22%)	58,95,113	1.54	7 (12%)
29	LHG	D	408	-	45,45,48	0.83	1 (2%)	48,51,54	1.37	5 (10%)
34	SQD	b	621	-	53,54,54	0.92	4 (7%)	62,65,65	1.72	11 (17%)
37	DGD	H	102	-	63,63,67	1.21	6 (9%)	77,77,81	1.52	10 (12%)
27	XAT	R	622	-	39,47,47	1.05	2 (5%)	54,74,74	2.72	19 (35%)
26	LUT	8	620	-	42,43,43	0.94	2 (4%)	51,60,60	2.09	15 (29%)
30	BCR	C	516	-	41,41,41	0.69	0	56,56,56	1.94	14 (25%)
29	LHG	b	2631	-	48,48,48	0.65	1 (2%)	51,54,54	1.23	5 (9%)
25	CLA	S	604	-	50,58,73	1.69	5 (10%)	58,95,113	1.62	8 (13%)
30	BCR	B	620	-	41,41,41	0.90	1 (2%)	56,56,56	2.01	15 (26%)
34	SQD	A	412	-	49,50,54	0.97	6 (12%)	58,61,65	1.67	9 (15%)
29	LHG	d	409	-	48,48,48	0.80	1 (2%)	51,54,54	1.33	7 (13%)
25	CLA	S	610	18	55,63,73	1.65	8 (14%)	64,101,113	1.43	9 (14%)
30	BCR	T	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.63	23 (41%)
28	NEX	N	1623	-	38,46,46	1.08	3 (7%)	50,70,70	2.42	16 (32%)
26	LUT	7	1621	-	42,43,43	0.93	1 (2%)	51,60,60	1.61	11 (21%)
30	BCR	C	514	-	41,41,41	0.78	0	56,56,56	1.72	12 (21%)
30	BCR	C	515	-	41,41,41	0.78	0	56,56,56	1.89	17 (30%)
25	CLA	3	610	2	60,68,73	1.54	10 (16%)	70,107,113	1.25	9 (12%)
26	LUT	S	1620	-	42,43,43	0.78	0	51,60,60	1.78	14 (27%)
26	LUT	n	1621	-	42,43,43	1.01	2 (4%)	51,60,60	1.85	15 (29%)
26	LUT	7	1620	-	42,43,43	0.96	3 (7%)	51,60,60	2.03	19 (37%)
25	CLA	B	615	5	65,73,73	1.42	11 (16%)	76,113,113	1.35	9 (11%)
29	LHG	C	523	-	48,48,48	0.65	1 (2%)	51,54,54	1.24	6 (11%)
24	CHL	7	601	2	64,72,74	1.88	13 (20%)	70,111,114	2.77	24 (34%)
30	BCR	8	623	-	41,41,41	0.79	0	56,56,56	2.18	15 (26%)
30	BCR	t	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.62	23 (41%)
30	BCR	h	101	-	41,41,41	0.92	0	56,56,56	2.02	13 (23%)
24	CHL	N	605	1	48,56,74	2.17	13 (27%)	51,92,114	3.11	23 (45%)
24	CHL	n	601	1	66,74,74	1.89	14 (21%)	73,114,114	2.70	23 (31%)
37	DGD	C	519	-	63,63,67	0.99	3 (4%)	77,77,81	1.39	9 (11%)
26	LUT	3	1621	-	42,43,43	0.93	1 (2%)	51,60,60	1.61	11 (21%)
29	LHG	c	2630	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	6 (11%)
27	XAT	3	1622	-	39,47,47	1.20	5 (12%)	54,74,74	3.06	27 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	a	410	4	60,68,73	1.50	10 (16%)	70,107,113	1.44	9 (12%)
24	CHL	g	605	1	46,54,74	2.26	14 (30%)	49,90,114	3.09	21 (42%)
30	BCR	H	101	-	41,41,41	0.92	0	56,56,56	2.02	13 (23%)
25	CLA	B	605	5	65,73,73	1.52	13 (20%)	76,113,113	1.86	18 (23%)
25	CLA	7	604	-	45,53,73	1.80	11 (24%)	52,89,113	1.48	6 (11%)
35	LMG	B	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.41	6 (10%)
25	CLA	a	406	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	9 (11%)
25	CLA	n	604	-	50,58,73	1.73	10 (20%)	58,95,113	1.59	9 (15%)
26	LUT	5	1621	-	42,43,43	1.02	3 (7%)	51,60,60	1.91	17 (33%)
25	CLA	S	612	18	49,57,73	1.69	7 (14%)	55,93,113	1.52	7 (12%)
25	CLA	C	512	6	65,73,73	1.46	6 (9%)	76,113,113	1.33	8 (10%)
26	LUT	G	1621	-	42,43,43	1.02	4 (9%)	51,60,60	1.94	18 (35%)
25	CLA	Y	610	1	60,68,73	1.55	9 (15%)	70,107,113	1.34	8 (11%)
25	CLA	5	613	1	55,63,73	1.61	11 (20%)	64,101,113	1.46	6 (9%)
27	XAT	Y	1622	-	39,47,47	1.14	4 (10%)	54,74,74	2.98	19 (35%)
24	CHL	n	609	1	66,74,74	1.85	16 (24%)	73,114,114	2.62	23 (31%)
24	CHL	G	601	1	66,74,74	1.83	13 (19%)	73,114,114	2.72	24 (32%)
25	CLA	b	615	5	65,73,73	1.42	11 (16%)	76,113,113	1.35	9 (11%)
25	CLA	R	601	17	49,57,73	1.71	9 (18%)	55,93,113	1.73	10 (18%)
26	LUT	Y	1620	-	42,43,43	1.08	5 (11%)	51,60,60	1.92	20 (39%)
25	CLA	n	611	29	60,68,73	1.52	9 (15%)	70,107,113	1.44	8 (11%)
29	LHG	D	409	-	48,48,48	0.79	1 (2%)	51,54,54	1.33	7 (13%)
37	DGD	h	102	-	63,63,67	1.21	7 (11%)	77,77,81	1.52	10 (12%)
25	CLA	b	614	5	65,73,73	1.50	11 (16%)	76,113,113	1.51	9 (11%)
24	CHL	g	601	1	66,74,74	1.83	13 (19%)	73,114,114	2.72	24 (32%)
25	CLA	1	613	1	55,63,73	1.62	11 (20%)	64,101,113	1.47	6 (9%)
25	CLA	r	612	17	49,57,73	1.70	9 (18%)	55,93,113	1.55	7 (12%)
24	CHL	Y	601	1	66,74,74	1.81	11 (16%)	73,114,114	2.83	23 (31%)
26	LUT	6	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.79	17 (33%)
24	CHL	G	605	1	46,54,74	2.26	15 (32%)	49,90,114	3.09	20 (40%)
27	XAT	6	1622	-	39,47,47	1.03	0	54,74,74	2.97	23 (42%)
25	CLA	A	410	4	60,68,73	1.50	10 (16%)	70,107,113	1.44	9 (12%)
25	CLA	R	609	17	58,66,73	1.53	11 (18%)	67,104,113	1.40	7 (10%)
25	CLA	d	403	7	65,73,73	1.42	10 (15%)	76,113,113	1.43	9 (11%)
24	CHL	R	614	17	42,50,74	2.39	15 (35%)	44,85,114	3.37	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	3	605	2	46,54,74	2.23	13 (28%)	49,90,114	3.19	22 (44%)
25	CLA	S	609	18	45,53,73	1.86	5 (11%)	52,89,113	1.45	9 (17%)
29	LHG	L	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	BCR	A	411	-	41,41,41	0.81	0	56,56,56	1.85	12 (21%)
25	CLA	y	611	29	60,68,73	1.61	9 (15%)	70,107,113	1.33	9 (12%)
30	BCR	C	517	-	41,41,41	0.80	0	56,56,56	2.10	13 (23%)
25	CLA	3	604	-	45,53,73	1.80	11 (24%)	52,89,113	1.48	7 (13%)
25	CLA	g	612	1	60,68,73	1.53	9 (15%)	70,107,113	1.38	9 (12%)
37	DGD	B	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.38	6 (8%)
25	CLA	r	602	17	60,68,73	1.49	10 (16%)	70,107,113	1.52	10 (14%)
25	CLA	Y	603	1	65,73,73	1.52	11 (16%)	76,113,113	1.41	12 (15%)
24	CHL	2	605	1	46,54,74	2.29	14 (30%)	49,90,114	3.11	19 (38%)
29	LHG	S	2630	25	48,48,48	0.65	1 (2%)	51,54,54	1.26	7 (13%)
25	CLA	B	613	5	65,73,73	1.48	11 (16%)	76,113,113	1.68	12 (15%)
36	PL9	A	414	-	13,13,55	0.75	0	17,17,69	2.08	4 (23%)
37	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.54	12 (17%)
25	CLA	R	613	17	60,68,73	1.56	8 (13%)	70,107,113	1.49	9 (12%)
25	CLA	C	510	6	65,73,73	1.46	7 (10%)	76,113,113	1.45	9 (11%)
25	CLA	N	604	-	50,58,73	1.73	10 (20%)	58,95,113	1.59	9 (15%)
25	CLA	1	602	1	61,69,73	1.54	10 (16%)	71,108,113	1.32	9 (12%)
25	CLA	7	614	2	48,56,73	1.79	7 (14%)	55,92,113	1.48	7 (12%)
30	BCR	B	619	-	41,41,41	0.87	1 (2%)	56,56,56	1.86	17 (30%)
28	NEX	R	623	-	38,46,46	1.08	3 (7%)	50,70,70	2.53	19 (38%)
24	CHL	G	607	-	66,74,74	1.83	12 (18%)	73,114,114	2.67	20 (27%)
25	CLA	B	607	5	65,73,73	1.52	11 (16%)	76,113,113	1.43	8 (10%)
37	DGD	c	520	-	61,61,67	0.98	3 (4%)	75,75,81	1.44	10 (13%)
24	CHL	y	605	1	48,56,74	2.14	12 (25%)	51,92,114	3.03	18 (35%)
24	CHL	G	609	1	61,69,74	1.92	15 (24%)	67,108,114	2.70	22 (32%)
24	CHL	R	606	-	66,74,74	1.86	13 (19%)	73,114,114	2.72	24 (32%)
24	CHL	r	608	-	61,69,74	1.82	10 (16%)	67,108,114	2.88	19 (28%)
25	CLA	n	614	1	48,56,73	1.64	9 (18%)	55,92,113	1.55	8 (14%)
24	CHL	8	601	3	44,53,74	2.44	16 (36%)	46,89,114	3.07	17 (36%)
24	CHL	6	609	1	61,69,74	1.95	13 (21%)	67,108,114	2.78	22 (32%)
37	DGD	b	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.38	6 (8%)
24	CHL	2	608	-	46,54,74	2.21	14 (30%)	49,90,114	3.23	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CHL	R	608	-	61,69,74	1.82	10 (16%)	67,108,114	2.88	19 (28%)
25	CLA	s	613	18	55,63,73	1.61	6 (10%)	64,101,113	1.41	6 (9%)
29	LHG	d	410	-	42,42,48	0.66	1 (2%)	45,48,54	1.23	4 (8%)
24	CHL	Y	609	1	66,74,74	1.86	14 (21%)	73,114,114	2.68	26 (35%)
29	LHG	7	2630	25	46,46,48	0.79	1 (2%)	49,52,54	1.31	4 (8%)
28	NEX	y	1623	-	38,46,46	1.12	3 (7%)	50,70,70	2.70	22 (44%)
25	CLA	B	606	5	65,73,73	1.53	12 (18%)	76,113,113	1.57	12 (15%)
25	CLA	C	507	-	65,73,73	1.43	8 (12%)	76,113,113	1.55	10 (13%)
25	CLA	N	602	1	65,73,73	1.46	10 (15%)	76,113,113	1.43	10 (13%)
25	CLA	3	612	2	45,53,73	1.76	11 (24%)	52,89,113	1.51	9 (17%)
25	CLA	c	512	6	65,73,73	1.46	6 (9%)	76,113,113	1.34	8 (10%)
25	CLA	B	603	5	65,73,73	1.46	10 (15%)	76,113,113	1.26	6 (7%)
24	CHL	s	608	-	46,54,74	2.29	15 (32%)	49,90,114	3.05	17 (34%)
24	CHL	6	605	1	46,54,74	2.29	14 (30%)	49,90,114	3.11	19 (38%)
25	CLA	C	513	6	65,73,73	1.43	7 (10%)	76,113,113	1.47	10 (13%)
28	NEX	S	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.36	16 (32%)
25	CLA	r	611	29	49,57,73	1.73	10 (20%)	55,93,113	1.37	8 (14%)
24	CHL	S	601	18	46,54,74	2.23	13 (28%)	49,90,114	3.20	22 (44%)
25	CLA	Y	614	1	48,56,73	1.73	11 (22%)	55,92,113	1.42	7 (12%)
25	CLA	1	610	1	56,64,73	1.53	10 (17%)	65,102,113	1.36	7 (10%)
24	CHL	7	607	-	53,61,74	2.09	16 (30%)	57,98,114	2.96	20 (35%)
27	XAT	2	1622	-	39,47,47	1.03	0	54,74,74	2.98	22 (40%)
35	LMG	d	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.37	6 (11%)
25	CLA	5	602	1	61,69,73	1.54	10 (16%)	71,108,113	1.32	8 (11%)
25	CLA	8	612	3	45,53,73	1.75	8 (17%)	52,89,113	1.61	7 (13%)
24	CHL	S	607	-	58,66,74	1.99	16 (27%)	63,104,114	2.78	22 (34%)
29	LHG	8	2630	25	20,20,48	0.87	0	23,26,54	1.32	1 (4%)
29	LHG	R	2630	25	41,41,48	0.73	1 (2%)	44,47,54	1.34	6 (13%)
25	CLA	B	602	-	65,73,73	1.47	11 (16%)	76,113,113	1.38	10 (13%)
24	CHL	r	606	-	66,74,74	1.86	12 (18%)	73,114,114	2.71	24 (32%)
25	CLA	4	612	3	45,53,73	1.74	8 (17%)	52,89,113	1.61	7 (13%)
24	CHL	G	606	-	50,58,74	2.14	13 (26%)	52,94,114	3.15	20 (38%)
35	LMG	b	2633	-	55,55,55	0.75	2 (3%)	63,63,63	1.36	6 (9%)
29	LHG	y	2630	25	48,48,48	0.81	2 (4%)	51,54,54	1.26	6 (11%)
25	CLA	b	605	5	65,73,73	1.52	14 (21%)	76,113,113	1.85	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	a	407	-	50,58,73	1.69	11 (22%)	58,95,113	1.48	8 (13%)
29	LHG	C	2630	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	6 (11%)
35	LMG	a	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.30	4 (7%)

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
25	CLA	n	613	1	1/1/14/20	6/31/109/115	-
35	LMG	A	415	-	-	11/35/55/70	0/1/1/1
25	CLA	d	402	7	1/1/15/20	5/37/115/115	-
24	CHL	y	607	-	4/4/20/26	15/39/137/137	-
29	LHG	D	410	-	-	24/47/47/53	-
25	CLA	c	510	6	1/1/15/20	17/37/115/115	-
25	CLA	r	603	17	1/1/14/20	13/31/109/115	-
25	CLA	g	604	-	-	5/19/97/115	-
25	CLA	1	612	1	1/1/11/20	4/13/91/115	-
29	LHG	n	2630	25	-	23/53/53/53	-
25	CLA	4	611	29	1/1/11/20	6/13/91/115	-
25	CLA	A	406	-	1/1/15/20	4/37/115/115	-
25	CLA	C	509	6	1/1/15/20	8/37/115/115	-
25	CLA	6	612	1	1/1/11/20	6/13/91/115	-
25	CLA	b	606	5	1/1/15/20	15/37/115/115	-
25	CLA	c	502	6	1/1/15/20	20/37/115/115	-
24	CHL	N	601	1	4/4/20/26	17/39/137/137	-
26	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	2	604	-	-	9/13/91/115	-
25	CLA	C	503	6	1/1/15/20	10/37/115/115	-
25	CLA	n	610	1	1/1/15/20	11/37/115/115	-
35	LMG	D	411	-	-	15/41/61/70	0/1/1/1
24	CHL	r	614	17	3/3/15/26	6/10/108/137	-
25	CLA	8	604	-	-	9/13/91/115	-
24	CHL	5	601	1	3/3/16/26	5/15/113/137	-
25	CLA	S	614	18	1/1/11/20	5/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	612	5	1/1/15/20	12/37/115/115	-
25	CLA	r	609	17	1/1/13/20	2/29/107/115	-
27	XAT	7	1622	-	-	1/31/93/93	0/4/4/4
24	CHL	g	607	-	4/4/20/26	13/39/137/137	-
28	NEX	g	1623	-	-	6/27/83/83	0/3/3/3
25	CLA	c	513	6	-	12/37/115/115	-
28	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	r	610	17	1/1/15/20	12/37/115/115	-
27	XAT	n	1622	-	-	3/31/93/93	0/4/4/4
25	CLA	5	610	1	1/1/13/20	3/27/105/115	-
30	BCR	c	514	-	-	2/29/63/63	0/2/2/2
25	CLA	b	613	5	1/1/15/20	15/37/115/115	-
30	BCR	B	618	-	-	4/29/63/63	0/2/2/2
25	CLA	G	610	1	1/1/14/20	13/36/114/115	-
25	CLA	b	602	-	1/1/15/20	15/37/115/115	-
24	CHL	8	606	-	3/3/16/26	7/15/113/137	-
25	CLA	B	608	-	1/1/15/20	13/37/115/115	-
25	CLA	y	604	-	1/1/12/20	5/19/97/115	-
25	CLA	C	505	6	-	13/37/115/115	-
24	CHL	n	608	-	4/4/20/26	14/39/137/137	-
25	CLA	1	611	29	1/1/11/20	5/13/91/115	-
25	CLA	B	616	5	1/1/15/20	12/37/115/115	-
25	CLA	B	604	5	1/1/15/20	9/37/115/115	-
24	CHL	y	606	-	3/3/16/26	5/20/118/137	-
25	CLA	D	402	7	1/1/15/20	5/37/115/115	-
25	CLA	5	612	1	1/1/11/20	4/13/91/115	-
33	PHO	a	409	-	-	8/37/103/103	0/5/6/6
25	CLA	1	614	1	1/1/11/20	4/13/91/115	-
24	CHL	7	606	-	3/3/16/26	5/15/113/137	-
25	CLA	G	611	29	1/1/14/20	11/31/109/115	-
24	CHL	7	609	2	4/4/19/26	14/33/131/137	-
24	CHL	6	601	1	3/3/16/26	8/15/113/137	-
25	CLA	s	612	18	1/1/11/20	3/18/96/115	-
25	CLA	3	602	2	1/1/14/20	15/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	b	620	-	-	6/29/63/63	0/2/2/2
30	BCR	a	411	-	-	2/29/63/63	0/2/2/2
26	LUT	Y	1621	-	-	2/29/67/67	0/2/2/2
24	CHL	4	608	-	3/3/16/26	8/15/113/137	-
35	LMG	A	413	-	-	17/43/63/70	0/1/1/1
36	PL9	a	414	-	-	1/5/18/73	0/1/1/1
26	LUT	5	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	g	611	29	1/1/14/20	11/31/109/115	-
25	CLA	s	614	18	1/1/11/20	5/18/96/115	-
25	CLA	2	612	1	1/1/11/20	6/13/91/115	-
25	CLA	b	617	5	1/1/15/20	17/37/115/115	-
25	CLA	s	602	18	1/1/14/20	14/33/111/115	-
25	CLA	c	507	-	1/1/15/20	21/37/115/115	-
26	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	n	606	-	3/3/16/26	8/20/118/137	-
27	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
29	LHG	c	522	-	-	20/53/53/53	-
25	CLA	C	501	6	1/1/15/20	15/37/115/115	-
25	CLA	b	603	5	1/1/15/20	10/37/115/115	-
24	CHL	Y	607	-	4/4/20/26	15/39/137/137	-
24	CHL	N	606	-	3/3/16/26	8/20/118/137	-
24	CHL	4	609	3	3/3/16/26	7/15/113/137	-
25	CLA	4	602	3	1/1/11/20	3/13/91/115	-
25	CLA	B	610	5	-	7/37/115/115	-
24	CHL	7	605	2	3/3/16/26	10/15/113/137	-
37	DGD	C	520	-	-	28/49/89/95	0/2/2/2
24	CHL	r	607	-	4/4/18/26	8/27/125/137	-
26	LUT	S	1621	-	-	4/29/67/67	0/2/2/2
24	CHL	g	609	1	4/4/19/26	11/33/131/137	-
25	CLA	C	508	6	1/1/15/20	8/37/115/115	-
25	CLA	S	613	18	1/1/13/20	6/25/103/115	-
29	LHG	N	2630	25	-	23/53/53/53	-
25	CLA	5	611	29	1/1/11/20	5/13/91/115	-
25	CLA	a	405	4	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	Y	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	5	614	1	1/1/11/20	4/13/91/115	-
25	CLA	B	611	-	1/1/15/20	9/37/115/115	-
24	CHL	S	608	-	3/3/16/26	3/15/113/137	-
25	CLA	C	511	6	-	13/37/115/115	-
25	CLA	8	610	3	1/1/11/20	6/13/91/115	-
33	PHO	A	408	-	-	6/37/103/103	0/5/6/6
24	CHL	Y	605	1	3/3/16/26	6/18/116/137	-
24	CHL	1	607	-	4/4/19/26	19/36/134/137	-
25	CLA	G	602	1	1/1/15/20	11/37/115/115	-
25	CLA	c	508	6	1/1/15/20	8/37/115/115	-
39	HEM	f	101	8,9	-	1/12/54/54	-
35	LMG	b	622	-	-	22/46/66/70	0/1/1/1
25	CLA	2	611	29	1/1/11/20	3/13/91/115	-
34	SQD	a	418	-	-	22/49/69/69	0/1/1/1
29	LHG	l	101	-	-	21/53/53/53	-
37	DGD	c	519	-	-	25/51/91/95	0/2/2/2
25	CLA	y	610	1	1/1/14/20	7/31/109/115	-
25	CLA	s	610	18	1/1/13/20	4/25/103/115	-
28	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
34	SQD	b	623	-	-	17/37/57/69	0/1/1/1
25	CLA	b	610	5	-	7/37/115/115	-
25	CLA	R	610	17	1/1/15/20	12/37/115/115	-
25	CLA	2	614	1	-	6/13/91/115	-
34	SQD	a	412	-	-	18/45/65/69	0/1/1/1
24	CHL	2	601	1	3/3/16/26	8/15/113/137	-
29	LHG	1	2630	25	-	9/45/45/53	-
25	CLA	8	611	29	1/1/11/20	6/13/91/115	-
25	CLA	Y	602	1	1/1/15/20	14/37/115/115	-
24	CHL	3	608	-	3/3/16/26	6/15/113/137	-
25	CLA	G	603	1	1/1/15/20	11/37/115/115	-
25	CLA	g	613	1	-	11/37/115/115	-
30	BCR	b	619	-	-	2/29/63/63	0/2/2/2
25	CLA	N	612	1	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	1	1623	-	-	9/27/83/83	0/3/3/3
25	CLA	b	611	-	1/1/15/20	9/37/115/115	-
24	CHL	Y	606	-	3/3/16/26	5/20/118/137	-
24	CHL	s	601	18	3/3/16/26	8/15/113/137	-
29	LHG	B	2631	-	-	20/53/53/53	-
30	BCR	4	623	-	-	12/29/63/63	0/2/2/2
28	NEX	6	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	7	603	2	1/1/13/20	9/25/103/115	-
25	CLA	y	614	1	1/1/11/20	3/17/95/115	-
39	HEM	F	101	8,9	-	1/12/54/54	-
24	CHL	2	609	1	4/4/19/26	15/33/131/137	-
33	PHO	a	408	-	-	6/37/103/103	0/5/6/6
24	CHL	6	607	-	4/4/19/26	18/33/131/137	-
24	CHL	y	601	1	4/4/20/26	15/39/137/137	-
25	CLA	R	602	17	1/1/14/20	7/31/109/115	-
29	LHG	G	2630	25	-	24/53/53/53	-
25	CLA	2	603	1	1/1/13/20	13/25/103/115	-
26	LUT	N	1621	-	-	1/29/67/67	0/2/2/2
35	LMG	Z	101	-	-	22/46/66/70	0/1/1/1
25	CLA	N	613	1	1/1/14/20	6/31/109/115	-
29	LHG	C	522	-	-	20/53/53/53	-
25	CLA	S	602	18	1/1/14/20	14/33/111/115	-
34	SQD	B	621	-	-	18/49/69/69	0/1/1/1
33	PHO	A	409	-	-	8/37/103/103	0/5/6/6
25	CLA	b	612	5	1/1/15/20	12/37/115/115	-
25	CLA	n	602	1	1/1/15/20	14/37/115/115	-
25	CLA	g	610	1	1/1/14/20	13/36/114/115	-
36	PL9	d	405	-	-	8/53/73/73	0/1/1/1
24	CHL	1	606	-	3/3/16/26	7/15/113/137	-
25	CLA	A	405	4	1/1/15/20	10/37/115/115	-
34	SQD	B	623	-	-	17/37/57/69	0/1/1/1
24	CHL	6	606	-	3/3/16/26	3/15/113/137	-
24	CHL	8	607	-	3/3/16/26	8/15/113/137	-
25	CLA	y	603	1	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	NEX	5	1623	-	-	9/27/83/83	0/3/3/3
24	CHL	R	607	-	4/4/18/26	8/27/125/137	-
26	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	5	2630	25	-	9/45/45/53	-
25	CLA	7	611	29	1/1/13/20	10/25/103/115	-
25	CLA	b	608	-	1/1/15/20	13/37/115/115	-
25	CLA	c	506	6	-	16/37/115/115	-
25	CLA	b	616	5	1/1/15/20	12/37/115/115	-
25	CLA	C	502	6	1/1/15/20	20/37/115/115	-
25	CLA	G	614	1	1/1/11/20	5/17/95/115	-
25	CLA	b	604	5	1/1/15/20	9/37/115/115	-
26	LUT	g	1621	-	-	2/29/67/67	0/2/2/2
29	LHG	B	2630	-	-	30/51/51/53	-
27	XAT	g	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	n	612	1	1/1/14/20	9/31/109/115	-
26	LUT	r	620	-	-	2/29/67/67	0/2/2/2
25	CLA	6	604	-	-	9/13/91/115	-
34	SQD	A	418	-	-	22/49/69/69	0/1/1/1
25	CLA	N	610	1	1/1/15/20	11/37/115/115	-
25	CLA	c	503	6	1/1/15/20	10/37/115/115	-
27	XAT	8	622	-	-	3/31/93/93	0/4/4/4
24	CHL	5	607	-	4/4/19/26	19/36/134/137	-
29	LHG	2	2630	25	-	14/41/41/53	-
24	CHL	Y	608	-	4/4/20/26	16/39/137/137	-
24	CHL	7	608	-	3/3/16/26	6/15/113/137	-
25	CLA	1	604	-	1/1/12/20	10/19/97/115	-
24	CHL	8	609	3	3/3/16/26	7/15/113/137	-
25	CLA	3	611	29	1/1/13/20	10/25/103/115	-
25	CLA	6	603	1	1/1/13/20	13/25/103/115	-
25	CLA	B	614	5	1/1/15/20	15/37/115/115	-
30	BCR	D	404	-	-	5/29/63/63	0/2/2/2
30	BCR	c	516	-	-	9/29/63/63	0/2/2/2
25	CLA	N	611	29	1/1/14/20	7/31/109/115	-
29	LHG	r	2630	25	-	16/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	s	611	29	1/1/13/20	9/27/105/115	-
26	LUT	4	620	-	-	5/29/67/67	0/2/2/2
25	CLA	7	613	2	1/1/13/20	8/29/107/115	-
27	XAT	N	1622	-	-	3/31/93/93	0/4/4/4
25	CLA	G	612	1	1/1/14/20	11/31/109/115	-
26	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	2	613	1	-	5/13/91/115	-
36	PL9	D	405	-	-	8/53/73/73	0/1/1/1
25	CLA	R	603	17	1/1/14/20	13/31/109/115	-
26	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	b	607	5	1/1/15/20	11/37/115/115	-
35	LMG	B	2633	-	-	21/50/70/70	0/1/1/1
30	BCR	d	404	-	-	5/29/63/63	0/2/2/2
25	CLA	R	612	17	1/1/11/20	6/18/96/115	-
29	LHG	g	2630	25	-	24/53/53/53	-
25	CLA	6	613	1	-	5/13/91/115	-
25	CLA	4	610	3	1/1/11/20	6/13/91/115	-
25	CLA	r	613	17	1/1/14/20	11/31/109/115	-
24	CHL	N	609	1	4/4/20/26	15/39/137/137	-
25	CLA	3	614	2	1/1/11/20	5/17/95/115	-
25	CLA	4	604	-	-	9/13/91/115	-
24	CHL	2	606	-	3/3/16/26	3/15/113/137	-
25	CLA	G	613	1	-	11/37/115/115	-
26	LUT	3	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	3	601	2	4/4/19/26	13/37/135/137	-
25	CLA	6	610	1	1/1/12/20	3/19/97/115	-
24	CHL	6	608	-	3/3/16/26	8/15/113/137	-
29	LHG	c	523	-	-	21/53/53/53	-
35	LMG	c	521	-	-	21/46/66/70	0/1/1/1
27	XAT	5	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	5	604	-	1/1/12/20	10/19/97/115	-
25	CLA	A	407	-	1/1/12/20	5/19/97/115	-
24	CHL	5	606	-	3/3/16/26	7/15/113/137	-
25	CLA	y	613	1	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	z	101	-	-	22/46/66/70	0/1/1/1
25	CLA	c	505	6	-	13/37/115/115	-
28	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
24	CHL	4	601	3	3/3/16/26	4/13/111/137	-
25	CLA	Y	613	1	1/1/15/20	9/37/115/115	-
25	CLA	N	614	1	1/1/11/20	7/17/95/115	-
25	CLA	s	603	18	1/1/11/20	3/13/91/115	-
25	CLA	g	614	1	1/1/11/20	5/17/95/115	-
25	CLA	Y	611	29	1/1/14/20	8/31/109/115	-
24	CHL	N	607	-	4/4/20/26	17/39/137/137	-
24	CHL	G	608	-	4/4/20/26	18/39/137/137	-
30	BCR	c	517	-	-	6/29/63/63	0/2/2/2
26	LUT	R	620	-	-	2/29/67/67	0/2/2/2
28	NEX	n	1623	-	-	5/27/83/83	0/3/3/3
29	LHG	3	2630	25	-	25/51/51/53	-
25	CLA	3	603	2	1/1/13/20	9/25/103/115	-
26	LUT	1	1621	-	-	5/29/67/67	0/2/2/2
24	CHL	3	609	2	4/4/19/26	14/33/131/137	-
24	CHL	5	605	1	3/3/16/26	8/15/113/137	-
25	CLA	R	611	29	1/1/11/20	9/18/96/115	-
29	LHG	s	2630	25	-	24/53/53/53	-
25	CLA	C	504	-	1/1/15/20	12/37/115/115	-
29	LHG	b	2630	-	-	30/51/51/53	-
25	CLA	c	509	6	1/1/15/20	8/37/115/115	-
27	XAT	G	1622	-	-	2/31/93/93	0/4/4/4
29	LHG	d	408	-	-	17/50/50/53	-
24	CHL	1	608	-	3/3/16/26	3/15/113/137	-
24	CHL	3	607	-	3/3/17/26	12/24/122/137	-
25	CLA	c	501	6	1/1/15/20	15/37/115/115	-
25	CLA	S	611	29	1/1/13/20	9/27/105/115	-
24	CHL	n	605	1	3/3/16/26	10/18/116/137	-
25	CLA	R	604	-	1/1/11/20	4/17/95/115	-
24	CHL	S	606	-	3/3/16/26	10/15/113/137	-
25	CLA	B	609	5	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	1	601	1	3/3/16/26	5/15/113/137	-
26	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	Y	2630	25	-	20/53/53/53	-
25	CLA	r	616	17	-	6/13/91/115	-
24	CHL	1	605	1	3/3/16/26	8/15/113/137	-
24	CHL	5	608	-	3/3/16/26	3/15/113/137	-
29	LHG	4	2630	25	-	8/23/23/53	-
30	BCR	b	618	-	-	4/29/63/63	0/2/2/2
24	CHL	s	607	-	4/4/18/26	11/30/128/137	-
25	CLA	2	610	1	1/1/12/20	3/19/97/115	-
35	LMG	a	415	-	-	11/35/55/70	0/1/1/1
25	CLA	g	602	1	1/1/15/20	11/37/115/115	-
26	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	6	602	1	1/1/14/20	15/33/111/115	-
25	CLA	B	617	5	1/1/15/20	17/37/115/115	-
26	LUT	2	1621	-	-	1/29/67/67	0/2/2/2
26	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	N	603	1	1/1/15/20	14/37/115/115	-
25	CLA	D	403	7	-	13/37/115/115	-
24	CHL	4	607	-	3/3/16/26	8/15/113/137	-
28	NEX	r	623	-	-	4/27/83/83	0/3/3/3
24	CHL	y	608	-	4/4/20/26	16/39/137/137	-
25	CLA	1	603	1	1/1/13/20	10/25/103/115	-
25	CLA	c	511	6	-	13/37/115/115	-
24	CHL	5	609	1	4/4/19/26	11/35/133/137	-
25	CLA	s	609	18	1/1/11/20	7/13/91/115	-
24	CHL	2	607	-	4/4/19/26	18/33/131/137	-
25	CLA	b	609	5	1/1/15/20	5/37/115/115	-
26	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	5	603	1	1/1/13/20	10/25/103/115	-
25	CLA	7	612	2	1/1/11/20	6/13/91/115	-
25	CLA	S	603	18	1/1/11/20	3/13/91/115	-
24	CHL	8	608	-	3/3/16/26	8/15/113/137	-
29	LHG	6	2630	25	-	14/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	1	609	1	4/4/19/26	11/35/133/137	-
28	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	R	616	17	-	6/13/91/115	-
26	LUT	y	1621	-	-	2/29/67/67	0/2/2/2
24	CHL	s	606	-	3/3/16/26	10/15/113/137	-
27	XAT	r	622	-	-	5/31/93/93	0/4/4/4
25	CLA	g	603	1	1/1/15/20	11/37/115/115	-
27	XAT	y	1622	-	-	3/31/93/93	0/4/4/4
24	CHL	g	608	-	4/4/20/26	18/39/137/137	-
25	CLA	c	504	-	1/1/15/20	12/37/115/115	-
25	CLA	n	603	1	1/1/15/20	14/37/115/115	-
27	XAT	4	622	-	-	3/31/93/93	0/4/4/4
28	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	3	606	-	3/3/16/26	5/15/113/137	-
25	CLA	8	603	3	1/1/11/20	4/13/91/115	-
24	CHL	n	607	-	4/4/20/26	17/39/137/137	-
25	CLA	y	602	1	1/1/15/20	14/37/115/115	-
25	CLA	s	604	-	1/1/12/20	6/19/97/115	-
25	CLA	6	611	29	1/1/11/20	3/13/91/115	-
25	CLA	r	601	17	1/1/11/20	9/18/96/115	-
30	BCR	c	515	-	-	6/29/63/63	0/2/2/2
25	CLA	C	506	6	-	16/37/115/115	-
25	CLA	7	602	2	1/1/14/20	14/31/109/115	-
25	CLA	Y	604	-	1/1/12/20	5/19/97/115	-
37	DGD	c	518	-	-	16/44/84/95	0/2/2/2
25	CLA	6	614	1	-	6/13/91/115	-
25	CLA	7	610	2	1/1/14/20	4/31/109/115	-
24	CHL	4	606	-	3/3/16/26	7/15/113/137	-
25	CLA	8	602	3	1/1/11/20	3/13/91/115	-
25	CLA	4	603	3	1/1/11/20	4/13/91/115	-
24	CHL	y	609	1	4/4/20/26	14/39/137/137	-
24	CHL	N	608	-	4/4/20/26	14/39/137/137	-
26	LUT	s	1621	-	-	4/29/67/67	0/2/2/2
35	LMG	C	521	-	-	21/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	3	613	2	1/1/13/20	8/29/107/115	-
25	CLA	2	602	1	1/1/14/20	15/33/111/115	-
25	CLA	y	612	1	1/1/14/20	13/31/109/115	-
25	CLA	r	604	-	1/1/11/20	4/17/95/115	-
24	CHL	g	606	-	3/3/16/26	8/20/118/137	-
25	CLA	Y	612	1	1/1/14/20	13/31/109/115	-
25	CLA	G	604	-	-	5/19/97/115	-
29	LHG	D	408	-	-	17/50/50/53	-
34	SQD	b	621	-	-	18/49/69/69	0/1/1/1
37	DGD	H	102	-	-	25/51/91/95	0/2/2/2
27	XAT	R	622	-	-	5/31/93/93	0/4/4/4
26	LUT	8	620	-	-	5/29/67/67	0/2/2/2
30	BCR	C	516	-	-	9/29/63/63	0/2/2/2
29	LHG	b	2631	-	-	20/53/53/53	-
25	CLA	S	604	-	1/1/12/20	6/19/97/115	-
30	BCR	B	620	-	-	6/29/63/63	0/2/2/2
34	SQD	A	412	-	-	18/45/65/69	0/1/1/1
29	LHG	d	409	-	-	20/53/53/53	-
25	CLA	S	610	18	1/1/13/20	4/25/103/115	-
30	BCR	T	101	-	-	13/29/63/63	0/2/2/2
28	NEX	N	1623	-	-	5/27/83/83	0/3/3/3
26	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
30	BCR	C	514	-	-	2/29/63/63	0/2/2/2
30	BCR	C	515	-	-	6/29/63/63	0/2/2/2
25	CLA	3	610	2	1/1/14/20	4/31/109/115	-
26	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
26	LUT	n	1621	-	-	1/29/67/67	0/2/2/2
26	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	B	615	5	1/1/15/20	15/37/115/115	-
29	LHG	C	523	-	-	21/53/53/53	-
24	CHL	7	601	2	4/4/19/26	13/37/135/137	-
30	BCR	8	623	-	-	12/29/63/63	0/2/2/2
30	BCR	t	101	-	-	13/29/63/63	0/2/2/2
30	BCR	h	101	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	N	605	1	3/3/16/26	10/18/116/137	-
24	CHL	n	601	1	4/4/20/26	17/39/137/137	-
37	DGD	C	519	-	-	25/51/91/95	0/2/2/2
26	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
29	LHG	c	2630	-	-	27/53/53/53	-
27	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
25	CLA	a	410	4	1/1/14/20	6/31/109/115	-
24	CHL	g	605	1	3/3/16/26	10/15/113/137	-
30	BCR	H	101	-	-	5/29/63/63	0/2/2/2
25	CLA	B	605	5	1/1/15/20	14/37/115/115	-
25	CLA	7	604	-	1/1/11/20	9/13/91/115	-
35	LMG	B	622	-	-	22/46/66/70	0/1/1/1
25	CLA	a	406	-	1/1/15/20	4/37/115/115	-
25	CLA	n	604	-	1/1/12/20	4/19/97/115	-
26	LUT	5	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	S	612	18	1/1/11/20	3/18/96/115	-
25	CLA	C	512	6	1/1/15/20	9/37/115/115	-
26	LUT	G	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	Y	610	1	1/1/14/20	7/31/109/115	-
25	CLA	5	613	1	-	7/25/103/115	-
27	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
24	CHL	n	609	1	4/4/20/26	15/39/137/137	-
24	CHL	G	601	1	4/4/20/26	17/39/137/137	-
25	CLA	b	615	5	1/1/15/20	15/37/115/115	-
25	CLA	R	601	17	1/1/11/20	9/18/96/115	-
26	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	n	611	29	1/1/14/20	7/31/109/115	-
29	LHG	D	409	-	-	20/53/53/53	-
37	DGD	h	102	-	-	25/51/91/95	0/2/2/2
25	CLA	b	614	5	1/1/15/20	15/37/115/115	-
24	CHL	g	601	1	4/4/20/26	17/39/137/137	-
25	CLA	1	613	1	-	7/25/103/115	-
25	CLA	r	612	17	1/1/11/20	6/18/96/115	-
24	CHL	Y	601	1	4/4/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	6	1621	-	-	1/29/67/67	0/2/2/2
24	CHL	G	605	1	3/3/16/26	9/15/113/137	-
27	XAT	6	1622	-	-	4/31/93/93	0/4/4/4
25	CLA	A	410	4	1/1/14/20	6/31/109/115	-
25	CLA	R	609	17	1/1/13/20	2/29/107/115	-
25	CLA	d	403	7	-	13/37/115/115	-
24	CHL	R	614	17	3/3/15/26	6/10/108/137	-
24	CHL	3	605	2	3/3/16/26	10/15/113/137	-
25	CLA	S	609	18	1/1/11/20	7/13/91/115	-
29	LHG	L	101	-	-	21/53/53/53	-
30	BCR	A	411	-	-	2/29/63/63	0/2/2/2
25	CLA	y	611	29	1/1/14/20	8/31/109/115	-
30	BCR	C	517	-	-	6/29/63/63	0/2/2/2
25	CLA	3	604	-	1/1/11/20	9/13/91/115	-
25	CLA	g	612	1	1/1/14/20	11/31/109/115	-
37	DGD	B	626	-	-	22/48/88/95	0/2/2/2
25	CLA	r	602	17	1/1/14/20	7/31/109/115	-
25	CLA	Y	603	1	1/1/15/20	14/37/115/115	-
24	CHL	2	605	1	3/3/16/26	8/15/113/137	-
29	LHG	S	2630	25	-	24/53/53/53	-
25	CLA	B	613	5	1/1/15/20	15/37/115/115	-
36	PL9	A	414	-	-	1/5/18/73	0/1/1/1
37	DGD	C	518	-	-	16/44/84/95	0/2/2/2
25	CLA	R	613	17	1/1/14/20	11/31/109/115	-
25	CLA	C	510	6	1/1/15/20	17/37/115/115	-
25	CLA	N	604	-	1/1/12/20	4/19/97/115	-
25	CLA	1	602	1	1/1/14/20	9/33/111/115	-
25	CLA	7	614	2	1/1/11/20	5/17/95/115	-
30	BCR	B	619	-	-	2/29/63/63	0/2/2/2
28	NEX	R	623	-	-	4/27/83/83	0/3/3/3
24	CHL	G	607	-	4/4/20/26	13/39/137/137	-
25	CLA	B	607	5	1/1/15/20	11/37/115/115	-
37	DGD	c	520	-	-	28/49/89/95	0/2/2/2
24	CHL	y	605	1	3/3/16/26	6/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	G	609	1	4/4/19/26	11/33/131/137	-
24	CHL	R	606	-	4/4/20/26	22/39/137/137	-
24	CHL	r	608	-	4/4/19/26	16/33/131/137	-
25	CLA	n	614	1	1/1/11/20	7/17/95/115	-
24	CHL	8	601	3	3/3/16/26	4/13/111/137	-
24	CHL	6	609	1	4/4/19/26	15/33/131/137	-
37	DGD	b	626	-	-	22/48/88/95	0/2/2/2
24	CHL	2	608	-	3/3/16/26	8/15/113/137	-
24	CHL	R	608	-	4/4/19/26	16/33/131/137	-
25	CLA	s	613	18	1/1/13/20	6/25/103/115	-
29	LHG	d	410	-	-	24/47/47/53	-
24	CHL	Y	609	1	4/4/20/26	14/39/137/137	-
29	LHG	7	2630	25	-	25/51/51/53	-
28	NEX	y	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	B	606	5	1/1/15/20	15/37/115/115	-
25	CLA	C	507	-	1/1/15/20	21/37/115/115	-
25	CLA	N	602	1	1/1/15/20	14/37/115/115	-
25	CLA	3	612	2	1/1/11/20	6/13/91/115	-
25	CLA	c	512	6	1/1/15/20	9/37/115/115	-
25	CLA	B	603	5	1/1/15/20	10/37/115/115	-
24	CHL	s	608	-	3/3/16/26	3/15/113/137	-
24	CHL	6	605	1	3/3/16/26	8/15/113/137	-
25	CLA	C	513	6	-	12/37/115/115	-
28	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	r	611	29	1/1/11/20	9/18/96/115	-
24	CHL	S	601	18	3/3/16/26	8/15/113/137	-
25	CLA	Y	614	1	1/1/11/20	3/17/95/115	-
25	CLA	1	610	1	1/1/13/20	3/27/105/115	-
24	CHL	7	607	-	3/3/17/26	12/24/122/137	-
27	XAT	2	1622	-	-	4/31/93/93	0/4/4/4
35	LMG	d	411	-	-	15/41/61/70	0/1/1/1
25	CLA	5	602	1	1/1/14/20	9/33/111/115	-
25	CLA	8	612	3	1/1/11/20	8/13/91/115	-
24	CHL	S	607	-	4/4/18/26	11/30/128/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	8	2630	25	-	8/23/23/53	-
29	LHG	R	2630	25	-	16/46/46/53	-
25	CLA	B	602	-	1/1/15/20	15/37/115/115	-
24	CHL	r	606	-	4/4/20/26	22/39/137/137	-
25	CLA	4	612	3	1/1/11/20	8/13/91/115	-
24	CHL	G	606	-	3/3/16/26	8/20/118/137	-
35	LMG	b	2633	-	-	21/50/70/70	0/1/1/1
29	LHG	y	2630	25	-	20/53/53/53	-
25	CLA	b	605	5	1/1/15/20	14/37/115/115	-
25	CLA	a	407	-	1/1/12/20	5/19/97/115	-
29	LHG	C	2630	-	-	27/53/53/53	-
35	LMG	a	413	-	-	17/43/63/70	0/1/1/1

All (3737) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	614	CLA	C4B-NB	8.15	1.42	1.35
25	7	614	CLA	C4B-NB	8.11	1.42	1.35
25	C	501	CLA	C4B-NB	7.90	1.42	1.35
25	s	602	CLA	C4B-NB	7.88	1.42	1.35
25	S	602	CLA	C4B-NB	7.88	1.42	1.35
25	c	501	CLA	C4B-NB	7.84	1.42	1.35
25	S	609	CLA	C4B-NB	7.80	1.42	1.35
25	s	609	CLA	C4B-NB	7.77	1.42	1.35
25	s	603	CLA	C4B-NB	7.70	1.42	1.35
25	G	603	CLA	C4B-NB	7.68	1.42	1.35
25	n	613	CLA	C4B-NB	7.67	1.42	1.35
25	S	603	CLA	C4B-NB	7.66	1.42	1.35
25	N	613	CLA	C4B-NB	7.65	1.42	1.35
25	g	603	CLA	C4B-NB	7.64	1.42	1.35
25	s	612	CLA	C4B-NB	7.57	1.42	1.35
25	S	612	CLA	C4B-NB	7.56	1.42	1.35
25	c	504	CLA	C4B-NB	7.50	1.41	1.35
25	S	610	CLA	C4B-NB	7.45	1.41	1.35
25	s	610	CLA	C4B-NB	7.44	1.41	1.35
25	S	613	CLA	C4B-NB	7.43	1.41	1.35
25	s	611	CLA	C4B-NB	7.43	1.41	1.35
25	C	504	CLA	C4B-NB	7.42	1.41	1.35
25	s	604	CLA	C4B-NB	7.42	1.41	1.35
25	S	611	CLA	C4B-NB	7.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	511	CLA	C4B-NB	7.41	1.41	1.35
25	s	613	CLA	C4B-NB	7.41	1.41	1.35
25	6	612	CLA	C4B-NB	7.41	1.41	1.35
25	S	604	CLA	C4B-NB	7.40	1.41	1.35
25	2	613	CLA	C4B-NB	7.36	1.41	1.35
25	2	612	CLA	C4B-NB	7.36	1.41	1.35
25	C	503	CLA	C4B-NB	7.35	1.41	1.35
25	c	503	CLA	C4B-NB	7.35	1.41	1.35
25	C	511	CLA	C4B-NB	7.34	1.41	1.35
25	C	506	CLA	C4B-NB	7.34	1.41	1.35
25	r	612	CLA	C4B-NB	7.31	1.41	1.35
25	c	506	CLA	C4B-NB	7.30	1.41	1.35
25	6	613	CLA	C4B-NB	7.28	1.41	1.35
25	C	512	CLA	C4B-NB	7.26	1.41	1.35
25	R	612	CLA	C4B-NB	7.26	1.41	1.35
25	c	512	CLA	C4B-NB	7.25	1.41	1.35
25	G	613	CLA	C4B-NB	7.21	1.41	1.35
25	g	613	CLA	C4B-NB	7.21	1.41	1.35
36	D	405	PL9	C3-C4	-7.20	1.37	1.49
36	d	405	PL9	C3-C4	-7.20	1.37	1.49
25	R	601	CLA	C4B-NB	7.19	1.41	1.35
25	c	505	CLA	C4B-NB	7.19	1.41	1.35
25	y	611	CLA	C4B-NB	7.19	1.41	1.35
25	Y	611	CLA	C4B-NB	7.17	1.41	1.35
25	S	614	CLA	C4B-NB	7.16	1.41	1.35
25	C	510	CLA	C4B-NB	7.15	1.41	1.35
25	G	604	CLA	C4B-NB	7.14	1.41	1.35
25	s	614	CLA	C4B-NB	7.14	1.41	1.35
25	C	505	CLA	C4B-NB	7.13	1.41	1.35
25	r	601	CLA	C4B-NB	7.13	1.41	1.35
25	g	604	CLA	C4B-NB	7.13	1.41	1.35
25	c	510	CLA	C4B-NB	7.11	1.41	1.35
25	4	603	CLA	C4B-NB	7.09	1.41	1.35
25	r	611	CLA	C4B-NB	7.05	1.41	1.35
25	R	616	CLA	C4B-NB	7.04	1.41	1.35
25	y	604	CLA	C4B-NB	7.04	1.41	1.35
25	N	604	CLA	C4B-NB	7.02	1.41	1.35
25	n	611	CLA	C4B-NB	7.02	1.41	1.35
25	7	604	CLA	C4B-NB	7.02	1.41	1.35
25	5	612	CLA	C4B-NB	7.01	1.41	1.35
25	8	603	CLA	C4B-NB	7.00	1.41	1.35
25	n	604	CLA	C4B-NB	7.00	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	611	CLA	C4B-NB	7.00	1.41	1.35
25	Y	604	CLA	C4B-NB	7.00	1.41	1.35
25	3	604	CLA	C4B-NB	7.00	1.41	1.35
25	1	612	CLA	C4B-NB	6.99	1.41	1.35
25	8	612	CLA	C4B-NB	6.99	1.41	1.35
25	7	613	CLA	C4B-NB	6.98	1.41	1.35
25	c	513	CLA	C4B-NB	6.98	1.41	1.35
25	c	502	CLA	C4B-NB	6.97	1.41	1.35
25	4	611	CLA	C4B-NB	6.95	1.41	1.35
25	4	612	CLA	C4B-NB	6.95	1.41	1.35
25	c	509	CLA	C4B-NB	6.95	1.41	1.35
25	G	612	CLA	C4B-NB	6.94	1.41	1.35
25	8	611	CLA	C4B-NB	6.94	1.41	1.35
25	r	616	CLA	C4B-NB	6.94	1.41	1.35
25	N	611	CLA	C4B-NB	6.93	1.41	1.35
25	C	502	CLA	C4B-NB	6.93	1.41	1.35
25	C	513	CLA	C4B-NB	6.92	1.41	1.35
25	C	509	CLA	C4B-NB	6.91	1.41	1.35
25	y	603	CLA	C4B-NB	6.91	1.41	1.35
25	3	613	CLA	C4B-NB	6.90	1.41	1.35
25	g	612	CLA	C4B-NB	6.90	1.41	1.35
25	2	614	CLA	C4B-NB	6.89	1.41	1.35
25	5	614	CLA	C4B-NB	6.88	1.41	1.35
25	1	614	CLA	C4B-NB	6.87	1.41	1.35
25	Y	603	CLA	C4B-NB	6.87	1.41	1.35
25	6	614	CLA	C4B-NB	6.86	1.41	1.35
25	1	613	CLA	C4B-NB	6.86	1.41	1.35
25	c	507	CLA	C4B-NB	6.84	1.41	1.35
25	A	407	CLA	C4B-NB	6.84	1.41	1.35
25	Y	613	CLA	C4B-NB	6.84	1.41	1.35
25	a	407	CLA	C4B-NB	6.84	1.41	1.35
25	b	607	CLA	C4B-NB	6.84	1.41	1.35
25	y	613	CLA	C4B-NB	6.84	1.41	1.35
25	N	612	CLA	C4B-NB	6.83	1.41	1.35
25	n	612	CLA	C4B-NB	6.82	1.41	1.35
25	5	613	CLA	C4B-NB	6.82	1.41	1.35
25	y	612	CLA	C4B-NB	6.82	1.41	1.35
25	6	611	CLA	C4B-NB	6.81	1.41	1.35
25	Y	612	CLA	C4B-NB	6.81	1.41	1.35
25	C	508	CLA	C4B-NB	6.78	1.41	1.35
25	2	611	CLA	C4B-NB	6.76	1.41	1.35
25	B	607	CLA	C4B-NB	6.76	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	614	CLA	C4B-NB	6.75	1.41	1.35
25	C	507	CLA	C4B-NB	6.75	1.41	1.35
25	g	614	CLA	C4B-NB	6.74	1.41	1.35
25	c	508	CLA	C4B-NB	6.74	1.41	1.35
25	4	602	CLA	C4B-NB	6.74	1.41	1.35
25	6	603	CLA	C4B-NB	6.74	1.41	1.35
25	2	603	CLA	C4B-NB	6.73	1.41	1.35
25	N	603	CLA	C4B-NB	6.73	1.41	1.35
25	A	406	CLA	C4B-NB	6.72	1.41	1.35
25	6	610	CLA	C4B-NB	6.70	1.41	1.35
25	8	602	CLA	C4B-NB	6.70	1.41	1.35
25	2	602	CLA	C4B-NB	6.70	1.41	1.35
25	B	616	CLA	C4B-NB	6.70	1.41	1.35
25	b	616	CLA	C4B-NB	6.70	1.41	1.35
25	R	603	CLA	C4B-NB	6.69	1.41	1.35
25	6	602	CLA	C4B-NB	6.68	1.41	1.35
25	7	611	CLA	C4B-NB	6.68	1.41	1.35
25	2	610	CLA	C4B-NB	6.67	1.41	1.35
25	G	611	CLA	C4B-NB	6.66	1.41	1.35
25	r	603	CLA	C4B-NB	6.66	1.41	1.35
25	3	611	CLA	C4B-NB	6.65	1.41	1.35
25	r	610	CLA	C4B-NB	6.64	1.41	1.35
25	n	603	CLA	C4B-NB	6.63	1.41	1.35
25	5	604	CLA	C4B-NB	6.63	1.41	1.35
25	y	614	CLA	C4B-NB	6.63	1.41	1.35
25	a	406	CLA	C4B-NB	6.62	1.41	1.35
25	g	611	CLA	C4B-NB	6.62	1.41	1.35
25	Y	614	CLA	C4B-NB	6.61	1.41	1.35
25	1	604	CLA	C4B-NB	6.59	1.41	1.35
25	R	610	CLA	C4B-NB	6.59	1.41	1.35
25	B	602	CLA	C4B-NB	6.58	1.41	1.35
25	b	602	CLA	C4B-NB	6.54	1.41	1.35
25	2	604	CLA	C4B-NB	6.54	1.41	1.35
25	N	614	CLA	C4B-NB	6.54	1.41	1.35
25	n	614	CLA	C4B-NB	6.52	1.41	1.35
36	D	405	PL9	C7-C3	-6.51	1.44	1.51
36	d	405	PL9	C7-C3	-6.49	1.44	1.51
25	1	611	CLA	C4B-NB	6.49	1.41	1.35
25	n	602	CLA	C4B-NB	6.49	1.41	1.35
25	6	604	CLA	C4B-NB	6.48	1.41	1.35
25	N	602	CLA	C4B-NB	6.48	1.41	1.35
25	3	610	CLA	C4B-NB	6.46	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	604	CLA	C4B-NB	6.45	1.41	1.35
25	R	613	CLA	C4B-NB	6.43	1.40	1.35
25	4	604	CLA	C4B-NB	6.42	1.40	1.35
25	5	611	CLA	C4B-NB	6.42	1.40	1.35
25	7	610	CLA	C4B-NB	6.41	1.40	1.35
25	8	610	CLA	C4B-NB	6.41	1.40	1.35
25	4	610	CLA	C4B-NB	6.41	1.40	1.35
25	r	613	CLA	C4B-NB	6.41	1.40	1.35
25	7	602	CLA	C4B-NB	6.40	1.40	1.35
25	r	604	CLA	C4B-NB	6.40	1.40	1.35
25	b	604	CLA	C4B-NB	6.38	1.40	1.35
25	B	608	CLA	C4B-NB	6.38	1.40	1.35
25	5	602	CLA	C4B-NB	6.38	1.40	1.35
25	R	609	CLA	C4B-NB	6.38	1.40	1.35
25	b	611	CLA	C4B-NB	6.37	1.40	1.35
25	b	608	CLA	C4B-NB	6.37	1.40	1.35
25	r	609	CLA	C4B-NB	6.36	1.40	1.35
25	R	604	CLA	C4B-NB	6.35	1.40	1.35
25	g	610	CLA	C4B-NB	6.35	1.40	1.35
25	A	410	CLA	C4B-NB	6.34	1.40	1.35
25	1	602	CLA	C4B-NB	6.33	1.40	1.35
25	b	603	CLA	C4B-NB	6.32	1.40	1.35
25	3	602	CLA	C4B-NB	6.31	1.40	1.35
25	B	603	CLA	C4B-NB	6.31	1.40	1.35
25	G	610	CLA	C4B-NB	6.31	1.40	1.35
25	B	604	CLA	C4B-NB	6.30	1.40	1.35
25	a	410	CLA	C4B-NB	6.30	1.40	1.35
25	B	611	CLA	C4B-NB	6.30	1.40	1.35
25	N	610	CLA	C4B-NB	6.30	1.40	1.35
25	n	610	CLA	C4B-NB	6.28	1.40	1.35
25	3	612	CLA	C4B-NB	6.26	1.40	1.35
25	A	405	CLA	C4B-NB	6.26	1.40	1.35
25	g	602	CLA	C4B-NB	6.25	1.40	1.35
25	r	602	CLA	C4B-NB	6.23	1.40	1.35
25	7	612	CLA	C4B-NB	6.21	1.40	1.35
25	G	602	CLA	C4B-NB	6.21	1.40	1.35
25	R	602	CLA	C4B-NB	6.20	1.40	1.35
25	a	405	CLA	C4B-NB	6.19	1.40	1.35
25	D	402	CLA	C4B-NB	6.19	1.40	1.35
25	d	402	CLA	C4B-NB	6.17	1.40	1.35
25	Y	610	CLA	C4B-NB	6.15	1.40	1.35
25	3	603	CLA	C4B-NB	6.13	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	C4B-NB	6.10	1.40	1.35
25	7	603	CLA	C4B-NB	6.09	1.40	1.35
25	y	610	CLA	C4B-NB	6.09	1.40	1.35
25	b	612	CLA	C4B-NB	6.09	1.40	1.35
25	D	403	CLA	C4B-NB	6.04	1.40	1.35
25	B	605	CLA	C4B-NB	6.03	1.40	1.35
25	B	610	CLA	C4B-NB	6.02	1.40	1.35
25	b	605	CLA	C4B-NB	6.02	1.40	1.35
25	d	403	CLA	C4B-NB	6.01	1.40	1.35
25	B	614	CLA	C4B-NB	5.98	1.40	1.35
25	b	610	CLA	C4B-NB	5.95	1.40	1.35
25	b	614	CLA	C4B-NB	5.94	1.40	1.35
25	1	610	CLA	C4B-NB	5.93	1.40	1.35
25	5	610	CLA	C4B-NB	5.87	1.40	1.35
25	b	617	CLA	C4B-NB	5.84	1.40	1.35
25	B	609	CLA	C4B-NB	5.83	1.40	1.35
24	Y	601	CHL	C3D-C4D	-5.82	1.31	1.44
25	B	606	CLA	C4B-NB	5.82	1.40	1.35
24	y	601	CHL	C3D-C4D	-5.81	1.31	1.44
25	b	609	CLA	C4B-NB	5.81	1.40	1.35
25	B	617	CLA	C4B-NB	5.81	1.40	1.35
25	Y	602	CLA	C4B-NB	5.81	1.40	1.35
25	5	603	CLA	C4B-NB	5.80	1.40	1.35
25	1	603	CLA	C4B-NB	5.79	1.40	1.35
25	b	606	CLA	C4B-NB	5.75	1.40	1.35
25	y	602	CLA	C4B-NB	5.74	1.40	1.35
25	b	615	CLA	C4B-NB	5.71	1.40	1.35
25	B	615	CLA	C4B-NB	5.68	1.40	1.35
24	7	606	CHL	C3D-C4D	-5.68	1.31	1.44
24	3	606	CHL	C3D-C4D	-5.65	1.31	1.44
24	Y	609	CHL	C3D-C4D	-5.65	1.31	1.44
24	1	601	CHL	C3D-C4D	-5.65	1.31	1.44
24	y	609	CHL	C3D-C4D	-5.64	1.31	1.44
24	3	601	CHL	C3D-C4D	-5.62	1.31	1.44
24	7	601	CHL	C3D-C4D	-5.62	1.31	1.44
24	5	601	CHL	C3D-C4D	-5.61	1.31	1.44
25	b	613	CLA	C4B-NB	5.60	1.40	1.35
24	5	608	CHL	C3D-C4D	-5.60	1.31	1.44
24	g	601	CHL	C3D-C4D	-5.60	1.31	1.44
24	G	601	CHL	C3D-C4D	-5.60	1.31	1.44
24	1	608	CHL	C3D-C4D	-5.59	1.31	1.44
24	5	609	CHL	C3D-C4D	-5.57	1.31	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	609	CHL	C3D-C4D	-5.56	1.31	1.44
24	n	608	CHL	C3D-C4D	-5.53	1.31	1.44
24	n	606	CHL	C3D-C4D	-5.52	1.31	1.44
24	N	608	CHL	C3D-C4D	-5.50	1.31	1.44
24	N	606	CHL	C3D-C4D	-5.50	1.31	1.44
25	B	613	CLA	C4B-NB	5.50	1.40	1.35
24	8	608	CHL	C3D-C4D	-5.48	1.31	1.44
24	4	608	CHL	C3D-C4D	-5.48	1.31	1.44
24	y	608	CHL	C3D-C4D	-5.48	1.31	1.44
24	y	606	CHL	C3D-C4D	-5.46	1.31	1.44
24	Y	608	CHL	C3D-C4D	-5.45	1.31	1.44
24	Y	606	CHL	C3D-C4D	-5.44	1.31	1.44
24	n	601	CHL	C3D-C4D	-5.44	1.31	1.44
24	n	609	CHL	C3D-C4D	-5.44	1.31	1.44
24	N	609	CHL	C3D-C4D	-5.43	1.31	1.44
24	N	601	CHL	C3D-C4D	-5.43	1.31	1.44
24	R	608	CHL	C3D-C4D	-5.42	1.31	1.44
24	r	608	CHL	C3D-C4D	-5.42	1.32	1.44
24	6	601	CHL	C3D-C4D	-5.39	1.32	1.44
24	2	601	CHL	C3D-C4D	-5.39	1.32	1.44
24	3	609	CHL	C3D-C4D	-5.37	1.32	1.44
36	D	405	PL9	C6-C1	-5.36	1.39	1.48
36	d	405	PL9	C6-C1	-5.35	1.39	1.48
24	7	609	CHL	C3D-C4D	-5.34	1.32	1.44
24	g	609	CHL	C3D-C4D	-5.32	1.32	1.44
24	G	609	CHL	C3D-C4D	-5.32	1.32	1.44
24	1	606	CHL	C3D-C4D	-5.31	1.32	1.44
24	G	608	CHL	C3D-C4D	-5.30	1.32	1.44
24	5	605	CHL	C3D-C4D	-5.30	1.32	1.44
24	5	606	CHL	C3D-C4D	-5.29	1.32	1.44
24	3	608	CHL	C3D-C4D	-5.29	1.32	1.44
24	2	607	CHL	C3D-C4D	-5.28	1.32	1.44
24	g	608	CHL	C3D-C4D	-5.28	1.32	1.44
24	7	608	CHL	C3D-C4D	-5.27	1.32	1.44
24	g	606	CHL	C3D-C4D	-5.27	1.32	1.44
24	6	607	CHL	C3D-C4D	-5.27	1.32	1.44
24	G	606	CHL	C3D-C4D	-5.26	1.32	1.44
24	2	609	CHL	C3D-C4D	-5.26	1.32	1.44
24	1	605	CHL	C3D-C4D	-5.26	1.32	1.44
24	6	609	CHL	C3D-C4D	-5.26	1.32	1.44
24	r	606	CHL	C3D-C4D	-5.25	1.32	1.44
24	y	607	CHL	C3D-C4D	-5.24	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	607	CHL	C3D-C4D	-5.24	1.32	1.44
24	1	607	CHL	C3D-C4D	-5.23	1.32	1.44
24	Y	607	CHL	C3D-C4D	-5.23	1.32	1.44
24	R	606	CHL	C3D-C4D	-5.22	1.32	1.44
24	8	601	CHL	C3B-C2B	5.22	1.47	1.40
24	8	609	CHL	C3D-C4D	-5.20	1.32	1.44
24	3	607	CHL	C3D-C4D	-5.20	1.32	1.44
24	5	607	CHL	C3D-C4D	-5.20	1.32	1.44
24	S	607	CHL	O2D-CGD	5.20	1.45	1.33
24	r	607	CHL	C3D-C4D	-5.20	1.32	1.44
24	R	607	CHL	C3D-C4D	-5.20	1.32	1.44
24	s	607	CHL	O2D-CGD	5.19	1.45	1.33
24	Y	605	CHL	C3D-C4D	-5.19	1.32	1.44
24	y	605	CHL	C3D-C4D	-5.18	1.32	1.44
24	4	609	CHL	C3D-C4D	-5.18	1.32	1.44
24	r	614	CHL	CHC-C1C	5.17	1.48	1.35
24	R	614	CHL	CHC-C1C	5.16	1.48	1.35
24	N	605	CHL	C3D-C4D	-5.16	1.32	1.44
24	n	605	CHL	C3D-C4D	-5.15	1.32	1.44
24	2	606	CHL	C3D-C4D	-5.15	1.32	1.44
24	4	601	CHL	C3B-C2B	5.14	1.47	1.40
24	4	601	CHL	CHC-C1C	5.13	1.48	1.35
24	8	601	CHL	CHC-C1C	5.13	1.48	1.35
24	6	607	CHL	O2D-CGD	5.12	1.45	1.33
24	6	606	CHL	C3D-C4D	-5.12	1.32	1.44
24	8	607	CHL	C3D-C4D	-5.12	1.32	1.44
24	4	606	CHL	C3D-C4D	-5.12	1.32	1.44
24	8	609	CHL	O2D-CGD	5.12	1.45	1.33
24	8	606	CHL	C3D-C4D	-5.12	1.32	1.44
24	4	607	CHL	C3D-C4D	-5.12	1.32	1.44
24	2	607	CHL	O2D-CGD	5.12	1.45	1.33
24	4	609	CHL	O2D-CGD	5.11	1.45	1.33
24	R	614	CHL	C3D-C4D	-5.10	1.32	1.44
24	7	605	CHL	C3D-C4D	-5.09	1.32	1.44
24	g	607	CHL	C3D-C4D	-5.09	1.32	1.44
24	6	608	CHL	C3D-C4D	-5.09	1.32	1.44
24	r	614	CHL	C3D-C4D	-5.09	1.32	1.44
24	S	601	CHL	O2D-CGD	5.08	1.45	1.33
24	2	608	CHL	C3D-C4D	-5.08	1.32	1.44
24	G	607	CHL	C3D-C4D	-5.07	1.32	1.44
24	3	605	CHL	C3D-C4D	-5.06	1.32	1.44
24	s	601	CHL	O2D-CGD	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	601	CHL	C3D-C4D	-5.06	1.32	1.44
24	S	601	CHL	C3D-C4D	-5.05	1.32	1.44
24	3	608	CHL	CHC-C1C	5.03	1.47	1.35
24	R	607	CHL	O2D-CGD	5.02	1.45	1.33
24	6	605	CHL	O2D-CGD	5.01	1.45	1.33
24	g	605	CHL	O2D-CGD	5.01	1.45	1.33
24	r	607	CHL	O2D-CGD	5.01	1.45	1.33
24	2	601	CHL	O2D-CGD	5.01	1.45	1.33
24	g	605	CHL	C3D-C4D	-5.01	1.32	1.44
24	n	601	CHL	O2D-CGD	5.01	1.45	1.33
24	N	601	CHL	O2D-CGD	5.01	1.45	1.33
24	2	605	CHL	O2D-CGD	5.00	1.45	1.33
24	7	608	CHL	CHC-C1C	5.00	1.47	1.35
24	6	601	CHL	O2D-CGD	5.00	1.45	1.33
24	G	605	CHL	O2D-CGD	5.00	1.45	1.33
24	s	606	CHL	O2D-CGD	5.00	1.45	1.33
24	g	608	CHL	O2D-CGD	4.99	1.45	1.33
24	S	601	CHL	CHC-C1C	4.99	1.47	1.35
24	G	605	CHL	C3D-C4D	-4.99	1.32	1.44
24	s	601	CHL	CHC-C1C	4.99	1.47	1.35
24	S	608	CHL	O2D-CGD	4.98	1.45	1.33
24	G	608	CHL	O2D-CGD	4.98	1.45	1.33
24	s	608	CHL	O2D-CGD	4.98	1.45	1.33
24	S	606	CHL	O2D-CGD	4.97	1.45	1.33
24	N	607	CHL	C3D-C4D	-4.97	1.33	1.44
24	6	606	CHL	O2D-CGD	4.97	1.45	1.33
24	g	608	CHL	CHC-C1C	4.97	1.47	1.35
24	3	605	CHL	O2D-CGD	4.97	1.45	1.33
24	6	605	CHL	C3D-C4D	-4.96	1.33	1.44
24	7	606	CHL	O2D-CGD	4.96	1.45	1.33
24	G	607	CHL	CHC-C1C	4.96	1.47	1.35
24	2	609	CHL	O2D-CGD	4.96	1.45	1.33
24	n	607	CHL	C3D-C4D	-4.96	1.33	1.44
24	3	606	CHL	O2D-CGD	4.96	1.45	1.33
24	7	605	CHL	O2D-CGD	4.96	1.45	1.33
24	2	605	CHL	C3D-C4D	-4.96	1.33	1.44
24	4	608	CHL	O2D-CGD	4.95	1.45	1.33
24	2	606	CHL	O2D-CGD	4.95	1.45	1.33
24	7	607	CHL	CHC-C1C	4.94	1.47	1.35
24	G	608	CHL	CHC-C1C	4.94	1.47	1.35
24	6	609	CHL	O2D-CGD	4.94	1.45	1.33
24	g	607	CHL	CHC-C1C	4.94	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	601	CHL	O2D-CGD	4.94	1.45	1.33
24	3	607	CHL	CHC-C1C	4.94	1.47	1.35
24	G	601	CHL	O2D-CGD	4.94	1.45	1.33
24	8	608	CHL	O2D-CGD	4.93	1.45	1.33
24	S	606	CHL	CHC-C1C	4.92	1.47	1.35
24	g	607	CHL	O2D-CGD	4.91	1.45	1.33
24	S	608	CHL	C3B-C2B	4.91	1.47	1.40
24	G	607	CHL	O2D-CGD	4.91	1.45	1.33
24	s	608	CHL	C3B-C2B	4.91	1.47	1.40
24	5	605	CHL	O2D-CGD	4.90	1.45	1.33
24	S	608	CHL	C3D-C4D	-4.89	1.33	1.44
24	s	606	CHL	CHC-C1C	4.89	1.47	1.35
24	1	605	CHL	O2D-CGD	4.89	1.45	1.33
24	8	606	CHL	O2D-CGD	4.89	1.45	1.33
24	G	606	CHL	O2D-CGD	4.89	1.45	1.33
24	g	606	CHL	O2D-CGD	4.89	1.45	1.33
24	s	608	CHL	C3D-C4D	-4.88	1.33	1.44
24	n	606	CHL	O2D-CGD	4.88	1.45	1.33
24	4	606	CHL	O2D-CGD	4.88	1.45	1.33
24	2	605	CHL	CHC-C1C	4.87	1.47	1.35
24	N	607	CHL	O2D-CGD	4.87	1.45	1.33
24	n	607	CHL	O2D-CGD	4.87	1.45	1.33
25	b	612	CLA	C4D-ND	-4.87	1.31	1.37
24	s	608	CHL	CHC-C1C	4.86	1.47	1.35
24	2	608	CHL	O2D-CGD	4.86	1.45	1.33
24	5	606	CHL	O2D-CGD	4.86	1.45	1.33
24	5	608	CHL	CHC-C1C	4.86	1.47	1.35
24	6	605	CHL	CHC-C1C	4.86	1.47	1.35
24	r	606	CHL	O2D-CGD	4.86	1.45	1.33
24	S	608	CHL	CHC-C1C	4.85	1.47	1.35
24	1	606	CHL	O2D-CGD	4.85	1.45	1.33
24	N	606	CHL	O2D-CGD	4.85	1.45	1.33
24	6	608	CHL	O2D-CGD	4.84	1.45	1.33
25	B	612	CLA	C4D-ND	-4.84	1.31	1.37
24	R	606	CHL	O2D-CGD	4.84	1.45	1.33
24	2	607	CHL	CHC-C1C	4.84	1.47	1.35
24	7	601	CHL	O2D-CGD	4.84	1.45	1.33
24	1	608	CHL	CHC-C1C	4.84	1.47	1.35
24	4	607	CHL	O2D-CGD	4.83	1.45	1.33
24	8	607	CHL	O2D-CGD	4.83	1.45	1.33
24	3	601	CHL	O2D-CGD	4.83	1.45	1.33
37	h	102	DGD	O2D-C2D	-4.83	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	607	CHL	CHC-C1C	4.83	1.47	1.35
24	4	601	CHL	C3D-C4D	-4.82	1.33	1.44
24	Y	605	CHL	O2D-CGD	4.82	1.45	1.33
37	H	102	DGD	O2D-C2D	-4.82	1.31	1.43
24	n	605	CHL	CHC-C1C	4.80	1.47	1.35
24	Y	606	CHL	O2D-CGD	4.80	1.44	1.33
24	8	601	CHL	C3D-C4D	-4.80	1.33	1.44
24	7	601	CHL	CHC-C1C	4.80	1.47	1.35
24	7	606	CHL	CHC-C1C	4.80	1.47	1.35
24	r	614	CHL	O2D-CGD	4.80	1.44	1.33
24	r	606	CHL	CHC-C1C	4.80	1.47	1.35
24	R	614	CHL	O2D-CGD	4.80	1.44	1.33
24	3	606	CHL	CHC-C1C	4.80	1.47	1.35
24	N	605	CHL	CHC-C1C	4.79	1.47	1.35
24	3	601	CHL	CHC-C1C	4.79	1.47	1.35
24	3	608	CHL	O2D-CGD	4.79	1.44	1.33
36	D	405	PL9	C7-C8	-4.79	1.43	1.50
24	g	609	CHL	O2D-CGD	4.78	1.44	1.33
24	y	606	CHL	O2D-CGD	4.78	1.44	1.33
24	y	605	CHL	O2D-CGD	4.78	1.44	1.33
24	R	606	CHL	CHC-C1C	4.78	1.47	1.35
24	S	606	CHL	C3B-C2B	4.78	1.47	1.40
24	n	608	CHL	O2D-CGD	4.78	1.44	1.33
24	N	608	CHL	O2D-CGD	4.78	1.44	1.33
24	7	608	CHL	O2D-CGD	4.77	1.44	1.33
25	Y	613	CLA	C4D-ND	-4.77	1.31	1.37
24	g	605	CHL	CHC-C1C	4.76	1.47	1.35
24	7	609	CHL	O2D-CGD	4.76	1.44	1.33
24	n	605	CHL	O2D-CGD	4.76	1.44	1.33
24	G	609	CHL	O2D-CGD	4.75	1.44	1.33
24	r	607	CHL	CHC-C1C	4.75	1.47	1.35
24	s	606	CHL	C3B-C2B	4.74	1.46	1.40
24	G	605	CHL	CHC-C1C	4.74	1.47	1.35
24	4	601	CHL	C2C-C3C	4.74	1.46	1.36
24	R	607	CHL	CHC-C1C	4.74	1.47	1.35
36	d	405	PL9	C7-C8	-4.73	1.43	1.50
24	8	606	CHL	CHC-C1C	4.73	1.47	1.35
25	y	613	CLA	C4D-ND	-4.73	1.31	1.37
24	S	606	CHL	C3D-C4D	-4.73	1.33	1.44
24	5	608	CHL	O2D-CGD	4.73	1.44	1.33
24	S	608	CHL	C2C-C3C	4.73	1.46	1.36
24	N	609	CHL	O2D-CGD	4.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	605	CHL	O2D-CGD	4.73	1.44	1.33
24	4	606	CHL	CHC-C1C	4.73	1.47	1.35
24	s	607	CHL	CHC-C1C	4.72	1.47	1.35
24	s	608	CHL	C2C-C3C	4.72	1.46	1.36
24	8	607	CHL	CHC-C1C	4.72	1.47	1.35
24	1	601	CHL	O2D-CGD	4.72	1.44	1.33
24	n	609	CHL	O2D-CGD	4.72	1.44	1.33
24	8	601	CHL	C2C-C3C	4.72	1.46	1.36
24	s	606	CHL	C3D-C4D	-4.72	1.33	1.44
24	3	609	CHL	O2D-CGD	4.72	1.44	1.33
24	4	607	CHL	CHC-C1C	4.71	1.47	1.35
24	1	607	CHL	O2D-CGD	4.71	1.44	1.33
24	N	608	CHL	CHC-C1C	4.71	1.47	1.35
24	S	607	CHL	CHC-C1C	4.71	1.47	1.35
24	y	601	CHL	O2D-CGD	4.70	1.44	1.33
24	5	607	CHL	O2D-CGD	4.70	1.44	1.33
24	7	607	CHL	O2D-CGD	4.70	1.44	1.33
24	y	609	CHL	O2D-CGD	4.69	1.44	1.33
24	n	608	CHL	CHC-C1C	4.69	1.47	1.35
24	2	609	CHL	CHC-C1C	4.69	1.47	1.35
24	1	608	CHL	O2D-CGD	4.69	1.44	1.33
24	5	601	CHL	O2D-CGD	4.68	1.44	1.33
24	3	607	CHL	O2D-CGD	4.68	1.44	1.33
24	Y	601	CHL	O2D-CGD	4.68	1.44	1.33
24	Y	609	CHL	O2D-CGD	4.68	1.44	1.33
24	G	606	CHL	CHC-C1C	4.68	1.47	1.35
24	g	606	CHL	CHC-C1C	4.68	1.47	1.35
24	1	606	CHL	CHC-C1C	4.66	1.46	1.35
24	6	609	CHL	CHC-C1C	4.66	1.46	1.35
24	5	606	CHL	CHC-C1C	4.66	1.46	1.35
24	y	607	CHL	CHC-C1C	4.66	1.46	1.35
24	Y	608	CHL	CHC-C1C	4.64	1.46	1.35
24	y	608	CHL	CHC-C1C	4.64	1.46	1.35
24	R	608	CHL	CHC-C1C	4.64	1.46	1.35
24	4	601	CHL	O2D-CGD	4.64	1.45	1.30
24	Y	607	CHL	CHC-C1C	4.64	1.46	1.35
24	8	601	CHL	O2D-CGD	4.64	1.45	1.30
24	4	601	CHL	CHD-C1D	4.64	1.47	1.38
24	s	607	CHL	C3B-C2B	4.63	1.46	1.40
24	y	607	CHL	O2D-CGD	4.63	1.44	1.33
24	5	605	CHL	CHC-C1C	4.62	1.46	1.35
24	Y	607	CHL	O2D-CGD	4.62	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	607	CHL	CHC-C1C	4.62	1.46	1.35
24	r	608	CHL	CHC-C1C	4.62	1.46	1.35
24	s	607	CHL	C3D-C4D	-4.62	1.33	1.44
24	Y	605	CHL	CHC-C1C	4.62	1.46	1.35
24	1	609	CHL	O2D-CGD	4.62	1.44	1.33
24	S	607	CHL	C3D-C4D	-4.61	1.33	1.44
24	y	605	CHL	CHC-C1C	4.61	1.46	1.35
24	8	601	CHL	CHD-C1D	4.61	1.47	1.38
24	2	605	CHL	C2C-C3C	4.61	1.46	1.36
24	N	607	CHL	CHC-C1C	4.61	1.46	1.35
24	R	608	CHL	O2D-CGD	4.61	1.44	1.33
24	R	614	CHL	C3B-C2B	4.60	1.46	1.40
24	1	605	CHL	CHC-C1C	4.60	1.46	1.35
24	3	609	CHL	CHC-C1C	4.60	1.46	1.35
24	6	605	CHL	C2C-C3C	4.60	1.46	1.36
24	y	601	CHL	CHC-C1C	4.60	1.46	1.35
24	3	609	CHL	C3B-C2B	4.60	1.46	1.40
24	G	605	CHL	C3B-C2B	4.60	1.46	1.40
24	r	614	CHL	C3B-C2B	4.60	1.46	1.40
24	2	605	CHL	C3B-C2B	4.60	1.46	1.40
24	7	609	CHL	CHC-C1C	4.60	1.46	1.35
24	S	607	CHL	C3B-C2B	4.59	1.46	1.40
24	g	605	CHL	C3B-C2B	4.59	1.46	1.40
24	5	609	CHL	O2D-CGD	4.59	1.44	1.33
24	N	601	CHL	CHC-C1C	4.59	1.46	1.35
24	r	608	CHL	O2D-CGD	4.59	1.44	1.33
24	S	601	CHL	O2A-CGA	4.58	1.46	1.30
24	Y	601	CHL	CHC-C1C	4.58	1.46	1.35
24	7	609	CHL	C3B-C2B	4.58	1.46	1.40
24	n	601	CHL	CHC-C1C	4.57	1.46	1.35
24	3	605	CHL	O2A-CGA	4.57	1.46	1.30
24	s	601	CHL	O2A-CGA	4.57	1.46	1.30
24	7	605	CHL	O2A-CGA	4.57	1.46	1.30
24	4	608	CHL	CHC-C1C	4.57	1.46	1.35
24	6	605	CHL	C3B-C2B	4.56	1.46	1.40
24	6	608	CHL	CHC-C1C	4.56	1.46	1.35
24	5	601	CHL	CHC-C1C	4.56	1.46	1.35
24	8	608	CHL	CHC-C1C	4.55	1.46	1.35
24	y	608	CHL	O2D-CGD	4.55	1.44	1.33
24	2	608	CHL	CHC-C1C	4.55	1.46	1.35
24	5	607	CHL	CHC-C1C	4.55	1.46	1.35
24	Y	608	CHL	O2D-CGD	4.55	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	601	CHL	CHC-C1C	4.54	1.46	1.35
24	1	607	CHL	CHC-C1C	4.53	1.46	1.35
24	s	606	CHL	O2A-CGA	4.53	1.46	1.30
24	3	608	CHL	C2C-C3C	4.53	1.46	1.36
24	G	605	CHL	O2A-CGA	4.53	1.46	1.30
24	6	608	CHL	C2C-C3C	4.53	1.46	1.36
24	g	605	CHL	O2A-CGA	4.52	1.46	1.30
24	S	606	CHL	O2A-CGA	4.52	1.45	1.30
24	2	608	CHL	C2C-C3C	4.52	1.46	1.36
24	8	609	CHL	CHC-C1C	4.51	1.46	1.35
24	7	608	CHL	C2C-C3C	4.51	1.46	1.36
24	5	601	CHL	O2A-CGA	4.51	1.45	1.30
24	6	608	CHL	O2A-CGA	4.50	1.45	1.30
24	2	608	CHL	O2A-CGA	4.50	1.45	1.30
24	n	601	CHL	C3B-C2B	4.50	1.46	1.40
24	6	605	CHL	O2A-CGA	4.50	1.45	1.30
24	2	606	CHL	O2A-CGA	4.50	1.45	1.30
24	G	608	CHL	C3B-C2B	4.50	1.46	1.40
24	2	605	CHL	O2A-CGA	4.50	1.45	1.30
24	4	609	CHL	CHC-C1C	4.50	1.46	1.35
24	3	605	CHL	CHC-C1C	4.49	1.46	1.35
24	S	608	CHL	O2A-CGA	4.49	1.45	1.30
24	8	601	CHL	O2A-CGA	4.49	1.45	1.30
24	g	608	CHL	C3B-C2B	4.49	1.46	1.40
24	6	607	CHL	C3B-C2B	4.49	1.46	1.40
24	7	605	CHL	CHC-C1C	4.49	1.46	1.35
24	1	609	CHL	CHD-C1D	4.49	1.47	1.38
24	4	601	CHL	O2A-CGA	4.49	1.45	1.30
24	1	601	CHL	O2A-CGA	4.49	1.45	1.30
24	3	609	CHL	C2C-C3C	4.49	1.46	1.36
24	s	608	CHL	O2A-CGA	4.48	1.45	1.30
24	6	606	CHL	O2A-CGA	4.48	1.45	1.30
24	6	601	CHL	O2A-CGA	4.48	1.45	1.30
24	7	609	CHL	C2C-C3C	4.48	1.46	1.36
24	N	606	CHL	O2A-CGA	4.48	1.46	1.33
24	n	606	CHL	O2A-CGA	4.47	1.46	1.33
24	4	606	CHL	C2C-C3C	4.47	1.46	1.36
24	2	606	CHL	CHC-C1C	4.47	1.46	1.35
24	8	609	CHL	O2A-CGA	4.47	1.45	1.30
24	5	606	CHL	O2A-CGA	4.47	1.45	1.30
24	8	607	CHL	O2A-CGA	4.46	1.45	1.30
25	g	613	CLA	C4D-ND	-4.46	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	601	CHL	O2A-CGA	4.46	1.45	1.30
24	6	606	CHL	CHC-C1C	4.46	1.46	1.35
24	2	607	CHL	C3B-C2B	4.46	1.46	1.40
24	4	607	CHL	O2A-CGA	4.46	1.45	1.30
24	8	606	CHL	C2C-C3C	4.46	1.46	1.36
24	4	609	CHL	O2A-CGA	4.46	1.45	1.30
24	5	609	CHL	CHD-C1D	4.46	1.47	1.38
24	1	606	CHL	O2A-CGA	4.46	1.45	1.30
24	2	606	CHL	C2C-C3C	4.45	1.46	1.36
24	s	606	CHL	C2C-C3C	4.45	1.46	1.36
24	6	607	CHL	C2C-C3C	4.45	1.46	1.36
24	r	606	CHL	C2C-C3C	4.45	1.46	1.36
25	G	613	CLA	C4D-ND	-4.45	1.31	1.37
24	4	607	CHL	C3B-C2B	4.45	1.46	1.40
24	1	608	CHL	O2A-CGA	4.45	1.45	1.30
24	7	608	CHL	O2A-CGA	4.45	1.45	1.30
24	3	606	CHL	O2A-CGA	4.44	1.45	1.30
24	S	606	CHL	C2C-C3C	4.44	1.46	1.36
24	N	606	CHL	CHC-C1C	4.44	1.46	1.35
24	3	608	CHL	O2A-CGA	4.44	1.45	1.30
24	N	601	CHL	C3B-C2B	4.44	1.46	1.40
24	2	607	CHL	C2C-C3C	4.44	1.46	1.36
24	1	609	CHL	CHC-C1C	4.44	1.46	1.35
24	n	606	CHL	CHC-C1C	4.44	1.46	1.35
24	7	606	CHL	O2A-CGA	4.44	1.45	1.30
24	2	601	CHL	C3B-C2B	4.44	1.46	1.40
24	6	606	CHL	C2C-C3C	4.44	1.46	1.36
24	5	609	CHL	CHC-C1C	4.43	1.46	1.35
24	3	609	CHL	O2A-CGA	4.43	1.46	1.33
24	5	608	CHL	O2A-CGA	4.43	1.45	1.30
24	5	605	CHL	C3B-C2B	4.42	1.46	1.40
24	6	601	CHL	CHC-C1C	4.42	1.46	1.35
24	2	601	CHL	CHC-C1C	4.42	1.46	1.35
24	G	601	CHL	CHC-C1C	4.42	1.46	1.35
24	7	609	CHL	O2A-CGA	4.42	1.46	1.33
24	6	601	CHL	C3B-C2B	4.42	1.46	1.40
24	R	606	CHL	C2C-C3C	4.42	1.46	1.36
24	1	605	CHL	O2A-CGA	4.41	1.45	1.30
24	g	601	CHL	CHC-C1C	4.41	1.46	1.35
24	5	605	CHL	O2A-CGA	4.41	1.45	1.30
24	1	605	CHL	C3B-C2B	4.41	1.46	1.40
24	s	607	CHL	O2A-CGA	4.40	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	607	CHL	O2A-CGA	4.40	1.46	1.33
24	8	607	CHL	C3B-C2B	4.40	1.46	1.40
24	3	609	CHL	CHD-C1D	4.39	1.46	1.38
24	7	605	CHL	C2C-C3C	4.39	1.46	1.36
24	7	609	CHL	CHD-C1D	4.38	1.46	1.38
24	2	607	CHL	CHD-C1D	4.38	1.46	1.38
24	4	606	CHL	O2A-CGA	4.38	1.45	1.30
24	7	605	CHL	C3B-C2B	4.37	1.46	1.40
24	8	606	CHL	O2A-CGA	4.37	1.45	1.30
24	3	605	CHL	C3B-C2B	4.37	1.46	1.40
24	6	607	CHL	CHD-C1D	4.37	1.46	1.38
24	3	605	CHL	C2C-C3C	4.36	1.46	1.36
24	N	609	CHL	O2A-CGA	4.36	1.46	1.33
24	n	609	CHL	O2A-CGA	4.35	1.46	1.33
24	5	609	CHL	C2C-C3C	4.34	1.46	1.36
24	1	605	CHL	C2C-C3C	4.34	1.46	1.36
24	1	609	CHL	C2C-C3C	4.34	1.46	1.36
24	8	608	CHL	O2A-CGA	4.34	1.45	1.30
25	N	613	CLA	C4D-ND	-4.33	1.31	1.37
24	4	608	CHL	O2A-CGA	4.33	1.45	1.30
25	n	613	CLA	C4D-ND	-4.33	1.31	1.37
24	1	606	CHL	C2C-C3C	4.33	1.46	1.36
24	r	614	CHL	C2C-C3C	4.32	1.46	1.36
24	5	605	CHL	C2C-C3C	4.32	1.46	1.36
24	7	607	CHL	O2A-CGA	4.32	1.46	1.33
24	R	614	CHL	C2C-C3C	4.32	1.46	1.36
24	G	605	CHL	C2C-C3C	4.31	1.46	1.36
24	N	605	CHL	CHD-C1D	4.31	1.46	1.38
24	N	601	CHL	O2A-CGA	4.31	1.45	1.33
24	n	605	CHL	CHD-C1D	4.31	1.46	1.38
24	n	601	CHL	O2A-CGA	4.31	1.45	1.33
24	3	607	CHL	O2A-CGA	4.31	1.45	1.33
24	g	605	CHL	C2C-C3C	4.30	1.46	1.36
24	R	614	CHL	CHD-C1D	4.30	1.46	1.38
24	Y	606	CHL	O2A-CGA	4.29	1.45	1.33
24	y	606	CHL	O2A-CGA	4.29	1.45	1.33
24	N	607	CHL	O2A-CGA	4.28	1.45	1.33
24	5	606	CHL	C2C-C3C	4.28	1.45	1.36
24	g	609	CHL	C2C-C3C	4.28	1.45	1.36
24	r	608	CHL	O2A-CGA	4.27	1.45	1.33
24	n	607	CHL	O2A-CGA	4.27	1.45	1.33
25	d	402	CLA	C4D-ND	-4.27	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	607	CHL	C3B-C2B	4.27	1.46	1.40
24	G	605	CHL	CHD-C1D	4.27	1.46	1.38
24	S	608	CHL	CHD-C1D	4.27	1.46	1.38
24	g	605	CHL	CHD-C1D	4.26	1.46	1.38
24	G	609	CHL	C2C-C3C	4.26	1.45	1.36
24	4	606	CHL	C3B-C2B	4.26	1.46	1.40
24	g	608	CHL	C2C-C3C	4.26	1.45	1.36
24	r	614	CHL	CHD-C1D	4.26	1.46	1.38
24	Y	609	CHL	CHC-C1C	4.26	1.45	1.35
24	y	609	CHL	CHC-C1C	4.26	1.45	1.35
24	s	607	CHL	C2C-C3C	4.25	1.45	1.36
24	G	608	CHL	C2C-C3C	4.25	1.45	1.36
24	s	608	CHL	CHD-C1D	4.24	1.46	1.38
24	2	601	CHL	C2C-C3C	4.24	1.45	1.36
24	S	607	CHL	C2C-C3C	4.24	1.45	1.36
24	R	608	CHL	O2A-CGA	4.24	1.45	1.33
24	R	607	CHL	C3B-C2B	4.24	1.46	1.40
24	1	607	CHL	O2A-CGA	4.24	1.45	1.33
24	5	608	CHL	C2C-C3C	4.24	1.45	1.36
24	5	609	CHL	O2A-CGA	4.24	1.45	1.33
24	R	606	CHL	O2A-CGA	4.23	1.45	1.33
25	D	402	CLA	C4D-ND	-4.23	1.31	1.37
24	r	606	CHL	O2A-CGA	4.23	1.45	1.33
24	N	605	CHL	O2A-CGA	4.23	1.45	1.33
24	1	608	CHL	C2C-C3C	4.23	1.45	1.36
24	y	609	CHL	O2A-CGA	4.23	1.45	1.33
24	n	605	CHL	O2A-CGA	4.23	1.45	1.33
24	1	609	CHL	O2A-CGA	4.22	1.45	1.33
24	Y	609	CHL	O2A-CGA	4.22	1.45	1.33
24	6	609	CHL	O2A-CGA	4.22	1.45	1.33
24	2	609	CHL	C3B-C2B	4.22	1.46	1.40
24	S	601	CHL	C2C-C3C	4.22	1.45	1.36
24	S	606	CHL	CHD-C1D	4.22	1.46	1.38
24	g	608	CHL	O2A-CGA	4.21	1.45	1.33
24	s	606	CHL	CHD-C1D	4.21	1.46	1.38
24	g	609	CHL	O2A-CGA	4.21	1.45	1.33
24	6	601	CHL	C2C-C3C	4.21	1.45	1.36
24	G	608	CHL	O2A-CGA	4.21	1.45	1.33
24	G	609	CHL	CHD-C1D	4.21	1.46	1.38
24	s	601	CHL	C2C-C3C	4.21	1.45	1.36
24	2	609	CHL	O2A-CGA	4.20	1.45	1.33
24	5	607	CHL	O2A-CGA	4.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	607	CHL	C2C-C3C	4.20	1.45	1.36
24	8	606	CHL	C3B-C2B	4.20	1.46	1.40
24	r	607	CHL	C2C-C3C	4.20	1.45	1.36
24	N	609	CHL	CHD-C1D	4.20	1.46	1.38
24	g	609	CHL	CHD-C1D	4.20	1.46	1.38
24	4	607	CHL	C2C-C3C	4.20	1.45	1.36
24	G	609	CHL	O2A-CGA	4.20	1.45	1.33
24	5	607	CHL	C2C-C3C	4.19	1.45	1.36
24	1	607	CHL	C2C-C3C	4.19	1.45	1.36
24	s	601	CHL	CHD-C1D	4.19	1.46	1.38
24	7	606	CHL	C2C-C3C	4.19	1.45	1.36
24	5	601	CHL	C3B-C2B	4.18	1.46	1.40
24	8	607	CHL	C2C-C3C	4.18	1.45	1.36
24	n	605	CHL	C2C-C3C	4.18	1.45	1.36
24	3	601	CHL	O2A-CGA	4.18	1.45	1.33
24	N	605	CHL	C2C-C3C	4.18	1.45	1.36
24	Y	609	CHL	CHD-C1D	4.18	1.46	1.38
24	n	609	CHL	CHD-C1D	4.18	1.46	1.38
24	y	609	CHL	CHD-C1D	4.17	1.46	1.38
24	g	606	CHL	O2A-CGA	4.17	1.45	1.33
24	Y	605	CHL	O2A-CGA	4.17	1.45	1.33
24	3	606	CHL	C2C-C3C	4.17	1.45	1.36
24	G	606	CHL	O2A-CGA	4.17	1.45	1.33
24	y	605	CHL	O2A-CGA	4.16	1.45	1.33
24	S	601	CHL	CHD-C1D	4.16	1.46	1.38
24	7	601	CHL	O2A-CGA	4.16	1.45	1.33
24	6	609	CHL	C3B-C2B	4.16	1.46	1.40
24	G	606	CHL	C3B-C2B	4.15	1.46	1.40
24	6	606	CHL	CHD-C1D	4.15	1.46	1.38
24	3	606	CHL	CHD-C1D	4.14	1.46	1.38
24	2	606	CHL	CHD-C1D	4.14	1.46	1.38
24	8	607	CHL	CHD-C1D	4.14	1.46	1.38
24	G	606	CHL	C2C-C3C	4.14	1.45	1.36
24	7	606	CHL	CHD-C1D	4.14	1.46	1.38
24	1	601	CHL	C3B-C2B	4.13	1.46	1.40
24	4	607	CHL	CHD-C1D	4.13	1.46	1.38
24	4	608	CHL	C3B-C2B	4.13	1.46	1.40
24	r	607	CHL	O2A-CGA	4.13	1.45	1.33
24	8	608	CHL	C3B-C2B	4.13	1.46	1.40
24	g	609	CHL	CHC-C1C	4.13	1.45	1.35
24	g	606	CHL	C2C-C3C	4.13	1.45	1.36
24	y	606	CHL	CHC-C1C	4.13	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	609	CHL	CHC-C1C	4.13	1.45	1.35
24	R	607	CHL	O2A-CGA	4.12	1.45	1.33
24	4	609	CHL	C2C-C3C	4.12	1.45	1.36
25	R	613	CLA	C1D-ND	4.12	1.42	1.37
25	r	613	CLA	C1D-ND	4.11	1.42	1.37
24	2	608	CHL	C3B-C2B	4.11	1.46	1.40
24	n	607	CHL	C2C-C3C	4.11	1.45	1.36
24	g	606	CHL	C3B-C2B	4.11	1.46	1.40
24	6	607	CHL	O2A-CGA	4.11	1.45	1.33
24	Y	606	CHL	CHC-C1C	4.10	1.45	1.35
24	N	601	CHL	C2C-C3C	4.10	1.45	1.36
24	R	614	CHL	C3A-C2A	-4.10	1.50	1.54
24	2	607	CHL	O2A-CGA	4.10	1.45	1.33
24	6	608	CHL	C3B-C2B	4.10	1.46	1.40
24	8	609	CHL	C2C-C3C	4.09	1.45	1.36
25	B	612	CLA	CMC-C2C	-4.09	1.42	1.50
25	b	612	CLA	CMC-C2C	-4.09	1.42	1.50
24	N	607	CHL	C2C-C3C	4.09	1.45	1.36
24	Y	607	CHL	C2C-C3C	4.09	1.45	1.36
24	S	607	CHL	CHD-C1D	4.09	1.46	1.38
24	r	614	CHL	C3A-C2A	-4.08	1.50	1.54
24	g	601	CHL	O2A-CGA	4.08	1.45	1.33
24	y	607	CHL	C2C-C3C	4.07	1.45	1.36
24	n	601	CHL	C2C-C3C	4.07	1.45	1.36
24	3	607	CHL	C3B-C2B	4.07	1.46	1.40
24	s	607	CHL	CHD-C1D	4.07	1.46	1.38
24	y	608	CHL	O2A-CGA	4.06	1.45	1.33
24	Y	608	CHL	O2A-CGA	4.06	1.45	1.33
24	1	601	CHL	C2C-C3C	4.06	1.45	1.36
24	G	607	CHL	O2A-CGA	4.06	1.45	1.33
24	N	608	CHL	O2A-CGA	4.06	1.45	1.33
24	r	607	CHL	CHD-C1D	4.06	1.46	1.38
24	G	601	CHL	O2A-CGA	4.06	1.45	1.33
24	Y	605	CHL	C2C-C3C	4.05	1.45	1.36
24	4	601	CHL	CHD-C4C	4.05	1.48	1.39
25	B	614	CLA	C4D-ND	-4.05	1.32	1.37
24	1	607	CHL	CHD-C1D	4.05	1.46	1.38
24	R	607	CHL	CHD-C1D	4.05	1.46	1.38
24	5	601	CHL	C2C-C3C	4.05	1.45	1.36
24	y	605	CHL	C2C-C3C	4.04	1.45	1.36
24	8	601	CHL	CHD-C4C	4.04	1.48	1.39
24	7	607	CHL	C3B-C2B	4.04	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	609	CLA	C1D-ND	4.04	1.42	1.37
24	n	608	CHL	O2A-CGA	4.04	1.45	1.33
25	S	609	CLA	C1D-ND	4.04	1.42	1.37
24	g	607	CHL	O2A-CGA	4.04	1.45	1.33
24	n	609	CHL	C2C-C3C	4.03	1.45	1.36
24	5	607	CHL	CHD-C1D	4.03	1.46	1.38
24	N	609	CHL	C2C-C3C	4.03	1.45	1.36
24	y	605	CHL	CHD-C1D	4.03	1.46	1.38
24	Y	605	CHL	CHD-C1D	4.03	1.46	1.38
24	y	608	CHL	C2C-C3C	4.03	1.45	1.36
24	Y	608	CHL	C2C-C3C	4.02	1.45	1.36
24	3	606	CHL	C3B-C2B	4.02	1.45	1.40
25	r	611	CLA	C4D-ND	-4.01	1.32	1.37
24	7	606	CHL	C3B-C2B	4.01	1.45	1.40
24	n	608	CHL	C2C-C3C	4.01	1.45	1.36
24	4	606	CHL	CHD-C1D	4.00	1.46	1.38
25	1	602	CLA	C4D-ND	-4.00	1.32	1.37
24	N	608	CHL	C2C-C3C	4.00	1.45	1.36
25	b	614	CLA	C4D-ND	-4.00	1.32	1.37
24	Y	605	CHL	C3B-C2B	4.00	1.45	1.40
25	R	611	CLA	C4D-ND	-4.00	1.32	1.37
25	5	602	CLA	C4D-ND	-4.00	1.32	1.37
24	n	605	CHL	C3B-C2B	4.00	1.45	1.40
25	b	611	CLA	C4D-ND	-3.99	1.32	1.37
24	r	608	CHL	C3B-C2B	3.99	1.45	1.40
25	a	405	CLA	C4D-ND	-3.99	1.32	1.37
24	Y	607	CHL	O2A-CGA	3.99	1.45	1.33
24	R	608	CHL	C3B-C2B	3.99	1.45	1.40
24	Y	601	CHL	O2A-CGA	3.99	1.45	1.33
24	y	605	CHL	C3B-C2B	3.99	1.45	1.40
24	2	609	CHL	C2C-C3C	3.99	1.45	1.36
24	6	609	CHL	C2C-C3C	3.98	1.45	1.36
24	s	601	CHL	C3B-C2B	3.98	1.45	1.40
24	7	608	CHL	C3B-C2B	3.98	1.45	1.40
24	2	609	CHL	CHD-C1D	3.98	1.46	1.38
25	A	405	CLA	C4D-ND	-3.98	1.32	1.37
24	y	601	CHL	O2A-CGA	3.98	1.45	1.33
24	g	606	CHL	CHD-C1D	3.97	1.46	1.38
24	y	607	CHL	O2A-CGA	3.97	1.45	1.33
25	B	611	CLA	C4D-ND	-3.97	1.32	1.37
24	8	606	CHL	CHD-C1D	3.97	1.46	1.38
24	G	606	CHL	CHD-C1D	3.97	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	607	CHL	C2C-C3C	3.96	1.45	1.36
25	s	604	CLA	C1D-ND	3.96	1.42	1.37
24	Y	609	CHL	C2C-C3C	3.96	1.45	1.36
24	6	609	CHL	CHD-C1D	3.96	1.46	1.38
39	F	101	HEM	C3C-CAC	3.95	1.55	1.47
24	7	607	CHL	C2C-C3C	3.95	1.45	1.36
24	G	601	CHL	C3B-C2B	3.95	1.45	1.40
39	f	101	HEM	C3C-CAC	3.95	1.55	1.47
25	7	603	CLA	C4D-ND	-3.95	1.32	1.37
25	r	602	CLA	C4D-ND	-3.95	1.32	1.37
25	R	602	CLA	C4D-ND	-3.95	1.32	1.37
24	3	607	CHL	C2C-C3C	3.95	1.45	1.36
25	Y	602	CLA	C4D-ND	-3.94	1.32	1.37
25	y	604	CLA	CMB-C2B	-3.94	1.43	1.51
24	G	607	CHL	C2C-C3C	3.94	1.45	1.36
24	N	605	CHL	C3B-C2B	3.94	1.45	1.40
24	S	601	CHL	C3B-C2B	3.94	1.45	1.40
24	g	601	CHL	C3B-C2B	3.94	1.45	1.40
24	y	609	CHL	C2C-C3C	3.94	1.45	1.36
25	b	606	CLA	C4D-ND	-3.93	1.32	1.37
25	8	610	CLA	C4D-ND	-3.93	1.32	1.37
24	3	608	CHL	C3B-C2B	3.93	1.45	1.40
24	3	607	CHL	CHD-C1D	3.93	1.46	1.38
24	5	606	CHL	C3B-C2B	3.93	1.45	1.40
25	B	606	CLA	C4D-ND	-3.93	1.32	1.37
25	1	604	CLA	C4D-ND	-3.93	1.32	1.37
25	5	611	CLA	C4D-ND	-3.93	1.32	1.37
25	4	610	CLA	C4D-ND	-3.93	1.32	1.37
25	Y	604	CLA	CMB-C2B	-3.92	1.43	1.51
25	y	602	CLA	C4D-ND	-3.92	1.32	1.37
24	2	605	CHL	CHD-C1D	3.92	1.46	1.38
24	R	606	CHL	CHD-C1D	3.92	1.46	1.38
25	B	613	CLA	C4D-ND	-3.92	1.32	1.37
24	7	607	CHL	CHD-C1D	3.91	1.46	1.38
24	N	607	CHL	C3B-C2B	3.91	1.45	1.40
25	3	603	CLA	C4D-ND	-3.91	1.32	1.37
24	1	606	CHL	C3B-C2B	3.91	1.45	1.40
24	6	605	CHL	CHD-C1D	3.91	1.46	1.38
25	6	602	CLA	C4D-ND	-3.91	1.32	1.37
24	r	606	CHL	CHD-C1D	3.91	1.46	1.38
25	1	611	CLA	C4D-ND	-3.90	1.32	1.37
25	b	613	CLA	C4D-ND	-3.90	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	604	CLA	C4D-ND	-3.90	1.32	1.37
24	n	609	CHL	CHC-C1C	3.90	1.45	1.35
25	2	602	CLA	C4D-ND	-3.89	1.32	1.37
24	r	606	CHL	C3B-C2B	3.89	1.45	1.40
24	7	601	CHL	C3B-C2B	3.89	1.45	1.40
24	R	606	CHL	C3B-C2B	3.88	1.45	1.40
24	N	609	CHL	CHC-C1C	3.88	1.44	1.35
24	n	601	CHL	CHD-C4C	3.88	1.48	1.39
25	S	604	CLA	C1D-ND	3.88	1.42	1.37
25	s	603	CLA	C1D-ND	3.87	1.42	1.37
24	1	609	CHL	C3B-C2B	3.87	1.45	1.40
24	6	606	CHL	C3B-C2B	3.87	1.45	1.40
24	5	609	CHL	CHD-C4C	3.86	1.48	1.39
25	b	608	CLA	C4D-ND	-3.86	1.32	1.37
24	1	601	CHL	CHD-C1D	3.86	1.45	1.38
25	r	609	CLA	C4D-ND	-3.86	1.32	1.37
24	1	609	CHL	CHD-C4C	3.86	1.48	1.39
24	5	601	CHL	CHD-C1D	3.86	1.45	1.38
25	D	403	CLA	C4D-ND	-3.86	1.32	1.37
24	Y	608	CHL	C3B-C2B	3.85	1.45	1.40
24	n	607	CHL	C3B-C2B	3.85	1.45	1.40
24	N	601	CHL	CHD-C4C	3.85	1.48	1.39
24	4	609	CHL	CHD-C1D	3.85	1.45	1.38
24	y	608	CHL	C3B-C2B	3.85	1.45	1.40
24	7	605	CHL	CHD-C1D	3.85	1.45	1.38
24	r	614	CHL	CHD-C4C	3.85	1.48	1.39
25	Y	610	CLA	C4D-ND	-3.84	1.32	1.37
25	B	608	CLA	C4D-ND	-3.84	1.32	1.37
25	S	603	CLA	C1D-ND	3.84	1.42	1.37
24	1	605	CHL	CHD-C1D	3.84	1.45	1.38
25	7	602	CLA	C4D-ND	-3.84	1.32	1.37
24	3	605	CHL	CHD-C1D	3.84	1.45	1.38
25	7	614	CLA	C1D-ND	3.84	1.42	1.37
25	R	609	CLA	C4D-ND	-3.83	1.32	1.37
24	3	601	CHL	C3B-C2B	3.83	1.45	1.40
24	5	609	CHL	C3B-C2B	3.83	1.45	1.40
25	1	603	CLA	C4D-ND	-3.83	1.32	1.37
24	2	601	CHL	CHD-C1D	3.83	1.45	1.38
25	7	611	CLA	C4D-ND	-3.83	1.32	1.37
24	4	608	CHL	C2C-C3C	3.83	1.45	1.36
25	S	610	CLA	C1D-ND	3.82	1.42	1.37
25	s	610	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	606	CHL	C3B-C2B	3.82	1.45	1.40
25	3	614	CLA	C1D-ND	3.82	1.42	1.37
25	3	602	CLA	C4D-ND	-3.82	1.32	1.37
24	R	614	CHL	CHD-C4C	3.81	1.47	1.39
24	Y	601	CHL	C3B-C2B	3.81	1.45	1.40
24	y	601	CHL	C3B-C2B	3.81	1.45	1.40
24	2	608	CHL	CHD-C1D	3.80	1.45	1.38
24	7	609	CHL	CHD-C4C	3.80	1.47	1.39
25	5	603	CLA	C4D-ND	-3.80	1.32	1.37
24	g	608	CHL	CHD-C1D	3.80	1.45	1.38
25	g	602	CLA	C4D-ND	-3.80	1.32	1.37
24	6	601	CHL	CHD-C1D	3.80	1.45	1.38
25	B	603	CLA	C4D-ND	-3.80	1.32	1.37
25	y	610	CLA	C4D-ND	-3.80	1.32	1.37
24	8	609	CHL	CHD-C1D	3.79	1.45	1.38
24	Y	609	CHL	C3B-C2B	3.79	1.45	1.40
24	5	605	CHL	CHD-C1D	3.79	1.45	1.38
24	4	607	CHL	CHD-C4C	3.79	1.47	1.39
24	n	601	CHL	CHD-C1D	3.79	1.45	1.38
24	g	601	CHL	CHD-C1D	3.79	1.45	1.38
24	G	608	CHL	CHD-C1D	3.79	1.45	1.38
25	3	611	CLA	C4D-ND	-3.79	1.32	1.37
24	8	608	CHL	C2C-C3C	3.79	1.44	1.36
25	s	602	CLA	C1D-ND	3.79	1.42	1.37
25	b	603	CLA	C4D-ND	-3.79	1.32	1.37
25	d	403	CLA	C4D-ND	-3.78	1.32	1.37
24	N	601	CHL	CHD-C1D	3.78	1.45	1.38
24	r	614	CHL	OBD-CAD	3.78	1.29	1.22
24	6	608	CHL	CHD-C1D	3.78	1.45	1.38
24	7	601	CHL	C2C-C3C	3.78	1.44	1.36
24	S	608	CHL	CHD-C4C	3.78	1.47	1.39
24	s	608	CHL	CHD-C4C	3.78	1.47	1.39
24	4	609	CHL	C3B-C2B	3.78	1.45	1.40
24	N	606	CHL	CHD-C1D	3.78	1.45	1.38
24	y	609	CHL	C3B-C2B	3.78	1.45	1.40
24	G	601	CHL	CHD-C1D	3.78	1.45	1.38
24	g	607	CHL	C3B-C2B	3.78	1.45	1.40
25	N	604	CLA	CMB-C2B	-3.77	1.43	1.51
24	G	609	CHL	C3B-C2B	3.77	1.45	1.40
25	G	602	CLA	C4D-ND	-3.77	1.32	1.37
24	G	607	CHL	C3B-C2B	3.77	1.45	1.40
24	3	609	CHL	CHD-C4C	3.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	607	CHL	CHD-C4C	3.77	1.47	1.39
25	8	604	CLA	C4D-ND	-3.77	1.32	1.37
24	s	607	CHL	OBD-CAD	3.77	1.29	1.22
25	B	604	CLA	C4D-ND	-3.76	1.32	1.37
25	g	614	CLA	C4D-ND	-3.76	1.32	1.37
25	Y	614	CLA	C4D-ND	-3.76	1.32	1.37
24	8	609	CHL	C3B-C2B	3.76	1.45	1.40
24	3	601	CHL	C2C-C3C	3.76	1.44	1.36
25	n	604	CLA	CMB-C2B	-3.76	1.43	1.51
25	b	604	CLA	C4D-ND	-3.76	1.32	1.37
24	n	605	CHL	OBD-CAD	3.76	1.29	1.22
25	y	614	CLA	C4D-ND	-3.75	1.32	1.37
24	2	607	CHL	CHD-C4C	3.75	1.47	1.39
24	n	606	CHL	CHD-C1D	3.75	1.45	1.38
24	R	614	CHL	OBD-CAD	3.75	1.28	1.22
24	N	605	CHL	OBD-CAD	3.75	1.28	1.22
24	S	607	CHL	OBD-CAD	3.75	1.28	1.22
25	4	604	CLA	C4D-ND	-3.74	1.32	1.37
25	r	613	CLA	C3B-C2B	-3.74	1.35	1.40
24	N	608	CHL	C3B-C2B	3.74	1.45	1.40
24	6	607	CHL	CHD-C4C	3.74	1.47	1.39
25	y	612	CLA	C4D-ND	-3.74	1.32	1.37
24	n	608	CHL	C3B-C2B	3.74	1.45	1.40
24	g	601	CHL	CHD-C4C	3.74	1.47	1.39
24	g	609	CHL	C3B-C2B	3.74	1.45	1.40
24	n	606	CHL	C3B-C2B	3.73	1.45	1.40
24	g	601	CHL	C2C-C3C	3.73	1.44	1.36
25	G	614	CLA	C4D-ND	-3.73	1.32	1.37
25	B	607	CLA	C4D-ND	-3.73	1.32	1.37
25	A	406	CLA	C4D-ND	-3.73	1.32	1.37
25	3	613	CLA	C4D-ND	-3.72	1.32	1.37
24	G	601	CHL	CHD-C4C	3.72	1.47	1.39
24	G	601	CHL	C2C-C3C	3.72	1.44	1.36
25	Y	612	CLA	C4D-ND	-3.72	1.32	1.37
25	n	602	CLA	C4D-ND	-3.72	1.32	1.37
25	R	613	CLA	C3B-C2B	-3.72	1.35	1.40
25	7	613	CLA	C4D-ND	-3.72	1.32	1.37
25	c	511	CLA	C1D-ND	3.72	1.42	1.37
24	S	601	CHL	CHD-C4C	3.72	1.47	1.39
25	a	406	CLA	C4D-ND	-3.71	1.32	1.37
25	R	603	CLA	C4D-ND	-3.71	1.32	1.37
24	s	601	CHL	CHD-C4C	3.71	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	C1D-ND	3.71	1.42	1.37
25	7	611	CLA	CMB-C2B	-3.71	1.43	1.51
25	c	507	CLA	C1D-ND	3.71	1.42	1.37
24	N	606	CHL	C3B-C2B	3.71	1.45	1.40
25	b	607	CLA	C4D-ND	-3.71	1.32	1.37
25	N	602	CLA	C4D-ND	-3.70	1.32	1.37
25	C	513	CLA	C1D-ND	3.70	1.42	1.37
25	3	604	CLA	C4D-ND	-3.70	1.32	1.37
25	S	602	CLA	C1D-ND	3.70	1.42	1.37
25	Y	604	CLA	C4D-ND	-3.70	1.32	1.37
25	C	507	CLA	C1D-ND	3.70	1.42	1.37
25	C	503	CLA	C1D-ND	3.70	1.42	1.37
25	3	611	CLA	CMB-C2B	-3.70	1.43	1.51
25	4	602	CLA	C4D-ND	-3.70	1.32	1.37
25	c	504	CLA	C1D-ND	3.69	1.42	1.37
24	y	606	CHL	C2C-C3C	3.68	1.44	1.36
25	c	502	CLA	C1D-ND	3.68	1.42	1.37
25	y	604	CLA	C4D-ND	-3.68	1.32	1.37
24	5	606	CHL	CHD-C1D	3.68	1.45	1.38
25	c	503	CLA	C1D-ND	3.68	1.42	1.37
24	g	607	CHL	CHD-C1D	3.68	1.45	1.38
25	C	508	CLA	C1D-ND	3.67	1.42	1.37
25	c	508	CLA	C1D-ND	3.67	1.42	1.37
24	Y	606	CHL	C2C-C3C	3.67	1.44	1.36
25	r	603	CLA	C4D-ND	-3.67	1.32	1.37
25	1	614	CLA	C4D-ND	-3.67	1.32	1.37
25	5	614	CLA	C4D-ND	-3.67	1.32	1.37
24	y	607	CHL	C3B-C2B	3.67	1.45	1.40
24	R	607	CHL	CHD-C4C	3.67	1.47	1.39
25	c	513	CLA	C1D-ND	3.67	1.42	1.37
25	G	604	CLA	CMB-C2B	-3.67	1.44	1.51
25	8	602	CLA	C4D-ND	-3.67	1.32	1.37
25	A	407	CLA	C4D-ND	-3.66	1.32	1.37
24	G	607	CHL	CHD-C1D	3.66	1.45	1.38
24	N	606	CHL	C2C-C3C	3.66	1.44	1.36
25	7	604	CLA	C4D-ND	-3.66	1.32	1.37
25	r	604	CLA	C4D-ND	-3.66	1.32	1.37
25	a	407	CLA	C4D-ND	-3.66	1.32	1.37
24	n	606	CHL	C2C-C3C	3.66	1.44	1.36
25	g	604	CLA	CMB-C2B	-3.66	1.44	1.51
24	Y	607	CHL	C3B-C2B	3.65	1.45	1.40
24	1	601	CHL	CHD-C4C	3.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	504	CLA	C1D-ND	3.65	1.42	1.37
24	r	607	CHL	CHD-C4C	3.65	1.47	1.39
25	c	506	CLA	C1D-ND	3.65	1.42	1.37
24	s	606	CHL	CHD-C4C	3.64	1.47	1.39
24	y	606	CHL	C3B-C2B	3.64	1.45	1.40
24	S	606	CHL	CHD-C4C	3.64	1.47	1.39
25	y	611	CLA	C4D-ND	-3.64	1.32	1.37
25	s	611	CLA	C1D-ND	3.64	1.42	1.37
25	S	611	CLA	C1D-ND	3.64	1.42	1.37
25	3	611	CLA	C3B-C2B	-3.64	1.35	1.40
24	r	608	CHL	C2C-C3C	3.64	1.44	1.36
24	5	601	CHL	CHD-C4C	3.64	1.47	1.39
24	1	606	CHL	CHD-C1D	3.63	1.45	1.38
24	R	608	CHL	C2C-C3C	3.63	1.44	1.36
25	R	604	CLA	C4D-ND	-3.63	1.32	1.37
24	6	605	CHL	CHD-C4C	3.63	1.47	1.39
25	6	614	CLA	C4D-ND	-3.62	1.32	1.37
24	2	605	CHL	CHD-C4C	3.62	1.47	1.39
24	R	607	CHL	OBD-CAD	3.62	1.28	1.22
24	N	605	CHL	CHD-C4C	3.62	1.47	1.39
24	Y	606	CHL	C3B-C2B	3.62	1.45	1.40
25	7	611	CLA	C3B-C2B	-3.62	1.35	1.40
25	Y	611	CLA	C4D-ND	-3.62	1.32	1.37
24	g	605	CHL	CHD-C4C	3.62	1.47	1.39
25	C	502	CLA	C1D-ND	3.62	1.42	1.37
25	N	603	CLA	C4D-ND	-3.62	1.32	1.37
25	2	603	CLA	C4D-ND	-3.62	1.32	1.37
25	6	603	CLA	C4D-ND	-3.62	1.32	1.37
24	r	607	CHL	OBD-CAD	3.61	1.28	1.22
25	C	506	CLA	C1D-ND	3.61	1.42	1.37
24	G	605	CHL	CHD-C4C	3.61	1.47	1.39
25	B	609	CLA	C4D-ND	-3.61	1.32	1.37
24	y	601	CHL	CHD-C4C	3.61	1.47	1.39
25	g	604	CLA	C4D-ND	-3.61	1.32	1.37
25	n	603	CLA	C4D-ND	-3.61	1.32	1.37
24	Y	601	CHL	C2C-C3C	3.61	1.44	1.36
24	n	605	CHL	CHD-C4C	3.61	1.47	1.39
24	y	601	CHL	C2C-C3C	3.60	1.44	1.36
25	a	410	CLA	C4D-ND	-3.60	1.32	1.37
24	4	601	CHL	OBD-CAD	3.60	1.28	1.22
25	y	603	CLA	C4D-ND	-3.60	1.32	1.37
25	5	610	CLA	C4D-ND	-3.60	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	601	CHL	CHD-C4C	3.60	1.47	1.39
25	4	611	CLA	C4D-ND	-3.59	1.32	1.37
24	1	608	CHL	CHD-C1D	3.59	1.45	1.38
25	1	610	CLA	C4D-ND	-3.59	1.32	1.37
25	G	611	CLA	C4D-ND	-3.59	1.32	1.37
24	6	601	CHL	CHD-C4C	3.59	1.47	1.39
24	2	601	CHL	CHD-C4C	3.59	1.47	1.39
24	S	607	CHL	CHD-C4C	3.59	1.47	1.39
25	1	613	CLA	C4D-ND	-3.58	1.32	1.37
24	6	605	CHL	OBD-CAD	3.58	1.28	1.22
25	g	611	CLA	C4D-ND	-3.58	1.32	1.37
25	b	604	CLA	CMB-C2B	-3.58	1.44	1.51
25	2	614	CLA	C4D-ND	-3.58	1.32	1.37
24	g	609	CHL	CHD-C4C	3.58	1.47	1.39
25	b	609	CLA	C4D-ND	-3.58	1.32	1.37
24	n	608	CHL	CHD-C1D	3.58	1.45	1.38
25	A	410	CLA	C4D-ND	-3.58	1.32	1.37
24	2	609	CHL	CHD-C4C	3.57	1.47	1.39
24	5	608	CHL	CHD-C1D	3.57	1.45	1.38
24	s	607	CHL	CHD-C4C	3.57	1.47	1.39
25	G	604	CLA	C4D-ND	-3.57	1.32	1.37
24	G	606	CHL	CHD-C4C	3.57	1.47	1.39
25	B	604	CLA	CMB-C2B	-3.57	1.44	1.51
24	6	609	CHL	CHD-C4C	3.57	1.47	1.39
24	N	608	CHL	CHD-C1D	3.57	1.45	1.38
24	7	606	CHL	CHD-C4C	3.56	1.47	1.39
37	h	102	DGD	O5D-C6D	-3.56	1.37	1.43
24	G	605	CHL	OBD-CAD	3.56	1.28	1.22
24	8	601	CHL	OBD-CAD	3.56	1.28	1.22
37	H	102	DGD	O5D-C6D	-3.56	1.37	1.43
24	g	605	CHL	OBD-CAD	3.56	1.28	1.22
24	2	605	CHL	OBD-CAD	3.55	1.28	1.22
25	g	603	CLA	C4D-ND	-3.55	1.32	1.37
24	n	609	CHL	CHD-C4C	3.55	1.47	1.39
25	b	610	CLA	C4D-ND	-3.55	1.32	1.37
24	G	609	CHL	CHD-C4C	3.55	1.47	1.39
25	8	611	CLA	C4D-ND	-3.55	1.32	1.37
24	n	609	CHL	C3B-C2B	3.55	1.45	1.40
25	5	613	CLA	C4D-ND	-3.55	1.32	1.37
24	1	607	CHL	C3B-C2B	3.54	1.45	1.40
24	3	601	CHL	CHD-C1D	3.54	1.45	1.38
25	G	603	CLA	C4D-ND	-3.54	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	604	CLA	C1D-ND	3.54	1.42	1.37
24	g	606	CHL	CHD-C4C	3.53	1.47	1.39
24	5	607	CHL	C3B-C2B	3.53	1.45	1.40
25	Y	603	CLA	C4D-ND	-3.53	1.32	1.37
25	6	611	CLA	C4D-ND	-3.53	1.32	1.37
24	N	609	CHL	CHD-C4C	3.53	1.47	1.39
24	S	606	CHL	OBD-CAD	3.53	1.28	1.22
24	7	601	CHL	CHD-C1D	3.53	1.45	1.38
25	2	611	CLA	C4D-ND	-3.52	1.32	1.37
24	s	606	CHL	OBD-CAD	3.52	1.28	1.22
24	n	607	CHL	CHD-C1D	3.52	1.45	1.38
24	N	609	CHL	C3B-C2B	3.52	1.45	1.40
25	c	505	CLA	C1D-ND	3.52	1.42	1.37
24	1	609	CHL	MG-NA	-3.52	1.97	2.06
25	7	610	CLA	C4D-ND	-3.51	1.32	1.37
24	3	606	CHL	CHD-C4C	3.51	1.47	1.39
29	d	409	LHG	O7-C5	-3.51	1.37	1.46
25	1	604	CLA	CMB-C2B	-3.51	1.44	1.51
25	5	604	CLA	CMB-C2B	-3.51	1.44	1.51
25	s	613	CLA	C1D-ND	3.51	1.42	1.37
24	N	607	CHL	CHD-C1D	3.51	1.45	1.38
24	5	607	CHL	CHD-C4C	3.51	1.47	1.39
25	3	612	CLA	C4D-ND	-3.50	1.32	1.37
25	b	616	CLA	C4D-ND	-3.50	1.32	1.37
24	5	609	CHL	MG-NA	-3.50	1.98	2.06
25	B	617	CLA	C4D-ND	-3.50	1.32	1.37
24	y	607	CHL	CHD-C1D	3.50	1.45	1.38
24	8	608	CHL	CHD-C1D	3.50	1.45	1.38
24	1	607	CHL	CHD-C4C	3.49	1.47	1.39
24	5	605	CHL	CHD-C4C	3.49	1.47	1.39
39	F	101	HEM	C3C-C2C	-3.49	1.35	1.40
25	7	612	CLA	C4D-ND	-3.49	1.32	1.37
25	C	505	CLA	C1D-ND	3.49	1.42	1.37
25	n	604	CLA	C4D-ND	-3.49	1.32	1.37
29	D	409	LHG	O7-C5	-3.49	1.37	1.46
24	G	607	CHL	OBD-CAD	3.49	1.28	1.22
25	B	610	CLA	C4D-ND	-3.49	1.32	1.37
25	r	610	CLA	C4D-ND	-3.49	1.32	1.37
25	3	610	CLA	C4D-ND	-3.49	1.32	1.37
25	2	604	CLA	C1D-ND	3.49	1.42	1.37
24	4	608	CHL	CHD-C1D	3.48	1.45	1.38
39	f	101	HEM	C3C-C2C	-3.48	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	605	CHL	CHD-C4C	3.48	1.47	1.39
25	R	610	CLA	C4D-ND	-3.48	1.32	1.37
24	1	605	CHL	CHD-C4C	3.48	1.47	1.39
25	1	604	CLA	C3B-C2B	-3.48	1.35	1.40
24	g	607	CHL	OBD-CAD	3.48	1.28	1.22
25	5	612	CLA	C1D-ND	3.47	1.42	1.37
24	Y	607	CHL	CHD-C1D	3.47	1.45	1.38
25	N	611	CLA	C4D-ND	-3.47	1.32	1.37
24	7	605	CHL	CHD-C4C	3.47	1.47	1.39
25	Y	603	CLA	C3B-C2B	-3.47	1.35	1.40
25	y	603	CLA	C3B-C2B	-3.47	1.35	1.40
25	B	616	CLA	C4D-ND	-3.47	1.32	1.37
25	n	611	CLA	C4D-ND	-3.47	1.32	1.37
36	D	405	PL9	C53-C6	-3.47	1.43	1.50
24	7	608	CHL	CHD-C4C	3.46	1.47	1.39
25	b	617	CLA	C4D-ND	-3.46	1.32	1.37
24	g	608	CHL	CHD-C4C	3.46	1.47	1.39
25	S	613	CLA	C1D-ND	3.46	1.42	1.37
24	G	608	CHL	CHD-C4C	3.46	1.47	1.39
24	y	609	CHL	CHD-C4C	3.46	1.47	1.39
25	G	612	CLA	C1D-ND	3.46	1.42	1.37
25	4	612	CLA	C4D-ND	-3.45	1.32	1.37
25	S	612	CLA	C1D-ND	3.45	1.42	1.37
24	4	606	CHL	CHD-C4C	3.45	1.47	1.39
25	g	612	CLA	C1D-ND	3.45	1.42	1.37
25	5	604	CLA	C3B-C2B	-3.45	1.35	1.40
24	3	608	CHL	CHD-C4C	3.45	1.47	1.39
25	N	614	CLA	C4D-ND	-3.45	1.33	1.37
25	b	602	CLA	C4D-ND	-3.45	1.33	1.37
25	S	614	CLA	C1D-ND	3.45	1.42	1.37
24	Y	609	CHL	CHD-C4C	3.45	1.47	1.39
25	8	612	CLA	C4D-ND	-3.44	1.33	1.37
25	4	603	CLA	C4D-ND	-3.44	1.33	1.37
25	n	614	CLA	C4D-ND	-3.44	1.33	1.37
29	l	101	LHG	O7-C5	-3.44	1.38	1.46
25	c	512	CLA	C1D-ND	3.44	1.42	1.37
25	B	604	CLA	C3B-C2B	-3.44	1.35	1.40
24	8	606	CHL	CHD-C4C	3.44	1.47	1.39
29	L	101	LHG	O7-C5	-3.44	1.38	1.46
25	s	612	CLA	C1D-ND	3.44	1.42	1.37
36	d	405	PL9	C53-C6	-3.44	1.43	1.50
28	1	1623	NEX	C7-C8	-3.44	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	606	CHL	CHD-C4C	3.44	1.47	1.39
25	6	613	CLA	C4D-ND	-3.43	1.33	1.37
25	y	613	CLA	C1D-ND	3.43	1.42	1.37
25	2	613	CLA	C4D-ND	-3.43	1.33	1.37
24	8	607	CHL	OBD-CAD	3.43	1.28	1.22
24	6	606	CHL	CHD-C4C	3.43	1.47	1.39
24	6	608	CHL	CHD-C4C	3.43	1.47	1.39
28	5	1623	NEX	C7-C8	-3.43	1.26	1.32
24	2	608	CHL	CHD-C4C	3.42	1.47	1.39
25	A	406	CLA	C1D-ND	3.42	1.42	1.37
25	C	506	CLA	CMB-C2B	-3.42	1.44	1.51
24	8	609	CHL	OBD-CAD	3.42	1.28	1.22
25	a	406	CLA	C1D-ND	3.42	1.42	1.37
24	4	607	CHL	OBD-CAD	3.42	1.28	1.22
25	N	604	CLA	C4D-ND	-3.42	1.33	1.37
25	r	616	CLA	C4D-ND	-3.42	1.33	1.37
24	7	605	CHL	OBD-CAD	3.42	1.28	1.22
25	c	501	CLA	C1D-ND	3.42	1.42	1.37
25	c	506	CLA	CMB-C2B	-3.42	1.44	1.51
25	b	604	CLA	C3B-C2B	-3.42	1.35	1.40
25	B	602	CLA	C4D-ND	-3.41	1.33	1.37
25	C	501	CLA	C1D-ND	3.41	1.42	1.37
24	3	605	CHL	OBD-CAD	3.41	1.28	1.22
24	6	607	CHL	MG-NA	-3.41	1.98	2.06
24	R	606	CHL	CHD-C4C	3.41	1.47	1.39
24	2	607	CHL	MG-NA	-3.41	1.98	2.06
25	B	605	CLA	C4D-ND	-3.41	1.33	1.37
24	4	609	CHL	OBD-CAD	3.41	1.28	1.22
24	4	609	CHL	CHD-C4C	3.41	1.47	1.39
25	6	610	CLA	C4D-ND	-3.41	1.33	1.37
25	s	614	CLA	C1D-ND	3.41	1.42	1.37
24	1	605	CHL	OBD-CAD	3.41	1.28	1.22
24	4	601	CHL	MG-NA	-3.41	1.98	2.06
25	b	605	CLA	C4D-ND	-3.41	1.33	1.37
25	C	512	CLA	C1D-ND	3.40	1.42	1.37
24	Y	606	CHL	CHD-C1D	3.40	1.45	1.38
24	5	605	CHL	OBD-CAD	3.40	1.28	1.22
25	1	612	CLA	C1D-ND	3.40	1.42	1.37
24	r	606	CHL	CHD-C4C	3.40	1.47	1.39
24	y	606	CHL	CHD-C1D	3.39	1.45	1.38
24	8	609	CHL	CHD-C4C	3.39	1.47	1.39
24	y	605	CHL	CHD-C4C	3.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	607	CHL	MG-NA	-3.39	1.98	2.06
25	2	610	CLA	C4D-ND	-3.39	1.33	1.37
24	8	606	CHL	OBD-CAD	3.39	1.28	1.22
24	8	601	CHL	MG-NA	-3.38	1.98	2.06
25	b	615	CLA	C4D-ND	-3.38	1.33	1.37
24	6	607	CHL	OBD-CAD	3.38	1.28	1.22
25	Y	613	CLA	C1D-ND	3.38	1.41	1.37
25	B	616	CLA	C3B-C2B	-3.38	1.35	1.40
25	R	616	CLA	C4D-ND	-3.38	1.33	1.37
24	Y	605	CHL	CHD-C4C	3.38	1.46	1.39
24	4	606	CHL	OBD-CAD	3.38	1.28	1.22
25	8	603	CLA	C4D-ND	-3.37	1.33	1.37
25	B	615	CLA	C4D-ND	-3.37	1.33	1.37
24	7	609	CHL	OBD-CAD	3.36	1.28	1.22
25	b	616	CLA	C3B-C2B	-3.36	1.35	1.40
25	B	612	CLA	CMB-C2B	-3.36	1.44	1.51
24	7	607	CHL	MG-NA	-3.36	1.98	2.06
24	y	601	CHL	CHD-C1D	3.36	1.44	1.38
25	b	612	CLA	CMB-C2B	-3.36	1.44	1.51
25	B	613	CLA	CMD-C2D	-3.36	1.43	1.50
25	B	606	CLA	C3B-C2B	-3.35	1.35	1.40
24	Y	601	CHL	CHD-C1D	3.35	1.44	1.38
24	6	606	CHL	OBD-CAD	3.35	1.28	1.22
24	7	606	CHL	OBD-CAD	3.35	1.28	1.22
24	N	608	CHL	CHD-C4C	3.35	1.46	1.39
24	2	607	CHL	OBD-CAD	3.35	1.28	1.22
24	6	609	CHL	OBD-CAD	3.34	1.28	1.22
24	2	606	CHL	OBD-CAD	3.34	1.28	1.22
24	5	608	CHL	C3B-C2B	3.34	1.45	1.40
24	3	609	CHL	OBD-CAD	3.34	1.28	1.22
25	c	509	CLA	C1D-ND	3.34	1.41	1.37
28	s	1623	NEX	C7-C8	-3.34	1.26	1.32
25	6	612	CLA	C4D-ND	-3.34	1.33	1.37
24	2	609	CHL	OBD-CAD	3.34	1.28	1.22
25	b	613	CLA	CMD-C2D	-3.34	1.43	1.50
25	C	509	CLA	C1D-ND	3.34	1.41	1.37
25	R	612	CLA	C4D-ND	-3.34	1.33	1.37
24	S	601	CHL	OBD-CAD	3.34	1.28	1.22
24	s	601	CHL	OBD-CAD	3.33	1.28	1.22
24	y	607	CHL	OBD-CAD	3.33	1.28	1.22
24	1	608	CHL	C3B-C2B	3.33	1.45	1.40
25	4	611	CLA	C1D-ND	3.33	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	612	CLA	C1D-ND	3.33	1.41	1.37
25	Y	612	CLA	C3B-C2B	-3.33	1.35	1.40
24	y	608	CHL	CHD-C1D	3.33	1.44	1.38
24	3	607	CHL	OBD-CAD	3.33	1.28	1.22
25	C	510	CLA	C1D-ND	3.33	1.41	1.37
24	n	608	CHL	CHD-C4C	3.33	1.46	1.39
24	r	606	CHL	OBD-CAD	3.33	1.28	1.22
28	S	1623	NEX	C7-C8	-3.33	1.26	1.32
25	c	501	CLA	C4D-ND	-3.33	1.33	1.37
25	b	606	CLA	C3B-C2B	-3.33	1.35	1.40
24	1	607	CHL	OBD-CAD	3.32	1.28	1.22
25	y	612	CLA	C3B-C2B	-3.32	1.35	1.40
24	7	601	CHL	CHD-C4C	3.32	1.46	1.39
24	Y	608	CHL	CHD-C1D	3.32	1.44	1.38
24	g	606	CHL	OBD-CAD	3.32	1.28	1.22
24	3	606	CHL	OBD-CAD	3.32	1.28	1.22
24	N	607	CHL	OBD-CAD	3.31	1.28	1.22
25	8	611	CLA	C1D-ND	3.31	1.41	1.37
24	3	601	CHL	CHD-C4C	3.31	1.46	1.39
25	N	612	CLA	C1D-ND	3.31	1.41	1.37
25	2	612	CLA	C4D-ND	-3.31	1.33	1.37
24	y	605	CHL	OBD-CAD	3.30	1.28	1.22
25	g	610	CLA	C4D-ND	-3.30	1.33	1.37
24	R	606	CHL	OBD-CAD	3.30	1.28	1.22
25	c	510	CLA	C1D-ND	3.30	1.41	1.37
24	Y	605	CHL	OBD-CAD	3.30	1.28	1.22
25	6	612	CLA	C1D-ND	3.30	1.41	1.37
25	C	501	CLA	C4D-ND	-3.30	1.33	1.37
25	c	508	CLA	C4D-ND	-3.30	1.33	1.37
24	3	608	CHL	CHD-C1D	3.30	1.44	1.38
24	G	606	CHL	OBD-CAD	3.29	1.28	1.22
24	5	606	CHL	OBD-CAD	3.29	1.28	1.22
24	7	607	CHL	OBD-CAD	3.29	1.28	1.22
24	1	606	CHL	OBD-CAD	3.29	1.28	1.22
25	R	612	CLA	C1D-ND	3.29	1.41	1.37
25	b	605	CLA	CMB-C2B	-3.29	1.44	1.51
24	5	607	CHL	OBD-CAD	3.29	1.28	1.22
25	N	614	CLA	C1D-ND	3.29	1.41	1.37
24	Y	607	CHL	OBD-CAD	3.29	1.28	1.22
25	C	508	CLA	C4D-ND	-3.28	1.33	1.37
24	6	601	CHL	OBD-CAD	3.28	1.28	1.22
25	r	612	CLA	C4D-ND	-3.28	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	604	CLA	C4D-ND	-3.28	1.33	1.37
25	1	603	CLA	C3B-C2B	-3.28	1.35	1.40
25	A	407	CLA	C1D-ND	3.28	1.41	1.37
24	n	607	CHL	OBD-CAD	3.28	1.28	1.22
24	2	601	CHL	OBD-CAD	3.27	1.28	1.22
25	s	610	CLA	C4D-ND	-3.27	1.33	1.37
25	c	507	CLA	C4D-ND	-3.27	1.33	1.37
24	1	605	CHL	MG-NA	-3.27	1.98	2.06
24	4	608	CHL	CHD-C4C	3.26	1.46	1.39
25	n	612	CLA	C1D-ND	3.26	1.41	1.37
25	N	611	CLA	C1D-ND	3.26	1.41	1.37
24	S	608	CHL	OBD-CAD	3.26	1.28	1.22
24	s	608	CHL	OBD-CAD	3.26	1.28	1.22
25	B	605	CLA	CMB-C2B	-3.26	1.44	1.51
25	5	603	CLA	C3B-C2B	-3.26	1.35	1.40
25	n	612	CLA	C4D-ND	-3.26	1.33	1.37
25	B	607	CLA	C1D-ND	3.25	1.41	1.37
25	B	602	CLA	C1D-ND	3.25	1.41	1.37
25	C	507	CLA	C4D-ND	-3.25	1.33	1.37
25	2	612	CLA	C3B-C2B	-3.25	1.35	1.40
25	R	601	CLA	C4D-ND	-3.25	1.33	1.37
25	N	613	CLA	C1D-ND	3.25	1.41	1.37
25	n	614	CLA	C1D-ND	3.25	1.41	1.37
25	b	602	CLA	C1D-ND	3.25	1.41	1.37
28	r	623	NEX	C7-C8	-3.25	1.26	1.32
36	d	405	PL9	C36-C34	-3.24	1.44	1.51
24	1	609	CHL	OBD-CAD	3.24	1.28	1.22
24	5	605	CHL	MG-NA	-3.24	1.98	2.06
25	b	607	CLA	C1D-ND	3.24	1.41	1.37
25	G	610	CLA	C4D-ND	-3.24	1.33	1.37
24	7	608	CHL	CHD-C1D	3.24	1.44	1.38
25	r	601	CLA	C4D-ND	-3.24	1.33	1.37
36	D	405	PL9	C36-C34	-3.24	1.44	1.51
25	n	610	CLA	C4D-ND	-3.24	1.33	1.37
25	6	604	CLA	C4D-ND	-3.23	1.33	1.37
25	y	611	CLA	C3B-C2B	-3.23	1.35	1.40
24	8	608	CHL	CHD-C4C	3.23	1.46	1.39
28	2	1623	NEX	C7-C8	-3.23	1.26	1.32
24	7	607	CHL	CHD-C4C	3.23	1.46	1.39
36	d	405	PL9	C52-C5	-3.23	1.44	1.50
25	a	407	CLA	C1D-ND	3.23	1.41	1.37
25	N	612	CLA	C4D-ND	-3.23	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	609	CHL	OBD-CAD	3.23	1.28	1.22
36	D	405	PL9	C52-C5	-3.22	1.44	1.50
24	g	608	CHL	OBD-CAD	3.22	1.28	1.22
24	n	606	CHL	CHD-C4C	3.22	1.46	1.39
25	6	612	CLA	C3B-C2B	-3.22	1.35	1.40
24	G	607	CHL	CHD-C4C	3.22	1.46	1.39
28	R	623	NEX	C7-C8	-3.22	1.26	1.32
25	N	610	CLA	C4D-ND	-3.22	1.33	1.37
24	N	606	CHL	CHD-C4C	3.22	1.46	1.39
25	B	606	CLA	C1D-ND	3.22	1.41	1.37
25	G	603	CLA	C3B-C2B	-3.21	1.35	1.40
24	G	608	CHL	OBD-CAD	3.21	1.28	1.22
25	N	610	CLA	C1D-ND	3.21	1.41	1.37
24	2	605	CHL	MG-NA	-3.21	1.98	2.06
24	5	608	CHL	CHD-C4C	3.21	1.46	1.39
25	n	611	CLA	C1D-ND	3.21	1.41	1.37
29	G	2630	LHG	O7-C5	-3.21	1.38	1.46
24	6	605	CHL	MG-NA	-3.21	1.98	2.06
37	h	102	DGD	O2G-C2G	-3.21	1.38	1.46
25	n	613	CLA	C1D-ND	3.21	1.41	1.37
25	b	606	CLA	C1D-ND	3.21	1.41	1.37
29	g	2630	LHG	O7-C5	-3.21	1.38	1.46
24	g	607	CHL	CHD-C4C	3.21	1.46	1.39
25	S	610	CLA	C4D-ND	-3.21	1.33	1.37
25	r	612	CLA	C1D-ND	3.20	1.41	1.37
25	G	612	CLA	C4D-ND	-3.20	1.33	1.37
25	R	601	CLA	CHC-C1C	3.20	1.43	1.35
24	1	608	CHL	CHD-C4C	3.20	1.46	1.39
28	6	1623	NEX	C7-C8	-3.20	1.26	1.32
25	s	602	CLA	C4D-ND	-3.20	1.33	1.37
25	3	614	CLA	C4D-ND	-3.19	1.33	1.37
25	c	506	CLA	C4D-ND	-3.19	1.33	1.37
37	H	102	DGD	O2G-C2G	-3.19	1.38	1.46
25	g	610	CLA	C1D-ND	3.19	1.41	1.37
24	3	607	CHL	CHD-C4C	3.19	1.46	1.39
25	g	612	CLA	C4D-ND	-3.19	1.33	1.37
24	7	609	CHL	MG-NA	-3.19	1.98	2.06
25	C	506	CLA	C4D-ND	-3.19	1.33	1.37
25	s	613	CLA	C4D-ND	-3.18	1.33	1.37
25	r	611	CLA	C1D-ND	3.18	1.41	1.37
25	Y	611	CLA	C3B-C2B	-3.18	1.36	1.40
25	n	602	CLA	C1D-ND	3.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	610	CLA	C1D-ND	3.18	1.41	1.37
25	7	614	CLA	C4D-ND	-3.18	1.33	1.37
25	Y	610	CLA	C3B-C2B	-3.18	1.36	1.40
25	g	603	CLA	C3B-C2B	-3.18	1.36	1.40
25	r	601	CLA	CHC-C1C	3.18	1.43	1.35
25	G	614	CLA	C1D-ND	3.17	1.41	1.37
24	3	609	CHL	MG-NA	-3.17	1.98	2.06
25	N	602	CLA	C1D-ND	3.17	1.41	1.37
24	5	609	CHL	C1B-NB	-3.17	1.32	1.35
25	R	611	CLA	C1D-ND	3.17	1.41	1.37
25	S	613	CLA	C4D-ND	-3.17	1.33	1.37
25	y	610	CLA	C3B-C2B	-3.17	1.36	1.40
25	C	502	CLA	C4D-ND	-3.16	1.33	1.37
25	C	513	CLA	C4D-ND	-3.16	1.33	1.37
25	5	612	CLA	C4D-ND	-3.16	1.33	1.37
24	2	608	CHL	OBD-CAD	3.16	1.27	1.22
25	n	610	CLA	C1D-ND	3.16	1.41	1.37
25	5	614	CLA	C1D-ND	3.15	1.41	1.37
25	S	602	CLA	C4D-ND	-3.15	1.33	1.37
25	3	612	CLA	C3B-C2B	-3.15	1.36	1.40
25	7	612	CLA	C3B-C2B	-3.15	1.36	1.40
24	1	601	CHL	OBD-CAD	3.15	1.27	1.22
25	r	613	CLA	CMB-C2B	-3.15	1.45	1.51
25	2	614	CLA	C1D-ND	3.14	1.41	1.37
25	c	502	CLA	C4D-ND	-3.14	1.33	1.37
25	c	513	CLA	C4D-ND	-3.14	1.33	1.37
25	g	614	CLA	C1D-ND	3.14	1.41	1.37
24	6	608	CHL	OBD-CAD	3.14	1.27	1.22
24	5	601	CHL	OBD-CAD	3.14	1.27	1.22
25	G	604	CLA	C1D-ND	3.13	1.41	1.37
25	6	603	CLA	C1D-ND	3.13	1.41	1.37
25	R	613	CLA	CMB-C2B	-3.13	1.45	1.51
25	1	614	CLA	C1D-ND	3.13	1.41	1.37
25	6	611	CLA	C1D-ND	3.13	1.41	1.37
25	1	612	CLA	C4D-ND	-3.12	1.33	1.37
25	2	611	CLA	C1D-ND	3.12	1.41	1.37
25	b	607	CLA	CMB-C2B	-3.12	1.45	1.51
25	b	608	CLA	CMB-C2B	-3.12	1.45	1.51
25	c	504	CLA	C4D-ND	-3.12	1.33	1.37
25	g	604	CLA	C1D-ND	3.12	1.41	1.37
25	B	614	CLA	CMB-C2B	-3.11	1.45	1.51
25	B	617	CLA	CMC-C2C	-3.11	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	604	CLA	C1D-ND	3.11	1.41	1.37
25	7	610	CLA	C3B-C2B	-3.11	1.36	1.40
24	r	608	CHL	CHD-C1D	3.11	1.44	1.38
25	s	614	CLA	C4D-ND	-3.11	1.33	1.37
25	b	617	CLA	CMC-C2C	-3.10	1.44	1.50
25	B	607	CLA	CMB-C2B	-3.10	1.45	1.51
25	g	613	CLA	C1D-ND	3.10	1.41	1.37
25	S	614	CLA	C4D-ND	-3.10	1.33	1.37
25	r	601	CLA	C1D-ND	3.10	1.41	1.37
25	4	604	CLA	C1D-ND	3.10	1.41	1.37
24	1	609	CHL	C1B-NB	-3.10	1.32	1.35
24	R	608	CHL	CHD-C1D	3.10	1.44	1.38
25	A	405	CLA	C1D-ND	3.10	1.41	1.37
25	3	610	CLA	C3B-C2B	-3.09	1.36	1.40
25	B	608	CLA	CMB-C2B	-3.09	1.45	1.51
25	7	604	CLA	C1D-ND	3.09	1.41	1.37
25	8	604	CLA	C1D-ND	3.09	1.41	1.37
25	7	613	CLA	C3B-C2B	-3.09	1.36	1.40
25	C	504	CLA	C4D-ND	-3.09	1.33	1.37
25	R	604	CLA	C1D-ND	3.09	1.41	1.37
28	N	1623	NEX	C7-C8	-3.09	1.26	1.32
24	Y	608	CHL	CHD-C4C	3.09	1.46	1.39
25	5	612	CLA	C3B-C2B	-3.09	1.36	1.40
25	2	603	CLA	C1D-ND	3.09	1.41	1.37
24	y	608	CHL	CHD-C4C	3.09	1.46	1.39
25	r	604	CLA	C1D-ND	3.09	1.41	1.37
25	6	614	CLA	C1D-ND	3.08	1.41	1.37
25	c	508	CLA	CMB-C2B	-3.08	1.45	1.51
25	C	508	CLA	CMB-C2B	-3.08	1.45	1.51
25	b	614	CLA	CMB-C2B	-3.08	1.45	1.51
25	C	503	CLA	C4D-ND	-3.08	1.33	1.37
24	1	606	CHL	CHD-C4C	3.08	1.46	1.39
25	4	603	CLA	C1D-ND	3.07	1.41	1.37
28	n	1623	NEX	C7-C8	-3.07	1.26	1.32
25	g	602	CLA	C1D-ND	3.07	1.41	1.37
25	r	616	CLA	CMB-C2B	-3.07	1.45	1.51
25	8	603	CLA	C1D-ND	3.07	1.41	1.37
24	5	606	CHL	CHD-C4C	3.07	1.46	1.39
29	D	408	LHG	O7-C5	-3.07	1.38	1.46
24	y	607	CHL	CHD-C4C	3.07	1.46	1.39
25	7	613	CLA	C1D-ND	3.07	1.41	1.37
25	3	613	CLA	C1D-ND	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	611	CLA	C1D-ND	3.06	1.41	1.37
25	1	611	CLA	C1D-ND	3.06	1.41	1.37
25	y	611	CLA	C1D-ND	3.06	1.41	1.37
25	3	613	CLA	C3B-C2B	-3.06	1.36	1.40
25	G	613	CLA	C1D-ND	3.06	1.41	1.37
39	f	101	HEM	CAB-C3B	3.06	1.55	1.47
25	1	612	CLA	C3B-C2B	-3.06	1.36	1.40
24	Y	607	CHL	CHD-C4C	3.06	1.46	1.39
25	B	605	CLA	CMD-C2D	-3.06	1.44	1.50
25	G	602	CLA	C1D-ND	3.06	1.41	1.37
34	b	623	SQD	O48-C23	3.05	1.42	1.33
25	c	503	CLA	C4D-ND	-3.05	1.33	1.37
25	b	605	CLA	CMD-C2D	-3.05	1.44	1.50
34	B	623	SQD	O48-C23	3.05	1.42	1.33
24	7	601	CHL	MG-NA	-3.05	1.99	2.06
39	F	101	HEM	CAB-C3B	3.05	1.55	1.47
25	2	610	CLA	C1D-ND	3.05	1.41	1.37
25	B	615	CLA	CMD-C2D	-3.05	1.44	1.50
25	b	606	CLA	CMB-C2B	-3.05	1.45	1.51
29	d	408	LHG	O7-C5	-3.04	1.39	1.46
25	6	610	CLA	C1D-ND	3.04	1.41	1.37
24	N	607	CHL	CHD-C4C	3.04	1.46	1.39
25	B	606	CLA	CMB-C2B	-3.04	1.45	1.51
25	R	613	CLA	C4D-ND	-3.04	1.33	1.37
25	g	611	CLA	C1D-ND	3.04	1.41	1.37
25	R	616	CLA	CMB-C2B	-3.04	1.45	1.51
25	a	405	CLA	C1D-ND	3.03	1.41	1.37
25	n	603	CLA	C1D-ND	3.03	1.41	1.37
25	5	611	CLA	C1D-ND	3.03	1.41	1.37
24	Y	601	CHL	MG-NA	-3.03	1.99	2.06
25	R	601	CLA	C1D-ND	3.03	1.41	1.37
25	1	603	CLA	CMB-C2B	-3.03	1.45	1.51
24	y	606	CHL	CHD-C4C	3.03	1.46	1.39
25	n	603	CLA	C3B-C2B	-3.02	1.36	1.40
25	B	617	CLA	C1D-ND	3.02	1.41	1.37
24	5	607	CHL	MG-NA	-3.02	1.99	2.06
24	3	601	CHL	MG-NA	-3.02	1.99	2.06
25	r	610	CLA	C1D-ND	3.02	1.41	1.37
25	C	510	CLA	CHC-C1C	3.02	1.42	1.35
25	C	505	CLA	C4D-ND	-3.02	1.33	1.37
34	b	623	SQD	O47-C7	3.02	1.42	1.34
24	n	607	CHL	CHD-C4C	3.02	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	603	CLA	C3B-C2B	-3.02	1.36	1.40
24	Y	606	CHL	CHD-C4C	3.02	1.46	1.39
25	5	603	CLA	CMB-C2B	-3.02	1.45	1.51
25	c	510	CLA	CHC-C1C	3.02	1.42	1.35
25	Y	602	CLA	C1D-ND	3.01	1.41	1.37
24	y	601	CHL	MG-NA	-3.01	1.99	2.06
34	B	623	SQD	O47-C7	3.01	1.42	1.34
24	n	601	CHL	OBD-CAD	3.01	1.27	1.22
25	b	615	CLA	CMD-C2D	-3.01	1.44	1.50
25	5	613	CLA	C1D-ND	3.01	1.41	1.37
25	s	610	CLA	CHC-C1C	3.01	1.42	1.35
25	c	510	CLA	C4D-ND	-3.01	1.33	1.37
24	1	607	CHL	MG-NA	-3.01	1.99	2.06
25	s	602	CLA	CHC-C1C	3.01	1.42	1.35
25	r	613	CLA	C4D-ND	-3.01	1.33	1.37
25	S	610	CLA	CHC-C1C	3.01	1.42	1.35
25	Y	611	CLA	C1D-ND	3.01	1.41	1.37
25	8	612	CLA	C1D-ND	3.01	1.41	1.37
24	R	608	CHL	CHD-C4C	3.01	1.46	1.39
25	b	611	CLA	C3B-C2B	-3.01	1.36	1.40
25	c	509	CLA	C4D-ND	-3.01	1.33	1.37
25	b	613	CLA	CMB-C2B	-3.01	1.45	1.51
24	N	601	CHL	OBD-CAD	3.01	1.27	1.22
25	S	602	CLA	CHC-C1C	3.00	1.42	1.35
25	N	603	CLA	C1D-ND	3.00	1.41	1.37
24	g	609	CHL	OBD-CAD	3.00	1.27	1.22
25	r	616	CLA	C1D-ND	3.00	1.41	1.37
25	R	610	CLA	C1D-ND	3.00	1.41	1.37
25	b	617	CLA	C1D-ND	3.00	1.41	1.37
25	B	613	CLA	CMB-C2B	-3.00	1.45	1.51
25	c	511	CLA	CHC-C1C	3.00	1.42	1.35
24	G	609	CHL	OBD-CAD	3.00	1.27	1.22
25	y	602	CLA	C1D-ND	2.99	1.41	1.37
25	c	505	CLA	C4D-ND	-2.99	1.33	1.37
25	B	613	CLA	MG-ND	-2.99	1.99	2.05
25	C	509	CLA	C4D-ND	-2.99	1.33	1.37
24	3	601	CHL	OBD-CAD	2.99	1.27	1.22
24	3	606	CHL	MG-NA	-2.99	1.99	2.06
25	S	611	CLA	C4D-ND	-2.99	1.33	1.37
25	R	616	CLA	C1D-ND	2.99	1.41	1.37
25	s	609	CLA	C4D-ND	-2.99	1.33	1.37
24	r	608	CHL	CHD-C4C	2.99	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y	2630	LHG	O7-C5	-2.98	1.39	1.46
25	C	510	CLA	C4D-ND	-2.98	1.33	1.37
25	b	613	CLA	MG-ND	-2.98	1.99	2.05
24	7	606	CHL	MG-NA	-2.98	1.99	2.06
25	4	612	CLA	C1D-ND	2.98	1.41	1.37
25	B	608	CLA	C1D-ND	2.98	1.41	1.37
25	D	403	CLA	C1D-ND	2.98	1.41	1.37
25	G	611	CLA	CHC-C1C	2.98	1.42	1.35
25	g	611	CLA	CHC-C1C	2.98	1.42	1.35
25	S	609	CLA	C4D-ND	-2.98	1.33	1.37
25	C	511	CLA	CHC-C1C	2.97	1.42	1.35
24	7	601	CHL	OBD-CAD	2.97	1.27	1.22
25	C	512	CLA	C4D-ND	-2.97	1.33	1.37
25	n	604	CLA	C3B-C2B	-2.97	1.36	1.40
25	8	604	CLA	C3B-C2B	-2.97	1.36	1.40
28	y	1623	NEX	C7-C8	-2.97	1.27	1.32
25	B	611	CLA	C3B-C2B	-2.97	1.36	1.40
25	5	610	CLA	C1D-ND	2.97	1.41	1.37
25	1	613	CLA	C1D-ND	2.97	1.41	1.37
25	b	608	CLA	C1D-ND	2.97	1.41	1.37
25	a	405	CLA	CMC-C2C	-2.97	1.44	1.50
25	N	604	CLA	C3B-C2B	-2.96	1.36	1.40
29	3	2630	LHG	O7-C5	-2.96	1.39	1.46
25	s	604	CLA	C4D-ND	-2.96	1.33	1.37
25	B	605	CLA	C1D-ND	2.96	1.41	1.37
25	3	604	CLA	CMB-C2B	-2.96	1.45	1.51
25	7	604	CLA	CMB-C2B	-2.96	1.45	1.51
25	b	605	CLA	C1D-ND	2.95	1.41	1.37
29	7	2630	LHG	O7-C5	-2.95	1.39	1.46
29	Y	2630	LHG	O7-C5	-2.95	1.39	1.46
36	d	405	PL9	C26-C24	-2.95	1.45	1.51
29	n	2630	LHG	O7-C5	-2.95	1.39	1.46
25	d	403	CLA	C1D-ND	2.95	1.41	1.37
25	B	608	CLA	C3B-C2B	-2.95	1.36	1.40
25	c	512	CLA	C4D-ND	-2.95	1.33	1.37
25	c	501	CLA	CHC-C1C	2.95	1.42	1.35
25	1	610	CLA	C1D-ND	2.95	1.41	1.37
25	A	405	CLA	CMC-C2C	-2.95	1.44	1.50
25	s	612	CLA	C4D-ND	-2.94	1.33	1.37
25	c	503	CLA	CHC-C1C	2.94	1.42	1.35
25	s	611	CLA	C4D-ND	-2.94	1.33	1.37
25	2	610	CLA	C3B-C2B	-2.94	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	501	CLA	CHC-C1C	2.94	1.42	1.35
25	S	612	CLA	C4D-ND	-2.94	1.33	1.37
29	N	2630	LHG	O7-C5	-2.94	1.39	1.46
25	S	604	CLA	CHC-C1C	2.94	1.42	1.35
25	y	610	CLA	CMB-C2B	-2.94	1.45	1.51
34	a	418	SQD	O47-C7	2.94	1.42	1.34
36	d	405	PL9	C16-C14	-2.94	1.45	1.51
36	D	405	PL9	C26-C24	-2.94	1.45	1.51
28	Y	1623	NEX	C7-C8	-2.94	1.27	1.32
25	C	503	CLA	CHC-C1C	2.94	1.42	1.35
25	s	604	CLA	CHC-C1C	2.93	1.42	1.35
25	r	604	CLA	CMB-C2B	-2.93	1.45	1.51
34	B	621	SQD	O47-C7	2.93	1.42	1.34
25	B	610	CLA	CMB-C2B	-2.93	1.45	1.51
25	b	608	CLA	C3B-C2B	-2.93	1.36	1.40
24	Y	609	CHL	OBD-CAD	2.93	1.27	1.22
25	4	604	CLA	C3B-C2B	-2.93	1.36	1.40
25	A	406	CLA	CMB-C2B	-2.93	1.45	1.51
25	d	402	CLA	CMB-C2B	-2.93	1.45	1.51
25	y	612	CLA	CMB-C2B	-2.93	1.45	1.51
24	7	608	CHL	OBD-CAD	2.93	1.27	1.22
25	4	604	CLA	CMB-C2B	-2.93	1.45	1.51
25	D	402	CLA	CMB-C2B	-2.93	1.45	1.51
33	A	409	PHO	CAC-C3C	-2.93	1.47	1.52
25	B	616	CLA	C1D-ND	2.93	1.41	1.37
25	6	610	CLA	C3B-C2B	-2.93	1.36	1.40
25	a	406	CLA	CMB-C2B	-2.92	1.45	1.51
24	4	607	CHL	MG-NA	-2.92	1.99	2.06
25	b	610	CLA	CMB-C2B	-2.92	1.45	1.51
24	3	608	CHL	OBD-CAD	2.92	1.27	1.22
25	C	511	CLA	C4D-ND	-2.92	1.33	1.37
34	A	418	SQD	O47-C7	2.92	1.42	1.34
25	Y	610	CLA	CMB-C2B	-2.92	1.45	1.51
25	R	604	CLA	CMB-C2B	-2.91	1.45	1.51
24	g	607	CHL	MG-NA	-2.91	1.99	2.06
34	b	621	SQD	O47-C7	2.91	1.42	1.34
25	Y	602	CLA	CMB-C2B	-2.91	1.45	1.51
36	D	405	PL9	C16-C14	-2.91	1.45	1.51
25	y	604	CLA	C3B-C2B	-2.91	1.36	1.40
25	b	617	CLA	CMB-C2B	-2.91	1.45	1.51
24	r	614	CHL	C1D-C2D	2.91	1.51	1.45
24	8	607	CHL	MG-NA	-2.91	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	609	CHL	OBD-CAD	2.91	1.27	1.22
24	n	601	CHL	MG-NA	-2.91	1.99	2.06
25	7	604	CLA	C3B-C2B	-2.90	1.36	1.40
33	a	409	PHO	CAC-C3C	-2.90	1.47	1.52
25	r	609	CLA	C3B-C2B	-2.90	1.36	1.40
25	c	513	CLA	CHC-C1C	2.90	1.42	1.35
25	8	604	CLA	CMB-C2B	-2.90	1.45	1.51
25	2	614	CLA	CHC-C1C	2.90	1.42	1.35
25	Y	611	CLA	CMB-C2B	-2.90	1.45	1.51
25	B	614	CLA	CHC-C1C	2.90	1.42	1.35
25	4	610	CLA	C1D-ND	2.90	1.41	1.37
34	b	621	SQD	O48-C23	2.90	1.41	1.33
25	3	604	CLA	C3B-C2B	-2.90	1.36	1.40
25	1	602	CLA	C1D-ND	2.90	1.41	1.37
25	c	511	CLA	C4D-ND	-2.89	1.33	1.37
25	Y	604	CLA	C3B-C2B	-2.89	1.36	1.40
25	y	611	CLA	CMB-C2B	-2.89	1.45	1.51
25	S	604	CLA	C4D-ND	-2.89	1.33	1.37
24	n	609	CHL	OBD-CAD	2.89	1.27	1.22
24	y	607	CHL	MG-NA	-2.89	1.99	2.06
25	Y	612	CLA	CMB-C2B	-2.89	1.45	1.51
24	G	607	CHL	MG-NA	-2.89	1.99	2.06
36	d	405	PL9	C11-C9	-2.89	1.45	1.51
24	N	601	CHL	MG-NA	-2.89	1.99	2.06
25	Y	610	CLA	C1D-ND	2.89	1.41	1.37
24	y	609	CHL	OBD-CAD	2.89	1.27	1.22
34	B	621	SQD	O48-C23	2.89	1.41	1.33
25	B	617	CLA	CMB-C2B	-2.89	1.45	1.51
25	Y	603	CLA	C1D-ND	2.89	1.41	1.37
25	S	609	CLA	CHC-C1C	2.89	1.42	1.35
25	y	602	CLA	CMB-C2B	-2.89	1.45	1.51
25	C	513	CLA	CHC-C1C	2.89	1.42	1.35
25	1	614	CLA	CHC-C1C	2.89	1.42	1.35
25	2	602	CLA	CHC-C1C	2.89	1.42	1.35
25	y	603	CLA	C1D-ND	2.88	1.41	1.37
25	8	602	CLA	CHC-C1C	2.88	1.42	1.35
25	R	609	CLA	C3B-C2B	-2.88	1.36	1.40
24	4	608	CHL	MG-NA	-2.88	1.99	2.06
25	4	602	CLA	CHC-C1C	2.88	1.42	1.35
24	8	608	CHL	MG-NA	-2.88	1.99	2.06
25	y	614	CLA	C1D-ND	2.88	1.41	1.37
25	6	614	CLA	CHC-C1C	2.88	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	609	CLA	CHC-C1C	2.88	1.42	1.35
25	S	614	CLA	CHC-C1C	2.88	1.42	1.35
25	b	614	CLA	CHC-C1C	2.88	1.42	1.35
25	b	611	CLA	CMB-C2B	-2.88	1.45	1.51
24	R	614	CHL	C1D-C2D	2.88	1.51	1.45
25	8	610	CLA	C1D-ND	2.88	1.41	1.37
25	6	602	CLA	CHC-C1C	2.87	1.42	1.35
25	Y	614	CLA	C1D-ND	2.87	1.41	1.37
24	Y	606	CHL	OBD-CAD	2.87	1.27	1.22
25	6	603	CLA	C3B-C2B	-2.87	1.36	1.40
24	y	606	CHL	OBD-CAD	2.87	1.27	1.22
25	7	614	CLA	CHC-C1C	2.87	1.42	1.35
36	d	405	PL9	C41-C39	-2.87	1.45	1.51
25	5	602	CLA	C1D-ND	2.87	1.41	1.37
25	2	603	CLA	C3B-C2B	-2.87	1.36	1.40
25	s	611	CLA	CHC-C1C	2.87	1.42	1.35
25	B	611	CLA	CMB-C2B	-2.87	1.45	1.51
25	a	407	CLA	CMB-C2B	-2.87	1.45	1.51
25	s	614	CLA	CHC-C1C	2.87	1.42	1.35
25	8	612	CLA	CHC-C1C	2.87	1.42	1.35
25	y	610	CLA	C1D-ND	2.87	1.41	1.37
25	d	402	CLA	CMD-C2D	-2.86	1.44	1.50
25	3	603	CLA	C3B-C2B	-2.86	1.36	1.40
25	4	612	CLA	CHC-C1C	2.86	1.42	1.35
36	D	405	PL9	C41-C39	-2.86	1.45	1.51
24	s	606	CHL	C1D-C2D	2.86	1.51	1.45
24	N	606	CHL	OBD-CAD	2.86	1.27	1.22
25	7	610	CLA	C1D-ND	2.86	1.41	1.37
25	g	602	CLA	CMC-C2C	-2.86	1.44	1.50
25	Y	614	CLA	C3B-C2B	-2.86	1.36	1.40
34	a	412	SQD	O48-C23	2.86	1.41	1.33
25	s	612	CLA	CHC-C1C	2.86	1.42	1.35
25	s	603	CLA	C4D-ND	-2.86	1.33	1.37
25	G	603	CLA	C1D-ND	2.86	1.41	1.37
25	5	614	CLA	CHC-C1C	2.86	1.42	1.35
34	A	412	SQD	O48-C23	2.86	1.41	1.33
37	h	102	DGD	O4D-C4D	-2.86	1.36	1.43
36	D	405	PL9	C11-C9	-2.86	1.45	1.51
25	S	603	CLA	CHC-C1C	2.86	1.42	1.35
25	N	604	CLA	C1D-ND	2.86	1.41	1.37
25	n	604	CLA	C1D-ND	2.86	1.41	1.37
24	y	609	CHL	MG-NA	-2.85	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	610	CLA	CHC-C1C	2.85	1.42	1.35
25	3	610	CLA	C1D-ND	2.85	1.41	1.37
25	S	603	CLA	C4D-ND	-2.85	1.33	1.37
34	a	418	SQD	O48-C23	2.85	1.41	1.33
25	b	616	CLA	C1D-ND	2.85	1.41	1.37
25	4	610	CLA	CHC-C1C	2.85	1.42	1.35
25	s	603	CLA	CHC-C1C	2.85	1.42	1.35
37	H	102	DGD	O4D-C4D	-2.85	1.36	1.43
24	y	605	CHL	MG-NA	-2.85	1.99	2.06
25	3	614	CLA	CHC-C1C	2.85	1.42	1.35
25	G	614	CLA	CHC-C1C	2.85	1.42	1.35
25	S	611	CLA	CHC-C1C	2.85	1.42	1.35
24	1	608	CHL	OBD-CAD	2.85	1.27	1.22
25	S	612	CLA	CHC-C1C	2.84	1.42	1.35
24	S	606	CHL	C1D-C2D	2.84	1.50	1.45
24	Y	607	CHL	MG-NA	-2.84	1.99	2.06
25	D	402	CLA	CMD-C2D	-2.84	1.44	1.50
25	7	603	CLA	C3B-C2B	-2.84	1.36	1.40
25	r	603	CLA	CMB-C2B	-2.84	1.45	1.51
24	8	601	CHL	C3D-C2D	2.84	1.46	1.39
24	5	608	CHL	OBD-CAD	2.84	1.27	1.22
25	A	407	CLA	CMB-C2B	-2.84	1.45	1.51
34	A	418	SQD	O48-C23	2.84	1.41	1.33
25	g	614	CLA	CHC-C1C	2.83	1.42	1.35
24	Y	605	CHL	MG-NA	-2.83	1.99	2.06
25	8	602	CLA	C1D-ND	2.83	1.41	1.37
24	s	608	CHL	C1D-C2D	2.83	1.50	1.45
25	7	610	CLA	CMB-C2B	-2.83	1.45	1.51
24	Y	609	CHL	MG-NA	-2.83	1.99	2.06
24	S	608	CHL	C1D-C2D	2.83	1.50	1.45
25	C	509	CLA	CHC-C1C	2.83	1.42	1.35
24	G	601	CHL	MG-NA	-2.83	1.99	2.06
24	5	601	CHL	MG-NA	-2.83	1.99	2.06
25	N	602	CLA	CMB-C2B	-2.83	1.45	1.51
26	y	1621	LUT	C22-C21	-2.82	1.51	1.54
24	8	609	CHL	MG-NA	-2.82	1.99	2.06
24	4	601	CHL	C3D-C2D	2.82	1.46	1.39
25	3	610	CLA	CMB-C2B	-2.82	1.45	1.51
25	R	603	CLA	CMB-C2B	-2.82	1.45	1.51
24	g	601	CHL	MG-NA	-2.82	1.99	2.06
24	n	606	CHL	OBD-CAD	2.82	1.27	1.22
25	y	614	CLA	C3B-C2B	-2.82	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	CLA	CMC-C2C	-2.82	1.44	1.50
25	1	610	CLA	C3B-C2B	-2.82	1.36	1.40
24	y	608	CHL	MG-NA	-2.82	1.99	2.06
25	G	602	CLA	CMC-C2C	-2.81	1.44	1.50
25	a	410	CLA	C1D-ND	2.81	1.41	1.37
25	1	602	CLA	CHC-C1C	2.81	1.42	1.35
25	5	603	CLA	C1D-ND	2.81	1.41	1.37
25	n	602	CLA	CMB-C2B	-2.81	1.45	1.51
25	G	602	CLA	CMB-C2B	-2.81	1.45	1.51
25	Y	603	CLA	CMB-C2B	-2.81	1.45	1.51
25	D	402	CLA	CMC-C2C	-2.81	1.44	1.50
24	Y	608	CHL	MG-NA	-2.80	1.99	2.06
25	5	610	CLA	C3B-C2B	-2.80	1.36	1.40
25	b	615	CLA	C1D-ND	2.80	1.41	1.37
24	1	601	CHL	MG-NA	-2.80	1.99	2.06
24	4	609	CHL	MG-NA	-2.80	1.99	2.06
25	4	602	CLA	C1D-ND	2.80	1.41	1.37
25	g	603	CLA	C1D-ND	2.80	1.41	1.37
25	C	501	CLA	C3B-C2B	-2.80	1.36	1.40
25	Y	612	CLA	C1D-ND	2.80	1.41	1.37
25	c	509	CLA	CHC-C1C	2.80	1.42	1.35
27	7	1622	XAT	C10-C9	-2.80	1.32	1.35
28	7	1623	NEX	C7-C8	-2.80	1.27	1.32
25	y	613	CLA	MG-ND	-2.80	2.00	2.05
25	b	604	CLA	MG-ND	-2.80	2.00	2.05
25	7	603	CLA	C1D-ND	2.79	1.41	1.37
24	6	609	CHL	MG-NA	-2.79	1.99	2.06
25	c	501	CLA	C3B-C2B	-2.79	1.36	1.40
25	G	604	CLA	C3B-C2B	-2.79	1.36	1.40
28	3	1623	NEX	C7-C8	-2.79	1.27	1.32
25	B	603	CLA	CHC-C1C	2.79	1.42	1.35
24	2	609	CHL	MG-NA	-2.79	1.99	2.06
25	n	603	CLA	CMD-C2D	-2.79	1.44	1.50
25	y	603	CLA	CMB-C2B	-2.79	1.45	1.51
25	3	611	CLA	CMD-C2D	-2.79	1.44	1.50
25	y	612	CLA	C1D-ND	2.79	1.41	1.37
24	y	608	CHL	OBD-CAD	2.79	1.27	1.22
25	3	603	CLA	C1D-ND	2.79	1.41	1.37
25	B	615	CLA	C1D-ND	2.79	1.41	1.37
25	s	613	CLA	CHC-C1C	2.79	1.42	1.35
26	Y	1621	LUT	C22-C21	-2.78	1.51	1.54
25	8	610	CLA	CMC-C2C	-2.78	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	613	CLA	CHC-C1C	2.78	1.42	1.35
25	g	604	CLA	C3B-C2B	-2.78	1.36	1.40
25	g	602	CLA	CMB-C2B	-2.78	1.45	1.51
25	3	610	CLA	C3B-CAB	-2.78	1.42	1.47
25	1	603	CLA	C1D-ND	2.78	1.41	1.37
25	7	611	CLA	CMD-C2D	-2.78	1.44	1.50
29	R	2630	LHG	O7-C5	-2.78	1.39	1.46
25	y	610	CLA	CMC-C2C	-2.78	1.44	1.50
29	r	2630	LHG	O7-C5	-2.78	1.39	1.46
25	B	604	CLA	MG-ND	-2.78	2.00	2.05
25	G	603	CLA	CMB-C2B	-2.77	1.45	1.51
25	Y	602	CLA	CMC-C2C	-2.77	1.44	1.50
25	Y	610	CLA	CHC-C1C	2.77	1.42	1.35
29	c	522	LHG	O7-C5	-2.77	1.39	1.46
25	c	512	CLA	CHC-C1C	2.77	1.42	1.35
25	y	611	CLA	CHC-C1C	2.77	1.42	1.35
25	5	602	CLA	CHC-C1C	2.77	1.42	1.35
25	3	613	CLA	CMB-C2B	-2.77	1.45	1.51
25	N	603	CLA	CMB-C2B	-2.77	1.45	1.51
25	g	603	CLA	CMB-C2B	-2.77	1.45	1.51
25	B	603	CLA	C1D-ND	2.77	1.41	1.37
25	4	610	CLA	CMC-C2C	-2.77	1.44	1.50
25	G	603	CLA	CHC-C1C	2.77	1.42	1.35
25	Y	611	CLA	CHC-C1C	2.77	1.42	1.35
25	b	603	CLA	CHC-C1C	2.77	1.42	1.35
24	R	607	CHL	MG-NA	-2.77	1.99	2.06
29	C	522	LHG	O7-C5	-2.77	1.39	1.46
25	g	603	CLA	CHC-C1C	2.76	1.42	1.35
24	r	607	CHL	MG-NA	-2.76	1.99	2.06
25	6	610	CLA	CMB-C2B	-2.76	1.45	1.51
24	n	605	CHL	MG-NA	-2.76	1.99	2.06
25	b	610	CLA	C1D-ND	2.76	1.41	1.37
25	B	612	CLA	C3B-C2B	-2.76	1.36	1.40
25	Y	613	CLA	MG-ND	-2.76	2.00	2.05
25	R	602	CLA	C1D-ND	2.76	1.41	1.37
25	c	510	CLA	CMD-C2D	-2.76	1.44	1.50
25	1	610	CLA	C3B-CAB	-2.76	1.42	1.47
25	r	602	CLA	C1D-ND	2.76	1.41	1.37
25	A	410	CLA	CMB-C2B	-2.76	1.45	1.51
25	C	512	CLA	CHC-C1C	2.76	1.42	1.35
25	N	602	CLA	CHC-C1C	2.76	1.42	1.35
25	5	610	CLA	C3B-CAB	-2.76	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	410	CLA	C1D-ND	2.76	1.41	1.37
25	b	603	CLA	C1D-ND	2.76	1.41	1.37
25	2	610	CLA	CMB-C2B	-2.76	1.45	1.51
25	7	610	CLA	C3B-CAB	-2.76	1.42	1.47
25	2	611	CLA	CHC-C1C	2.76	1.42	1.35
25	R	609	CLA	C1D-ND	2.76	1.41	1.37
25	y	602	CLA	CMC-C2C	-2.76	1.45	1.50
25	2	610	CLA	CHC-C1C	2.76	1.42	1.35
25	N	603	CLA	CMD-C2D	-2.76	1.45	1.50
25	n	602	CLA	CHC-C1C	2.76	1.42	1.35
25	y	614	CLA	CMB-C2B	-2.76	1.45	1.51
24	Y	608	CHL	OBD-CAD	2.76	1.27	1.22
25	B	610	CLA	C1D-ND	2.76	1.41	1.37
25	3	610	CLA	CHC-C1C	2.75	1.42	1.35
25	7	610	CLA	CHC-C1C	2.75	1.42	1.35
25	b	612	CLA	C3B-C2B	-2.75	1.36	1.40
25	r	610	CLA	CMB-C2B	-2.75	1.45	1.51
25	b	607	CLA	C3B-C2B	-2.75	1.36	1.40
24	G	605	CHL	MG-NA	-2.75	1.99	2.06
25	y	610	CLA	CHC-C1C	2.75	1.42	1.35
25	7	612	CLA	CMB-C2B	-2.75	1.45	1.51
25	n	603	CLA	CMB-C2B	-2.75	1.45	1.51
25	B	615	CLA	CMB-C2B	-2.75	1.45	1.51
25	b	615	CLA	CMB-C2B	-2.75	1.45	1.51
25	R	610	CLA	CMB-C2B	-2.75	1.45	1.51
25	C	510	CLA	CMD-C2D	-2.75	1.45	1.50
25	6	613	CLA	C1D-ND	2.75	1.41	1.37
24	N	605	CHL	MG-NA	-2.75	1.99	2.06
25	r	604	CLA	CHC-C1C	2.74	1.42	1.35
25	Y	614	CLA	CMB-C2B	-2.74	1.45	1.51
25	2	613	CLA	C1D-ND	2.74	1.41	1.37
27	3	1622	XAT	C10-C9	-2.74	1.32	1.35
25	6	611	CLA	CHC-C1C	2.74	1.42	1.35
25	1	613	CLA	CMB-C2B	-2.74	1.45	1.51
25	D	403	CLA	CMB-C2B	-2.74	1.45	1.51
25	5	611	CLA	CMB-C2B	-2.74	1.45	1.51
25	b	613	CLA	CMC-C2C	-2.74	1.45	1.50
29	s	2630	LHG	O7-C5	-2.74	1.39	1.46
25	2	612	CLA	CMB-C2B	-2.74	1.45	1.51
25	3	611	CLA	C1D-ND	2.74	1.41	1.37
25	r	609	CLA	C1D-ND	2.74	1.41	1.37
29	S	2630	LHG	O7-C5	-2.74	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	613	CLA	CMB-C2B	-2.74	1.46	1.51
24	S	606	CHL	C3D-C2D	2.73	1.46	1.39
25	Y	610	CLA	CMC-C2C	-2.73	1.45	1.50
25	a	410	CLA	CMB-C2B	-2.73	1.46	1.51
25	b	610	CLA	CMD-C2D	-2.73	1.45	1.50
25	3	612	CLA	CMB-C2B	-2.73	1.46	1.51
25	5	613	CLA	CMB-C2B	-2.73	1.46	1.51
24	n	608	CHL	OBD-CAD	2.73	1.27	1.22
25	6	612	CLA	CMB-C2B	-2.73	1.46	1.51
25	g	613	CLA	MG-ND	-2.73	2.00	2.05
24	R	614	CHL	MG-NA	-2.73	1.99	2.06
24	s	606	CHL	C3D-C2D	2.73	1.46	1.39
25	6	610	CLA	CHC-C1C	2.73	1.42	1.35
24	N	608	CHL	OBD-CAD	2.73	1.27	1.22
25	g	610	CLA	CMB-C2B	-2.73	1.46	1.51
25	B	613	CLA	CMC-C2C	-2.73	1.45	1.50
25	c	509	CLA	CMB-C2B	-2.73	1.46	1.51
25	8	611	CLA	CHC-C1C	2.73	1.42	1.35
25	d	403	CLA	CMB-C2B	-2.73	1.46	1.51
25	G	610	CLA	CMB-C2B	-2.72	1.46	1.51
25	4	610	CLA	CMD-C2D	-2.72	1.45	1.50
24	n	607	CHL	MG-NA	-2.72	1.99	2.06
25	4	611	CLA	CHC-C1C	2.72	1.41	1.35
25	7	602	CLA	CMC-C2C	-2.72	1.45	1.50
25	R	604	CLA	CHC-C1C	2.72	1.41	1.35
24	r	614	CHL	MG-NA	-2.72	1.99	2.06
25	B	613	CLA	CMA-C3A	-2.72	1.47	1.53
24	N	607	CHL	MG-NA	-2.72	1.99	2.06
25	8	610	CLA	CMD-C2D	-2.72	1.45	1.50
25	R	602	CLA	CHC-C1C	2.72	1.41	1.35
25	R	612	CLA	CMB-C2B	-2.72	1.46	1.51
25	r	603	CLA	MG-ND	-2.72	2.00	2.05
24	g	605	CHL	MG-NA	-2.72	1.99	2.06
25	C	501	CLA	CMB-C2B	-2.71	1.46	1.51
24	n	606	CHL	MG-NA	-2.71	1.99	2.06
25	g	611	CLA	CMB-C2B	-2.71	1.46	1.51
25	R	609	CLA	CMB-C2B	-2.71	1.46	1.51
25	6	604	CLA	CMB-C2B	-2.71	1.46	1.51
30	b	618	BCR	C21-C22	-2.71	1.32	1.35
25	2	604	CLA	CMB-C2B	-2.71	1.46	1.51
25	B	607	CLA	C3B-C2B	-2.71	1.36	1.40
25	c	504	CLA	CHC-C1C	2.71	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	613	CLA	MG-ND	-2.71	2.00	2.05
25	3	612	CLA	CMD-C2D	-2.71	1.45	1.50
25	C	509	CLA	CMB-C2B	-2.71	1.46	1.51
25	c	501	CLA	CMB-C2B	-2.71	1.46	1.51
24	g	606	CHL	MG-NA	-2.71	1.99	2.06
25	1	612	CLA	CMB-C2B	-2.71	1.46	1.51
25	1	611	CLA	CMB-C2B	-2.71	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.71	1.46	1.51
34	A	412	SQD	O47-C7	2.71	1.41	1.34
24	S	608	CHL	MG-NA	-2.71	1.99	2.06
24	G	606	CHL	MG-NA	-2.71	1.99	2.06
25	B	610	CLA	CMD-C2D	-2.70	1.45	1.50
25	6	613	CLA	MG-ND	-2.70	2.00	2.05
25	C	504	CLA	CMB-C2B	-2.70	1.46	1.51
25	G	611	CLA	CMB-C2B	-2.70	1.46	1.51
24	N	606	CHL	MG-NA	-2.70	1.99	2.06
25	R	603	CLA	MG-ND	-2.70	2.00	2.05
25	r	602	CLA	CHC-C1C	2.70	1.41	1.35
25	5	613	CLA	MG-ND	-2.70	2.00	2.05
25	b	613	CLA	CMA-C3A	-2.70	1.47	1.53
25	s	613	CLA	CMB-C2B	-2.70	1.46	1.51
25	B	604	CLA	C1D-ND	2.70	1.41	1.37
25	r	612	CLA	CMB-C2B	-2.70	1.46	1.51
25	7	612	CLA	CMD-C2D	-2.70	1.45	1.50
25	g	602	CLA	CHC-C1C	2.70	1.41	1.35
34	a	412	SQD	O47-C7	2.70	1.41	1.34
25	3	602	CLA	CMC-C2C	-2.70	1.45	1.50
25	B	608	CLA	CMC-C2C	-2.70	1.45	1.50
24	8	601	CHL	C1D-C2D	2.70	1.50	1.45
25	C	504	CLA	CHC-C1C	2.70	1.41	1.35
25	r	609	CLA	CMB-C2B	-2.70	1.46	1.51
25	5	602	CLA	CMB-C2B	-2.69	1.46	1.51
25	1	602	CLA	CMB-C2B	-2.69	1.46	1.51
25	r	603	CLA	CHC-C1C	2.69	1.41	1.35
25	b	616	CLA	CMB-C2B	-2.69	1.46	1.51
24	s	601	CHL	C1D-C2D	2.69	1.50	1.45
25	7	603	CLA	CMB-C2B	-2.69	1.46	1.51
25	b	604	CLA	C1D-ND	2.69	1.41	1.37
24	s	608	CHL	MG-NA	-2.69	1.99	2.06
24	S	601	CHL	C1D-C2D	2.69	1.50	1.45
25	r	610	CLA	C3B-C2B	-2.69	1.36	1.40
26	N	1621	LUT	C22-C21	-2.69	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	609	CHL	C1B-NB	-2.69	1.32	1.35
25	1	613	CLA	MG-ND	-2.69	2.00	2.05
25	C	502	CLA	CMB-C2B	-2.69	1.46	1.51
35	b	622	LMG	O8-C9	-2.69	1.39	1.45
25	c	504	CLA	CMB-C2B	-2.69	1.46	1.51
25	G	602	CLA	CHC-C1C	2.69	1.41	1.35
25	N	611	CLA	CHC-C1C	2.69	1.41	1.35
30	B	618	BCR	C21-C22	-2.69	1.32	1.35
25	R	610	CLA	C3B-C2B	-2.68	1.36	1.40
25	B	607	CLA	CMC-C2C	-2.68	1.45	1.50
25	b	608	CLA	CMC-C2C	-2.68	1.45	1.50
26	n	1621	LUT	C22-C21	-2.68	1.51	1.54
25	2	613	CLA	MG-ND	-2.68	2.00	2.05
25	2	602	CLA	CMC-C2C	-2.68	1.45	1.50
24	4	601	CHL	C1D-C2D	2.68	1.50	1.45
25	A	410	CLA	CHC-C1C	2.68	1.41	1.35
25	7	611	CLA	C1D-ND	2.68	1.41	1.37
25	y	614	CLA	CMD-C2D	-2.68	1.45	1.50
25	Y	614	CLA	CMD-C2D	-2.68	1.45	1.50
25	3	614	CLA	CMB-C2B	-2.68	1.46	1.51
25	g	612	CLA	CHC-C1C	2.68	1.41	1.35
25	1	604	CLA	C1D-ND	2.68	1.41	1.37
25	n	610	CLA	CMB-C2B	-2.68	1.46	1.51
25	Y	611	CLA	CMD-C2D	-2.68	1.45	1.50
25	G	612	CLA	CHC-C1C	2.68	1.41	1.35
25	3	603	CLA	CMD-C2D	-2.68	1.45	1.50
25	5	604	CLA	C1D-ND	2.67	1.41	1.37
25	b	609	CLA	C1D-ND	2.67	1.41	1.37
25	R	603	CLA	CHC-C1C	2.67	1.41	1.35
25	B	603	CLA	CMB-C2B	-2.67	1.46	1.51
25	b	615	CLA	C3B-C2B	-2.67	1.36	1.40
25	b	612	CLA	CMD-C2D	-2.67	1.45	1.50
25	n	603	CLA	CHC-C1C	2.67	1.41	1.35
25	y	611	CLA	CMD-C2D	-2.67	1.45	1.50
25	n	611	CLA	CHC-C1C	2.67	1.41	1.35
25	b	603	CLA	CMB-C2B	-2.67	1.46	1.51
25	3	612	CLA	C1D-ND	2.67	1.41	1.37
25	b	614	CLA	C1D-ND	2.67	1.41	1.37
25	B	602	CLA	CMD-C2D	-2.67	1.45	1.50
35	B	622	LMG	O8-C9	-2.67	1.39	1.45
24	S	607	CHL	C3D-C2D	2.67	1.46	1.39
26	y	1620	LUT	C22-C21	-2.67	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	601	CHL	OBD-CAD	2.67	1.27	1.22
25	N	610	CLA	CMB-C2B	-2.67	1.46	1.51
25	6	602	CLA	CMC-C2C	-2.67	1.45	1.50
24	6	601	CHL	C1D-C2D	2.66	1.50	1.45
25	b	605	CLA	MG-ND	-2.66	2.00	2.05
25	N	603	CLA	CHC-C1C	2.66	1.41	1.35
25	r	603	CLA	C1D-ND	2.66	1.41	1.37
25	N	611	CLA	CMB-C2B	-2.66	1.46	1.51
25	B	615	CLA	C3B-C2B	-2.66	1.36	1.40
25	7	603	CLA	CMD-C2D	-2.66	1.45	1.50
25	1	611	CLA	C3B-C2B	-2.66	1.36	1.40
25	2	613	CLA	CHC-C1C	2.66	1.41	1.35
25	a	410	CLA	CHC-C1C	2.66	1.41	1.35
25	A	405	CLA	CHC-C1C	2.66	1.41	1.35
25	B	602	CLA	CMB-C2B	-2.66	1.46	1.51
25	S	613	CLA	CMB-C2B	-2.66	1.46	1.51
25	a	405	CLA	CHC-C1C	2.66	1.41	1.35
26	8	620	LUT	C22-C21	-2.66	1.51	1.54
25	b	607	CLA	CMC-C2C	-2.66	1.45	1.50
24	G	601	CHL	OBD-CAD	2.66	1.27	1.22
25	B	614	CLA	C1D-ND	2.66	1.41	1.37
25	4	602	CLA	CMB-C2B	-2.66	1.46	1.51
24	2	608	CHL	MG-NA	-2.66	2.00	2.06
25	y	613	CLA	CMB-C2B	-2.66	1.46	1.51
25	y	602	CLA	CHC-C1C	2.66	1.41	1.35
25	5	612	CLA	CMB-C2B	-2.66	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.66	1.46	1.51
25	3	603	CLA	CMB-C2B	-2.65	1.46	1.51
25	b	602	CLA	CMB-C2B	-2.65	1.46	1.51
24	s	607	CHL	C3D-C2D	2.65	1.46	1.39
25	6	613	CLA	CHC-C1C	2.65	1.41	1.35
25	n	613	CLA	CHC-C1C	2.65	1.41	1.35
25	B	605	CLA	MG-ND	-2.65	2.00	2.05
25	R	603	CLA	C1D-ND	2.65	1.41	1.37
25	Y	602	CLA	CHC-C1C	2.65	1.41	1.35
25	Y	613	CLA	CMB-C2B	-2.65	1.46	1.51
25	8	602	CLA	CMB-C2B	-2.65	1.46	1.51
25	B	609	CLA	C1D-ND	2.65	1.41	1.37
25	y	604	CLA	CHC-C1C	2.65	1.41	1.35
25	R	610	CLA	CHC-C1C	2.65	1.41	1.35
25	Y	603	CLA	CMD-C2D	-2.65	1.45	1.50
24	5	607	CHL	C1D-C2D	2.64	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	7	1622	XAT	C14-C13	-2.64	1.32	1.35
26	4	620	LUT	C22-C21	-2.64	1.51	1.54
24	N	609	CHL	MG-NA	-2.64	2.00	2.06
26	Y	1620	LUT	C22-C21	-2.64	1.51	1.54
25	N	612	CLA	CMB-C2B	-2.64	1.46	1.51
25	n	614	CLA	CMB-C2B	-2.64	1.46	1.51
24	6	608	CHL	MG-NA	-2.64	2.00	2.06
24	n	609	CHL	MG-NA	-2.64	2.00	2.06
25	b	602	CLA	CMD-C2D	-2.64	1.45	1.50
25	B	612	CLA	CMD-C2D	-2.64	1.45	1.50
25	Y	604	CLA	CHC-C1C	2.64	1.41	1.35
25	6	614	CLA	CMB-C2B	-2.64	1.46	1.51
25	r	610	CLA	CHC-C1C	2.64	1.41	1.35
24	2	601	CHL	C1D-C2D	2.63	1.50	1.45
24	Y	606	CHL	MG-NA	-2.63	2.00	2.06
25	7	614	CLA	CMB-C2B	-2.63	1.46	1.51
25	2	614	CLA	CMB-C2B	-2.63	1.46	1.51
24	y	606	CHL	MG-NA	-2.63	2.00	2.06
24	n	608	CHL	MG-NA	-2.63	2.00	2.06
25	n	612	CLA	CMB-C2B	-2.63	1.46	1.51
25	5	614	CLA	CMB-C2B	-2.63	1.46	1.51
25	r	616	CLA	C3B-C2B	-2.63	1.36	1.40
24	G	605	CHL	C1D-C2D	2.63	1.50	1.45
25	8	604	CLA	CHC-C1C	2.63	1.41	1.35
26	G	1621	LUT	C22-C21	-2.63	1.51	1.54
25	5	613	CLA	C3B-C2B	-2.63	1.36	1.40
25	n	611	CLA	CMB-C2B	-2.63	1.46	1.51
25	N	613	CLA	CHC-C1C	2.63	1.41	1.35
25	2	613	CLA	CMB-C2B	-2.63	1.46	1.51
25	7	602	CLA	CMB-C2B	-2.63	1.46	1.51
25	1	614	CLA	CMB-C2B	-2.62	1.46	1.51
25	4	604	CLA	CHC-C1C	2.62	1.41	1.35
24	2	601	CHL	MG-NA	-2.62	2.00	2.06
25	y	603	CLA	CMD-C2D	-2.62	1.45	1.50
25	3	602	CLA	CHC-C1C	2.62	1.41	1.35
26	g	1621	LUT	C22-C21	-2.62	1.51	1.54
25	G	611	CLA	C3B-C2B	-2.62	1.36	1.40
24	g	608	CHL	MG-NA	-2.62	2.00	2.06
25	8	603	CLA	CMB-C2B	-2.62	1.46	1.51
25	c	505	CLA	CHC-C1C	2.62	1.41	1.35
25	7	612	CLA	C1D-ND	2.62	1.41	1.37
24	1	607	CHL	C1D-C2D	2.62	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	605	CLA	C3B-C2B	-2.62	1.36	1.40
25	4	603	CLA	CMB-C2B	-2.62	1.46	1.51
25	Y	614	CLA	CHC-C1C	2.62	1.41	1.35
25	A	407	CLA	CHC-C1C	2.62	1.41	1.35
25	C	502	CLA	CHC-C1C	2.62	1.41	1.35
25	R	613	CLA	CHC-C1C	2.62	1.41	1.35
27	3	1622	XAT	C34-C33	-2.62	1.32	1.35
25	B	611	CLA	MG-ND	-2.62	2.00	2.05
25	5	611	CLA	C3B-C2B	-2.62	1.36	1.40
25	7	602	CLA	CHC-C1C	2.62	1.41	1.35
25	R	611	CLA	CMB-C2B	-2.62	1.46	1.51
25	R	612	CLA	CHC-C1C	2.62	1.41	1.35
25	a	410	CLA	C3B-C2B	-2.62	1.36	1.40
26	5	1621	LUT	C10-C9	-2.62	1.32	1.35
24	G	608	CHL	MG-NA	-2.62	2.00	2.06
24	R	606	CHL	MG-NA	-2.62	2.00	2.06
24	8	606	CHL	MG-NA	-2.61	2.00	2.06
24	5	607	CHL	C1C-NC	-2.61	1.33	1.37
25	y	614	CLA	CHC-C1C	2.61	1.41	1.35
24	4	606	CHL	MG-NA	-2.61	2.00	2.06
25	c	502	CLA	CHC-C1C	2.61	1.41	1.35
25	b	611	CLA	MG-ND	-2.61	2.00	2.05
25	a	407	CLA	CHC-C1C	2.61	1.41	1.35
25	N	614	CLA	CMB-C2B	-2.61	1.46	1.51
25	b	611	CLA	CHC-C1C	2.61	1.41	1.35
25	r	611	CLA	CMB-C2B	-2.61	1.46	1.51
25	r	613	CLA	CHC-C1C	2.61	1.41	1.35
36	D	405	PL9	C46-C44	-2.61	1.45	1.51
27	3	1622	XAT	C14-C13	-2.61	1.32	1.35
24	5	609	CHL	C1D-C2D	2.61	1.50	1.45
25	c	507	CLA	CHC-C1C	2.61	1.41	1.35
36	d	405	PL9	C46-C44	-2.61	1.45	1.51
25	c	508	CLA	CHC-C1C	2.61	1.41	1.35
25	r	612	CLA	CHC-C1C	2.61	1.41	1.35
25	R	616	CLA	C3B-C2B	-2.61	1.36	1.40
25	b	611	CLA	C1D-ND	2.61	1.41	1.37
25	3	602	CLA	CMB-C2B	-2.61	1.46	1.51
24	6	601	CHL	MG-NA	-2.61	2.00	2.06
24	r	606	CHL	MG-NA	-2.61	2.00	2.06
24	7	608	CHL	MG-NA	-2.61	2.00	2.06
25	6	613	CLA	CMB-C2B	-2.61	1.46	1.51
25	b	606	CLA	CMD-C2D	-2.61	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	CHC-C1C	2.60	1.41	1.35
24	1	609	CHL	C1D-C2D	2.60	1.50	1.45
24	g	605	CHL	C1D-C2D	2.60	1.50	1.45
36	D	405	PL9	C21-C19	-2.60	1.45	1.51
24	N	608	CHL	MG-NA	-2.60	2.00	2.06
24	Y	601	CHL	OBD-CAD	2.60	1.27	1.22
26	1	1621	LUT	C10-C9	-2.60	1.32	1.35
25	1	613	CLA	C3B-C2B	-2.60	1.36	1.40
25	c	506	CLA	CHC-C1C	2.60	1.41	1.35
25	b	609	CLA	CHC-C1C	2.60	1.41	1.35
37	c	519	DGD	O1G-C1G	-2.60	1.39	1.45
25	B	609	CLA	CHC-C1C	2.60	1.41	1.35
25	1	610	CLA	CMB-C2B	-2.60	1.46	1.51
36	d	405	PL9	C21-C19	-2.60	1.45	1.51
25	y	614	CLA	C3B-CAB	-2.60	1.42	1.47
25	N	613	CLA	MG-ND	-2.59	2.00	2.05
25	N	604	CLA	CHC-C1C	2.59	1.41	1.35
37	C	519	DGD	O1G-C1G	-2.59	1.39	1.45
25	8	603	CLA	CHC-C1C	2.59	1.41	1.35
25	B	611	CLA	C3B-CAB	-2.59	1.42	1.47
25	B	611	CLA	CHC-C1C	2.59	1.41	1.35
25	b	614	CLA	C3B-C2B	-2.59	1.36	1.40
25	C	505	CLA	CHC-C1C	2.59	1.41	1.35
25	C	507	CLA	CHC-C1C	2.59	1.41	1.35
25	Y	614	CLA	C3B-CAB	-2.59	1.42	1.47
24	3	608	CHL	MG-NA	-2.59	2.00	2.06
24	N	609	CHL	C1B-NB	-2.59	1.32	1.35
27	7	1622	XAT	C34-C33	-2.59	1.32	1.35
25	5	610	CLA	CMB-C2B	-2.59	1.46	1.51
25	4	603	CLA	CHC-C1C	2.59	1.41	1.35
25	B	602	CLA	C3B-C2B	-2.59	1.36	1.40
36	d	405	PL9	C2-C1	-2.59	1.37	1.44
25	B	606	CLA	CMD-C2D	-2.59	1.45	1.50
25	B	616	CLA	CMC-C2C	-2.59	1.45	1.50
25	b	616	CLA	CMC-C2C	-2.59	1.45	1.50
25	B	605	CLA	C3B-C2B	-2.59	1.36	1.40
24	S	608	CHL	C3D-C2D	2.59	1.46	1.39
25	b	602	CLA	C3B-C2B	-2.59	1.36	1.40
24	8	608	CHL	OBD-CAD	2.58	1.26	1.22
25	N	602	CLA	CMC-C2C	-2.58	1.45	1.50
25	n	602	CLA	CMC-C2C	-2.58	1.45	1.50
25	g	611	CLA	C3B-C2B	-2.58	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	607	CHL	C1D-C2D	2.58	1.50	1.45
25	B	614	CLA	CMC-C2C	-2.58	1.45	1.50
25	1	610	CLA	CHC-C1C	2.58	1.41	1.35
25	n	604	CLA	CHC-C1C	2.58	1.41	1.35
25	2	613	CLA	CMD-C2D	-2.58	1.45	1.50
25	5	610	CLA	CHC-C1C	2.58	1.41	1.35
25	B	606	CLA	CMC-C2C	-2.58	1.45	1.50
25	6	613	CLA	CMD-C2D	-2.58	1.45	1.50
25	g	610	CLA	CHC-C1C	2.58	1.41	1.35
24	1	607	CHL	C1C-NC	-2.58	1.34	1.37
25	r	604	CLA	CMD-C2D	-2.58	1.45	1.50
25	C	506	CLA	CHC-C1C	2.58	1.41	1.35
25	R	604	CLA	CMD-C2D	-2.58	1.45	1.50
24	4	608	CHL	OBD-CAD	2.57	1.26	1.22
28	g	1623	NEX	C7-C8	-2.57	1.27	1.32
25	6	603	CLA	CHC-C1C	2.57	1.41	1.35
25	b	615	CLA	CMC-C2C	-2.57	1.45	1.50
24	y	601	CHL	OBD-CAD	2.57	1.26	1.22
25	Y	604	CLA	C1D-ND	2.57	1.40	1.37
25	G	614	CLA	CMB-C2B	-2.57	1.46	1.51
24	r	607	CHL	C1D-C2D	2.57	1.50	1.45
25	2	611	CLA	CMB-C2B	-2.57	1.46	1.51
25	n	613	CLA	MG-ND	-2.57	2.00	2.05
26	3	1620	LUT	C22-C21	-2.57	1.51	1.54
24	7	605	CHL	MG-NA	-2.57	2.00	2.06
25	B	604	CLA	CMD-C2D	-2.57	1.45	1.50
37	c	518	DGD	O1G-C1G	-2.57	1.39	1.45
25	b	611	CLA	CMD-C2D	-2.57	1.45	1.50
25	g	614	CLA	CMB-C2B	-2.57	1.46	1.51
25	n	614	CLA	CHC-C1C	2.57	1.41	1.35
36	D	405	PL9	C2-C1	-2.57	1.37	1.44
25	2	603	CLA	CMB-C2B	-2.57	1.46	1.51
25	6	603	CLA	CMB-C2B	-2.57	1.46	1.51
24	s	601	CHL	MG-NA	-2.57	2.00	2.06
24	s	608	CHL	C3D-C2D	2.57	1.46	1.39
25	b	611	CLA	C3B-CAB	-2.56	1.42	1.47
25	G	610	CLA	CHC-C1C	2.56	1.41	1.35
25	b	614	CLA	CMC-C2C	-2.56	1.45	1.50
37	C	518	DGD	O1G-C1G	-2.56	1.39	1.45
25	B	611	CLA	C1D-ND	2.56	1.40	1.37
25	B	611	CLA	CMD-C2D	-2.56	1.45	1.50
25	A	410	CLA	C3B-C2B	-2.56	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	1621	LUT	C1-C6	-2.56	1.50	1.53
25	a	405	CLA	CMD-C2D	-2.56	1.45	1.50
25	3	603	CLA	MG-ND	-2.56	2.00	2.05
24	S	601	CHL	MG-NA	-2.56	2.00	2.06
25	2	603	CLA	CHC-C1C	2.56	1.41	1.35
25	b	604	CLA	CMD-C2D	-2.56	1.45	1.50
24	g	609	CHL	MG-NA	-2.56	2.00	2.06
25	G	604	CLA	CHC-C1C	2.56	1.41	1.35
25	6	611	CLA	CMB-C2B	-2.56	1.46	1.51
25	b	606	CLA	CMC-C2C	-2.56	1.45	1.50
24	7	609	CHL	C1D-C2D	2.56	1.50	1.45
37	c	520	DGD	O5D-C6D	-2.56	1.39	1.43
25	7	611	CLA	MG-ND	-2.55	2.00	2.05
25	5	604	CLA	MG-ND	-2.55	2.00	2.05
24	3	605	CHL	C3D-C2D	2.55	1.46	1.39
25	b	608	CLA	CMD-C2D	-2.55	1.45	1.50
24	6	605	CHL	C3D-C2D	2.55	1.46	1.39
26	7	1620	LUT	C22-C21	-2.55	1.51	1.54
25	r	612	CLA	C3B-C2B	-2.55	1.36	1.40
25	6	602	CLA	CMB-C2B	-2.55	1.46	1.51
25	Y	612	CLA	CMD-C2D	-2.55	1.45	1.50
28	G	1623	NEX	C7-C8	-2.55	1.27	1.32
25	1	602	CLA	C3B-C2B	-2.55	1.36	1.40
25	s	610	CLA	CMB-C2B	-2.55	1.46	1.51
25	7	603	CLA	MG-ND	-2.54	2.00	2.05
25	8	603	CLA	CMD-C2D	-2.54	1.45	1.50
25	4	603	CLA	CMD-C2D	-2.54	1.45	1.50
25	c	505	CLA	CMD-C2D	-2.54	1.45	1.50
25	b	609	CLA	CMD-C2D	-2.54	1.45	1.50
25	3	611	CLA	MG-ND	-2.54	2.00	2.05
29	c	2630	LHG	O7-C5	-2.54	1.40	1.46
33	a	408	PHO	CAC-C3C	-2.54	1.47	1.52
25	5	604	CLA	C3B-CAB	-2.54	1.42	1.47
25	b	609	CLA	CMB-C2B	-2.54	1.46	1.51
24	5	605	CHL	C3D-C2D	2.54	1.46	1.39
37	C	520	DGD	O5D-C6D	-2.54	1.39	1.43
25	g	604	CLA	CHC-C1C	2.54	1.41	1.35
25	r	601	CLA	CMB-C2B	-2.54	1.46	1.51
24	6	609	CHL	C1D-C2D	2.54	1.50	1.45
25	N	614	CLA	CHC-C1C	2.54	1.41	1.35
24	3	605	CHL	MG-NA	-2.54	2.00	2.06
25	R	601	CLA	CMB-C2B	-2.54	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	615	CLA	CHC-C1C	2.54	1.41	1.35
25	5	603	CLA	MG-ND	-2.54	2.00	2.05
25	B	615	CLA	CMC-C2C	-2.54	1.45	1.50
29	C	2630	LHG	O7-C5	-2.54	1.40	1.46
25	B	609	CLA	CMD-C2D	-2.54	1.45	1.50
33	A	408	PHO	CAC-C3C	-2.54	1.47	1.52
25	B	603	CLA	C3B-C2B	-2.54	1.36	1.40
25	B	608	CLA	CMD-C2D	-2.53	1.45	1.50
24	7	605	CHL	C3D-C2D	2.53	1.46	1.39
25	y	604	CLA	C1D-ND	2.53	1.40	1.37
25	y	603	CLA	MG-ND	-2.53	2.00	2.05
25	D	403	CLA	CMD-C2D	-2.53	1.45	1.50
25	B	608	CLA	CHC-C1C	2.53	1.41	1.35
24	G	609	CHL	MG-NA	-2.53	2.00	2.06
25	A	405	CLA	CMD-C2D	-2.53	1.45	1.50
25	B	604	CLA	CHC-C1C	2.53	1.41	1.35
25	s	611	CLA	CMB-C2B	-2.53	1.46	1.51
24	2	609	CHL	C1D-C2D	2.53	1.50	1.45
24	s	607	CHL	C1D-C2D	2.53	1.50	1.45
24	S	607	CHL	C1D-C2D	2.53	1.50	1.45
35	B	622	LMG	O7-C8	-2.53	1.40	1.46
25	b	615	CLA	CHC-C1C	2.53	1.41	1.35
36	d	405	PL9	C35-C34	-2.53	1.44	1.50
24	2	605	CHL	C3D-C2D	2.53	1.46	1.39
25	B	609	CLA	CMB-C2B	-2.53	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.53	1.46	1.51
24	1	605	CHL	C3D-C2D	2.53	1.46	1.39
25	1	603	CLA	MG-ND	-2.53	2.00	2.05
25	1	604	CLA	MG-ND	-2.53	2.00	2.05
25	7	602	CLA	CMD-C2D	-2.53	1.45	1.50
25	4	611	CLA	CMB-C2B	-2.52	1.46	1.51
27	Y	1622	XAT	C10-C9	-2.52	1.32	1.35
24	s	606	CHL	C4B-CHC	2.52	1.48	1.41
25	C	511	CLA	CMB-C2B	-2.52	1.46	1.51
25	8	611	CLA	CMB-C2B	-2.52	1.46	1.51
25	Y	603	CLA	MG-ND	-2.52	2.00	2.05
25	R	612	CLA	C3B-C2B	-2.52	1.36	1.40
25	1	604	CLA	C3B-CAB	-2.52	1.42	1.47
24	S	606	CHL	C4B-CHC	2.52	1.48	1.41
25	S	610	CLA	CMB-C2B	-2.52	1.46	1.51
25	8	610	CLA	CMB-C2B	-2.52	1.46	1.51
25	b	604	CLA	C3B-CAB	-2.52	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	604	CLA	CHC-C1C	2.52	1.41	1.35
25	B	614	CLA	C3B-C2B	-2.52	1.36	1.40
25	5	602	CLA	C3B-C2B	-2.52	1.36	1.40
25	B	616	CLA	CHC-C1C	2.52	1.41	1.35
25	6	603	CLA	MG-ND	-2.52	2.00	2.05
25	r	611	CLA	CHC-C1C	2.52	1.41	1.35
26	y	1620	LUT	C14-C13	-2.52	1.32	1.35
35	b	622	LMG	O7-C8	-2.52	1.40	1.46
24	4	607	CHL	C1D-C2D	2.52	1.50	1.45
25	G	613	CLA	CHC-C1C	2.52	1.41	1.35
25	2	602	CLA	CMB-C2B	-2.52	1.46	1.51
36	D	405	PL9	C35-C34	-2.52	1.44	1.50
25	2	603	CLA	MG-ND	-2.52	2.00	2.05
25	b	613	CLA	CHC-C1C	2.52	1.41	1.35
25	4	610	CLA	CMB-C2B	-2.52	1.46	1.51
25	g	613	CLA	CHC-C1C	2.52	1.41	1.35
25	b	608	CLA	CHC-C1C	2.52	1.41	1.35
25	s	602	CLA	CMB-C2B	-2.51	1.46	1.51
25	C	509	CLA	CMD-C2D	-2.51	1.45	1.50
24	3	609	CHL	C1D-C2D	2.51	1.50	1.45
25	S	604	CLA	CMB-C2B	-2.51	1.46	1.51
25	3	602	CLA	CMD-C2D	-2.51	1.45	1.50
25	d	402	CLA	CHC-C1C	2.51	1.41	1.35
24	3	605	CHL	C1D-C2D	2.51	1.50	1.45
24	2	606	CHL	MG-NA	-2.51	2.00	2.06
25	b	616	CLA	CHC-C1C	2.51	1.41	1.35
25	c	505	CLA	CMB-C2B	-2.51	1.46	1.51
25	b	604	CLA	CHC-C1C	2.51	1.41	1.35
25	R	611	CLA	CHC-C1C	2.51	1.41	1.35
25	B	613	CLA	CHC-C1C	2.51	1.41	1.35
25	A	407	CLA	C3B-C2B	-2.51	1.36	1.40
25	Y	602	CLA	CMD-C2D	-2.51	1.45	1.50
25	3	604	CLA	CHC-C1C	2.51	1.41	1.35
25	d	403	CLA	CMD-C2D	-2.50	1.45	1.50
25	y	612	CLA	CMD-C2D	-2.50	1.45	1.50
24	5	606	CHL	MG-NA	-2.50	2.00	2.06
25	c	511	CLA	CMB-C2B	-2.50	1.46	1.51
25	a	407	CLA	C3B-C2B	-2.50	1.36	1.40
24	6	606	CHL	MG-NA	-2.50	2.00	2.06
25	Y	612	CLA	MG-ND	-2.50	2.00	2.05
25	y	612	CLA	MG-ND	-2.50	2.00	2.05
25	D	402	CLA	CHC-C1C	2.50	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	CMD-C2D	-2.50	1.45	1.50
25	R	602	CLA	CMB-C2B	-2.50	1.46	1.51
24	7	605	CHL	C1D-C2D	2.50	1.50	1.45
25	B	604	CLA	C3B-CAB	-2.50	1.42	1.47
25	S	611	CLA	CMB-C2B	-2.49	1.46	1.51
25	7	613	CLA	MG-ND	-2.49	2.00	2.05
25	N	613	CLA	CMB-C2B	-2.49	1.46	1.51
24	g	605	CHL	C3D-C2D	2.49	1.45	1.39
24	S	606	CHL	MG-NA	-2.49	2.00	2.06
24	6	607	CHL	C3D-C2D	2.49	1.45	1.39
25	y	602	CLA	CMD-C2D	-2.49	1.45	1.50
24	G	605	CHL	C3D-C2D	2.49	1.45	1.39
24	8	606	CHL	C1D-C2D	2.49	1.50	1.45
25	b	607	CLA	CMD-C2D	-2.49	1.45	1.50
27	y	1622	XAT	C10-C9	-2.49	1.32	1.35
25	r	602	CLA	CMB-C2B	-2.49	1.46	1.51
26	1	1621	LUT	C1-C6	-2.49	1.50	1.53
25	5	611	CLA	CHC-C1C	2.49	1.41	1.35
25	3	613	CLA	MG-ND	-2.49	2.00	2.05
25	A	410	CLA	CMD-C2D	-2.49	1.45	1.50
26	Y	1620	LUT	C14-C13	-2.49	1.32	1.35
25	B	607	CLA	CMD-C2D	-2.49	1.45	1.50
25	1	611	CLA	CHC-C1C	2.49	1.41	1.35
25	S	602	CLA	CMB-C2B	-2.49	1.46	1.51
25	s	604	CLA	CMB-C2B	-2.49	1.46	1.51
25	1	602	CLA	CMC-C2C	-2.49	1.45	1.50
25	r	604	CLA	C3B-C2B	-2.49	1.36	1.40
25	5	602	CLA	C3B-CAB	-2.49	1.42	1.47
25	3	603	CLA	CHC-C1C	2.48	1.41	1.35
24	2	607	CHL	C3D-C2D	2.48	1.45	1.39
25	4	603	CLA	MG-ND	-2.48	2.00	2.05
25	D	403	CLA	CHC-C1C	2.48	1.41	1.35
30	b	620	BCR	C1-C6	-2.48	1.50	1.53
25	Y	610	CLA	CMD-C2D	-2.48	1.45	1.50
25	c	509	CLA	CMD-C2D	-2.48	1.45	1.50
25	n	613	CLA	CMB-C2B	-2.48	1.46	1.51
25	b	613	CLA	C3B-CAB	-2.48	1.42	1.47
24	1	606	CHL	MG-NA	-2.48	2.00	2.06
24	1	601	CHL	C1D-C2D	2.47	1.50	1.45
25	8	603	CLA	MG-ND	-2.47	2.00	2.05
30	B	620	BCR	C1-C6	-2.47	1.50	1.53
25	r	602	CLA	CMC-C2C	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	607	CHL	C1D-C2D	2.47	1.50	1.45
25	b	610	CLA	CHC-C1C	2.47	1.41	1.35
25	r	611	CLA	C3B-C2B	-2.47	1.36	1.40
37	H	102	DGD	O3E-C3E	-2.47	1.37	1.43
25	c	507	CLA	CMB-C2B	-2.47	1.46	1.51
25	a	410	CLA	CMD-C2D	-2.47	1.45	1.50
25	C	503	CLA	CMB-C2B	-2.47	1.46	1.51
25	d	403	CLA	CHC-C1C	2.47	1.41	1.35
25	R	604	CLA	C3B-C2B	-2.47	1.36	1.40
25	c	508	CLA	CMC-C2C	-2.47	1.45	1.50
25	N	604	CLA	CMD-C2D	-2.47	1.45	1.50
25	c	503	CLA	CMB-C2B	-2.47	1.46	1.51
24	R	614	CHL	C3D-C2D	2.47	1.45	1.39
25	b	603	CLA	C3B-C2B	-2.47	1.36	1.40
25	G	612	CLA	CMD-C2D	-2.47	1.45	1.50
25	Y	614	CLA	MG-ND	-2.47	2.00	2.05
25	1	602	CLA	C3B-CAB	-2.47	1.42	1.47
25	Y	610	CLA	C3B-CAB	-2.46	1.42	1.47
37	h	102	DGD	O3E-C3E	-2.46	1.37	1.43
25	A	405	CLA	CMB-C2B	-2.46	1.46	1.51
25	B	610	CLA	CHC-C1C	2.46	1.41	1.35
25	y	610	CLA	CMD-C2D	-2.46	1.45	1.50
24	8	609	CHL	C1D-C2D	2.46	1.50	1.45
25	5	614	CLA	CMD-C2D	-2.46	1.45	1.50
25	5	602	CLA	CMC-C2C	-2.46	1.45	1.50
24	5	601	CHL	C1D-C2D	2.46	1.50	1.45
25	5	604	CLA	CHC-C1C	2.46	1.41	1.35
25	3	612	CLA	MG-ND	-2.46	2.00	2.05
25	B	613	CLA	C3B-CAB	-2.46	1.42	1.47
25	1	602	CLA	MG-ND	-2.46	2.00	2.05
25	b	602	CLA	CHC-C1C	2.46	1.41	1.35
25	1	604	CLA	CHC-C1C	2.46	1.41	1.35
25	6	611	CLA	MG-ND	-2.46	2.00	2.05
24	s	606	CHL	MG-NA	-2.46	2.00	2.06
25	7	603	CLA	CHC-C1C	2.46	1.41	1.35
24	N	601	CHL	C1D-C2D	2.46	1.50	1.45
25	G	612	CLA	CMB-C2B	-2.46	1.46	1.51
25	C	508	CLA	CMC-C2C	-2.46	1.45	1.50
25	y	614	CLA	MG-ND	-2.46	2.00	2.05
25	g	612	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	617	CLA	CMD-C2D	-2.45	1.45	1.50
25	R	611	CLA	C3B-C2B	-2.45	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	612	CLA	C3B-C2B	-2.45	1.37	1.40
36	d	405	PL9	C31-C29	-2.45	1.46	1.51
25	y	610	CLA	C3B-CAB	-2.45	1.42	1.47
25	5	602	CLA	MG-ND	-2.45	2.00	2.05
25	y	604	CLA	CMC-C2C	-2.45	1.45	1.50
24	4	607	CHL	C3D-C2D	2.45	1.45	1.39
25	g	612	CLA	CMD-C2D	-2.45	1.45	1.50
24	4	606	CHL	C1D-C2D	2.45	1.50	1.45
24	y	609	CHL	C1B-NB	-2.45	1.33	1.35
25	N	612	CLA	C3B-C2B	-2.45	1.37	1.40
25	C	507	CLA	CMB-C2B	-2.45	1.46	1.51
25	a	405	CLA	CMB-C2B	-2.45	1.46	1.51
25	2	611	CLA	MG-ND	-2.45	2.00	2.05
24	S	601	CHL	C3D-C2D	2.45	1.45	1.39
25	r	613	CLA	C3B-CAB	-2.45	1.42	1.47
29	5	2630	LHG	O7-C5	-2.45	1.40	1.46
25	7	612	CLA	MG-ND	-2.45	2.00	2.05
25	R	610	CLA	CMD-C2D	-2.45	1.45	1.50
25	7	613	CLA	CMD-C2D	-2.45	1.45	1.50
25	b	617	CLA	CMD-C2D	-2.45	1.45	1.50
24	n	601	CHL	C1D-C2D	2.45	1.50	1.45
25	3	612	CLA	CHC-C1C	2.45	1.41	1.35
25	B	602	CLA	CHC-C1C	2.44	1.41	1.35
25	b	612	CLA	C3B-CAB	-2.44	1.43	1.47
25	Y	603	CLA	CHC-C1C	2.44	1.41	1.35
25	7	612	CLA	CHC-C1C	2.44	1.41	1.35
25	Y	613	CLA	C4B-CHC	-2.44	1.34	1.41
24	s	601	CHL	C3D-C2D	2.44	1.45	1.39
36	D	405	PL9	C31-C29	-2.44	1.46	1.51
24	5	605	CHL	C1C-NC	-2.44	1.34	1.37
25	G	613	CLA	CMB-C2B	-2.44	1.46	1.51
24	Y	606	CHL	C1B-NB	-2.44	1.33	1.35
25	R	602	CLA	CMC-C2C	-2.44	1.45	1.50
25	6	612	CLA	CHC-C1C	2.44	1.41	1.35
25	a	406	CLA	CHC-C1C	2.44	1.41	1.35
25	2	613	CLA	C3B-C2B	-2.44	1.37	1.40
25	y	613	CLA	C4B-CHC	-2.44	1.34	1.41
25	1	613	CLA	CHC-C1C	2.44	1.41	1.35
29	1	2630	LHG	O7-C5	-2.44	1.40	1.46
25	A	407	CLA	CMD-C2D	-2.44	1.45	1.50
25	6	602	CLA	CMD-C2D	-2.44	1.45	1.50
25	y	612	CLA	CHC-C1C	2.44	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	613	CLA	C3B-CAB	-2.44	1.43	1.47
29	B	2630	LHG	O7-C5	-2.44	1.40	1.46
25	5	604	CLA	CMD-C2D	-2.44	1.45	1.50
25	n	604	CLA	CMD-C2D	-2.44	1.45	1.50
25	S	610	CLA	C3B-CAB	-2.44	1.43	1.47
24	4	609	CHL	C1D-C2D	2.43	1.50	1.45
25	B	612	CLA	C3B-CAB	-2.43	1.43	1.47
25	B	609	CLA	CMC-C2C	-2.43	1.45	1.50
24	r	614	CHL	C3D-C2D	2.43	1.45	1.39
25	2	610	CLA	C3B-CAB	-2.43	1.43	1.47
25	2	602	CLA	CMD-C2D	-2.43	1.45	1.50
25	s	610	CLA	C3B-CAB	-2.43	1.43	1.47
26	3	1621	LUT	C22-C21	-2.43	1.51	1.54
24	8	607	CHL	C3D-C2D	2.43	1.45	1.39
24	1	605	CHL	C1C-NC	-2.43	1.34	1.37
25	1	614	CLA	CMD-C2D	-2.43	1.45	1.50
25	5	613	CLA	CHC-C1C	2.43	1.41	1.35
24	Y	606	CHL	C1D-ND	-2.43	1.34	1.37
25	2	602	CLA	C1D-ND	2.43	1.40	1.37
25	d	402	CLA	C3B-C2B	-2.43	1.37	1.40
26	7	1621	LUT	C22-C21	-2.43	1.51	1.54
24	y	606	CHL	C1D-ND	-2.43	1.34	1.37
25	3	602	CLA	C1D-ND	2.43	1.40	1.37
25	3	613	CLA	CMD-C2D	-2.43	1.45	1.50
24	g	608	CHL	C1D-C2D	2.43	1.50	1.45
25	Y	604	CLA	CMC-C2C	-2.43	1.45	1.50
25	b	609	CLA	MG-ND	-2.43	2.01	2.05
25	y	603	CLA	CHC-C1C	2.43	1.41	1.35
25	7	602	CLA	C1D-ND	2.42	1.40	1.37
25	s	609	CLA	CMB-C2B	-2.42	1.46	1.51
25	5	602	CLA	CMD-C2D	-2.42	1.45	1.50
25	8	612	CLA	CMB-C2B	-2.42	1.46	1.51
25	b	609	CLA	CMC-C2C	-2.42	1.45	1.50
25	A	406	CLA	CHC-C1C	2.42	1.41	1.35
25	6	602	CLA	C1D-ND	2.42	1.40	1.37
25	B	616	CLA	CMD-C2D	-2.42	1.45	1.50
25	3	604	CLA	C3B-CAB	-2.42	1.43	1.47
24	r	608	CHL	OBD-CAD	2.42	1.26	1.22
25	7	602	CLA	MG-ND	-2.42	2.01	2.05
25	4	612	CLA	CMB-C2B	-2.42	1.46	1.51
24	R	608	CHL	OBD-CAD	2.42	1.26	1.22
25	Y	612	CLA	CHC-C1C	2.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	611	CLA	C4B-CHC	-2.42	1.34	1.41
25	7	604	CLA	C3B-CAB	-2.42	1.43	1.47
25	a	407	CLA	CMD-C2D	-2.42	1.45	1.50
25	6	603	CLA	CMD-C2D	-2.42	1.45	1.50
25	A	410	CLA	C3B-CAB	-2.42	1.43	1.47
29	b	2630	LHG	O7-C5	-2.42	1.40	1.46
25	6	610	CLA	C3B-CAB	-2.42	1.43	1.47
25	r	610	CLA	CMD-C2D	-2.42	1.45	1.50
26	G	1621	LUT	C1-C6	-2.42	1.50	1.53
24	G	608	CHL	C1D-C2D	2.42	1.50	1.45
25	1	602	CLA	CMD-C2D	-2.41	1.45	1.50
25	g	613	CLA	CMB-C2B	-2.41	1.46	1.51
35	Z	101	LMG	C7-C8	2.41	1.58	1.50
35	D	411	LMG	O7-C8	-2.41	1.40	1.46
25	7	612	CLA	C3B-CAB	-2.41	1.43	1.47
25	B	617	CLA	CHC-C1C	2.41	1.41	1.35
26	y	1620	LUT	C10-C9	-2.41	1.32	1.35
24	G	606	CHL	C1D-C2D	2.41	1.50	1.45
25	7	611	CLA	C4B-CHC	-2.41	1.34	1.41
37	C	520	DGD	O1G-C1G	-2.41	1.39	1.45
25	2	612	CLA	CHC-C1C	2.41	1.41	1.35
25	4	612	CLA	CMD-C2D	-2.41	1.45	1.50
25	6	613	CLA	C3B-C2B	-2.41	1.37	1.40
25	6	604	CLA	CHC-C1C	2.41	1.41	1.35
25	A	406	CLA	CMD-C2D	-2.41	1.45	1.50
24	6	608	CHL	C1D-C2D	2.41	1.50	1.45
25	S	609	CLA	CMB-C2B	-2.41	1.46	1.51
24	5	608	CHL	MG-NA	-2.41	2.00	2.06
24	N	609	CHL	C1D-C2D	2.41	1.50	1.45
25	2	603	CLA	CMD-C2D	-2.41	1.45	1.50
26	g	1621	LUT	C1-C6	-2.41	1.50	1.53
33	a	408	PHO	CBD-CGD	-2.41	1.49	1.52
24	g	606	CHL	C1D-C2D	2.41	1.50	1.45
25	b	616	CLA	CMD-C2D	-2.41	1.45	1.50
26	R	620	LUT	C1-C6	-2.41	1.50	1.53
25	3	612	CLA	C3B-CAB	-2.40	1.43	1.47
24	G	609	CHL	C1B-NB	-2.40	1.33	1.35
25	5	612	CLA	C4B-CHC	-2.40	1.34	1.41
25	8	612	CLA	CMD-C2D	-2.40	1.45	1.50
25	Y	612	CLA	CMC-C2C	-2.40	1.45	1.50
25	B	614	CLA	CMD-C2D	-2.40	1.45	1.50
25	3	602	CLA	MG-ND	-2.40	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	608	CHL	MG-NA	-2.40	2.00	2.06
37	c	520	DGD	O1G-C1G	-2.40	1.39	1.45
25	D	402	CLA	C3B-C2B	-2.40	1.37	1.40
25	5	603	CLA	C4B-CHC	-2.40	1.34	1.41
25	r	604	CLA	MG-ND	-2.40	2.01	2.05
24	g	609	CHL	C1B-NB	-2.40	1.33	1.35
25	b	617	CLA	CHC-C1C	2.40	1.41	1.35
25	1	604	CLA	CMD-C2D	-2.40	1.45	1.50
24	n	609	CHL	C1D-C2D	2.40	1.50	1.45
25	7	612	CLA	CMC-C2C	-2.40	1.45	1.50
24	2	608	CHL	C1D-C2D	2.40	1.50	1.45
24	3	607	CHL	C1D-C2D	2.40	1.50	1.45
35	z	101	LMG	C7-C8	2.40	1.58	1.50
25	6	614	CLA	CMD-C2D	-2.39	1.45	1.50
25	1	603	CLA	C4B-CHC	-2.39	1.34	1.41
25	1	612	CLA	C4B-CHC	-2.39	1.34	1.41
25	b	614	CLA	MG-ND	-2.39	2.01	2.05
25	a	406	CLA	CMD-C2D	-2.39	1.45	1.50
25	g	603	CLA	MG-ND	-2.39	2.01	2.05
25	b	614	CLA	CMD-C2D	-2.39	1.45	1.50
25	a	410	CLA	C3B-CAB	-2.39	1.43	1.47
25	N	612	CLA	CMD-C2D	-2.39	1.45	1.50
25	g	614	CLA	CMD-C2D	-2.39	1.45	1.50
24	y	605	CHL	C3D-C2D	2.39	1.45	1.39
24	Y	609	CHL	C1B-NB	-2.39	1.33	1.35
25	B	617	CLA	C4B-CHC	-2.39	1.34	1.41
24	4	606	CHL	C3D-C2D	2.39	1.45	1.39
25	G	614	CLA	CMD-C2D	-2.39	1.45	1.50
25	C	512	CLA	CMB-C2B	-2.39	1.46	1.51
25	R	604	CLA	MG-ND	-2.39	2.01	2.05
24	r	606	CHL	C1D-C2D	2.39	1.50	1.45
27	7	1622	XAT	O4-C5	-2.39	1.42	1.46
25	2	604	CLA	CHC-C1C	2.39	1.41	1.35
25	r	603	CLA	CMD-C2D	-2.39	1.45	1.50
25	G	603	CLA	MG-ND	-2.39	2.01	2.05
35	d	411	LMG	O7-C8	-2.38	1.40	1.46
25	r	602	CLA	CMD-C2D	-2.38	1.45	1.50
25	y	612	CLA	CMC-C2C	-2.38	1.45	1.50
24	4	601	CHL	C4C-C3C	2.38	1.49	1.45
25	r	609	CLA	CMD-C2D	-2.38	1.45	1.50
24	6	605	CHL	C1D-C2D	2.38	1.50	1.45
24	6	609	CHL	C3D-C2D	2.38	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	613	CLA	C4B-CHC	-2.38	1.34	1.41
25	B	612	CLA	CHC-C1C	2.38	1.41	1.35
25	N	610	CLA	CHC-C1C	2.38	1.41	1.35
25	n	610	CLA	CHC-C1C	2.38	1.41	1.35
24	2	609	CHL	C3D-C2D	2.38	1.45	1.39
25	R	603	CLA	CMD-C2D	-2.38	1.45	1.50
25	b	612	CLA	CHC-C1C	2.38	1.41	1.35
25	R	609	CLA	CMD-C2D	-2.38	1.45	1.50
25	7	613	CLA	C4B-CHC	-2.38	1.34	1.41
25	s	603	CLA	CMB-C2B	-2.38	1.46	1.51
24	G	601	CHL	C1D-C2D	2.38	1.50	1.45
25	B	609	CLA	MG-ND	-2.38	2.01	2.05
25	b	617	CLA	C4B-CHC	-2.38	1.34	1.41
25	R	602	CLA	CMD-C2D	-2.38	1.45	1.50
24	8	606	CHL	C3D-C2D	2.37	1.45	1.39
27	3	1622	XAT	O4-C5	-2.37	1.42	1.46
25	g	610	CLA	CMC-C2C	-2.37	1.45	1.50
25	B	614	CLA	MG-ND	-2.37	2.01	2.05
24	2	605	CHL	C1D-C2D	2.37	1.50	1.45
24	S	607	CHL	MG-NA	-2.37	2.00	2.06
25	5	612	CLA	MG-ND	-2.37	2.01	2.05
25	g	602	CLA	CMD-C2D	-2.37	1.45	1.50
25	n	610	CLA	CMC-C2C	-2.37	1.45	1.50
25	G	602	CLA	CMD-C2D	-2.37	1.45	1.50
25	Y	602	CLA	C3B-CAB	-2.37	1.43	1.47
25	B	606	CLA	CHC-C1C	2.37	1.41	1.35
24	8	601	CHL	C4C-C3C	2.37	1.49	1.45
25	2	614	CLA	CMD-C2D	-2.37	1.45	1.50
24	Y	605	CHL	C3D-C2D	2.37	1.45	1.39
25	S	603	CLA	CMB-C2B	-2.37	1.46	1.51
24	g	601	CHL	C1D-C2D	2.37	1.50	1.45
26	Y	1620	LUT	C10-C9	-2.37	1.32	1.35
25	G	610	CLA	C3B-C2B	-2.37	1.37	1.40
25	B	603	CLA	CMD-C2D	-2.37	1.45	1.50
25	1	603	CLA	CMD-C2D	-2.37	1.45	1.50
24	y	606	CHL	C1B-NB	-2.37	1.33	1.35
25	3	613	CLA	CHC-C1C	2.37	1.41	1.35
25	N	610	CLA	CMC-C2C	-2.37	1.45	1.50
25	4	604	CLA	C3B-CAB	-2.37	1.43	1.47
25	y	602	CLA	C3B-CAB	-2.37	1.43	1.47
25	b	603	CLA	C3B-CAB	-2.37	1.43	1.47
25	7	613	CLA	CHC-C1C	2.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	1620	LUT	C22-C21	-2.36	1.51	1.54
25	b	606	CLA	CHC-C1C	2.36	1.41	1.35
25	N	612	CLA	CHC-C1C	2.36	1.41	1.35
25	g	610	CLA	C3B-C2B	-2.36	1.37	1.40
25	g	604	CLA	CMD-C2D	-2.36	1.45	1.50
24	g	609	CHL	C1D-C2D	2.36	1.50	1.45
33	A	409	PHO	CMD-C2D	-2.36	1.45	1.51
25	3	612	CLA	CMC-C2C	-2.36	1.45	1.50
25	G	610	CLA	CMC-C2C	-2.36	1.45	1.50
25	g	613	CLA	C4B-CHC	-2.36	1.34	1.41
25	B	605	CLA	C4B-CHC	-2.36	1.34	1.41
25	r	610	CLA	C3B-CAB	-2.36	1.43	1.47
25	b	605	CLA	C4B-CHC	-2.36	1.34	1.41
24	R	608	CHL	MG-NA	-2.36	2.00	2.06
25	S	614	CLA	CMB-C2B	-2.36	1.46	1.51
25	5	603	CLA	CMD-C2D	-2.36	1.45	1.50
25	G	613	CLA	C4B-CHC	-2.36	1.34	1.41
27	r	622	XAT	O4-C5	-2.36	1.42	1.46
25	s	614	CLA	CMB-C2B	-2.36	1.46	1.51
25	N	610	CLA	C3B-CAB	-2.36	1.43	1.47
33	A	409	PHO	CMC-C2C	-2.36	1.46	1.51
26	r	620	LUT	C1-C6	-2.36	1.50	1.53
25	Y	602	CLA	C3B-C2B	-2.36	1.37	1.40
25	G	604	CLA	CMD-C2D	-2.36	1.45	1.50
25	n	612	CLA	CMD-C2D	-2.36	1.45	1.50
25	6	604	CLA	C3B-C2B	-2.36	1.37	1.40
25	A	405	CLA	MG-ND	-2.35	2.01	2.05
25	d	403	CLA	MG-ND	-2.35	2.01	2.05
24	7	607	CHL	C3D-C2D	2.35	1.45	1.39
25	D	402	CLA	MG-ND	-2.35	2.01	2.05
33	A	408	PHO	CBD-CGD	-2.35	1.49	1.52
25	5	613	CLA	CMD-C2D	-2.35	1.45	1.50
33	a	409	PHO	CMC-C2C	-2.35	1.46	1.51
24	s	607	CHL	MG-NA	-2.35	2.00	2.06
24	3	606	CHL	C1D-C2D	2.35	1.50	1.45
25	n	610	CLA	C3B-CAB	-2.35	1.43	1.47
25	2	604	CLA	C3B-C2B	-2.35	1.37	1.40
25	D	402	CLA	C3B-CAB	-2.35	1.43	1.47
28	R	623	NEX	C30-C29	-2.35	1.32	1.35
26	1	1621	LUT	C22-C21	-2.35	1.51	1.54
25	c	512	CLA	CMB-C2B	-2.35	1.46	1.51
25	y	602	CLA	C3B-C2B	-2.35	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	603	CLA	CMC-C2C	-2.35	1.45	1.50
24	7	606	CHL	C1D-C2D	2.35	1.50	1.45
24	N	605	CHL	C1D-C2D	2.35	1.50	1.45
25	y	611	CLA	MG-ND	-2.35	2.01	2.05
27	R	622	XAT	O4-C5	-2.35	1.42	1.46
25	1	613	CLA	CMD-C2D	-2.35	1.45	1.50
25	B	615	CLA	C3B-CAB	-2.35	1.43	1.47
24	7	607	CHL	C1D-C2D	2.35	1.50	1.45
25	8	604	CLA	C3B-CAB	-2.35	1.43	1.47
24	G	609	CHL	C1D-C2D	2.35	1.50	1.45
24	g	607	CHL	C1D-C2D	2.34	1.49	1.45
25	n	612	CLA	CHC-C1C	2.34	1.41	1.35
28	r	623	NEX	C30-C29	-2.34	1.32	1.35
24	1	605	CHL	C1D-C2D	2.34	1.49	1.45
33	a	409	PHO	CMD-C2D	-2.34	1.46	1.51
25	1	612	CLA	CMC-C2C	-2.34	1.45	1.50
25	R	603	CLA	CMC-C2C	-2.34	1.45	1.50
24	N	606	CHL	C1B-NB	-2.34	1.33	1.35
24	r	608	CHL	MG-NA	-2.34	2.00	2.06
25	b	603	CLA	CMD-C2D	-2.34	1.45	1.50
25	a	405	CLA	MG-ND	-2.34	2.01	2.05
25	d	402	CLA	MG-ND	-2.34	2.01	2.05
25	N	604	CLA	CMC-C2C	-2.34	1.45	1.50
25	R	610	CLA	C3B-CAB	-2.34	1.43	1.47
25	r	612	CLA	CMD-C2D	-2.34	1.45	1.50
24	R	606	CHL	C1D-C2D	2.34	1.49	1.45
25	1	612	CLA	MG-ND	-2.34	2.01	2.05
24	3	607	CHL	C3D-C2D	2.34	1.45	1.39
28	1	1623	NEX	O24-C25	-2.34	1.42	1.46
33	a	408	PHO	C3B-C2B	-2.34	1.37	1.40
24	1	605	CHL	C1D-ND	-2.34	1.34	1.37
25	d	402	CLA	C3B-CAB	-2.34	1.43	1.47
25	B	607	CLA	CHC-C1C	2.34	1.41	1.35
25	B	611	CLA	CMC-C2C	-2.33	1.45	1.50
25	B	605	CLA	C3B-CAB	-2.33	1.43	1.47
24	r	607	CHL	C3D-C2D	2.33	1.45	1.39
25	b	605	CLA	C3B-CAB	-2.33	1.43	1.47
25	N	604	CLA	MG-ND	-2.33	2.01	2.05
25	D	403	CLA	MG-ND	-2.33	2.01	2.05
25	5	612	CLA	CMC-C2C	-2.33	1.45	1.50
25	R	612	CLA	CMD-C2D	-2.33	1.45	1.50
25	B	603	CLA	C3B-CAB	-2.33	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	607	CHL	C3D-C2D	2.33	1.45	1.39
25	2	604	CLA	C4B-CHC	-2.33	1.34	1.41
25	6	604	CLA	C4B-CHC	-2.33	1.34	1.41
25	5	603	CLA	CMC-C2C	-2.33	1.45	1.50
25	2	610	CLA	CMC-C2C	-2.33	1.45	1.50
25	B	616	CLA	C3B-CAB	-2.33	1.43	1.47
25	b	615	CLA	C3B-CAB	-2.33	1.43	1.47
24	7	606	CHL	C4B-CHC	2.33	1.47	1.41
25	n	603	CLA	MG-ND	-2.33	2.01	2.05
25	6	603	CLA	CMC-C2C	-2.33	1.45	1.50
24	4	601	CHL	C4B-CHC	2.33	1.47	1.41
24	7	601	CHL	C1D-C2D	2.33	1.49	1.45
24	n	605	CHL	C1D-C2D	2.33	1.49	1.45
24	n	605	CHL	C3D-C2D	2.32	1.45	1.39
25	2	603	CLA	CMC-C2C	-2.32	1.45	1.50
27	Y	1622	XAT	C34-C33	-2.32	1.32	1.35
24	n	606	CHL	C1D-ND	-2.32	1.34	1.37
25	7	610	CLA	MG-ND	-2.32	2.01	2.05
25	b	607	CLA	CHC-C1C	2.32	1.40	1.35
33	A	408	PHO	C3B-C2B	-2.32	1.37	1.40
28	5	1623	NEX	O24-C25	-2.32	1.42	1.46
25	n	604	CLA	MG-ND	-2.32	2.01	2.05
25	b	616	CLA	C3B-CAB	-2.32	1.43	1.47
33	A	408	PHO	CMC-C2C	-2.32	1.46	1.51
25	g	611	CLA	CMD-C2D	-2.32	1.45	1.50
27	y	1622	XAT	C34-C33	-2.32	1.32	1.35
25	n	612	CLA	C4B-CHC	-2.32	1.34	1.41
25	n	604	CLA	CMC-C2C	-2.32	1.45	1.50
25	N	612	CLA	C4B-CHC	-2.32	1.34	1.41
25	B	606	CLA	C3B-CAB	-2.32	1.43	1.47
24	5	605	CHL	C1D-ND	-2.32	1.34	1.37
24	R	607	CHL	C3D-C2D	2.32	1.45	1.39
24	g	607	CHL	C3D-C2D	2.32	1.45	1.39
25	R	609	CLA	CHC-C1C	2.32	1.40	1.35
25	R	611	CLA	MG-ND	-2.32	2.01	2.05
24	3	609	CHL	C3D-C2D	2.32	1.45	1.39
24	n	606	CHL	C1B-NB	-2.32	1.33	1.35
25	1	603	CLA	CHC-C1C	2.32	1.40	1.35
25	1	603	CLA	CMC-C2C	-2.32	1.45	1.50
24	8	601	CHL	C4B-CHC	2.32	1.47	1.41
25	N	603	CLA	MG-ND	-2.32	2.01	2.05
25	b	606	CLA	C3B-CAB	-2.31	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	603	CLA	CHC-C1C	2.31	1.40	1.35
25	1	612	CLA	CHC-C1C	2.31	1.40	1.35
25	Y	604	CLA	CMD-C2D	-2.31	1.45	1.50
33	A	408	PHO	CMD-C2D	-2.31	1.46	1.51
25	B	606	CLA	C4B-CHC	-2.31	1.34	1.41
34	A	412	SQD	O2-C2	-2.31	1.37	1.43
25	3	610	CLA	MG-ND	-2.31	2.01	2.05
25	C	510	CLA	CMB-C2B	-2.31	1.46	1.51
26	n	1620	LUT	C22-C21	-2.31	1.51	1.54
24	Y	605	CHL	C1D-C2D	2.31	1.49	1.45
25	b	606	CLA	C4B-CHC	-2.31	1.34	1.41
25	r	613	CLA	C4B-CHC	-2.31	1.34	1.41
25	y	604	CLA	CMD-C2D	-2.31	1.45	1.50
25	Y	611	CLA	MG-ND	-2.31	2.01	2.05
24	5	605	CHL	C1D-C2D	2.31	1.49	1.45
24	N	606	CHL	C1D-ND	-2.31	1.34	1.37
25	1	613	CLA	C4B-CHC	-2.31	1.34	1.41
34	a	412	SQD	O2-C2	-2.31	1.37	1.43
24	3	601	CHL	C1D-C2D	2.31	1.49	1.45
25	5	612	CLA	CHC-C1C	2.31	1.40	1.35
25	6	610	CLA	CMC-C2C	-2.31	1.45	1.50
24	y	605	CHL	C1D-C2D	2.31	1.49	1.45
25	5	603	CLA	C3B-CAB	-2.31	1.43	1.47
25	C	501	CLA	CMD-C2D	-2.31	1.45	1.50
25	y	604	CLA	MG-ND	-2.31	2.01	2.05
24	y	609	CHL	C1D-C2D	2.31	1.49	1.45
25	D	402	CLA	CAA-C2A	-2.31	1.49	1.54
33	a	408	PHO	CMD-C2D	-2.31	1.46	1.51
25	r	611	CLA	MG-ND	-2.31	2.01	2.05
24	G	607	CHL	C1D-C2D	2.31	1.49	1.45
25	y	613	CLA	C3B-C2B	-2.31	1.37	1.40
25	C	512	CLA	CMD-C2D	-2.31	1.45	1.50
25	Y	611	CLA	CMC-C2C	-2.30	1.45	1.50
24	3	606	CHL	C4B-CHC	2.30	1.47	1.41
24	N	609	CHL	C3D-C2D	2.30	1.45	1.39
25	c	513	CLA	CMB-C2B	-2.30	1.46	1.51
25	b	611	CLA	CMC-C2C	-2.30	1.45	1.50
24	Y	609	CHL	C1D-C2D	2.30	1.49	1.45
26	R	620	LUT	C22-C21	-2.30	1.51	1.54
25	C	513	CLA	CMB-C2B	-2.30	1.46	1.51
25	4	604	CLA	MG-ND	-2.30	2.01	2.05
25	b	604	CLA	CMC-C2C	-2.30	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R	623	NEX	O24-C25	-2.30	1.42	1.46
33	a	408	PHO	CMC-C2C	-2.30	1.46	1.51
24	N	605	CHL	C3D-C2D	2.30	1.45	1.39
25	B	604	CLA	CMC-C2C	-2.30	1.45	1.50
24	7	609	CHL	C3D-C2D	2.30	1.45	1.39
25	R	610	CLA	CMC-C2C	-2.30	1.45	1.50
25	R	613	CLA	C4B-CHC	-2.30	1.34	1.41
25	S	612	CLA	CMB-C2B	-2.30	1.46	1.51
25	s	612	CLA	CMB-C2B	-2.30	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.30	1.46	1.51
25	Y	604	CLA	MG-ND	-2.30	2.01	2.05
25	1	603	CLA	C3B-CAB	-2.30	1.43	1.47
24	Y	601	CHL	C1D-C2D	2.30	1.49	1.45
25	G	611	CLA	MG-ND	-2.29	2.01	2.05
25	y	611	CLA	CMC-C2C	-2.29	1.45	1.50
26	5	1621	LUT	C22-C21	-2.29	1.51	1.54
24	S	601	CHL	C4B-CHC	2.29	1.47	1.41
28	Y	1623	NEX	O24-C25	-2.29	1.42	1.46
25	6	611	CLA	CMD-C2D	-2.29	1.45	1.50
37	H	102	DGD	O2E-C2E	-2.29	1.37	1.43
25	r	609	CLA	CHC-C1C	2.29	1.40	1.35
37	h	102	DGD	O2E-C2E	-2.29	1.37	1.43
24	S	608	CHL	C4C-C3C	2.29	1.49	1.45
24	y	606	CHL	C1C-NC	-2.29	1.34	1.37
25	2	611	CLA	CMD-C2D	-2.29	1.46	1.50
25	1	612	CLA	CMD-C2D	-2.29	1.46	1.50
25	3	610	CLA	CMC-C2C	-2.28	1.46	1.50
25	7	612	CLA	C4B-CHC	-2.28	1.34	1.41
25	B	617	CLA	C3B-C2B	-2.28	1.37	1.40
27	g	1622	XAT	O4-C5	-2.28	1.42	1.46
25	B	605	CLA	CMC-C2C	-2.28	1.46	1.50
25	1	603	CLA	CAC-C3C	-2.28	1.45	1.51
25	5	603	CLA	CAC-C3C	-2.28	1.45	1.51
25	3	603	CLA	C4B-CHC	-2.28	1.34	1.41
33	A	408	PHO	CMB-C2B	-2.28	1.46	1.51
25	d	402	CLA	CAA-C2A	-2.28	1.49	1.54
25	c	512	CLA	CMD-C2D	-2.28	1.46	1.50
33	a	408	PHO	CMB-C2B	-2.28	1.46	1.51
25	8	604	CLA	MG-ND	-2.28	2.01	2.05
25	3	612	CLA	C4B-CHC	-2.28	1.34	1.41
25	g	614	CLA	C3B-C2B	-2.28	1.37	1.40
25	B	610	CLA	MG-ND	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	611	CLA	MG-ND	-2.28	2.01	2.05
25	6	604	CLA	CMC-C2C	-2.28	1.46	1.50
24	7	601	CHL	C1D-ND	-2.28	1.35	1.37
25	5	613	CLA	C4B-CHC	-2.28	1.34	1.41
25	7	603	CLA	C4B-CHC	-2.28	1.34	1.41
25	b	616	CLA	C4B-CHC	-2.28	1.34	1.41
25	B	616	CLA	C4B-CHC	-2.28	1.34	1.41
25	b	617	CLA	C3B-C2B	-2.28	1.37	1.40
25	5	610	CLA	CMC-C2C	-2.28	1.46	1.50
30	b	618	BCR	C17-C18	-2.28	1.32	1.35
24	4	608	CHL	C1B-CHB	2.28	1.47	1.41
25	r	610	CLA	CMC-C2C	-2.28	1.46	1.50
25	B	608	CLA	MG-ND	-2.28	2.01	2.05
25	B	610	CLA	C4B-CHC	-2.28	1.34	1.41
24	s	608	CHL	C4C-C3C	2.28	1.49	1.45
24	6	608	CHL	C3D-C2D	2.28	1.45	1.39
25	8	610	CLA	MG-ND	-2.27	2.01	2.05
25	4	610	CLA	MG-ND	-2.27	2.01	2.05
24	Y	606	CHL	C1C-NC	-2.27	1.34	1.37
25	g	604	CLA	CMC-C2C	-2.27	1.46	1.50
24	s	601	CHL	C4B-CHC	2.27	1.47	1.41
25	4	611	CLA	CMD-C2D	-2.27	1.46	1.50
25	a	406	CLA	CAC-C3C	-2.27	1.45	1.51
25	A	406	CLA	CAC-C3C	-2.27	1.45	1.51
29	B	2631	LHG	O7-C5	-2.27	1.40	1.46
25	G	611	CLA	CMD-C2D	-2.27	1.46	1.50
24	n	609	CHL	C3D-C2D	2.27	1.45	1.39
25	c	501	CLA	CMD-C2D	-2.27	1.46	1.50
25	7	610	CLA	CMD-C2D	-2.27	1.46	1.50
24	2	608	CHL	C3D-C2D	2.27	1.45	1.39
25	3	610	CLA	CMD-C2D	-2.27	1.46	1.50
25	G	604	CLA	CMC-C2C	-2.27	1.46	1.50
25	r	609	CLA	CMC-C2C	-2.27	1.46	1.50
25	Y	613	CLA	C3B-C2B	-2.27	1.37	1.40
25	b	605	CLA	CMC-C2C	-2.26	1.46	1.50
24	6	606	CHL	C3D-C2D	2.26	1.45	1.39
25	N	602	CLA	CMD-C2D	-2.26	1.46	1.50
25	n	602	CLA	CMD-C2D	-2.26	1.46	1.50
29	b	2631	LHG	O7-C5	-2.26	1.40	1.46
26	G	1621	LUT	C30-C29	-2.26	1.32	1.35
25	G	612	CLA	C3B-C2B	-2.26	1.37	1.40
25	G	614	CLA	C3B-C2B	-2.26	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	y	1623	NEX	O24-C25	-2.26	1.43	1.46
24	2	607	CHL	C1D-ND	-2.26	1.35	1.37
37	C	518	DGD	O5D-C6D	-2.26	1.39	1.43
25	n	612	CLA	CMC-C2C	-2.26	1.46	1.50
25	b	610	CLA	CMC-C2C	-2.26	1.46	1.50
24	s	606	CHL	C1B-CHB	2.26	1.47	1.41
24	y	601	CHL	C1D-C2D	2.26	1.49	1.45
27	G	1622	XAT	O4-C5	-2.26	1.43	1.46
25	b	608	CLA	MG-ND	-2.26	2.01	2.05
37	C	518	DGD	O3E-C3E	-2.26	1.37	1.43
25	g	610	CLA	CMD-C2D	-2.26	1.46	1.50
25	b	610	CLA	MG-ND	-2.26	2.01	2.05
25	Y	613	CLA	CHC-C1C	2.26	1.40	1.35
25	5	604	CLA	C4B-CHC	-2.26	1.34	1.41
25	1	610	CLA	CMC-C2C	-2.26	1.46	1.50
26	g	1621	LUT	C30-C29	-2.26	1.32	1.35
25	7	603	CLA	CMC-C2C	-2.26	1.46	1.50
24	2	606	CHL	C3D-C2D	2.26	1.45	1.39
24	8	608	CHL	C1B-CHB	2.26	1.47	1.41
25	R	616	CLA	CHC-C1C	2.26	1.40	1.35
25	4	610	CLA	C3B-C2B	-2.26	1.37	1.40
25	R	616	CLA	C4B-CHC	-2.26	1.34	1.41
25	b	610	CLA	C4B-CHC	-2.26	1.34	1.41
25	S	614	CLA	CMD-C2D	-2.26	1.46	1.50
24	6	605	CHL	C4B-CHC	2.26	1.47	1.41
25	g	612	CLA	C3B-C2B	-2.26	1.37	1.40
25	N	612	CLA	CMC-C2C	-2.26	1.46	1.50
25	N	602	CLA	MG-ND	-2.26	2.01	2.05
25	2	610	CLA	CMD-C2D	-2.25	1.46	1.50
25	3	603	CLA	CMC-C2C	-2.25	1.46	1.50
25	7	610	CLA	CMC-C2C	-2.25	1.46	1.50
25	8	611	CLA	CMD-C2D	-2.25	1.46	1.50
35	Z	101	LMG	C4-C5	2.25	1.57	1.53
25	1	611	CLA	MG-ND	-2.25	2.01	2.05
25	2	602	CLA	MG-ND	-2.25	2.01	2.05
25	2	604	CLA	CMC-C2C	-2.25	1.46	1.50
24	6	607	CHL	C4C-C3C	2.25	1.48	1.45
37	c	518	DGD	O3E-C3E	-2.25	1.37	1.43
24	2	605	CHL	C4B-CHC	2.25	1.47	1.41
25	r	616	CLA	CHC-C1C	2.25	1.40	1.35
25	r	616	CLA	C4B-CHC	-2.25	1.34	1.41
25	5	612	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	613	CLA	CMC-C2C	-2.25	1.46	1.50
25	n	603	CLA	CMC-C2C	-2.25	1.46	1.50
24	2	607	CHL	C4C-C3C	2.25	1.48	1.45
25	6	602	CLA	MG-ND	-2.25	2.01	2.05
25	R	609	CLA	CMC-C2C	-2.25	1.46	1.50
25	s	614	CLA	CMD-C2D	-2.25	1.46	1.50
34	B	623	SQD	O3-C3	-2.25	1.37	1.43
30	B	618	BCR	C17-C18	-2.25	1.32	1.35
25	c	506	CLA	C3B-C2B	-2.25	1.37	1.40
28	r	623	NEX	O24-C25	-2.25	1.43	1.46
24	S	606	CHL	C1B-CHB	2.25	1.47	1.41
25	N	611	CLA	C3B-C2B	-2.24	1.37	1.40
34	b	623	SQD	O3-C3	-2.24	1.37	1.43
25	A	407	CLA	C3B-CAB	-2.24	1.43	1.47
25	a	407	CLA	C3B-CAB	-2.24	1.43	1.47
25	3	613	CLA	CMC-C2C	-2.24	1.46	1.50
25	s	610	CLA	C3B-C2B	-2.24	1.37	1.40
25	G	610	CLA	C3B-CAB	-2.24	1.43	1.47
25	B	612	CLA	MG-ND	-2.24	2.01	2.05
25	1	604	CLA	C4B-CHC	-2.24	1.34	1.41
25	6	610	CLA	CMD-C2D	-2.24	1.46	1.50
25	B	608	CLA	C4B-CHC	-2.24	1.34	1.41
25	1	614	CLA	MG-ND	-2.24	2.01	2.05
25	B	610	CLA	CMC-C2C	-2.24	1.46	1.50
37	c	518	DGD	O5D-C6D	-2.24	1.39	1.43
25	b	605	CLA	CHC-C1C	2.24	1.40	1.35
29	6	2630	LHG	O7-C5	-2.24	1.41	1.46
25	n	602	CLA	MG-ND	-2.24	2.01	2.05
25	C	506	CLA	C3B-C2B	-2.24	1.37	1.40
35	z	101	LMG	C4-C5	2.24	1.57	1.53
25	B	605	CLA	CHC-C1C	2.24	1.40	1.35
25	y	613	CLA	CHC-C1C	2.24	1.40	1.35
25	5	614	CLA	MG-ND	-2.24	2.01	2.05
24	3	601	CHL	C1D-ND	-2.24	1.35	1.37
25	B	612	CLA	C1D-ND	2.24	1.40	1.37
25	s	602	CLA	CMC-C2C	-2.24	1.46	1.50
25	G	604	CLA	MG-ND	-2.24	2.01	2.05
25	8	604	CLA	CMD-C2D	-2.24	1.46	1.50
24	g	608	CHL	C4B-CHC	2.24	1.47	1.41
35	Z	101	LMG	C4-C3	2.24	1.58	1.52
24	3	608	CHL	C1D-ND	-2.24	1.35	1.37
25	3	611	CLA	C3B-CAB	-2.24	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	614	CHL	C4B-CHC	2.24	1.47	1.41
25	Y	602	CLA	MG-ND	-2.24	2.01	2.05
25	b	608	CLA	C4B-CHC	-2.24	1.34	1.41
27	4	622	XAT	O4-C5	-2.24	1.43	1.46
29	2	2630	LHG	O7-C5	-2.24	1.41	1.46
25	g	613	CLA	C3B-C2B	-2.23	1.37	1.40
26	r	620	LUT	C22-C21	-2.23	1.51	1.54
25	4	604	CLA	CMD-C2D	-2.23	1.46	1.50
24	R	614	CHL	C4B-CHC	2.23	1.47	1.41
25	d	403	CLA	CMC-C2C	-2.23	1.46	1.50
25	N	603	CLA	CMC-C2C	-2.23	1.46	1.50
27	8	622	XAT	O4-C5	-2.23	1.43	1.46
24	N	601	CHL	C3D-C2D	2.23	1.45	1.39
24	6	607	CHL	C1D-ND	-2.23	1.35	1.37
34	b	623	SQD	O2-C2	-2.23	1.37	1.43
25	g	611	CLA	C3B-CAB	-2.23	1.43	1.47
25	8	612	CLA	CMC-C2C	-2.23	1.46	1.50
27	y	1622	XAT	O4-C5	-2.23	1.43	1.46
24	y	607	CHL	C1B-NB	-2.23	1.33	1.35
25	A	406	CLA	C3B-C2B	-2.23	1.37	1.40
24	G	608	CHL	C4B-CHC	2.23	1.47	1.41
24	N	608	CHL	C1D-C2D	2.23	1.49	1.45
25	8	610	CLA	C3B-C2B	-2.23	1.37	1.40
25	g	610	CLA	C3B-CAB	-2.23	1.43	1.47
25	n	610	CLA	C3B-C2B	-2.23	1.37	1.40
25	r	603	CLA	C3B-C2B	-2.23	1.37	1.40
25	S	602	CLA	CMC-C2C	-2.23	1.46	1.50
27	r	622	XAT	C2-C1	-2.23	1.51	1.54
24	s	606	CHL	C4C-C3C	2.23	1.48	1.45
29	c	523	LHG	O7-C5	-2.23	1.41	1.46
25	N	610	CLA	C3B-C2B	-2.22	1.37	1.40
24	R	606	CHL	C3D-C2D	2.22	1.45	1.39
25	S	610	CLA	C3B-C2B	-2.22	1.37	1.40
25	2	604	CLA	CMD-C2D	-2.22	1.46	1.50
25	B	604	CLA	C4B-CHC	-2.22	1.34	1.41
25	4	612	CLA	CMC-C2C	-2.22	1.46	1.50
25	y	602	CLA	MG-ND	-2.22	2.01	2.05
25	y	603	CLA	CAC-C3C	-2.22	1.45	1.51
24	n	601	CHL	C3D-C2D	2.22	1.45	1.39
25	n	613	CLA	C4B-CHC	-2.22	1.34	1.41
26	y	1621	LUT	C1-C6	-2.22	1.50	1.53
34	B	623	SQD	O2-C2	-2.22	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	1622	XAT	O4-C5	-2.22	1.43	1.46
25	G	610	CLA	CMD-C2D	-2.22	1.46	1.50
25	5	611	CLA	CMC-C2C	-2.22	1.46	1.50
24	S	606	CHL	C4C-C3C	2.22	1.48	1.45
24	2	606	CHL	C1D-C2D	2.22	1.49	1.45
25	G	603	CLA	CAC-C3C	-2.22	1.45	1.51
35	z	101	LMG	C4-C3	2.22	1.58	1.52
24	2	607	CHL	C1D-C2D	2.22	1.49	1.45
24	g	609	CHL	C3D-C2D	2.22	1.45	1.39
25	G	614	CLA	MG-ND	-2.22	2.01	2.05
25	1	611	CLA	CMC-C2C	-2.22	1.46	1.50
25	8	602	CLA	CMC-C2C	-2.22	1.46	1.50
25	R	603	CLA	C3B-C2B	-2.22	1.37	1.40
25	g	613	CLA	CMD-C2D	-2.22	1.46	1.50
25	g	603	CLA	CAC-C3C	-2.22	1.45	1.51
25	r	603	CLA	C3B-CAB	-2.22	1.43	1.47
27	Y	1622	XAT	O4-C5	-2.22	1.43	1.46
27	R	622	XAT	C2-C1	-2.22	1.51	1.54
25	n	611	CLA	C3B-C2B	-2.22	1.37	1.40
25	y	614	CLA	CMC-C2C	-2.22	1.46	1.50
25	r	616	CLA	CMD-C2D	-2.22	1.46	1.50
25	G	611	CLA	C3B-CAB	-2.22	1.43	1.47
25	b	604	CLA	C4B-CHC	-2.22	1.34	1.41
25	Y	614	CLA	CMC-C2C	-2.21	1.46	1.50
26	Y	1621	LUT	C10-C9	-2.21	1.32	1.35
24	5	606	CHL	MG-ND	-2.21	2.01	2.05
27	n	1622	XAT	O4-C5	-2.21	1.43	1.46
34	B	623	SQD	O4-C4	-2.21	1.37	1.43
26	y	1621	LUT	C10-C9	-2.21	1.32	1.35
24	r	606	CHL	C3D-C2D	2.21	1.45	1.39
24	1	606	CHL	C1B-NB	-2.21	1.33	1.35
24	7	608	CHL	C1D-ND	-2.21	1.35	1.37
24	n	601	CHL	C4B-CHC	2.21	1.47	1.41
25	Y	603	CLA	CMC-C2C	-2.21	1.46	1.50
25	g	612	CLA	CMC-C2C	-2.21	1.46	1.50
25	n	610	CLA	CMD-C2D	-2.21	1.46	1.50
25	R	612	CLA	MG-ND	-2.21	2.01	2.05
25	6	604	CLA	MG-ND	-2.21	2.01	2.05
24	7	608	CHL	C1D-C2D	2.21	1.49	1.45
25	7	611	CLA	C3B-CAB	-2.21	1.43	1.47
25	3	603	CLA	CAC-C3C	-2.21	1.45	1.51
34	b	623	SQD	O4-C4	-2.21	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	1620	LUT	C30-C29	-2.21	1.32	1.35
25	3	613	CLA	C3B-CAB	-2.21	1.43	1.47
25	G	613	CLA	CMD-C2D	-2.21	1.46	1.50
25	B	615	CLA	MG-ND	-2.21	2.01	2.05
27	1	1622	XAT	O4-C5	-2.21	1.43	1.46
25	D	403	CLA	CMC-C2C	-2.21	1.46	1.50
24	7	607	CHL	C1C-NC	-2.21	1.34	1.37
25	4	602	CLA	CMC-C2C	-2.21	1.46	1.50
25	G	603	CLA	CMD-C2D	-2.21	1.46	1.50
25	5	611	CLA	MG-ND	-2.21	2.01	2.05
25	b	612	CLA	MG-ND	-2.20	2.01	2.05
24	n	608	CHL	C1D-C2D	2.20	1.49	1.45
24	S	608	CHL	C1B-CHB	2.20	1.47	1.41
24	8	609	CHL	C3D-C2D	2.20	1.45	1.39
25	7	603	CLA	CAC-C3C	-2.20	1.45	1.51
25	a	406	CLA	C3B-C2B	-2.20	1.37	1.40
24	1	606	CHL	C1D-ND	-2.20	1.35	1.37
25	g	603	CLA	CMD-C2D	-2.20	1.46	1.50
25	s	612	CLA	CMD-C2D	-2.20	1.46	1.50
25	N	613	CLA	C4B-CHC	-2.20	1.34	1.41
24	1	609	CHL	C4B-NB	-2.20	1.33	1.35
24	4	601	CHL	C1B-CHB	2.20	1.47	1.41
25	R	603	CLA	C3B-CAB	-2.20	1.43	1.47
24	N	609	CHL	C1C-NC	-2.20	1.34	1.37
25	Y	603	CLA	CAC-C3C	-2.20	1.45	1.51
24	N	601	CHL	C4B-CHC	2.20	1.47	1.41
25	G	614	CLA	CMC-C2C	-2.20	1.46	1.50
37	C	519	DGD	O2G-C2G	-2.20	1.41	1.46
25	1	604	CLA	CMC-C2C	-2.20	1.46	1.50
25	N	610	CLA	CMD-C2D	-2.20	1.46	1.50
25	S	612	CLA	CMD-C2D	-2.20	1.46	1.50
24	G	609	CHL	C3D-C2D	2.20	1.45	1.39
24	8	608	CHL	C3D-C2D	2.20	1.45	1.39
25	R	604	CLA	CMC-C2C	-2.20	1.46	1.50
25	n	603	CLA	CAC-C3C	-2.20	1.45	1.51
37	C	518	DGD	O2G-C2G	-2.20	1.41	1.46
34	A	418	SQD	O2-C2	-2.20	1.37	1.43
25	8	611	CLA	C3B-CAB	-2.20	1.43	1.47
25	g	614	CLA	MG-ND	-2.20	2.01	2.05
29	C	523	LHG	O7-C5	-2.20	1.41	1.46
25	g	604	CLA	C4B-CHC	-2.20	1.34	1.41
25	g	604	CLA	MG-ND	-2.20	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	612	CLA	CMC-C2C	-2.20	1.46	1.50
25	C	507	CLA	C4B-CHC	-2.19	1.34	1.41
25	4	603	CLA	CMC-C2C	-2.19	1.46	1.50
25	b	615	CLA	MG-ND	-2.19	2.01	2.05
24	3	609	CHL	C1C-NC	-2.19	1.34	1.37
25	G	613	CLA	C3B-C2B	-2.19	1.37	1.40
25	c	507	CLA	C4B-CHC	-2.19	1.34	1.41
24	1	609	CHL	C3D-C2D	2.19	1.45	1.39
25	N	603	CLA	CAC-C3C	-2.19	1.45	1.51
24	6	606	CHL	C1D-C2D	2.19	1.49	1.45
37	c	519	DGD	O2G-C2G	-2.19	1.41	1.46
24	6	607	CHL	C1D-C2D	2.19	1.49	1.45
24	8	601	CHL	C1B-CHB	2.19	1.47	1.41
24	Y	607	CHL	C1B-NB	-2.19	1.33	1.35
24	4	608	CHL	C3D-C2D	2.19	1.45	1.39
25	N	614	CLA	CMD-C2D	-2.19	1.46	1.50
25	5	604	CLA	CMC-C2C	-2.19	1.46	1.50
25	g	614	CLA	CMC-C2C	-2.19	1.46	1.50
25	8	603	CLA	C3B-C2B	-2.19	1.37	1.40
25	R	609	CLA	C4B-CHC	-2.19	1.34	1.41
25	8	603	CLA	CMC-C2C	-2.19	1.46	1.50
34	a	418	SQD	O2-C2	-2.19	1.37	1.43
25	5	611	CLA	CMD-C2D	-2.19	1.46	1.50
24	5	609	CHL	C3D-C2D	2.19	1.45	1.39
24	4	608	CHL	C1D-C2D	2.19	1.49	1.45
25	R	616	CLA	CMC-C2C	-2.19	1.46	1.50
24	1	606	CHL	MG-ND	-2.19	2.01	2.05
25	B	614	CLA	CAA-C2A	-2.19	1.50	1.54
25	G	603	CLA	CMC-C2C	-2.19	1.46	1.50
24	r	614	CHL	C1B-CHB	2.19	1.47	1.41
25	G	614	CLA	C3B-CAB	-2.19	1.43	1.47
24	3	608	CHL	C1D-C2D	2.19	1.49	1.45
24	4	609	CHL	C3D-C2D	2.19	1.45	1.39
25	6	604	CLA	CMD-C2D	-2.19	1.46	1.50
27	7	1622	XAT	O24-C25	-2.18	1.43	1.46
25	2	614	CLA	C3B-C2B	-2.18	1.37	1.40
25	r	612	CLA	MG-ND	-2.18	2.01	2.05
25	N	611	CLA	CMD-C2D	-2.18	1.46	1.50
25	D	403	CLA	C4B-CHC	-2.18	1.34	1.41
25	7	603	CLA	C3B-CAB	-2.18	1.43	1.47
25	1	611	CLA	C3B-CAB	-2.18	1.43	1.47
24	n	609	CHL	C1C-NC	-2.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	612	CLA	C3B-CAB	-2.18	1.43	1.47
24	5	606	CHL	C1B-NB	-2.18	1.33	1.35
24	5	608	CHL	C4B-CHC	2.18	1.47	1.41
25	a	410	CLA	CMC-C2C	-2.18	1.46	1.50
25	y	603	CLA	CMC-C2C	-2.18	1.46	1.50
25	A	410	CLA	CMC-C2C	-2.18	1.46	1.50
24	s	608	CHL	C1B-CHB	2.18	1.47	1.41
25	g	614	CLA	C3B-CAB	-2.18	1.43	1.47
26	Y	1621	LUT	C1-C6	-2.18	1.50	1.53
37	c	518	DGD	O2G-C2G	-2.18	1.41	1.46
25	G	602	CLA	MG-ND	-2.18	2.01	2.05
25	b	614	CLA	CAA-C2A	-2.18	1.50	1.54
25	d	403	CLA	C4B-CHC	-2.18	1.34	1.41
36	D	405	PL9	C5-C4	-2.18	1.39	1.47
25	6	612	CLA	MG-ND	-2.18	2.01	2.05
25	4	611	CLA	C3B-CAB	-2.18	1.43	1.47
25	3	611	CLA	CHC-C1C	2.18	1.40	1.35
25	r	604	CLA	CMC-C2C	-2.18	1.46	1.50
24	n	609	CHL	C4C-C3C	2.18	1.48	1.45
25	7	613	CLA	C3B-CAB	-2.18	1.43	1.47
24	1	608	CHL	C4B-CHC	2.18	1.47	1.41
24	R	614	CHL	C1B-CHB	2.18	1.47	1.41
25	6	614	CLA	C3B-C2B	-2.18	1.37	1.40
25	B	614	CLA	C3B-CAB	-2.18	1.43	1.47
25	R	616	CLA	CMD-C2D	-2.18	1.46	1.50
25	G	604	CLA	C4B-CHC	-2.18	1.34	1.41
24	7	609	CHL	C1C-NC	-2.18	1.34	1.37
25	b	612	CLA	C1D-ND	2.18	1.40	1.37
25	B	607	CLA	C3B-CAB	-2.18	1.43	1.47
25	r	616	CLA	CMC-C2C	-2.17	1.46	1.50
24	g	609	CHL	C1C-NC	-2.17	1.34	1.37
25	b	606	CLA	CAC-C3C	-2.17	1.45	1.51
25	a	406	CLA	C4B-CHC	-2.17	1.34	1.41
24	5	609	CHL	C4B-NB	-2.17	1.33	1.35
28	7	1623	NEX	O24-C25	-2.17	1.43	1.46
25	6	612	CLA	CMD-C2D	-2.17	1.46	1.50
25	2	612	CLA	MG-ND	-2.17	2.01	2.05
25	A	406	CLA	C4B-CHC	-2.17	1.35	1.41
25	B	606	CLA	CAC-C3C	-2.17	1.45	1.51
25	5	611	CLA	C3B-CAB	-2.17	1.43	1.47
24	5	606	CHL	C1D-ND	-2.17	1.35	1.37
25	n	614	CLA	CMD-C2D	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	609	CLA	C4B-CHC	-2.17	1.35	1.41
25	C	506	CLA	CMD-C2D	-2.17	1.46	1.50
25	b	602	CLA	CMC-C2C	-2.17	1.46	1.50
24	6	606	CHL	C4C-C3C	2.17	1.48	1.45
37	c	519	DGD	C4E-C3E	2.17	1.57	1.52
24	7	608	CHL	C4B-CHC	2.17	1.47	1.41
25	A	407	CLA	C4B-CHC	-2.17	1.35	1.41
36	d	405	PL9	C5-C4	-2.17	1.39	1.47
24	N	609	CHL	C4C-C3C	2.17	1.48	1.45
25	N	604	CLA	C4B-CHC	-2.17	1.35	1.41
28	n	1623	NEX	O24-C25	-2.17	1.43	1.46
25	n	604	CLA	C4B-CHC	-2.17	1.35	1.41
25	b	607	CLA	C4B-CHC	-2.17	1.35	1.41
25	1	612	CLA	C3B-CAB	-2.17	1.43	1.47
25	c	506	CLA	CMD-C2D	-2.17	1.46	1.50
28	3	1623	NEX	O24-C25	-2.17	1.43	1.46
25	b	614	CLA	C3B-CAB	-2.17	1.43	1.47
24	3	607	CHL	C1C-NC	-2.17	1.34	1.37
37	C	519	DGD	C4E-C3E	2.17	1.57	1.52
34	a	412	SQD	O47-C45	-2.17	1.41	1.46
26	5	1620	LUT	C10-C9	-2.16	1.32	1.35
25	7	604	CLA	CMC-C2C	-2.16	1.46	1.50
24	5	608	CHL	C1D-C2D	2.16	1.49	1.45
25	8	602	CLA	C3B-C2B	-2.16	1.37	1.40
25	a	407	CLA	C4B-CHC	-2.16	1.35	1.41
24	4	606	CHL	C4B-CHC	2.16	1.47	1.41
25	2	604	CLA	MG-ND	-2.16	2.01	2.05
25	3	603	CLA	C3B-CAB	-2.16	1.43	1.47
25	C	508	CLA	C4B-CHC	-2.16	1.35	1.41
25	1	610	CLA	CMD-C2D	-2.16	1.46	1.50
26	y	1620	LUT	C34-C33	-2.16	1.32	1.35
28	N	1623	NEX	O24-C25	-2.16	1.43	1.46
25	1	613	CLA	CMC-C2C	-2.16	1.46	1.50
25	8	604	CLA	CMC-C2C	-2.16	1.46	1.50
24	7	601	CHL	C1B-NB	-2.16	1.33	1.35
24	1	608	CHL	C1D-C2D	2.16	1.49	1.45
24	3	608	CHL	C4B-CHC	2.16	1.47	1.41
25	5	610	CLA	CMD-C2D	-2.16	1.46	1.50
25	n	611	CLA	CMD-C2D	-2.16	1.46	1.50
24	y	607	CHL	C1C-NC	-2.16	1.34	1.37
25	3	604	CLA	CMC-C2C	-2.16	1.46	1.50
25	4	611	CLA	C3B-C2B	-2.16	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	C4B-CHC	-2.16	1.35	1.41
25	g	603	CLA	CMC-C2C	-2.16	1.46	1.50
25	3	604	CLA	C4B-CHC	-2.16	1.35	1.41
25	1	611	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	603	CLA	CMC-C2C	-2.16	1.46	1.50
24	8	608	CHL	C1D-C2D	2.16	1.49	1.45
25	4	612	CLA	MG-ND	-2.15	2.01	2.05
25	B	603	CLA	CMC-C2C	-2.15	1.46	1.50
25	4	602	CLA	C3B-C2B	-2.15	1.37	1.40
25	7	614	CLA	C3B-C2B	-2.15	1.37	1.40
24	3	609	CHL	C4C-C3C	2.15	1.48	1.45
24	3	601	CHL	C1B-NB	-2.15	1.33	1.35
25	8	612	CLA	MG-ND	-2.15	2.01	2.05
25	4	604	CLA	CMC-C2C	-2.15	1.46	1.50
25	7	604	CLA	C4B-CHC	-2.15	1.35	1.41
25	2	614	CLA	MG-ND	-2.15	2.01	2.05
25	b	607	CLA	C3B-CAB	-2.15	1.43	1.47
24	2	606	CHL	C4C-C3C	2.15	1.48	1.45
25	r	611	CLA	CMD-C2D	-2.15	1.46	1.50
25	d	402	CLA	C1D-ND	2.15	1.40	1.37
34	A	412	SQD	O47-C45	-2.15	1.41	1.46
25	N	612	CLA	MG-ND	-2.15	2.01	2.05
25	4	603	CLA	C3B-C2B	-2.15	1.37	1.40
27	N	1622	XAT	O4-C5	-2.15	1.43	1.46
25	2	612	CLA	CMD-C2D	-2.15	1.46	1.50
25	B	606	CLA	MG-ND	-2.15	2.01	2.05
25	B	602	CLA	CMC-C2C	-2.15	1.46	1.50
25	S	602	CLA	CMD-C2D	-2.15	1.46	1.50
25	s	602	CLA	CMD-C2D	-2.15	1.46	1.50
24	5	607	CHL	C4C-C3C	2.15	1.48	1.45
24	8	606	CHL	C4B-CHC	2.15	1.47	1.41
25	b	606	CLA	MG-ND	-2.15	2.01	2.05
24	1	609	CHL	C1C-NC	-2.15	1.34	1.37
37	b	626	DGD	O2G-C2G	-2.15	1.41	1.46
25	B	610	CLA	C3B-C2B	-2.15	1.37	1.40
25	3	604	CLA	CMD-C2D	-2.14	1.46	1.50
25	7	604	CLA	CMD-C2D	-2.14	1.46	1.50
25	5	613	CLA	CMC-C2C	-2.14	1.46	1.50
26	3	1620	LUT	C14-C13	-2.14	1.32	1.35
24	Y	609	CHL	C3D-C2D	2.14	1.45	1.39
26	Y	1620	LUT	C30-C29	-2.14	1.32	1.35
24	8	607	CHL	C4C-C3C	2.14	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	602	CLA	MG-ND	-2.14	2.01	2.05
25	7	611	CLA	CHC-C1C	2.14	1.40	1.35
24	Y	607	CHL	C1C-NC	-2.14	1.34	1.37
25	N	614	CLA	CMC-C2C	-2.14	1.46	1.50
24	y	609	CHL	C3D-C2D	2.14	1.45	1.39
25	C	511	CLA	CMD-C2D	-2.14	1.46	1.50
26	7	1620	LUT	C14-C13	-2.14	1.32	1.35
24	N	606	CHL	MG-ND	-2.14	2.01	2.05
24	y	606	CHL	MG-ND	-2.14	2.01	2.05
25	g	612	CLA	MG-ND	-2.14	2.01	2.05
25	R	611	CLA	CMD-C2D	-2.14	1.46	1.50
24	g	601	CHL	C3D-C2D	2.14	1.45	1.39
24	G	609	CHL	C1C-NC	-2.14	1.34	1.37
24	1	607	CHL	C4C-C3C	2.14	1.48	1.45
25	G	612	CLA	MG-ND	-2.14	2.01	2.05
25	R	609	CLA	MG-ND	-2.14	2.01	2.05
25	6	614	CLA	MG-ND	-2.14	2.01	2.05
24	r	614	CHL	C2C-C1C	2.14	1.49	1.44
25	B	602	CLA	MG-ND	-2.13	2.01	2.05
24	7	609	CHL	C4C-C3C	2.13	1.48	1.45
37	B	626	DGD	O2G-C2G	-2.13	1.41	1.46
25	G	613	CLA	C3B-CAB	-2.13	1.43	1.47
24	G	606	CHL	C3D-C2D	2.13	1.44	1.39
25	a	410	CLA	MG-ND	-2.13	2.01	2.05
30	b	618	BCR	C30-C25	-2.13	1.50	1.53
25	c	507	CLA	CMD-C2D	-2.13	1.46	1.50
25	B	612	CLA	C4B-CHC	-2.13	1.35	1.41
26	G	1621	LUT	C10-C9	-2.13	1.33	1.35
24	n	606	CHL	MG-ND	-2.13	2.01	2.05
25	n	612	CLA	MG-ND	-2.13	2.01	2.05
25	g	613	CLA	CMC-C2C	-2.13	1.46	1.50
25	g	610	CLA	C4B-CHC	-2.13	1.35	1.41
34	A	412	SQD	O4-C4	-2.13	1.38	1.43
34	a	412	SQD	O4-C4	-2.13	1.38	1.43
24	4	607	CHL	C4C-C3C	2.13	1.48	1.45
26	Y	1621	LUT	C30-C29	-2.13	1.33	1.35
30	B	618	BCR	C30-C25	-2.13	1.50	1.53
25	b	602	CLA	MG-ND	-2.13	2.01	2.05
25	g	613	CLA	C3B-CAB	-2.13	1.43	1.47
28	5	1623	NEX	C22-C21	-2.13	1.51	1.54
34	B	621	SQD	O2-C2	-2.13	1.38	1.43
35	a	413	LMG	O7-C8	-2.13	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	1620	LUT	C10-C9	-2.13	1.33	1.35
26	Y	1620	LUT	C34-C33	-2.13	1.33	1.35
25	1	611	CLA	C4B-CHC	-2.13	1.35	1.41
25	c	511	CLA	CMD-C2D	-2.13	1.46	1.50
26	N	1621	LUT	C10-C9	-2.13	1.33	1.35
33	A	409	PHO	CMB-C2B	-2.13	1.46	1.51
24	5	606	CHL	C4B-CHC	2.13	1.46	1.41
25	A	410	CLA	MG-ND	-2.12	2.01	2.05
25	n	614	CLA	CMC-C2C	-2.12	1.46	1.50
25	c	508	CLA	C4B-CHC	-2.12	1.35	1.41
26	y	1621	LUT	C30-C29	-2.12	1.33	1.35
25	s	613	CLA	CMD-C2D	-2.12	1.46	1.50
25	2	613	CLA	C3B-CAB	-2.12	1.43	1.47
26	G	1620	LUT	C30-C29	-2.12	1.33	1.35
35	A	413	LMG	O7-C8	-2.12	1.41	1.46
27	3	1622	XAT	O24-C25	-2.12	1.43	1.46
25	G	613	CLA	CMC-C2C	-2.12	1.46	1.50
25	n	611	CLA	CMC-C2C	-2.12	1.46	1.50
25	b	610	CLA	C3B-C2B	-2.12	1.37	1.40
25	b	612	CLA	C4B-CHC	-2.12	1.35	1.41
28	g	1623	NEX	O24-C25	-2.12	1.43	1.46
24	R	614	CHL	C2C-C1C	2.12	1.49	1.44
28	1	1623	NEX	C22-C21	-2.12	1.51	1.54
25	S	611	CLA	CMD-C2D	-2.12	1.46	1.50
24	G	601	CHL	C3D-C2D	2.12	1.44	1.39
24	1	606	CHL	C4B-CHC	2.12	1.46	1.41
25	G	610	CLA	C4B-CHC	-2.12	1.35	1.41
34	A	412	SQD	O3-C3	-2.12	1.38	1.43
25	b	602	CLA	C3B-CAB	-2.12	1.43	1.47
25	7	604	CLA	MG-ND	-2.12	2.01	2.05
25	2	613	CLA	CMC-C2C	-2.12	1.46	1.50
25	C	506	CLA	CMC-C2C	-2.12	1.46	1.50
25	r	612	CLA	CMC-C2C	-2.12	1.46	1.50
25	N	610	CLA	C4B-CHC	-2.12	1.35	1.41
25	7	614	CLA	CMD-C2D	-2.11	1.46	1.50
24	g	606	CHL	C3D-C2D	2.11	1.44	1.39
24	5	609	CHL	C1C-NC	-2.11	1.34	1.37
25	6	613	CLA	C3B-CAB	-2.11	1.43	1.47
25	8	611	CLA	C3B-C2B	-2.11	1.37	1.40
25	B	602	CLA	C3B-CAB	-2.11	1.43	1.47
25	r	609	CLA	MG-ND	-2.11	2.01	2.05
25	2	603	CLA	C4B-CHC	-2.11	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	621	SQD	O2-C2	-2.11	1.38	1.43
25	n	610	CLA	C4B-CHC	-2.11	1.35	1.41
25	C	507	CLA	CMD-C2D	-2.11	1.46	1.50
25	2	611	CLA	CMC-C2C	-2.11	1.46	1.50
25	c	505	CLA	C4B-CHC	-2.11	1.35	1.41
25	R	612	CLA	CMC-C2C	-2.11	1.46	1.50
25	6	613	CLA	CMC-C2C	-2.11	1.46	1.50
33	a	409	PHO	CMB-C2B	-2.11	1.46	1.51
26	g	1621	LUT	C10-C9	-2.11	1.33	1.35
25	5	611	CLA	C4B-CHC	-2.11	1.35	1.41
25	C	513	CLA	CMC-C2C	-2.11	1.46	1.50
25	c	506	CLA	CMC-C2C	-2.11	1.46	1.50
25	g	604	CLA	C3B-CAB	-2.11	1.43	1.47
25	D	402	CLA	C1D-ND	2.11	1.40	1.37
24	Y	609	CHL	C1C-NC	-2.11	1.34	1.37
33	A	408	PHO	C1C-NC	-2.11	1.32	1.38
26	4	620	LUT	C1-C6	-2.11	1.50	1.53
33	a	408	PHO	C1C-NC	-2.11	1.32	1.38
25	6	603	CLA	C4B-CHC	-2.10	1.35	1.41
25	S	613	CLA	CMD-C2D	-2.10	1.46	1.50
25	6	611	CLA	CMC-C2C	-2.10	1.46	1.50
25	Y	612	CLA	C3B-CAB	-2.10	1.43	1.47
25	s	611	CLA	CMD-C2D	-2.10	1.46	1.50
25	n	602	CLA	C3B-CAB	-2.10	1.43	1.47
34	a	412	SQD	O3-C3	-2.10	1.38	1.43
24	y	608	CHL	C1C-NC	-2.10	1.34	1.37
25	3	614	CLA	C3B-C2B	-2.10	1.37	1.40
24	s	607	CHL	C4C-C3C	2.10	1.48	1.45
24	1	608	CHL	C1D-ND	-2.10	1.35	1.37
24	2	601	CHL	C1B-CHB	2.10	1.46	1.41
25	B	605	CLA	CAC-C3C	-2.10	1.45	1.51
25	y	612	CLA	C3B-CAB	-2.10	1.43	1.47
24	n	607	CHL	C1C-NC	-2.10	1.34	1.37
25	C	501	CLA	CMC-C2C	-2.10	1.46	1.50
25	1	610	CLA	C4B-CHC	-2.10	1.35	1.41
25	2	603	CLA	C3B-CAB	-2.10	1.43	1.47
36	D	405	PL9	C10-C9	-2.10	1.45	1.50
25	3	604	CLA	MG-ND	-2.10	2.01	2.05
24	y	609	CHL	C1C-NC	-2.10	1.34	1.37
26	1	1620	LUT	C30-C29	-2.10	1.33	1.35
25	r	609	CLA	C3B-CAB	-2.09	1.43	1.47
25	c	513	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	405	PL9	C10-C9	-2.09	1.45	1.50
24	8	609	CHL	C1C-NC	-2.09	1.34	1.37
25	5	610	CLA	C4B-CHC	-2.09	1.35	1.41
29	B	2630	LHG	P-O6	2.09	1.67	1.59
25	B	615	CLA	C4B-CHC	-2.09	1.35	1.41
25	C	503	CLA	CMD-C2D	-2.09	1.46	1.50
25	b	605	CLA	CAC-C3C	-2.09	1.45	1.51
24	6	601	CHL	C1B-CHB	2.09	1.46	1.41
24	n	607	CHL	C3D-C2D	2.09	1.44	1.39
25	3	614	CLA	CMD-C2D	-2.09	1.46	1.50
24	1	605	CHL	C1B-CHB	2.09	1.46	1.41
25	G	604	CLA	C3B-CAB	-2.09	1.43	1.47
25	N	602	CLA	C3B-CAB	-2.09	1.43	1.47
25	r	601	CLA	C3B-CAB	-2.09	1.43	1.47
24	4	607	CHL	C1B-CHB	2.09	1.46	1.41
24	N	601	CHL	C1B-CHB	2.09	1.46	1.41
24	Y	608	CHL	C1C-NC	-2.09	1.34	1.37
25	5	613	CLA	C3B-CAB	-2.09	1.43	1.47
29	d	410	LHG	O7-C5	-2.09	1.41	1.46
35	d	411	LMG	O4-C4	-2.09	1.38	1.43
26	n	1621	LUT	C10-C9	-2.09	1.33	1.35
25	8	604	CLA	C4B-CHC	-2.09	1.35	1.41
25	1	614	CLA	CMC-C2C	-2.09	1.46	1.50
25	b	615	CLA	C4B-CHC	-2.09	1.35	1.41
25	c	504	CLA	CMC-C2C	-2.09	1.46	1.50
24	Y	606	CHL	MG-ND	-2.09	2.01	2.05
25	C	505	CLA	C4B-CHC	-2.09	1.35	1.41
24	5	605	CHL	C1B-CHB	2.08	1.46	1.41
25	G	611	CLA	CMC-C2C	-2.08	1.46	1.50
25	5	614	CLA	CMC-C2C	-2.08	1.46	1.50
24	7	607	CHL	C4B-CHC	2.08	1.46	1.41
25	6	614	CLA	CMC-C2C	-2.08	1.46	1.50
25	3	602	CLA	C4B-CHC	-2.08	1.35	1.41
24	S	607	CHL	C4C-C3C	2.08	1.48	1.45
25	7	602	CLA	C4B-CHC	-2.08	1.35	1.41
25	C	505	CLA	CMC-C2C	-2.08	1.46	1.50
25	R	601	CLA	CMD-C2D	-2.08	1.46	1.50
25	C	508	CLA	CMD-C2D	-2.08	1.46	1.50
29	y	2630	LHG	O8-C6	-2.08	1.40	1.45
25	4	602	CLA	MG-ND	-2.08	2.01	2.05
25	5	611	CLA	O2A-CGA	2.08	1.37	1.30
24	2	607	CHL	MG-ND	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	609	CLA	C4B-CHC	-2.08	1.35	1.41
25	1	613	CLA	C3B-CAB	-2.08	1.43	1.47
26	r	620	LUT	C34-C33	-2.08	1.33	1.35
25	2	612	CLA	C4B-CHC	-2.08	1.35	1.41
28	G	1623	NEX	O24-C25	-2.08	1.43	1.46
25	g	611	CLA	CMC-C2C	-2.08	1.46	1.50
25	b	613	CLA	C3B-C2B	-2.08	1.37	1.40
25	c	503	CLA	CMD-C2D	-2.08	1.46	1.50
24	N	607	CHL	C3D-C2D	2.08	1.44	1.39
24	N	608	CHL	C4B-CHC	2.08	1.46	1.41
25	5	614	CLA	C3B-C2B	-2.08	1.37	1.40
25	c	509	CLA	MG-ND	-2.08	2.01	2.05
25	C	513	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	613	CLA	C3B-C2B	-2.08	1.37	1.40
25	r	601	CLA	CMD-C2D	-2.08	1.46	1.50
25	Y	612	CLA	C4B-CHC	-2.08	1.35	1.41
24	n	608	CHL	C4B-CHC	2.08	1.46	1.41
25	1	614	CLA	C3B-C2B	-2.08	1.37	1.40
25	R	609	CLA	C3B-CAB	-2.08	1.43	1.47
24	1	606	CHL	C3D-C2D	2.08	1.44	1.39
25	N	611	CLA	CMC-C2C	-2.08	1.46	1.50
24	6	607	CHL	MG-ND	-2.08	2.01	2.05
25	C	509	CLA	MG-ND	-2.08	2.01	2.05
24	4	601	CHL	C4D-CHA	2.07	1.45	1.38
29	b	2630	LHG	P-O6	2.07	1.67	1.59
24	8	607	CHL	C1B-CHB	2.07	1.46	1.41
25	B	609	CLA	C4B-CHC	-2.07	1.35	1.41
24	4	609	CHL	C1C-NC	-2.07	1.34	1.37
25	1	611	CLA	O2A-CGA	2.07	1.37	1.30
25	S	603	CLA	CMD-C2D	-2.07	1.46	1.50
25	c	501	CLA	CMC-C2C	-2.07	1.46	1.50
25	c	505	CLA	CMC-C2C	-2.07	1.46	1.50
25	c	508	CLA	CMD-C2D	-2.07	1.46	1.50
25	s	603	CLA	CMD-C2D	-2.07	1.46	1.50
25	C	504	CLA	CMC-C2C	-2.07	1.46	1.50
24	5	601	CHL	MG-ND	-2.07	2.01	2.05
25	8	610	CLA	C3B-CAB	-2.07	1.43	1.47
25	y	612	CLA	C4B-CHC	-2.07	1.35	1.41
24	3	607	CHL	C4B-CHC	2.07	1.46	1.41
35	D	411	LMG	O4-C4	-2.07	1.38	1.43
25	4	604	CLA	C4B-CHC	-2.07	1.35	1.41
25	8	602	CLA	MG-ND	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Y	1622	XAT	C14-C13	-2.07	1.33	1.35
25	r	602	CLA	CAC-C3C	-2.07	1.45	1.51
24	N	607	CHL	C1C-NC	-2.07	1.34	1.37
24	n	601	CHL	C1B-CHB	2.07	1.46	1.41
24	8	601	CHL	C4D-CHA	2.07	1.45	1.38
25	B	602	CLA	C4B-CHC	-2.07	1.35	1.41
25	R	601	CLA	C3B-CAB	-2.07	1.43	1.47
25	c	506	CLA	MG-ND	-2.07	2.01	2.05
25	R	616	CLA	CAC-C3C	-2.07	1.45	1.51
25	7	611	CLA	CMC-C2C	-2.07	1.46	1.50
25	4	610	CLA	C3B-CAB	-2.07	1.43	1.47
25	y	613	CLA	CMC-C2C	-2.07	1.46	1.50
29	Y	2630	LHG	O8-C6	-2.07	1.40	1.45
28	n	1623	NEX	C10-C9	-2.07	1.33	1.35
25	r	616	CLA	CAC-C3C	-2.06	1.45	1.51
25	A	407	CLA	CMC-C2C	-2.06	1.46	1.50
24	n	605	CHL	C4B-CHC	2.06	1.46	1.41
25	r	601	CLA	C3B-C2B	-2.06	1.37	1.40
25	6	612	CLA	C4B-CHC	-2.06	1.35	1.41
24	5	608	CHL	C1D-ND	-2.06	1.35	1.37
25	b	603	CLA	MG-ND	-2.06	2.01	2.05
25	a	407	CLA	CMC-C2C	-2.06	1.46	1.50
25	B	603	CLA	MG-ND	-2.06	2.01	2.05
25	b	613	CLA	C4B-CHC	-2.06	1.35	1.41
24	2	601	CHL	C1C-NC	-2.06	1.34	1.37
26	8	620	LUT	C1-C6	-2.06	1.50	1.53
24	3	609	CHL	C1B-CHB	2.06	1.46	1.41
25	2	614	CLA	CMC-C2C	-2.06	1.46	1.50
25	R	602	CLA	CAC-C3C	-2.06	1.45	1.51
24	6	601	CHL	C1C-NC	-2.06	1.34	1.37
25	6	603	CLA	C3B-CAB	-2.06	1.43	1.47
26	R	620	LUT	C34-C33	-2.06	1.33	1.35
24	3	609	CHL	C1B-NB	-2.06	1.33	1.35
25	b	602	CLA	C4B-CHC	-2.06	1.35	1.41
25	C	504	CLA	CMD-C2D	-2.06	1.46	1.50
25	c	513	CLA	CMD-C2D	-2.06	1.46	1.50
39	f	101	HEM	CMB-C2B	2.06	1.55	1.50
24	3	607	CHL	C1D-ND	-2.06	1.35	1.37
26	7	1620	LUT	C30-C29	-2.06	1.33	1.35
37	c	520	DGD	O2G-C2G	-2.06	1.41	1.46
24	N	605	CHL	C4B-CHC	2.06	1.46	1.41
30	T	101	BCR	C1-C6	-2.06	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	606	CHL	C3D-C2D	2.06	1.44	1.39
25	C	506	CLA	MG-ND	-2.06	2.01	2.05
25	b	607	CLA	MG-ND	-2.06	2.01	2.05
25	S	612	CLA	CMC-C2C	-2.06	1.46	1.50
29	D	410	LHG	O7-C5	-2.05	1.41	1.46
30	t	101	BCR	C1-C6	-2.05	1.50	1.53
26	5	1620	LUT	C30-C29	-2.05	1.33	1.35
28	N	1623	NEX	C10-C9	-2.05	1.33	1.35
25	Y	613	CLA	CMC-C2C	-2.05	1.46	1.50
25	3	611	CLA	CMC-C2C	-2.05	1.46	1.50
25	c	506	CLA	C4B-CHC	-2.05	1.35	1.41
25	r	602	CLA	C3B-CAB	-2.05	1.43	1.47
27	8	622	XAT	O24-C25	-2.05	1.43	1.46
24	8	609	CHL	C4C-C3C	2.05	1.48	1.45
25	B	613	CLA	C4B-CHC	-2.05	1.35	1.41
26	g	1620	LUT	C30-C29	-2.05	1.33	1.35
24	S	607	CHL	C4D-CHA	2.05	1.45	1.38
25	C	509	CLA	CMC-C2C	-2.05	1.46	1.50
25	c	504	CLA	CMD-C2D	-2.05	1.46	1.50
24	Y	606	CHL	C3D-C2D	2.05	1.44	1.39
25	s	612	CLA	CMC-C2C	-2.05	1.46	1.50
26	3	1620	LUT	C30-C29	-2.05	1.33	1.35
24	3	606	CHL	C4C-C3C	2.04	1.48	1.45
34	b	621	SQD	O4-C4	-2.04	1.38	1.43
25	C	502	CLA	CMC-C2C	-2.04	1.46	1.50
25	Y	613	CLA	CMD-C2D	-2.04	1.46	1.50
25	a	406	CLA	CMC-C2C	-2.04	1.46	1.50
39	F	101	HEM	CMB-C2B	2.04	1.55	1.50
24	7	607	CHL	C1D-ND	-2.04	1.35	1.37
25	n	614	CLA	C4B-CHC	-2.04	1.35	1.41
24	7	608	CHL	C2C-C1C	2.04	1.49	1.44
25	R	602	CLA	C3B-CAB	-2.04	1.43	1.47
37	C	520	DGD	O2G-C2G	-2.04	1.41	1.46
24	4	609	CHL	C4C-C3C	2.04	1.48	1.45
25	B	607	CLA	MG-ND	-2.04	2.01	2.05
24	y	606	CHL	C3D-C2D	2.04	1.44	1.39
25	A	406	CLA	CMC-C2C	-2.04	1.46	1.50
24	7	609	CHL	C1B-CHB	2.04	1.46	1.41
24	N	607	CHL	C1D-C2D	2.04	1.49	1.45
25	B	605	CLA	CAA-C2A	-2.04	1.50	1.54
24	1	601	CHL	MG-ND	-2.04	2.01	2.05
24	G	609	CHL	C4C-C3C	2.04	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	402	CLA	C4B-CHC	-2.04	1.35	1.41
25	R	601	CLA	C3B-C2B	-2.04	1.37	1.40
25	4	602	CLA	CMD-C2D	-2.04	1.46	1.50
25	C	507	CLA	CMC-C2C	-2.04	1.46	1.50
35	b	2633	LMG	O2-C2	-2.04	1.38	1.43
24	g	605	CHL	C1B-CHB	2.04	1.46	1.41
24	s	607	CHL	C4D-CHA	2.04	1.45	1.38
25	6	611	CLA	C4B-CHC	-2.04	1.35	1.41
24	g	608	CHL	C3D-C2D	2.04	1.44	1.39
34	B	621	SQD	O4-C4	-2.04	1.38	1.43
24	y	608	CHL	C4B-CHC	2.04	1.46	1.41
25	C	506	CLA	C4B-CHC	-2.04	1.35	1.41
25	a	405	CLA	C4B-CHC	-2.04	1.35	1.41
26	R	620	LUT	C30-C29	-2.04	1.33	1.35
25	c	502	CLA	CMC-C2C	-2.04	1.46	1.50
24	2	606	CHL	C1C-NC	-2.03	1.34	1.37
34	A	418	SQD	O4-C4	-2.03	1.38	1.43
30	b	619	BCR	C14-C13	-2.03	1.33	1.35
30	B	619	BCR	C14-C13	-2.03	1.33	1.35
25	Y	602	CLA	C4B-CHC	-2.03	1.35	1.41
25	3	613	CLA	CAC-C3C	-2.03	1.45	1.51
24	7	606	CHL	C4C-C3C	2.03	1.48	1.45
25	R	611	CLA	CMC-C2C	-2.03	1.46	1.50
35	c	521	LMG	O7-C8	-2.03	1.41	1.46
25	d	402	CLA	C4B-CHC	-2.03	1.35	1.41
34	a	418	SQD	O4-C4	-2.03	1.38	1.43
28	1	1623	NEX	C30-C29	-2.03	1.33	1.35
25	y	613	CLA	CMD-C2D	-2.03	1.46	1.50
24	3	608	CHL	C2C-C1C	2.03	1.48	1.44
24	6	606	CHL	C1C-NC	-2.03	1.34	1.37
24	2	601	CHL	C4B-CHC	2.03	1.46	1.41
24	1	601	CHL	C1B-CHB	2.03	1.46	1.41
25	b	605	CLA	CAA-C2A	-2.03	1.50	1.54
25	7	613	CLA	CAC-C3C	-2.03	1.45	1.51
26	6	1621	LUT	C22-C21	-2.03	1.52	1.54
24	2	609	CHL	C1B-CHB	2.03	1.46	1.41
24	g	601	CHL	C4B-CHC	2.03	1.46	1.41
25	A	405	CLA	C4B-CHC	-2.03	1.35	1.41
27	1	1622	XAT	O24-C25	-2.03	1.43	1.46
25	A	407	CLA	MG-ND	-2.03	2.01	2.05
25	N	614	CLA	MG-ND	-2.03	2.01	2.05
25	r	604	CLA	C4B-CHC	-2.03	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	614	CLA	C4B-CHC	-2.03	1.35	1.41
24	7	605	CHL	C4B-CHC	2.03	1.46	1.41
35	b	2633	LMG	C3-C2	2.03	1.57	1.52
25	R	601	CLA	MG-ND	-2.03	2.01	2.05
25	c	510	CLA	MG-ND	-2.03	2.01	2.05
24	6	608	CHL	C4C-C3C	2.03	1.48	1.45
24	6	605	CHL	C1B-CHB	2.03	1.46	1.41
24	S	606	CHL	C4D-CHA	2.03	1.45	1.38
24	s	606	CHL	C4D-CHA	2.03	1.45	1.38
24	N	606	CHL	C1D-C2D	2.03	1.49	1.45
24	n	607	CHL	C1D-C2D	2.02	1.49	1.45
25	c	509	CLA	CMC-C2C	-2.02	1.46	1.50
24	2	605	CHL	C1B-CHB	2.02	1.46	1.41
25	r	601	CLA	MG-ND	-2.02	2.01	2.05
26	n	1620	LUT	C14-C13	-2.02	1.33	1.35
24	G	606	CHL	C4B-CHC	2.02	1.46	1.41
25	S	603	CLA	C3B-C2B	-2.02	1.37	1.40
25	7	602	CLA	C3B-C2B	-2.02	1.37	1.40
35	B	2633	LMG	C3-C2	2.02	1.57	1.52
25	8	602	CLA	CMD-C2D	-2.02	1.46	1.50
24	6	601	CHL	C4B-CHC	2.02	1.46	1.41
27	y	1622	XAT	C14-C13	-2.02	1.33	1.35
24	g	609	CHL	C4C-C3C	2.02	1.48	1.45
24	G	601	CHL	C4B-CHC	2.02	1.46	1.41
24	S	607	CHL	C1B-CHB	2.02	1.46	1.41
24	R	606	CHL	C4B-CHC	2.02	1.46	1.41
25	C	510	CLA	MG-ND	-2.02	2.01	2.05
25	R	602	CLA	C4B-CHC	-2.02	1.35	1.41
24	g	605	CHL	C4B-CHC	2.02	1.46	1.41
24	G	608	CHL	C3D-C2D	2.02	1.44	1.39
33	A	409	PHO	C1C-NC	-2.02	1.32	1.38
24	6	609	CHL	C1B-CHB	2.02	1.46	1.41
24	7	606	CHL	C1D-ND	-2.02	1.35	1.37
24	G	605	CHL	C4B-CHC	2.02	1.46	1.41
33	A	408	PHO	C3B-CAB	-2.02	1.43	1.47
25	R	604	CLA	C4B-CHC	-2.02	1.35	1.41
30	b	619	BCR	C21-C22	-2.02	1.33	1.35
24	S	607	CHL	C4B-CHC	2.02	1.46	1.41
24	g	606	CHL	C4B-CHC	2.02	1.46	1.41
33	a	409	PHO	C1C-NC	-2.02	1.32	1.38
25	2	612	CLA	CMC-C2C	-2.02	1.46	1.50
25	S	610	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	603	CLA	C3B-C2B	-2.02	1.37	1.40
25	r	602	CLA	C4B-CHC	-2.02	1.35	1.41
24	Y	608	CHL	C4B-CHC	2.02	1.46	1.41
25	S	613	CLA	CMC-C2C	-2.02	1.46	1.50
24	3	605	CHL	C4B-CHC	2.02	1.46	1.41
24	2	608	CHL	C4C-C3C	2.02	1.48	1.45
35	B	2633	LMG	O2-C2	-2.02	1.38	1.43
25	n	602	CLA	C3B-C2B	-2.01	1.37	1.40
24	G	605	CHL	C1B-CHB	2.01	1.46	1.41
26	r	620	LUT	C30-C29	-2.01	1.33	1.35
25	d	403	CLA	C3B-CAB	-2.01	1.43	1.47
25	y	602	CLA	C4B-CHC	-2.01	1.35	1.41
24	s	607	CHL	C4B-CHC	2.01	1.46	1.41
26	N	1620	LUT	C14-C13	-2.01	1.33	1.35
33	a	408	PHO	C3B-CAB	-2.01	1.43	1.47
25	n	614	CLA	MG-ND	-2.01	2.01	2.05
25	r	611	CLA	C3B-CAB	-2.01	1.43	1.47
24	s	607	CHL	C1B-CHB	2.01	1.46	1.41
25	c	507	CLA	CMC-C2C	-2.01	1.46	1.50
24	1	607	CHL	C3D-C2D	2.01	1.44	1.39
25	a	407	CLA	MG-ND	-2.01	2.01	2.05
28	y	1623	NEX	C22-C21	-2.01	1.51	1.54
25	r	611	CLA	CMC-C2C	-2.01	1.46	1.50
24	n	609	CHL	C3A-C2A	-2.01	1.48	1.54
24	N	608	CHL	C3D-C2D	2.01	1.44	1.39
25	Y	614	CLA	C4B-CHC	-2.01	1.35	1.41
24	3	606	CHL	C1D-ND	-2.01	1.35	1.37
25	Y	603	CLA	C4B-CHC	-2.01	1.35	1.41
24	5	601	CHL	C1B-CHB	2.01	1.46	1.41
24	7	609	CHL	C1B-NB	-2.01	1.33	1.35
25	D	403	CLA	C3B-CAB	-2.01	1.43	1.47
25	b	605	CLA	CMA-C3A	-2.01	1.48	1.53
27	5	1622	XAT	O24-C25	-2.01	1.43	1.46
24	n	606	CHL	C1D-C2D	2.01	1.49	1.45
37	h	102	DGD	O3D-C3D	-2.01	1.38	1.43
25	y	603	CLA	C4B-CHC	-2.01	1.35	1.41
24	6	608	CHL	C4B-CHC	2.01	1.46	1.41
25	S	611	CLA	C3B-C2B	-2.01	1.37	1.40
25	g	602	CLA	C3B-C2B	-2.01	1.37	1.40
27	4	622	XAT	O24-C25	-2.01	1.43	1.46
25	N	602	CLA	C3B-C2B	-2.00	1.37	1.40
25	s	610	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	608	CHL	C4D-CHA	2.00	1.45	1.38
24	s	608	CHL	C4D-CHA	2.00	1.45	1.38
25	b	608	CLA	C3B-CAB	-2.00	1.43	1.47
25	2	611	CLA	C4B-CHC	-2.00	1.35	1.41
24	G	605	CHL	C4C-C3C	2.00	1.48	1.45
26	2	1621	LUT	C22-C21	-2.00	1.52	1.54
24	1	601	CHL	C1D-ND	-2.00	1.35	1.37
24	g	608	CHL	C1B-CHB	2.00	1.46	1.41
25	C	504	CLA	C4B-CHC	-2.00	1.35	1.41
24	8	607	CHL	C4B-CHC	2.00	1.46	1.41
24	2	608	CHL	C4B-CHC	2.00	1.46	1.41
25	B	608	CLA	C3B-CAB	-2.00	1.43	1.47
24	7	607	CHL	C1B-NB	-2.00	1.33	1.35
25	6	604	CLA	C3B-CAB	-2.00	1.43	1.47
25	4	611	CLA	CMC-C2C	-2.00	1.46	1.50
24	5	607	CHL	C3D-C2D	2.00	1.44	1.39
25	n	611	CLA	C3B-CAB	-2.00	1.43	1.47

All (5869) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	1622	XAT	O24-C25-C24	10.52	121.28	113.38
27	1	1622	XAT	O24-C25-C24	10.51	121.28	113.38
24	y	601	CHL	CMD-C2D-C1D	10.18	142.65	124.71
24	Y	601	CHL	CMD-C2D-C1D	10.16	142.62	124.71
24	2	601	CHL	CMD-C2D-C1D	9.95	142.25	124.71
24	6	601	CHL	CMD-C2D-C1D	9.94	142.22	124.71
24	1	601	CHL	CMD-C2D-C1D	9.91	142.18	124.71
24	5	601	CHL	CMD-C2D-C1D	9.89	142.14	124.71
28	6	1623	NEX	O24-C25-C24	9.83	120.76	113.38
27	2	1622	XAT	O4-C5-C4	9.81	120.75	113.38
27	6	1622	XAT	O4-C5-C4	9.81	120.75	113.38
28	G	1623	NEX	O24-C25-C24	9.78	120.73	113.38
28	g	1623	NEX	O24-C25-C24	9.78	120.73	113.38
28	2	1623	NEX	O24-C25-C24	9.73	120.69	113.38
24	5	607	CHL	C2C-C3C-C4C	-9.67	99.59	106.49
24	1	607	CHL	C2C-C3C-C4C	-9.66	99.60	106.49
28	5	1623	NEX	O24-C25-C24	9.56	120.57	113.38
28	1	1623	NEX	O24-C25-C24	9.52	120.53	113.38
27	2	1622	XAT	O24-C25-C24	9.41	120.45	113.38
24	g	601	CHL	CMD-C2D-C1D	9.38	141.25	124.71
27	6	1622	XAT	O24-C25-C24	9.37	120.42	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	601	CHL	CMD-C2D-C1D	9.36	141.21	124.71
24	G	601	CHL	CMD-C2D-C1D	9.35	141.20	124.71
24	7	601	CHL	CMD-C2D-C1D	9.34	141.18	124.71
25	Y	613	CLA	C4A-NA-C1A	9.33	110.90	106.71
24	N	607	CHL	C2C-C3C-C4C	-9.32	99.85	106.49
25	y	613	CLA	C4A-NA-C1A	9.30	110.89	106.71
24	n	607	CHL	C2C-C3C-C4C	-9.30	99.86	106.49
28	3	1623	NEX	O24-C25-C24	9.28	120.35	113.38
28	7	1623	NEX	O24-C25-C24	9.27	120.35	113.38
24	y	607	CHL	C2C-C3C-C4C	-9.26	99.89	106.49
24	Y	607	CHL	C2C-C3C-C4C	-9.24	99.90	106.49
24	Y	601	CHL	C1D-ND-C4D	-9.24	99.77	106.33
24	3	606	CHL	CMD-C2D-C1D	9.23	140.98	124.71
27	G	1622	XAT	O24-C25-C24	9.22	120.31	113.38
24	7	606	CHL	CMD-C2D-C1D	9.22	140.97	124.71
24	4	609	CHL	CMD-C2D-C1D	9.22	140.97	124.71
27	g	1622	XAT	O24-C25-C24	9.22	120.31	113.38
24	y	601	CHL	C1D-ND-C4D	-9.20	99.80	106.33
24	8	609	CHL	CMD-C2D-C1D	9.20	140.93	124.71
24	N	601	CHL	CMD-C2D-C1D	9.12	140.79	124.71
24	n	601	CHL	CMD-C2D-C1D	9.11	140.78	124.71
24	g	608	CHL	CMD-C2D-C1D	9.10	140.75	124.71
24	5	607	CHL	CMD-C2D-C1D	9.10	140.75	124.71
24	1	607	CHL	CMD-C2D-C1D	9.10	140.75	124.71
24	G	608	CHL	CMD-C2D-C1D	9.09	140.73	124.71
24	y	608	CHL	C1D-ND-C4D	-9.07	99.90	106.33
24	R	614	CHL	CMD-C2D-C1D	9.05	140.67	124.71
24	Y	608	CHL	C1D-ND-C4D	-9.05	99.91	106.33
24	r	614	CHL	CMD-C2D-C1D	9.03	140.62	124.71
24	r	607	CHL	CMD-C2D-C1D	8.92	140.43	124.71
24	1	608	CHL	CMD-C2D-C1D	8.90	140.40	124.71
24	R	607	CHL	CMD-C2D-C1D	8.90	140.40	124.71
24	5	608	CHL	CMD-C2D-C1D	8.90	140.39	124.71
24	y	609	CHL	CMD-C2D-C1D	8.87	140.35	124.71
24	Y	609	CHL	CMD-C2D-C1D	8.86	140.33	124.71
24	7	609	CHL	CMD-C2D-C1D	8.83	140.28	124.71
24	5	609	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	n	608	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	1	609	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	N	608	CHL	CMD-C2D-C1D	8.82	140.25	124.71
24	R	606	CHL	CMD-C2D-C1D	8.82	140.25	124.71
24	3	609	CHL	CMD-C2D-C1D	8.81	140.24	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	1622	XAT	O4-C5-C4	8.80	120.00	113.38
24	N	609	CHL	CMD-C2D-C1D	8.80	140.22	124.71
27	7	1622	XAT	O4-C5-C4	8.79	119.98	113.38
24	r	606	CHL	CMD-C2D-C1D	8.79	140.20	124.71
24	n	609	CHL	CMD-C2D-C1D	8.78	140.19	124.71
24	1	605	CHL	C2C-C3C-C4C	-8.78	100.23	106.49
24	3	608	CHL	CMD-C2D-C1D	8.76	140.15	124.71
24	5	605	CHL	C2C-C3C-C4C	-8.75	100.25	106.49
24	3	607	CHL	C2C-C3C-C4C	-8.74	100.26	106.49
24	7	608	CHL	CMD-C2D-C1D	8.73	140.11	124.71
24	7	607	CHL	C2C-C3C-C4C	-8.73	100.27	106.49
24	y	606	CHL	C2C-C3C-C4C	-8.72	100.27	106.49
25	n	613	CLA	C4A-NA-C1A	8.72	110.63	106.71
24	3	608	CHL	C1D-ND-C4D	-8.70	100.16	106.33
24	Y	606	CHL	C2C-C3C-C4C	-8.69	100.29	106.49
24	8	608	CHL	C1D-ND-C4D	-8.69	100.16	106.33
24	g	609	CHL	CMD-C2D-C1D	8.68	140.01	124.71
24	G	609	CHL	CMD-C2D-C1D	8.66	139.97	124.71
24	G	606	CHL	CMD-C2D-C1D	8.66	139.97	124.71
25	N	613	CLA	C4A-NA-C1A	8.66	110.60	106.71
24	7	608	CHL	C1D-ND-C4D	-8.65	100.19	106.33
24	g	606	CHL	CMD-C2D-C1D	8.64	139.93	124.71
24	4	608	CHL	C1D-ND-C4D	-8.63	100.21	106.33
24	G	608	CHL	C1D-ND-C4D	-8.62	100.21	106.33
24	g	608	CHL	C1D-ND-C4D	-8.61	100.22	106.33
24	R	608	CHL	CMD-C2D-C1D	8.60	139.88	124.71
24	n	606	CHL	CMD-C2D-C1D	8.60	139.87	124.71
24	2	608	CHL	CMD-C2D-C1D	8.60	139.86	124.71
24	N	606	CHL	CMD-C2D-C1D	8.59	139.86	124.71
24	4	608	CHL	CMD-C2D-C1D	8.59	139.86	124.71
24	r	608	CHL	CMD-C2D-C1D	8.59	139.85	124.71
24	6	608	CHL	CMD-C2D-C1D	8.59	139.85	124.71
24	8	608	CHL	CMD-C2D-C1D	8.59	139.85	124.71
24	y	608	CHL	CMD-C2D-C1D	8.55	139.79	124.71
24	3	601	CHL	C1D-ND-C4D	-8.55	100.26	106.33
24	g	606	CHL	C2C-C3C-C4C	-8.54	100.40	106.49
24	G	606	CHL	C2C-C3C-C4C	-8.54	100.40	106.49
24	y	607	CHL	CMD-C2D-C1D	8.54	139.76	124.71
24	Y	608	CHL	CMD-C2D-C1D	8.53	139.75	124.71
24	s	601	CHL	C1D-ND-C4D	-8.52	100.28	106.33
24	Y	607	CHL	CMD-C2D-C1D	8.51	139.71	124.71
24	7	601	CHL	C1D-ND-C4D	-8.49	100.30	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	608	CHL	CMD-C2D-C1D	8.47	139.64	124.71
24	S	601	CHL	C1D-ND-C4D	-8.47	100.32	106.33
24	s	608	CHL	CMD-C2D-C1D	8.46	139.63	124.71
24	6	606	CHL	C2C-C3C-C4C	-8.45	100.47	106.49
24	2	606	CHL	C2C-C3C-C4C	-8.45	100.47	106.49
24	N	601	CHL	C1D-ND-C4D	-8.44	100.34	106.33
24	n	608	CHL	C1D-ND-C4D	-8.44	100.34	106.33
24	N	607	CHL	CMD-C2D-C1D	8.43	139.57	124.71
24	2	609	CHL	CMD-C2D-C1D	8.43	139.57	124.71
24	n	607	CHL	CMD-C2D-C1D	8.43	139.57	124.71
24	1	606	CHL	C2C-C3C-C4C	-8.43	100.48	106.49
24	n	601	CHL	C1D-ND-C4D	-8.42	100.35	106.33
24	6	609	CHL	CMD-C2D-C1D	8.42	139.54	124.71
24	n	605	CHL	CMD-C2D-C1D	8.42	139.54	124.71
24	N	608	CHL	C1D-ND-C4D	-8.42	100.36	106.33
24	n	606	CHL	C2C-C3C-C4C	-8.41	100.50	106.49
28	n	1623	NEX	O24-C25-C24	8.41	119.70	113.38
24	N	606	CHL	C2C-C3C-C4C	-8.40	100.50	106.49
24	5	606	CHL	C2C-C3C-C4C	-8.40	100.50	106.49
28	N	1623	NEX	O24-C25-C24	8.40	119.69	113.38
24	1	606	CHL	CMD-C2D-C1D	8.40	139.51	124.71
24	s	601	CHL	CMD-C2D-C1D	8.39	139.50	124.71
24	N	605	CHL	CMD-C2D-C1D	8.39	139.49	124.71
24	S	601	CHL	CMD-C2D-C1D	8.37	139.46	124.71
24	5	606	CHL	CMD-C2D-C1D	8.37	139.46	124.71
24	r	608	CHL	C1D-ND-C4D	-8.36	100.40	106.33
24	R	608	CHL	C1D-ND-C4D	-8.35	100.40	106.33
24	2	608	CHL	C1D-ND-C4D	-8.35	100.40	106.33
24	G	601	CHL	C1D-ND-C4D	-8.35	100.40	106.33
24	g	607	CHL	C2C-C3C-C4C	-8.33	100.55	106.49
24	g	601	CHL	C1D-ND-C4D	-8.32	100.42	106.33
24	4	606	CHL	CMD-C2D-C1D	8.32	139.37	124.71
24	4	607	CHL	CMD-C2D-C1D	8.31	139.36	124.71
24	8	606	CHL	CMD-C2D-C1D	8.30	139.34	124.71
24	6	608	CHL	C1D-ND-C4D	-8.29	100.44	106.33
24	8	607	CHL	CMD-C2D-C1D	8.29	139.32	124.71
24	G	605	CHL	CMD-C2D-C1D	8.28	139.31	124.71
24	g	605	CHL	CMD-C2D-C1D	8.28	139.31	124.71
24	5	608	CHL	C1D-ND-C4D	-8.28	100.45	106.33
24	G	607	CHL	C2C-C3C-C4C	-8.27	100.59	106.49
24	1	608	CHL	C1D-ND-C4D	-8.25	100.47	106.33
24	7	605	CHL	C1D-ND-C4D	-8.25	100.47	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	605	CHL	C1D-ND-C4D	-8.25	100.47	106.33
24	4	609	CHL	C2C-C3C-C4C	-8.24	100.61	106.49
24	8	609	CHL	C2C-C3C-C4C	-8.22	100.63	106.49
24	2	601	CHL	C1D-ND-C4D	-8.20	100.51	106.33
24	6	601	CHL	C1D-ND-C4D	-8.19	100.52	106.33
24	G	607	CHL	CMD-C2D-C1D	8.17	139.10	124.71
24	g	607	CHL	CMD-C2D-C1D	8.14	139.06	124.71
24	y	608	CHL	C2D-C1D-ND	8.13	116.09	110.10
24	3	605	CHL	CMD-C2D-C1D	8.13	139.04	124.71
24	7	605	CHL	CMD-C2D-C1D	8.13	139.03	124.71
24	5	605	CHL	CMD-C2D-C1D	8.12	139.01	124.71
24	1	605	CHL	CMD-C2D-C1D	8.11	139.00	124.71
24	7	607	CHL	CMD-C2D-C1D	8.10	139.00	124.71
24	3	607	CHL	CMD-C2D-C1D	8.10	138.99	124.71
24	Y	608	CHL	C2C-C3C-C4C	-8.10	100.72	106.49
24	y	608	CHL	C2C-C3C-C4C	-8.10	100.72	106.49
24	y	605	CHL	CMD-C2D-C1D	8.09	138.98	124.71
24	n	607	CHL	C1D-ND-C4D	-8.09	100.59	106.33
24	G	606	CHL	C1D-ND-C4D	-8.09	100.59	106.33
24	1	607	CHL	C1D-ND-C4D	-8.09	100.59	106.33
24	Y	608	CHL	C2D-C1D-ND	8.08	116.06	110.10
24	Y	605	CHL	CMD-C2D-C1D	8.07	138.93	124.71
24	N	607	CHL	C1D-ND-C4D	-8.07	100.60	106.33
24	2	606	CHL	CMD-C2D-C1D	8.06	138.92	124.71
24	6	606	CHL	CMD-C2D-C1D	8.06	138.92	124.71
24	8	601	CHL	CMD-C2D-C1D	8.05	138.91	124.71
24	4	601	CHL	CMD-C2D-C1D	8.05	138.90	124.71
24	5	607	CHL	C1D-ND-C4D	-8.05	100.62	106.33
24	g	606	CHL	C1D-ND-C4D	-8.03	100.63	106.33
24	2	605	CHL	CMD-C2D-C1D	8.02	138.85	124.71
24	6	605	CHL	CMD-C2D-C1D	8.02	138.85	124.71
24	s	606	CHL	CMD-C2D-C1D	8.01	138.84	124.71
24	2	607	CHL	CMD-C2D-C1D	8.00	138.82	124.71
24	S	606	CHL	CMD-C2D-C1D	8.00	138.81	124.71
25	c	502	CLA	C4A-NA-C1A	7.99	110.30	106.71
24	R	606	CHL	C2C-C3C-C4C	-7.99	100.79	106.49
24	6	607	CHL	CMD-C2D-C1D	7.99	138.79	124.71
24	5	601	CHL	C1D-ND-C4D	-7.98	100.66	106.33
24	4	606	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
25	C	502	CLA	C4A-NA-C1A	7.97	110.29	106.71
24	2	607	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
24	8	606	CHL	C2C-C3C-C4C	-7.97	100.81	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	608	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
24	r	606	CHL	C2C-C3C-C4C	-7.96	100.81	106.49
24	1	601	CHL	C1D-ND-C4D	-7.95	100.68	106.33
24	S	606	CHL	C2C-C3C-C4C	-7.95	100.82	106.49
24	R	608	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
24	6	608	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
24	r	608	CHL	C2C-C3C-C4C	-7.93	100.83	106.49
24	6	607	CHL	C2C-C3C-C4C	-7.93	100.84	106.49
24	s	606	CHL	C2C-C3C-C4C	-7.92	100.84	106.49
24	4	606	CHL	C1D-ND-C4D	-7.91	100.72	106.33
24	g	607	CHL	C1D-ND-C4D	-7.91	100.72	106.33
24	R	608	CHL	C2D-C1D-ND	7.90	115.92	110.10
24	G	607	CHL	C1D-ND-C4D	-7.89	100.73	106.33
24	r	608	CHL	C2D-C1D-ND	7.89	115.92	110.10
24	8	609	CHL	C1D-ND-C4D	-7.86	100.75	106.33
24	Y	607	CHL	C1D-ND-C4D	-7.86	100.75	106.33
24	R	614	CHL	CHD-C1D-ND	-7.85	117.24	124.45
24	4	609	CHL	C1D-ND-C4D	-7.84	100.76	106.33
24	8	606	CHL	C1D-ND-C4D	-7.84	100.76	106.33
24	y	607	CHL	C1D-ND-C4D	-7.82	100.78	106.33
24	r	614	CHL	CHD-C1D-ND	-7.82	117.27	124.45
24	S	607	CHL	C1D-ND-C4D	-7.82	100.78	106.33
28	S	1623	NEX	O24-C25-C24	7.82	119.25	113.38
24	R	606	CHL	C1D-ND-C4D	-7.81	100.78	106.33
27	1	1622	XAT	O4-C5-C4	7.81	119.25	113.38
24	n	605	CHL	C1D-ND-C4D	-7.80	100.79	106.33
24	Y	605	CHL	C1D-ND-C4D	-7.80	100.80	106.33
24	y	605	CHL	C1D-ND-C4D	-7.79	100.80	106.33
28	s	1623	NEX	O24-C25-C24	7.79	119.23	113.38
24	s	607	CHL	C1D-ND-C4D	-7.78	100.81	106.33
24	r	606	CHL	C1D-ND-C4D	-7.77	100.81	106.33
24	2	609	CHL	C1D-ND-C4D	-7.76	100.82	106.33
24	3	608	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
24	7	608	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
27	5	1622	XAT	O4-C5-C4	7.75	119.20	113.38
24	R	614	CHL	C1D-ND-C4D	-7.75	100.83	106.33
24	3	608	CHL	C2D-C1D-ND	7.74	115.81	110.10
24	r	607	CHL	C1D-ND-C4D	-7.74	100.84	106.33
24	N	605	CHL	C1D-ND-C4D	-7.73	100.84	106.33
27	n	1622	XAT	O24-C25-C24	7.73	119.19	113.38
24	5	608	CHL	C2C-C3C-C4C	-7.72	100.98	106.49
24	6	609	CHL	C1D-ND-C4D	-7.72	100.85	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	607	CHL	C1D-ND-C4D	-7.71	100.86	106.33
24	r	614	CHL	C1D-ND-C4D	-7.70	100.86	106.33
24	S	607	CHL	CMD-C2D-C1D	7.70	138.28	124.71
27	N	1622	XAT	O24-C25-C24	7.70	119.17	113.38
24	1	608	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
24	S	606	CHL	C1D-ND-C4D	-7.69	100.87	106.33
24	g	608	CHL	C2C-C3C-C4C	-7.68	101.01	106.49
24	s	607	CHL	CMD-C2D-C1D	7.68	138.25	124.71
24	g	605	CHL	C1D-ND-C4D	-7.67	100.88	106.33
24	G	608	CHL	C2C-C3C-C4C	-7.67	101.02	106.49
24	2	605	CHL	C1D-ND-C4D	-7.67	100.89	106.33
24	6	605	CHL	C1D-ND-C4D	-7.66	100.89	106.33
24	7	608	CHL	C2D-C1D-ND	7.66	115.75	110.10
24	4	601	CHL	CHD-C1D-ND	-7.66	117.42	124.45
24	s	606	CHL	C1D-ND-C4D	-7.65	100.90	106.33
24	n	605	CHL	C2C-C3C-C4C	-7.65	101.04	106.49
24	3	605	CHL	C2C-C3C-C4C	-7.65	101.04	106.49
24	N	605	CHL	C2C-C3C-C4C	-7.65	101.04	106.49
24	7	605	CHL	C2C-C3C-C4C	-7.65	101.04	106.49
30	8	623	BCR	C24-C23-C22	-7.63	114.70	126.23
24	G	605	CHL	C1D-ND-C4D	-7.63	100.91	106.33
24	8	601	CHL	CHD-C1D-ND	-7.63	117.44	124.45
24	2	605	CHL	C2C-C3C-C4C	-7.62	101.06	106.49
24	y	606	CHL	CMD-C2D-C1D	7.62	138.14	124.71
30	4	623	BCR	C24-C23-C22	-7.61	114.73	126.23
24	Y	606	CHL	CMD-C2D-C1D	7.61	138.13	124.71
24	6	605	CHL	C2C-C3C-C4C	-7.58	101.09	106.49
27	N	1622	XAT	C15-C14-C13	-7.55	116.54	127.31
24	R	607	CHL	C2C-C3C-C4C	-7.54	101.12	106.49
24	r	607	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
24	S	608	CHL	C1D-ND-C4D	-7.52	100.99	106.33
27	n	1622	XAT	C15-C14-C13	-7.52	116.58	127.31
24	S	608	CHL	C2C-C3C-C4C	-7.51	101.13	106.49
24	4	607	CHL	C2C-C3C-C4C	-7.50	101.15	106.49
24	8	607	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
24	G	605	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
24	g	605	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
24	s	608	CHL	C1D-ND-C4D	-7.45	101.05	106.33
24	s	608	CHL	C2C-C3C-C4C	-7.43	101.19	106.49
24	7	606	CHL	C2C-C3C-C4C	-7.42	101.20	106.49
24	8	608	CHL	C2D-C1D-ND	7.41	115.57	110.10
24	Y	605	CHL	C2C-C3C-C4C	-7.41	101.21	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	608	CHL	C2D-C1D-ND	7.41	115.56	110.10
24	7	606	CHL	C1D-ND-C4D	-7.40	101.08	106.33
24	3	606	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
27	R	622	XAT	O24-C25-C24	7.39	118.94	113.38
24	2	608	CHL	C2D-C1D-ND	7.37	115.54	110.10
27	r	622	XAT	O24-C25-C24	7.36	118.91	113.38
24	y	605	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
24	7	607	CHL	C1D-ND-C4D	-7.36	101.10	106.33
24	3	606	CHL	C1D-ND-C4D	-7.36	101.11	106.33
24	y	606	CHL	C1D-ND-C4D	-7.35	101.12	106.33
24	6	608	CHL	C2D-C1D-ND	7.34	115.52	110.10
24	n	607	CHL	C2D-C1D-ND	7.34	115.51	110.10
24	N	607	CHL	C2D-C1D-ND	7.32	115.50	110.10
24	3	609	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
24	7	609	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
25	g	613	CLA	C4A-NA-C1A	7.30	109.99	106.71
25	G	613	CLA	C4A-NA-C1A	7.30	109.99	106.71
24	3	607	CHL	C1D-ND-C4D	-7.30	101.15	106.33
24	8	607	CHL	C1D-ND-C4D	-7.29	101.16	106.33
27	n	1622	XAT	O4-C5-C4	7.28	118.85	113.38
24	4	607	CHL	C1D-ND-C4D	-7.28	101.17	106.33
24	s	601	CHL	C2C-C3C-C4C	-7.28	101.30	106.49
24	Y	606	CHL	C1D-ND-C4D	-7.28	101.17	106.33
28	R	623	NEX	O24-C25-C24	7.27	118.84	113.38
24	1	609	CHL	CHD-C1D-ND	-7.26	117.78	124.45
24	S	601	CHL	C2C-C3C-C4C	-7.26	101.31	106.49
27	N	1622	XAT	O4-C5-C4	7.25	118.83	113.38
24	4	601	CHL	C2C-C3C-C4C	-7.24	101.33	106.49
28	r	623	NEX	O24-C25-C24	7.23	118.81	113.38
24	5	609	CHL	CHD-C1D-ND	-7.23	117.81	124.45
24	5	606	CHL	C1D-ND-C4D	-7.23	101.20	106.33
24	n	606	CHL	C1D-ND-C4D	-7.23	101.20	106.33
24	2	606	CHL	C1D-ND-C4D	-7.23	101.20	106.33
25	n	611	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	N	608	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
25	N	611	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	1	609	CHL	C1D-ND-C4D	-7.22	101.21	106.33
24	6	606	CHL	C1D-ND-C4D	-7.22	101.21	106.33
24	5	609	CHL	C1D-ND-C4D	-7.21	101.22	106.33
24	N	606	CHL	C1D-ND-C4D	-7.21	101.22	106.33
25	B	613	CLA	C4A-NA-C1A	7.20	109.94	106.71
24	8	601	CHL	C2C-C3C-C4C	-7.20	101.36	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	601	CHL	CHD-C1D-ND	-7.19	117.84	124.45
24	Y	601	CHL	C2D-C1D-ND	7.19	115.40	110.10
25	b	613	CLA	C4A-NA-C1A	7.19	109.94	106.71
24	y	601	CHL	CHD-C1D-ND	-7.19	117.85	124.45
24	8	607	CHL	CHD-C1D-ND	-7.18	117.85	124.45
24	n	608	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
24	y	601	CHL	C2D-C1D-ND	7.17	115.39	110.10
24	1	608	CHL	C2D-C1D-ND	7.17	115.39	110.10
24	4	607	CHL	CHD-C1D-ND	-7.17	117.86	124.45
24	g	609	CHL	C2C-C3C-C4C	-7.16	101.38	106.49
24	5	608	CHL	C2D-C1D-ND	7.16	115.38	110.10
24	1	606	CHL	C1D-ND-C4D	-7.15	101.26	106.33
24	3	601	CHL	CHD-C1D-ND	-7.14	117.89	124.45
24	G	609	CHL	C2C-C3C-C4C	-7.13	101.41	106.49
24	7	601	CHL	CHD-C1D-ND	-7.13	117.90	124.45
24	n	608	CHL	C2D-C1D-ND	7.12	115.35	110.10
24	s	607	CHL	C2C-C3C-C4C	-7.12	101.42	106.49
24	N	608	CHL	C2D-C1D-ND	7.11	115.34	110.10
24	S	607	CHL	C2C-C3C-C4C	-7.06	101.46	106.49
30	t	101	BCR	C24-C23-C22	-7.04	115.60	126.23
30	T	101	BCR	C24-C23-C22	-7.04	115.60	126.23
27	Y	1622	XAT	C15-C14-C13	-7.03	117.28	127.31
27	y	1622	XAT	C15-C14-C13	-7.03	117.28	127.31
24	5	609	CHL	C2C-C3C-C4C	-7.02	101.48	106.49
24	5	605	CHL	CHD-C1D-ND	-7.02	118.00	124.45
24	8	608	CHL	C2C-C3C-C4C	-7.02	101.48	106.49
24	Y	609	CHL	C1D-ND-C4D	-7.01	101.35	106.33
24	1	605	CHL	CHD-C1D-ND	-7.01	118.01	124.45
24	5	605	CHL	C1D-ND-C4D	-7.01	101.36	106.33
24	4	608	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
24	Y	609	CHL	C2C-C3C-C4C	-7.01	101.50	106.49
24	G	609	CHL	C1D-ND-C4D	-7.00	101.36	106.33
24	g	609	CHL	C1D-ND-C4D	-7.00	101.36	106.33
24	1	605	CHL	C1D-ND-C4D	-7.00	101.36	106.33
24	y	609	CHL	C1D-ND-C4D	-6.99	101.37	106.33
24	g	608	CHL	C2D-C1D-ND	6.99	115.25	110.10
24	6	609	CHL	C2C-C3C-C4C	-6.98	101.51	106.49
24	1	609	CHL	C2C-C3C-C4C	-6.98	101.51	106.49
24	2	609	CHL	C2C-C3C-C4C	-6.97	101.52	106.49
24	R	614	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
24	r	614	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
24	y	609	CHL	C2C-C3C-C4C	-6.96	101.53	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	608	CHL	C2D-C1D-ND	6.94	115.22	110.10
24	N	601	CHL	CHD-C1D-ND	-6.89	118.12	124.45
24	n	609	CHL	C2C-C3C-C4C	-6.88	101.58	106.49
24	N	601	CHL	C2D-C1D-ND	6.87	115.17	110.10
24	G	607	CHL	C2D-C1D-ND	6.86	115.16	110.10
24	n	601	CHL	C2D-C1D-ND	6.86	115.16	110.10
24	n	601	CHL	CHD-C1D-ND	-6.85	118.16	124.45
24	N	609	CHL	C2C-C3C-C4C	-6.85	101.61	106.49
24	S	607	CHL	C2D-C1D-ND	6.84	115.14	110.10
24	4	606	CHL	C2D-C1D-ND	6.83	115.14	110.10
24	g	607	CHL	C2D-C1D-ND	6.82	115.13	110.10
24	s	607	CHL	C2D-C1D-ND	6.81	115.12	110.10
27	y	1622	XAT	O24-C25-C24	6.80	118.49	113.38
25	B	605	CLA	C4A-NA-C1A	6.79	109.76	106.71
27	r	622	XAT	O4-C5-C4	6.79	118.48	113.38
24	8	606	CHL	C2D-C1D-ND	6.78	115.10	110.10
24	3	605	CHL	C2D-C1D-ND	6.78	115.10	110.10
24	r	607	CHL	CHD-C1D-ND	-6.77	118.24	124.45
25	b	614	CLA	C4A-NA-C1A	6.76	109.74	106.71
25	B	614	CLA	C4A-NA-C1A	6.75	109.74	106.71
27	R	622	XAT	O4-C5-C4	6.74	118.45	113.38
24	g	601	CHL	C2D-C1D-ND	6.74	115.07	110.10
25	b	605	CLA	C4A-NA-C1A	6.74	109.74	106.71
27	Y	1622	XAT	O24-C25-C24	6.73	118.44	113.38
24	7	605	CHL	C2D-C1D-ND	6.72	115.06	110.10
25	C	507	CLA	C4A-NA-C1A	6.71	109.72	106.71
24	y	607	CHL	C2D-C1D-ND	6.70	115.05	110.10
25	c	507	CLA	C4A-NA-C1A	6.69	109.71	106.71
24	R	607	CHL	CHD-C1D-ND	-6.69	118.31	124.45
24	s	601	CHL	C2D-C1D-ND	6.69	115.03	110.10
24	G	601	CHL	C2D-C1D-ND	6.68	115.02	110.10
24	3	609	CHL	CHD-C1D-ND	-6.67	118.32	124.45
24	Y	607	CHL	C2D-C1D-ND	6.65	115.00	110.10
24	5	601	CHL	CHD-C1D-ND	-6.65	118.35	124.45
25	B	612	CLA	C4A-NA-C1A	6.64	109.69	106.71
24	3	601	CHL	C2D-C1D-ND	6.64	114.99	110.10
24	7	609	CHL	CHD-C1D-ND	-6.62	118.37	124.45
24	S	601	CHL	C2D-C1D-ND	6.62	114.98	110.10
25	b	617	CLA	C4A-NA-C1A	6.62	109.68	106.71
24	7	601	CHL	C2D-C1D-ND	6.62	114.98	110.10
24	N	609	CHL	C1D-ND-C4D	-6.62	101.64	106.33
25	b	612	CLA	C4A-NA-C1A	6.62	109.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	601	CHL	CHD-C1D-ND	-6.61	118.38	124.45
24	n	609	CHL	C1D-ND-C4D	-6.61	101.64	106.33
24	g	601	CHL	CHD-C1D-ND	-6.60	118.39	124.45
24	1	601	CHL	CHD-C1D-ND	-6.60	118.39	124.45
25	Y	604	CLA	CMB-C2B-C1B	-6.57	118.37	128.46
25	B	617	CLA	C4A-NA-C1A	6.56	109.65	106.71
25	y	604	CLA	CMB-C2B-C1B	-6.55	118.39	128.46
27	8	622	XAT	O4-C5-C4	6.53	118.29	113.38
24	3	609	CHL	C1D-ND-C4D	-6.52	101.70	106.33
30	t	101	BCR	C16-C17-C18	-6.52	118.00	127.31
24	2	601	CHL	C2C-C3C-C4C	-6.52	101.84	106.49
30	T	101	BCR	C16-C17-C18	-6.52	118.01	127.31
27	4	622	XAT	O4-C5-C4	6.52	118.28	113.38
24	S	606	CHL	CHD-C1D-ND	-6.51	118.47	124.45
24	S	606	CHL	C2D-C1D-ND	6.51	114.90	110.10
24	s	606	CHL	C2D-C1D-ND	6.50	114.89	110.10
24	4	601	CHL	C1B-CHB-C4A	-6.50	117.25	130.12
24	8	601	CHL	C1B-CHB-C4A	-6.50	117.25	130.12
24	4	609	CHL	CHD-C1D-ND	-6.49	118.49	124.45
24	8	609	CHL	CHD-C1D-ND	-6.49	118.49	124.45
24	6	601	CHL	C2C-C3C-C4C	-6.49	101.87	106.49
24	s	606	CHL	CHD-C1D-ND	-6.48	118.50	124.45
24	7	609	CHL	C1D-ND-C4D	-6.48	101.73	106.33
25	5	611	CLA	C4A-NA-C1A	6.48	109.62	106.71
25	b	606	CLA	C4A-NA-C1A	6.48	109.62	106.71
28	Y	1623	NEX	O24-C25-C24	6.48	118.25	113.38
24	s	601	CHL	CHD-C1D-ND	-6.45	118.53	124.45
24	2	601	CHL	CHD-C1D-ND	-6.44	118.54	124.45
30	T	101	BCR	C20-C21-C22	-6.43	118.13	127.31
28	y	1623	NEX	O24-C25-C24	6.43	118.21	113.38
24	6	601	CHL	CHD-C1D-ND	-6.43	118.55	124.45
30	t	101	BCR	C20-C21-C22	-6.43	118.14	127.31
25	1	611	CLA	C4A-NA-C1A	6.43	109.59	106.71
27	n	1622	XAT	C31-C30-C29	-6.42	118.15	127.31
27	N	1622	XAT	C31-C30-C29	-6.41	118.16	127.31
24	S	608	CHL	C2D-C1D-ND	6.41	114.83	110.10
24	y	606	CHL	C2D-C1D-ND	6.41	114.83	110.10
24	y	605	CHL	C2D-C1D-ND	6.41	114.83	110.10
24	2	609	CHL	C2D-C1D-ND	6.40	114.82	110.10
24	S	601	CHL	CHD-C1D-ND	-6.40	118.57	124.45
25	B	606	CLA	C4A-NA-C1A	6.40	109.58	106.71
24	2	605	CHL	C2D-C1D-ND	6.38	114.81	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	G	1622	XAT	C15-C14-C13	-6.38	118.20	127.31
24	6	609	CHL	C2D-C1D-ND	6.38	114.81	110.10
27	g	1622	XAT	C15-C14-C13	-6.38	118.21	127.31
24	6	605	CHL	C2D-C1D-ND	6.37	114.80	110.10
24	5	601	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
24	Y	605	CHL	C2D-C1D-ND	6.37	114.80	110.10
24	2	609	CHL	CHD-C1D-ND	-6.37	118.60	124.45
24	1	601	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
24	Y	606	CHL	C2D-C1D-ND	6.35	114.79	110.10
24	7	607	CHL	CHD-C1D-ND	-6.35	118.62	124.45
24	s	608	CHL	C2D-C1D-ND	6.35	114.78	110.10
24	6	609	CHL	CHD-C1D-ND	-6.34	118.62	124.45
24	6	607	CHL	CHD-C1D-ND	-6.34	118.63	124.45
27	8	622	XAT	O24-C25-C24	6.33	118.14	113.38
27	4	622	XAT	O24-C25-C24	6.33	118.13	113.38
24	3	607	CHL	CHD-C1D-ND	-6.29	118.67	124.45
24	2	607	CHL	CHD-C1D-ND	-6.29	118.68	124.45
24	S	608	CHL	CHD-C1D-ND	-6.26	118.70	124.45
25	C	505	CLA	C4A-NA-C1A	6.26	109.52	106.71
25	c	505	CLA	C4A-NA-C1A	6.25	109.52	106.71
24	1	607	CHL	CHD-C1D-ND	-6.24	118.72	124.45
24	4	606	CHL	CHD-C1D-ND	-6.24	118.72	124.45
24	3	608	CHL	CHD-C1D-ND	-6.24	118.72	124.45
25	5	603	CLA	C4A-NA-C1A	6.23	109.51	106.71
24	Y	609	CHL	CHD-C1D-ND	-6.23	118.73	124.45
25	g	611	CLA	C4A-NA-C1A	6.23	109.51	106.71
25	1	603	CLA	C4A-NA-C1A	6.23	109.51	106.71
24	4	609	CHL	C2D-C1D-ND	6.23	114.69	110.10
25	A	410	CLA	C4A-NA-C1A	6.22	109.50	106.71
24	s	608	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	8	606	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	G	606	CHL	C2D-C1D-ND	6.21	114.68	110.10
25	G	611	CLA	C4A-NA-C1A	6.20	109.49	106.71
25	a	410	CLA	C4A-NA-C1A	6.20	109.49	106.71
24	y	609	CHL	CHD-C1D-ND	-6.19	118.76	124.45
25	S	604	CLA	C4A-NA-C1A	6.19	109.49	106.71
24	7	608	CHL	CHD-C1D-ND	-6.19	118.76	124.45
24	8	609	CHL	C2D-C1D-ND	6.19	114.67	110.10
25	s	604	CLA	C4A-NA-C1A	6.19	109.49	106.71
24	5	607	CHL	CHD-C1D-ND	-6.19	118.77	124.45
25	r	612	CLA	C4A-NA-C1A	6.17	109.48	106.71
24	3	606	CHL	CHD-C1D-ND	-6.17	118.78	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	612	CLA	C4A-NA-C1A	6.17	109.48	106.71
24	R	606	CHL	C2D-C1D-ND	6.17	114.65	110.10
25	r	616	CLA	C4A-NA-C1A	6.17	109.48	106.71
25	R	616	CLA	C4A-NA-C1A	6.16	109.48	106.71
24	1	601	CHL	C2D-C1D-ND	6.16	114.64	110.10
24	R	606	CHL	CHD-C1D-ND	-6.16	118.80	124.45
24	g	606	CHL	CHD-C1D-ND	-6.16	118.80	124.45
24	g	606	CHL	C2D-C1D-ND	6.15	114.64	110.10
24	7	606	CHL	CHD-C1D-ND	-6.15	118.80	124.45
24	G	606	CHL	CHD-C1D-ND	-6.15	118.81	124.45
24	2	601	CHL	C2D-C1D-ND	6.14	114.63	110.10
24	5	601	CHL	C2D-C1D-ND	6.13	114.62	110.10
25	r	613	CLA	C4A-NA-C1A	6.13	109.46	106.71
25	A	406	CLA	C4A-NA-C1A	6.12	109.46	106.71
24	R	614	CHL	C2D-C1D-ND	6.12	114.61	110.10
24	6	601	CHL	C2D-C1D-ND	6.11	114.61	110.10
24	r	606	CHL	CHD-C1D-ND	-6.11	118.84	124.45
26	3	1620	LUT	C7-C8-C9	-6.10	117.02	126.23
24	n	605	CHL	C2D-C1D-ND	6.10	114.60	110.10
26	7	1620	LUT	C7-C8-C9	-6.10	117.02	126.23
25	R	613	CLA	C4A-NA-C1A	6.10	109.45	106.71
24	2	607	CHL	C1D-ND-C4D	-6.10	102.00	106.33
24	6	607	CHL	C1D-ND-C4D	-6.10	102.00	106.33
24	r	606	CHL	C2D-C1D-ND	6.09	114.59	110.10
24	r	614	CHL	C2D-C1D-ND	6.07	114.58	110.10
24	R	608	CHL	C3C-C4C-NC	6.07	117.37	110.57
24	r	607	CHL	C2D-C1D-ND	6.05	114.56	110.10
30	d	404	BCR	C7-C8-C9	-6.05	117.10	126.23
24	r	608	CHL	C3C-C4C-NC	6.05	117.35	110.57
24	1	605	CHL	C2D-C1D-ND	6.04	114.56	110.10
24	3	605	CHL	CHD-C1D-ND	-6.04	118.91	124.45
24	N	607	CHL	C3C-C4C-NC	6.04	117.34	110.57
24	N	601	CHL	C2C-C3C-C4C	-6.04	102.19	106.49
24	4	607	CHL	C2D-C1D-ND	6.03	114.55	110.10
24	n	607	CHL	C3C-C4C-NC	6.02	117.33	110.57
24	N	605	CHL	C2D-C1D-ND	6.02	114.54	110.10
30	D	404	BCR	C7-C8-C9	-6.02	117.14	126.23
24	5	605	CHL	C2D-C1D-ND	6.02	114.54	110.10
24	7	605	CHL	CHD-C1D-ND	-6.01	118.93	124.45
24	y	609	CHL	O2D-CGD-CBD	6.01	121.95	111.27
24	r	608	CHL	C3D-C2D-C1D	-6.01	97.63	105.83
24	G	607	CHL	CHD-C1D-ND	-6.01	118.93	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	609	CHL	O2D-CGD-CBD	6.01	121.95	111.27
24	n	601	CHL	C2C-C3C-C4C	-6.00	102.21	106.49
24	8	607	CHL	C2D-C1D-ND	6.00	114.53	110.10
24	R	608	CHL	C3D-C2D-C1D	-6.00	97.64	105.83
30	C	516	BCR	C24-C23-C22	-6.00	117.17	126.23
30	c	516	BCR	C24-C23-C22	-6.00	117.18	126.23
25	a	406	CLA	C4A-NA-C1A	5.99	109.40	106.71
24	R	607	CHL	C2D-C1D-ND	5.98	114.51	110.10
25	3	603	CLA	C4A-NA-C1A	5.97	109.39	106.71
24	g	607	CHL	CHD-C1D-ND	-5.97	118.96	124.45
24	2	608	CHL	CHD-C1D-ND	-5.96	118.98	124.45
27	Y	1622	XAT	O4-C5-C18	5.96	122.19	115.06
25	N	604	CLA	CMB-C2B-C1B	-5.95	119.31	128.46
24	g	608	CHL	CHD-C1D-ND	-5.95	118.98	124.45
27	y	1622	XAT	O4-C5-C18	5.95	122.19	115.06
25	n	604	CLA	CMB-C2B-C1B	-5.95	119.32	128.46
24	6	608	CHL	CHD-C1D-ND	-5.94	118.99	124.45
24	y	608	CHL	CHD-C1D-ND	-5.93	119.01	124.45
24	1	607	CHL	C2D-C1D-ND	5.93	114.47	110.10
24	3	609	CHL	O2D-CGD-CBD	5.92	121.79	111.27
24	Y	606	CHL	C3C-C4C-NC	5.91	117.20	110.57
25	7	603	CLA	C4A-NA-C1A	5.91	109.36	106.71
28	y	1623	NEX	C17-C1-C6	-5.91	105.18	110.47
24	N	609	CHL	CHD-C1D-ND	-5.91	119.03	124.45
24	5	606	CHL	C2D-C1D-ND	5.91	114.46	110.10
24	5	607	CHL	C2D-C1D-ND	5.91	114.46	110.10
28	Y	1623	NEX	C17-C1-C6	-5.91	105.19	110.47
24	y	608	CHL	C3D-C2D-C1D	-5.91	97.77	105.83
24	y	606	CHL	C3C-C4C-NC	5.90	117.19	110.57
24	n	606	CHL	C2D-C1D-ND	5.90	114.45	110.10
24	G	608	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	5	608	CHL	C3C-C4C-NC	5.90	117.19	110.57
24	Y	608	CHL	C3D-C2D-C1D	-5.90	97.78	105.83
24	n	609	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	8	608	CHL	CHD-C1D-ND	-5.90	119.03	124.45
27	y	1622	XAT	C31-C30-C29	-5.89	118.90	127.31
27	Y	1622	XAT	C6-C7-C8	-5.89	113.53	125.99
24	7	609	CHL	O2D-CGD-CBD	5.89	121.74	111.27
24	Y	608	CHL	CHD-C1D-ND	-5.89	119.04	124.45
24	N	606	CHL	C2D-C1D-ND	5.89	114.44	110.10
24	1	606	CHL	C2D-C1D-ND	5.88	114.44	110.10
27	Y	1622	XAT	C31-C30-C29	-5.88	118.92	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	y	1622	XAT	C6-C7-C8	-5.87	113.58	125.99
24	G	601	CHL	C2C-C3C-C4C	-5.87	102.31	106.49
25	b	609	CLA	CMB-C2B-C1B	-5.86	119.46	128.46
24	1	608	CHL	C3C-C4C-NC	5.85	117.14	110.57
24	g	605	CHL	C2D-C1D-ND	5.85	114.42	110.10
27	8	622	XAT	C6-C7-C8	-5.85	113.62	125.99
24	4	608	CHL	CHD-C1D-ND	-5.85	119.08	124.45
24	G	605	CHL	C2D-C1D-ND	5.85	114.41	110.10
25	B	609	CLA	CMB-C2B-C1B	-5.85	119.47	128.46
24	g	601	CHL	C2C-C3C-C4C	-5.85	102.32	106.49
27	4	622	XAT	C6-C7-C8	-5.84	113.65	125.99
27	7	1622	XAT	C31-C30-C29	-5.84	118.98	127.31
25	B	609	CLA	C4A-NA-C1A	5.83	109.33	106.71
24	Y	608	CHL	C3C-C4C-NC	5.80	117.08	110.57
27	3	1622	XAT	C31-C30-C29	-5.80	119.03	127.31
24	y	608	CHL	C3C-C4C-NC	5.79	117.06	110.57
24	1	606	CHL	C3C-C4C-NC	5.78	117.06	110.57
24	2	608	CHL	C3C-C4C-NC	5.78	117.05	110.57
24	6	606	CHL	C2D-C1D-ND	5.78	114.36	110.10
24	5	606	CHL	C3C-C4C-NC	5.78	117.05	110.57
25	b	609	CLA	C4A-NA-C1A	5.77	109.30	106.71
24	2	606	CHL	C2D-C1D-ND	5.77	114.36	110.10
30	4	623	BCR	C28-C27-C26	-5.77	103.78	114.08
30	8	623	BCR	C28-C27-C26	-5.76	103.80	114.08
24	N	606	CHL	C3C-C4C-NC	5.75	117.02	110.57
24	n	606	CHL	C3C-C4C-NC	5.75	117.02	110.57
25	B	605	CLA	CAA-C2A-C3A	-5.75	97.03	112.78
25	b	605	CLA	CAA-C2A-C3A	-5.75	97.04	112.78
30	c	517	BCR	C7-C8-C9	-5.75	117.55	126.23
24	6	608	CHL	C3C-C4C-NC	5.75	117.01	110.57
27	G	1622	XAT	C6-C7-C8	-5.74	113.85	125.99
25	3	611	CLA	C4A-NA-C1A	5.74	109.29	106.71
25	7	611	CLA	C4A-NA-C1A	5.74	109.29	106.71
27	g	1622	XAT	C6-C7-C8	-5.74	113.86	125.99
24	G	609	CHL	CHD-C1D-ND	-5.73	119.18	124.45
30	C	517	BCR	C7-C8-C9	-5.73	117.57	126.23
27	3	1622	XAT	C27-C28-C29	-5.73	116.64	125.53
24	1	608	CHL	CHD-C1D-ND	-5.73	119.19	124.45
24	7	607	CHL	C2D-C1D-ND	5.72	114.32	110.10
24	4	608	CHL	C3D-C2D-C1D	-5.72	98.02	105.83
27	7	1622	XAT	C27-C28-C29	-5.72	116.66	125.53
24	n	608	CHL	CHD-C1D-ND	-5.71	119.20	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	608	CHL	CHD-C1D-ND	-5.71	119.21	124.45
24	1	608	CHL	C3D-C2D-C1D	-5.71	98.04	105.83
24	3	608	CHL	C3D-C2D-C1D	-5.70	98.05	105.83
25	C	508	CLA	CMB-C2B-C1B	-5.70	119.70	128.46
24	5	608	CHL	C3D-C2D-C1D	-5.70	98.05	105.83
25	c	508	CLA	CMB-C2B-C1B	-5.70	119.70	128.46
24	5	608	CHL	CHD-C1D-ND	-5.70	119.22	124.45
24	3	606	CHL	O2D-CGD-CBD	5.70	121.39	111.27
24	g	609	CHL	CHD-C1D-ND	-5.70	119.22	124.45
24	8	608	CHL	C3D-C2D-C1D	-5.70	98.06	105.83
24	7	606	CHL	O2D-CGD-CBD	5.69	121.38	111.27
24	3	607	CHL	C2D-C1D-ND	5.69	114.30	110.10
24	7	608	CHL	C3D-C2D-C1D	-5.68	98.09	105.83
24	g	609	CHL	C2D-C1D-ND	5.67	114.28	110.10
25	c	509	CLA	C4A-NA-C1A	5.67	109.25	106.71
24	Y	607	CHL	C3C-C4C-NC	5.66	116.92	110.57
24	y	607	CHL	C3C-C4C-NC	5.66	116.92	110.57
24	G	609	CHL	C2D-C1D-ND	5.66	114.28	110.10
25	S	603	CLA	C4A-NA-C1A	5.65	109.25	106.71
24	4	601	CHL	C1D-ND-C4D	-5.64	102.33	106.33
27	7	1622	XAT	O24-C25-C24	5.64	117.62	113.38
27	7	1622	XAT	C6-C7-C8	-5.64	114.07	125.99
28	1	1623	NEX	C27-C28-C29	-5.64	116.78	125.53
25	B	612	CLA	CMB-C2B-C1B	-5.63	119.81	128.46
25	N	612	CLA	C4A-NA-C1A	5.63	109.24	106.71
25	n	612	CLA	C4A-NA-C1A	5.63	109.24	106.71
25	b	612	CLA	CMB-C2B-C1B	-5.63	119.81	128.46
24	4	606	CHL	C3C-C4C-NC	5.63	116.88	110.57
24	8	601	CHL	C1D-ND-C4D	-5.63	102.34	106.33
27	r	622	XAT	C6-C7-C8	-5.62	114.12	125.99
27	3	1622	XAT	O24-C25-C24	5.61	117.60	113.38
25	s	603	CLA	C4A-NA-C1A	5.61	109.23	106.71
27	3	1622	XAT	C6-C7-C8	-5.61	114.13	125.99
27	R	622	XAT	C26-C27-C28	-5.61	114.13	125.99
28	5	1623	NEX	C27-C28-C29	-5.61	116.83	125.53
27	r	622	XAT	C26-C27-C28	-5.61	114.13	125.99
24	G	605	CHL	CHD-C1D-ND	-5.61	119.30	124.45
24	Y	605	CHL	CHD-C1D-ND	-5.61	119.30	124.45
27	R	622	XAT	C6-C7-C8	-5.60	114.15	125.99
30	H	101	BCR	C11-C10-C9	-5.60	119.32	127.31
24	8	606	CHL	C3C-C4C-NC	5.60	116.85	110.57
27	8	622	XAT	C38-C25-C26	-5.60	112.88	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	509	CLA	C4A-NA-C1A	5.59	109.22	106.71
24	Y	601	CHL	C3D-C2D-C1D	-5.59	98.20	105.83
30	h	101	BCR	C11-C10-C9	-5.59	119.33	127.31
24	g	605	CHL	CHD-C1D-ND	-5.59	119.32	124.45
24	n	606	CHL	CHD-C1D-ND	-5.59	119.32	124.45
24	s	607	CHL	CHD-C1D-ND	-5.58	119.32	124.45
24	y	601	CHL	C3D-C2D-C1D	-5.58	98.21	105.83
25	b	608	CLA	C4A-NA-C1A	5.58	109.22	106.71
24	1	609	CHL	C2D-C1D-ND	5.58	114.22	110.10
27	4	622	XAT	C38-C25-C26	-5.58	112.91	122.26
24	y	605	CHL	CHD-C1D-ND	-5.57	119.33	124.45
25	7	614	CLA	C4A-NA-C1A	5.57	109.21	106.71
24	S	607	CHL	CHD-C1D-ND	-5.57	119.33	124.45
24	N	606	CHL	CHD-C1D-ND	-5.57	119.34	124.45
24	n	608	CHL	C3D-C2D-C1D	-5.57	98.23	105.83
25	3	614	CLA	C4A-NA-C1A	5.57	109.21	106.71
24	5	609	CHL	C2D-C1D-ND	5.56	114.20	110.10
27	7	1622	XAT	C15-C14-C13	-5.56	119.37	127.31
27	R	622	XAT	O4-C5-C18	5.56	121.72	115.06
24	N	608	CHL	C3D-C2D-C1D	-5.56	98.25	105.83
27	r	622	XAT	O4-C5-C18	5.56	121.72	115.06
24	n	605	CHL	CHD-C1D-ND	-5.55	119.36	124.45
24	6	609	CHL	O2D-CGD-CBD	5.55	121.12	111.27
28	6	1623	NEX	C27-C28-C29	-5.55	116.92	125.53
25	B	608	CLA	C4A-NA-C1A	5.55	109.20	106.71
27	3	1622	XAT	C15-C14-C13	-5.54	119.40	127.31
25	8	603	CLA	C4A-NA-C1A	5.54	109.20	106.71
28	3	1623	NEX	C15-C14-C13	-5.54	119.41	127.31
24	6	608	CHL	C3D-C2D-C1D	-5.54	98.28	105.83
28	2	1623	NEX	C27-C28-C29	-5.53	116.94	125.53
28	7	1623	NEX	C15-C14-C13	-5.53	119.42	127.31
38	D	401	BCT	O2-C-O1	5.53	133.89	119.55
24	2	606	CHL	C3C-C4C-NC	5.53	116.77	110.57
24	2	609	CHL	O2D-CGD-CBD	5.53	121.09	111.27
25	4	603	CLA	C4A-NA-C1A	5.52	109.19	106.71
25	b	610	CLA	C4A-NA-C1A	5.52	109.19	106.71
25	b	611	CLA	C4A-NA-C1A	5.52	109.19	106.71
27	R	622	XAT	C38-C25-C26	-5.52	113.01	122.26
24	2	608	CHL	C3D-C2D-C1D	-5.51	98.31	105.83
24	y	609	CHL	C2D-C1D-ND	5.51	114.17	110.10
38	d	401	BCT	O2-C-O1	5.51	133.84	119.55
24	4	609	CHL	C3C-C4C-NC	5.51	116.75	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	606	CHL	C3C-C4C-NC	5.51	116.75	110.57
24	R	606	CHL	C3C-C4C-NC	5.50	116.74	110.57
27	r	622	XAT	C38-C25-C26	-5.50	113.04	122.26
24	r	606	CHL	C3C-C4C-NC	5.50	116.74	110.57
25	B	611	CLA	C4A-NA-C1A	5.49	109.18	106.71
24	N	605	CHL	CHD-C1D-ND	-5.49	119.41	124.45
24	Y	609	CHL	C2D-C1D-ND	5.48	114.15	110.10
25	B	610	CLA	C4A-NA-C1A	5.48	109.17	106.71
24	8	609	CHL	C3C-C4C-NC	5.48	116.72	110.57
30	B	620	BCR	C7-C8-C9	-5.48	117.96	126.23
24	G	606	CHL	C3C-C4C-NC	5.48	116.71	110.57
30	b	620	BCR	C7-C8-C9	-5.47	117.97	126.23
24	3	608	CHL	C3C-C4C-NC	5.46	116.70	110.57
25	r	603	CLA	C4A-NA-C1A	5.46	109.16	106.71
24	n	601	CHL	O2D-CGD-CBD	5.46	120.96	111.27
25	R	603	CLA	C4A-NA-C1A	5.45	109.15	106.71
24	7	608	CHL	C3C-C4C-NC	5.44	116.68	110.57
24	g	606	CHL	C3C-C4C-NC	5.44	116.67	110.57
24	N	601	CHL	O2D-CGD-CBD	5.43	120.92	111.27
28	Y	1623	NEX	C35-C34-C33	-5.42	119.58	127.31
24	g	607	CHL	C3C-C4C-NC	5.41	116.63	110.57
24	3	601	CHL	O2D-CGD-CBD	5.39	120.85	111.27
30	C	517	BCR	C11-C10-C9	-5.39	119.62	127.31
28	y	1623	NEX	C35-C34-C33	-5.39	119.62	127.31
24	G	607	CHL	C3C-C4C-NC	5.38	116.61	110.57
24	6	605	CHL	CHD-C1D-ND	-5.38	119.51	124.45
30	c	517	BCR	C11-C10-C9	-5.38	119.63	127.31
24	1	605	CHL	C3C-C4C-NC	5.37	116.60	110.57
24	g	608	CHL	C3C-C4C-NC	5.37	116.60	110.57
24	4	601	CHL	C2D-C1D-ND	5.37	114.06	110.10
24	g	608	CHL	C3D-C2D-C1D	-5.37	98.51	105.83
34	B	621	SQD	O9-S-C6	5.36	113.31	106.94
24	g	601	CHL	C3D-C2D-C1D	-5.36	98.52	105.83
27	n	1622	XAT	C38-C25-C26	-5.36	113.28	122.26
24	2	605	CHL	CHD-C1D-ND	-5.36	119.53	124.45
25	b	616	CLA	C4A-NA-C1A	5.36	109.11	106.71
24	7	601	CHL	O2D-CGD-CBD	5.35	120.78	111.27
24	n	607	CHL	C3D-C2D-C1D	-5.35	98.53	105.83
25	2	611	CLA	C4A-NA-C1A	5.35	109.11	106.71
27	N	1622	XAT	C38-C25-C26	-5.35	113.30	122.26
24	G	608	CHL	C3D-C2D-C1D	-5.35	98.53	105.83
24	N	607	CHL	C3D-C2D-C1D	-5.35	98.54	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	G	608	CHL	C3C-C4C-NC	5.35	116.57	110.57
24	8	601	CHL	C2D-C1D-ND	5.34	114.04	110.10
24	5	605	CHL	C3C-C4C-NC	5.34	116.56	110.57
34	b	621	SQD	O9-S-C6	5.34	113.28	106.94
28	y	1623	NEX	C11-C10-C9	-5.33	119.70	127.31
30	D	404	BCR	C24-C23-C22	-5.33	118.19	126.23
24	S	606	CHL	C3C-C4C-NC	5.33	116.54	110.57
24	G	601	CHL	C3D-C2D-C1D	-5.33	98.56	105.83
24	S	608	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
30	d	404	BCR	C24-C23-C22	-5.32	118.19	126.23
24	N	601	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
24	N	608	CHL	C3C-C4C-NC	5.32	116.54	110.57
24	n	601	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
24	r	608	CHL	CHD-C1D-ND	-5.32	119.57	124.45
25	A	405	CLA	CMB-C2B-C1B	-5.32	120.29	128.46
28	Y	1623	NEX	C38-C25-C26	-5.32	113.35	122.26
24	n	608	CHL	O2D-CGD-CBD	5.32	120.72	111.27
24	N	608	CHL	O2D-CGD-CBD	5.32	120.71	111.27
28	Y	1623	NEX	C11-C10-C9	-5.31	119.73	127.31
24	R	608	CHL	CHD-C1D-ND	-5.31	119.57	124.45
24	8	606	CHL	C3D-C2D-C1D	-5.31	98.58	105.83
28	y	1623	NEX	C38-C25-C26	-5.31	113.36	122.26
24	4	606	CHL	C3D-C2D-C1D	-5.31	98.59	105.83
24	1	601	CHL	C3D-C2D-C1D	-5.31	98.59	105.83
24	N	605	CHL	O2D-CGD-CBD	5.31	120.69	111.27
24	s	606	CHL	C3C-C4C-NC	5.30	116.52	110.57
25	c	511	CLA	C4A-NA-C1A	5.30	109.09	106.71
25	a	405	CLA	CMB-C2B-C1B	-5.30	120.32	128.46
24	s	608	CHL	C3D-C2D-C1D	-5.30	98.60	105.83
25	1	613	CLA	C4A-NA-C1A	5.29	109.08	106.71
25	6	611	CLA	C4A-NA-C1A	5.29	109.08	106.71
24	n	605	CHL	O2D-CGD-CBD	5.28	120.66	111.27
24	n	608	CHL	C3C-C4C-NC	5.28	116.50	110.57
27	8	622	XAT	C18-C5-C6	-5.28	113.42	122.26
24	n	607	CHL	CHD-C1D-ND	-5.28	119.61	124.45
24	Y	601	CHL	C2C-C3C-C4C	-5.28	102.73	106.49
25	B	616	CLA	C4A-NA-C1A	5.28	109.08	106.71
24	y	601	CHL	C2C-C3C-C4C	-5.27	102.73	106.49
28	G	1623	NEX	C27-C28-C29	-5.27	117.35	125.53
28	g	1623	NEX	C27-C28-C29	-5.27	117.36	125.53
24	g	609	CHL	C3C-C4C-NC	5.27	116.48	110.57
24	5	601	CHL	C3D-C2D-C1D	-5.27	98.64	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	4	622	XAT	C18-C5-C6	-5.26	113.44	122.26
24	N	607	CHL	CHD-C1D-ND	-5.25	119.63	124.45
24	N	609	CHL	C2D-C1D-ND	5.25	113.97	110.10
24	G	609	CHL	C3C-C4C-NC	5.25	116.46	110.57
25	R	602	CLA	CMB-C2B-C1B	-5.24	120.40	128.46
24	5	609	CHL	O2D-CGD-CBD	5.24	120.59	111.27
24	1	609	CHL	O2D-CGD-CBD	5.24	120.58	111.27
27	r	622	XAT	C18-C5-C6	-5.24	113.48	122.26
24	r	608	CHL	CHD-C4C-C3C	-5.24	117.14	124.84
25	7	613	CLA	C4A-NA-C1A	5.23	109.06	106.71
25	r	602	CLA	CMB-C2B-C1B	-5.23	120.43	128.46
25	3	604	CLA	C4A-NA-C1A	5.23	109.06	106.71
25	C	511	CLA	C4A-NA-C1A	5.23	109.06	106.71
28	y	1623	NEX	O24-C25-C38	5.23	121.32	115.06
24	R	608	CHL	CHD-C4C-C3C	-5.22	117.16	124.84
27	R	622	XAT	C18-C5-C6	-5.22	113.50	122.26
34	A	418	SQD	O7-S-C6	5.21	113.13	106.94
28	Y	1623	NEX	O24-C25-C38	5.21	121.30	115.06
24	6	606	CHL	CHD-C1D-ND	-5.21	119.67	124.45
25	c	506	CLA	C4A-NA-C1A	5.20	109.05	106.71
34	a	418	SQD	O7-S-C6	5.20	113.12	106.94
24	G	607	CHL	C3D-C2D-C1D	-5.20	98.74	105.83
25	6	603	CLA	C4A-NA-C1A	5.20	109.04	106.71
25	7	604	CLA	C4A-NA-C1A	5.20	109.04	106.71
25	5	613	CLA	C4A-NA-C1A	5.19	109.04	106.71
25	C	506	CLA	C4A-NA-C1A	5.19	109.04	106.71
24	g	607	CHL	C3D-C2D-C1D	-5.19	98.75	105.83
24	n	609	CHL	C2D-C1D-ND	5.19	113.93	110.10
24	2	609	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
28	G	1623	NEX	C35-C34-C33	-5.18	119.91	127.31
24	1	607	CHL	C3C-C4C-NC	5.18	116.38	110.57
24	6	605	CHL	C3C-C4C-NC	5.18	116.38	110.57
25	R	601	CLA	CAC-C3C-C4C	5.18	131.53	124.81
28	G	1623	NEX	C11-C10-C9	-5.18	119.92	127.31
24	6	609	CHL	C3D-C2D-C1D	-5.17	98.77	105.83
25	N	614	CLA	C4A-NA-C1A	5.17	109.03	106.71
24	2	605	CHL	C3C-C4C-NC	5.17	116.37	110.57
28	R	623	NEX	C15-C14-C13	-5.17	119.93	127.31
25	3	613	CLA	C4A-NA-C1A	5.17	109.03	106.71
24	2	606	CHL	CHD-C1D-ND	-5.17	119.71	124.45
24	4	608	CHL	C3C-C4C-NC	5.17	116.36	110.57
25	C	513	CLA	CMB-C2B-C1B	-5.17	120.53	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	7	609	CHL	C2D-C1D-ND	5.16	113.91	110.10
27	4	622	XAT	C26-C27-C28	-5.16	115.08	125.99
24	5	607	CHL	C3C-C4C-NC	5.16	116.36	110.57
28	g	1623	NEX	C35-C34-C33	-5.15	119.95	127.31
28	r	623	NEX	C15-C14-C13	-5.15	119.96	127.31
25	r	601	CLA	CAC-C3C-C4C	5.15	131.49	124.81
27	8	622	XAT	C26-C27-C28	-5.15	115.11	125.99
24	3	609	CHL	C2D-C1D-ND	5.15	113.90	110.10
28	g	1623	NEX	C11-C10-C9	-5.14	119.97	127.31
25	c	513	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
25	g	602	CLA	CMB-C2B-C1B	-5.14	120.57	128.46
24	7	601	CHL	C3D-C2D-C1D	-5.14	98.82	105.83
25	G	604	CLA	CMB-C2B-C1B	-5.13	120.57	128.46
25	2	603	CLA	C4A-NA-C1A	5.13	109.01	106.71
24	S	607	CHL	C3C-C4C-NC	5.13	116.33	110.57
27	Y	1622	XAT	C38-C25-C26	-5.13	113.66	122.26
27	y	1622	XAT	C38-C25-C26	-5.13	113.66	122.26
24	y	607	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
24	s	607	CHL	C3C-C4C-NC	5.13	116.32	110.57
24	3	601	CHL	C3D-C2D-C1D	-5.12	98.84	105.83
25	G	602	CLA	CMB-C2B-C1B	-5.12	120.59	128.46
24	N	609	CHL	O2D-CGD-CBD	5.12	120.36	111.27
24	8	608	CHL	C3C-C4C-NC	5.11	116.31	110.57
25	g	604	CLA	CMB-C2B-C1B	-5.11	120.61	128.46
24	n	609	CHL	O2D-CGD-CBD	5.11	120.35	111.27
25	n	614	CLA	C4A-NA-C1A	5.11	109.00	106.71
24	1	609	CHL	C3D-C2D-C1D	-5.11	98.86	105.83
28	r	623	NEX	C38-C25-C26	-5.11	113.70	122.26
24	G	605	CHL	C3C-C4C-NC	5.10	116.30	110.57
27	G	1622	XAT	O4-C5-C4	5.10	117.22	113.38
24	g	605	CHL	C3C-C4C-NC	5.10	116.29	110.57
28	R	623	NEX	C38-C25-C26	-5.10	113.71	122.26
24	S	601	CHL	C3D-C4D-ND	5.10	118.49	110.24
24	8	609	CHL	C3D-C2D-C1D	-5.10	98.87	105.83
25	C	508	CLA	C4A-NA-C1A	5.10	109.00	106.71
24	4	609	CHL	C3D-C2D-C1D	-5.10	98.87	105.83
24	s	601	CHL	C3D-C4D-ND	5.10	118.49	110.24
24	Y	605	CHL	C3C-C4C-NC	5.10	116.29	110.57
25	c	508	CLA	C4A-NA-C1A	5.10	109.00	106.71
24	Y	607	CHL	C3D-C2D-C1D	-5.10	98.88	105.83
27	N	1622	XAT	C6-C7-C8	-5.09	115.22	125.99
24	5	609	CHL	C3D-C2D-C1D	-5.09	98.88	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	n	1622	XAT	C6-C7-C8	-5.09	115.23	125.99
24	3	605	CHL	C3D-C4D-ND	5.09	118.47	110.24
25	g	602	CLA	C4A-NA-C1A	5.08	108.99	106.71
24	R	606	CHL	O2D-CGD-CBD	5.08	120.30	111.27
24	7	605	CHL	C3D-C4D-ND	5.08	118.46	110.24
27	g	1622	XAT	O4-C5-C4	5.08	117.20	113.38
25	G	602	CLA	C4A-NA-C1A	5.08	108.99	106.71
25	S	613	CLA	C4A-NA-C1A	5.08	108.99	106.71
24	r	606	CHL	O2D-CGD-CBD	5.08	120.30	111.27
25	c	506	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
25	b	613	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
25	b	608	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
24	y	605	CHL	C3C-C4C-NC	5.07	116.26	110.57
25	C	506	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
24	3	605	CHL	C3C-C4C-NC	5.07	116.26	110.57
25	y	614	CLA	C4A-NA-C1A	5.07	108.98	106.71
24	7	606	CHL	C3C-C4C-NC	5.07	116.25	110.57
25	B	608	CLA	CMB-C2B-C1B	-5.07	120.68	128.46
25	S	614	CLA	CMB-C2B-C1B	-5.07	120.68	128.46
24	Y	608	CHL	CHD-C4C-C3C	-5.06	117.40	124.84
24	N	605	CHL	C3C-C4C-NC	5.06	116.25	110.57
24	7	605	CHL	C3C-C4C-NC	5.06	116.24	110.57
30	c	517	BCR	C24-C23-C22	-5.06	118.59	126.23
24	6	601	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
24	2	601	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
25	s	613	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	B	613	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
24	y	607	CHL	CHD-C1D-ND	-5.04	119.82	124.45
24	Y	607	CHL	CHD-C1D-ND	-5.04	119.82	124.45
24	y	608	CHL	CHD-C4C-C3C	-5.04	117.43	124.84
25	s	614	CLA	CMB-C2B-C1B	-5.04	120.72	128.46
30	C	516	BCR	C16-C17-C18	-5.04	120.12	127.31
24	3	606	CHL	C3C-C4C-NC	5.04	116.22	110.57
24	Y	601	CHL	O2D-CGD-CBD	5.03	120.21	111.27
24	n	605	CHL	C3C-C4C-NC	5.03	116.21	110.57
26	G	1620	LUT	C35-C34-C33	-5.03	120.13	127.31
24	y	601	CHL	O2D-CGD-CBD	5.03	120.20	111.27
26	g	1620	LUT	C35-C34-C33	-5.03	120.13	127.31
30	C	517	BCR	C24-C23-C22	-5.03	118.64	126.23
24	4	601	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
24	7	606	CHL	C3D-C4D-ND	5.02	118.36	110.24
30	c	516	BCR	C16-C17-C18	-5.02	120.15	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	601	CHL	C2C-C3C-C4C	-5.02	102.91	106.49
24	3	601	CHL	C3D-C4D-ND	5.02	118.35	110.24
24	7	601	CHL	C2C-C3C-C4C	-5.01	102.92	106.49
24	8	601	CHL	C3D-C2D-C1D	-5.01	99.00	105.83
24	3	606	CHL	C3D-C4D-ND	5.01	118.34	110.24
24	1	605	CHL	C3D-C2D-C1D	-5.00	99.00	105.83
25	b	614	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
28	3	1623	NEX	C38-C25-C26	-5.00	113.88	122.26
25	C	504	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
24	R	614	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
27	y	1622	XAT	O24-C25-C38	4.99	121.04	115.06
24	y	605	CHL	C3D-C2D-C1D	-4.99	99.02	105.83
25	c	504	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
24	Y	605	CHL	C3D-C2D-C1D	-4.99	99.02	105.83
24	5	605	CHL	C3D-C2D-C1D	-4.99	99.03	105.83
24	r	614	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
24	7	601	CHL	C3D-C4D-ND	4.98	118.30	110.24
24	3	605	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
28	7	1623	NEX	C38-C25-C26	-4.98	113.91	122.26
24	R	614	CHL	C3D-C4D-ND	4.98	118.30	110.24
24	2	605	CHL	O2D-CGD-CBD	4.98	120.12	111.27
25	Y	614	CLA	C4A-NA-C1A	4.98	108.94	106.71
30	4	623	BCR	C11-C10-C9	-4.98	120.20	127.31
24	S	606	CHL	O2D-CGD-CBD	4.98	120.11	111.27
25	C	512	CLA	C4A-NA-C1A	4.98	108.94	106.71
27	Y	1622	XAT	O24-C25-C38	4.97	121.02	115.06
30	8	623	BCR	C11-C10-C9	-4.97	120.21	127.31
25	c	512	CLA	C4A-NA-C1A	4.97	108.94	106.71
30	T	101	BCR	C7-C8-C9	-4.97	118.72	126.23
24	s	606	CHL	O2D-CGD-CBD	4.97	120.10	111.27
24	S	607	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
25	b	609	CLA	CMB-C2B-C3B	4.97	133.97	124.68
25	B	614	CLA	CMB-C2B-C1B	-4.97	120.83	128.46
24	7	605	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
24	s	607	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
28	r	623	NEX	C11-C10-C9	-4.97	120.22	127.31
30	t	101	BCR	C7-C8-C9	-4.96	118.73	126.23
24	y	609	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
24	r	614	CHL	C3D-C4D-ND	4.96	118.26	110.24
27	6	1622	XAT	C38-C25-C26	-4.96	113.95	122.26
30	4	623	BCR	C15-C14-C13	-4.96	120.24	127.31
24	6	605	CHL	O2D-CGD-CBD	4.96	120.07	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	7	1622	XAT	C38-C25-C26	-4.95	113.96	122.26
24	s	601	CHL	C3D-C2D-C1D	-4.95	99.07	105.83
27	3	1622	XAT	C38-C25-C26	-4.95	113.96	122.26
28	R	623	NEX	C11-C10-C9	-4.95	120.24	127.31
24	Y	609	CHL	C3D-C2D-C1D	-4.95	99.07	105.83
24	s	606	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
24	Y	609	CHL	C3C-C4C-NC	4.95	116.12	110.57
25	d	403	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
25	B	609	CLA	CMB-C2B-C3B	4.95	133.94	124.68
25	7	602	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
24	G	609	CHL	O2D-CGD-CBD	4.95	120.06	111.27
24	N	601	CHL	C3D-C4D-ND	4.95	118.24	110.24
24	S	606	CHL	C3D-C2D-C1D	-4.94	99.08	105.83
27	2	1622	XAT	C38-C25-C26	-4.94	113.97	122.26
27	N	1622	XAT	C27-C28-C29	-4.94	117.86	125.53
28	r	623	NEX	C27-C28-C29	-4.94	117.86	125.53
27	n	1622	XAT	C27-C28-C29	-4.94	117.86	125.53
24	g	609	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
24	N	606	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
24	G	609	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
25	3	602	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
24	n	601	CHL	C3D-C4D-ND	4.94	118.22	110.24
24	n	606	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
24	g	609	CHL	O2D-CGD-CBD	4.94	120.04	111.27
30	8	623	BCR	C15-C14-C13	-4.93	120.27	127.31
37	c	518	DGD	O3G-C3G-C2G	-4.93	99.00	110.90
24	S	601	CHL	C3D-C2D-C1D	-4.93	99.10	105.83
24	Y	601	CHL	C3D-C4D-ND	4.93	118.21	110.24
28	R	623	NEX	C27-C28-C29	-4.93	117.89	125.53
25	D	403	CLA	CMB-C2B-C1B	-4.92	120.89	128.46
37	C	518	DGD	O3G-C3G-C2G	-4.92	99.02	110.90
27	2	1622	XAT	C15-C35-C34	-4.92	113.39	123.47
24	y	609	CHL	C3C-C4C-NC	4.92	116.09	110.57
24	2	607	CHL	C2D-C1D-ND	4.92	113.73	110.10
24	6	607	CHL	C2D-C1D-ND	4.92	113.73	110.10
27	6	1622	XAT	C15-C35-C34	-4.92	113.40	123.47
24	4	607	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
24	y	601	CHL	C3D-C4D-ND	4.92	118.19	110.24
24	1	607	CHL	C3D-C4D-ND	4.91	118.19	110.24
24	5	607	CHL	C3D-C4D-ND	4.91	118.18	110.24
24	7	609	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
27	g	1622	XAT	C31-C30-C29	-4.90	120.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	510	CLA	C4A-NA-C1A	4.90	108.91	106.71
24	G	606	CHL	C3D-C4D-ND	4.90	118.16	110.24
27	G	1622	XAT	C31-C30-C29	-4.90	120.32	127.31
24	N	609	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
24	6	605	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
25	a	407	CLA	C4A-NA-C1A	4.89	108.91	106.71
24	r	607	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
24	3	609	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
24	8	607	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
24	2	605	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
30	c	517	BCR	C15-C14-C13	-4.88	120.34	127.31
24	g	605	CHL	C3D-C4D-ND	4.88	118.14	110.24
24	7	607	CHL	C3C-C4C-NC	4.88	116.05	110.57
24	r	607	CHL	O2D-CGD-CBD	4.88	119.94	111.27
24	1	606	CHL	O2D-CGD-CBD	4.88	119.94	111.27
24	R	606	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
27	y	1622	XAT	C15-C35-C34	-4.88	113.48	123.47
24	n	609	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
24	3	607	CHL	C3C-C4C-NC	4.88	116.04	110.57
24	g	601	CHL	O2D-CGD-CBD	4.88	119.94	111.27
30	C	517	BCR	C15-C14-C13	-4.88	120.35	127.31
25	B	602	CLA	C4A-NA-C1A	4.88	108.90	106.71
25	c	510	CLA	C4A-NA-C1A	4.88	108.90	106.71
24	s	601	CHL	C3C-C4C-NC	4.88	116.04	110.57
24	r	614	CHL	C3C-C4C-NC	4.88	116.04	110.57
25	y	612	CLA	C4A-NA-C1A	4.87	108.90	106.71
24	5	606	CHL	O2D-CGD-CBD	4.87	119.93	111.27
24	r	606	CHL	C3D-C2D-C1D	-4.87	99.18	105.83
24	N	606	CHL	O2D-CGD-CBD	4.87	119.93	111.27
24	n	606	CHL	O2D-CGD-CBD	4.87	119.93	111.27
25	n	613	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
27	Y	1622	XAT	C15-C35-C34	-4.87	113.50	123.47
24	G	601	CHL	O2D-CGD-CBD	4.87	119.92	111.27
24	g	606	CHL	C3D-C4D-ND	4.87	118.12	110.24
25	Y	612	CLA	C4A-NA-C1A	4.87	108.89	106.71
25	N	613	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
24	R	607	CHL	C3D-C2D-C1D	-4.87	99.19	105.83
24	g	605	CHL	O2D-CGD-CBD	4.86	119.91	111.27
24	y	606	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
24	S	601	CHL	C3C-C4C-NC	4.86	116.03	110.57
24	R	607	CHL	O2D-CGD-CBD	4.86	119.91	111.27
25	S	611	CLA	C4A-NA-C1A	4.86	108.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	1620	LUT	C35-C34-C33	-4.86	120.37	127.31
24	R	606	CHL	C3D-C4D-ND	4.86	118.10	110.24
24	2	609	CHL	C3C-C4C-NC	4.86	116.02	110.57
25	C	510	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
24	7	607	CHL	C3D-C4D-ND	4.86	118.10	110.24
24	r	606	CHL	C3D-C4D-ND	4.86	118.10	110.24
24	6	609	CHL	C3C-C4C-NC	4.86	116.02	110.57
24	G	605	CHL	O2D-CGD-CBD	4.85	119.89	111.27
24	G	606	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
24	1	607	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
24	R	607	CHL	C3C-C4C-NC	4.85	116.01	110.57
36	a	414	PL9	C7-C3-C2	-4.85	116.92	123.30
24	g	606	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
25	A	407	CLA	C4A-NA-C1A	4.85	108.89	106.71
24	r	607	CHL	C3C-C4C-NC	4.85	116.01	110.57
24	5	607	CHL	C3D-C2D-C1D	-4.85	99.22	105.83
24	6	609	CHL	C3D-C4D-ND	4.85	118.08	110.24
26	1	1620	LUT	C35-C34-C33	-4.85	120.39	127.31
24	Y	606	CHL	C3D-C2D-C1D	-4.84	99.22	105.83
24	3	607	CHL	C3D-C4D-ND	4.84	118.07	110.24
24	2	609	CHL	C3D-C4D-ND	4.84	118.07	110.24
24	G	605	CHL	C3D-C4D-ND	4.84	118.07	110.24
24	2	601	CHL	C3D-C4D-ND	4.84	118.07	110.24
25	c	510	CLA	CMB-C2B-C1B	-4.84	121.03	128.46
24	S	606	CHL	C3D-C4D-ND	4.84	118.06	110.24
24	R	614	CHL	C3C-C4C-NC	4.84	115.99	110.57
24	6	601	CHL	C3D-C4D-ND	4.83	118.05	110.24
24	8	608	CHL	C3D-C4D-ND	4.83	118.05	110.24
24	S	608	CHL	C3C-C4C-NC	4.83	115.99	110.57
24	s	606	CHL	C3D-C4D-ND	4.83	118.05	110.24
25	A	405	CLA	C4A-NA-C1A	4.83	108.88	106.71
27	2	1622	XAT	C31-C30-C29	-4.82	120.42	127.31
27	5	1622	XAT	C15-C14-C13	-4.82	120.43	127.31
27	7	1622	XAT	C11-C10-C9	-4.82	120.43	127.31
27	6	1622	XAT	C31-C30-C29	-4.82	120.43	127.31
27	3	1622	XAT	C11-C10-C9	-4.82	120.43	127.31
24	G	601	CHL	C3D-C4D-ND	4.82	118.03	110.24
36	A	414	PL9	C7-C3-C2	-4.82	116.97	123.30
27	1	1622	XAT	C15-C14-C13	-4.82	120.44	127.31
24	4	607	CHL	C3C-C4C-NC	4.82	115.97	110.57
26	4	620	LUT	C35-C34-C33	-4.81	120.44	127.31
30	b	618	BCR	C15-C14-C13	-4.81	120.44	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	504	CLA	C4A-NA-C1A	4.81	108.87	106.71
24	R	607	CHL	C3D-C4D-ND	4.81	118.02	110.24
25	g	612	CLA	C4A-NA-C1A	4.81	108.87	106.71
28	N	1623	NEX	C15-C14-C13	-4.81	120.45	127.31
30	c	515	BCR	C15-C14-C13	-4.81	120.45	127.31
25	s	611	CLA	C4A-NA-C1A	4.80	108.87	106.71
24	1	609	CHL	C3D-C4D-ND	4.80	118.01	110.24
24	r	607	CHL	C3D-C4D-ND	4.80	118.01	110.24
24	4	609	CHL	O2D-CGD-CBD	4.80	119.80	111.27
24	7	606	CHL	C2D-C1D-ND	4.80	113.64	110.10
24	4	608	CHL	C3D-C4D-ND	4.80	118.00	110.24
25	c	504	CLA	C4A-NA-C1A	4.80	108.86	106.71
24	n	609	CHL	C3C-C4C-NC	4.80	115.95	110.57
24	8	607	CHL	C3C-C4C-NC	4.80	115.95	110.57
24	5	609	CHL	C3D-C4D-ND	4.80	118.00	110.24
24	2	605	CHL	C3D-C4D-ND	4.80	118.00	110.24
30	B	618	BCR	C15-C14-C13	-4.79	120.47	127.31
30	C	515	BCR	C15-C14-C13	-4.79	120.47	127.31
24	s	608	CHL	C3C-C4C-NC	4.79	115.94	110.57
24	6	605	CHL	C3D-C4D-ND	4.79	117.99	110.24
24	g	601	CHL	C3D-C4D-ND	4.79	117.99	110.24
28	n	1623	NEX	C15-C14-C13	-4.79	120.47	127.31
25	n	602	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
26	8	620	LUT	C35-C34-C33	-4.79	120.48	127.31
24	3	606	CHL	C2D-C1D-ND	4.79	113.63	110.10
24	G	608	CHL	C3D-C4D-ND	4.79	117.98	110.24
30	C	514	BCR	C15-C14-C13	-4.78	120.48	127.31
24	y	605	CHL	C3D-C4D-ND	4.78	117.98	110.24
25	b	602	CLA	C4A-NA-C1A	4.78	108.86	106.71
30	T	101	BCR	C11-C10-C9	-4.78	120.48	127.31
24	8	607	CHL	O2D-CGD-CBD	4.78	119.76	111.27
25	b	610	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
24	4	607	CHL	O2D-CGD-CBD	4.78	119.76	111.27
24	8	609	CHL	O2D-CGD-CBD	4.78	119.76	111.27
24	5	605	CHL	C3D-C4D-ND	4.78	117.97	110.24
24	Y	605	CHL	C3D-C4D-ND	4.78	117.96	110.24
25	C	513	CLA	C4A-NA-C1A	4.77	108.85	106.71
24	g	608	CHL	C3D-C4D-ND	4.77	117.96	110.24
30	t	101	BCR	C11-C10-C9	-4.77	120.50	127.31
28	N	1623	NEX	C38-C25-C26	-4.77	114.27	122.26
24	r	608	CHL	O2D-CGD-CBD	4.77	119.74	111.27
24	N	609	CHL	C3C-C4C-NC	4.77	115.92	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	610	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
28	n	1623	NEX	C38-C25-C26	-4.77	114.27	122.26
24	R	608	CHL	O2D-CGD-CBD	4.77	119.74	111.27
24	1	605	CHL	C3D-C4D-ND	4.76	117.94	110.24
24	n	605	CHL	C3D-C4D-ND	4.76	117.94	110.24
30	c	514	BCR	C15-C14-C13	-4.76	120.51	127.31
25	G	612	CLA	C4A-NA-C1A	4.76	108.85	106.71
26	4	620	LUT	C21-C26-C27	-4.76	106.68	112.70
25	N	602	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
27	y	1622	XAT	C18-C5-C6	-4.76	114.28	122.26
24	8	607	CHL	C3D-C4D-ND	4.75	117.93	110.24
26	8	620	LUT	C21-C26-C27	-4.75	106.70	112.70
24	5	606	CHL	CHD-C1D-ND	-4.75	120.09	124.45
24	N	605	CHL	C3D-C4D-ND	4.75	117.92	110.24
28	6	1623	NEX	C15-C14-C13	-4.75	120.54	127.31
28	y	1623	NEX	C27-C28-C29	-4.74	118.17	125.53
28	s	1623	NEX	C27-C28-C29	-4.74	118.17	125.53
24	4	608	CHL	CHD-C4C-C3C	-4.74	117.87	124.84
24	4	607	CHL	C3D-C4D-ND	4.74	117.90	110.24
27	1	1622	XAT	C27-C28-C29	-4.74	118.18	125.53
27	Y	1622	XAT	C18-C5-C6	-4.73	114.33	122.26
24	4	606	CHL	C3D-C4D-ND	4.73	117.89	110.24
28	2	1623	NEX	C15-C14-C13	-4.73	120.56	127.31
25	s	612	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
24	n	605	CHL	C3D-C2D-C1D	-4.73	99.38	105.83
27	2	1622	XAT	C27-C28-C29	-4.73	118.20	125.53
24	8	608	CHL	CHD-C4C-C3C	-4.73	117.89	124.84
24	N	605	CHL	C3D-C2D-C1D	-4.73	99.38	105.83
28	S	1623	NEX	C27-C28-C29	-4.73	118.20	125.53
25	S	614	CLA	C4A-NA-C1A	4.72	108.83	106.71
25	a	405	CLA	C4A-NA-C1A	4.72	108.83	106.71
24	5	601	CHL	C3D-C4D-ND	4.72	117.88	110.24
30	b	619	BCR	C15-C14-C13	-4.72	120.57	127.31
25	S	612	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
27	6	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
25	c	513	CLA	C4A-NA-C1A	4.72	108.83	106.71
24	s	601	CHL	O2D-CGD-CBD	4.72	119.65	111.27
24	1	601	CHL	C3D-C4D-ND	4.72	117.87	110.24
27	5	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
24	2	608	CHL	C3D-C4D-ND	4.71	117.86	110.24
27	g	1622	XAT	O4-C5-C18	4.71	120.70	115.06
24	G	607	CHL	O2D-CGD-CBD	4.71	119.64	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	620	LUT	C7-C8-C9	-4.71	119.12	126.23
30	B	619	BCR	C15-C14-C13	-4.71	120.59	127.31
27	y	1622	XAT	C11-C10-C9	-4.71	120.59	127.31
26	N	1621	LUT	C15-C14-C13	-4.71	120.59	127.31
24	S	601	CHL	O2D-CGD-CBD	4.71	119.63	111.27
24	1	606	CHL	C3D-C2D-C1D	-4.71	99.41	105.83
25	2	602	CLA	CMB-C2B-C1B	-4.70	121.23	128.46
25	C	503	CLA	C4A-NA-C1A	4.70	108.82	106.71
25	5	612	CLA	C4A-NA-C1A	4.70	108.82	106.71
24	8	606	CHL	C3D-C4D-ND	4.70	117.85	110.24
26	n	1621	LUT	C15-C14-C13	-4.70	120.60	127.31
26	4	620	LUT	C7-C8-C9	-4.70	119.13	126.23
24	g	607	CHL	C3D-C4D-ND	4.70	117.84	110.24
27	2	1622	XAT	C7-C8-C9	-4.70	118.24	125.53
24	g	607	CHL	O2D-CGD-CBD	4.70	119.61	111.27
25	6	602	CLA	CMB-C2B-C1B	-4.70	121.25	128.46
24	8	609	CHL	C3D-C4D-ND	4.69	117.83	110.24
24	6	608	CHL	C3D-C4D-ND	4.69	117.83	110.24
28	Y	1623	NEX	C27-C28-C29	-4.69	118.25	125.53
25	B	604	CLA	CMB-C2B-C1B	-4.69	121.25	128.46
25	S	602	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
36	d	405	PL9	C7-C3-C4	4.69	120.69	116.88
30	H	101	BCR	C16-C17-C18	-4.68	120.62	127.31
24	3	608	CHL	C3D-C4D-ND	4.68	117.81	110.24
26	4	620	LUT	C15-C14-C13	-4.68	120.63	127.31
24	1	606	CHL	CHD-C1D-ND	-4.68	120.15	124.45
25	D	402	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
36	D	405	PL9	C7-C3-C4	4.68	120.68	116.88
27	6	1622	XAT	C7-C8-C9	-4.68	118.27	125.53
24	G	607	CHL	C3D-C4D-ND	4.68	117.80	110.24
25	8	612	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
25	b	604	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
26	8	620	LUT	C15-C14-C13	-4.67	120.64	127.31
24	5	606	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
27	G	1622	XAT	O4-C5-C18	4.67	120.65	115.06
25	s	602	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
27	Y	1622	XAT	C11-C10-C9	-4.67	120.65	127.31
24	3	605	CHL	O2D-CGD-CBD	4.67	119.56	111.27
24	4	609	CHL	C3D-C4D-ND	4.67	117.79	110.24
24	7	608	CHL	C3D-C4D-ND	4.66	117.78	110.24
25	d	402	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
28	S	1623	NEX	C15-C14-C13	-4.66	120.66	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	s	604	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
27	g	1622	XAT	C38-C25-C26	-4.66	114.45	122.26
30	h	101	BCR	C16-C17-C18	-4.66	120.67	127.31
24	G	605	CHL	C3D-C2D-C1D	-4.66	99.48	105.83
25	1	612	CLA	C4A-NA-C1A	4.65	108.80	106.71
24	y	608	CHL	C3D-C4D-ND	4.65	117.76	110.24
24	r	614	CHL	O2D-CGD-CBD	4.65	119.53	111.27
24	7	609	CHL	C3C-C4C-NC	4.65	115.79	110.57
25	r	604	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
24	R	614	CHL	O2D-CGD-CBD	4.65	119.53	111.27
24	N	608	CHL	C3D-C4D-ND	4.65	117.76	110.24
24	2	606	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
28	6	1623	NEX	C38-C25-C26	-4.65	114.47	122.26
28	N	1623	NEX	C35-C34-C33	-4.65	120.68	127.31
25	4	612	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
24	3	609	CHL	C3C-C4C-NC	4.65	115.78	110.57
24	7	605	CHL	O2D-CGD-CBD	4.65	119.52	111.27
24	g	605	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
27	G	1622	XAT	C38-C25-C26	-4.64	114.48	122.26
24	Y	608	CHL	C3D-C4D-ND	4.64	117.75	110.24
25	R	604	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
24	n	608	CHL	C3D-C4D-ND	4.64	117.74	110.24
25	B	615	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
28	S	1623	NEX	C38-C25-C26	-4.63	114.49	122.26
28	s	1623	NEX	C15-C14-C13	-4.63	120.70	127.31
25	b	615	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
28	2	1623	NEX	C38-C25-C26	-4.63	114.50	122.26
28	n	1623	NEX	C35-C34-C33	-4.63	120.71	127.31
24	6	606	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
25	S	604	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
25	s	614	CLA	C4A-NA-C1A	4.62	108.78	106.71
25	d	403	CLA	C4A-NA-C1A	4.62	108.78	106.71
24	2	606	CHL	C3D-C4D-ND	4.62	117.71	110.24
24	2	601	CHL	C3C-C4C-NC	4.62	115.75	110.57
24	5	601	CHL	C3C-C4C-NC	4.62	115.75	110.57
28	s	1623	NEX	C38-C25-C26	-4.61	114.53	122.26
25	Y	603	CLA	C4A-NA-C1A	4.61	108.78	106.71
24	6	606	CHL	C3D-C4D-ND	4.61	117.70	110.24
25	c	503	CLA	C4A-NA-C1A	4.61	108.78	106.71
24	3	607	CHL	C3D-C2D-C1D	-4.61	99.55	105.83
25	D	403	CLA	C4A-NA-C1A	4.60	108.78	106.71
25	8	602	CLA	CMB-C2B-C1B	-4.60	121.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	608	CHL	C3D-C4D-ND	4.60	117.68	110.24
24	6	601	CHL	C3C-C4C-NC	4.60	115.73	110.57
28	G	1623	NEX	C15-C14-C13	-4.60	120.75	127.31
24	7	607	CHL	C3D-C2D-C1D	-4.59	99.56	105.83
24	y	606	CHL	CHD-C1D-ND	-4.59	120.23	124.45
24	Y	605	CHL	O2D-CGD-CBD	4.59	119.42	111.27
25	y	602	CLA	C4A-NA-C1A	4.59	108.77	106.71
24	1	601	CHL	C3C-C4C-NC	4.59	115.72	110.57
25	R	610	CLA	C4A-NA-C1A	4.59	108.77	106.71
25	B	607	CLA	C4A-NA-C1A	4.58	108.77	106.71
24	y	605	CHL	O2D-CGD-CBD	4.58	119.41	111.27
24	S	607	CHL	C3D-C4D-ND	4.58	117.65	110.24
28	1	1623	NEX	C35-C34-C33	-4.58	120.77	127.31
25	4	602	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
24	1	608	CHL	C3D-C4D-ND	4.58	117.64	110.24
28	5	1623	NEX	C35-C34-C33	-4.57	120.78	127.31
25	y	603	CLA	C4A-NA-C1A	4.57	108.76	106.71
28	g	1623	NEX	C15-C14-C13	-4.57	120.78	127.31
25	s	613	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
24	1	605	CHL	O2D-CGD-CBD	4.57	119.39	111.27
26	S	1620	LUT	C35-C34-C33	-4.56	120.80	127.31
25	S	613	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
24	5	605	CHL	O2D-CGD-CBD	4.56	119.38	111.27
26	s	1620	LUT	C35-C34-C33	-4.56	120.80	127.31
24	Y	606	CHL	CHD-C1D-ND	-4.56	120.26	124.45
25	r	610	CLA	C4A-NA-C1A	4.56	108.75	106.71
27	y	1622	XAT	O4-C5-C4	4.56	116.81	113.38
25	B	612	CLA	CMB-C2B-C3B	4.56	133.20	124.68
25	C	509	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
24	n	609	CHL	CAC-C3C-C4C	4.55	130.72	124.81
24	s	607	CHL	C3D-C4D-ND	4.55	117.60	110.24
28	y	1623	NEX	C15-C14-C13	-4.55	120.82	127.31
37	C	520	DGD	O3G-C3G-C2G	-4.55	99.93	110.90
30	A	411	BCR	C7-C8-C9	-4.55	119.37	126.23
37	c	520	DGD	O3G-C3G-C2G	-4.54	99.94	110.90
25	Y	602	CLA	C4A-NA-C1A	4.54	108.75	106.71
25	b	612	CLA	CMB-C2B-C3B	4.54	133.18	124.68
25	n	602	CLA	C4A-NA-C1A	4.54	108.75	106.71
24	3	607	CHL	O2D-CGD-CBD	4.54	119.33	111.27
30	a	411	BCR	C7-C8-C9	-4.54	119.38	126.23
27	7	1622	XAT	O24-C25-C38	4.54	120.49	115.06
24	N	609	CHL	CAC-C3C-C4C	4.53	130.69	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	509	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
25	C	513	CLA	CMB-C2B-C3B	4.53	133.16	124.68
28	Y	1623	NEX	C15-C14-C13	-4.53	120.84	127.31
24	N	607	CHL	CHD-C4C-C3C	-4.53	118.18	124.84
24	7	607	CHL	O2D-CGD-CBD	4.52	119.30	111.27
30	h	101	BCR	C15-C14-C13	-4.52	120.86	127.31
24	n	607	CHL	CHD-C4C-C3C	-4.52	118.19	124.84
27	3	1622	XAT	O24-C25-C38	4.52	120.47	115.06
30	H	101	BCR	C15-C14-C13	-4.51	120.87	127.31
25	c	513	CLA	CMB-C2B-C3B	4.51	133.12	124.68
25	N	602	CLA	C4A-NA-C1A	4.51	108.73	106.71
25	R	602	CLA	CMB-C2B-C3B	4.51	133.11	124.68
25	b	607	CLA	C4A-NA-C1A	4.51	108.73	106.71
24	2	606	CHL	O2D-CGD-CBD	4.51	119.28	111.27
25	R	609	CLA	C4A-NA-C1A	4.50	108.73	106.71
25	S	612	CLA	C4A-NA-C1A	4.50	108.73	106.71
25	s	612	CLA	C4A-NA-C1A	4.50	108.73	106.71
30	4	623	BCR	C16-C17-C18	-4.50	120.89	127.31
24	6	606	CHL	O2D-CGD-CBD	4.50	119.26	111.27
27	Y	1622	XAT	O4-C5-C4	4.50	116.76	113.38
30	8	623	BCR	C16-C17-C18	-4.50	120.89	127.31
24	g	601	CHL	CAC-C3C-C4C	4.50	130.64	124.81
25	r	602	CLA	CMB-C2B-C3B	4.49	133.09	124.68
27	n	1622	XAT	C18-C5-C6	-4.49	114.73	122.26
26	S	1621	LUT	C35-C34-C33	-4.49	120.90	127.31
27	N	1622	XAT	C18-C5-C6	-4.49	114.73	122.26
27	g	1622	XAT	C18-C5-C6	-4.49	114.73	122.26
25	4	602	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
25	b	613	CLA	CMB-C2B-C3B	4.49	133.07	124.68
26	s	1621	LUT	C35-C34-C33	-4.48	120.91	127.31
27	G	1622	XAT	C18-C5-C6	-4.48	114.75	122.26
30	T	101	BCR	C33-C5-C4	4.48	122.23	113.62
26	G	1621	LUT	C15-C14-C13	-4.48	120.92	127.31
24	S	608	CHL	C3D-C4D-ND	4.48	117.48	110.24
24	n	606	CHL	C3D-C4D-ND	4.48	117.48	110.24
24	2	607	CHL	C3D-C4D-ND	4.48	117.48	110.24
26	g	1621	LUT	C15-C14-C13	-4.48	120.92	127.31
25	8	604	CLA	C4A-NA-C1A	4.48	108.72	106.71
30	H	101	BCR	C24-C23-C22	-4.47	119.48	126.23
28	G	1623	NEX	C38-C25-C26	-4.47	114.76	122.26
30	h	101	BCR	C24-C23-C22	-4.47	119.48	126.23
25	A	405	CLA	CMB-C2B-C3B	4.47	133.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	613	CLA	CMB-C2B-C3B	4.47	133.04	124.68
24	G	601	CHL	CAC-C3C-C4C	4.47	130.61	124.81
28	g	1623	NEX	C38-C25-C26	-4.47	114.77	122.26
25	4	604	CLA	C4A-NA-C1A	4.47	108.72	106.71
24	6	607	CHL	C3D-C4D-ND	4.47	117.47	110.24
25	R	602	CLA	C4A-NA-C1A	4.46	108.71	106.71
26	1	1621	LUT	C15-C14-C13	-4.46	120.94	127.31
24	N	606	CHL	C3D-C4D-ND	4.46	117.46	110.24
24	2	607	CHL	C3C-C4C-NC	4.46	115.58	110.57
30	t	101	BCR	C33-C5-C4	4.46	122.19	113.62
25	8	602	CLA	O2D-CGD-O1D	-4.46	115.12	123.84
29	D	408	LHG	O4-P-O5	4.46	134.28	112.24
29	d	408	LHG	O4-P-O5	4.45	134.26	112.24
24	3	609	CHL	C3D-C4D-ND	4.45	117.44	110.24
25	r	609	CLA	C4A-NA-C1A	4.45	108.71	106.71
25	a	405	CLA	CMB-C2B-C3B	4.45	133.00	124.68
24	1	601	CHL	O2D-CGD-CBD	4.45	119.17	111.27
24	y	606	CHL	O2D-CGD-CBD	4.45	119.17	111.27
24	s	608	CHL	C3D-C4D-ND	4.45	117.44	110.24
25	6	604	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
24	5	601	CHL	O2D-CGD-CBD	4.44	119.17	111.27
24	6	607	CHL	C3C-C4C-NC	4.44	115.56	110.57
26	5	1621	LUT	C15-C14-C13	-4.44	120.97	127.31
24	Y	607	CHL	CHD-C4C-C3C	-4.44	118.31	124.84
24	G	608	CHL	CHD-C4C-C3C	-4.44	118.31	124.84
25	A	406	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
27	8	622	XAT	O24-C25-C38	4.44	120.38	115.06
28	5	1623	NEX	C38-C25-C26	-4.44	114.82	122.26
24	y	607	CHL	CHD-C4C-C3C	-4.44	118.31	124.84
24	g	609	CHL	C3D-C4D-ND	4.44	117.42	110.24
24	G	608	CHL	O2D-CGD-CBD	4.44	119.16	111.27
25	Y	604	CLA	CMB-C2B-C3B	4.44	132.98	124.68
24	g	608	CHL	CHD-C4C-C3C	-4.44	118.32	124.84
27	4	622	XAT	C35-C34-C33	-4.43	120.98	127.31
27	2	1622	XAT	C15-C14-C13	-4.43	120.98	127.31
30	H	101	BCR	C7-C8-C9	-4.43	119.54	126.23
25	y	604	CLA	CMB-C2B-C3B	4.43	132.97	124.68
27	4	622	XAT	O24-C25-C38	4.43	120.36	115.06
25	N	610	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
25	b	605	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
24	Y	606	CHL	O2D-CGD-CBD	4.43	119.14	111.27
24	5	606	CHL	C3D-C4D-ND	4.43	117.40	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	406	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
24	S	607	CHL	O2D-CGD-CBD	4.43	119.13	111.27
25	2	604	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
25	R	603	CLA	CMB-C2B-C1B	-4.42	121.66	128.46
25	n	610	CLA	CMB-C2B-C1B	-4.42	121.66	128.46
24	G	609	CHL	C3D-C4D-ND	4.42	117.39	110.24
24	g	608	CHL	O2D-CGD-CBD	4.42	119.13	111.27
25	D	402	CLA	C4A-NA-C1A	4.42	108.69	106.71
27	1	1622	XAT	C31-C30-C29	-4.42	121.00	127.31
24	Y	609	CHL	C3D-C4D-ND	4.42	117.39	110.24
25	B	605	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
25	r	603	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
24	2	607	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
28	1	1623	NEX	C38-C25-C26	-4.42	114.85	122.26
24	7	609	CHL	C3D-C4D-ND	4.42	117.39	110.24
27	6	1622	XAT	C15-C14-C13	-4.42	121.00	127.31
24	1	606	CHL	C3D-C4D-ND	4.42	117.38	110.24
24	1	609	CHL	C3C-C4C-NC	4.41	115.52	110.57
30	h	101	BCR	C7-C8-C9	-4.41	119.57	126.23
36	a	414	PL9	C7-C3-C4	4.41	123.65	118.08
24	5	609	CHL	C3C-C4C-NC	4.40	115.51	110.57
24	y	609	CHL	C3D-C4D-ND	4.40	117.36	110.24
26	N	1620	LUT	C35-C34-C33	-4.40	121.03	127.31
36	A	414	PL9	C7-C3-C4	4.40	123.64	118.08
24	s	607	CHL	O2D-CGD-CBD	4.40	119.09	111.27
24	6	607	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
24	Y	607	CHL	C3D-C4D-ND	4.40	117.36	110.24
27	5	1622	XAT	C31-C30-C29	-4.40	121.03	127.31
24	n	607	CHL	C3D-C4D-ND	4.40	117.36	110.24
26	n	1620	LUT	C35-C34-C33	-4.40	121.03	127.31
27	8	622	XAT	C35-C34-C33	-4.39	121.04	127.31
25	n	603	CLA	C4A-NA-C1A	4.39	108.68	106.71
24	N	607	CHL	C3D-C4D-ND	4.39	117.33	110.24
24	1	608	CHL	O2D-CGD-CBD	4.38	119.06	111.27
24	y	607	CHL	C3D-C4D-ND	4.38	117.33	110.24
25	c	508	CLA	CMB-C2B-C3B	4.38	132.88	124.68
25	1	614	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
25	r	602	CLA	C4A-NA-C1A	4.38	108.67	106.71
25	R	610	CLA	C1B-CHB-C4A	-4.38	121.45	130.12
25	S	614	CLA	CMB-C2B-C3B	4.38	132.87	124.68
25	d	402	CLA	C4A-NA-C1A	4.38	108.67	106.71
24	5	608	CHL	O2D-CGD-CBD	4.37	119.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	614	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
25	r	610	CLA	C1B-CHB-C4A	-4.37	121.46	130.12
27	5	1622	XAT	C38-C25-C26	-4.37	114.94	122.26
25	C	508	CLA	CMB-C2B-C3B	4.36	132.84	124.68
27	1	1622	XAT	C38-C25-C26	-4.36	114.96	122.26
30	D	404	BCR	C11-C10-C9	-4.36	121.09	127.31
24	n	606	CHL	CAC-C3C-C4C	4.35	130.46	124.81
25	s	614	CLA	CMB-C2B-C3B	4.35	132.82	124.68
24	S	608	CHL	O2D-CGD-CBD	4.35	119.00	111.27
25	N	603	CLA	C4A-NA-C1A	4.35	108.66	106.71
25	C	510	CLA	CMB-C2B-C3B	4.35	132.81	124.68
24	Y	606	CHL	C3D-C4D-ND	4.34	117.27	110.24
24	y	606	CHL	C3D-C4D-ND	4.34	117.27	110.24
24	N	606	CHL	CAC-C3C-C4C	4.34	130.45	124.81
30	c	515	BCR	C7-C8-C9	-4.34	119.67	126.23
26	Y	1621	LUT	C35-C34-C33	-4.34	121.12	127.31
25	c	502	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
26	y	1621	LUT	C35-C34-C33	-4.34	121.12	127.31
25	c	510	CLA	CMB-C2B-C3B	4.33	132.78	124.68
30	d	404	BCR	C11-C10-C9	-4.33	121.13	127.31
25	Y	602	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
25	4	612	CLA	C4A-NA-C1A	4.33	108.65	106.71
25	C	505	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
30	c	515	BCR	C21-C20-C19	-4.33	109.71	123.22
29	l	101	LHG	O4-P-O5	4.33	133.64	112.24
30	C	515	BCR	C7-C8-C9	-4.33	119.70	126.23
24	n	609	CHL	C3D-C4D-ND	4.33	117.24	110.24
24	N	609	CHL	C3D-C4D-ND	4.32	117.23	110.24
30	C	515	BCR	C21-C20-C19	-4.32	109.72	123.22
25	c	505	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
29	L	101	LHG	O4-P-O5	4.32	133.60	112.24
24	s	608	CHL	O2D-CGD-CBD	4.32	118.94	111.27
25	N	614	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
25	8	612	CLA	C4A-NA-C1A	4.32	108.65	106.71
25	g	602	CLA	CMB-C2B-C3B	4.31	132.75	124.68
29	4	2630	LHG	O4-P-O5	4.31	133.57	112.24
25	y	602	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
29	8	2630	LHG	O4-P-O5	4.31	133.55	112.24
25	C	502	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
25	n	614	CLA	CMB-C2B-C1B	-4.31	121.85	128.46
25	G	602	CLA	CMB-C2B-C3B	4.30	132.72	124.68
26	Y	1621	LUT	C15-C14-C13	-4.30	121.18	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	y	1621	LUT	C15-C14-C13	-4.29	121.19	127.31
29	Y	2630	LHG	O4-P-O5	4.29	133.45	112.24
29	y	2630	LHG	O4-P-O5	4.29	133.45	112.24
30	t	101	BCR	C20-C19-C18	-4.29	114.36	126.42
30	T	101	BCR	C20-C19-C18	-4.28	114.38	126.42
24	7	606	CHL	C3D-C2D-C1D	-4.27	100.00	105.83
24	3	606	CHL	C3D-C2D-C1D	-4.27	100.00	105.83
24	5	608	CHL	CHD-C4C-C3C	-4.27	118.56	124.84
29	c	523	LHG	O4-P-O5	4.27	133.34	112.24
24	1	608	CHL	CHD-C4C-C3C	-4.27	118.57	124.84
24	g	601	CHL	C3C-C4C-NC	4.26	115.35	110.57
24	G	601	CHL	C3C-C4C-NC	4.26	115.35	110.57
24	N	601	CHL	C3C-C4C-NC	4.26	115.35	110.57
29	C	523	LHG	O4-P-O5	4.26	133.31	112.24
33	a	409	PHO	CMB-C2B-C3B	4.26	132.65	124.68
29	R	2630	LHG	O4-P-O5	4.26	133.28	112.24
29	d	410	LHG	O4-P-O5	4.26	133.28	112.24
25	4	610	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
27	g	1622	XAT	C4-C3-C2	-4.25	102.56	110.77
24	n	601	CHL	C3C-C4C-NC	4.25	115.34	110.57
29	D	410	LHG	O4-P-O5	4.25	133.26	112.24
29	r	2630	LHG	O4-P-O5	4.25	133.26	112.24
33	A	409	PHO	CMB-C2B-C3B	4.25	132.63	124.68
25	D	403	CLA	CMB-C2B-C3B	4.25	132.63	124.68
25	d	403	CLA	CMB-C2B-C3B	4.24	132.61	124.68
27	1	1622	XAT	C18-C5-C6	-4.24	115.16	122.26
27	1	1622	XAT	C11-C10-C9	-4.23	121.27	127.31
27	G	1622	XAT	C4-C3-C2	-4.23	102.60	110.77
24	Y	606	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
29	d	409	LHG	O4-P-O5	4.22	133.12	112.24
29	D	409	LHG	O4-P-O5	4.22	133.12	112.24
29	s	2630	LHG	O4-P-O5	4.22	133.10	112.24
27	5	1622	XAT	C18-C5-C6	-4.22	115.19	122.26
29	n	2630	LHG	O4-P-O5	4.22	133.09	112.24
30	b	618	BCR	C16-C17-C18	-4.22	121.29	127.31
24	4	601	CHL	C3C-C4C-NC	4.22	115.30	110.57
25	8	610	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
29	N	2630	LHG	O4-P-O5	4.21	133.08	112.24
29	S	2630	LHG	O4-P-O5	4.21	133.07	112.24
27	5	1622	XAT	C11-C10-C9	-4.21	121.30	127.31
27	n	1622	XAT	C11-C10-C9	-4.21	121.30	127.31
26	1	1621	LUT	C2-C3-C4	4.21	116.07	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	602	CLA	C4A-NA-C1A	4.21	108.60	106.71
25	g	604	CLA	C4A-NA-C1A	4.21	108.60	106.71
29	C	522	LHG	O4-P-O5	4.21	133.04	112.24
29	6	2630	LHG	O4-P-O5	4.21	133.04	112.24
24	N	609	CHL	C3B-C4B-NB	4.21	114.65	109.21
29	c	522	LHG	O4-P-O5	4.21	133.03	112.24
27	4	622	XAT	C15-C14-C13	-4.20	121.31	127.31
24	5	607	CHL	O2D-CGD-CBD	4.20	118.74	111.27
29	2	2630	LHG	O4-P-O5	4.20	133.02	112.24
25	B	617	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
24	y	606	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
27	8	622	XAT	C15-C14-C13	-4.20	121.32	127.31
27	N	1622	XAT	C11-C10-C9	-4.20	121.32	127.31
25	b	617	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
24	n	609	CHL	C3B-C4B-NB	4.19	114.63	109.21
25	C	511	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
26	5	1621	LUT	C2-C3-C4	4.19	116.04	110.30
24	8	601	CHL	C3C-C4C-NC	4.19	115.27	110.57
30	B	618	BCR	C16-C17-C18	-4.18	121.34	127.31
24	1	607	CHL	O2D-CGD-CBD	4.18	118.70	111.27
28	1	1623	NEX	C17-C1-C6	-4.18	106.73	110.47
27	G	1622	XAT	C27-C28-C29	-4.18	119.04	125.53
24	3	601	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
27	g	1622	XAT	C27-C28-C29	-4.18	119.04	125.53
24	N	608	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
24	7	601	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
25	4	603	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
25	G	604	CLA	C4A-NA-C1A	4.18	108.58	106.71
25	5	613	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
25	8	603	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
30	c	516	BCR	C28-C27-C26	-4.17	106.62	114.08
30	C	516	BCR	C28-C27-C26	-4.17	106.62	114.08
25	1	613	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
25	b	607	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
29	c	2630	LHG	O4-P-O5	4.17	132.84	112.24
24	n	608	CHL	CHD-C4C-C3C	-4.17	118.72	124.84
27	Y	1622	XAT	C4-C3-C2	-4.17	102.73	110.77
28	5	1623	NEX	C17-C1-C6	-4.16	106.75	110.47
37	c	519	DGD	O3G-C3G-C2G	-4.16	100.86	110.90
29	1	2630	LHG	O4-P-O5	4.16	132.80	112.24
29	C	2630	LHG	O4-P-O5	4.16	132.80	112.24
29	5	2630	LHG	O4-P-O5	4.16	132.80	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	6	1622	XAT	O24-C25-C38	4.16	120.04	115.06
25	g	610	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
24	R	608	CHL	C3D-C4D-ND	4.15	116.96	110.24
25	c	511	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
24	3	608	CHL	O2D-CGD-CBD	4.15	118.65	111.27
27	2	1622	XAT	O24-C25-C38	4.15	120.03	115.06
24	2	608	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
37	C	519	DGD	O3G-C3G-C2G	-4.15	100.89	110.90
27	y	1622	XAT	C4-C3-C2	-4.15	102.76	110.77
29	B	2630	LHG	O4-P-O5	4.15	132.74	112.24
24	n	606	CHL	CHD-C4C-C3C	-4.15	118.75	124.84
25	4	602	CLA	C4A-NA-C1A	4.15	108.57	106.71
26	n	1621	LUT	C22-C23-C24	-4.15	107.02	111.74
24	r	608	CHL	C3D-C4D-ND	4.14	116.94	110.24
25	B	607	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
29	b	2630	LHG	O4-P-O5	4.14	132.72	112.24
27	7	1622	XAT	C4-C3-C2	-4.14	102.77	110.77
24	N	606	CHL	CHD-C4C-C3C	-4.14	118.75	124.84
24	g	607	CHL	CHD-C4C-C3C	-4.14	118.75	124.84
24	7	606	CHL	CAC-C3C-C4C	4.14	130.18	124.81
25	G	610	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
24	n	605	CHL	O2D-CGD-O1D	-4.14	115.75	123.84
25	C	507	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
27	3	1622	XAT	C4-C3-C2	-4.13	102.79	110.77
26	g	1621	LUT	C35-C34-C33	-4.13	121.41	127.31
26	N	1621	LUT	C22-C23-C24	-4.13	107.04	111.74
30	c	514	BCR	C16-C17-C18	-4.13	121.42	127.31
24	7	608	CHL	O2D-CGD-CBD	4.13	118.60	111.27
24	6	608	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
25	c	507	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
25	7	602	CLA	CMB-C2B-C3B	4.12	132.39	124.68
24	N	605	CHL	O2D-CGD-O1D	-4.12	115.78	123.84
30	A	411	BCR	C11-C10-C9	-4.12	121.43	127.31
24	n	607	CHL	O2D-CGD-CBD	4.12	118.59	111.27
25	3	614	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
26	G	1621	LUT	C35-C34-C33	-4.12	121.43	127.31
30	a	411	BCR	C11-C10-C9	-4.11	121.44	127.31
25	7	614	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
29	B	2631	LHG	O4-P-O5	4.11	132.56	112.24
29	b	2631	LHG	O4-P-O5	4.11	132.55	112.24
24	4	606	CHL	O2D-CGD-CBD	4.10	118.56	111.27
30	C	514	BCR	C16-C17-C18	-4.10	121.45	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	607	CHL	O2D-CGD-CBD	4.10	118.56	111.27
25	3	602	CLA	CMB-C2B-C3B	4.10	132.35	124.68
24	2	607	CHL	O2D-CGD-CBD	4.10	118.56	111.27
24	G	607	CHL	CHD-C4C-C3C	-4.10	118.81	124.84
24	3	606	CHL	CAC-C3C-C4C	4.10	130.13	124.81
30	C	517	BCR	C20-C21-C22	-4.10	121.46	127.31
26	6	1621	LUT	C22-C23-C24	-4.10	107.08	111.74
25	Y	610	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
25	5	610	CLA	C1B-CHB-C4A	-4.09	122.01	130.12
25	r	604	CLA	CAA-C2A-C3A	-4.09	101.57	112.78
25	R	604	CLA	CAA-C2A-C3A	-4.09	101.57	112.78
24	N	607	CHL	O2D-CGD-CBD	4.09	118.54	111.27
25	s	610	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
25	1	614	CLA	C4A-NA-C1A	4.09	108.55	106.71
30	c	517	BCR	C20-C21-C22	-4.09	121.47	127.31
25	S	610	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
26	2	1621	LUT	C35-C34-C33	-4.09	121.47	127.31
25	B	615	CLA	C4A-NA-C1A	4.09	108.54	106.71
24	8	606	CHL	O2D-CGD-CBD	4.09	118.53	111.27
25	n	610	CLA	CMB-C2B-C3B	4.09	132.32	124.68
26	N	1621	LUT	C35-C34-C33	-4.09	121.48	127.31
24	Y	607	CHL	O2D-CGD-CBD	4.08	118.53	111.27
25	R	604	CLA	C4A-NA-C1A	4.08	108.54	106.71
26	2	1621	LUT	C22-C23-C24	-4.08	107.09	111.74
24	r	606	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
25	B	611	CLA	CAA-C2A-C3A	-4.08	101.60	112.78
24	y	607	CHL	O2D-CGD-CBD	4.08	118.52	111.27
25	8	612	CLA	CMB-C2B-C3B	4.08	132.31	124.68
24	R	606	CHL	CHD-C4C-C3C	-4.08	118.84	124.84
26	n	1621	LUT	C35-C34-C33	-4.08	121.49	127.31
25	Y	613	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
25	y	613	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
27	r	622	XAT	C35-C34-C33	-4.08	121.49	127.31
25	1	610	CLA	C1B-CHB-C4A	-4.07	122.05	130.12
25	s	612	CLA	CMB-C2B-C3B	4.07	132.30	124.68
25	b	611	CLA	CAA-C2A-C3A	-4.07	101.63	112.78
27	2	1622	XAT	C18-C5-C6	-4.07	115.44	122.26
25	N	610	CLA	CMB-C2B-C3B	4.07	132.29	124.68
25	8	602	CLA	CMB-C2B-C3B	4.07	132.29	124.68
24	4	606	CHL	CHD-C4C-C3C	-4.07	118.86	124.84
25	y	610	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
25	b	615	CLA	C4A-NA-C1A	4.07	108.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	602	CLA	CMB-C2B-C3B	4.06	132.28	124.68
25	S	612	CLA	CMB-C2B-C3B	4.06	132.28	124.68
24	2	608	CHL	O2D-CGD-CBD	4.06	118.49	111.27
27	6	1622	XAT	C18-C5-C6	-4.06	115.45	122.26
26	6	1621	LUT	C35-C34-C33	-4.06	121.51	127.31
25	4	612	CLA	CMB-C2B-C3B	4.06	132.27	124.68
27	R	622	XAT	C35-C34-C33	-4.06	121.52	127.31
28	N	1623	NEX	C27-C28-C29	-4.05	119.24	125.53
25	G	612	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
29	G	2630	LHG	O4-P-O5	4.05	132.27	112.24
24	6	608	CHL	O2D-CGD-CBD	4.05	118.47	111.27
24	8	608	CHL	O2D-CGD-CBD	4.05	118.47	111.27
29	g	2630	LHG	O4-P-O5	4.05	132.27	112.24
25	4	611	CLA	C4A-NA-C1A	4.05	108.53	106.71
24	8	606	CHL	CHD-C4C-C3C	-4.05	118.89	124.84
26	3	1621	LUT	C10-C11-C12	-4.05	110.59	123.22
24	4	608	CHL	O2D-CGD-CBD	4.05	118.46	111.27
25	B	614	CLA	CMB-C2B-C3B	4.05	132.25	124.68
24	G	609	CHL	C3B-C4B-NB	4.05	114.44	109.21
24	g	609	CHL	C1C-C2C-C3C	-4.04	103.91	107.11
26	6	1620	LUT	C15-C14-C13	-4.04	121.54	127.31
24	G	609	CHL	C1C-C2C-C3C	-4.04	103.91	107.11
25	b	614	CLA	CMB-C2B-C3B	4.04	132.24	124.68
25	5	614	CLA	C4A-NA-C1A	4.04	108.52	106.71
25	C	503	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
25	g	612	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
26	7	1621	LUT	C10-C11-C12	-4.03	110.63	123.22
30	B	620	BCR	C28-C27-C26	-4.03	106.87	114.08
26	G	1621	LUT	C2-C3-C4	4.03	115.83	110.30
26	2	1620	LUT	C15-C14-C13	-4.03	121.55	127.31
28	n	1623	NEX	C27-C28-C29	-4.03	119.28	125.53
25	2	602	CLA	CMB-C2B-C3B	4.03	132.22	124.68
25	5	610	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
24	G	606	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
30	b	620	BCR	C28-C27-C26	-4.03	106.89	114.08
25	6	602	CLA	CMB-C2B-C3B	4.02	132.21	124.68
25	1	610	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
24	S	606	CHL	CAC-C3C-C4C	4.02	130.03	124.81
30	B	620	BCR	C16-C17-C18	-4.02	121.57	127.31
25	1	604	CLA	C4A-NA-C1A	4.02	108.51	106.71
29	7	2630	LHG	O4-P-O5	4.02	132.12	112.24
24	g	609	CHL	C3B-C4B-NB	4.02	114.41	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	601	CHL	O2D-CGD-CBD	4.02	118.41	111.27
25	6	614	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
29	3	2630	LHG	O4-P-O5	4.02	132.09	112.24
24	s	606	CHL	CAC-C3C-C4C	4.01	130.02	124.81
28	R	623	NEX	C31-C30-C29	-4.01	121.58	127.31
30	T	101	BCR	C28-C27-C26	-4.01	106.91	114.08
26	g	1621	LUT	C2-C3-C4	4.01	115.80	110.30
30	t	101	BCR	C28-C27-C26	-4.01	106.92	114.08
24	g	606	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
24	Y	606	CHL	CAC-C3C-C4C	4.01	130.01	124.81
24	2	601	CHL	O2D-CGD-CBD	4.01	118.39	111.27
25	c	503	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
25	B	605	CLA	CAA-CBA-CGA	-4.01	101.55	113.25
25	r	604	CLA	C4A-NA-C1A	4.01	108.51	106.71
25	C	504	CLA	CMB-C2B-C3B	4.01	132.17	124.68
24	7	601	CHL	C3C-C4C-NC	4.01	115.06	110.57
24	y	606	CHL	C3B-C4B-NB	4.00	114.38	109.21
25	b	605	CLA	CAA-CBA-CGA	-4.00	101.56	113.25
27	G	1622	XAT	O24-C25-C38	4.00	119.85	115.06
30	C	517	BCR	C33-C5-C6	-4.00	120.04	124.53
30	b	620	BCR	C16-C17-C18	-4.00	121.60	127.31
24	3	601	CHL	C3C-C4C-NC	4.00	115.05	110.57
24	2	605	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
24	Y	606	CHL	C3B-C4B-NB	3.99	114.37	109.21
24	8	601	CHL	C4A-NA-C1A	3.99	108.50	106.71
28	3	1623	NEX	C11-C10-C9	-3.99	121.61	127.31
25	c	504	CLA	CMB-C2B-C3B	3.99	132.15	124.68
24	y	606	CHL	CAC-C3C-C4C	3.99	129.99	124.81
28	7	1623	NEX	C11-C10-C9	-3.99	121.61	127.31
24	8	601	CHL	C3D-C4D-ND	3.99	116.69	110.24
24	Y	609	CHL	CAC-C3C-C4C	3.99	129.99	124.81
25	2	614	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
27	3	1622	XAT	C18-C5-C6	-3.99	115.58	122.26
25	r	610	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
30	c	517	BCR	C33-C5-C6	-3.99	120.05	124.53
24	4	601	CHL	C3D-C4D-ND	3.99	116.69	110.24
24	6	605	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
25	5	604	CLA	C4A-NA-C1A	3.99	108.50	106.71
27	4	622	XAT	C4-C3-C2	-3.99	103.08	110.77
25	b	615	CLA	CMB-C2B-C3B	3.98	132.13	124.68
27	n	1622	XAT	C15-C35-C34	-3.98	115.31	123.47
25	8	611	CLA	C4A-NA-C1A	3.98	108.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	609	CLA	C1B-CHB-C4A	-3.98	122.23	130.12
25	b	611	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
27	N	1622	XAT	C15-C35-C34	-3.98	115.33	123.47
24	y	609	CHL	CAC-C3C-C4C	3.98	129.97	124.81
27	Y	1622	XAT	C27-C28-C29	-3.98	119.36	125.53
27	8	622	XAT	C4-C3-C2	-3.98	103.09	110.77
28	r	623	NEX	C31-C30-C29	-3.97	121.64	127.31
25	G	614	CLA	C4A-NA-C1A	3.97	108.49	106.71
26	r	620	LUT	C35-C34-C33	-3.97	121.64	127.31
25	R	609	CLA	C1B-CHB-C4A	-3.97	122.26	130.12
25	B	615	CLA	CMB-C2B-C3B	3.97	132.10	124.68
26	R	620	LUT	C35-C34-C33	-3.97	121.65	127.31
25	B	603	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
27	7	1622	XAT	C18-C5-C6	-3.96	115.62	122.26
25	B	611	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
25	R	610	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
28	7	1623	NEX	C27-C28-C29	-3.96	119.38	125.53
24	1	606	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
27	g	1622	XAT	O24-C25-C38	3.96	119.80	115.06
24	7	608	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
24	3	608	CHL	CHD-C4C-C3C	-3.96	119.03	124.84
30	c	517	BCR	C16-C17-C18	-3.95	121.67	127.31
24	Y	608	CHL	O2D-CGD-CBD	3.95	118.29	111.27
24	s	607	CHL	C3B-C4B-NB	3.95	114.32	109.21
26	1	1621	LUT	C35-C34-C33	-3.95	121.68	127.31
24	5	606	CHL	CHD-C4C-C3C	-3.95	119.04	124.84
27	y	1622	XAT	C27-C28-C29	-3.94	119.41	125.53
25	b	610	CLA	CMB-C2B-C3B	3.94	132.06	124.68
24	y	608	CHL	O2D-CGD-CBD	3.94	118.27	111.27
28	3	1623	NEX	C27-C28-C29	-3.94	119.42	125.53
25	5	602	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
24	S	607	CHL	C3B-C4B-NB	3.94	114.30	109.21
25	B	610	CLA	CMB-C2B-C3B	3.94	132.04	124.68
25	b	603	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
30	C	517	BCR	C16-C17-C18	-3.93	121.70	127.31
24	8	607	CHL	CAC-C3C-C4C	3.93	129.91	124.81
24	4	607	CHL	CAC-C3C-C4C	3.93	129.91	124.81
26	5	1621	LUT	C35-C34-C33	-3.93	121.70	127.31
34	b	623	SQD	O47-C7-C8	3.93	119.97	111.50
24	g	607	CHL	CAC-C3C-C4C	3.93	129.91	124.81
25	S	602	CLA	C4A-NA-C1A	3.93	108.47	106.71
30	b	619	BCR	C11-C10-C9	-3.93	121.70	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	611	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
24	4	601	CHL	C4A-NA-C1A	3.93	108.47	106.71
25	3	602	CLA	C4A-NA-C1A	3.92	108.47	106.71
25	1	602	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
25	N	604	CLA	CMB-C2B-C3B	3.92	132.02	124.68
24	s	601	CHL	CHD-C4C-C3C	-3.92	119.08	124.84
34	B	623	SQD	O47-C7-C8	3.92	119.95	111.50
25	2	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
27	7	1622	XAT	C15-C35-C34	-3.92	115.45	123.47
24	7	605	CHL	CHD-C4C-C3C	-3.92	119.08	124.84
25	s	602	CLA	C4A-NA-C1A	3.91	108.47	106.71
30	B	619	BCR	C11-C10-C9	-3.91	121.73	127.31
25	n	604	CLA	CMB-C2B-C3B	3.91	131.99	124.68
25	2	604	CLA	C4A-NA-C1A	3.91	108.46	106.71
25	s	604	CLA	CMB-C2B-C3B	3.91	131.99	124.68
25	S	604	CLA	CMB-C2B-C3B	3.91	131.99	124.68
24	3	605	CHL	CHD-C4C-C3C	-3.90	119.10	124.84
25	g	614	CLA	C4A-NA-C1A	3.90	108.46	106.71
30	b	619	BCR	C16-C17-C18	-3.90	121.75	127.31
27	N	1622	XAT	C4-C3-C2	-3.90	103.24	110.77
24	G	607	CHL	CAC-C3C-C4C	3.90	129.87	124.81
24	S	601	CHL	CHD-C4C-C3C	-3.90	119.11	124.84
25	r	601	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
27	3	1622	XAT	C15-C35-C34	-3.90	115.49	123.47
25	5	610	CLA	CMB-C2B-C3B	3.89	131.96	124.68
27	n	1622	XAT	C4-C3-C2	-3.89	103.25	110.77
25	R	601	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
24	N	609	CHL	CHB-C4A-NA	3.89	129.89	124.51
30	b	618	BCR	C24-C23-C22	-3.89	120.36	126.23
24	N	609	CHL	C1C-C2C-C3C	-3.89	104.03	107.11
24	g	606	CHL	O2D-CGD-CBD	3.88	118.17	111.27
30	B	619	BCR	C16-C17-C18	-3.88	121.77	127.31
24	S	608	CHL	C3B-C4B-NB	3.88	114.23	109.21
28	r	623	NEX	C26-C27-C28	-3.88	117.79	125.99
24	s	608	CHL	C3B-C4B-NB	3.88	114.23	109.21
24	n	609	CHL	C1C-C2C-C3C	-3.88	104.03	107.11
34	b	623	SQD	C1-O5-C5	3.88	121.30	113.69
25	G	603	CLA	C4A-NA-C1A	3.88	108.45	106.71
26	r	620	LUT	C15-C14-C13	-3.87	121.78	127.31
25	1	610	CLA	CMB-C2B-C3B	3.87	131.92	124.68
30	B	618	BCR	C24-C23-C22	-3.87	120.38	126.23
37	c	520	DGD	O6D-C1D-O3G	-3.87	100.81	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R	620	LUT	C15-C14-C13	-3.87	121.79	127.31
30	h	101	BCR	C20-C21-C22	-3.87	121.79	127.31
24	n	609	CHL	CHB-C4A-NA	3.87	129.86	124.51
24	G	606	CHL	O2D-CGD-CBD	3.87	118.14	111.27
28	R	623	NEX	C26-C27-C28	-3.87	117.81	125.99
34	B	623	SQD	C1-O5-C5	3.87	121.28	113.69
25	8	604	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
25	n	602	CLA	CMB-C2B-C3B	3.87	131.91	124.68
25	7	602	CLA	C4A-NA-C1A	3.87	108.44	106.71
25	N	602	CLA	CMB-C2B-C3B	3.86	131.90	124.68
24	y	601	CHL	C3C-C4C-NC	3.86	114.90	110.57
28	s	1623	NEX	O24-C25-C38	3.86	119.68	115.06
30	C	516	BCR	C20-C21-C22	-3.86	121.80	127.31
25	4	604	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
24	Y	601	CHL	C3C-C4C-NC	3.86	114.89	110.57
37	C	520	DGD	O6D-C1D-O3G	-3.85	100.85	109.97
30	C	515	BCR	C11-C10-C9	-3.85	121.81	127.31
24	Y	605	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
27	y	1622	XAT	C10-C11-C12	-3.85	111.20	123.22
30	c	515	BCR	C11-C10-C9	-3.85	121.81	127.31
30	c	516	BCR	C20-C21-C22	-3.85	121.81	127.31
30	T	101	BCR	C4-C5-C6	-3.85	117.14	122.73
24	s	607	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
28	Y	1623	NEX	C2-C1-C6	3.85	112.95	109.21
24	S	607	CHL	CHD-C4C-C3C	-3.85	119.19	124.84
25	1	604	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
30	H	101	BCR	C20-C21-C22	-3.84	121.83	127.31
34	B	623	SQD	O9-S-C6	3.84	111.50	106.94
27	r	622	XAT	O24-C25-C38	3.84	119.66	115.06
24	N	605	CHL	CHD-C4C-C3C	-3.84	119.19	124.84
34	b	623	SQD	O9-S-C6	3.84	111.50	106.94
24	y	605	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
27	Y	1622	XAT	C10-C11-C12	-3.84	111.25	123.22
34	a	412	SQD	O9-S-O7	-3.84	100.67	113.95
28	y	1623	NEX	C2-C1-C6	3.84	112.94	109.21
25	5	604	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
25	r	613	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
25	s	610	CLA	CMB-C2B-C3B	3.83	131.85	124.68
25	g	603	CLA	C4A-NA-C1A	3.83	108.43	106.71
27	R	622	XAT	O24-C25-C38	3.83	119.65	115.06
25	S	602	CLA	CMB-C2B-C3B	3.83	131.85	124.68
30	t	101	BCR	C4-C5-C6	-3.83	117.17	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	A	412	SQD	O9-S-O7	-3.83	100.69	113.95
24	7	607	CHL	CAC-C3C-C4C	3.83	129.78	124.81
25	C	505	CLA	CMB-C2B-C3B	3.83	131.84	124.68
30	b	618	BCR	C21-C20-C19	-3.83	111.27	123.22
25	s	602	CLA	CMB-C2B-C3B	3.83	131.84	124.68
24	N	601	CHL	CAC-C3C-C4C	3.83	129.78	124.81
24	Y	605	CHL	C3B-C4B-NB	3.83	114.16	109.21
24	2	601	CHL	CMD-C2D-C3D	-3.83	118.81	127.61
26	R	620	LUT	C10-C11-C12	-3.82	111.29	123.22
24	n	605	CHL	CHD-C4C-C3C	-3.82	119.22	124.84
26	r	620	LUT	C10-C11-C12	-3.82	111.29	123.22
25	B	603	CLA	C4A-NA-C1A	3.82	108.42	106.71
24	n	601	CHL	CAC-C3C-C4C	3.82	129.76	124.81
25	r	601	CLA	CBC-CAC-C3C	3.82	122.96	112.43
28	S	1623	NEX	O24-C25-C38	3.82	119.63	115.06
30	B	618	BCR	C21-C20-C19	-3.82	111.31	123.22
25	D	402	CLA	CMB-C2B-C3B	3.82	131.82	124.68
25	n	613	CLA	CMB-C2B-C3B	3.82	131.82	124.68
24	6	601	CHL	CMD-C2D-C3D	-3.81	118.84	127.61
25	S	610	CLA	CMB-C2B-C3B	3.81	131.81	124.68
30	A	411	BCR	C15-C14-C13	-3.81	121.87	127.31
25	R	601	CLA	CBC-CAC-C3C	3.81	122.94	112.43
25	N	613	CLA	CMB-C2B-C3B	3.81	131.80	124.68
25	2	612	CLA	C4A-NA-C1A	3.81	108.42	106.71
34	b	623	SQD	O9-S-O7	-3.81	100.77	113.95
28	N	1623	NEX	C11-C10-C9	-3.81	121.88	127.31
30	C	516	BCR	C33-C5-C6	-3.81	120.25	124.53
30	c	516	BCR	C33-C5-C6	-3.81	120.25	124.53
24	2	607	CHL	C1B-CHB-C4A	-3.80	122.58	130.12
25	c	505	CLA	CMB-C2B-C3B	3.80	131.80	124.68
28	R	623	NEX	O24-C25-C38	3.80	119.61	115.06
26	Y	1620	LUT	C35-C34-C33	-3.80	121.88	127.31
30	a	411	BCR	C15-C14-C13	-3.80	121.88	127.31
24	N	607	CHL	C3B-C4B-NB	3.80	114.13	109.21
25	R	613	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
28	r	623	NEX	O24-C25-C38	3.80	119.61	115.06
24	3	607	CHL	CAC-C3C-C4C	3.80	129.74	124.81
25	Y	610	CLA	C1B-CHB-C4A	-3.80	122.59	130.12
37	H	102	DGD	C3D-C4D-C5D	-3.80	103.46	110.24
26	y	1620	LUT	C35-C34-C33	-3.80	121.89	127.31
24	y	605	CHL	C3B-C4B-NB	3.80	114.12	109.21
34	B	623	SQD	O9-S-O7	-3.80	100.81	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	601	CHL	CAC-C3C-C4C	3.80	129.73	124.81
30	a	411	BCR	C24-C23-C22	-3.79	120.50	126.23
25	2	613	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
24	G	605	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
25	d	402	CLA	CMB-C2B-C3B	3.79	131.77	124.68
37	h	102	DGD	C3D-C4D-C5D	-3.79	103.47	110.24
28	s	1623	NEX	C24-C23-C22	-3.79	103.45	110.77
30	A	411	BCR	C24-C23-C22	-3.79	120.51	126.23
24	y	601	CHL	CAC-C3C-C4C	3.79	129.73	124.81
30	A	411	BCR	C20-C21-C22	-3.79	121.90	127.31
25	c	512	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	y	610	CLA	C1B-CHB-C4A	-3.79	122.62	130.12
30	d	404	BCR	C38-C26-C25	-3.79	120.28	124.53
25	g	613	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	6	613	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
24	6	607	CHL	C1B-CHB-C4A	-3.79	122.62	130.12
30	D	404	BCR	C38-C26-C25	-3.78	120.28	124.53
24	n	607	CHL	C3B-C4B-NB	3.78	114.10	109.21
28	Y	1623	NEX	C5-C4-C3	-3.78	107.27	111.75
24	N	607	CHL	CHB-C4A-NA	3.78	129.74	124.51
28	7	1623	NEX	O24-C25-C38	3.78	119.58	115.06
25	C	512	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
24	g	605	CHL	C3B-C4B-NB	3.78	114.09	109.21
24	g	605	CHL	CHD-C4C-C3C	-3.77	119.29	124.84
28	3	1623	NEX	O24-C25-C38	3.77	119.58	115.06
30	H	101	BCR	C31-C1-C6	-3.77	104.18	110.30
30	h	101	BCR	C31-C1-C6	-3.77	104.18	110.30
30	a	411	BCR	C20-C21-C22	-3.77	121.93	127.31
28	n	1623	NEX	C11-C10-C9	-3.77	121.93	127.31
28	S	1623	NEX	C24-C23-C22	-3.77	103.50	110.77
30	C	516	BCR	C16-C15-C14	-3.77	115.76	123.47
25	6	612	CLA	C4A-NA-C1A	3.76	108.40	106.71
30	c	516	BCR	C16-C15-C14	-3.76	115.77	123.47
25	6	604	CLA	C4A-NA-C1A	3.76	108.40	106.71
28	y	1623	NEX	C5-C4-C3	-3.76	107.29	111.75
24	n	607	CHL	CHB-C4A-NA	3.76	129.71	124.51
34	A	412	SQD	O8-S-C6	3.76	111.73	105.74
25	G	613	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
25	B	608	CLA	CMB-C2B-C3B	3.76	131.71	124.68
25	b	603	CLA	C4A-NA-C1A	3.75	108.39	106.71
25	b	608	CLA	CMB-C2B-C3B	3.75	131.69	124.68
24	R	607	CHL	CAC-C3C-C4C	3.74	129.67	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	412	SQD	O8-S-C6	3.74	111.70	105.74
24	4	609	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
24	3	606	CHL	CMD-C2D-C3D	-3.74	119.02	127.61
34	A	412	SQD	O5-C5-C4	3.73	116.47	109.69
24	7	606	CHL	CMD-C2D-C3D	-3.73	119.03	127.61
25	5	614	CLA	CMB-C2B-C3B	3.73	131.66	124.68
24	G	605	CHL	C3B-C4B-NB	3.73	114.03	109.21
27	7	1622	XAT	C35-C34-C33	-3.72	122.00	127.31
28	N	1623	NEX	O24-C25-C38	3.72	119.52	115.06
25	C	509	CLA	CMB-C2B-C3B	3.72	131.64	124.68
26	7	1620	LUT	C35-C34-C33	-3.72	122.00	127.31
25	1	614	CLA	CMB-C2B-C3B	3.72	131.64	124.68
25	Y	602	CLA	CMB-C2B-C3B	3.72	131.63	124.68
26	3	1620	LUT	C35-C34-C33	-3.72	122.00	127.31
25	c	509	CLA	CMB-C2B-C3B	3.72	131.63	124.68
28	n	1623	NEX	O24-C25-C38	3.72	119.51	115.06
28	s	1623	NEX	C11-C10-C9	-3.72	122.00	127.31
24	r	607	CHL	CAC-C3C-C4C	3.72	129.63	124.81
26	1	1620	LUT	C35-C15-C14	-3.72	115.86	123.47
34	a	412	SQD	O5-C5-C4	3.71	116.43	109.69
26	5	1620	LUT	C35-C15-C14	-3.71	115.87	123.47
39	f	101	HEM	CMC-C2C-C3C	3.71	131.62	124.68
25	6	602	CLA	C4A-NA-C1A	3.71	108.37	106.71
25	y	602	CLA	CMB-C2B-C3B	3.70	131.61	124.68
25	g	610	CLA	CMB-C2B-C3B	3.70	131.61	124.68
25	4	610	CLA	CMB-C2B-C3B	3.70	131.60	124.68
39	F	101	HEM	CMC-C2C-C3C	3.70	131.60	124.68
27	1	1622	XAT	C6-C7-C8	-3.70	118.17	125.99
24	5	609	CHL	C3B-C4B-NB	3.70	113.99	109.21
25	R	601	CLA	CMB-C2B-C3B	3.70	131.60	124.68
24	G	606	CHL	CAC-C3C-C4C	3.70	129.61	124.81
30	b	620	BCR	C11-C10-C9	-3.70	122.03	127.31
25	2	604	CLA	C1B-CHB-C4A	-3.70	122.80	130.12
25	6	604	CLA	C1B-CHB-C4A	-3.70	122.80	130.12
27	5	1622	XAT	C6-C7-C8	-3.70	118.18	125.99
25	G	614	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
24	y	601	CHL	CMD-C2D-C3D	-3.69	119.11	127.61
34	A	418	SQD	O9-S-O7	-3.69	101.16	113.95
25	r	604	CLA	CMB-C2B-C3B	3.69	131.59	124.68
25	2	613	CLA	C1B-CHB-C4A	-3.69	122.81	130.12
25	g	614	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
25	r	601	CLA	CMB-C2B-C3B	3.69	131.58	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	3	1622	XAT	C35-C34-C33	-3.69	122.04	127.31
26	1	1620	LUT	C10-C11-C12	-3.69	111.70	123.22
24	1	609	CHL	C3B-C4B-NB	3.69	113.98	109.21
25	2	614	CLA	O2D-CGD-O1D	-3.69	116.63	123.84
25	8	610	CLA	CMB-C2B-C3B	3.69	131.58	124.68
25	G	610	CLA	CMB-C2B-C3B	3.69	131.58	124.68
34	a	418	SQD	O9-S-O7	-3.69	101.19	113.95
24	8	609	CHL	CHD-C4C-C3C	-3.68	119.42	124.84
30	B	620	BCR	C24-C23-C22	-3.68	120.67	126.23
25	2	602	CLA	C4A-NA-C1A	3.68	108.36	106.71
24	6	609	CHL	CAC-C3C-C4C	3.68	129.59	124.81
30	b	620	BCR	C24-C23-C22	-3.68	120.67	126.23
28	S	1623	NEX	C11-C10-C9	-3.68	122.05	127.31
26	5	1620	LUT	C10-C11-C12	-3.68	111.73	123.22
25	6	614	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
24	Y	601	CHL	CMD-C2D-C3D	-3.68	119.15	127.61
27	n	1622	XAT	O24-C25-C38	3.68	119.47	115.06
34	b	621	SQD	O47-C7-C8	3.68	119.43	111.50
25	R	604	CLA	CMB-C2B-C3B	3.68	131.56	124.68
25	1	604	CLA	C1B-CHB-C4A	-3.68	122.83	130.12
24	2	609	CHL	CAC-C3C-C4C	3.68	129.58	124.81
25	2	604	CLA	CMB-C2B-C3B	3.68	131.56	124.68
25	C	501	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
28	2	1623	NEX	O24-C25-C38	3.68	119.46	115.06
25	c	501	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
27	2	1622	XAT	C11-C10-C9	-3.68	122.06	127.31
28	s	1623	NEX	C35-C34-C33	-3.68	122.06	127.31
25	6	613	CLA	C1B-CHB-C4A	-3.67	122.84	130.12
34	B	621	SQD	O47-C7-C8	3.67	119.42	111.50
24	4	609	CHL	CAC-C3C-C4C	3.67	129.57	124.81
24	1	609	CHL	CMB-C2B-C3B	3.67	131.55	124.68
25	6	604	CLA	CMB-C2B-C3B	3.67	131.54	124.68
27	N	1622	XAT	O24-C25-C38	3.67	119.45	115.06
25	A	407	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
24	g	606	CHL	CAC-C3C-C4C	3.67	129.57	124.81
24	1	605	CHL	CHD-C4C-C3C	-3.67	119.45	124.84
28	R	623	NEX	C15-C35-C34	-3.67	115.96	123.47
26	1	1620	LUT	C15-C14-C13	-3.67	122.08	127.31
30	B	620	BCR	C11-C10-C9	-3.67	122.08	127.31
26	5	1620	LUT	C15-C14-C13	-3.66	122.08	127.31
25	5	604	CLA	C1B-CHB-C4A	-3.66	122.86	130.12
27	6	1622	XAT	C11-C10-C9	-3.66	122.09	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	407	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
24	5	609	CHL	CMB-C2B-C3B	3.66	131.52	124.68
24	5	601	CHL	CMD-C2D-C3D	-3.66	119.20	127.61
28	3	1623	NEX	C19-C9-C10	-3.66	117.80	122.92
34	a	412	SQD	C1-O5-C5	3.65	120.86	113.69
28	6	1623	NEX	O24-C25-C38	3.65	119.43	115.06
24	7	601	CHL	C1C-C2C-C3C	-3.65	104.22	107.11
24	Y	609	CHL	C3B-C4B-NB	3.65	113.93	109.21
24	1	601	CHL	CMD-C2D-C3D	-3.65	119.22	127.61
25	1	602	CLA	CMB-C2B-C3B	3.65	131.50	124.68
28	7	1623	NEX	C19-C9-C10	-3.65	117.81	122.92
24	s	607	CHL	CAC-C3C-C4C	3.65	129.54	124.81
25	g	610	CLA	C4A-NA-C1A	3.65	108.34	106.71
28	r	623	NEX	C15-C35-C34	-3.65	116.01	123.47
24	8	609	CHL	CAC-C3C-C4C	3.64	129.54	124.81
25	5	602	CLA	CMB-C2B-C3B	3.64	131.49	124.68
24	5	605	CHL	CHD-C4C-C3C	-3.64	119.49	124.84
28	1	1623	NEX	O24-C25-C38	3.64	119.42	115.06
25	n	614	CLA	CMB-C2B-C3B	3.64	131.48	124.68
25	2	614	CLA	C1B-CHB-C4A	-3.64	122.92	130.12
37	c	518	DGD	O6D-C1D-O3G	-3.63	101.37	109.97
24	S	607	CHL	CAC-C3C-C4C	3.63	129.53	124.81
24	y	609	CHL	C3B-C4B-NB	3.63	113.91	109.21
26	y	1620	LUT	C10-C11-C12	-3.63	111.88	123.22
26	Y	1620	LUT	C10-C11-C12	-3.63	111.88	123.22
28	S	1623	NEX	C35-C34-C33	-3.63	122.12	127.31
34	A	412	SQD	C1-O5-C5	3.63	120.82	113.69
24	5	607	CHL	CHB-C4A-NA	3.63	129.53	124.51
24	Y	607	CHL	CHB-C4A-NA	3.63	129.53	124.51
25	S	610	CLA	C1B-CHB-C4A	-3.63	122.93	130.12
24	y	607	CHL	CHB-C4A-NA	3.63	129.53	124.51
37	H	102	DGD	C1D-C2D-C3D	-3.63	102.44	110.00
24	7	607	CHL	CHD-C4C-C3C	-3.63	119.51	124.84
25	N	614	CLA	CMB-C2B-C3B	3.63	131.47	124.68
34	b	621	SQD	O7-S-C6	3.63	111.25	106.94
37	h	102	DGD	C1D-C2D-C3D	-3.63	102.44	110.00
25	5	613	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
37	C	518	DGD	O6D-C1D-O3G	-3.62	101.39	109.97
30	A	411	BCR	C16-C17-C18	-3.62	122.14	127.31
25	1	613	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
25	6	614	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
25	s	610	CLA	C1B-CHB-C4A	-3.62	122.95	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	601	CHL	CAC-C3C-C4C	3.62	129.51	124.81
25	b	605	CLA	CMB-C2B-C3B	3.62	131.45	124.68
25	r	611	CLA	C4A-NA-C1A	3.62	108.33	106.71
24	8	601	CHL	CAC-C3C-C4C	3.62	129.50	124.81
24	3	607	CHL	CHD-C4C-C3C	-3.62	119.52	124.84
24	6	601	CHL	C1C-C2C-C3C	-3.62	104.24	107.11
24	Y	607	CHL	CAC-C3C-C4C	3.62	129.50	124.81
25	A	406	CLA	CMB-C2B-C3B	3.62	131.44	124.68
30	a	411	BCR	C16-C17-C18	-3.61	122.15	127.31
24	5	607	CHL	CAC-C3C-C4C	3.61	129.50	124.81
24	3	601	CHL	C1C-C2C-C3C	-3.61	104.25	107.11
24	2	601	CHL	C1C-C2C-C3C	-3.61	104.25	107.11
24	1	607	CHL	CAC-C3C-C4C	3.61	129.50	124.81
25	y	610	CLA	CMB-C2B-C3B	3.61	131.43	124.68
27	r	622	XAT	C15-C14-C13	-3.61	122.16	127.31
27	4	622	XAT	O4-C5-C18	3.61	119.38	115.06
24	1	607	CHL	CHB-C4A-NA	3.61	129.50	124.51
24	1	601	CHL	CHD-C4C-C3C	-3.61	119.54	124.84
25	B	605	CLA	CMB-C2B-C3B	3.60	131.42	124.68
24	y	607	CHL	CAC-C3C-C4C	3.60	129.49	124.81
25	Y	610	CLA	CMB-C2B-C3B	3.60	131.42	124.68
25	a	406	CLA	CMB-C2B-C3B	3.60	131.42	124.68
28	5	1623	NEX	O24-C25-C38	3.60	119.37	115.06
25	C	507	CLA	CMB-C2B-C3B	3.60	131.41	124.68
26	7	1620	LUT	C16-C1-C6	-3.60	104.46	110.30
25	g	603	CLA	CBC-CAC-C3C	-3.60	102.51	112.43
25	s	613	CLA	CMB-C2B-C3B	3.60	131.41	124.68
27	Y	1622	XAT	C26-C27-C28	-3.60	118.39	125.99
25	G	603	CLA	CBC-CAC-C3C	-3.60	102.52	112.43
24	5	601	CHL	CHD-C4C-C3C	-3.60	119.56	124.84
25	1	611	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
27	N	1622	XAT	O4-C5-C18	3.59	119.36	115.06
24	1	601	CHL	CAC-C3C-C4C	3.59	129.47	124.81
25	c	505	CLA	C1B-CHB-C4A	-3.59	123.00	130.12
34	B	621	SQD	O7-S-C6	3.59	111.21	106.94
27	n	1622	XAT	O4-C5-C18	3.59	119.36	115.06
24	y	607	CHL	C3B-C4B-NB	3.59	113.85	109.21
30	b	619	BCR	C20-C21-C22	-3.59	122.19	127.31
25	c	507	CLA	CMB-C2B-C3B	3.59	131.39	124.68
26	3	1620	LUT	C16-C1-C6	-3.59	104.48	110.30
26	8	620	LUT	C31-C30-C29	-3.59	122.19	127.31
24	6	607	CHL	CAC-C3C-C4C	3.59	129.46	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	8	622	XAT	O4-C5-C18	3.59	119.35	115.06
25	5	611	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
27	R	622	XAT	C15-C14-C13	-3.58	122.20	127.31
24	2	607	CHL	CAC-C3C-C4C	3.58	129.46	124.81
27	8	622	XAT	C24-C23-C22	-3.58	103.86	110.77
26	Y	1620	LUT	C35-C15-C14	-3.58	116.14	123.47
30	B	619	BCR	C20-C21-C22	-3.58	122.20	127.31
30	B	618	BCR	C7-C8-C9	-3.58	120.82	126.23
24	5	601	CHL	CAC-C3C-C4C	3.58	129.46	124.81
26	4	620	LUT	C31-C30-C29	-3.58	122.20	127.31
25	C	513	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
25	y	611	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
26	g	1620	LUT	C30-C31-C32	-3.58	112.06	123.22
25	C	511	CLA	CMB-C2B-C3B	3.57	131.37	124.68
25	S	613	CLA	CMB-C2B-C3B	3.57	131.37	124.68
25	C	505	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
27	y	1622	XAT	C26-C27-C28	-3.57	118.44	125.99
24	Y	607	CHL	C3B-C4B-NB	3.57	113.83	109.21
26	G	1620	LUT	C30-C31-C32	-3.57	112.07	123.22
25	c	513	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
24	r	614	CHL	C1B-CHB-C4A	-3.57	123.05	130.12
28	1	1623	NEX	C15-C35-C34	-3.57	116.16	123.47
28	5	1623	NEX	C15-C35-C34	-3.57	116.16	123.47
24	R	614	CHL	C1B-CHB-C4A	-3.57	123.05	130.12
26	y	1620	LUT	C35-C15-C14	-3.57	116.16	123.47
25	n	603	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
27	1	1622	XAT	C4-C3-C2	-3.56	103.89	110.77
25	G	603	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
27	5	1622	XAT	C4-C3-C2	-3.56	103.89	110.77
25	R	603	CLA	CMB-C2B-C3B	3.56	131.34	124.68
24	8	608	CHL	C3B-C4B-NB	3.56	113.81	109.21
27	4	622	XAT	C24-C23-C22	-3.56	103.90	110.77
25	Y	611	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
30	b	620	BCR	C15-C14-C13	-3.56	122.23	127.31
25	r	603	CLA	CMB-C2B-C3B	3.55	131.33	124.68
25	c	511	CLA	CMB-C2B-C3B	3.55	131.33	124.68
25	G	610	CLA	C4A-NA-C1A	3.55	108.30	106.71
25	r	609	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	r	613	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	g	603	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	R	609	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
24	4	608	CHL	C3B-C4B-NB	3.54	113.79	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	618	BCR	C7-C8-C9	-3.54	120.88	126.23
34	a	412	SQD	O9-S-C6	3.54	111.15	106.94
34	A	412	SQD	O9-S-C6	3.54	111.14	106.94
24	S	606	CHL	CHD-C4C-C3C	-3.54	119.64	124.84
34	B	621	SQD	O9-S-O7	-3.54	101.71	113.95
25	b	602	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
26	G	1620	LUT	C35-C15-C14	-3.53	116.23	123.47
25	c	502	CLA	CMB-C2B-C3B	3.53	131.29	124.68
25	4	610	CLA	C1B-CHB-C4A	-3.53	123.12	130.12
25	8	610	CLA	C1B-CHB-C4A	-3.53	123.12	130.12
24	7	606	CHL	CHD-C4C-C3C	-3.53	119.65	124.84
34	b	621	SQD	O9-S-O7	-3.53	101.74	113.95
25	R	611	CLA	C4A-NA-C1A	3.53	108.29	106.71
25	N	603	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	R	613	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
24	7	605	CHL	C3B-C4B-NB	3.53	113.77	109.21
26	Y	1620	LUT	C15-C14-C13	-3.52	122.28	127.31
24	R	607	CHL	CHD-C4C-C3C	-3.52	119.66	124.84
25	r	610	CLA	CHB-C4A-NA	3.52	129.38	124.51
30	B	620	BCR	C15-C14-C13	-3.52	122.29	127.31
25	8	602	CLA	O2D-CGD-CBD	3.52	117.52	111.27
25	R	610	CLA	CHB-C4A-NA	3.52	129.38	124.51
34	a	412	SQD	O7-S-C6	3.52	111.12	106.94
24	s	606	CHL	CHD-C4C-C3C	-3.52	119.67	124.84
25	4	602	CLA	O2D-CGD-CBD	3.52	117.52	111.27
25	n	610	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
24	3	605	CHL	C3B-C4B-NB	3.51	113.75	109.21
26	g	1620	LUT	C35-C15-C14	-3.51	116.28	123.47
26	y	1620	LUT	C15-C14-C13	-3.51	122.30	127.31
25	Y	613	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
25	B	602	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
25	N	612	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
25	C	502	CLA	CMB-C2B-C3B	3.51	131.24	124.68
25	7	612	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
25	N	610	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
30	B	619	BCR	C39-C30-C25	-3.50	104.61	110.30
28	s	1623	NEX	C31-C30-C29	-3.50	122.31	127.31
24	r	607	CHL	CHD-C4C-C3C	-3.50	119.69	124.84
30	b	619	BCR	C39-C30-C25	-3.50	104.62	110.30
25	3	610	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
25	n	612	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
25	3	612	CLA	O2D-CGD-O1D	-3.50	117.00	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	604	CLA	CMB-C2B-C3B	3.50	131.22	124.68
34	A	412	SQD	O7-S-C6	3.50	111.09	106.94
28	S	1623	NEX	C31-C30-C29	-3.50	122.32	127.31
24	4	609	CHL	C3B-C4B-NB	3.50	113.73	109.21
24	g	606	CHL	CMB-C2B-C3B	3.50	131.22	124.68
25	g	612	CLA	CMB-C2B-C3B	3.50	131.22	124.68
25	B	608	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
24	8	609	CHL	C3B-C4B-NB	3.49	113.73	109.21
30	t	101	BCR	C1-C6-C7	3.49	125.66	115.78
26	5	1621	LUT	C19-C9-C8	3.49	123.58	118.08
26	G	1620	LUT	C15-C14-C13	-3.49	122.33	127.31
24	3	606	CHL	CHD-C4C-C3C	-3.49	119.71	124.84
30	T	101	BCR	C1-C6-C7	3.49	125.65	115.78
25	n	610	CLA	C4A-NA-C1A	3.49	108.27	106.71
25	y	613	CLA	C1B-CHB-C4A	-3.49	123.21	130.12
25	G	612	CLA	CMB-C2B-C3B	3.49	131.20	124.68
24	y	601	CHL	C1C-C2C-C3C	-3.49	104.35	107.11
26	1	1621	LUT	C19-C9-C8	3.49	123.57	118.08
24	g	601	CHL	C1C-C2C-C3C	-3.48	104.35	107.11
25	2	610	CLA	C1B-CHB-C4A	-3.48	123.22	130.12
25	G	613	CLA	C1B-CHB-C4A	-3.48	123.22	130.12
24	S	608	CHL	CHD-C4C-C3C	-3.48	119.72	124.84
28	N	1623	NEX	C39-C29-C30	-3.48	118.05	122.92
27	G	1622	XAT	C10-C11-C12	-3.48	112.35	123.22
30	T	101	BCR	C33-C5-C6	-3.48	120.62	124.53
24	5	607	CHL	CHD-C4C-C3C	-3.48	119.72	124.84
25	b	612	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
24	G	606	CHL	CMB-C2B-C3B	3.48	131.19	124.68
27	g	1622	XAT	C10-C11-C12	-3.48	112.36	123.22
26	s	1621	LUT	C10-C11-C12	-3.48	112.36	123.22
27	7	1622	XAT	C35-C15-C14	-3.48	116.35	123.47
26	S	1621	LUT	C10-C11-C12	-3.48	112.37	123.22
25	B	612	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
25	C	506	CLA	CMB-C2B-C3B	3.47	131.18	124.68
24	1	607	CHL	C3B-C4B-NB	3.47	113.70	109.21
26	g	1620	LUT	C15-C14-C13	-3.47	122.35	127.31
24	1	607	CHL	CHD-C4C-C3C	-3.47	119.74	124.84
25	N	604	CLA	C4A-NA-C1A	3.47	108.27	106.71
34	A	412	SQD	O47-C7-C8	3.47	118.98	111.50
25	c	506	CLA	CMB-C2B-C3B	3.47	131.17	124.68
24	Y	601	CHL	C1C-C2C-C3C	-3.47	104.36	107.11
25	7	610	CLA	C1B-CHB-C4A	-3.47	123.24	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	412	SQD	O47-C7-C8	3.47	118.98	111.50
25	6	610	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	g	613	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	B	613	CLA	CHB-C4A-NA	3.47	129.31	124.51
28	n	1623	NEX	C39-C29-C30	-3.47	118.06	122.92
30	t	101	BCR	C33-C5-C6	-3.47	120.63	124.53
25	b	608	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
26	N	1620	LUT	C35-C15-C14	-3.47	116.37	123.47
36	d	405	PL9	C7-C3-C2	-3.47	118.74	123.30
25	g	604	CLA	CMB-C2B-C3B	3.47	131.16	124.68
25	a	410	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
24	g	609	CHL	CAC-C3C-C4C	3.47	129.31	124.81
27	3	1622	XAT	C35-C15-C14	-3.47	116.38	123.47
24	s	608	CHL	CHD-C4C-C3C	-3.46	119.75	124.84
36	D	405	PL9	C7-C3-C2	-3.46	118.75	123.30
25	5	613	CLA	CMB-C2B-C3B	3.46	131.15	124.68
37	b	626	DGD	C3G-C2G-C1G	-3.46	103.61	111.79
25	1	613	CLA	CMB-C2B-C3B	3.46	131.15	124.68
24	G	601	CHL	C1C-C2C-C3C	-3.46	104.37	107.11
25	b	613	CLA	CHB-C4A-NA	3.46	129.29	124.51
25	s	611	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
26	n	1620	LUT	C35-C15-C14	-3.46	116.39	123.47
24	G	609	CHL	CAC-C3C-C4C	3.45	129.29	124.81
24	5	607	CHL	C3B-C4B-NB	3.45	113.67	109.21
25	S	611	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
28	2	1623	NEX	C11-C10-C9	-3.45	122.39	127.31
25	2	612	CLA	C1B-CHB-C4A	-3.45	123.29	130.12
30	B	618	BCR	C29-C28-C27	-3.44	103.68	111.38
25	6	612	CLA	C1B-CHB-C4A	-3.44	123.30	130.12
30	C	514	BCR	C10-C11-C12	-3.44	112.47	123.22
25	4	603	CLA	CMB-C2B-C3B	3.44	131.12	124.68
37	B	626	DGD	C3G-C2G-C1G	-3.44	103.65	111.79
24	y	601	CHL	C3B-C4B-NB	3.44	113.66	109.21
30	b	618	BCR	C29-C28-C27	-3.44	103.69	111.38
25	N	610	CLA	C4A-NA-C1A	3.44	108.25	106.71
25	8	602	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
25	3	603	CLA	CHB-C4A-NA	3.44	129.26	124.51
30	c	514	BCR	C10-C11-C12	-3.44	112.49	123.22
25	4	602	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
24	S	607	CHL	CHB-C4A-NA	3.44	129.26	124.51
25	7	603	CLA	CHB-C4A-NA	3.43	129.26	124.51
37	h	102	DGD	O2D-C2D-C3D	-3.43	102.41	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	H	102	DGD	O2D-C2D-C3D	-3.43	102.42	110.35
28	6	1623	NEX	C11-C10-C9	-3.43	122.42	127.31
26	S	1620	LUT	C15-C14-C13	-3.43	122.42	127.31
25	A	410	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
28	5	1623	NEX	C39-C29-C30	-3.42	118.13	122.92
25	7	610	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
25	8	603	CLA	CMB-C2B-C3B	3.42	131.08	124.68
24	Y	601	CHL	C3B-C4B-NB	3.42	113.63	109.21
28	G	1623	NEX	C39-C29-C30	-3.42	118.14	122.92
26	6	1620	LUT	C35-C34-C33	-3.42	122.43	127.31
24	s	607	CHL	CHB-C4A-NA	3.42	129.24	124.51
24	n	605	CHL	C3B-C4B-NB	3.41	113.62	109.21
25	r	610	CLA	CMB-C2B-C3B	3.41	131.07	124.68
26	2	1620	LUT	C35-C34-C33	-3.41	122.44	127.31
27	7	1622	XAT	O4-C5-C18	3.41	119.14	115.06
26	N	1621	LUT	C10-C11-C12	-3.41	112.57	123.22
25	4	604	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
25	R	610	CLA	CMB-C2B-C3B	3.41	131.06	124.68
25	8	604	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
25	3	610	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
25	n	604	CLA	C4A-NA-C1A	3.41	108.24	106.71
26	G	1621	LUT	C10-C11-C12	-3.41	112.58	123.22
24	r	614	CHL	CHD-C4C-C3C	-3.41	119.83	124.84
24	y	601	CHL	CHD-C4C-C3C	-3.41	119.83	124.84
24	S	601	CHL	CAC-C3C-C4C	3.41	129.23	124.81
24	s	601	CHL	CAC-C3C-C4C	3.41	129.23	124.81
25	7	604	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
24	3	609	CHL	C1B-CHB-C4A	-3.41	123.37	130.12
34	b	621	SQD	C1-O5-C5	3.41	120.37	113.69
25	C	507	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
25	3	613	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
28	1	1623	NEX	C39-C29-C30	-3.40	118.16	122.92
25	r	612	CLA	CAA-C2A-C3A	-3.40	103.46	112.78
26	s	1620	LUT	C15-C14-C13	-3.40	122.45	127.31
25	c	508	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
24	3	609	CHL	C3B-C4B-NB	3.40	113.61	109.21
27	3	1622	XAT	O4-C5-C18	3.40	119.13	115.06
25	3	604	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
24	7	609	CHL	C1B-CHB-C4A	-3.40	123.38	130.12
25	c	507	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
24	Y	601	CHL	CHD-C4C-C3C	-3.40	119.84	124.84
26	g	1621	LUT	C10-C11-C12	-3.40	112.61	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	608	CHL	C3B-C4B-NB	3.40	113.60	109.21
26	n	1621	LUT	C10-C11-C12	-3.40	112.62	123.22
27	g	1622	XAT	C15-C35-C34	-3.40	116.52	123.47
24	6	606	CHL	C3B-C4B-NB	3.40	113.60	109.21
25	c	507	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
34	B	621	SQD	C1-O5-C5	3.40	120.35	113.69
25	C	507	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
25	R	612	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
26	1	1621	LUT	C18-C5-C6	-3.39	120.72	124.53
24	2	601	CHL	CHD-C4C-C3C	-3.39	119.85	124.84
25	C	508	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
28	g	1623	NEX	C39-C29-C30	-3.39	118.17	122.92
24	R	614	CHL	CHD-C4C-C3C	-3.39	119.86	124.84
27	G	1622	XAT	C15-C35-C34	-3.39	116.53	123.47
25	6	614	CLA	CMB-C2B-C3B	3.39	131.02	124.68
26	n	1621	LUT	C7-C8-C9	-3.39	121.11	126.23
24	6	601	CHL	CHD-C4C-C3C	-3.39	119.86	124.84
24	6	601	CHL	CAC-C3C-C4C	3.39	129.21	124.81
25	5	612	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
24	2	601	CHL	CAC-C3C-C4C	3.39	129.21	124.81
26	N	1621	LUT	C7-C8-C9	-3.39	121.11	126.23
25	7	613	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
24	6	606	CHL	CHD-C4C-C3C	-3.39	119.86	124.84
24	3	608	CHL	CAC-C3C-C4C	3.39	129.20	124.81
25	B	603	CLA	CMB-C2B-C3B	3.39	131.01	124.68
25	B	604	CLA	CMB-C2B-C3B	3.39	131.01	124.68
26	3	1620	LUT	C11-C10-C9	-3.39	122.48	127.31
24	2	606	CHL	CHD-C4C-C3C	-3.38	119.86	124.84
24	G	608	CHL	C3B-C4B-NB	3.38	113.58	109.21
24	6	609	CHL	CHD-C4C-C3C	-3.38	119.87	124.84
24	2	606	CHL	C3B-C4B-NB	3.38	113.58	109.21
24	R	608	CHL	CAC-C3C-C4C	3.38	129.19	124.81
27	5	1622	XAT	O4-C5-C18	3.38	119.10	115.06
24	7	608	CHL	CAC-C3C-C4C	3.38	129.19	124.81
25	Y	611	CLA	C4A-NA-C1A	3.38	108.22	106.71
26	3	1621	LUT	C7-C8-C9	-3.38	121.13	126.23
25	2	614	CLA	CMB-C2B-C3B	3.38	130.99	124.68
26	g	1620	LUT	C16-C1-C6	-3.38	104.82	110.30
25	B	602	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
25	b	603	CLA	CMB-C2B-C3B	3.37	130.99	124.68
26	5	1621	LUT	C18-C5-C6	-3.37	120.74	124.53
30	B	618	BCR	C11-C10-C9	-3.37	122.50	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	604	CLA	CMB-C2B-C3B	3.37	130.99	124.68
25	C	503	CLA	CMB-C2B-C3B	3.37	130.98	124.68
25	C	501	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
25	y	604	CLA	C4A-NA-C1A	3.37	108.22	106.71
26	7	1621	LUT	C7-C8-C9	-3.37	121.15	126.23
24	2	609	CHL	CHD-C4C-C3C	-3.37	119.89	124.84
24	N	605	CHL	C3B-C4B-NB	3.37	113.56	109.21
25	1	612	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
28	5	1623	NEX	C11-C10-C9	-3.37	122.51	127.31
25	S	609	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
25	y	611	CLA	C4A-NA-C1A	3.37	108.22	106.71
24	N	608	CHL	CAC-C3C-C4C	3.36	129.18	124.81
34	A	418	SQD	C45-O47-C7	3.36	126.07	117.79
25	S	609	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
26	7	1620	LUT	C11-C10-C9	-3.36	122.51	127.31
28	7	1623	NEX	C39-C29-C30	-3.36	118.21	122.92
26	G	1620	LUT	C16-C1-C6	-3.36	104.85	110.30
24	G	601	CHL	C3B-C4B-NB	3.36	113.56	109.21
25	b	602	CLA	C1B-CHB-C4A	-3.36	123.46	130.12
24	r	608	CHL	CAC-C3C-C4C	3.36	129.17	124.81
34	a	418	SQD	C45-O47-C7	3.36	126.05	117.79
24	7	609	CHL	C3B-C4B-NB	3.36	113.55	109.21
24	g	601	CHL	C3B-C4B-NB	3.35	113.55	109.21
28	2	1623	NEX	C39-C29-C30	-3.35	118.22	122.92
25	b	617	CLA	CMB-C2B-C3B	3.35	130.95	124.68
25	c	501	CLA	C1B-CHB-C4A	-3.35	123.47	130.12
27	1	1622	XAT	O4-C5-C18	3.35	119.07	115.06
28	1	1623	NEX	C11-C10-C9	-3.35	122.53	127.31
25	C	512	CLA	CMB-C2B-C3B	3.35	130.95	124.68
25	s	609	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
34	B	621	SQD	O5-C5-C4	3.35	115.78	109.69
25	c	512	CLA	CMB-C2B-C3B	3.35	130.94	124.68
25	B	617	CLA	CMB-C2B-C3B	3.35	130.94	124.68
24	N	605	CHL	CAC-C3C-C4C	3.35	129.16	124.81
24	N	607	CHL	CAC-C3C-C4C	3.35	129.16	124.81
25	c	503	CLA	CMB-C2B-C3B	3.35	130.94	124.68
25	s	609	CLA	C1B-CHB-C4A	-3.35	123.49	130.12
24	Y	605	CHL	CAC-C3C-C4C	3.35	129.15	124.81
24	n	607	CHL	CAC-C3C-C4C	3.34	129.15	124.81
24	R	607	CHL	C3B-C4B-NB	3.34	113.53	109.21
28	3	1623	NEX	C39-C29-C30	-3.34	118.24	122.92
34	b	621	SQD	O5-C5-C4	3.34	115.77	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	606	CLA	CHB-C4A-NA	3.34	129.13	124.51
24	n	605	CHL	CAC-C3C-C4C	3.34	129.15	124.81
30	b	618	BCR	C11-C10-C9	-3.34	122.54	127.31
24	3	601	CHL	CMD-C2D-C3D	-3.34	119.93	127.61
25	B	604	CLA	C1B-CHB-C4A	-3.34	123.50	130.12
25	b	604	CLA	C4A-NA-C1A	3.34	108.21	106.71
25	G	604	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
30	B	618	BCR	C28-C27-C26	-3.34	108.12	114.08
30	4	623	BCR	C11-C12-C13	-3.34	117.05	126.42
25	b	607	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
24	n	608	CHL	CAC-C3C-C4C	3.33	129.14	124.81
25	b	604	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
30	d	404	BCR	C21-C20-C19	-3.33	112.81	123.22
27	6	1622	XAT	O4-C5-C18	3.33	119.05	115.06
30	b	618	BCR	C28-C27-C26	-3.33	108.13	114.08
28	6	1623	NEX	C39-C29-C30	-3.33	118.26	122.92
25	G	603	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
24	N	601	CHL	C1C-C2C-C3C	-3.33	104.47	107.11
27	2	1622	XAT	O4-C5-C18	3.33	119.05	115.06
37	c	519	DGD	O6D-C1D-O3G	-3.33	102.09	109.97
25	g	603	CLA	CAA-C2A-C3A	-3.33	103.67	112.78
30	8	623	BCR	C11-C12-C13	-3.33	117.07	126.42
25	g	604	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
25	y	604	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
25	B	605	CLA	C2D-C1D-ND	-3.33	107.65	110.10
25	B	607	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
30	t	101	BCR	C15-C14-C13	-3.33	122.56	127.31
30	T	101	BCR	C15-C14-C13	-3.32	122.56	127.31
26	5	1620	LUT	C30-C31-C32	-3.32	112.84	123.22
25	g	610	CLA	C1B-CHB-C4A	-3.32	123.53	130.12
25	b	606	CLA	C1B-CHB-C4A	-3.32	123.53	130.12
26	N	1620	LUT	C15-C14-C13	-3.32	122.57	127.31
37	C	519	DGD	O6D-C1D-O3G	-3.32	102.10	109.97
26	1	1620	LUT	C30-C31-C32	-3.32	112.85	123.22
30	D	404	BCR	C21-C20-C19	-3.32	112.86	123.22
24	7	601	CHL	CMD-C2D-C3D	-3.32	119.98	127.61
26	3	1620	LUT	C21-C26-C27	-3.32	108.50	112.70
26	3	1621	LUT	C35-C34-C33	-3.32	122.57	127.31
24	r	607	CHL	C3B-C4B-NB	3.32	113.50	109.21
25	Y	611	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
25	R	601	CLA	C4A-NA-C1A	3.32	108.20	106.71
25	Y	604	CLA	C4A-NA-C1A	3.32	108.20	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	608	CHL	CAC-C3C-C4C	3.32	129.11	124.81
30	b	620	BCR	C33-C5-C4	3.32	119.99	113.62
27	N	1622	XAT	C10-C11-C12	-3.32	112.87	123.22
25	6	611	CLA	CMB-C2B-C3B	3.32	130.88	124.68
25	B	606	CLA	CHB-C4A-NA	3.32	129.10	124.51
25	G	610	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
25	Y	604	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
24	n	601	CHL	C1C-C2C-C3C	-3.31	104.48	107.11
26	r	620	LUT	C30-C31-C32	-3.31	112.87	123.22
24	y	605	CHL	CAC-C3C-C4C	3.31	129.11	124.81
26	R	620	LUT	C30-C31-C32	-3.31	112.88	123.22
25	2	611	CLA	CMB-C2B-C3B	3.31	130.88	124.68
30	c	515	BCR	C16-C17-C18	-3.31	122.58	127.31
27	Y	1622	XAT	C24-C23-C22	-3.31	104.38	110.77
27	n	1622	XAT	C10-C11-C12	-3.31	112.89	123.22
26	n	1620	LUT	C15-C14-C13	-3.31	122.59	127.31
30	c	515	BCR	C15-C16-C17	-3.31	116.70	123.47
25	2	613	CLA	C4A-NA-C1A	3.31	108.19	106.71
24	r	614	CHL	CAC-C3C-C4C	3.31	129.10	124.81
25	n	604	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
25	y	611	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
26	y	1621	LUT	C10-C11-C12	-3.31	112.90	123.22
30	C	515	BCR	C16-C17-C18	-3.31	122.59	127.31
25	R	612	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	r	612	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
27	y	1622	XAT	C24-C23-C22	-3.30	104.39	110.77
26	3	1620	LUT	C35-C15-C14	-3.30	116.71	123.47
30	b	618	BCR	C15-C16-C17	-3.30	116.71	123.47
25	B	606	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
26	7	1620	LUT	C35-C15-C14	-3.30	116.71	123.47
25	b	615	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
26	Y	1621	LUT	C10-C11-C12	-3.30	112.91	123.22
25	B	617	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
24	1	601	CHL	C1C-C2C-C3C	-3.30	104.50	107.11
25	N	604	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
26	7	1620	LUT	C21-C26-C27	-3.30	108.53	112.70
24	2	606	CHL	CAC-C3C-C4C	3.30	129.09	124.81
24	2	609	CHL	C3B-C4B-NB	3.30	113.47	109.21
25	b	617	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
30	B	620	BCR	C33-C5-C4	3.30	119.95	113.62
24	5	607	CHL	CMD-C2D-C3D	-3.29	120.03	127.61
25	B	604	CLA	C4A-NA-C1A	3.29	108.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	6	613	CLA	C4A-NA-C1A	3.29	108.19	106.71
25	n	603	CLA	CAA-C2A-C3A	-3.29	103.76	112.78
30	C	515	BCR	C15-C16-C17	-3.29	116.73	123.47
24	1	607	CHL	CMD-C2D-C3D	-3.29	120.05	127.61
24	7	601	CHL	C3B-C4B-NB	3.29	113.46	109.21
30	B	618	BCR	C15-C16-C17	-3.29	116.74	123.47
35	d	411	LMG	C1-C2-C3	-3.29	103.15	110.00
24	6	606	CHL	CAC-C3C-C4C	3.29	129.07	124.81
25	N	603	CLA	CAA-C2A-C3A	-3.29	103.78	112.78
35	D	411	LMG	C1-C2-C3	-3.29	103.15	110.00
25	b	605	CLA	C2D-C1D-ND	-3.29	107.68	110.10
24	s	608	CHL	CAC-C3C-C4C	3.28	129.07	124.81
26	7	1621	LUT	C35-C34-C33	-3.28	122.62	127.31
25	B	615	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
25	2	612	CLA	CAA-C2A-C3A	-3.28	103.79	112.78
28	6	1623	NEX	C24-C23-C22	-3.28	104.44	110.77
24	5	601	CHL	C1C-C2C-C3C	-3.28	104.51	107.11
24	N	608	CHL	C3B-C4B-NB	3.28	113.45	109.21
30	t	101	BCR	C1-C6-C5	-3.28	118.00	122.61
24	r	608	CHL	C3B-C4B-NB	3.28	113.44	109.21
26	8	620	LUT	C11-C10-C9	-3.28	122.64	127.31
25	6	612	CLA	CAA-C2A-C3A	-3.27	103.81	112.78
24	y	609	CHL	C1C-C2C-C3C	-3.27	104.52	107.11
30	T	101	BCR	C1-C6-C5	-3.27	118.00	122.61
24	R	614	CHL	CAC-C3C-C4C	3.27	129.05	124.81
25	7	614	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
24	g	605	CHL	CAC-C3C-C4C	3.27	129.05	124.81
36	a	414	PL9	O2-C1-C2	-3.27	116.74	121.41
28	2	1623	NEX	C24-C23-C22	-3.26	104.47	110.77
24	Y	609	CHL	C1C-C2C-C3C	-3.26	104.53	107.11
26	n	1620	LUT	C21-C26-C27	-3.26	108.58	112.70
26	4	620	LUT	C11-C10-C9	-3.26	122.66	127.31
24	G	605	CHL	CAC-C3C-C4C	3.26	129.04	124.81
25	b	611	CLA	CMB-C2B-C3B	3.26	130.78	124.68
25	B	611	CLA	CMB-C2B-C3B	3.26	130.78	124.68
25	s	610	CLA	C4A-NA-C1A	3.26	108.17	106.71
24	R	608	CHL	C3B-C4B-NB	3.26	113.42	109.21
25	r	602	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
25	2	603	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
24	n	608	CHL	C3B-C4B-NB	3.25	113.42	109.21
28	1	1623	NEX	C24-C23-C22	-3.25	104.49	110.77
26	1	1621	LUT	C15-C35-C34	-3.25	116.81	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	608	CHL	C3B-C4B-NB	3.25	113.42	109.21
25	1	614	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
28	5	1623	NEX	C24-C23-C22	-3.25	104.49	110.77
25	A	410	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
26	3	1620	LUT	C15-C14-C13	-3.25	122.67	127.31
25	S	610	CLA	C4A-NA-C1A	3.25	108.17	106.71
25	R	602	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
26	7	1620	LUT	C15-C14-C13	-3.25	122.67	127.31
24	G	607	CHL	C3B-C4B-NB	3.25	113.41	109.21
25	5	614	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
30	B	619	BCR	C15-C16-C17	-3.25	116.82	123.47
30	b	619	BCR	C15-C16-C17	-3.25	116.82	123.47
24	n	607	CHL	CAA-C2A-C3A	-3.25	103.88	112.78
26	N	1620	LUT	C21-C26-C27	-3.25	108.59	112.70
24	N	607	CHL	CAA-C2A-C3A	-3.25	103.88	112.78
24	5	605	CHL	OMC-CMC-C2C	-3.25	118.34	125.69
24	6	609	CHL	C3B-C4B-NB	3.25	113.41	109.21
25	3	603	CLA	CBC-CAC-C3C	-3.25	103.48	112.43
30	b	619	BCR	C24-C23-C22	-3.25	121.33	126.23
25	3	614	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
26	5	1621	LUT	C15-C35-C34	-3.24	116.83	123.47
24	3	601	CHL	C3B-C4B-NB	3.24	113.41	109.21
25	7	603	CLA	CBC-CAC-C3C	-3.24	103.49	112.43
25	C	506	CLA	C1B-CHB-C4A	-3.24	123.69	130.12
24	4	609	CHL	CMD-C2D-C3D	-3.24	120.15	127.61
25	6	603	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
25	b	609	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
25	c	506	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
25	a	410	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
25	6	611	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
25	2	611	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
25	S	603	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
25	a	406	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
24	n	606	CHL	C3B-C4B-NB	3.23	113.39	109.21
24	5	608	CHL	CAC-C3C-C4C	3.23	129.01	124.81
25	G	611	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
24	Y	608	CHL	C3B-C4B-NB	3.23	113.39	109.21
36	A	414	PL9	O2-C1-C2	-3.23	116.79	121.41
24	1	605	CHL	OMC-CMC-C2C	-3.23	118.39	125.69
24	8	609	CHL	CMD-C2D-C3D	-3.23	120.19	127.61
25	B	609	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
25	r	601	CLA	C1B-CHB-C4A	-3.23	123.73	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	1622	XAT	O24-C25-C38	3.22	118.92	115.06
24	2	605	CHL	C1B-CHB-C4A	-3.22	123.73	130.12
25	4	612	CLA	CAA-C2A-C3A	-3.22	103.95	112.78
30	c	517	BCR	C15-C16-C17	-3.22	116.87	123.47
25	Y	613	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	r	613	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
30	C	517	BCR	C15-C16-C17	-3.22	116.88	123.47
25	G	614	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	R	601	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
24	6	608	CHL	C3B-C4B-NB	3.22	113.37	109.21
25	g	611	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
24	N	606	CHL	C3B-C4B-NB	3.22	113.37	109.21
24	1	608	CHL	CAC-C3C-C4C	3.22	128.99	124.81
26	N	1620	LUT	C16-C1-C6	-3.22	105.08	110.30
25	C	501	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
25	c	501	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
26	n	1620	LUT	C16-C1-C6	-3.22	105.08	110.30
26	n	1620	LUT	C10-C11-C12	-3.22	113.18	123.22
25	y	613	CLA	CMB-C2B-C3B	3.22	130.70	124.68
24	g	607	CHL	C3B-C4B-NB	3.22	113.37	109.21
27	5	1622	XAT	O24-C25-C38	3.22	118.91	115.06
34	B	623	SQD	O7-S-C6	3.22	110.76	106.94
24	y	608	CHL	C3B-C4B-NB	3.21	113.37	109.21
24	g	601	CHL	CMD-C2D-C3D	-3.21	120.22	127.61
25	A	406	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
25	8	612	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
30	B	619	BCR	C24-C23-C22	-3.21	121.38	126.23
24	G	601	CHL	CMD-C2D-C3D	-3.21	120.22	127.61
26	N	1620	LUT	C10-C11-C12	-3.21	113.19	123.22
25	y	604	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
25	g	614	CLA	CMB-C2B-C3B	3.21	130.69	124.68
25	R	613	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
24	6	605	CHL	C1B-CHB-C4A	-3.21	123.76	130.12
25	s	603	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
30	A	411	BCR	C33-C5-C6	-3.21	120.92	124.53
27	g	1622	XAT	C24-C23-C22	-3.21	104.58	110.77
25	Y	604	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
25	s	602	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
25	a	410	CLA	CMB-C2B-C3B	3.21	130.68	124.68
34	b	623	SQD	O7-S-C6	3.21	110.75	106.94
25	3	603	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
28	N	1623	NEX	C24-C23-C22	-3.20	104.59	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	1620	LUT	C31-C30-C29	-3.20	122.74	127.31
24	1	601	CHL	C3B-C4B-NB	3.20	113.35	109.21
25	2	613	CLA	CMB-C2B-C3B	3.20	130.67	124.68
26	y	1621	LUT	C7-C8-C9	-3.20	121.40	126.23
27	7	1622	XAT	C30-C31-C32	-3.20	113.23	123.22
25	S	602	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
25	2	603	CLA	CHB-C4A-NA	3.20	128.94	124.51
24	1	605	CHL	C3B-C4B-NB	3.20	113.34	109.21
25	c	504	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
26	5	1620	LUT	C31-C30-C29	-3.20	122.75	127.31
25	7	603	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
25	r	611	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
28	n	1623	NEX	C24-C23-C22	-3.20	104.60	110.77
25	R	611	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
25	6	613	CLA	CMB-C2B-C3B	3.19	130.65	124.68
27	Y	1622	XAT	C35-C34-C33	-3.19	122.75	127.31
30	a	411	BCR	C33-C5-C6	-3.19	120.94	124.53
26	1	1621	LUT	C10-C11-C12	-3.19	113.25	123.22
25	Y	610	CLA	C4A-NA-C1A	3.19	108.14	106.71
25	6	603	CLA	CHB-C4A-NA	3.19	128.93	124.51
26	5	1621	LUT	C10-C11-C12	-3.19	113.26	123.22
25	G	614	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
25	r	611	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
34	A	418	SQD	O6-C1-C2	3.19	113.28	108.30
24	5	601	CHL	C3B-C4B-NB	3.19	113.33	109.21
24	g	609	CHL	CHD-C4C-C3C	-3.19	120.16	124.84
25	3	611	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
25	A	410	CLA	CMB-C2B-C3B	3.18	130.63	124.68
24	6	607	CHL	C3B-C4B-NB	3.18	113.33	109.21
24	1	607	CHL	OMC-CMC-C2C	-3.18	118.49	125.69
26	Y	1621	LUT	C7-C8-C9	-3.18	121.43	126.23
30	C	514	BCR	C15-C16-C17	-3.18	116.95	123.47
24	2	601	CHL	C3B-C4B-NB	3.18	113.32	109.21
27	G	1622	XAT	C24-C23-C22	-3.18	104.63	110.77
27	3	1622	XAT	C30-C31-C32	-3.18	113.29	123.22
30	c	514	BCR	C15-C16-C17	-3.18	116.96	123.47
24	6	601	CHL	C3B-C4B-NB	3.18	113.32	109.21
24	G	609	CHL	CHD-C4C-C3C	-3.18	120.17	124.84
25	R	611	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
27	y	1622	XAT	C35-C34-C33	-3.18	122.78	127.31
25	4	611	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
25	C	508	CLA	O2D-CGD-O1D	-3.18	117.63	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	1620	LUT	C35-C15-C14	-3.18	116.97	123.47
24	R	614	CHL	CMD-C2D-C3D	-3.17	120.31	127.61
24	Y	607	CHL	CMB-C2B-C3B	3.17	130.62	124.68
25	7	611	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
25	C	504	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
30	b	619	BCR	C8-C7-C6	-3.17	118.29	127.20
30	B	619	BCR	C8-C7-C6	-3.17	118.30	127.20
28	5	1623	NEX	C15-C14-C13	-3.17	122.79	127.31
24	5	607	CHL	OMC-CMC-C2C	-3.17	118.52	125.69
25	Y	612	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
25	y	610	CLA	C4A-NA-C1A	3.17	108.13	106.71
34	a	418	SQD	O6-C1-C2	3.16	113.24	108.30
25	r	601	CLA	C4A-NA-C1A	3.16	108.13	106.71
24	2	607	CHL	C3B-C4B-NB	3.16	113.30	109.21
24	6	608	CHL	CHB-C4A-NA	3.16	128.88	124.51
24	5	605	CHL	C3B-C4B-NB	3.16	113.30	109.21
24	g	606	CHL	C3B-C4B-NB	3.16	113.30	109.21
24	y	607	CHL	CMB-C2B-C3B	3.16	130.59	124.68
33	a	408	PHO	O1D-CGD-CBD	3.16	130.00	124.74
28	Y	1623	NEX	C24-C23-C22	-3.16	104.67	110.77
25	8	611	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
24	r	614	CHL	CMD-C2D-C3D	-3.16	120.34	127.61
24	n	606	CHL	CMB-C2B-C3B	3.16	130.59	124.68
28	N	1623	NEX	C26-C27-C28	-3.16	119.31	125.99
37	b	626	DGD	O6D-C1D-O3G	-3.16	102.49	109.97
37	B	626	DGD	O6D-C1D-O3G	-3.16	102.49	109.97
26	s	1620	LUT	C35-C15-C14	-3.16	117.00	123.47
24	3	609	CHL	C1C-C2C-C3C	-3.16	104.61	107.11
26	7	1620	LUT	C30-C31-C32	-3.16	113.36	123.22
28	y	1623	NEX	C24-C23-C22	-3.16	104.68	110.77
25	R	610	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
28	1	1623	NEX	C15-C14-C13	-3.16	122.81	127.31
25	1	612	CLA	CMB-C2B-C3B	3.15	130.58	124.68
30	b	618	BCR	C20-C21-C22	-3.15	122.81	127.31
37	H	102	DGD	O3E-C3E-C2E	-3.15	103.06	110.35
28	n	1623	NEX	C26-C27-C28	-3.15	119.33	125.99
25	y	603	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
24	G	606	CHL	C3B-C4B-NB	3.15	113.29	109.21
25	g	614	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
27	N	1622	XAT	C24-C23-C22	-3.15	104.69	110.77
24	2	608	CHL	CHB-C4A-NA	3.15	128.87	124.51
25	c	508	CLA	O2D-CGD-O1D	-3.15	117.68	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	613	CLA	CMD-C2D-C1D	-3.15	119.16	124.71
25	n	603	CLA	CBC-CAC-C3C	-3.15	103.75	112.43
26	r	620	LUT	C39-C29-C28	3.15	123.04	118.08
27	n	1622	XAT	C24-C23-C22	-3.15	104.70	110.77
24	7	609	CHL	C1C-C2C-C3C	-3.15	104.62	107.11
33	A	408	PHO	O1D-CGD-CBD	3.15	129.98	124.74
26	y	1621	LUT	C21-C26-C27	-3.15	108.72	112.70
25	D	403	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
30	B	618	BCR	C3-C4-C5	-3.15	108.46	114.08
25	d	403	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
26	R	620	LUT	C39-C29-C28	3.14	123.03	118.08
25	5	612	CLA	CMB-C2B-C3B	3.14	130.56	124.68
37	h	102	DGD	O3E-C3E-C2E	-3.14	103.08	110.35
26	3	1620	LUT	C30-C31-C32	-3.14	113.41	123.22
28	n	1623	NEX	C16-C1-C6	3.14	113.28	110.47
24	N	606	CHL	CMB-C2B-C3B	3.14	130.56	124.68
25	y	612	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
30	b	618	BCR	C3-C4-C5	-3.14	108.47	114.08
25	c	505	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	r	604	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
25	r	610	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	N	603	CLA	CBC-CAC-C3C	-3.14	103.78	112.43
25	B	611	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
24	r	614	CHL	O2D-CGD-O1D	-3.14	117.70	123.84
24	Y	601	CHL	C4-C3-C5	3.14	120.55	115.27
27	4	622	XAT	C10-C11-C12	-3.14	113.43	123.22
25	Y	603	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
24	y	601	CHL	C4-C3-C5	3.13	120.54	115.27
24	R	607	CHL	O2A-CGA-CBA	3.13	121.74	111.91
26	Y	1621	LUT	C21-C26-C27	-3.13	108.74	112.70
25	4	604	CLA	CMB-C2B-C3B	3.13	130.54	124.68
24	G	609	CHL	CHB-C4A-NA	3.13	128.84	124.51
25	b	611	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
30	B	618	BCR	C20-C21-C22	-3.13	122.84	127.31
24	R	607	CHL	CMD-C2D-C3D	-3.13	120.41	127.61
24	r	607	CHL	CMD-C2D-C3D	-3.13	120.41	127.61
24	r	607	CHL	O2A-CGA-CBA	3.13	121.73	111.91
25	C	505	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
27	8	622	XAT	C10-C11-C12	-3.13	113.45	123.22
25	R	604	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
24	R	614	CHL	O2D-CGD-O1D	-3.13	117.72	123.84
28	N	1623	NEX	C16-C1-C6	3.13	113.27	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	601	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
25	8	604	CLA	CMB-C2B-C3B	3.12	130.52	124.68
30	c	515	BCR	C37-C22-C23	3.12	123.00	118.08
26	G	1621	LUT	C39-C29-C28	3.12	123.00	118.08
24	g	609	CHL	CHB-C4A-NA	3.12	128.83	124.51
25	A	407	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	b	613	CLA	CMD-C2D-C1D	-3.12	119.21	124.71
25	2	611	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	a	407	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
26	Y	1620	LUT	C30-C31-C32	-3.12	113.48	123.22
25	B	603	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
24	2	605	CHL	C3B-C4B-NB	3.12	113.24	109.21
26	S	1620	LUT	C11-C10-C9	-3.12	122.86	127.31
24	1	605	CHL	CAC-C3C-C4C	3.12	128.85	124.81
34	A	418	SQD	O8-S-C6	3.12	110.70	105.74
24	6	605	CHL	C3B-C4B-NB	3.12	113.24	109.21
26	3	1620	LUT	C22-C23-C24	3.11	115.28	111.74
28	6	1623	NEX	C35-C34-C33	-3.11	122.87	127.31
29	D	408	LHG	O8-C23-C24	3.11	121.68	111.91
25	2	603	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
25	6	603	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
25	b	603	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
34	a	418	SQD	O8-S-C6	3.11	110.70	105.74
25	N	612	CLA	CHB-C4A-NA	3.11	128.81	124.51
26	y	1620	LUT	C30-C31-C32	-3.11	113.51	123.22
30	C	515	BCR	C37-C22-C23	3.11	122.98	118.08
24	n	601	CHL	CHD-C4C-C3C	-3.11	120.27	124.84
37	b	626	DGD	O3G-C3G-C2G	-3.11	103.40	110.90
25	S	609	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
26	n	1620	LUT	C30-C31-C32	-3.11	113.53	123.22
25	s	609	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
25	6	611	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
26	g	1620	LUT	C21-C26-C27	-3.10	108.78	112.70
26	g	1621	LUT	C39-C29-C28	3.10	122.97	118.08
26	N	1620	LUT	C30-C31-C32	-3.10	113.54	123.22
25	C	509	CLA	CHB-C4A-NA	3.10	128.80	124.51
26	7	1620	LUT	C22-C23-C24	3.10	115.27	111.74
26	r	620	LUT	C18-C5-C6	-3.10	121.05	124.53
29	d	408	LHG	O8-C23-C24	3.10	121.63	111.91
25	G	603	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
24	5	606	CHL	C3B-C4B-NB	3.10	113.21	109.21
24	8	607	CHL	C3B-C4B-NB	3.10	113.21	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	605	CHL	CAC-C3C-C4C	3.10	128.83	124.81
25	c	509	CLA	CHB-C4A-NA	3.10	128.79	124.51
25	n	612	CLA	CHB-C4A-NA	3.10	128.79	124.51
26	s	1620	LUT	C11-C10-C9	-3.10	122.89	127.31
30	D	404	BCR	C16-C17-C18	-3.09	122.89	127.31
24	4	607	CHL	C1B-CHB-C4A	-3.09	123.99	130.12
25	g	603	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
26	s	1621	LUT	C17-C1-C6	3.09	115.32	110.30
25	Y	614	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
30	d	404	BCR	C16-C17-C18	-3.09	122.90	127.31
37	B	626	DGD	O3G-C3G-C2G	-3.09	103.45	110.90
37	h	102	DGD	O3G-C3G-C2G	-3.09	103.45	110.90
28	2	1623	NEX	C35-C34-C33	-3.09	122.91	127.31
37	H	102	DGD	O3G-C3G-C2G	-3.09	103.45	110.90
26	G	1620	LUT	C21-C26-C27	-3.08	108.80	112.70
27	g	1622	XAT	C18-C5-C4	3.08	117.75	114.28
25	7	610	CLA	CMB-C2B-C3B	3.08	130.44	124.68
27	G	1622	XAT	C18-C5-C4	3.08	117.75	114.28
25	4	604	CLA	CHB-C4A-NA	3.08	128.77	124.51
25	b	607	CLA	CMB-C2B-C3B	3.08	130.44	124.68
25	y	612	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
27	1	1622	XAT	C35-C34-C33	-3.08	122.92	127.31
24	4	607	CHL	C3B-C4B-NB	3.08	113.19	109.21
30	C	514	BCR	C21-C20-C19	-3.08	113.61	123.22
25	s	609	CLA	C4A-NA-C1A	3.08	108.09	106.71
30	c	514	BCR	C21-C20-C19	-3.08	113.61	123.22
25	N	614	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
34	a	418	SQD	C4-C3-C2	3.08	116.19	110.82
24	1	609	CHL	C1C-C2C-C3C	-3.08	104.67	107.11
26	r	620	LUT	C15-C35-C34	-3.07	117.17	123.47
26	R	620	LUT	C15-C35-C34	-3.07	117.18	123.47
26	S	1621	LUT	C17-C1-C6	3.07	115.28	110.30
25	n	614	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	y	614	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	Y	612	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
28	r	623	NEX	C24-C23-C22	-3.07	104.84	110.77
24	8	607	CHL	C1B-CHB-C4A	-3.07	124.04	130.12
24	s	601	CHL	CHB-C4A-NA	3.07	128.76	124.51
25	8	604	CLA	CHB-C4A-NA	3.07	128.76	124.51
25	7	603	CLA	CMB-C2B-C3B	3.07	130.42	124.68
24	S	608	CHL	C1B-CHB-C4A	-3.07	124.04	130.12
25	y	612	CLA	C1B-CHB-C4A	-3.07	124.04	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	1622	XAT	C7-C8-C9	-3.07	120.77	125.53
28	y	1623	NEX	C39-C29-C30	-3.07	118.63	122.92
28	R	623	NEX	C24-C23-C22	-3.07	104.85	110.77
25	3	610	CLA	CMB-C2B-C3B	3.07	130.41	124.68
25	Y	612	CLA	C1B-CHB-C4A	-3.07	124.05	130.12
25	N	614	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
27	G	1622	XAT	C11-C10-C9	-3.06	122.94	127.31
24	g	601	CHL	CHD-C4C-C3C	-3.06	120.34	124.84
24	4	609	CHL	OMC-CMC-C2C	-3.06	118.76	125.69
24	S	601	CHL	CHB-C4A-NA	3.06	128.75	124.51
24	y	609	CHL	CMD-C2D-C3D	-3.06	120.57	127.61
25	S	614	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
27	g	1622	XAT	C11-C10-C9	-3.06	122.94	127.31
24	7	609	CHL	CMD-C2D-C3D	-3.06	120.57	127.61
25	S	609	CLA	C4A-NA-C1A	3.06	108.08	106.71
24	R	606	CHL	CMD-C2D-C3D	-3.06	120.57	127.61
24	1	606	CHL	C3B-C4B-NB	3.06	113.17	109.21
24	Y	609	CHL	CMD-C2D-C3D	-3.06	120.58	127.61
25	B	607	CLA	CAA-CBA-CGA	-3.06	104.31	113.25
24	8	609	CHL	OMC-CMC-C2C	-3.06	118.77	125.69
25	3	612	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
24	r	606	CHL	C3B-C4B-NB	3.06	113.16	109.21
25	B	607	CLA	CMB-C2B-C3B	3.06	130.40	124.68
34	A	418	SQD	C4-C3-C2	3.06	116.16	110.82
30	B	620	BCR	C1-C6-C5	-3.06	118.31	122.61
24	3	609	CHL	CMD-C2D-C3D	-3.06	120.59	127.61
25	3	603	CLA	CMB-C2B-C3B	3.05	130.39	124.68
24	s	608	CHL	C1B-CHB-C4A	-3.05	124.07	130.12
25	b	607	CLA	CAA-CBA-CGA	-3.05	104.33	113.25
30	b	620	BCR	C1-C6-C5	-3.05	118.32	122.61
24	N	609	CHL	CMD-C2D-C3D	-3.05	120.60	127.61
24	n	609	CHL	CMD-C2D-C3D	-3.05	120.60	127.61
28	3	1623	NEX	C11-C12-C13	-3.05	117.85	126.42
24	G	601	CHL	CHD-C4C-C3C	-3.05	120.36	124.84
25	y	614	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
25	7	612	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
25	s	614	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
25	r	613	CLA	CHB-C4A-NA	3.05	128.73	124.51
25	G	613	CLA	CMB-C2B-C3B	3.05	130.38	124.68
25	1	604	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
28	y	1623	NEX	C26-C27-C28	-3.05	119.55	125.99
25	7	604	CLA	C1B-CHB-C4A	-3.04	124.09	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	1622	XAT	C7-C8-C9	-3.04	120.81	125.53
25	5	603	CLA	CHB-C4A-NA	3.04	128.72	124.51
27	5	1622	XAT	C35-C34-C33	-3.04	122.97	127.31
24	r	606	CHL	CMD-C2D-C3D	-3.04	120.61	127.61
26	g	1621	LUT	C7-C8-C9	-3.04	121.64	126.23
28	7	1623	NEX	C11-C12-C13	-3.04	117.87	126.42
25	n	614	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	1	603	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
27	3	1622	XAT	C7-C8-C9	-3.04	120.81	125.53
25	1	612	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
24	7	601	CHL	C4D-CHA-C1A	-3.04	117.55	121.25
25	g	613	CLA	CMB-C2B-C3B	3.04	130.36	124.68
26	R	620	LUT	C18-C5-C6	-3.04	121.12	124.53
24	R	606	CHL	C3B-C4B-NB	3.04	113.14	109.21
28	Y	1623	NEX	C39-C29-C30	-3.04	118.67	122.92
25	5	603	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
25	5	612	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
24	N	601	CHL	CMD-C2D-C3D	-3.04	120.63	127.61
25	3	612	CLA	CAA-C2A-C3A	-3.04	104.47	112.78
24	5	609	CHL	C1C-C2C-C3C	-3.04	104.70	107.11
25	b	616	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	7	612	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
27	1	1622	XAT	C15-C35-C34	-3.03	117.26	123.47
25	5	604	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
25	b	616	CLA	CHB-C4A-NA	3.03	128.71	124.51
24	n	601	CHL	CMD-C2D-C3D	-3.03	120.64	127.61
25	B	616	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
27	7	1622	XAT	C7-C8-C9	-3.03	120.83	125.53
24	n	601	CHL	C3B-C4B-NB	3.03	113.13	109.21
28	S	1623	NEX	C39-C29-C30	-3.03	118.68	122.92
28	s	1623	NEX	C39-C29-C30	-3.03	118.68	122.92
25	Y	614	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	1	603	CLA	CHB-C4A-NA	3.03	128.70	124.51
25	R	613	CLA	CHB-C4A-NA	3.02	128.69	124.51
24	Y	606	CHL	O2A-CGA-CBA	3.02	121.39	111.91
25	B	616	CLA	CHB-C4A-NA	3.02	128.69	124.51
24	3	601	CHL	C4D-CHA-C1A	-3.02	117.57	121.25
25	N	612	CLA	CMB-C2B-C3B	3.02	130.32	124.68
28	Y	1623	NEX	C26-C27-C28	-3.02	119.62	125.99
25	3	604	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
28	G	1623	NEX	O24-C25-C38	3.02	118.67	115.06
24	y	609	CHL	CHB-C4A-NA	3.01	128.68	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	407	CLA	CMB-C2B-C3B	3.01	130.32	124.68
25	3	603	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
25	2	603	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
26	G	1621	LUT	C7-C8-C9	-3.01	121.68	126.23
25	a	407	CLA	CMB-C2B-C3B	3.01	130.31	124.68
25	6	603	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
30	c	515	BCR	C23-C22-C21	-3.01	114.32	118.94
37	H	102	DGD	CDB-CCB-CBB	-3.01	99.14	114.42
37	h	102	DGD	CDB-CCB-CBB	-3.01	99.14	114.42
25	7	603	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
24	y	606	CHL	O2A-CGA-CBA	3.01	121.35	111.91
26	8	620	LUT	C18-C5-C6	-3.01	121.15	124.53
27	7	1622	XAT	C40-C33-C32	3.01	122.82	118.08
35	A	413	LMG	O6-C1-O1	-3.01	102.86	109.97
27	7	1622	XAT	C24-C23-C22	-3.01	104.97	110.77
26	6	1621	LUT	C10-C11-C12	-3.00	113.84	123.22
35	a	413	LMG	O6-C1-O1	-3.00	102.86	109.97
25	C	507	CLA	CHB-C4A-NA	3.00	128.66	124.51
28	g	1623	NEX	C24-C23-C22	-3.00	104.97	110.77
25	g	611	CLA	CHB-C4A-NA	3.00	128.66	124.51
36	d	405	PL9	C7-C8-C9	-3.00	121.79	126.79
34	b	621	SQD	C4-C3-C2	3.00	116.06	110.82
24	4	609	CHL	CHB-C4A-NA	3.00	128.66	124.51
26	4	620	LUT	C18-C5-C6	-3.00	121.16	124.53
24	2	609	CHL	CMB-C2B-C3B	3.00	130.29	124.68
27	3	1622	XAT	C40-C33-C32	3.00	122.80	118.08
25	C	512	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
25	G	611	CLA	CHB-C4A-NA	3.00	128.66	124.51
27	5	1622	XAT	C15-C35-C34	-3.00	117.34	123.47
28	G	1623	NEX	C24-C23-C22	-3.00	104.99	110.77
26	2	1621	LUT	C10-C11-C12	-3.00	113.87	123.22
24	6	606	CHL	CHB-C4A-NA	3.00	128.65	124.51
25	6	604	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
36	D	405	PL9	C7-C8-C9	-2.99	121.81	126.79
24	G	608	CHL	CMD-C2D-C3D	-2.99	120.73	127.61
24	G	601	CHL	C1-C2-C3	-2.99	120.86	126.04
25	c	507	CLA	CHB-C4A-NA	2.99	128.65	124.51
35	B	2633	LMG	O2-C2-C1	-2.99	102.77	110.05
25	G	611	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
25	c	512	CLA	CAA-C2A-C3A	-2.99	104.58	112.78
24	6	608	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
24	N	605	CHL	O2A-CGA-CBA	2.99	121.30	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	608	CHL	CMD-C2D-C3D	-2.99	120.73	127.61
25	S	614	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	n	612	CLA	CMB-C2B-C3B	2.99	130.27	124.68
28	S	1623	NEX	C19-C9-C10	-2.99	118.73	122.92
25	g	611	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
24	N	601	CHL	C3B-C4B-NB	2.99	113.08	109.21
24	Y	609	CHL	CHB-C4A-NA	2.99	128.65	124.51
24	5	609	CHL	C1B-CHB-C4A	-2.99	124.20	130.12
25	5	614	CLA	CHB-C4A-NA	2.99	128.64	124.51
24	1	609	CHL	C1B-CHB-C4A	-2.99	124.20	130.12
28	g	1623	NEX	O24-C25-C38	2.99	118.64	115.06
24	n	605	CHL	O2A-CGA-CBA	2.99	121.28	111.91
30	C	515	BCR	C23-C22-C21	-2.99	114.36	118.94
25	B	609	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	s	614	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	B	616	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
24	G	608	CHL	CAC-C3C-C4C	2.98	128.68	124.81
34	B	621	SQD	C4-C3-C2	2.98	116.03	110.82
24	7	601	CHL	CBC-CAC-C3C	-2.98	104.20	112.43
25	R	604	CLA	O2D-CGD-CBD	2.98	116.57	111.27
26	2	1621	LUT	C15-C14-C13	-2.98	123.05	127.31
30	b	620	BCR	C4-C5-C6	-2.98	118.40	122.73
25	b	609	CLA	CHB-C4A-NA	2.98	128.64	124.51
26	2	1621	LUT	C30-C31-C32	-2.98	113.91	123.22
26	4	620	LUT	C15-C35-C34	-2.98	117.36	123.47
25	n	603	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
24	6	609	CHL	CMB-C2B-C3B	2.98	130.26	124.68
25	b	616	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
24	2	606	CHL	CHB-C4A-NA	2.98	128.63	124.51
35	b	2633	LMG	O2-C2-C1	-2.98	102.81	110.05
24	4	607	CHL	CHD-C4C-C3C	-2.98	120.46	124.84
27	3	1622	XAT	C24-C23-C22	-2.98	105.02	110.77
25	C	501	CLA	C4A-NA-C1A	2.98	108.05	106.71
25	B	605	CLA	C1-C2-C3	-2.98	120.89	126.04
28	r	623	NEX	C11-C12-C13	-2.98	118.05	126.42
25	B	605	CLA	C6-C5-C3	-2.98	105.65	113.45
25	b	605	CLA	C6-C5-C3	-2.98	105.65	113.45
25	1	614	CLA	CHB-C4A-NA	2.98	128.63	124.51
26	S	1621	LUT	C30-C31-C32	-2.98	113.93	123.22
24	g	608	CHL	CAC-C3C-C4C	2.97	128.67	124.81
28	y	1623	NEX	C11-C12-C13	-2.97	118.06	126.42
25	b	605	CLA	C1-C2-C3	-2.97	120.90	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	1621	LUT	C30-C31-C32	-2.97	113.94	123.22
25	c	501	CLA	C4A-NA-C1A	2.97	108.04	106.71
26	6	1621	LUT	C15-C14-C13	-2.97	123.07	127.31
24	g	601	CHL	C1-C2-C3	-2.97	120.90	126.04
28	R	623	NEX	C11-C12-C13	-2.97	118.06	126.42
24	8	609	CHL	CHB-C4A-NA	2.97	128.62	124.51
26	6	1621	LUT	C30-C31-C32	-2.97	113.94	123.22
24	8	607	CHL	CHD-C4C-C3C	-2.97	120.47	124.84
24	G	601	CHL	CHB-C4A-NA	2.97	128.62	124.51
25	3	602	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
24	3	601	CHL	CBC-CAC-C3C	-2.97	104.24	112.43
30	C	514	BCR	C20-C21-C22	-2.97	123.07	127.31
25	B	609	CLA	CHB-C4A-NA	2.97	128.62	124.51
25	r	604	CLA	O2D-CGD-CBD	2.97	116.55	111.27
25	Y	603	CLA	CBC-CAC-C3C	-2.97	104.25	112.43
25	b	602	CLA	CMB-C2B-C3B	2.97	130.23	124.68
28	Y	1623	NEX	C11-C12-C13	-2.97	118.08	126.42
25	1	602	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
24	4	606	CHL	C3B-C4B-NB	2.97	113.05	109.21
24	g	601	CHL	CHB-C4A-NA	2.97	128.62	124.51
30	t	101	BCR	C16-C15-C14	-2.97	117.40	123.47
25	N	603	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	S	602	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
26	6	1620	LUT	C31-C30-C29	-2.96	123.08	127.31
25	b	609	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	n	612	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	8	602	CLA	CHB-C4A-NA	2.96	128.61	124.51
28	s	1623	NEX	C19-C9-C10	-2.96	118.78	122.92
30	B	620	BCR	C4-C5-C6	-2.96	118.43	122.73
26	8	620	LUT	C15-C35-C34	-2.96	117.41	123.47
24	g	605	CHL	O2D-CGD-O1D	-2.96	118.05	123.84
25	R	601	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	B	602	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	2	604	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	3	613	CLA	CHB-C4A-NA	2.96	128.60	124.51
26	y	1621	LUT	C22-C23-C24	-2.96	108.37	111.74
25	b	614	CLA	C4-C3-C5	2.96	120.25	115.27
25	N	612	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
25	a	410	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
24	Y	609	CHL	CHD-C4C-C3C	-2.95	120.50	124.84
24	G	606	CHL	CMD-C2D-C3D	-2.95	120.82	127.61
25	r	601	CLA	O2D-CGD-O1D	-2.95	118.06	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	D	404	BCR	C16-C15-C14	-2.95	117.43	123.47
25	5	602	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	s	602	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	C	513	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
24	3	608	CHL	C3B-C4B-NB	2.95	113.02	109.21
30	c	514	BCR	C20-C21-C22	-2.95	123.10	127.31
25	4	602	CLA	CHB-C4A-NA	2.95	128.59	124.51
24	s	601	CHL	C3B-C4B-NB	2.95	113.02	109.21
30	T	101	BCR	C16-C15-C14	-2.95	117.44	123.47
25	y	603	CLA	CBC-CAC-C3C	-2.95	104.31	112.43
26	4	620	LUT	C30-C31-C32	-2.95	114.02	123.22
26	2	1620	LUT	C31-C30-C29	-2.95	123.11	127.31
25	C	511	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	S	610	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	7	602	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
24	2	608	CHL	C1C-C2C-C3C	-2.95	104.78	107.11
24	8	606	CHL	C3B-C4B-NB	2.94	113.02	109.21
25	7	613	CLA	CHB-C4A-NA	2.94	128.58	124.51
24	G	605	CHL	O2D-CGD-O1D	-2.94	118.08	123.84
26	4	620	LUT	C18-C5-C4	2.94	119.81	114.36
24	5	609	CHL	CMD-C2D-C3D	-2.94	120.84	127.61
26	Y	1621	LUT	C22-C23-C24	-2.94	108.39	111.74
26	Y	1621	LUT	C30-C31-C32	-2.94	114.03	123.22
26	8	620	LUT	C30-C31-C32	-2.94	114.03	123.22
24	S	601	CHL	C3B-C4B-NB	2.94	113.01	109.21
30	d	404	BCR	C16-C15-C14	-2.94	117.45	123.47
24	7	608	CHL	C3B-C4B-NB	2.94	113.01	109.21
25	r	603	CLA	CAA-C2A-C3A	-2.94	104.72	112.78
25	B	614	CLA	C4-C3-C5	2.94	120.22	115.27
25	5	611	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
24	y	609	CHL	CHD-C4C-C3C	-2.94	120.52	124.84
25	R	616	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
25	d	402	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
24	g	606	CHL	CMD-C2D-C3D	-2.94	120.85	127.61
25	R	609	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	C	502	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	c	513	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
25	A	410	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
25	4	611	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	R	603	CLA	CAA-C2A-C3A	-2.94	104.74	112.78
27	8	622	XAT	C31-C30-C29	-2.94	123.12	127.31
25	b	611	CLA	CAA-CBA-CGA	-2.94	104.67	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	620	LUT	C18-C5-C4	2.94	119.79	114.36
25	7	611	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
24	y	606	CHL	OMC-CMC-C2C	-2.93	119.05	125.69
25	s	610	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	N	611	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
25	n	611	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
24	1	609	CHL	CMD-C2D-C3D	-2.93	120.87	127.61
30	4	623	BCR	C20-C21-C22	-2.93	123.12	127.31
26	y	1621	LUT	C30-C31-C32	-2.93	114.07	123.22
25	c	511	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	c	502	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	r	616	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
27	4	622	XAT	C31-C30-C29	-2.93	123.13	127.31
30	8	623	BCR	C20-C21-C22	-2.93	123.13	127.31
24	Y	606	CHL	OMC-CMC-C2C	-2.93	119.06	125.69
25	g	602	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	6	602	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
25	B	611	CLA	CAA-CBA-CGA	-2.93	104.69	113.25
25	3	611	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
25	2	602	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
25	r	609	CLA	CHB-C4A-NA	2.93	128.56	124.51
24	g	609	CHL	CMD-C2D-C3D	-2.93	120.88	127.61
28	3	1623	NEX	C28-C29-C30	2.92	123.43	118.94
25	C	503	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
24	3	605	CHL	CAC-C3C-C4C	2.92	128.60	124.81
25	2	614	CLA	CHB-C4A-NA	2.92	128.55	124.51
25	Y	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
27	6	1622	XAT	C40-C33-C32	2.92	122.68	118.08
25	A	405	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
28	R	623	NEX	C17-C1-C6	-2.92	107.86	110.47
25	c	513	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
25	C	513	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	S	603	CLA	CHB-C4A-NA	2.92	128.55	124.51
28	1	1623	NEX	C26-C27-C28	-2.92	119.82	125.99
25	8	611	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	7	605	CHL	CAC-C3C-C4C	2.92	128.59	124.81
26	3	1621	LUT	C15-C14-C13	-2.92	123.15	127.31
25	D	402	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	2	612	CLA	CHB-C4A-NA	2.92	128.54	124.51
24	1	608	CHL	C1C-C2C-C3C	-2.92	104.80	107.11
25	1	611	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	6	612	CLA	CHB-C4A-NA	2.92	128.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	603	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
25	G	602	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	G	609	CHL	CMD-C2D-C3D	-2.91	120.92	127.61
26	G	1621	LUT	C28-C29-C30	-2.91	114.47	118.94
25	a	405	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
25	G	612	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
25	c	503	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
26	S	1620	LUT	C10-C11-C12	-2.91	114.14	123.22
28	7	1623	NEX	C28-C29-C30	2.91	123.40	118.94
26	7	1621	LUT	C15-C14-C13	-2.91	123.16	127.31
25	C	505	CLA	O2D-CGD-CBD	2.90	116.43	111.27
27	2	1622	XAT	C40-C33-C32	2.90	122.65	118.08
25	c	507	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
26	g	1620	LUT	C10-C11-C12	-2.90	114.16	123.22
25	y	602	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	4	612	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	c	505	CLA	O2D-CGD-CBD	2.90	116.42	111.27
25	8	603	CLA	CHB-C4A-NA	2.90	128.52	124.51
26	1	1620	LUT	C8-C9-C10	-2.90	114.49	118.94
28	r	623	NEX	C17-C1-C6	-2.90	107.88	110.47
26	s	1620	LUT	C10-C11-C12	-2.90	114.17	123.22
25	8	612	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
28	5	1623	NEX	C26-C27-C28	-2.90	119.87	125.99
24	5	608	CHL	C1C-C2C-C3C	-2.90	104.82	107.11
25	3	614	CLA	CMB-C2B-C3B	2.90	130.09	124.68
25	g	612	CLA	CAA-C2A-C3A	-2.89	104.85	112.78
25	Y	612	CLA	CHB-C4A-NA	2.89	128.51	124.51
30	h	101	BCR	C38-C26-C25	-2.89	121.28	124.53
25	g	602	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
25	G	611	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	S	603	CLA	CMB-C2B-C3B	2.89	130.09	124.68
25	g	602	CLA	CAC-C3C-C4C	2.89	128.56	124.81
26	G	1620	LUT	C10-C11-C12	-2.89	114.20	123.22
25	s	603	CLA	CMB-C2B-C3B	2.89	130.09	124.68
25	y	612	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	1	603	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
24	6	605	CHL	CAC-C3C-C4C	2.89	128.56	124.81
25	C	507	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
30	c	515	BCR	C33-C5-C4	2.89	119.16	113.62
25	6	614	CLA	CHB-C4A-NA	2.89	128.50	124.51
24	2	605	CHL	CAC-C3C-C4C	2.89	128.56	124.81
25	s	603	CLA	CHB-C4A-NA	2.89	128.50	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	609	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
25	s	611	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
26	5	1620	LUT	C8-C9-C10	-2.88	114.52	118.94
26	g	1621	LUT	C28-C29-C30	-2.88	114.52	118.94
25	G	602	CLA	CAC-C3C-C4C	2.88	128.55	124.81
26	3	1620	LUT	C10-C11-C12	-2.88	114.23	123.22
25	2	604	CLA	CHB-C4A-NA	2.88	128.50	124.51
24	2	606	CHL	CMB-C2B-C3B	2.88	130.06	124.68
25	B	612	CLA	CAC-C3C-C4C	2.88	128.54	124.81
34	a	418	SQD	O47-C7-C8	2.88	117.70	111.50
24	3	607	CHL	C3B-C4B-NB	2.88	112.93	109.21
25	S	611	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
24	N	607	CHL	CMB-C2B-C3B	2.88	130.06	124.68
25	g	612	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
25	g	611	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
24	s	601	CHL	OMC-CMC-C2C	-2.87	119.19	125.69
25	G	602	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
25	S	611	CLA	CMB-C2B-C3B	2.87	130.05	124.68
24	n	601	CHL	C1-C2-C3	-2.87	121.08	126.04
34	A	418	SQD	O47-C7-C8	2.87	117.69	111.50
30	C	515	BCR	C33-C5-C4	2.87	119.13	113.62
24	4	606	CHL	CMB-C2B-C3B	2.87	130.05	124.68
25	5	611	CLA	CMB-C2B-C3B	2.87	130.05	124.68
24	6	606	CHL	CMB-C2B-C3B	2.87	130.05	124.68
25	n	603	CLA	CMB-C2B-C3B	2.87	130.05	124.68
24	n	607	CHL	CMB-C2B-C3B	2.87	130.05	124.68
24	S	606	CHL	C3B-C4B-NB	2.87	112.92	109.21
25	4	611	CLA	CMB-C2B-C3B	2.87	130.04	124.68
26	7	1620	LUT	C10-C11-C12	-2.87	114.27	123.22
25	s	611	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	7	614	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	4	603	CLA	CHB-C4A-NA	2.87	128.48	124.51
24	R	614	CHL	C3B-C4B-NB	2.87	112.92	109.21
24	N	601	CHL	C1-C2-C3	-2.87	121.09	126.04
25	6	603	CLA	CMB-C2B-C3B	2.87	130.04	124.68
34	a	418	SQD	O9-S-C6	2.87	110.34	106.94
24	S	607	CHL	C1C-C2C-C3C	-2.87	104.84	107.11
24	7	605	CHL	C4A-NA-C1A	-2.86	105.42	106.71
25	R	604	CLA	CHB-C4A-NA	2.86	128.47	124.51
24	7	607	CHL	C3B-C4B-NB	2.86	112.91	109.21
25	b	612	CLA	CAC-C3C-C4C	2.86	128.53	124.81
24	6	609	CHL	C1C-C2C-C3C	-2.86	104.84	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	613	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
27	r	622	XAT	C35-C15-C14	-2.86	117.61	123.47
24	y	608	CHL	C1-C2-C3	-2.86	121.09	126.04
27	r	622	XAT	C10-C11-C12	-2.86	114.29	123.22
29	d	409	LHG	C11-C10-C9	-2.86	99.91	114.42
35	a	415	LMG	O6-C1-O1	-2.86	103.20	109.97
24	8	606	CHL	CMB-C2B-C3B	2.86	130.03	124.68
30	H	101	BCR	C38-C26-C25	-2.86	121.32	124.53
25	G	612	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
29	D	410	LHG	O8-C23-C24	2.86	120.88	111.91
29	D	409	LHG	C11-C10-C9	-2.86	99.91	114.42
24	n	606	CHL	CMD-C2D-C3D	-2.86	121.04	127.61
25	R	601	CLA	CAC-C3C-C2C	-2.86	122.64	127.53
25	6	604	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	s	612	CLA	CHB-C4A-NA	2.86	128.46	124.51
26	S	1621	LUT	C15-C14-C13	-2.86	123.23	127.31
25	s	609	CLA	CMB-C2B-C3B	2.86	130.02	124.68
29	d	410	LHG	O8-C23-C24	2.86	120.87	111.91
24	s	606	CHL	C3B-C4B-NB	2.85	112.90	109.21
25	S	609	CLA	CMB-C2B-C3B	2.85	130.02	124.68
25	8	611	CLA	CMB-C2B-C3B	2.85	130.02	124.68
27	R	622	XAT	C10-C11-C12	-2.85	114.31	123.22
24	r	614	CHL	C3B-C4B-NB	2.85	112.90	109.21
30	c	515	BCR	C33-C5-C6	-2.85	121.32	124.53
24	N	606	CHL	CMD-C2D-C3D	-2.85	121.05	127.61
25	1	611	CLA	CMB-C2B-C3B	2.85	130.02	124.68
25	B	607	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	3	613	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
25	B	612	CLA	CHB-C4A-NA	2.85	128.46	124.51
27	R	622	XAT	C35-C15-C14	-2.85	117.63	123.47
25	B	608	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	b	607	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	b	612	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	r	604	CLA	CHB-C4A-NA	2.85	128.46	124.51
35	A	415	LMG	O6-C1-O1	-2.85	103.22	109.97
25	3	612	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	N	603	CLA	CMB-C2B-C3B	2.85	130.01	124.68
26	S	1621	LUT	C35-C15-C14	-2.85	117.64	123.47
25	2	603	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	n	612	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
27	R	622	XAT	C24-C23-C22	-2.85	105.28	110.77
24	s	606	CHL	O2D-CGD-O1D	-2.85	118.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	606	CHL	CMD-C2D-C3D	-2.85	121.07	127.61
26	N	1620	LUT	C17-C1-C6	2.85	114.91	110.30
24	S	601	CHL	OMC-CMC-C2C	-2.85	119.25	125.69
24	7	606	CHL	CMB-C2B-C3B	2.84	130.00	124.68
30	C	517	BCR	C33-C5-C4	2.84	119.08	113.62
27	r	622	XAT	C24-C23-C22	-2.84	105.28	110.77
30	C	515	BCR	C33-C5-C6	-2.84	121.33	124.53
24	5	606	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
24	n	605	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
25	7	612	CLA	CMB-C2B-C3B	2.84	130.00	124.68
25	B	615	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
28	R	623	NEX	C35-C34-C33	-2.84	123.26	127.31
24	7	606	CHL	C4A-NA-C1A	-2.84	105.43	106.71
25	r	601	CLA	CAC-C3C-C2C	-2.84	122.67	127.53
26	s	1621	LUT	C15-C14-C13	-2.84	123.26	127.31
25	C	502	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	B	616	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
25	b	616	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
24	N	608	CHL	C1-C2-C3	-2.84	121.14	126.04
30	c	517	BCR	C33-C5-C4	2.84	119.07	113.62
34	A	418	SQD	O9-S-C6	2.84	110.31	106.94
25	b	615	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	b	608	CLA	CHB-C4A-NA	2.84	128.43	124.51
34	b	621	SQD	C44-O6-C1	2.84	119.28	113.74
25	N	612	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
28	R	623	NEX	C39-C29-C30	-2.83	118.95	122.92
27	3	1622	XAT	C38-C25-C24	2.83	117.47	114.28
24	S	606	CHL	O2D-CGD-O1D	-2.83	118.30	123.84
37	c	520	DGD	C3G-C2G-C1G	-2.83	105.09	111.79
25	y	611	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
26	s	1621	LUT	C35-C15-C14	-2.83	117.67	123.47
34	B	621	SQD	C44-O6-C1	2.83	119.27	113.74
24	Y	608	CHL	C1-C2-C3	-2.83	121.15	126.04
24	n	608	CHL	C1-C2-C3	-2.83	121.15	126.04
24	g	606	CHL	O2A-CGA-CBA	2.83	120.79	111.91
25	S	612	CLA	CHB-C4A-NA	2.83	128.42	124.51
26	r	620	LUT	C21-C26-C27	-2.83	109.13	112.70
25	2	610	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
24	Y	607	CHL	CAA-C2A-C3A	-2.83	105.04	112.78
25	c	502	CLA	CHB-C4A-NA	2.83	128.42	124.51
26	y	1620	LUT	C38-C25-C24	-2.82	117.52	123.56
25	r	609	CLA	CMB-C2B-C3B	2.82	129.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	406	CLA	CHB-C4A-NA	2.82	128.42	124.51
29	b	2631	LHG	O8-C23-C24	2.82	120.77	111.91
37	C	520	DGD	C3G-C2G-C1G	-2.82	105.11	111.79
24	3	606	CHL	CMB-C2B-C3B	2.82	129.96	124.68
29	B	2631	LHG	O8-C23-C24	2.82	120.77	111.91
26	6	1620	LUT	C15-C35-C34	-2.82	117.69	123.47
25	n	613	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
25	g	612	CLA	CHB-C4A-NA	2.82	128.41	124.51
26	6	1620	LUT	C30-C31-C32	-2.82	114.41	123.22
34	b	623	SQD	O5-C1-C2	2.82	116.32	110.35
24	N	605	CHL	CMD-C2D-C3D	-2.82	121.12	127.61
25	6	610	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
26	n	1620	LUT	C17-C1-C6	2.82	114.87	110.30
25	a	406	CLA	CHB-C4A-NA	2.82	128.41	124.51
24	S	607	CHL	CBC-CAC-C3C	-2.82	104.66	112.43
25	2	613	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
27	8	622	XAT	C18-C5-C4	2.82	117.45	114.28
25	D	402	CLA	CAC-C3C-C4C	2.82	128.47	124.81
24	Y	601	CHL	CHB-C4A-NA	2.82	128.41	124.51
26	g	1620	LUT	C38-C25-C24	-2.82	117.53	123.56
24	s	607	CHL	CBC-CAC-C3C	-2.82	104.66	112.43
26	2	1620	LUT	C30-C31-C32	-2.82	114.42	123.22
24	y	607	CHL	CAA-C2A-C3A	-2.82	105.06	112.78
28	5	1623	NEX	C31-C30-C29	-2.82	123.29	127.31
25	A	410	CLA	CAA-CBA-CGA	-2.82	105.03	113.25
37	c	518	DGD	CDB-CCB-CBB	-2.82	100.13	114.42
25	a	410	CLA	CAA-CBA-CGA	-2.81	105.03	113.25
25	N	613	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
25	5	612	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	d	403	CLA	CHB-C4A-NA	2.81	128.40	124.51
34	B	623	SQD	O5-C1-C2	2.81	116.31	110.35
26	Y	1620	LUT	C38-C25-C24	-2.81	117.54	123.56
28	r	623	NEX	C35-C34-C33	-2.81	123.29	127.31
37	C	518	DGD	CDB-CCB-CBB	-2.81	100.14	114.42
24	G	606	CHL	O2A-CGA-CBA	2.81	120.74	111.91
25	C	504	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
28	r	623	NEX	C39-C29-C30	-2.81	118.98	122.92
24	3	609	CHL	CAC-C3C-C4C	2.81	128.46	124.81
28	1	1623	NEX	C31-C30-C29	-2.81	123.30	127.31
25	y	610	CLA	C1D-ND-C4D	-2.81	104.34	106.33
37	C	520	DGD	O5D-C6D-C5D	-2.81	103.85	109.05
24	1	609	CHL	O2A-CGA-CBA	2.81	120.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	403	CLA	CHB-C4A-NA	2.81	128.40	124.51
24	s	607	CHL	C1C-C2C-C3C	-2.81	104.89	107.11
25	c	504	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	R	609	CLA	CMB-C2B-C3B	2.81	129.93	124.68
25	G	612	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	Y	611	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	c	505	CLA	CHB-C4A-NA	2.81	128.39	124.51
24	n	609	CHL	CMB-C2B-C3B	2.80	129.92	124.68
25	6	613	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	7	609	CHL	CAC-C3C-C4C	2.80	128.45	124.81
24	N	608	CHL	O2A-CGA-CBA	2.80	120.70	111.91
27	7	1622	XAT	C38-C25-C24	2.80	117.43	114.28
24	5	609	CHL	O2A-CGA-CBA	2.80	120.70	111.91
25	5	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
27	2	1622	XAT	C35-C34-C33	-2.80	123.31	127.31
24	n	608	CHL	O2A-CGA-CBA	2.80	120.69	111.91
24	3	606	CHL	C3B-C4B-NB	2.80	112.83	109.21
26	2	1620	LUT	C15-C35-C34	-2.80	117.74	123.47
25	c	510	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
27	6	1622	XAT	C35-C34-C33	-2.80	123.32	127.31
25	C	510	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
25	s	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
27	4	622	XAT	C18-C5-C4	2.79	117.42	114.28
25	r	604	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
30	t	101	BCR	C35-C13-C12	2.79	122.48	118.08
37	B	626	DGD	CDB-CCB-CBB	-2.79	100.24	114.42
25	C	505	CLA	CHB-C4A-NA	2.79	128.38	124.51
25	D	403	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	1	612	CLA	CHB-C4A-NA	2.79	128.37	124.51
24	5	609	CHL	C4-C3-C5	2.79	119.97	115.27
24	7	606	CHL	C3B-C4B-NB	2.79	112.82	109.21
26	R	620	LUT	C21-C26-C27	-2.79	109.17	112.70
37	b	626	DGD	CDB-CCB-CBB	-2.79	100.25	114.42
25	S	611	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	d	402	CLA	CAC-C3C-C4C	2.79	128.43	124.81
25	b	606	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
25	Y	610	CLA	C1D-ND-C4D	-2.79	104.35	106.33
25	d	403	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
24	N	609	CHL	CMB-C2B-C3B	2.79	129.90	124.68
25	R	604	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
26	G	1620	LUT	C38-C25-C24	-2.79	117.59	123.56
25	g	603	CLA	O2D-CGD-O1D	-2.79	118.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	605	CHL	CMD-C2D-C3D	-2.79	121.20	127.61
25	B	606	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
30	T	101	BCR	C35-C13-C12	2.79	122.47	118.08
34	a	412	SQD	O48-C23-C24	2.79	120.65	111.91
24	1	609	CHL	C4-C3-C5	2.78	119.95	115.27
24	G	605	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
25	c	508	CLA	CHB-C4A-NA	2.78	128.36	124.51
26	s	1620	LUT	C30-C31-C32	-2.78	114.54	123.22
25	N	611	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	3	614	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
28	R	623	NEX	C4-C3-C2	-2.78	105.40	110.77
26	N	1620	LUT	C38-C25-C24	-2.78	117.61	123.56
24	1	608	CHL	C4A-NA-C1A	-2.78	105.46	106.71
29	n	2630	LHG	C11-C10-C9	-2.78	100.31	114.42
24	2	608	CHL	CAC-C3C-C4C	2.78	128.42	124.81
24	y	601	CHL	CHB-C4A-NA	2.78	128.35	124.51
25	c	503	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	B	602	CLA	CHB-C4A-NA	2.78	128.35	124.51
28	R	623	NEX	C30-C31-C32	-2.78	114.55	123.22
25	C	508	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	N	2630	LHG	C11-C10-C9	-2.78	100.32	114.42
25	C	503	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
37	c	520	DGD	O5D-C6D-C5D	-2.78	103.91	109.05
34	A	412	SQD	O48-C23-C24	2.78	120.62	111.91
28	r	623	NEX	C4-C3-C2	-2.78	105.41	110.77
26	n	1620	LUT	C38-C25-C24	-2.78	117.62	123.56
26	S	1620	LUT	C30-C31-C32	-2.78	114.55	123.22
25	G	603	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	N	604	CLA	C1-C2-C3	-2.77	122.26	126.75
25	n	611	CLA	CHB-C4A-NA	2.77	128.35	124.51
25	B	602	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
25	B	614	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
24	5	605	CHL	O2D-CGD-O1D	-2.77	118.42	123.84
30	A	411	BCR	C16-C15-C14	-2.77	117.79	123.47
25	b	602	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	7	614	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
24	6	609	CHL	O2A-CGA-CBA	2.77	120.61	111.91
25	c	510	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	n	603	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	1	604	CLA	CMB-C2B-C3B	2.77	129.86	124.68
25	S	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	N	606	CHL	OMC-CMC-C2C	-2.77	119.42	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	608	CHL	O2A-CGA-CBA	2.77	120.60	111.91
25	s	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	n	606	CHL	OMC-CMC-C2C	-2.77	119.43	125.69
24	r	608	CHL	O2A-CGA-CBA	2.77	120.60	111.91
29	b	2630	LHG	O8-C23-C24	2.77	120.60	111.91
29	B	2630	LHG	O8-C23-C24	2.77	120.60	111.91
26	r	620	LUT	C20-C13-C12	2.77	122.44	118.08
24	6	608	CHL	CAC-C3C-C4C	2.77	128.40	124.81
28	1	1623	NEX	C11-C12-C13	-2.77	118.64	126.42
25	1	612	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
25	7	612	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
24	5	608	CHL	C4A-NA-C1A	-2.77	105.46	106.71
28	5	1623	NEX	C11-C12-C13	-2.77	118.64	126.42
24	2	609	CHL	O2A-CGA-CBA	2.77	120.59	111.91
25	B	608	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
24	Y	601	CHL	C1-C2-C3	-2.77	121.26	126.04
28	r	623	NEX	C30-C31-C32	-2.77	114.59	123.22
28	3	1623	NEX	C15-C35-C34	-2.76	117.81	123.47
25	B	606	CLA	C6-C5-C3	-2.76	106.21	113.45
25	1	613	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	5	604	CLA	CMB-C2B-C3B	2.76	129.85	124.68
29	d	408	LHG	C11-C10-C9	-2.76	100.40	114.42
25	8	603	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
24	r	608	CHL	CHB-C4A-NA	2.76	128.33	124.51
25	n	604	CLA	C1-C2-C3	-2.76	122.28	126.75
25	B	616	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
25	N	611	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	R	603	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	r	603	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
29	D	408	LHG	C11-C10-C9	-2.76	100.41	114.42
25	b	606	CLA	C6-C5-C3	-2.76	106.22	113.45
27	r	622	XAT	C19-C9-C8	2.76	122.42	118.08
25	b	614	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	2	614	CLA	C4A-NA-C1A	2.76	107.95	106.71
25	b	613	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
24	r	606	CHL	CHB-C4A-NA	2.76	128.32	124.51
26	Y	1620	LUT	C11-C10-C9	-2.76	123.38	127.31
30	a	411	BCR	C16-C15-C14	-2.76	117.83	123.47
25	n	611	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
24	R	606	CHL	CHB-C4A-NA	2.75	128.32	124.51
25	N	603	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	1	605	CHL	O2D-CGD-O1D	-2.75	118.45	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	402	CLA	CBA-CAA-C2A	-2.75	105.73	113.86
25	b	602	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	7	607	CHL	C1B-CHB-C4A	-2.75	124.67	130.12
25	3	612	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
24	R	614	CHL	CAA-C2A-C3A	-2.75	109.67	116.10
25	d	402	CLA	CBA-CAA-C2A	-2.75	105.74	113.86
27	R	622	XAT	C19-C9-C8	2.75	122.41	118.08
24	1	609	CHL	CAC-C3C-C4C	2.75	128.38	124.81
25	C	510	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
25	b	608	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
24	y	601	CHL	C1-C2-C3	-2.75	121.29	126.04
25	4	603	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
24	3	609	CHL	CHD-C4C-C3C	-2.75	120.80	124.84
25	b	616	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
26	R	620	LUT	C20-C13-C12	2.75	122.41	118.08
24	5	609	CHL	CAC-C3C-C4C	2.75	128.38	124.81
26	6	1620	LUT	C10-C11-C12	-2.75	114.64	123.22
24	3	608	CHL	CMB-C2B-C3B	2.75	129.82	124.68
25	Y	614	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
24	6	601	CHL	CHB-C4A-NA	2.75	128.31	124.51
26	y	1620	LUT	C11-C10-C9	-2.75	123.39	127.31
24	3	606	CHL	C4A-NA-C1A	-2.74	105.47	106.71
24	n	608	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
28	3	1623	NEX	C35-C34-C33	-2.74	123.39	127.31
27	N	1622	XAT	C18-C5-C4	2.74	117.37	114.28
24	r	614	CHL	CAA-C2A-C3A	-2.74	109.70	116.10
25	5	611	CLA	CHB-C4A-NA	2.74	128.31	124.51
25	B	613	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	7	609	CHL	CHD-C4C-C3C	-2.74	120.81	124.84
24	R	608	CHL	CHB-C4A-NA	2.74	128.30	124.51
24	3	605	CHL	C4A-NA-C1A	-2.74	105.47	106.71
24	3	607	CHL	C1B-CHB-C4A	-2.74	124.69	130.12
25	5	603	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
25	1	603	CLA	CBC-CAC-C3C	-2.74	104.88	112.43
26	5	1621	LUT	C31-C30-C29	-2.74	123.40	127.31
25	S	613	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	A	410	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	c	511	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	R	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
24	G	608	CHL	C1-C2-C3	-2.74	121.31	126.04
28	7	1623	NEX	C15-C35-C34	-2.73	117.87	123.47
24	g	601	CHL	C4D-CHA-C1A	-2.73	117.92	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	606	CHL	O2A-CGA-CBA	2.73	120.49	111.91
24	6	609	CHL	O1D-CGD-CBD	-2.73	118.89	124.48
26	2	1620	LUT	C10-C11-C12	-2.73	114.69	123.22
25	6	612	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
24	G	601	CHL	C4D-CHA-C1A	-2.73	117.92	121.25
24	7	608	CHL	CMB-C2B-C3B	2.73	129.79	124.68
25	g	610	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
25	5	613	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	g	608	CHL	C1-C2-C3	-2.73	121.32	126.04
28	5	1623	NEX	C30-C31-C32	-2.73	114.70	123.22
25	G	610	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
24	G	607	CHL	CHB-C4A-NA	2.73	128.29	124.51
27	n	1622	XAT	C18-C5-C4	2.73	117.35	114.28
24	N	608	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
25	1	611	CLA	CHB-C4A-NA	2.73	128.28	124.51
26	1	1620	LUT	C19-C9-C8	2.73	122.37	118.08
24	n	606	CHL	O2A-CGA-CBA	2.73	120.46	111.91
29	c	2630	LHG	O8-C23-C24	2.73	120.46	111.91
24	R	607	CHL	CHB-C4A-NA	2.73	128.28	124.51
28	1	1623	NEX	C30-C31-C32	-2.73	114.71	123.22
24	y	609	CHL	C1B-CHB-C4A	-2.72	124.72	130.12
24	2	601	CHL	CHB-C4A-NA	2.72	128.28	124.51
25	c	504	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	R	620	LUT	C28-C29-C30	-2.72	114.76	118.94
25	y	614	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
25	y	611	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
29	C	2630	LHG	O8-C23-C24	2.72	120.45	111.91
25	7	602	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
24	4	606	CHL	CHB-C4A-NA	2.72	128.27	124.51
24	6	607	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
25	r	612	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	A	407	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	2	1621	LUT	C39-C29-C28	2.72	122.36	118.08
26	r	620	LUT	C28-C29-C30	-2.72	114.77	118.94
25	B	605	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
24	2	607	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
25	2	612	CLA	CMB-C2B-C1B	-2.72	124.29	128.46
24	Y	605	CHL	CHB-C4A-NA	2.72	128.27	124.51
25	s	613	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
25	7	612	CLA	CHB-C4A-NA	2.72	128.27	124.51
30	b	620	BCR	C29-C30-C25	2.72	114.66	110.48
24	Y	609	CHL	C1B-CHB-C4A	-2.72	124.74	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	620	BCR	C20-C21-C22	-2.71	123.44	127.31
26	5	1620	LUT	C19-C9-C8	2.71	122.35	118.08
26	6	1621	LUT	C39-C29-C28	2.71	122.35	118.08
25	2	610	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
26	g	1621	LUT	C11-C10-C9	-2.71	123.44	127.31
24	1	606	CHL	CAC-C3C-C4C	2.71	128.33	124.81
28	7	1623	NEX	C35-C34-C33	-2.71	123.44	127.31
25	6	610	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
25	a	410	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	8	606	CHL	CHB-C4A-NA	2.71	128.26	124.51
25	c	509	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	1	1621	LUT	C31-C30-C29	-2.71	123.44	127.31
25	3	602	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
26	G	1621	LUT	C11-C10-C9	-2.71	123.44	127.31
25	C	511	CLA	CHB-C4A-NA	2.71	128.26	124.51
37	c	519	DGD	O5D-C6D-C5D	-2.71	104.03	109.05
25	Y	611	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
24	7	606	CHL	C1C-C2C-C3C	-2.71	104.97	107.11
25	N	614	CLA	CHB-C4A-NA	2.71	128.26	124.51
28	G	1623	NEX	C31-C30-C29	-2.71	123.45	127.31
24	N	608	CHL	CHB-C4A-NA	2.71	128.25	124.51
25	C	504	CLA	CHB-C4A-NA	2.71	128.25	124.51
24	2	609	CHL	O1D-CGD-CBD	-2.71	118.95	124.48
26	r	620	LUT	C37-C21-C22	-2.70	104.31	109.44
25	C	509	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
25	b	605	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
24	G	608	CHL	O2A-CGA-CBA	2.70	120.39	111.91
30	B	620	BCR	C29-C30-C25	2.70	114.64	110.48
26	4	620	LUT	C35-C15-C14	-2.70	117.94	123.47
29	Y	2630	LHG	O8-C23-C24	2.70	120.39	111.91
25	7	604	CLA	CMB-C2B-C3B	2.70	129.73	124.68
24	y	605	CHL	CHB-C4A-NA	2.70	128.25	124.51
29	y	2630	LHG	O8-C23-C24	2.70	120.38	111.91
30	C	516	BCR	C7-C8-C9	-2.70	122.15	126.23
25	6	614	CLA	C4A-NA-C1A	2.70	107.92	106.71
25	3	612	CLA	CHB-C4A-NA	2.70	128.25	124.51
25	n	614	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	y	607	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
24	n	608	CHL	CHB-C4A-NA	2.70	128.24	124.51
25	a	407	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	g	608	CHL	O2A-CGA-CBA	2.70	120.37	111.91
24	g	607	CHL	CHB-C4A-NA	2.70	128.24	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	614	CLA	CHB-C4A-NA	2.70	128.24	124.51
25	b	610	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
37	c	519	DGD	CDB-CCB-CBB	-2.69	100.75	114.42
24	4	608	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
25	y	603	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
24	Y	607	CHL	CMD-C2D-C3D	-2.69	121.42	127.61
35	D	411	LMG	O6-C1-O1	-2.69	103.60	109.97
37	C	519	DGD	CDB-CCB-CBB	-2.69	100.75	114.42
25	C	512	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
25	B	605	CLA	CHB-C4A-NA	2.69	128.24	124.51
25	c	506	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	y	601	CHL	C4D-CHA-C1A	-2.69	117.97	121.25
24	n	607	CHL	O2A-CGA-CBA	2.69	120.35	111.91
25	G	611	CLA	CMB-C2B-C3B	2.69	129.71	124.68
25	D	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	8	620	LUT	C35-C15-C14	-2.69	117.96	123.47
25	s	604	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	A	414	PL9	C8-C7-C3	2.69	119.58	111.98
24	s	601	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
24	r	607	CHL	CHB-C4A-NA	2.69	128.23	124.51
24	S	601	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
24	3	609	CHL	CMB-C2B-C3B	2.69	129.71	124.68
25	C	506	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	B	610	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
26	R	620	LUT	C37-C21-C22	-2.69	104.35	109.44
25	c	512	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
37	C	519	DGD	O5D-C6D-C5D	-2.69	104.08	109.05
25	d	402	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
27	N	1622	XAT	C35-C34-C33	-2.69	123.48	127.31
35	d	411	LMG	O6-C1-O1	-2.68	103.62	109.97
24	N	607	CHL	O2A-CGA-CBA	2.68	120.33	111.91
24	8	601	CHL	C3B-C4B-NB	2.68	112.68	109.21
28	g	1623	NEX	C31-C30-C29	-2.68	123.48	127.31
25	S	604	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	7	607	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
25	D	402	CLA	CHD-C1D-ND	-2.68	121.99	124.45
29	c	523	LHG	O8-C23-C24	2.68	120.33	111.91
30	B	620	BCR	C20-C21-C22	-2.68	123.48	127.31
25	R	601	CLA	CHB-C4A-NA	2.68	128.22	124.51
28	3	1623	NEX	C24-C23-C22	-2.68	105.59	110.77
25	Y	603	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
24	7	605	CHL	C1C-C2C-C3C	-2.68	104.99	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	614	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	7	609	CHL	CMB-C2B-C3B	2.68	129.69	124.68
30	b	618	BCR	C10-C11-C12	-2.68	114.86	123.22
30	c	516	BCR	C7-C8-C9	-2.68	122.19	126.23
25	3	604	CLA	CMB-C2B-C3B	2.68	129.69	124.68
29	C	523	LHG	O8-C23-C24	2.68	120.31	111.91
25	c	504	CLA	CHD-C1D-ND	-2.68	122.00	124.45
28	7	1623	NEX	C24-C23-C22	-2.68	105.61	110.77
25	g	611	CLA	CMB-C2B-C3B	2.68	129.68	124.68
24	s	606	CHL	OMC-CMC-C2C	-2.67	119.64	125.69
27	4	622	XAT	C15-C35-C34	-2.67	118.00	123.47
27	n	1622	XAT	C35-C34-C33	-2.67	123.49	127.31
30	B	618	BCR	C10-C11-C12	-2.67	114.87	123.22
36	a	414	PL9	C8-C7-C3	2.67	119.54	111.98
24	3	607	CHL	CMD-C2D-C3D	-2.67	121.46	127.61
24	5	606	CHL	CAC-C3C-C4C	2.67	128.28	124.81
25	C	504	CLA	CHD-C1D-ND	-2.67	122.00	124.45
27	7	1622	XAT	C10-C11-C12	-2.67	114.88	123.22
24	S	606	CHL	OMC-CMC-C2C	-2.67	119.64	125.69
25	B	617	CLA	CHB-C4A-NA	2.67	128.21	124.51
24	N	605	CHL	C4D-CHA-C1A	-2.67	118.00	121.25
27	3	1622	XAT	C10-C11-C12	-2.67	114.88	123.22
24	y	609	CHL	C4-C3-C5	2.67	119.76	115.27
36	D	405	PL9	C8-C7-C3	2.67	119.52	111.98
29	G	2630	LHG	O8-C23-C24	2.67	120.28	111.91
25	C	509	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
30	b	620	BCR	C33-C5-C6	-2.67	121.53	124.53
24	g	605	CHL	C1C-C2C-C3C	-2.67	105.00	107.11
24	y	605	CHL	C1C-C2C-C3C	-2.67	105.00	107.11
25	b	617	CLA	CHB-C4A-NA	2.67	128.20	124.51
30	t	101	BCR	C8-C9-C10	2.67	123.03	118.94
27	y	1622	XAT	C31-C32-C33	-2.67	118.92	126.42
25	b	605	CLA	CHB-C4A-NA	2.67	128.20	124.51
24	6	605	CHL	C1C-C2C-C3C	-2.67	105.00	107.11
26	6	1620	LUT	C21-C26-C27	-2.67	109.33	112.70
30	A	411	BCR	C38-C26-C25	-2.66	121.54	124.53
25	c	509	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
25	6	603	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
25	1	612	CLA	C2A-C1A-CHA	2.66	128.52	123.86
25	B	613	CLA	CMD-C2D-C3D	2.66	133.74	127.61
30	b	618	BCR	C16-C15-C14	-2.66	118.02	123.47
25	c	501	CLA	CMB-C2B-C3B	2.66	129.66	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	510	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
25	5	602	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
25	G	603	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	R	607	CHL	C4-C3-C5	2.66	119.75	115.27
26	2	1620	LUT	C21-C26-C27	-2.66	109.34	112.70
25	c	510	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
25	r	601	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	1	602	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	B	620	BCR	C33-C5-C6	-2.66	121.54	124.53
36	d	405	PL9	C8-C7-C3	2.66	119.50	111.98
24	Y	601	CHL	C4D-CHA-C1A	-2.66	118.01	121.25
25	C	501	CLA	CMB-C2B-C3B	2.66	129.66	124.68
29	g	2630	LHG	O8-C23-C24	2.66	120.26	111.91
35	b	622	LMG	O6-C1-O1	-2.66	103.67	109.97
30	A	411	BCR	C21-C20-C19	-2.66	114.92	123.22
27	Y	1622	XAT	C31-C32-C33	-2.66	118.94	126.42
25	n	602	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
25	d	402	CLA	CHD-C1D-ND	-2.66	122.01	124.45
24	N	608	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
30	T	101	BCR	C8-C9-C10	2.66	123.02	118.94
24	Y	609	CHL	C4-C3-C5	2.66	119.74	115.27
24	4	601	CHL	C3B-C4B-NB	2.66	112.65	109.21
24	3	605	CHL	C1C-C2C-C3C	-2.66	105.00	107.11
25	8	610	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
25	N	603	CLA	C2D-C1D-ND	-2.66	108.15	110.10
35	b	622	LMG	C38-C37-C36	-2.66	100.94	114.42
24	G	608	CHL	CMB-C2B-C3B	2.66	129.65	124.68
25	4	603	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
24	n	608	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
35	B	622	LMG	C38-C37-C36	-2.66	100.94	114.42
26	N	1621	LUT	C31-C30-C29	-2.65	123.52	127.31
26	n	1621	LUT	C31-C30-C29	-2.65	123.52	127.31
28	1	1623	NEX	C16-C1-C6	2.65	112.85	110.47
25	S	614	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	C	513	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	4	604	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
25	6	602	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
24	y	601	CHL	C2A-C1A-CHA	-2.65	119.22	123.86
30	d	404	BCR	C38-C26-C27	2.65	118.71	113.62
25	N	602	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
25	6	612	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
25	8	603	CLA	CAA-C2A-C3A	-2.65	105.52	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	603	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	r	607	CHL	C4-C3-C5	2.65	119.73	115.27
30	a	411	BCR	C21-C20-C19	-2.65	114.95	123.22
24	8	607	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
26	g	1621	LUT	C30-C31-C32	-2.65	114.95	123.22
24	4	607	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
25	5	612	CLA	C2A-C1A-CHA	2.65	128.49	123.86
25	y	603	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	G	605	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
27	R	622	XAT	C4-C3-C2	-2.65	105.66	110.77
25	b	613	CLA	CMD-C2D-C3D	2.65	133.71	127.61
30	B	618	BCR	C16-C15-C14	-2.65	118.05	123.47
36	d	405	PL9	O1-C4-C3	-2.65	117.80	120.72
24	2	609	CHL	C4-C3-C5	2.65	119.72	115.27
25	c	513	CLA	CHB-C4A-NA	2.65	128.17	124.51
24	5	607	CHL	CMB-C2B-C3B	2.65	129.63	124.68
24	1	609	CHL	CHD-C4C-C3C	-2.65	120.95	124.84
25	B	607	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
35	B	622	LMG	O6-C1-O1	-2.65	103.71	109.97
24	r	606	CHL	CMB-C2B-C3B	2.65	129.63	124.68
24	Y	601	CHL	C2A-C1A-CHA	-2.65	119.23	123.86
24	3	606	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
29	c	522	LHG	O8-C23-C24	2.64	120.21	111.91
30	C	516	BCR	C10-C11-C12	-2.64	114.97	123.22
24	G	609	CHL	CAA-C2A-C3A	-2.64	105.54	112.78
25	2	603	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
24	Y	605	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
27	8	622	XAT	C15-C35-C34	-2.64	118.06	123.47
25	4	610	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
28	2	1623	NEX	C16-C1-C6	2.64	112.84	110.47
24	n	605	CHL	C4D-CHA-C1A	-2.64	118.03	121.25
24	5	609	CHL	CHD-C4C-C3C	-2.64	120.96	124.84
24	n	609	CHL	CHD-C4C-C3C	-2.64	120.96	124.84
25	s	612	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
25	2	602	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
25	g	603	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	g	608	CHL	CMB-C2B-C3B	2.64	129.62	124.68
30	D	404	BCR	C38-C26-C27	2.64	118.69	113.62
26	g	1620	LUT	C39-C29-C28	2.64	122.23	118.08
26	1	1620	LUT	C21-C26-C27	-2.64	109.36	112.70
30	a	411	BCR	C38-C26-C25	-2.64	121.57	124.53
25	B	610	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	604	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	S	603	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
29	c	522	LHG	C11-C10-C9	-2.64	101.05	114.42
25	G	603	CLA	CHD-C1D-ND	-2.64	122.03	124.45
35	A	413	LMG	O3-C3-C2	-2.64	104.26	110.35
24	6	606	CHL	CMD-C2D-C3D	-2.63	121.55	127.61
30	4	623	BCR	C1-C6-C5	-2.63	118.90	122.61
25	s	604	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
25	b	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
28	y	1623	NEX	C35-C15-C14	-2.63	118.08	123.47
24	5	607	CHL	O2A-CGA-CBA	2.63	120.17	111.91
24	2	607	CHL	CAA-C2A-C3A	-2.63	105.57	112.78
24	5	608	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
29	C	522	LHG	C11-C10-C9	-2.63	101.06	114.42
24	1	608	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
25	B	604	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
24	g	609	CHL	CAA-C2A-C3A	-2.63	105.57	112.78
24	5	605	CHL	CMB-C2B-C3B	2.63	129.60	124.68
28	s	1623	NEX	C11-C12-C13	-2.63	119.03	126.42
29	C	522	LHG	O8-C23-C24	2.63	120.16	111.91
25	s	603	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
24	R	606	CHL	O2A-CGA-CBA	2.63	120.16	111.91
24	1	605	CHL	CMB-C2B-C3B	2.63	129.60	124.68
24	8	607	CHL	CMB-C2B-C3B	2.63	129.60	124.68
24	r	606	CHL	C1C-C2C-C3C	-2.63	105.03	107.11
25	S	604	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
25	2	612	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
24	6	607	CHL	CBA-CAA-C2A	-2.63	106.11	113.86
25	s	614	CLA	CHB-C4A-NA	2.63	128.15	124.51
27	r	622	XAT	C4-C3-C2	-2.63	105.70	110.77
24	3	609	CHL	O2A-CGA-CBA	2.63	120.15	111.91
36	d	405	PL9	C40-C39-C41	2.63	119.69	115.27
24	6	607	CHL	CAA-C2A-C3A	-2.63	105.58	112.78
25	N	613	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
35	a	413	LMG	O3-C3-C2	-2.63	104.28	110.35
25	S	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	7	609	CHL	O2A-CGA-CBA	2.63	120.15	111.91
24	s	601	CHL	CMB-C2B-C3B	2.63	129.59	124.68
26	5	1620	LUT	C21-C26-C27	-2.63	109.38	112.70
25	B	613	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
24	6	609	CHL	C4-C3-C5	2.63	119.69	115.27
25	a	406	CLA	O2D-CGD-O1D	-2.62	118.71	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	607	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
24	2	605	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
26	G	1621	LUT	C30-C31-C32	-2.62	115.03	123.22
28	6	1623	NEX	C16-C1-C6	2.62	112.82	110.47
24	1	607	CHL	CMB-C2B-C3B	2.62	129.59	124.68
24	N	609	CHL	CHD-C4C-C3C	-2.62	120.98	124.84
36	D	405	PL9	O1-C4-C3	-2.62	117.83	120.72
24	4	607	CHL	CMB-C2B-C3B	2.62	129.59	124.68
25	g	602	CLA	CHB-C4A-NA	2.62	128.14	124.51
25	S	612	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
24	G	601	CHL	C4-C3-C5	2.62	119.68	115.27
25	a	407	CLA	CHB-C4A-NA	2.62	128.14	124.51
25	n	602	CLA	CAC-C3C-C4C	2.62	128.21	124.81
25	6	610	CLA	CMB-C2B-C3B	2.62	129.59	124.68
28	g	1623	NEX	C11-C12-C13	-2.62	119.05	126.42
24	2	607	CHL	CMB-C2B-C3B	2.62	129.58	124.68
28	Y	1623	NEX	C35-C15-C14	-2.62	118.11	123.47
24	2	606	CHL	CMD-C2D-C3D	-2.62	121.59	127.61
24	s	601	CHL	C4A-NA-C1A	-2.62	105.53	106.71
24	1	607	CHL	O2A-CGA-CBA	2.62	120.13	111.91
25	s	610	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	b	604	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	r	602	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
24	3	607	CHL	OMC-CMC-C2C	-2.62	119.77	125.69
30	c	516	BCR	C10-C11-C12	-2.62	115.05	123.22
28	G	1623	NEX	C11-C12-C13	-2.62	119.06	126.42
24	3	607	CHL	C4-C3-C5	2.62	119.67	115.27
25	A	407	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	S	601	CHL	CMB-C2B-C3B	2.62	129.57	124.68
26	y	1621	LUT	C8-C9-C10	-2.62	114.93	118.94
24	8	608	CHL	C1C-C2C-C3C	-2.62	105.04	107.11
25	S	613	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	6	613	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	7	607	CHL	C4-C3-C5	2.62	119.67	115.27
24	R	606	CHL	CMB-C2B-C3B	2.62	129.57	124.68
25	5	603	CLA	CMB-C2B-C3B	2.62	129.57	124.68
25	n	610	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
24	2	607	CHL	CBA-CAA-C2A	-2.62	106.14	113.86
25	2	610	CLA	CMB-C2B-C3B	2.61	129.57	124.68
25	N	604	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
29	g	2630	LHG	C20-C19-C18	-2.61	101.16	114.42
24	r	606	CHL	O2A-CGA-CBA	2.61	120.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	613	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	g	601	CHL	C4-C3-C5	2.61	119.66	115.27
24	7	608	CHL	C4A-NA-C1A	-2.61	105.53	106.71
30	8	623	BCR	C1-C6-C5	-2.61	118.94	122.61
28	5	1623	NEX	C16-C1-C6	2.61	112.81	110.47
29	L	101	LHG	O8-C23-C24	2.61	120.10	111.91
24	6	607	CHL	CED-O2D-CGD	2.61	121.84	115.94
25	3	611	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
30	4	623	BCR	C7-C8-C9	-2.61	122.29	126.23
28	s	1623	NEX	C15-C35-C34	-2.61	118.13	123.47
28	S	1623	NEX	C11-C12-C13	-2.61	119.09	126.42
36	D	405	PL9	C40-C39-C41	2.61	119.66	115.27
29	l	101	LHG	O8-C23-C24	2.61	120.09	111.91
30	8	623	BCR	C7-C8-C9	-2.61	122.30	126.23
25	1	603	CLA	CMB-C2B-C3B	2.61	129.56	124.68
25	A	406	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	n	613	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
24	6	607	CHL	CMB-C2B-C3B	2.61	129.55	124.68
25	3	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	Y	1620	LUT	C19-C9-C8	2.60	122.18	118.08
25	R	602	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
24	5	608	CHL	C3B-C4B-NB	2.60	112.58	109.21
29	G	2630	LHG	C20-C19-C18	-2.60	101.21	114.42
24	2	607	CHL	CED-O2D-CGD	2.60	121.83	115.94
34	b	623	SQD	O8-S-C6	2.60	109.89	105.74
25	7	611	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
30	B	619	BCR	C28-C27-C26	-2.60	109.43	114.08
25	n	603	CLA	C2D-C1D-ND	-2.60	108.19	110.10
25	7	604	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	g	603	CLA	CHD-C1D-ND	-2.60	122.06	124.45
24	g	609	CHL	O2D-CGD-O1D	-2.60	118.75	123.84
26	G	1620	LUT	C39-C29-C28	2.60	122.17	118.08
24	s	608	CHL	CMB-C2B-C3B	2.60	129.54	124.68
25	b	613	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
35	B	622	LMG	C40-C39-C38	-2.60	101.23	114.42
24	5	607	CHL	CAA-C2A-C3A	-2.60	105.66	112.78
24	1	608	CHL	C3B-C4B-NB	2.60	112.57	109.21
25	c	511	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
35	b	622	LMG	C40-C39-C38	-2.60	101.24	114.42
24	3	601	CHL	CHB-C4A-NA	2.60	128.10	124.51
34	B	623	SQD	O8-S-C6	2.60	109.88	105.74
24	7	607	CHL	OMC-CMC-C2C	-2.60	119.82	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	S	608	CHL	CMB-C2B-C3B	2.60	129.53	124.68
34	A	418	SQD	O5-C5-C4	2.60	114.41	109.69
29	l	101	LHG	C11-C10-C9	-2.60	101.25	114.42
25	G	602	CLA	CHB-C4A-NA	2.59	128.10	124.51
28	S	1623	NEX	C15-C35-C34	-2.59	118.16	123.47
26	R	620	LUT	C38-C25-C24	-2.59	118.01	123.56
25	7	611	CLA	CHB-C4A-NA	2.59	128.10	124.51
35	z	101	LMG	C1-O6-C5	-2.59	108.60	113.69
24	8	608	CHL	OMC-CMC-C2C	-2.59	119.83	125.69
25	Y	602	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	L	101	LHG	C11-C10-C9	-2.59	101.27	114.42
27	2	1622	XAT	C6-C7-C8	-2.59	120.51	125.99
26	Y	1621	LUT	C8-C9-C10	-2.59	114.96	118.94
25	N	610	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
25	n	604	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
25	s	613	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
30	C	517	BCR	C21-C20-C19	-2.59	115.13	123.22
30	c	517	BCR	C21-C20-C19	-2.59	115.13	123.22
35	Z	101	LMG	C1-O6-C5	-2.59	108.60	113.69
26	7	1621	LUT	C30-C31-C32	-2.59	115.14	123.22
25	c	513	CLA	CBA-CAA-C2A	2.59	121.51	113.86
26	Y	1621	LUT	C15-C35-C34	-2.59	118.17	123.47
25	g	603	CLA	C3C-C4C-NC	-2.59	107.67	110.57
24	g	609	CHL	C4-C3-C5	2.59	119.62	115.27
26	y	1620	LUT	C19-C9-C8	2.59	122.16	118.08
24	7	601	CHL	CHB-C4A-NA	2.59	128.09	124.51
24	G	609	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
30	b	619	BCR	C28-C27-C26	-2.59	109.46	114.08
25	1	604	CLA	CHB-C4A-NA	2.59	128.09	124.51
27	6	1622	XAT	C6-C7-C8	-2.59	120.52	125.99
25	y	603	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
26	1	1621	LUT	C8-C7-C6	-2.59	119.94	127.20
24	4	608	CHL	OMC-CMC-C2C	-2.59	119.84	125.69
24	y	609	CHL	C4D-CHA-C1A	-2.58	118.10	121.25
25	1	612	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
25	7	614	CLA	CHB-C4A-NA	2.58	128.09	124.51
24	6	605	CHL	C2A-C3A-C4A	-2.58	97.70	101.87
24	2	605	CHL	C2A-C3A-C4A	-2.58	97.70	101.87
24	2	609	CHL	CMD-C2D-C3D	-2.58	121.67	127.61
26	5	1621	LUT	C8-C7-C6	-2.58	119.95	127.20
24	R	607	CHL	CMB-C2B-C3B	2.58	129.51	124.68
25	G	603	CLA	C3C-C4C-NC	-2.58	107.68	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	r	613	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	5	612	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
29	g	2630	LHG	C11-C10-C9	-2.58	101.32	114.42
24	6	609	CHL	CMD-C2D-C3D	-2.58	121.68	127.61
29	d	409	LHG	O8-C23-C24	2.58	120.00	111.91
25	R	613	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	3	603	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
24	Y	609	CHL	C4D-CHA-C1A	-2.58	118.11	121.25
26	g	1621	LUT	C31-C30-C29	-2.58	123.63	127.31
24	y	609	CHL	O2D-CGD-O1D	-2.58	118.80	123.84
25	3	614	CLA	CHB-C4A-NA	2.58	128.07	124.51
24	G	609	CHL	C4-C3-C5	2.58	119.61	115.27
26	3	1621	LUT	C30-C31-C32	-2.58	115.18	123.22
24	1	607	CHL	CAA-C2A-C3A	-2.58	105.73	112.78
25	Y	613	CLA	CAC-C3C-C4C	2.57	128.15	124.81
29	D	409	LHG	O8-C23-C24	2.57	119.99	111.91
24	Y	609	CHL	O2D-CGD-O1D	-2.57	118.80	123.84
25	Y	613	CLA	CHB-C4A-NA	2.57	128.07	124.51
34	a	418	SQD	O5-C5-C4	2.57	114.37	109.69
26	r	620	LUT	C38-C25-C24	-2.57	118.05	123.56
25	B	610	CLA	C7-C6-C5	-2.57	106.37	113.36
24	7	607	CHL	O2A-CGA-CBA	2.57	119.98	111.91
25	y	602	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
29	C	2630	LHG	C11-C10-C9	-2.57	101.36	114.42
25	b	615	CLA	C2D-C1D-ND	-2.57	108.21	110.10
24	4	601	CHL	CMB-C2B-C3B	2.57	129.49	124.68
25	3	613	CLA	CMB-C2B-C3B	2.57	129.49	124.68
29	G	2630	LHG	C11-C10-C9	-2.57	101.37	114.42
24	N	605	CHL	CHB-C4A-NA	2.57	128.07	124.51
29	d	410	LHG	C11-C10-C9	-2.57	101.37	114.42
25	C	511	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
24	1	606	CHL	CMB-C2B-C3B	2.57	129.49	124.68
25	C	513	CLA	CBA-CAA-C2A	2.57	121.45	113.86
24	n	605	CHL	CHB-C4A-NA	2.57	128.07	124.51
25	3	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
25	N	602	CLA	CAC-C3C-C4C	2.57	128.14	124.81
29	c	2630	LHG	C11-C10-C9	-2.57	101.38	114.42
25	R	603	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	y	613	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	r	608	CHL	CMB-C2B-C3B	2.57	129.49	124.68
29	D	410	LHG	C11-C10-C9	-2.57	101.38	114.42
25	7	603	CLA	CAA-C2A-C3A	-2.57	105.74	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	1621	LUT	C31-C30-C29	-2.57	123.64	127.31
25	4	612	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	8	601	CHL	CMB-C2B-C3B	2.57	129.48	124.68
25	g	602	CLA	C6-C7-C8	-2.57	107.62	115.92
25	4	611	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
26	y	1621	LUT	C15-C35-C34	-2.57	118.22	123.47
25	Y	603	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
25	5	604	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	5	605	CHL	C1B-CHB-C4A	-2.57	125.03	130.12
26	y	1621	LUT	C28-C29-C30	-2.57	115.00	118.94
24	n	601	CHL	C4D-CHA-C1A	-2.57	118.13	121.25
24	5	606	CHL	CMB-C2B-C3B	2.57	129.48	124.68
25	A	406	CLA	CHD-C1D-ND	-2.57	122.10	124.45
27	r	622	XAT	C38-C25-C24	2.56	117.17	114.28
24	s	608	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
25	8	612	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	Y	1620	LUT	C15-C35-C34	-2.56	118.22	123.47
24	2	606	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
25	b	610	CLA	C7-C6-C5	-2.56	106.40	113.36
35	d	411	LMG	C6-C5-C4	-2.56	107.00	113.00
30	B	620	BCR	C16-C15-C14	-2.56	118.23	123.47
25	3	604	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	B	606	CLA	C1-C2-C3	-2.56	121.61	126.04
36	D	405	PL9	C22-C23-C24	-2.56	121.49	127.66
24	R	606	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
24	3	607	CHL	O2A-CGA-CBA	2.56	119.94	111.91
24	y	609	CHL	O1D-CGD-CBD	-2.56	119.25	124.48
26	n	1621	LUT	C30-C31-C32	-2.56	115.23	123.22
25	6	611	CLA	O2D-CGD-CBD	2.56	115.82	111.27
24	Y	609	CHL	O1D-CGD-CBD	-2.56	119.25	124.48
25	y	602	CLA	CAA-CBA-CGA	-2.56	105.77	113.25
25	r	603	CLA	CHB-C4A-NA	2.56	128.05	124.51
27	y	1622	XAT	C7-C8-C9	-2.56	121.56	125.53
35	D	411	LMG	C6-C5-C4	-2.56	107.01	113.00
30	b	620	BCR	C16-C15-C14	-2.56	118.23	123.47
25	7	613	CLA	CMB-C2B-C3B	2.56	129.47	124.68
25	g	603	CLA	CMB-C2B-C3B	2.56	129.47	124.68
27	Y	1622	XAT	C7-C8-C9	-2.56	121.56	125.53
26	s	1620	LUT	C38-C25-C24	-2.56	118.09	123.56
24	R	608	CHL	CMB-C2B-C3B	2.56	129.46	124.68
24	r	607	CHL	CMB-C2B-C3B	2.56	129.46	124.68
25	1	603	CLA	CAA-C2A-C3A	-2.56	105.78	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	1621	LUT	C30-C31-C32	-2.56	115.24	123.22
26	Y	1621	LUT	C28-C29-C30	-2.56	115.02	118.94
25	2	604	CLA	O2A-CGA-O1A	-2.56	116.93	123.30
24	S	601	CHL	C4A-NA-C1A	-2.56	105.56	106.71
24	n	609	CHL	CAA-C2A-C3A	-2.56	105.78	112.78
24	3	609	CHL	O1D-CGD-CBD	-2.56	119.26	124.48
25	Y	602	CLA	CAA-CBA-CGA	-2.55	105.79	113.25
25	G	603	CLA	CMB-C2B-C3B	2.55	129.46	124.68
25	G	602	CLA	C6-C7-C8	-2.55	107.66	115.92
24	3	608	CHL	C4A-NA-C1A	-2.55	105.56	106.71
36	D	405	PL9	C50-C49-C48	-2.55	115.27	122.65
27	3	1622	XAT	C19-C9-C8	2.55	122.10	118.08
26	y	1620	LUT	C15-C35-C34	-2.55	118.25	123.47
25	5	603	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
24	1	605	CHL	C1B-CHB-C4A	-2.55	125.06	130.12
25	6	604	CLA	O2A-CGA-O1A	-2.55	116.94	123.30
24	N	609	CHL	CAA-C2A-C3A	-2.55	105.79	112.78
25	7	604	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
25	8	611	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
27	R	622	XAT	C38-C25-C24	2.55	117.15	114.28
30	h	101	BCR	C3-C4-C5	-2.55	109.53	114.08
24	Y	605	CHL	CMB-C2B-C3B	2.55	129.44	124.68
24	2	607	CHL	O2A-CGA-CBA	2.55	119.90	111.91
24	G	608	CHL	CHB-C4A-NA	2.55	128.03	124.51
36	d	405	PL9	C50-C49-C48	-2.55	115.28	122.65
25	b	606	CLA	C1-C2-C3	-2.55	121.64	126.04
25	7	612	CLA	C4A-NA-C1A	2.55	107.85	106.71
29	3	2630	LHG	C11-C10-C9	-2.55	101.50	114.42
26	S	1620	LUT	C38-C25-C24	-2.55	118.11	123.56
36	d	405	PL9	C22-C23-C24	-2.54	121.53	127.66
26	S	1620	LUT	C31-C30-C29	-2.54	123.68	127.31
24	s	608	CHL	CMD-C2D-C3D	-2.54	121.76	127.61
26	7	1620	LUT	C31-C30-C29	-2.54	123.68	127.31
26	7	1620	LUT	C37-C21-C22	-2.54	104.62	109.44
29	6	2630	LHG	O8-C23-C24	2.54	119.89	111.91
30	C	516	BCR	C11-C10-C9	-2.54	123.68	127.31
29	7	2630	LHG	C11-C10-C9	-2.54	101.53	114.42
26	r	620	LUT	C35-C15-C14	-2.54	118.27	123.47
26	3	1620	LUT	C31-C30-C29	-2.54	123.69	127.31
25	B	615	CLA	C2D-C1D-ND	-2.54	108.23	110.10
29	2	2630	LHG	O8-C23-C24	2.54	119.87	111.91
26	R	620	LUT	C35-C15-C14	-2.54	118.28	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	613	CLA	CAC-C3C-C4C	2.54	128.10	124.81
26	2	1620	LUT	C8-C7-C6	-2.54	120.08	127.20
25	r	613	CLA	CMB-C2B-C3B	2.54	129.42	124.68
26	4	620	LUT	C8-C7-C6	-2.54	120.08	127.20
24	S	608	CHL	CMD-C2D-C3D	-2.53	121.78	127.61
24	6	607	CHL	O2A-CGA-CBA	2.53	119.86	111.91
30	C	517	BCR	C38-C26-C25	-2.53	121.68	124.53
30	H	101	BCR	C3-C4-C5	-2.53	109.55	114.08
24	N	601	CHL	C4D-CHA-C1A	-2.53	118.17	121.25
25	C	502	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
25	G	612	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
24	s	607	CHL	C4-C3-C5	2.53	119.53	115.27
24	y	605	CHL	CMB-C2B-C3B	2.53	129.42	124.68
25	g	612	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
35	C	521	LMG	O6-C1-O1	-2.53	103.98	109.97
26	3	1620	LUT	C37-C21-C22	-2.53	104.64	109.44
24	S	607	CHL	C4-C3-C5	2.53	119.53	115.27
29	D	409	LHG	C20-C19-C18	-2.53	101.57	114.42
25	c	502	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
25	N	602	CLA	C1-C2-C3	-2.53	121.67	126.04
25	2	611	CLA	O2D-CGD-CBD	2.53	115.77	111.27
24	7	609	CHL	O1D-CGD-CBD	-2.53	119.31	124.48
35	c	521	LMG	O6-C1-O1	-2.53	103.98	109.97
25	r	602	CLA	CAA-CBA-CGA	-2.53	105.86	113.25
25	4	603	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
25	B	615	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	6	1620	LUT	C8-C7-C6	-2.53	120.10	127.20
29	c	2630	LHG	C20-C19-C18	-2.53	101.58	114.42
29	C	2630	LHG	C20-C19-C18	-2.53	101.58	114.42
27	7	1622	XAT	C19-C9-C8	2.53	122.06	118.08
26	s	1620	LUT	C16-C1-C6	-2.53	106.20	110.30
25	B	610	CLA	C1-C2-C3	-2.53	121.67	126.04
26	8	620	LUT	C8-C7-C6	-2.53	120.11	127.20
25	b	615	CLA	CHB-C4A-NA	2.53	128.00	124.51
29	d	409	LHG	C20-C19-C18	-2.53	101.60	114.42
25	n	602	CLA	C1-C2-C3	-2.53	121.67	126.04
26	y	1621	LUT	C39-C29-C28	2.53	122.06	118.08
25	b	610	CLA	C1-C2-C3	-2.52	121.68	126.04
24	7	608	CHL	CMD-C2D-C3D	-2.52	121.81	127.61
24	3	608	CHL	CMD-C2D-C3D	-2.52	121.81	127.61
26	s	1620	LUT	C21-C26-C27	-2.52	109.51	112.70
26	Y	1621	LUT	C39-C29-C28	2.52	122.05	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	7	1621	LUT	C38-C25-C24	-2.52	118.16	123.56
25	3	612	CLA	C4A-NA-C1A	2.52	107.84	106.71
28	n	1623	NEX	C19-C9-C10	-2.52	119.39	122.92
25	R	602	CLA	CAA-CBA-CGA	-2.52	105.88	113.25
26	s	1620	LUT	C31-C30-C29	-2.52	123.71	127.31
25	S	614	CLA	CHD-C1D-ND	-2.52	122.14	124.45
26	S	1620	LUT	C21-C26-C27	-2.52	109.51	112.70
30	c	517	BCR	C38-C26-C25	-2.52	121.70	124.53
26	5	1621	LUT	C30-C31-C32	-2.52	115.35	123.22
25	4	612	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
25	g	610	CLA	CHB-C4A-NA	2.52	127.99	124.51
25	R	613	CLA	CMB-C2B-C3B	2.52	129.39	124.68
24	6	606	CHL	C1C-C2C-C3C	-2.52	105.12	107.11
24	g	609	CHL	CMB-C2B-C3B	2.52	129.39	124.68
25	8	603	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
26	1	1621	LUT	C30-C31-C32	-2.52	115.36	123.22
25	4	610	CLA	C4A-NA-C1A	2.52	107.84	106.71
28	y	1623	NEX	C31-C30-C29	-2.52	123.72	127.31
24	g	608	CHL	CHB-C4A-NA	2.51	127.99	124.51
26	S	1620	LUT	C16-C1-C6	-2.51	106.22	110.30
24	2	608	CHL	CMD-C2D-C3D	-2.51	121.83	127.61
25	S	612	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
25	G	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	d	409	LHG	C18-C17-C16	-2.51	101.68	114.42
29	D	409	LHG	C18-C17-C16	-2.51	101.68	114.42
26	G	1620	LUT	C19-C9-C8	2.51	122.03	118.08
28	Y	1623	NEX	C31-C30-C29	-2.51	123.73	127.31
26	3	1621	LUT	C38-C25-C24	-2.51	118.19	123.56
35	a	413	LMG	C40-C39-C38	-2.51	101.70	114.42
24	S	608	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
24	r	614	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
25	R	612	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
25	B	606	CLA	CHD-C1D-ND	-2.51	122.15	124.45
25	g	604	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
26	g	1620	LUT	C19-C9-C8	2.50	122.02	118.08
25	a	406	CLA	CHD-C1D-ND	-2.50	122.15	124.45
25	s	604	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
25	R	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	b	606	CLA	CMB-C2B-C3B	2.50	129.36	124.68
25	N	612	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
25	B	612	CLA	CHC-C1C-NC	2.50	128.00	124.20
35	A	413	LMG	C40-C39-C38	-2.50	101.72	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	602	CLA	C1-C2-C3	-2.50	121.72	126.04
25	N	611	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
26	G	1621	LUT	C22-C23-C24	-2.50	108.89	111.74
25	6	602	CLA	C1-C2-C3	-2.50	121.72	126.04
24	Y	606	CHL	CHB-C4A-NA	2.50	127.97	124.51
26	Y	1620	LUT	C8-C9-C10	-2.50	115.11	118.94
24	3	609	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
33	A	409	PHO	O2D-CGD-O1D	-2.50	118.95	123.84
25	s	614	CLA	CHD-C1D-ND	-2.50	122.16	124.45
24	G	609	CHL	CMB-C2B-C3B	2.50	129.35	124.68
28	7	1623	NEX	C12-C13-C14	2.50	122.78	118.94
25	b	602	CLA	C2D-C1D-ND	-2.50	108.26	110.10
24	7	609	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
25	s	612	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
25	r	602	CLA	CHD-C1D-ND	-2.50	122.16	124.45
25	n	612	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
24	6	608	CHL	CMD-C2D-C3D	-2.50	121.87	127.61
25	r	602	CLA	CHB-C4A-NA	2.50	127.96	124.51
26	6	1620	LUT	C19-C9-C8	2.49	122.01	118.08
24	g	605	CHL	CMB-C2B-C3B	2.49	129.34	124.68
26	1	1621	LUT	O3-C3-C2	-2.49	104.85	109.80
29	r	2630	LHG	C11-C10-C9	-2.49	101.77	114.42
28	N	1623	NEX	C19-C9-C10	-2.49	119.43	122.92
25	b	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	r	612	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	S	1620	LUT	C39-C29-C28	2.49	122.00	118.08
24	3	601	CHL	O1D-CGD-CBD	-2.49	119.39	124.48
26	2	1620	LUT	C19-C9-C8	2.49	122.00	118.08
24	1	608	CHL	CHB-C4A-NA	2.49	127.95	124.51
25	2	610	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	R	2630	LHG	C11-C10-C9	-2.49	101.79	114.42
35	Z	101	LMG	O8-C28-O10	-2.49	117.31	123.59
24	7	601	CHL	O1D-CGD-CBD	-2.49	119.39	124.48
24	G	605	CHL	CMB-C2B-C3B	2.49	129.33	124.68
24	G	601	CHL	O2A-CGA-CBA	2.49	119.72	111.91
24	N	607	CHL	CMD-C2D-C3D	-2.49	121.89	127.61
26	5	1620	LUT	C39-C29-C28	2.49	122.00	118.08
25	G	604	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
24	2	605	CHL	O1D-CGD-CBD	-2.49	119.39	124.48
25	B	606	CLA	CMB-C2B-C3B	2.49	129.33	124.68
25	8	612	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
25	S	604	CLA	O2D-CGD-O1D	-2.49	118.98	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g	1621	LUT	C22-C23-C24	-2.49	108.91	111.74
24	g	601	CHL	O2A-CGA-CBA	2.49	119.71	111.91
24	y	606	CHL	CHB-C4A-NA	2.49	127.95	124.51
25	c	503	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	s	607	CHL	CMB-C2B-C3B	2.49	129.33	124.68
27	n	1622	XAT	C39-C29-C30	-2.48	119.44	122.92
26	y	1620	LUT	C8-C9-C10	-2.48	115.13	118.94
25	B	613	CLA	CAA-CBA-CGA	-2.48	105.99	113.25
25	B	611	CLA	CHB-C4A-NA	2.48	127.95	124.51
26	6	1621	LUT	C3-C4-C5	-2.48	106.91	111.85
24	n	607	CHL	CMD-C2D-C3D	-2.48	121.90	127.61
24	Y	608	CHL	O2A-CGA-CBA	2.48	119.70	111.91
25	C	503	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	s	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	R	602	CLA	CHD-C1D-ND	-2.48	122.17	124.45
26	5	1621	LUT	O3-C3-C2	-2.48	104.87	109.80
25	r	609	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
28	3	1623	NEX	C12-C13-C14	2.48	122.75	118.94
26	s	1621	LUT	C38-C25-C24	-2.48	118.25	123.56
30	c	516	BCR	C11-C10-C9	-2.48	123.77	127.31
25	8	610	CLA	C4A-NA-C1A	2.48	107.82	106.71
27	N	1622	XAT	C39-C29-C30	-2.48	119.45	122.92
24	7	605	CHL	CMD-C2D-C3D	-2.48	121.91	127.61
24	S	607	CHL	CMB-C2B-C3B	2.48	129.32	124.68
25	n	611	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
26	2	1621	LUT	C3-C4-C5	-2.48	106.92	111.85
27	R	622	XAT	C8-C9-C10	-2.48	115.14	118.94
29	1	2630	LHG	O8-C23-C24	2.48	119.69	111.91
25	b	613	CLA	CAA-CBA-CGA	-2.48	106.01	113.25
26	s	1620	LUT	C39-C29-C28	2.48	121.98	118.08
26	n	1620	LUT	C39-C29-C28	2.48	121.98	118.08
26	7	1620	LUT	C38-C25-C24	-2.48	118.26	123.56
30	B	619	BCR	C29-C30-C25	2.48	114.29	110.48
24	5	608	CHL	CHB-C4A-NA	2.48	127.94	124.51
25	Y	610	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	1	613	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	R	612	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
27	r	622	XAT	C8-C9-C10	-2.48	115.14	118.94
25	8	602	CLA	CHD-C1D-ND	-2.48	122.18	124.45
25	Y	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	6	610	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	y	602	CLA	CHB-C4A-NA	2.48	127.94	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	1622	XAT	C5-C4-C3	-2.48	107.85	112.75
24	n	605	CHL	CMB-C2B-C3B	2.48	129.31	124.68
24	6	605	CHL	O1D-CGD-CBD	-2.47	119.42	124.48
35	z	101	LMG	O8-C28-O10	-2.47	117.35	123.59
33	a	408	PHO	CMB-C2B-C3B	2.47	129.31	124.68
33	a	409	PHO	O2D-CGD-O1D	-2.47	119.00	123.84
37	c	518	DGD	O3E-C3E-C2E	-2.47	104.63	110.35
28	2	1623	NEX	C28-C29-C30	2.47	122.74	118.94
37	h	102	DGD	O2D-C2D-C1D	-2.47	104.04	110.05
25	S	611	CLA	CHB-C4A-NA	2.47	127.93	124.51
37	H	102	DGD	O2D-C2D-C1D	-2.47	104.04	110.05
30	b	619	BCR	C29-C30-C25	2.47	114.29	110.48
24	3	605	CHL	CMD-C2D-C3D	-2.47	121.93	127.61
36	D	405	PL9	C27-C28-C29	-2.47	121.71	127.66
25	5	613	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
36	d	405	PL9	C46-C47-C48	-2.47	103.76	111.88
26	g	1621	LUT	C19-C9-C8	2.47	121.97	118.08
29	5	2630	LHG	O8-C23-C24	2.47	119.66	111.91
26	2	1621	LUT	C35-C15-C14	-2.47	118.41	123.47
25	r	610	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
24	2	605	CHL	OMC-CMC-C2C	-2.47	120.10	125.69
35	b	2633	LMG	C40-C39-C38	-2.47	101.89	114.42
25	r	612	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
24	7	606	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
24	3	606	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
25	a	406	CLA	O2D-CGD-CBD	2.47	115.66	111.27
33	A	408	PHO	CMB-C2B-C3B	2.47	129.30	124.68
25	R	609	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
25	Y	614	CLA	CMB-C2B-C3B	2.47	129.30	124.68
24	G	606	CHL	CHB-C4A-NA	2.47	127.92	124.51
35	B	2633	LMG	C40-C39-C38	-2.47	101.90	114.42
26	r	620	LUT	C12-C13-C14	-2.47	115.15	118.94
36	d	405	PL9	C27-C28-C29	-2.47	121.72	127.66
26	1	1620	LUT	C39-C29-C28	2.47	121.97	118.08
24	y	608	CHL	O2A-CGA-CBA	2.47	119.65	111.91
25	5	610	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	g	602	CLA	C1-C2-C3	-2.47	121.78	126.04
24	g	606	CHL	CHB-C4A-NA	2.47	127.92	124.51
25	d	402	CLA	CAA-CBA-CGA	-2.47	106.05	113.25
25	n	602	CLA	CAA-CBA-CGA	-2.47	106.05	113.25
37	c	518	DGD	C1E-O6E-C5E	2.47	118.53	113.69
26	R	620	LUT	C12-C13-C14	-2.46	115.16	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	n	603	CLA	C3C-C4C-NC	-2.46	107.81	110.57
25	R	610	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
26	S	1621	LUT	C38-C25-C24	-2.46	118.29	123.56
25	1	611	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
36	D	405	PL9	C46-C47-C48	-2.46	103.78	111.88
25	n	610	CLA	CHB-C4A-NA	2.46	127.92	124.51
37	C	518	DGD	O3E-C3E-C2E	-2.46	104.65	110.35
25	R	616	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
25	G	602	CLA	C1-C2-C3	-2.46	121.78	126.04
25	N	602	CLA	CAA-CBA-CGA	-2.46	106.05	113.25
25	S	604	CLA	C1-C2-C3	-2.46	122.77	126.75
26	6	1621	LUT	C35-C15-C14	-2.46	118.43	123.47
29	N	2630	LHG	C20-C19-C18	-2.46	101.92	114.42
24	7	601	CHL	CMB-C2B-C3B	2.46	129.28	124.68
29	n	2630	LHG	C20-C19-C18	-2.46	101.93	114.42
26	3	1620	LUT	C38-C25-C24	-2.46	118.29	123.56
37	C	518	DGD	C1E-O6E-C5E	2.46	118.52	113.69
25	b	606	CLA	CHD-C1D-ND	-2.46	122.19	124.45
24	4	606	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
25	s	604	CLA	C1-C2-C3	-2.46	122.77	126.75
25	D	402	CLA	CAA-CBA-CGA	-2.46	106.07	113.25
25	1	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	5	605	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
25	A	406	CLA	O2D-CGD-CBD	2.46	115.64	111.27
24	N	606	CHL	CHB-C4A-NA	2.46	127.91	124.51
26	6	1620	LUT	C35-C15-C14	-2.46	118.44	123.47
26	N	1620	LUT	C39-C29-C28	2.46	121.95	118.08
26	n	1621	LUT	C19-C9-C8	2.46	121.95	118.08
24	8	601	CHL	CHD-C4C-C3C	-2.46	121.23	124.84
25	b	612	CLA	CHC-C1C-NC	2.46	127.93	124.20
27	5	1622	XAT	C5-C4-C3	-2.46	107.89	112.75
29	1	2630	LHG	C18-C17-C16	-2.45	101.96	114.42
25	y	614	CLA	CMB-C2B-C3B	2.45	129.27	124.68
30	C	517	BCR	C11-C12-C13	-2.45	119.52	126.42
29	5	2630	LHG	C18-C17-C16	-2.45	101.97	114.42
25	y	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	4	601	CHL	CHD-C4C-C3C	-2.45	121.23	124.84
24	7	605	CHL	CMB-C2B-C3B	2.45	129.26	124.68
25	r	616	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
25	7	603	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
25	R	616	CLA	CHD-C1D-ND	-2.45	122.20	124.45
24	n	606	CHL	CHB-C4A-NA	2.45	127.90	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	611	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
30	8	623	BCR	C27-C26-C25	-2.45	119.17	122.73
24	R	614	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
25	N	603	CLA	C3C-C4C-NC	-2.45	107.83	110.57
24	N	605	CHL	CMB-C2B-C3B	2.45	129.26	124.68
25	b	611	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
26	N	1621	LUT	C15-C35-C34	-2.45	118.46	123.47
24	6	605	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
26	S	1621	LUT	C19-C9-C8	2.45	121.93	118.08
27	G	1622	XAT	C5-C4-C3	-2.45	107.91	112.75
24	Y	609	CHL	CMB-C2B-C3B	2.45	129.26	124.68
24	3	605	CHL	CMB-C2B-C3B	2.45	129.26	124.68
24	3	601	CHL	CMB-C2B-C3B	2.45	129.25	124.68
24	2	605	CHL	CMD-C2D-C3D	-2.45	121.99	127.61
24	s	601	CHL	C2A-C1A-CHA	-2.45	119.58	123.86
26	6	1621	LUT	C8-C7-C6	-2.45	120.33	127.20
24	6	605	CHL	CMB-C2B-C3B	2.45	129.25	124.68
24	1	609	CHL	O1D-CGD-CBD	-2.45	119.48	124.48
25	N	610	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	G	1621	LUT	C19-C9-C8	2.44	121.93	118.08
26	2	1620	LUT	C35-C15-C14	-2.44	118.47	123.47
25	R	611	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
27	g	1622	XAT	C5-C4-C3	-2.44	107.91	112.75
25	n	602	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
25	R	611	CLA	CMB-C2B-C3B	2.44	129.25	124.68
26	n	1621	LUT	C8-C9-C10	-2.44	115.19	118.94
28	6	1623	NEX	C28-C29-C30	2.44	122.69	118.94
37	C	518	DGD	C3G-C2G-C1G	-2.44	106.01	111.79
24	1	605	CHL	CMD-C2D-C3D	-2.44	122.00	127.61
30	c	517	BCR	C11-C12-C13	-2.44	119.56	126.42
26	N	1621	LUT	C19-C9-C8	2.44	121.92	118.08
25	b	614	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
25	3	603	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
25	N	602	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
25	Y	611	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	S	601	CHL	C2A-C1A-CHA	-2.44	119.59	123.86
29	S	2630	LHG	O8-C23-C24	2.44	119.56	111.91
24	y	605	CHL	CMD-C2D-C3D	-2.44	122.00	127.61
24	8	606	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
35	D	411	LMG	O1-C7-C8	-2.44	105.01	110.90
27	6	1622	XAT	C39-C29-C30	-2.44	119.51	122.92
25	3	612	CLA	CMD-C2D-C1D	-2.44	120.41	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	605	CHL	CMD-C2D-C3D	-2.44	122.00	127.61
26	n	1621	LUT	C15-C35-C34	-2.44	118.48	123.47
24	4	609	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
37	c	518	DGD	C3G-C2G-C1G	-2.44	106.02	111.79
27	3	1622	XAT	C39-C29-C30	-2.44	119.51	122.92
28	3	1623	NEX	C20-C13-C14	-2.44	119.51	122.92
25	B	602	CLA	C2D-C1D-ND	-2.44	108.31	110.10
24	5	609	CHL	O1D-CGD-CBD	-2.44	119.50	124.48
29	3	2630	LHG	O8-C6-C5	-2.44	101.34	108.43
24	y	609	CHL	CMB-C2B-C3B	2.44	129.24	124.68
28	Y	1623	NEX	C30-C31-C32	-2.44	115.61	123.22
33	a	408	PHO	O2A-CGA-O1A	-2.44	117.44	123.59
26	r	620	LUT	C19-C9-C8	2.44	121.92	118.08
25	B	614	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
25	y	603	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
29	s	2630	LHG	O8-C23-C24	2.43	119.55	111.91
29	7	2630	LHG	O8-C6-C5	-2.43	101.35	108.43
25	Y	603	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
28	1	1623	NEX	C19-C9-C10	-2.43	119.51	122.92
30	b	619	BCR	C21-C20-C19	-2.43	115.62	123.22
24	8	609	CHL	C1C-C2C-C3C	-2.43	105.18	107.11
26	3	1621	LUT	C15-C35-C34	-2.43	118.49	123.47
25	r	611	CLA	CMB-C2B-C3B	2.43	129.23	124.68
26	2	1621	LUT	C8-C7-C6	-2.43	120.37	127.20
25	N	613	CLA	CHB-C4A-NA	2.43	127.88	124.51
29	L	101	LHG	C20-C19-C18	-2.43	102.08	114.42
34	b	623	SQD	O6-C44-C45	-2.43	105.03	110.90
29	y	2630	LHG	C20-C19-C18	-2.43	102.09	114.42
24	2	605	CHL	CMB-C2B-C3B	2.43	129.22	124.68
25	B	616	CLA	CMB-C2B-C3B	2.43	129.22	124.68
25	r	611	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
25	C	510	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	n	613	CLA	CHB-C4A-NA	2.43	127.87	124.51
35	d	411	LMG	O1-C7-C8	-2.43	105.04	110.90
29	Y	2630	LHG	C20-C19-C18	-2.43	102.09	114.42
30	B	619	BCR	C21-C20-C19	-2.43	115.64	123.22
25	r	612	CLA	CMB-C2B-C3B	2.43	129.22	124.68
25	y	612	CLA	CMB-C2B-C3B	2.43	129.22	124.68
29	D	408	LHG	O8-C23-O10	-2.43	117.46	123.59
28	y	1623	NEX	C30-C31-C32	-2.43	115.64	123.22
25	c	512	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	Y	612	CLA	CMB-C2B-C3B	2.43	129.22	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	603	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
25	n	613	CLA	CAC-C3C-C4C	2.43	127.96	124.81
25	c	510	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	N	1621	LUT	C8-C9-C10	-2.43	115.22	118.94
26	S	1620	LUT	C7-C8-C9	-2.43	122.57	126.23
25	B	611	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
28	5	1623	NEX	C19-C9-C10	-2.43	119.53	122.92
33	A	409	PHO	O1D-CGD-CBD	2.43	128.78	124.74
25	7	612	CLA	CMD-C2D-C1D	-2.43	120.44	124.71
25	1	610	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
26	s	1621	LUT	C19-C9-C8	2.42	121.90	118.08
26	7	1621	LUT	C15-C35-C34	-2.42	118.51	123.47
34	B	623	SQD	C44-O6-C1	2.42	118.47	113.74
25	b	617	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
27	7	1622	XAT	C39-C29-C30	-2.42	119.53	122.92
25	r	616	CLA	CHD-C1D-ND	-2.42	122.23	124.45
24	4	606	CHL	CMD-C2D-C3D	-2.42	122.04	127.61
29	l	101	LHG	C20-C19-C18	-2.42	102.13	114.42
27	2	1622	XAT	C39-C29-C30	-2.42	119.53	122.92
33	A	408	PHO	O2A-CGA-O1A	-2.42	117.48	123.59
25	Y	610	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
28	1	1623	NEX	C2-C1-C6	2.42	111.56	109.21
24	Y	605	CHL	CMD-C2D-C3D	-2.42	122.05	127.61
24	6	609	CHL	C1B-CHB-C4A	-2.42	125.32	130.12
24	2	601	CHL	C2A-C1A-CHA	-2.42	119.63	123.86
25	N	613	CLA	CAC-C3C-C4C	2.42	127.95	124.81
28	7	1623	NEX	C20-C13-C14	-2.42	119.53	122.92
26	Y	1621	LUT	C16-C1-C6	-2.42	106.37	110.30
26	g	1620	LUT	C28-C29-C30	-2.42	115.23	118.94
30	4	623	BCR	C27-C26-C25	-2.42	119.22	122.73
34	a	418	SQD	O47-C45-C44	2.42	117.16	108.40
25	4	611	CLA	CHD-C1D-ND	-2.42	122.23	124.45
29	d	408	LHG	O8-C23-O10	-2.42	117.49	123.59
26	R	620	LUT	C19-C9-C8	2.42	121.89	118.08
25	R	612	CLA	CMB-C2B-C3B	2.42	129.20	124.68
25	y	611	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	R	603	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	Y	601	CHL	O2A-CGA-CBA	2.42	119.49	111.91
29	n	2630	LHG	C27-C26-C25	-2.42	102.16	114.42
26	2	1621	LUT	C31-C30-C29	-2.42	123.86	127.31
25	n	603	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
27	5	1622	XAT	C31-C32-C33	-2.41	119.63	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	4	602	CLA	CHD-C1D-ND	-2.41	122.23	124.45
27	7	1622	XAT	C25-C24-C23	-2.41	107.97	112.75
25	8	604	CLA	O2A-CGA-O1A	-2.41	117.28	123.30
24	2	609	CHL	C1B-CHB-C4A	-2.41	125.33	130.12
26	8	620	LUT	C1-C6-C5	-2.41	119.21	122.61
24	S	606	CHL	CMB-C2B-C3B	2.41	129.19	124.68
30	B	619	BCR	C10-C11-C12	-2.41	115.68	123.22
25	C	512	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	s	606	CHL	CMB-C2B-C3B	2.41	129.19	124.68
26	S	1620	LUT	C19-C9-C8	2.41	121.88	118.08
25	7	610	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
33	a	409	PHO	O1D-CGD-CBD	2.41	128.76	124.74
34	b	623	SQD	O48-C23-C24	2.41	119.48	111.91
25	B	617	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
27	1	1622	XAT	C31-C32-C33	-2.41	119.64	126.42
29	B	2631	LHG	C11-C10-C9	-2.41	102.18	114.42
29	N	2630	LHG	C27-C26-C25	-2.41	102.18	114.42
27	3	1622	XAT	C25-C24-C23	-2.41	107.98	112.75
25	2	602	CLA	CAA-CBA-CGA	-2.41	106.21	113.25
34	B	623	SQD	O6-C44-C45	-2.41	105.08	110.90
24	2	609	CHL	C1-C2-C3	-2.41	121.87	126.04
27	2	1622	XAT	C10-C11-C12	-2.41	115.69	123.22
29	n	2630	LHG	C18-C17-C16	-2.41	102.19	114.42
24	y	601	CHL	O2A-CGA-CBA	2.41	119.47	111.91
30	b	619	BCR	C10-C11-C12	-2.41	115.70	123.22
29	N	2630	LHG	C18-C17-C16	-2.41	102.20	114.42
25	y	610	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
25	y	611	CLA	CAA-CBA-CGA	-2.41	106.22	113.25
27	6	1622	XAT	C10-C11-C12	-2.41	115.70	123.22
24	6	601	CHL	C2A-C1A-CHA	-2.41	119.65	123.86
34	A	418	SQD	O47-C45-C44	2.41	117.12	108.40
24	8	606	CHL	CMD-C2D-C3D	-2.41	122.08	127.61
25	4	604	CLA	O2A-CGA-O1A	-2.41	117.30	123.30
24	2	608	CHL	CMB-C2B-C3B	2.41	129.18	124.68
25	b	616	CLA	CMB-C2B-C3B	2.41	129.18	124.68
26	4	620	LUT	C1-C6-C5	-2.41	119.22	122.61
25	5	610	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
27	5	1622	XAT	C24-C23-C22	-2.41	106.13	110.77
26	s	1620	LUT	C19-C9-C8	2.40	121.87	118.08
24	S	607	CHL	O2A-CGA-CBA	2.40	119.45	111.91
26	s	1620	LUT	C7-C8-C9	-2.40	122.60	126.23
26	G	1620	LUT	C28-C29-C30	-2.40	115.25	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	5	2630	LHG	C20-C19-C18	-2.40	102.22	114.42
26	y	1620	LUT	C37-C21-C22	-2.40	104.88	109.44
26	N	1620	LUT	C19-C9-C8	2.40	121.86	118.08
27	1	1622	XAT	C24-C23-C22	-2.40	106.13	110.77
24	s	606	CHL	CMD-C2D-C3D	-2.40	122.09	127.61
25	g	614	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
34	b	623	SQD	C44-O6-C1	2.40	118.43	113.74
24	8	608	CHL	CMD-C2D-C3D	-2.40	122.09	127.61
25	8	611	CLA	CHD-C1D-ND	-2.40	122.25	124.45
34	B	623	SQD	O48-C23-C24	2.40	119.44	111.91
25	3	603	CLA	C2A-C1A-CHA	2.40	128.06	123.86
29	b	2631	LHG	C11-C10-C9	-2.40	102.24	114.42
28	5	1623	NEX	C2-C1-C6	2.40	111.54	109.21
26	Y	1620	LUT	C37-C21-C22	-2.40	104.89	109.44
26	Y	1620	LUT	C21-C26-C27	-2.40	109.67	112.70
29	S	2630	LHG	C11-C10-C9	-2.40	102.24	114.42
29	s	2630	LHG	C11-C10-C9	-2.40	102.24	114.42
24	8	601	CHL	CMD-C2D-C3D	-2.40	122.09	127.61
25	5	614	CLA	CHD-C1D-ND	-2.40	122.25	124.45
25	r	603	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
24	r	614	CHL	CMB-C2B-C3B	2.40	129.17	124.68
29	1	2630	LHG	C20-C19-C18	-2.40	102.25	114.42
26	y	1621	LUT	C16-C1-C6	-2.40	106.41	110.30
25	G	613	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	1	604	CLA	C1-C2-C3	-2.40	122.87	126.75
25	6	602	CLA	CAA-CBA-CGA	-2.40	106.25	113.25
25	2	610	CLA	C4A-NA-C1A	2.40	107.78	106.71
24	S	606	CHL	CMD-C2D-C3D	-2.40	122.10	127.61
25	6	613	CLA	CHD-C1D-ND	-2.40	122.25	124.45
24	8	609	CHL	CMB-C2B-C3B	2.40	129.16	124.68
25	y	604	CLA	C1-C2-C3	-2.39	122.88	126.75
25	g	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	N	610	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
25	Y	611	CLA	CAA-CBA-CGA	-2.39	106.26	113.25
25	C	509	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
24	g	605	CHL	C2A-C3A-C4A	-2.39	98.01	101.87
25	n	610	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
25	c	509	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
24	3	606	CHL	O1D-CGD-CBD	-2.39	119.59	124.48
24	4	608	CHL	CMD-C2D-C3D	-2.39	122.11	127.61
25	G	614	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
24	s	607	CHL	O2A-CGA-CBA	2.39	119.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	1620	LUT	C19-C9-C8	2.39	121.84	118.08
24	4	601	CHL	CMD-C2D-C3D	-2.39	122.12	127.61
33	a	409	PHO	CMC-C2C-C3C	2.39	129.45	124.94
25	6	610	CLA	C4A-NA-C1A	2.39	107.78	106.71
29	c	2630	LHG	C18-C17-C16	-2.39	102.30	114.42
29	C	2630	LHG	C18-C17-C16	-2.39	102.30	114.42
26	6	1621	LUT	C31-C30-C29	-2.39	123.90	127.31
26	n	1621	LUT	C16-C1-C6	-2.39	106.43	110.30
26	7	1620	LUT	C20-C13-C12	2.39	121.84	118.08
24	G	605	CHL	C2A-C3A-C4A	-2.39	98.01	101.87
24	6	609	CHL	C1-C2-C3	-2.39	121.92	126.04
30	b	620	BCR	C10-C11-C12	-2.39	115.77	123.22
28	r	623	NEX	C38-C25-C24	2.39	116.96	114.28
24	r	607	CHL	O1D-CGD-CBD	-2.38	119.60	124.48
25	3	610	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
24	7	606	CHL	O1D-CGD-CBD	-2.38	119.61	124.48
26	y	1620	LUT	C21-C26-C27	-2.38	109.69	112.70
25	1	614	CLA	CHD-C1D-ND	-2.38	122.26	124.45
24	G	607	CHL	O2A-CGA-CBA	2.38	119.39	111.91
25	Y	611	CLA	CMB-C2B-C3B	2.38	129.14	124.68
26	n	1620	LUT	C28-C29-C30	-2.38	115.28	118.94
24	6	608	CHL	CMB-C2B-C3B	2.38	129.14	124.68
25	2	602	CLA	CHB-C4A-NA	2.38	127.81	124.51
24	g	607	CHL	O2A-CGA-CBA	2.38	119.38	111.91
26	Y	1620	LUT	C39-C29-C28	2.38	121.83	118.08
25	6	602	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	N	611	CLA	CMB-C2B-C3B	2.38	129.13	124.68
26	N	1621	LUT	C16-C1-C6	-2.38	106.44	110.30
30	t	101	BCR	C39-C30-C25	-2.38	106.44	110.30
25	R	616	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	r	616	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
26	6	1621	LUT	C7-C8-C9	-2.38	122.64	126.23
24	2	601	CHL	C4D-C3D-CAD	2.38	110.90	108.10
24	5	601	CHL	C4D-CHA-C1A	-2.38	118.36	121.25
25	5	604	CLA	C1-C2-C3	-2.38	122.91	126.75
25	7	603	CLA	C2A-C1A-CHA	2.38	128.01	123.86
33	A	409	PHO	CMC-C2C-C3C	2.37	129.42	124.94
27	7	1622	XAT	C32-C33-C34	-2.37	115.30	118.94
24	G	607	CHL	CMD-C2D-C3D	-2.37	122.16	127.61
26	3	1620	LUT	C20-C13-C12	2.37	121.81	118.08
29	6	2630	LHG	C11-C10-C9	-2.37	102.38	114.42
25	4	604	CLA	CHD-C1D-ND	-2.37	122.27	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	609	CHL	CMB-C2B-C3B	2.37	129.12	124.68
25	y	611	CLA	CMB-C2B-C3B	2.37	129.12	124.68
30	c	516	BCR	C15-C14-C13	-2.37	123.93	127.31
30	B	620	BCR	C10-C11-C12	-2.37	115.82	123.22
25	Y	604	CLA	C1-C2-C3	-2.37	122.92	126.75
28	g	1623	NEX	O4-C5-C18	-2.37	105.18	109.39
24	R	614	CHL	CMB-C2B-C3B	2.37	129.11	124.68
27	5	1622	XAT	C18-C5-C4	2.37	116.94	114.28
34	B	621	SQD	O48-C23-C24	2.37	119.33	111.91
37	c	520	DGD	O3G-C1D-C2D	-2.37	104.61	108.30
26	5	1621	LUT	C8-C9-C10	-2.37	115.31	118.94
37	C	520	DGD	O3G-C1D-C2D	-2.37	104.61	108.30
25	g	604	CLA	C1-C2-C3	-2.37	122.92	126.75
26	1	1621	LUT	C8-C9-C10	-2.37	115.31	118.94
24	6	601	CHL	C4D-C3D-CAD	2.37	110.88	108.10
26	Y	1620	LUT	C8-C7-C6	-2.36	120.56	127.20
26	y	1620	LUT	C39-C29-C28	2.36	121.80	118.08
25	y	610	CLA	O2A-CGA-O1A	-2.36	117.62	123.59
25	8	604	CLA	CHD-C1D-ND	-2.36	122.28	124.45
24	4	609	CHL	O1D-CGD-CBD	-2.36	119.65	124.48
24	R	607	CHL	O1D-CGD-CBD	-2.36	119.65	124.48
29	2	2630	LHG	C11-C10-C9	-2.36	102.43	114.42
25	B	613	CLA	C16-C15-C13	-2.36	108.28	115.92
30	T	101	BCR	C39-C30-C25	-2.36	106.47	110.30
25	B	605	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	b	613	CLA	C16-C15-C13	-2.36	108.28	115.92
28	n	1623	NEX	C11-C12-C13	-2.36	119.78	126.42
25	G	604	CLA	C1-C2-C3	-2.36	122.93	126.75
28	N	1623	NEX	C11-C12-C13	-2.36	119.78	126.42
26	N	1620	LUT	C28-C29-C30	-2.36	115.32	118.94
24	1	606	CHL	O1D-CGD-CBD	-2.36	119.65	124.48
25	2	613	CLA	CHD-C1D-ND	-2.36	122.28	124.45
26	S	1621	LUT	C8-C9-C10	-2.36	115.32	118.94
27	1	1622	XAT	C18-C5-C4	2.36	116.94	114.28
25	n	611	CLA	CMB-C2B-C3B	2.36	129.09	124.68
25	S	603	CLA	C2A-C1A-CHA	2.36	127.98	123.86
29	c	523	LHG	C20-C19-C18	-2.36	102.45	114.42
24	6	607	CHL	C1-C2-C3	-2.36	121.96	126.04
25	Y	610	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
28	G	1623	NEX	O4-C5-C18	-2.36	105.19	109.39
25	s	603	CLA	C2A-C1A-CHA	2.36	127.98	123.86
24	g	607	CHL	CMD-C2D-C3D	-2.36	122.19	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	b	621	SQD	O48-C23-C24	2.36	119.31	111.91
24	N	601	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
24	8	609	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
26	y	1620	LUT	C8-C7-C6	-2.36	120.58	127.20
24	n	601	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
24	2	607	CHL	C1-C2-C3	-2.36	121.97	126.04
25	Y	612	CLA	C1-C2-C3	-2.36	121.97	126.04
30	T	101	BCR	C29-C30-C25	2.36	114.11	110.48
26	5	1621	LUT	C7-C8-C9	-2.36	122.68	126.23
25	6	611	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	b	605	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
35	b	622	LMG	O1-C7-C8	-2.35	105.22	110.90
30	C	516	BCR	C15-C14-C13	-2.35	123.95	127.31
27	8	622	XAT	C19-C9-C8	2.35	121.79	118.08
24	4	607	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
25	2	611	CLA	CHB-C4A-NA	2.35	127.77	124.51
29	C	523	LHG	C20-C19-C18	-2.35	102.48	114.42
29	d	408	LHG	C27-C26-C25	-2.35	102.48	114.42
25	y	612	CLA	C1-C2-C3	-2.35	121.97	126.04
25	S	609	CLA	CHD-C1D-ND	-2.35	122.29	124.45
24	2	606	CHL	CAA-C2A-C3A	-2.35	106.34	112.78
24	1	601	CHL	C4D-CHA-C1A	-2.35	118.39	121.25
24	6	606	CHL	CAA-C2A-C3A	-2.35	106.34	112.78
26	2	1621	LUT	C7-C8-C9	-2.35	122.68	126.23
27	3	1622	XAT	C32-C33-C34	-2.35	115.33	118.94
25	b	604	CLA	O2D-CGD-CBD	2.35	115.45	111.27
30	H	101	BCR	C2-C3-C4	-2.35	106.12	111.38
26	7	1620	LUT	C39-C29-C28	2.35	121.78	118.08
26	1	1621	LUT	C7-C8-C9	-2.35	122.69	126.23
37	h	102	DGD	O6D-C1D-O3G	-2.35	104.41	109.97
29	D	408	LHG	C27-C26-C25	-2.35	102.50	114.42
26	s	1621	LUT	C8-C9-C10	-2.35	115.34	118.94
24	5	608	CHL	CMB-C2B-C3B	2.35	129.07	124.68
24	5	606	CHL	O1D-CGD-CBD	-2.35	119.68	124.48
26	7	1620	LUT	C18-C5-C6	-2.35	121.89	124.53
24	4	608	CHL	CHB-C4A-NA	2.35	127.76	124.51
24	7	607	CHL	CMB-C2B-C3B	2.34	129.06	124.68
26	3	1620	LUT	C39-C29-C28	2.34	121.77	118.08
35	B	622	LMG	O1-C7-C8	-2.34	105.24	110.90
25	b	611	CLA	C3A-C2A-C1A	2.34	104.85	101.34
28	N	1623	NEX	C28-C29-C30	2.34	122.54	118.94
27	4	622	XAT	C19-C9-C8	2.34	121.77	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	612	CLA	C2A-C1A-CHA	2.34	127.95	123.86
25	R	601	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
26	Y	1620	LUT	C28-C29-C30	-2.34	115.35	118.94
25	B	611	CLA	C3A-C2A-C1A	2.34	104.85	101.34
25	B	617	CLA	CHC-C1C-NC	2.34	127.75	124.20
24	r	606	CHL	C4A-NA-C1A	-2.34	105.65	106.71
28	R	623	NEX	C38-C25-C24	2.34	116.91	114.28
25	B	604	CLA	O2D-CGD-CBD	2.34	115.42	111.27
30	h	101	BCR	C2-C3-C4	-2.34	106.15	111.38
26	S	1621	LUT	C7-C8-C9	-2.34	122.70	126.23
24	G	605	CHL	C4D-CHA-C1A	-2.34	118.41	121.25
35	D	411	LMG	O3-C3-C2	-2.34	104.95	110.35
25	1	604	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
25	r	604	CLA	CBA-CAA-C2A	2.34	120.76	113.86
25	5	604	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
24	r	608	CHL	C4-C3-C5	2.34	119.20	115.27
35	c	521	LMG	C40-C39-C38	-2.34	102.57	114.42
25	y	603	CLA	C1-C2-C3	-2.34	122.00	126.04
24	g	607	CHL	C6-C7-C8	-2.34	108.37	115.92
36	D	405	PL9	C41-C39-C38	-2.33	116.39	121.12
35	d	411	LMG	O3-C3-C2	-2.33	104.95	110.35
35	C	521	LMG	C40-C39-C38	-2.33	102.57	114.42
30	C	514	BCR	C34-C9-C8	2.33	121.75	118.08
24	3	607	CHL	CMB-C2B-C3B	2.33	129.04	124.68
26	3	1621	LUT	C18-C5-C6	-2.33	121.91	124.53
28	n	1623	NEX	C28-C29-C30	2.33	122.52	118.94
24	g	605	CHL	C4D-CHA-C1A	-2.33	118.41	121.25
24	1	608	CHL	CMB-C2B-C3B	2.33	129.04	124.68
30	c	514	BCR	C34-C9-C8	2.33	121.75	118.08
25	6	612	CLA	CMB-C2B-C3B	2.33	129.04	124.68
36	d	405	PL9	C41-C39-C38	-2.33	116.40	121.12
25	r	601	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
29	R	2630	LHG	C20-C19-C18	-2.33	102.59	114.42
25	b	605	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
26	G	1621	LUT	C18-C5-C6	-2.33	121.91	124.53
26	7	1621	LUT	C18-C5-C6	-2.33	121.91	124.53
37	H	102	DGD	O6D-C1D-O3G	-2.33	104.45	109.97
26	2	1621	LUT	C21-C26-C27	-2.33	109.75	112.70
30	t	101	BCR	C29-C30-C25	2.33	114.07	110.48
24	R	607	CHL	C1-C2-C3	-2.33	122.01	126.04
24	3	608	CHL	C1C-C2C-C3C	-2.33	105.27	107.11
25	6	612	CLA	C2A-C1A-CHA	2.33	127.93	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	1	2630	LHG	C11-C10-C9	-2.33	102.60	114.42
26	3	1620	LUT	C18-C5-C6	-2.33	121.91	124.53
25	R	616	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	2	612	CLA	CMB-C2B-C3B	2.33	129.04	124.68
24	8	608	CHL	CHB-C4A-NA	2.33	127.73	124.51
25	b	617	CLA	CHC-C1C-NC	2.33	127.73	124.20
24	R	606	CHL	C4A-NA-C1A	-2.33	105.66	106.71
25	b	605	CLA	C2A-C1A-CHA	2.33	127.93	123.86
25	R	604	CLA	CBA-CAA-C2A	2.33	120.73	113.86
25	B	605	CLA	C2A-C1A-CHA	2.33	127.93	123.86
25	S	612	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
25	4	610	CLA	CHB-C4A-NA	2.32	127.73	124.51
35	A	415	LMG	C40-C39-C38	-2.32	102.62	114.42
24	r	606	CHL	C1-C2-C3	-2.32	122.02	126.04
29	r	2630	LHG	C20-C19-C18	-2.32	102.63	114.42
24	Y	605	CHL	O2D-CGD-O1D	-2.32	119.29	123.84
25	Y	603	CLA	C1-C2-C3	-2.32	122.02	126.04
29	5	2630	LHG	C11-C10-C9	-2.32	102.63	114.42
35	B	2633	LMG	C6-C5-C4	-2.32	107.56	113.00
24	G	607	CHL	C6-C7-C8	-2.32	108.41	115.92
30	4	623	BCR	C29-C30-C25	2.32	114.06	110.48
35	b	2633	LMG	C6-C5-C4	-2.32	107.56	113.00
26	s	1621	LUT	C7-C8-C9	-2.32	122.73	126.23
25	r	616	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	6	601	CHL	CMB-C2B-C3B	2.32	129.02	124.68
37	C	519	DGD	C3G-C2G-C1G	-2.32	106.30	111.79
35	b	2633	LMG	C38-C37-C36	-2.32	102.65	114.42
27	8	622	XAT	C38-C25-C24	2.32	116.89	114.28
24	8	607	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
25	8	610	CLA	CHB-C4A-NA	2.32	127.72	124.51
35	a	415	LMG	C40-C39-C38	-2.32	102.65	114.42
37	C	520	DGD	C3D-C4D-C5D	-2.32	106.10	110.24
35	B	2633	LMG	C38-C37-C36	-2.32	102.65	114.42
27	n	1622	XAT	C26-C27-C28	-2.32	121.09	125.99
25	3	613	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
26	6	1621	LUT	C21-C26-C27	-2.32	109.77	112.70
24	7	608	CHL	C1C-C2C-C3C	-2.32	105.28	107.11
25	1	612	CLA	CHA-C1A-NA	-2.32	121.09	126.40
24	8	606	CHL	C4A-NA-C1A	-2.32	105.67	106.71
29	C	523	LHG	C11-C10-C9	-2.32	102.67	114.42
29	c	523	LHG	C11-C10-C9	-2.32	102.67	114.42
25	n	602	CLA	C6-C7-C8	-2.31	108.44	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	608	CHL	CAC-C3C-C4C	2.31	127.81	124.81
25	B	605	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
24	R	608	CHL	C4-C3-C5	2.31	119.16	115.27
25	s	612	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
24	N	608	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
26	6	1620	LUT	C39-C29-C28	2.31	121.72	118.08
26	y	1620	LUT	C28-C29-C30	-2.31	115.39	118.94
37	c	520	DGD	C3D-C4D-C5D	-2.31	106.12	110.24
24	r	607	CHL	C1-C2-C3	-2.31	122.05	126.04
25	A	407	CLA	C1-C2-C3	-2.31	123.01	126.75
25	7	613	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
25	B	614	CLA	CHB-C4A-NA	2.31	127.70	124.51
24	n	608	CHL	O2D-CGD-O1D	-2.31	119.32	123.84
24	R	606	CHL	C1-C2-C3	-2.31	122.05	126.04
30	8	623	BCR	C29-C30-C25	2.31	114.03	110.48
25	s	609	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	N	602	CLA	C6-C7-C8	-2.31	108.46	115.92
37	c	519	DGD	C3G-C2G-C1G	-2.31	106.33	111.79
25	R	611	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
27	4	622	XAT	C38-C25-C24	2.31	116.88	114.28
26	N	1621	LUT	C3-C4-C5	-2.31	107.26	111.85
26	1	1620	LUT	C40-C33-C32	2.31	121.71	118.08
24	N	601	CHL	CHB-C4A-NA	2.31	127.70	124.51
24	y	605	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
25	5	612	CLA	CHA-C1A-NA	-2.31	121.12	126.40
24	2	601	CHL	CMB-C2B-C3B	2.30	128.99	124.68
25	a	407	CLA	C1-C2-C3	-2.30	123.02	126.75
35	A	413	LMG	C38-C37-C36	-2.30	102.73	114.42
29	b	2631	LHG	C27-C26-C25	-2.30	102.73	114.42
27	3	1622	XAT	C26-C27-C28	-2.30	121.12	125.99
25	B	616	CLA	C3A-C2A-C1A	2.30	104.79	101.34
35	a	413	LMG	C38-C37-C36	-2.30	102.73	114.42
27	N	1622	XAT	C26-C27-C28	-2.30	121.12	125.99
34	B	621	SQD	O8-S-C6	2.30	109.41	105.74
29	B	2631	LHG	C27-C26-C25	-2.30	102.73	114.42
26	S	1620	LUT	C20-C13-C12	2.30	121.70	118.08
24	3	605	CHL	CAA-C2A-C3A	-2.30	106.47	112.78
25	b	614	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	s	601	CHL	C4D-CHA-C1A	-2.30	118.45	121.25
26	g	1621	LUT	C18-C5-C6	-2.30	121.94	124.53
26	R	620	LUT	C7-C8-C9	-2.30	122.76	126.23
28	s	1623	NEX	C26-C27-C28	-2.30	121.13	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n	1623	NEX	C30-C31-C32	-2.30	116.04	123.22
24	N	601	CHL	CMB-C2B-C3B	2.30	128.98	124.68
24	7	605	CHL	CAA-C2A-C3A	-2.30	106.48	112.78
25	y	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
25	1	610	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
26	2	1620	LUT	C39-C29-C28	2.30	121.70	118.08
27	2	1622	XAT	C4-C3-C2	-2.30	106.33	110.77
36	D	405	PL9	C36-C37-C38	-2.30	104.33	111.88
28	S	1623	NEX	C26-C27-C28	-2.30	121.14	125.99
24	Y	608	CHL	CAC-C3C-C4C	2.30	127.79	124.81
30	t	101	BCR	C11-C12-C13	-2.30	119.96	126.42
26	y	1620	LUT	C16-C1-C6	-2.30	106.57	110.30
36	d	405	PL9	C36-C37-C38	-2.30	104.33	111.88
24	3	601	CHL	C4-C3-C5	2.30	119.14	115.27
26	S	1621	LUT	C39-C29-C28	2.30	121.70	118.08
28	N	1623	NEX	C30-C31-C32	-2.30	116.05	123.22
29	r	2630	LHG	C18-C17-C16	-2.30	102.77	114.42
25	r	613	CLA	O1D-CGD-CBD	2.30	129.18	124.48
25	r	611	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
27	7	1622	XAT	C26-C27-C28	-2.29	121.14	125.99
30	T	101	BCR	C11-C12-C13	-2.29	119.97	126.42
37	C	518	DGD	O6E-C5E-C4E	2.29	113.86	109.69
24	S	601	CHL	C4D-CHA-C1A	-2.29	118.46	121.25
30	C	515	BCR	C23-C24-C25	-2.29	120.76	127.20
24	Y	608	CHL	CHB-C4A-NA	2.29	127.68	124.51
26	s	1621	LUT	C39-C29-C28	2.29	121.69	118.08
26	R	620	LUT	C1-C2-C3	2.29	118.82	113.64
26	s	1620	LUT	C20-C13-C12	2.29	121.69	118.08
24	y	606	CHL	CMB-C2B-C3B	2.29	128.97	124.68
27	N	1622	XAT	C40-C33-C32	2.29	121.69	118.08
26	5	1620	LUT	C40-C33-C32	2.29	121.68	118.08
24	n	601	CHL	CMB-C2B-C3B	2.29	128.96	124.68
29	B	2630	LHG	C20-C19-C18	-2.29	102.81	114.42
29	R	2630	LHG	C18-C17-C16	-2.29	102.81	114.42
26	r	620	LUT	C1-C2-C3	2.29	118.81	113.64
27	6	1622	XAT	C4-C3-C2	-2.29	106.36	110.77
24	7	601	CHL	C4-C3-C5	2.29	119.12	115.27
25	Y	612	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
24	Y	609	CHL	O2A-CGA-CBA	2.29	119.08	111.91
25	B	611	CLA	C2A-C1A-CHA	2.29	127.86	123.86
24	n	601	CHL	CHB-C4A-NA	2.29	127.67	124.51
25	1	614	CLA	O2D-CGD-O1D	-2.29	119.37	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	613	CLA	O1D-CGD-CBD	2.29	129.16	124.48
24	S	607	CHL	CED-O2D-CGD	2.29	121.11	115.94
24	n	601	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
34	b	621	SQD	O8-S-C6	2.28	109.38	105.74
24	g	605	CHL	CHB-C4A-NA	2.28	127.67	124.51
28	Y	1623	NEX	O4-C5-C18	-2.28	105.33	109.39
26	r	620	LUT	C7-C8-C9	-2.28	122.78	126.23
24	4	606	CHL	CAC-C3C-C4C	2.28	127.77	124.81
26	n	1621	LUT	C3-C4-C5	-2.28	107.31	111.85
37	c	519	DGD	CBB-CAB-C9B	-2.28	102.83	114.42
24	1	606	CHL	C1C-C2C-C3C	-2.28	105.30	107.11
24	5	606	CHL	CHB-C4A-NA	2.28	127.67	124.51
25	5	610	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
24	Y	606	CHL	CMB-C2B-C3B	2.28	128.95	124.68
24	y	601	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
24	4	606	CHL	C4A-NA-C1A	-2.28	105.68	106.71
24	6	607	CHL	C4-C3-C5	2.28	119.11	115.27
26	7	1621	LUT	C1-C2-C3	2.28	118.80	113.64
24	g	607	CHL	CAA-C2A-C3A	-2.28	106.53	112.78
29	y	2630	LHG	C27-C26-C25	-2.28	102.84	114.42
29	b	2630	LHG	C20-C19-C18	-2.28	102.84	114.42
24	4	601	CHL	C1C-C2C-C3C	-2.28	105.30	107.11
25	b	612	CLA	CGD-CBD-CAD	-2.28	103.35	110.73
24	y	609	CHL	O2A-CGA-CBA	2.28	119.06	111.91
24	5	601	CHL	O1D-CGD-CBD	-2.28	119.82	124.48
24	6	601	CHL	O2A-CGA-CBA	2.28	121.35	114.03
37	c	518	DGD	O6E-C5E-C4E	2.28	113.83	109.69
26	y	1621	LUT	C19-C9-C8	2.28	121.67	118.08
30	c	515	BCR	C23-C24-C25	-2.28	120.80	127.20
26	Y	1620	LUT	C16-C1-C6	-2.28	106.61	110.30
27	N	1622	XAT	C38-C25-C24	2.28	116.84	114.28
37	C	519	DGD	CBB-CAB-C9B	-2.28	102.87	114.42
24	8	601	CHL	C1C-C2C-C3C	-2.28	105.31	107.11
27	5	1622	XAT	C39-C29-C30	-2.28	119.73	122.92
25	8	611	CLA	O2A-CGA-O1A	-2.28	117.63	123.30
26	N	1621	LUT	C28-C29-C30	-2.27	115.45	118.94
24	2	601	CHL	O2A-CGA-CBA	2.27	121.34	114.03
24	G	607	CHL	CAA-C2A-C3A	-2.27	106.55	112.78
26	n	1621	LUT	C28-C29-C30	-2.27	115.45	118.94
29	g	2630	LHG	C27-C26-C25	-2.27	102.88	114.42
26	2	1621	LUT	C36-C21-C26	2.27	112.99	109.55
29	Y	2630	LHG	C27-C26-C25	-2.27	102.88	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	1620	LUT	C1-C2-C3	2.27	118.78	113.64
25	5	614	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
30	D	404	BCR	C3-C4-C5	-2.27	110.02	114.08
25	B	612	CLA	CGD-CBD-CAD	-2.27	103.37	110.73
29	L	101	LHG	C18-C17-C16	-2.27	102.89	114.42
27	n	1622	XAT	C28-C29-C30	2.27	122.43	118.94
26	Y	1621	LUT	C19-C9-C8	2.27	121.66	118.08
25	b	616	CLA	C3A-C2A-C1A	2.27	104.74	101.34
24	s	607	CHL	CED-O2D-CGD	2.27	121.07	115.94
29	l	101	LHG	C18-C17-C16	-2.27	102.90	114.42
25	b	611	CLA	C2A-C1A-CHA	2.27	127.83	123.86
24	1	601	CHL	CHB-C4A-NA	2.27	127.65	124.51
27	R	622	XAT	C20-C13-C12	2.27	121.65	118.08
27	n	1622	XAT	C40-C33-C32	2.27	121.65	118.08
39	F	101	HEM	CMB-C2B-C1B	-2.27	121.58	125.04
27	1	1622	XAT	C39-C29-C30	-2.27	119.75	122.92
24	2	607	CHL	C4-C3-C5	2.27	119.09	115.27
24	y	608	CHL	CHB-C4A-NA	2.27	127.65	124.51
25	r	611	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	3	1621	LUT	C1-C2-C3	2.27	118.76	113.64
26	y	1620	LUT	C1-C2-C3	2.27	118.76	113.64
24	G	607	CHL	CMB-C2B-C3B	2.27	128.92	124.68
35	Z	101	LMG	C38-C37-C36	-2.27	102.92	114.42
25	S	602	CLA	O1D-CGD-CBD	2.27	129.12	124.48
25	b	606	CLA	CHC-C1C-NC	2.27	127.64	124.20
24	1	601	CHL	O1D-CGD-CBD	-2.27	119.85	124.48
28	y	1623	NEX	O4-C5-C18	-2.26	105.36	109.39
29	G	2630	LHG	C27-C26-C25	-2.26	102.93	114.42
27	8	622	XAT	C8-C9-C10	-2.26	115.47	118.94
25	Y	603	CLA	CMB-C2B-C3B	2.26	128.91	124.68
27	g	1622	XAT	C39-C29-C30	-2.26	119.75	122.92
24	1	606	CHL	CHB-C4A-NA	2.26	127.64	124.51
27	n	1622	XAT	C38-C25-C24	2.26	116.82	114.28
35	z	101	LMG	C38-C37-C36	-2.26	102.94	114.42
24	N	601	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
24	g	609	CHL	CBC-CAC-C3C	-2.26	106.20	112.43
24	8	606	CHL	CAC-C3C-C4C	2.26	127.74	124.81
24	7	606	CHL	C2A-C1A-CHA	-2.26	119.91	123.86
26	G	1620	LUT	C8-C9-C10	-2.26	115.47	118.94
27	4	622	XAT	C8-C9-C10	-2.26	115.47	118.94
25	5	603	CLA	C2A-C1A-CHA	2.26	127.81	123.86
25	s	609	CLA	O2D-CGD-CBD	2.26	115.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	2	607	CHL	CHD-C4C-C3C	-2.26	121.52	124.84
24	g	607	CHL	CMB-C2B-C3B	2.26	128.90	124.68
35	b	2633	LMG	C42-C41-C40	-2.26	102.96	114.42
24	n	605	CHL	C4D-C3D-CAD	2.26	110.76	108.10
27	r	622	XAT	C20-C13-C12	2.26	121.63	118.08
35	B	2633	LMG	C42-C41-C40	-2.26	102.97	114.42
25	N	611	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
29	R	2630	LHG	O8-C23-C24	2.26	118.99	111.91
25	r	613	CLA	C1-C2-C3	-2.26	122.14	126.04
30	c	515	BCR	C8-C7-C6	-2.26	120.87	127.20
25	b	603	CLA	CHD-C1D-ND	-2.26	122.38	124.45
25	n	611	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
25	1	603	CLA	C2A-C1A-CHA	2.26	127.80	123.86
25	4	611	CLA	CHB-C4A-NA	2.26	127.63	124.51
25	y	603	CLA	CMB-C2B-C3B	2.26	128.90	124.68
30	c	514	BCR	C3-C4-C5	-2.26	110.05	114.08
26	6	1621	LUT	C36-C21-C26	2.26	112.96	109.55
35	A	415	LMG	O3-C3-C2	-2.25	105.14	110.35
25	4	611	CLA	O2A-CGA-O1A	-2.25	117.68	123.30
24	5	606	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
25	r	611	CLA	CHA-C1A-NA	-2.25	121.23	126.40
24	1	601	CHL	CMB-C2B-C3B	2.25	128.90	124.68
30	C	514	BCR	C3-C4-C5	-2.25	110.05	114.08
24	Y	601	CHL	O2D-CGD-O1D	-2.25	119.43	123.84
36	D	405	PL9	C20-C19-C21	2.25	119.06	115.27
25	S	609	CLA	O2D-CGD-CBD	2.25	115.27	111.27
30	C	516	BCR	C29-C30-C25	2.25	113.95	110.48
29	r	2630	LHG	O8-C23-C24	2.25	118.97	111.91
30	C	516	BCR	C8-C7-C6	-2.25	120.88	127.20
24	y	608	CHL	CMD-C2D-C3D	-2.25	122.44	127.61
25	s	602	CLA	O1D-CGD-CBD	2.25	129.09	124.48
39	f	101	HEM	CMB-C2B-C1B	-2.25	121.61	125.04
24	Y	609	CHL	C2A-C1A-CHA	-2.25	119.92	123.86
36	d	405	PL9	C20-C19-C21	2.25	119.06	115.27
24	7	601	CHL	C2A-C1A-CHA	-2.25	119.92	123.86
27	N	1622	XAT	C28-C29-C30	2.25	122.39	118.94
25	B	610	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	R	611	CLA	CHA-C1A-NA	-2.25	121.25	126.40
27	g	1622	XAT	C26-C27-C28	-2.25	121.24	125.99
25	y	603	CLA	C2D-C1D-ND	-2.25	108.45	110.10
30	c	516	BCR	C29-C30-C25	2.25	113.94	110.48
24	N	605	CHL	C4D-C3D-CAD	2.25	110.75	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	404	BCR	C3-C4-C5	-2.25	110.06	114.08
24	8	601	CHL	OMC-CMC-C2C	-2.25	120.60	125.69
25	R	613	CLA	C1-C2-C3	-2.25	122.15	126.04
26	1	1620	LUT	C8-C7-C6	-2.25	120.89	127.20
30	C	515	BCR	C8-C7-C6	-2.25	120.89	127.20
24	4	601	CHL	OMC-CMC-C2C	-2.25	120.60	125.69
25	a	410	CLA	O2D-CGD-CBD	2.25	115.26	111.27
24	6	607	CHL	CHD-C4C-C3C	-2.25	121.54	124.84
24	n	601	CHL	C2A-C1A-CHA	-2.25	119.93	123.86
25	3	610	CLA	C1-C2-C3	-2.25	122.16	126.04
24	1	608	CHL	O1D-CGD-CBD	-2.25	119.89	124.48
25	b	610	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
26	g	1620	LUT	C8-C9-C10	-2.25	115.50	118.94
24	G	609	CHL	CBC-CAC-C3C	-2.25	106.24	112.43
30	c	516	BCR	C8-C7-C6	-2.25	120.90	127.20
28	2	1623	NEX	C20-C13-C14	-2.25	119.78	122.92
25	B	606	CLA	CHC-C1C-NC	2.24	127.61	124.20
27	G	1622	XAT	C26-C27-C28	-2.24	121.25	125.99
29	d	409	LHG	C27-C26-C25	-2.24	103.04	114.42
26	Y	1621	LUT	C38-C25-C24	-2.24	118.76	123.56
24	5	601	CHL	CMB-C2B-C3B	2.24	128.87	124.68
24	n	605	CHL	OMC-CMC-C2C	-2.24	120.62	125.69
24	3	606	CHL	C2A-C1A-CHA	-2.24	119.94	123.86
26	5	1620	LUT	C8-C7-C6	-2.24	120.91	127.20
35	a	415	LMG	O3-C3-C2	-2.24	105.17	110.35
24	Y	608	CHL	CMD-C2D-C3D	-2.24	122.46	127.61
25	7	610	CLA	C1-C2-C3	-2.24	122.17	126.04
24	3	601	CHL	C2A-C1A-CHA	-2.24	119.94	123.86
24	2	601	CHL	CED-O2D-CGD	2.24	121.00	115.94
30	B	619	BCR	C33-C5-C6	-2.24	122.02	124.53
24	y	609	CHL	C2A-C1A-CHA	-2.24	119.95	123.86
26	2	1621	LUT	C38-C25-C24	-2.24	118.77	123.56
25	5	603	CLA	CHD-C1D-ND	-2.24	122.40	124.45
33	A	408	PHO	C1B-NB-C4B	2.24	111.68	107.09
24	N	605	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
29	D	409	LHG	C27-C26-C25	-2.24	103.07	114.42
24	r	607	CHL	CED-O2D-CGD	2.24	120.99	115.94
29	d	410	LHG	C27-C26-C25	-2.24	103.08	114.42
24	G	605	CHL	CHB-C4A-NA	2.24	127.60	124.51
24	N	609	CHL	C4-C3-C5	2.24	119.03	115.27
25	7	610	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
24	R	607	CHL	CED-O2D-CGD	2.23	120.99	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	609	CHL	C4-C3-C5	2.23	119.03	115.27
24	Y	606	CHL	O2A-CGA-O1A	-2.23	117.95	123.59
25	b	606	CLA	C2D-C1D-ND	-2.23	108.46	110.10
26	S	1621	LUT	C2-C3-C4	2.23	113.36	110.30
24	R	608	CHL	CMD-C2D-C3D	-2.23	122.48	127.61
27	G	1622	XAT	C39-C29-C30	-2.23	119.80	122.92
26	y	1621	LUT	C38-C25-C24	-2.23	118.78	123.56
25	R	611	CLA	CHB-C4A-NA	2.23	127.60	124.51
26	6	1621	LUT	C38-C25-C24	-2.23	118.78	123.56
30	t	101	BCR	C31-C1-C6	-2.23	106.68	110.30
29	D	410	LHG	C27-C26-C25	-2.23	103.09	114.42
33	a	408	PHO	C1B-NB-C4B	2.23	111.67	107.09
29	y	2630	LHG	C18-C17-C16	-2.23	103.10	114.42
25	G	614	CLA	CHB-C4A-NA	2.23	127.60	124.51
29	Y	2630	LHG	C18-C17-C16	-2.23	103.10	114.42
25	3	611	CLA	C2C-C1C-NC	2.23	112.06	109.97
24	s	607	CHL	OMC-CMC-C2C	-2.23	120.64	125.69
24	N	601	CHL	C2A-C1A-CHA	-2.23	119.96	123.86
24	5	601	CHL	CHB-C4A-NA	2.23	127.59	124.51
36	D	405	PL9	C11-C12-C13	-2.23	104.56	111.88
25	3	602	CLA	CHB-C4A-NA	2.23	127.59	124.51
24	n	608	CHL	O1D-CGD-CBD	-2.23	119.93	124.48
25	N	611	CLA	CAA-CBA-CGA	-2.23	106.75	113.25
25	8	611	CLA	CHB-C4A-NA	2.23	127.59	124.51
30	c	515	BCR	C4-C5-C6	-2.23	119.50	122.73
25	S	609	CLA	CHB-C4A-NA	2.23	127.59	124.51
35	C	521	LMG	C38-C37-C36	-2.23	103.12	114.42
35	c	521	LMG	C38-C37-C36	-2.23	103.13	114.42
30	T	101	BCR	C31-C1-C6	-2.23	106.69	110.30
25	B	604	CLA	C2D-C1D-ND	-2.22	108.47	110.10
24	N	609	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
25	s	609	CLA	CHB-C4A-NA	2.22	127.59	124.51
30	b	619	BCR	C33-C5-C6	-2.22	122.03	124.53
28	r	623	NEX	C2-C1-C6	2.22	111.37	109.21
25	3	612	CLA	CMD-C2D-C3D	2.22	132.73	127.61
24	N	608	CHL	O1D-CGD-CBD	-2.22	119.94	124.48
30	A	411	BCR	C15-C16-C17	-2.22	118.92	123.47
24	y	607	CHL	O2A-CGA-CBA	2.22	118.88	111.91
25	b	604	CLA	C2D-C1D-ND	-2.22	108.47	110.10
35	c	521	LMG	C1-C2-C3	-2.22	105.37	110.00
24	3	609	CHL	C4-C3-C5	2.22	119.01	115.27
27	6	1622	XAT	C24-C23-C22	-2.22	106.48	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	1621	LUT	C37-C21-C22	-2.22	105.23	109.44
25	n	611	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
24	3	605	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
24	6	601	CHL	CED-O2D-CGD	2.22	120.96	115.94
24	N	605	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
24	N	601	CHL	O2A-CGA-CBA	2.22	118.88	111.91
24	S	607	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
36	d	405	PL9	C11-C12-C13	-2.22	104.58	111.88
38	D	401	BCT	O3-C-O1	-2.22	113.79	119.55
24	5	608	CHL	O1D-CGD-CBD	-2.22	119.94	124.48
25	A	410	CLA	C1-C2-C3	-2.22	122.20	126.04
25	b	612	CLA	C11-C12-C13	-2.22	108.75	115.92
28	6	1623	NEX	C20-C13-C14	-2.22	119.81	122.92
27	2	1622	XAT	C24-C23-C22	-2.22	106.49	110.77
24	g	606	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
25	A	407	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	1	601	CHL	C4D-C3D-CAD	2.22	110.71	108.10
26	8	620	LUT	C10-C11-C12	-2.22	116.29	123.22
35	C	521	LMG	C1-C2-C3	-2.22	105.38	110.00
24	Y	607	CHL	O2A-CGA-CBA	2.22	118.87	111.91
24	7	609	CHL	C4-C3-C5	2.22	119.00	115.27
25	A	410	CLA	O2D-CGD-CBD	2.22	115.21	111.27
25	B	603	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	7	605	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
28	g	1623	NEX	C16-C1-C6	2.22	112.46	110.47
25	a	410	CLA	C1-C2-C3	-2.22	122.21	126.04
24	G	606	CHL	OMC-CMC-C2C	-2.22	120.68	125.69
24	y	605	CHL	O2A-CGA-CBA	2.22	118.86	111.91
24	3	606	CHL	CHB-C4A-NA	2.22	127.58	124.51
25	7	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
25	7	611	CLA	C2C-C1C-NC	2.21	112.05	109.97
26	4	620	LUT	C10-C11-C12	-2.21	116.31	123.22
24	2	601	CHL	C4D-CHA-C1A	-2.21	118.55	121.25
30	C	515	BCR	C4-C5-C6	-2.21	119.52	122.73
37	c	520	DGD	CAB-C9B-C8B	-2.21	103.18	114.42
24	G	601	CHL	C1-O2A-CGA	2.21	122.25	116.44
24	r	608	CHL	CMD-C2D-C3D	-2.21	122.52	127.61
24	G	601	CHL	C2A-C1A-CHA	-2.21	119.99	123.86
24	N	609	CHL	CBC-CAC-C3C	-2.21	106.33	112.43
25	B	612	CLA	C11-C12-C13	-2.21	108.77	115.92
35	c	521	LMG	O1-C7-C8	-2.21	105.56	110.90
25	5	612	CLA	O2D-CGD-CBD	2.21	115.20	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	610	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
37	C	520	DGD	CAB-C9B-C8B	-2.21	103.20	114.42
24	4	607	CHL	OMC-CMC-C2C	-2.21	120.69	125.69
25	1	612	CLA	O2D-CGD-CBD	2.21	115.20	111.27
30	D	404	BCR	C33-C5-C6	-2.21	122.05	124.53
24	g	601	CHL	C2A-C1A-CHA	-2.21	120.00	123.86
25	3	610	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
24	n	606	CHL	O2D-CGD-O1D	-2.21	119.52	123.84
24	Y	605	CHL	O2A-CGA-CBA	2.21	118.84	111.91
24	n	609	CHL	CBC-CAC-C3C	-2.21	106.34	112.43
24	8	607	CHL	OMC-CMC-C2C	-2.21	120.69	125.69
35	C	521	LMG	O1-C7-C8	-2.21	105.57	110.90
24	g	601	CHL	C1-O2A-CGA	2.21	122.24	116.44
25	G	604	CLA	CHB-C4A-NA	2.21	127.56	124.51
24	g	606	CHL	O2A-CGA-O1A	-2.21	118.02	123.59
29	G	2630	LHG	C18-C17-C16	-2.21	103.22	114.42
24	4	608	CHL	CAC-C3C-C4C	2.21	127.67	124.81
24	n	601	CHL	O2A-CGA-CBA	2.21	118.83	111.91
26	s	1621	LUT	C2-C3-C4	2.21	113.33	110.30
26	g	1621	LUT	C38-C25-C24	-2.21	118.84	123.56
24	8	608	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
25	Y	613	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
38	d	401	BCT	O3-C-O1	-2.21	113.82	119.55
30	a	411	BCR	C15-C16-C17	-2.21	118.95	123.47
25	n	603	CLA	CHD-C1D-ND	-2.21	122.43	124.45
25	5	602	CLA	C1-C2-C3	-2.21	122.23	126.04
24	5	601	CHL	C4D-C3D-CAD	2.21	110.69	108.10
29	C	522	LHG	C27-C26-C25	-2.20	103.23	114.42
26	N	1620	LUT	C36-C21-C26	2.20	112.89	109.55
30	C	515	BCR	C1-C6-C5	-2.20	119.51	122.61
24	n	609	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
24	4	608	CHL	O1D-CGD-CBD	-2.20	119.97	124.48
25	6	603	CLA	O2A-C1-C2	-2.20	102.84	108.64
25	N	604	CLA	CHB-C4A-NA	2.20	127.56	124.51
24	y	606	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
29	g	2630	LHG	C18-C17-C16	-2.20	103.25	114.42
24	6	601	CHL	C4D-CHA-C1A	-2.20	118.57	121.25
26	G	1621	LUT	C38-C25-C24	-2.20	118.85	123.56
28	R	623	NEX	C2-C1-C6	2.20	111.35	109.21
24	N	606	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
37	C	518	DGD	CBB-CAB-C9B	-2.20	103.25	114.42
29	c	522	LHG	C27-C26-C25	-2.20	103.25	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	608	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
25	3	611	CLA	CAA-CBA-CGA	2.20	119.68	113.25
25	6	604	CLA	O1A-CGA-CBA	2.20	130.15	123.08
29	Y	2630	LHG	C11-C10-C9	-2.20	103.26	114.42
25	c	502	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
24	8	608	CHL	O2A-CGA-O1A	-2.20	117.82	123.30
25	2	604	CLA	O1A-CGA-CBA	2.20	130.15	123.08
25	b	607	CLA	C6-C7-C8	-2.20	108.81	115.92
29	y	2630	LHG	C11-C10-C9	-2.20	103.26	114.42
24	4	608	CHL	O2A-CGA-O1A	-2.20	117.82	123.30
37	c	518	DGD	CBB-CAB-C9B	-2.20	103.26	114.42
25	7	612	CLA	CMD-C2D-C3D	2.20	132.67	127.61
28	G	1623	NEX	C35-C15-C14	-2.20	118.97	123.47
26	5	1620	LUT	C38-C25-C24	-2.20	118.86	123.56
25	B	607	CLA	C6-C7-C8	-2.20	108.81	115.92
25	n	604	CLA	CHB-C4A-NA	2.20	127.55	124.51
37	B	626	DGD	C3D-C4D-C5D	-2.20	106.32	110.24
25	1	602	CLA	CHD-C1D-ND	-2.20	122.44	124.45
26	1	1620	LUT	C38-C25-C24	-2.20	118.86	123.56
28	g	1623	NEX	C35-C15-C14	-2.20	118.97	123.47
26	6	1620	LUT	C8-C9-C10	-2.20	115.57	118.94
25	1	602	CLA	C1-C2-C3	-2.20	122.25	126.04
24	7	607	CHL	C4A-NA-C1A	2.20	107.69	106.71
29	7	2630	LHG	C18-C17-C16	-2.20	103.28	114.42
25	b	616	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
25	y	613	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
24	R	606	CHL	CAA-C2A-C3A	-2.19	106.77	112.78
25	B	606	CLA	C2D-C1D-ND	-2.19	108.49	110.10
30	c	515	BCR	C1-C6-C5	-2.19	119.52	122.61
25	D	402	CLA	O2D-CGD-CBD	2.19	115.17	111.27
25	d	402	CLA	O2D-CGD-CBD	2.19	115.17	111.27
29	3	2630	LHG	C18-C17-C16	-2.19	103.29	114.42
24	n	605	CHL	C2A-C3A-C4A	-2.19	98.33	101.87
29	c	523	LHG	C18-C17-C16	-2.19	103.29	114.42
25	g	614	CLA	CHB-C4A-NA	2.19	127.55	124.51
25	r	602	CLA	O2D-CGD-CBD	2.19	115.16	111.27
25	2	603	CLA	O2A-C1-C2	-2.19	102.87	108.64
25	A	405	CLA	CHB-C4A-NA	2.19	127.54	124.51
30	H	101	BCR	C16-C15-C14	-2.19	118.98	123.47
26	n	1620	LUT	C36-C21-C26	2.19	112.86	109.55
24	n	605	CHL	C1C-C2C-C3C	-2.19	105.38	107.11
25	g	602	CLA	CAA-CBA-CGA	-2.19	106.85	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	1622	XAT	C16-C1-C2	-2.19	105.18	108.98
24	R	606	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
24	r	606	CHL	CAA-C2A-C3A	-2.19	106.78	112.78
25	s	610	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
25	7	611	CLA	CAA-CBA-CGA	2.19	119.65	113.25
26	R	620	LUT	C31-C30-C29	-2.19	124.19	127.31
28	G	1623	NEX	C16-C1-C6	2.19	112.43	110.47
25	C	502	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
30	B	620	BCR	C21-C20-C19	-2.19	116.39	123.22
26	r	620	LUT	C31-C30-C29	-2.19	124.19	127.31
24	7	606	CHL	CHB-C4A-NA	2.19	127.54	124.51
25	c	510	CLA	C2D-C1D-ND	-2.19	108.49	110.10
24	n	609	CHL	O2A-CGA-CBA	2.19	118.77	111.91
25	g	604	CLA	CHB-C4A-NA	2.19	127.54	124.51
26	G	1621	LUT	C37-C21-C22	-2.19	105.29	109.44
26	N	1621	LUT	C37-C21-C22	-2.19	105.29	109.44
29	C	523	LHG	C18-C17-C16	-2.19	103.32	114.42
30	b	620	BCR	C21-C20-C19	-2.19	116.39	123.22
37	b	626	DGD	C3D-C4D-C5D	-2.19	106.34	110.24
24	R	608	CHL	C1C-C2C-C3C	-2.19	105.38	107.11
25	n	610	CLA	C2A-C1A-CHA	2.19	127.68	123.86
25	n	604	CLA	O1D-CGD-CBD	2.19	128.96	124.48
24	6	606	CHL	CED-O2D-CGD	2.18	120.88	115.94
25	N	604	CLA	O1D-CGD-CBD	2.18	128.95	124.48
24	6	609	CHL	C6-C5-C3	-2.18	107.73	113.45
25	a	407	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	6	1620	LUT	C38-C25-C24	-2.18	118.89	123.56
24	G	606	CHL	O2A-CGA-O1A	-2.18	118.08	123.59
24	G	601	CHL	CMB-C2B-C3B	2.18	128.76	124.68
24	2	609	CHL	C6-C5-C3	-2.18	107.73	113.45
30	h	101	BCR	C16-C15-C14	-2.18	119.00	123.47
34	A	418	SQD	C44-O6-C1	2.18	118.00	113.74
25	B	616	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
24	8	608	CHL	O2A-CGA-CBA	2.18	121.04	114.03
25	c	513	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	b	605	CLA	CHA-C1A-NA	-2.18	121.41	126.40
24	4	608	CHL	O2A-CGA-CBA	2.18	121.03	114.03
24	y	609	CHL	C11-C12-C13	-2.18	108.87	115.92
25	G	602	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
24	y	608	CHL	CMB-C2B-C3B	2.18	128.75	124.68
24	4	606	CHL	O2A-CGA-CBA	2.18	121.03	114.03
36	D	405	PL9	O2-C1-C2	-2.18	116.79	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	R	622	XAT	O24-C25-C26	-2.18	57.16	58.96
24	2	606	CHL	CED-O2D-CGD	2.18	120.86	115.94
24	r	606	CHL	O1D-CGD-CBD	-2.18	120.03	124.48
25	7	611	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
24	Y	608	CHL	CMB-C2B-C3B	2.18	128.75	124.68
24	g	601	CHL	CMB-C2B-C3B	2.18	128.75	124.68
24	N	609	CHL	O2A-CGA-CBA	2.18	118.73	111.91
29	l	101	LHG	C27-C26-C25	-2.18	103.38	114.42
24	8	606	CHL	O2A-CGA-CBA	2.18	121.02	114.03
25	B	605	CLA	CHA-C1A-NA	-2.17	121.42	126.40
26	Y	1620	LUT	C31-C30-C29	-2.17	124.21	127.31
26	2	1621	LUT	C16-C1-C6	-2.17	106.77	110.30
30	4	623	BCR	C3-C4-C5	-2.17	110.19	114.08
30	8	623	BCR	C3-C4-C5	-2.17	110.19	114.08
29	S	2630	LHG	C18-C17-C16	-2.17	103.39	114.42
26	2	1620	LUT	C8-C9-C10	-2.17	115.61	118.94
30	d	404	BCR	C33-C5-C6	-2.17	122.09	124.53
25	1	603	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
24	3	608	CHL	CHB-C4A-NA	2.17	127.52	124.51
25	n	602	CLA	CHB-C4A-NA	2.17	127.52	124.51
25	5	602	CLA	CHD-C1D-ND	-2.17	122.46	124.45
24	N	605	CHL	C2A-C3A-C4A	-2.17	98.36	101.87
24	8	608	CHL	CAC-C3C-C4C	2.17	127.63	124.81
27	6	1622	XAT	C16-C1-C2	-2.17	105.21	108.98
27	r	622	XAT	O24-C25-C26	-2.17	57.16	58.96
29	L	101	LHG	C27-C26-C25	-2.17	103.40	114.42
24	r	606	CHL	CAC-C3C-C4C	2.17	127.63	124.81
25	c	507	CLA	C2A-C1A-CHA	2.17	127.66	123.86
26	g	1621	LUT	C37-C21-C22	-2.17	105.33	109.44
25	C	507	CLA	C2A-C1A-CHA	2.17	127.65	123.86
30	H	101	BCR	C15-C16-C17	-2.17	119.03	123.47
25	B	616	CLA	O2D-CGD-CBD	2.17	115.12	111.27
26	2	1620	LUT	C38-C25-C24	-2.17	118.92	123.56
34	a	418	SQD	C44-O6-C1	2.17	117.98	113.74
25	Y	603	CLA	C2D-C1D-ND	-2.17	108.51	110.10
24	R	607	CHL	CAA-CBA-CGA	-2.17	106.92	113.25
25	B	609	CLA	CAC-C3C-C4C	2.17	127.62	124.81
29	s	2630	LHG	C18-C17-C16	-2.17	103.42	114.42
25	c	501	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
24	n	608	CHL	OBD-CAD-C3D	-2.17	123.31	128.52
24	7	606	CHL	C4D-C3D-CAD	2.17	110.65	108.10
26	2	1620	LUT	C2-C3-C4	2.17	113.27	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	N	610	CLA	C2A-C1A-CHA	2.17	127.65	123.86
24	Y	609	CHL	C11-C12-C13	-2.17	108.92	115.92
24	7	608	CHL	O2A-CGA-CBA	2.17	120.99	114.03
25	3	611	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
24	G	606	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
24	g	608	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
25	R	602	CLA	O2D-CGD-CBD	2.16	115.11	111.27
24	R	606	CHL	CAC-C3C-C4C	2.16	127.62	124.81
25	C	513	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	N	608	CHL	OBD-CAD-C3D	-2.16	123.32	128.52
24	3	607	CHL	C4A-NA-C1A	2.16	107.68	106.71
25	y	602	CLA	CAC-C3C-C4C	2.16	127.61	124.81
35	a	415	LMG	C38-C37-C36	-2.16	103.45	114.42
25	n	614	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
25	C	510	CLA	C2D-C1D-ND	-2.16	108.51	110.10
33	a	408	PHO	O2A-C1-C2	-2.16	102.95	108.64
35	A	415	LMG	C38-C37-C36	-2.16	103.46	114.42
30	A	411	BCR	C10-C11-C12	-2.16	116.47	123.22
24	r	607	CHL	CAA-CBA-CGA	-2.16	106.94	113.25
36	d	405	PL9	O2-C1-C2	-2.16	116.83	121.78
24	3	606	CHL	C4D-C3D-CAD	2.16	110.64	108.10
24	Y	606	CHL	CMD-C2D-C3D	-2.16	122.65	127.61
25	b	603	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
25	N	603	CLA	CHD-C1D-ND	-2.16	122.47	124.45
34	A	418	SQD	O48-C23-C24	2.16	118.68	111.91
26	6	1621	LUT	C16-C1-C6	-2.16	106.80	110.30
30	a	411	BCR	C10-C11-C12	-2.16	116.48	123.22
25	C	501	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
25	B	603	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
25	1	602	CLA	CHA-C1A-NA	-2.16	121.46	126.40
29	2	2630	LHG	C27-C26-C25	-2.16	103.48	114.42
24	2	607	CHL	C4A-NA-C1A	2.16	107.67	106.71
29	C	2630	LHG	C27-C26-C25	-2.16	103.48	114.42
25	N	614	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
26	y	1620	LUT	C36-C21-C26	2.15	112.81	109.55
25	a	405	CLA	C16-C15-C13	-2.15	108.96	115.92
25	b	616	CLA	O2D-CGD-CBD	2.15	115.09	111.27
33	A	408	PHO	O2A-C1-C2	-2.15	102.97	108.64
25	s	602	CLA	CHB-C4A-NA	2.15	127.49	124.51
25	1	603	CLA	CHD-C1D-ND	-2.15	122.47	124.45
25	G	602	CLA	CHD-C1D-ND	-2.15	122.47	124.45
29	6	2630	LHG	C27-C26-C25	-2.15	103.50	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	3	608	CHL	O2A-CGA-CBA	2.15	120.95	114.03
33	a	408	PHO	CMC-C2C-C3C	2.15	129.00	124.94
26	7	1620	LUT	C15-C35-C34	-2.15	119.06	123.47
25	5	602	CLA	CHA-C1A-NA	-2.15	121.47	126.40
25	c	510	CLA	C1-C2-C3	-2.15	122.32	126.04
25	N	602	CLA	CHB-C4A-NA	2.15	127.49	124.51
29	n	2630	LHG	O8-C23-C24	2.15	118.66	111.91
24	N	601	CHL	C1-O2A-CGA	2.15	122.09	116.44
24	S	607	CHL	CMD-C2D-C3D	-2.15	122.67	127.61
24	y	606	CHL	CMD-C2D-C3D	-2.15	122.67	127.61
24	g	608	CHL	C4D-CHA-C1A	-2.15	118.63	121.25
25	A	405	CLA	C16-C15-C13	-2.15	108.97	115.92
29	c	2630	LHG	C27-C26-C25	-2.15	103.51	114.42
24	G	608	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
24	7	608	CHL	CHB-C4A-NA	2.15	127.49	124.51
24	r	606	CHL	C2A-C1A-CHA	-2.15	120.10	123.86
25	1	602	CLA	CHB-C4A-NA	2.15	127.48	124.51
25	C	506	CLA	CHB-C4A-NA	2.15	127.48	124.51
26	6	1620	LUT	C2-C3-C4	2.15	113.25	110.30
24	g	606	CHL	C2A-C1A-CHA	-2.15	120.10	123.86
24	n	601	CHL	C1-O2A-CGA	2.15	122.08	116.44
26	3	1620	LUT	C15-C35-C34	-2.15	119.07	123.47
24	5	607	CHL	CBA-CAA-C2A	-2.15	107.52	113.86
34	a	418	SQD	O48-C23-C24	2.15	118.65	111.91
29	N	2630	LHG	O8-C23-C24	2.15	118.65	111.91
33	A	408	PHO	CMC-C2C-C3C	2.15	128.99	124.94
24	8	607	CHL	CAA-CBA-CGA	-2.15	106.81	112.51
30	h	101	BCR	C15-C16-C17	-2.15	119.08	123.47
30	B	619	BCR	C40-C30-C25	2.15	113.78	110.30
25	1	604	CLA	C2D-C1D-ND	-2.15	108.52	110.10
25	5	603	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
24	4	607	CHL	CAA-CBA-CGA	-2.15	106.81	112.51
26	y	1620	LUT	C31-C30-C29	-2.15	124.25	127.31
24	r	607	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
30	b	619	BCR	C40-C30-C25	2.15	113.78	110.30
29	B	2630	LHG	C27-C26-C25	-2.15	103.53	114.42
29	5	2630	LHG	C27-C26-C25	-2.15	103.53	114.42
25	a	405	CLA	CHB-C4A-NA	2.15	127.48	124.51
29	b	2630	LHG	C27-C26-C25	-2.15	103.53	114.42
25	y	611	CLA	C2D-C1D-ND	-2.15	108.52	110.10
25	g	610	CLA	C2A-C1A-CHA	2.15	127.61	123.86
26	Y	1621	LUT	C35-C15-C14	-2.15	119.08	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	603	CLA	CHA-C1A-NA	-2.14	121.49	126.40
25	g	602	CLA	CHD-C1D-ND	-2.14	122.48	124.45
26	y	1620	LUT	O3-C3-C4	-2.14	105.08	109.68
24	1	608	CHL	C2A-C1A-CHA	-2.14	120.11	123.86
25	3	603	CLA	CHA-C1A-NA	-2.14	121.49	126.40
25	5	614	CLA	O2A-CGA-O1A	-2.14	117.95	123.30
26	5	1620	LUT	C20-C13-C12	2.14	121.45	118.08
37	c	518	DGD	O6D-C5D-C6D	-2.14	102.34	106.67
34	b	623	SQD	O5-C5-C4	2.14	113.59	109.69
24	G	608	CHL	C1C-C2C-C3C	-2.14	105.41	107.11
25	d	402	CLA	C3C-C4C-NC	-2.14	108.17	110.57
24	1	607	CHL	CBA-CAA-C2A	-2.14	107.54	113.86
25	S	602	CLA	CHB-C4A-NA	2.14	127.48	124.51
26	y	1621	LUT	C31-C30-C29	-2.14	124.25	127.31
37	C	518	DGD	CAB-C9B-C8B	-2.14	103.55	114.42
34	B	623	SQD	O5-C5-C4	2.14	113.58	109.69
25	N	614	CLA	CHD-C1D-ND	-2.14	122.49	124.45
26	1	1620	LUT	C20-C13-C12	2.14	121.45	118.08
25	c	506	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	Y	602	CLA	CAC-C3C-C4C	2.14	127.59	124.81
24	g	608	CHL	O2D-CGD-O1D	-2.14	119.65	123.84
25	b	609	CLA	CAC-C3C-C4C	2.14	127.59	124.81
26	Y	1620	LUT	C36-C21-C26	2.14	112.79	109.55
30	C	516	BCR	C35-C13-C12	2.14	121.45	118.08
25	1	614	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
35	B	2633	LMG	O6-C1-O1	-2.14	104.91	109.97
25	5	602	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	B	605	CLA	C1D-ND-C4D	2.14	107.86	106.33
24	4	606	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
30	C	515	BCR	C3-C4-C5	-2.14	110.26	114.08
25	c	508	CLA	CHC-C1C-NC	2.14	127.45	124.20
30	c	515	BCR	C3-C4-C5	-2.14	110.26	114.08
29	1	2630	LHG	C27-C26-C25	-2.14	103.57	114.42
30	c	516	BCR	C35-C13-C12	2.14	121.45	118.08
24	s	607	CHL	CMD-C2D-C3D	-2.14	122.70	127.61
26	Y	1621	LUT	C31-C30-C29	-2.14	124.26	127.31
24	G	609	CHL	C1-C2-C3	-2.14	122.35	126.04
37	c	518	DGD	CAB-C9B-C8B	-2.14	103.58	114.42
37	c	520	DGD	CBB-CAB-C9B	-2.14	103.58	114.42
25	C	513	CLA	O2D-CGD-CBD	2.14	115.06	111.27
29	c	522	LHG	C18-C17-C16	-2.14	103.58	114.42
29	b	2630	LHG	C11-C10-C9	-2.14	103.58	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	d	405	PL9	C31-C32-C33	-2.14	104.86	111.88
25	C	508	CLA	CHC-C1C-NC	2.13	127.44	124.20
29	B	2630	LHG	C11-C10-C9	-2.13	103.59	114.42
24	n	609	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
25	c	512	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
26	Y	1620	LUT	O3-C3-C4	-2.13	105.10	109.68
25	r	609	CLA	C2C-C1C-NC	2.13	111.97	109.97
30	t	101	BCR	C7-C6-C5	-2.13	116.29	121.46
37	C	520	DGD	CBB-CAB-C9B	-2.13	103.59	114.42
25	G	610	CLA	C2A-C1A-CHA	2.13	127.59	123.86
37	C	518	DGD	O6D-C5D-C6D	-2.13	102.36	106.67
25	n	614	CLA	CHD-C1D-ND	-2.13	122.49	124.45
37	H	102	DGD	O1G-C1A-O1A	-2.13	118.21	123.59
24	8	609	CHL	O2A-CGA-CBA	2.13	120.88	114.03
25	Y	611	CLA	C2D-C1D-ND	-2.13	108.53	110.10
30	T	101	BCR	C7-C6-C5	-2.13	116.30	121.46
24	4	609	CHL	O2A-CGA-CBA	2.13	120.88	114.03
26	6	1621	LUT	C11-C10-C9	-2.13	124.27	127.31
36	D	405	PL9	C31-C32-C33	-2.13	104.88	111.88
24	r	606	CHL	O2D-CGD-O1D	-2.13	119.67	123.84
35	c	521	LMG	O3-C3-C2	-2.13	105.42	110.35
24	7	601	CHL	O2A-CGA-CBA	2.13	118.59	111.91
30	c	515	BCR	C36-C18-C19	2.13	121.43	118.08
25	c	513	CLA	O2D-CGD-CBD	2.13	115.05	111.27
24	8	606	CHL	OMC-CMC-C2C	-2.13	120.87	125.69
25	c	507	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	3	606	CHL	C1B-CHB-C4A	-2.13	125.90	130.12
25	D	402	CLA	C3C-C4C-NC	-2.13	108.18	110.57
24	R	606	CHL	C2A-C1A-CHA	-2.13	120.14	123.86
29	C	522	LHG	C18-C17-C16	-2.13	103.62	114.42
37	c	519	DGD	CAB-C9B-C8B	-2.13	103.62	114.42
25	R	609	CLA	C2C-C1C-NC	2.13	111.97	109.97
24	n	607	CHL	C4D-C3D-CAD	2.13	110.60	108.10
35	b	2633	LMG	O6-C1-O1	-2.13	104.94	109.97
37	C	518	DGD	O3G-C1D-C2D	-2.13	104.98	108.30
37	c	518	DGD	O3G-C1D-C2D	-2.13	104.98	108.30
26	3	1620	LUT	C17-C1-C6	2.13	113.75	110.30
24	S	601	CHL	C1C-C2C-C3C	-2.13	105.43	107.11
25	b	609	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
24	8	606	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
24	8	607	CHL	O2D-CGD-O1D	-2.12	119.68	123.84
35	B	622	LMG	O2-C2-C1	-2.12	104.89	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	514	BCR	C7-C8-C9	-2.12	123.03	126.23
25	C	510	CLA	C1-C2-C3	-2.12	122.37	126.04
26	y	1621	LUT	C35-C15-C14	-2.12	119.12	123.47
35	A	415	LMG	O2-C2-C1	-2.12	104.89	110.05
24	G	608	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
28	y	1623	NEX	C40-C33-C34	-2.12	119.95	122.92
25	Y	603	CLA	C11-C10-C8	-2.12	109.06	115.92
35	b	622	LMG	O2-C2-C1	-2.12	104.89	110.05
24	3	609	CHL	OMC-CMC-C2C	-2.12	120.89	125.69
29	S	2630	LHG	C27-C26-C25	-2.12	103.65	114.42
24	R	607	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
29	B	2631	LHG	C20-C19-C18	-2.12	103.66	114.42
24	R	608	CHL	O2D-CGD-O1D	-2.12	119.69	123.84
28	r	623	NEX	C40-C33-C32	2.12	121.42	118.08
35	C	521	LMG	O3-C3-C2	-2.12	105.45	110.35
25	C	501	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	g	609	CHL	C1-C2-C3	-2.12	122.38	126.04
24	4	606	CHL	OMC-CMC-C2C	-2.12	120.89	125.69
37	h	102	DGD	CBB-CAB-C9B	-2.12	103.66	114.42
24	g	606	CHL	O2D-CGD-O1D	-2.12	119.69	123.84
24	G	607	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
26	2	1621	LUT	C11-C10-C9	-2.12	124.28	127.31
24	7	606	CHL	C1B-CHB-C4A	-2.12	125.92	130.12
24	7	609	CHL	OMC-CMC-C2C	-2.12	120.89	125.69
24	Y	601	CHL	CGD-CBD-CAD	-2.12	103.87	110.73
24	R	606	CHL	O2D-CGD-O1D	-2.12	119.69	123.84
37	H	102	DGD	CBB-CAB-C9B	-2.12	103.67	114.42
24	N	609	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
37	h	102	DGD	O1G-C1A-O1A	-2.12	118.25	123.59
24	r	608	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
30	C	514	BCR	C7-C8-C9	-2.12	123.03	126.23
25	B	609	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
24	3	601	CHL	O2A-CGA-CBA	2.12	118.55	111.91
24	y	601	CHL	CGD-CBD-CAD	-2.12	103.87	110.73
29	r	2630	LHG	C27-C26-C25	-2.12	103.67	114.42
37	C	519	DGD	CAB-C9B-C8B	-2.12	103.67	114.42
39	F	101	HEM	C4B-CHC-C1C	2.12	125.35	122.56
25	y	603	CLA	C11-C10-C8	-2.12	109.08	115.92
29	s	2630	LHG	C27-C26-C25	-2.12	103.68	114.42
27	g	1622	XAT	C35-C34-C33	-2.12	124.29	127.31
28	g	1623	NEX	C19-C9-C10	-2.12	119.96	122.92
26	7	1620	LUT	C17-C1-C6	2.12	113.73	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	2630	LHG	C27-C26-C25	-2.12	103.68	114.42
25	C	507	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
30	C	515	BCR	C36-C18-C19	2.11	121.41	118.08
26	y	1621	LUT	C37-C21-C22	-2.11	105.43	109.44
25	b	608	CLA	CHC-C1C-NC	2.11	127.41	124.20
24	5	608	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
25	S	613	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	2	603	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
29	b	2631	LHG	C20-C19-C18	-2.11	103.70	114.42
26	n	1620	LUT	C8-C9-C10	-2.11	115.70	118.94
25	c	501	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	C	505	CLA	C1-C2-C3	-2.11	122.39	126.04
24	G	606	CHL	O2D-CGD-O1D	-2.11	119.71	123.84
27	G	1622	XAT	O24-C25-C26	-2.11	57.21	58.96
24	s	601	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
24	8	608	CHL	CBC-CAC-C3C	-2.11	106.61	112.43
26	5	1621	LUT	C22-C23-C24	-2.11	109.34	111.74
37	B	626	DGD	C1D-C2D-C3D	-2.11	105.60	110.00
35	a	415	LMG	O2-C2-C1	-2.11	104.92	110.05
36	D	405	PL9	O2-C1-C6	2.11	124.24	120.59
25	5	612	CLA	CHC-C1C-NC	2.11	127.40	124.20
27	G	1622	XAT	C35-C34-C33	-2.11	124.30	127.31
28	y	1623	NEX	C4-C3-C2	-2.11	106.70	110.77
30	b	619	BCR	C37-C22-C23	2.11	121.40	118.08
26	1	1621	LUT	C31-C32-C33	-2.11	120.49	126.42
24	3	605	CHL	CHB-C4A-NA	2.11	127.43	124.51
25	s	609	CLA	O2A-CGA-O1A	-2.11	118.05	123.30
24	5	601	CHL	C2A-C1A-CHA	-2.11	120.17	123.86
26	s	1621	LUT	C21-C26-C27	-2.11	110.04	112.70
28	Y	1623	NEX	C4-C3-C2	-2.11	106.70	110.77
39	f	101	HEM	C4B-CHC-C1C	2.11	125.34	122.56
24	g	607	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
30	8	623	BCR	C21-C20-C19	-2.11	116.64	123.22
28	R	623	NEX	C40-C33-C32	2.11	121.39	118.08
27	g	1622	XAT	O24-C25-C26	-2.11	57.22	58.96
28	7	1623	NEX	C30-C31-C32	-2.10	116.65	123.22
24	r	606	CHL	C4-C3-C5	2.10	118.81	115.27
25	6	603	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
25	Y	602	CLA	CHD-C1D-ND	-2.10	122.52	124.45
25	3	610	CLA	CHB-C4A-NA	2.10	127.42	124.51
30	D	404	BCR	C36-C18-C19	2.10	121.39	118.08
24	n	607	CHL	CAA-CBA-CGA	-2.10	107.11	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	605	CHL	OMC-CMC-C2C	-2.10	120.93	125.69
24	1	607	CHL	C4-C3-C5	2.10	118.81	115.27
25	b	604	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
26	S	1621	LUT	C21-C26-C27	-2.10	110.04	112.70
29	s	2630	LHG	C5-O7-C7	-2.10	112.61	117.79
25	Y	612	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
24	N	608	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
37	b	626	DGD	C1D-C2D-C3D	-2.10	105.62	110.00
25	g	610	CLA	CAA-C2A-C1A	2.10	118.86	111.97
24	N	607	CHL	CAA-CBA-CGA	-2.10	107.11	113.25
24	N	607	CHL	C4D-C3D-CAD	2.10	110.57	108.10
28	Y	1623	NEX	C40-C33-C34	-2.10	119.98	122.92
24	4	607	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
26	5	1621	LUT	C31-C32-C33	-2.10	120.51	126.42
25	C	512	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
25	b	605	CLA	C1D-ND-C4D	2.10	107.83	106.33
26	1	1621	LUT	C22-C23-C24	-2.10	109.35	111.74
25	n	604	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	B	604	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	1	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
25	D	403	CLA	CHA-C1A-NA	-2.10	121.59	126.40
26	Y	1621	LUT	C37-C21-C22	-2.10	105.46	109.44
29	C	522	LHG	C20-C19-C18	-2.10	103.76	114.42
24	6	608	CHL	C2A-C1A-CHA	-2.10	120.19	123.86
30	4	623	BCR	C21-C20-C19	-2.10	116.66	123.22
24	6	607	CHL	C4A-NA-C1A	2.10	107.65	106.71
25	5	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	R	606	CHL	C4-C3-C5	2.10	118.80	115.27
24	g	608	CHL	C4D-C3D-CAD	2.10	110.57	108.10
27	7	1622	XAT	C11-C12-C13	-2.10	120.52	126.42
24	S	608	CHL	O2D-CGD-O1D	-2.10	119.74	123.84
24	4	608	CHL	CBC-CAC-C3C	-2.10	106.65	112.43
29	S	2630	LHG	C5-O7-C7	-2.10	112.63	117.79
24	n	608	CHL	C4D-CHA-C1A	-2.10	118.70	121.25
25	G	610	CLA	CAA-C2A-C1A	2.10	118.85	111.97
25	y	602	CLA	CHD-C1D-ND	-2.10	122.53	124.45
25	B	608	CLA	CHC-C1C-NC	2.10	127.38	124.20
25	s	613	CLA	CHB-C4A-NA	2.10	127.41	124.51
37	C	519	DGD	C5B-C4B-C3B	-2.10	103.79	114.42
29	c	522	LHG	C20-C19-C18	-2.10	103.79	114.42
24	G	605	CHL	OMC-CMC-C2C	-2.10	120.95	125.69
26	N	1620	LUT	C8-C9-C10	-2.10	115.73	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	606	CHL	O2A-CGA-CBA	2.09	120.76	114.03
24	G	608	CHL	C4D-C3D-CAD	2.09	110.56	108.10
37	c	519	DGD	C5B-C4B-C3B	-2.09	103.80	114.42
28	3	1623	NEX	C30-C31-C32	-2.09	116.68	123.22
26	g	1621	LUT	C1-C2-C3	2.09	118.37	113.64
25	S	609	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
25	B	614	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
36	d	405	PL9	O2-C1-C6	2.09	124.21	120.59
26	g	1621	LUT	C15-C35-C34	-2.09	119.19	123.47
24	1	601	CHL	C2A-C1A-CHA	-2.09	120.20	123.86
24	2	608	CHL	C2A-C1A-CHA	-2.09	120.20	123.86
28	G	1623	NEX	C19-C9-C10	-2.09	119.99	122.92
30	B	619	BCR	C37-C22-C23	2.09	121.37	118.08
28	6	1623	NEX	C30-C31-C32	-2.09	116.69	123.22
25	c	505	CLA	C1-C2-C3	-2.09	122.43	126.04
25	C	508	CLA	CMC-C2C-C1C	-2.09	121.86	125.04
35	a	415	LMG	O1-C7-C8	-2.09	105.86	110.90
30	d	404	BCR	C36-C18-C19	2.09	121.37	118.08
24	3	601	CHL	C4D-C3D-CAD	2.09	110.56	108.10
25	B	605	CLA	CHC-C1C-NC	2.09	127.37	124.20
26	3	1621	LUT	C39-C29-C28	2.09	121.37	118.08
24	3	601	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
25	3	610	CLA	CHD-C1D-ND	-2.09	122.53	124.45
28	2	1623	NEX	C30-C31-C32	-2.09	116.70	123.22
27	3	1622	XAT	C11-C12-C13	-2.09	120.55	126.42
29	S	2630	LHG	C20-C19-C18	-2.09	103.83	114.42
25	S	603	CLA	CHA-C1A-NA	-2.09	121.62	126.40
25	d	403	CLA	CHD-C1D-ND	-2.09	122.54	124.45
25	N	612	CLA	C2A-C1A-CHA	2.09	127.51	123.86
25	n	612	CLA	C2A-C1A-CHA	2.09	127.51	123.86
25	B	613	CLA	C9-C8-C10	-2.09	103.74	111.29
26	7	1621	LUT	C39-C29-C28	2.09	121.36	118.08
25	y	612	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	1	612	CLA	CHC-C1C-NC	2.09	127.37	124.20
24	g	601	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
25	N	604	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
25	b	605	CLA	CHC-C1C-NC	2.08	127.36	124.20
26	G	1621	LUT	C1-C2-C3	2.08	118.35	113.64
24	5	606	CHL	O2A-CGA-CBA	2.08	120.72	114.03
25	d	403	CLA	CHA-C1A-NA	-2.08	121.63	126.40
34	B	621	SQD	C3-C4-C5	2.08	113.95	110.24
25	C	512	CLA	O2A-CGA-O1A	-2.08	118.33	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	614	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
30	C	515	BCR	C10-C11-C12	-2.08	116.72	123.22
24	6	606	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
30	c	515	BCR	C10-C11-C12	-2.08	116.72	123.22
25	b	610	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
25	s	603	CLA	CHA-C1A-NA	-2.08	121.63	126.40
25	7	610	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	7	601	CHL	C4D-C3D-CAD	2.08	110.55	108.10
29	s	2630	LHG	C20-C19-C18	-2.08	103.86	114.42
35	A	415	LMG	O1-C7-C8	-2.08	105.88	110.90
24	Y	606	CHL	C1C-C2C-C3C	-2.08	105.46	107.11
37	C	518	DGD	C5B-C4B-C3B	-2.08	103.86	114.42
25	Y	614	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
39	F	101	HEM	C4D-ND-C1D	2.08	107.22	105.07
24	3	605	CHL	C2A-C1A-CHA	-2.08	120.22	123.86
26	G	1621	LUT	C15-C35-C34	-2.08	119.22	123.47
24	s	608	CHL	O2D-CGD-O1D	-2.08	119.78	123.84
25	b	613	CLA	C9-C8-C10	-2.08	103.77	111.29
25	B	610	CLA	CAA-CBA-CGA	-2.08	107.18	113.25
25	6	604	CLA	CAC-C3C-C4C	2.08	127.50	124.81
25	6	603	CLA	C2A-C1A-CHA	2.08	127.49	123.86
25	1	611	CLA	O2A-CGA-O1A	-2.08	118.12	123.30
30	b	619	BCR	C34-C9-C8	2.08	121.35	118.08
25	7	602	CLA	C1-C2-C3	-2.08	122.45	126.04
24	G	601	CHL	O1D-CGD-CBD	-2.08	120.24	124.48
25	c	512	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
24	Y	609	CHL	C1-C2-C3	-2.08	122.45	126.04
25	b	612	CLA	CAA-CBA-CGA	-2.07	107.19	113.25
37	c	518	DGD	C5B-C4B-C3B	-2.07	103.90	114.42
30	4	623	BCR	C15-C16-C17	-2.07	119.23	123.47
26	S	1621	LUT	C16-C1-C6	-2.07	106.94	110.30
25	G	610	CLA	CHA-C1A-NA	-2.07	121.65	126.40
25	g	610	CLA	CHA-C1A-NA	-2.07	121.65	126.40
30	D	404	BCR	C10-C11-C12	-2.07	116.75	123.22
25	5	611	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
27	g	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
24	7	605	CHL	CHB-C4A-NA	2.07	127.38	124.51
30	b	619	BCR	C16-C15-C14	-2.07	119.23	123.47
25	B	612	CLA	CAA-CBA-CGA	-2.07	107.20	113.25
37	c	519	DGD	O3E-C3E-C2E	-2.07	105.56	110.35
25	y	604	CLA	CHB-C4A-NA	2.07	127.38	124.51
30	B	619	BCR	C16-C15-C14	-2.07	119.23	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	523	LHG	C27-C26-C25	-2.07	103.92	114.42
30	c	516	BCR	C33-C5-C4	2.07	117.59	113.62
27	N	1622	XAT	C7-C8-C9	-2.07	122.32	125.53
24	5	607	CHL	C4-C3-C5	2.07	118.75	115.27
24	N	605	CHL	O2A-CGA-O1A	-2.07	118.37	123.59
24	R	607	CHL	CGD-CBD-CAD	-2.07	104.03	110.73
25	D	402	CLA	CAC-C3C-C2C	-2.07	123.99	127.53
35	B	622	LMG	O3-C3-C2	-2.07	105.57	110.35
25	b	614	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
29	D	409	LHG	O8-C6-C5	-2.07	102.41	108.43
39	f	101	HEM	C4D-ND-C1D	2.07	107.21	105.07
25	B	616	CLA	C2A-C1A-CHA	2.07	127.47	123.86
30	C	516	BCR	C33-C5-C4	2.07	117.59	113.62
25	7	610	CLA	CHD-C1D-ND	-2.07	122.55	124.45
29	d	409	LHG	O8-C6-C5	-2.07	102.42	108.43
26	s	1621	LUT	C16-C1-C6	-2.07	106.95	110.30
29	c	523	LHG	C27-C26-C25	-2.07	103.93	114.42
25	C	506	CLA	C1-C2-C3	-2.07	122.47	126.04
30	h	101	BCR	C2-C1-C6	2.07	113.66	110.48
24	7	605	CHL	C2A-C1A-CHA	-2.07	120.25	123.86
24	n	605	CHL	O2A-CGA-O1A	-2.07	118.38	123.59
35	Z	101	LMG	O3-C3-C2	-2.07	105.57	110.35
25	S	610	CLA	O2D-CGD-CBD	2.07	114.94	111.27
25	1	610	CLA	C4A-NA-C1A	2.07	107.64	106.71
30	c	517	BCR	C36-C18-C19	2.07	121.33	118.08
25	c	508	CLA	CMC-C2C-C1C	-2.07	121.89	125.04
35	z	101	LMG	O3-C3-C2	-2.07	105.57	110.35
25	B	610	CLA	O2D-CGD-O1D	-2.07	119.80	123.84
30	d	404	BCR	C10-C11-C12	-2.07	116.77	123.22
24	N	609	CHL	CED-O2D-CGD	2.07	120.61	115.94
25	B	611	CLA	CAA-C2A-C1A	-2.06	105.21	111.97
30	c	514	BCR	C37-C22-C23	2.06	121.33	118.08
26	1	1621	LUT	C38-C25-C24	-2.06	119.14	123.56
27	n	1622	XAT	C7-C8-C9	-2.06	122.33	125.53
26	7	1621	LUT	C31-C30-C29	-2.06	124.37	127.31
26	4	620	LUT	C20-C13-C12	2.06	121.33	118.08
30	C	517	BCR	C36-C18-C19	2.06	121.33	118.08
25	b	612	CLA	C1C-C2C-C3C	2.06	109.12	106.96
26	5	1621	LUT	C38-C25-C24	-2.06	119.15	123.56
30	C	514	BCR	C24-C23-C22	-2.06	123.12	126.23
25	c	509	CLA	C11-C12-C13	-2.06	109.25	115.92
26	g	1621	LUT	C8-C9-C10	-2.06	115.78	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	403	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	y	609	CHL	CMA-C3A-C4A	-2.06	106.23	111.77
35	b	622	LMG	O3-C3-C2	-2.06	105.58	110.35
27	G	1622	XAT	C7-C8-C9	-2.06	122.33	125.53
25	s	610	CLA	O2D-CGD-CBD	2.06	114.93	111.27
25	Y	602	CLA	C4-C3-C5	2.06	118.73	115.27
25	B	614	CLA	C3A-C2A-C1A	2.06	104.42	101.34
25	B	615	CLA	O1D-CGD-CBD	2.06	128.70	124.48
24	2	606	CHL	C4D-CHA-C1A	-2.06	118.74	121.25
24	r	607	CHL	CGD-CBD-CAD	-2.06	104.07	110.73
25	2	603	CLA	C2A-C1A-CHA	2.06	127.46	123.86
25	c	502	CLA	O1D-CGD-CBD	2.06	128.69	124.48
28	r	623	NEX	O24-C25-C26	-2.06	57.26	58.96
25	2	604	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	d	403	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	Y	604	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	3	605	CHL	C1B-CHB-C4A	-2.06	126.04	130.12
24	3	607	CHL	O2D-CGD-O1D	-2.06	119.82	123.84
26	8	620	LUT	C20-C13-C12	2.06	121.32	118.08
25	c	506	CLA	C1-C2-C3	-2.06	122.49	126.04
37	C	519	DGD	O3E-C3E-C2E	-2.06	105.59	110.35
30	c	514	BCR	C24-C23-C22	-2.06	123.13	126.23
30	t	101	BCR	C34-C9-C10	-2.06	120.04	122.92
25	C	509	CLA	C11-C12-C13	-2.06	109.27	115.92
28	N	1623	NEX	C40-C33-C34	-2.06	120.04	122.92
25	y	602	CLA	C6-C7-C8	-2.06	109.28	115.92
25	d	402	CLA	CAC-C3C-C2C	-2.06	124.01	127.53
25	b	611	CLA	CAA-C2A-C1A	-2.05	105.24	111.97
24	3	608	CHL	C2A-C1A-CHA	-2.05	120.27	123.86
25	B	612	CLA	C1C-C2C-C3C	2.05	109.12	106.96
30	H	101	BCR	C2-C1-C6	2.05	113.64	110.48
24	7	601	CHL	O2D-CGD-O1D	-2.05	119.82	123.84
24	Y	609	CHL	CMA-C3A-C4A	-2.05	106.25	111.77
24	R	607	CHL	C1B-CHB-C4A	-2.05	126.05	130.12
25	B	612	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
24	n	609	CHL	CED-O2D-CGD	2.05	120.58	115.94
30	D	404	BCR	C28-C27-C26	-2.05	110.41	114.08
24	Y	608	CHL	C1C-C2C-C3C	-2.05	105.48	107.11
24	y	606	CHL	C1C-C2C-C3C	-2.05	105.48	107.11
25	b	615	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
35	Z	101	LMG	O5-C6-C5	-2.05	104.25	111.29
26	N	1620	LUT	C20-C13-C12	2.05	121.31	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	1620	LUT	C20-C13-C12	2.05	121.31	118.08
29	N	2630	LHG	C29-C28-C27	-2.05	104.01	114.42
37	c	520	DGD	O2D-C2D-C1D	-2.05	105.06	110.05
30	8	623	BCR	C15-C16-C17	-2.05	119.27	123.47
28	G	1623	NEX	O24-C25-C26	-2.05	57.26	58.96
25	2	613	CLA	O1D-CGD-CBD	2.05	128.68	124.48
25	b	611	CLA	O1D-CGD-CBD	2.05	128.68	124.48
25	3	610	CLA	C7-C6-C5	-2.05	107.79	113.36
28	n	1623	NEX	C40-C33-C34	-2.05	120.05	122.92
25	6	612	CLA	CHA-C1A-NA	-2.05	121.70	126.40
30	B	619	BCR	C34-C9-C8	2.05	121.31	118.08
30	C	514	BCR	C37-C22-C23	2.05	121.31	118.08
25	B	615	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	N	1621	LUT	C38-C25-C24	-2.05	119.17	123.56
25	b	615	CLA	O1D-CGD-CBD	2.05	128.68	124.48
34	a	412	SQD	C44-O6-C1	2.05	117.74	113.74
34	b	621	SQD	C3-C4-C5	2.05	113.89	110.24
25	2	612	CLA	CHA-C1A-NA	-2.05	121.71	126.40
25	6	613	CLA	O1D-CGD-CBD	2.05	128.68	124.48
25	7	610	CLA	C7-C6-C5	-2.05	107.80	113.36
29	n	2630	LHG	C29-C28-C27	-2.05	104.03	114.42
25	g	612	CLA	C2A-C1A-CHA	2.05	127.44	123.86
24	1	607	CHL	C4D-C3D-CAD	2.05	110.51	108.10
28	g	1623	NEX	O24-C25-C26	-2.05	57.26	58.96
25	Y	602	CLA	C6-C7-C8	-2.05	109.30	115.92
25	6	604	CLA	C2D-C1D-ND	-2.05	108.60	110.10
25	b	612	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
24	8	608	CHL	CMA-C3A-C2A	-2.05	105.58	113.83
30	8	623	BCR	C4-C5-C6	-2.05	119.76	122.73
24	7	601	CHL	C1-O2A-CGA	2.05	121.81	116.44
24	5	607	CHL	C4D-C3D-CAD	2.05	110.51	108.10
35	z	101	LMG	O5-C6-C5	-2.05	104.27	111.29
30	T	101	BCR	C34-C9-C10	-2.05	120.06	122.92
24	G	601	CHL	O2D-CGD-O1D	-2.04	119.84	123.84
25	3	613	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	3	602	CLA	C1-C2-C3	-2.04	122.51	126.04
26	7	1620	LUT	C36-C21-C26	2.04	112.64	109.55
25	b	610	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
26	S	1621	LUT	C20-C13-C12	2.04	121.30	118.08
24	1	607	CHL	CMA-C3A-C4A	-2.04	106.28	111.77
30	T	101	BCR	C38-C26-C25	-2.04	122.23	124.53
34	A	412	SQD	C44-O6-C1	2.04	117.73	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	604	CLA	O1D-CGD-CBD	2.04	128.66	124.48
25	S	602	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	y	609	CHL	C1-C2-C3	-2.04	122.51	126.04
24	g	601	CHL	O2D-CGD-O1D	-2.04	119.84	123.84
25	B	609	CLA	C16-C15-C13	-2.04	109.32	115.92
26	n	1621	LUT	C38-C25-C24	-2.04	119.19	123.56
25	s	602	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	7	608	CHL	C2A-C1A-CHA	-2.04	120.29	123.86
24	R	607	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
25	C	502	CLA	O1D-CGD-CBD	2.04	128.66	124.48
24	5	607	CHL	CMA-C3A-C4A	-2.04	106.28	111.77
26	n	1620	LUT	C11-C10-C9	-2.04	124.40	127.31
24	4	608	CHL	CMA-C3A-C2A	-2.04	105.59	113.83
24	g	605	CHL	C4D-C3D-CAD	2.04	110.50	108.10
30	d	404	BCR	C28-C27-C26	-2.04	110.43	114.08
34	A	418	SQD	C3-C4-C5	2.04	113.88	110.24
30	D	404	BCR	C15-C14-C13	-2.04	124.40	127.31
30	d	404	BCR	C15-C14-C13	-2.04	124.40	127.31
25	y	602	CLA	C4-C3-C5	2.04	118.70	115.27
24	3	601	CHL	C1-O2A-CGA	2.04	121.80	116.44
24	Y	601	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
37	c	520	DGD	O6E-C1E-O5D	-2.04	105.14	109.97
25	G	612	CLA	C2A-C1A-CHA	2.04	127.43	123.86
25	C	507	CLA	O2D-CGD-CBD	2.04	114.89	111.27
28	y	1623	NEX	O24-C25-C26	-2.04	57.27	58.96
25	Y	604	CLA	O1D-CGD-CBD	2.04	128.66	124.48
25	b	616	CLA	C2A-C1A-CHA	2.04	127.42	123.86
35	d	411	LMG	O7-C10-O9	-2.04	118.78	123.70
25	R	603	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	t	101	BCR	C38-C26-C25	-2.04	122.24	124.53
25	B	602	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	y	603	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	7	605	CHL	C1B-CHB-C4A	-2.04	126.08	130.12
24	r	607	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
25	b	609	CLA	C16-C15-C13	-2.04	109.33	115.92
35	D	411	LMG	O7-C10-O9	-2.04	118.78	123.70
25	5	604	CLA	C2D-C1D-ND	-2.04	108.60	110.10
24	7	607	CHL	O2D-CGD-O1D	-2.04	119.86	123.84
25	B	605	CLA	C1-O2A-CGA	-2.04	111.10	116.44
28	6	1623	NEX	C15-C35-C34	-2.04	119.31	123.47
25	b	605	CLA	C1-O2A-CGA	-2.03	111.11	116.44
24	1	607	CHL	CAA-CBA-CGA	-2.03	107.31	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	C	520	DGD	O2D-C2D-C1D	-2.03	105.10	110.05
26	6	1620	LUT	C11-C10-C9	-2.03	124.41	127.31
25	b	602	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	4	609	CHL	CED-O2D-CGD	2.03	120.53	115.94
24	y	608	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
28	G	1623	NEX	C28-C29-C30	2.03	122.06	118.94
33	a	409	PHO	C1B-NB-C4B	2.03	111.27	107.09
24	g	609	CHL	C1-O2A-CGA	2.03	121.78	116.44
24	s	601	CHL	O2D-CGD-O1D	-2.03	119.86	123.84
25	r	610	CLA	C1-C2-C3	-2.03	122.53	126.04
26	G	1621	LUT	C8-C9-C10	-2.03	115.82	118.94
25	c	507	CLA	O2D-CGD-CBD	2.03	114.88	111.27
24	5	607	CHL	CAA-CBA-CGA	-2.03	107.32	113.25
24	s	606	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
25	r	603	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	B	611	CLA	O1D-CGD-CBD	2.03	128.64	124.48
24	S	601	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
30	d	404	BCR	C20-C21-C22	-2.03	124.41	127.31
28	Y	1623	NEX	O24-C25-C26	-2.03	57.28	58.96
24	G	609	CHL	C1-O2A-CGA	2.03	121.77	116.44
37	C	520	DGD	O6E-C1E-O5D	-2.03	105.17	109.97
26	N	1620	LUT	C11-C10-C9	-2.03	124.42	127.31
25	B	617	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	c	511	CLA	CAA-C2A-C1A	2.03	118.62	111.97
28	S	1623	NEX	C16-C1-C6	2.03	112.29	110.47
25	Y	603	CLA	CHA-C1A-NA	-2.03	121.76	126.40
25	R	616	CLA	O2D-CGD-CBD	2.03	114.87	111.27
24	r	607	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
27	6	1622	XAT	O24-C25-C26	-2.03	57.28	58.96
25	C	511	CLA	CAA-C2A-C1A	2.03	118.61	111.97
24	8	608	CHL	CED-O2D-CGD	2.03	120.52	115.94
30	4	623	BCR	C4-C5-C6	-2.03	119.79	122.73
27	5	1622	XAT	O24-C25-C26	-2.03	57.28	58.96
25	7	613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
24	2	606	CHL	O2A-CGA-CBA	2.02	120.53	114.03
33	A	409	PHO	C1B-NB-C4B	2.02	111.25	107.09
25	S	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45
27	2	1622	XAT	O24-C25-C26	-2.02	57.28	58.96
24	6	606	CHL	O2A-CGA-CBA	2.02	120.53	114.03
25	G	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	3	602	CLA	O1D-CGD-CBD	2.02	128.62	124.48
26	3	1620	LUT	C36-C21-C26	2.02	112.61	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	617	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
26	s	1621	LUT	C20-C13-C12	2.02	121.26	118.08
26	3	1621	LUT	C31-C30-C29	-2.02	124.43	127.31
33	a	408	PHO	O2D-CGD-O1D	-2.02	119.89	123.84
25	4	610	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
24	S	606	CHL	C1C-C2C-C3C	-2.02	105.51	107.11
25	s	604	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
34	a	418	SQD	C3-C4-C5	2.02	113.84	110.24
25	S	604	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	b	614	CLA	C3A-C2A-C1A	2.02	104.36	101.34
25	7	614	CLA	O2D-CGD-CBD	2.02	114.85	111.27
28	Y	1623	NEX	C5-C6-C1	2.02	121.70	119.70
25	B	602	CLA	CAC-C3C-C4C	2.02	127.42	124.81
25	r	616	CLA	O2D-CGD-CBD	2.02	114.85	111.27
25	3	611	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
25	B	606	CLA	C3C-C4C-NC	-2.02	108.31	110.57
27	6	1622	XAT	C31-C32-C33	-2.02	120.75	126.42
24	8	608	CHL	C2A-C1A-CHA	-2.01	120.34	123.86
30	c	514	BCR	C2-C3-C4	-2.01	106.88	111.38
27	1	1622	XAT	C10-C11-C12	-2.01	116.93	123.22
25	R	610	CLA	C1-C2-C3	-2.01	122.56	126.04
27	6	1622	XAT	C19-C9-C10	-2.01	120.10	122.92
28	r	623	NEX	C5-C4-C3	-2.01	109.36	111.75
27	y	1622	XAT	O24-C25-C26	-2.01	57.29	58.96
26	5	1621	LUT	C36-C21-C26	2.01	112.59	109.55
24	8	609	CHL	CED-O2D-CGD	2.01	120.49	115.94
25	8	610	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
25	b	602	CLA	CAC-C3C-C4C	2.01	127.42	124.81
25	1	612	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
28	2	1623	NEX	C15-C35-C34	-2.01	119.35	123.47
25	s	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	S	607	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
24	5	609	CHL	O2D-CGD-O1D	-2.01	119.91	123.84
25	D	403	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	2	1621	LUT	C18-C5-C6	-2.01	122.27	124.53
25	A	406	CLA	CHD-C4C-NC	2.01	127.37	124.20
25	B	612	CLA	C7-C6-C5	-2.01	107.90	113.36
28	n	1623	NEX	O24-C25-C26	-2.01	57.29	58.96
24	4	608	CHL	C1D-CHD-C4C	-2.01	121.72	126.06
30	C	514	BCR	C2-C3-C4	-2.01	106.89	111.38
25	8	604	CLA	O1A-CGA-CBA	2.01	129.54	123.08
24	y	601	CHL	O1D-CGD-CBD	-2.01	120.37	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	608	CHL	CED-O2D-CGD	2.01	120.48	115.94
27	8	622	XAT	C39-C29-C28	2.01	121.24	118.08
28	y	1623	NEX	C5-C6-C1	2.01	121.69	119.70
25	r	602	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	Y	613	CLA	O2D-CGD-CBD	2.01	114.84	111.27
25	7	610	CLA	C2D-C1D-ND	-2.01	108.62	110.10
25	S	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	6	614	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
25	7	611	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
25	B	602	CLA	CHD-C1D-ND	-2.01	122.61	124.45
25	b	605	CLA	CAA-C2A-C1A	2.01	118.55	111.97
24	S	601	CHL	CED-O2D-CGD	2.01	120.48	115.94
25	2	604	CLA	C2D-C1D-ND	-2.01	108.62	110.10
25	R	602	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
25	7	602	CLA	O1D-CGD-CBD	2.01	128.59	124.48
25	5	612	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
28	S	1623	NEX	C38-C25-C24	2.01	116.54	114.28
27	5	1622	XAT	C10-C11-C12	-2.01	116.96	123.22
26	1	1621	LUT	C36-C21-C26	2.01	112.58	109.55
25	g	612	CLA	CHA-C1A-NA	-2.01	121.80	126.40
28	g	1623	NEX	C28-C29-C30	2.01	122.02	118.94
27	1	1622	XAT	O24-C25-C26	-2.01	57.30	58.96
25	B	613	CLA	C11-C12-C13	-2.01	109.44	115.92
27	2	1622	XAT	C31-C32-C33	-2.01	120.78	126.42
25	2	614	CLA	O2D-CGD-CBD	2.01	114.83	111.27
25	b	606	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
26	2	1620	LUT	C11-C10-C9	-2.00	124.45	127.31
26	6	1621	LUT	C18-C5-C6	-2.00	122.28	124.53
25	b	606	CLA	C3C-C4C-NC	-2.00	108.32	110.57
25	B	606	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
24	G	607	CHL	C1B-CHB-C4A	-2.00	126.15	130.12
24	s	601	CHL	CED-O2D-CGD	2.00	120.47	115.94
25	1	602	CLA	C4A-NA-C1A	2.00	107.61	106.71
24	3	605	CHL	CGD-CBD-CAD	-2.00	104.24	110.73
27	8	622	XAT	C30-C31-C32	-2.00	116.97	123.22
28	s	1623	NEX	C38-C25-C24	2.00	116.53	114.28
24	2	609	CHL	CBC-CAC-C3C	-2.00	106.91	112.43
25	3	614	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	b	604	CLA	CHA-C1A-NA	-2.00	121.81	126.40
25	3	604	CLA	O1A-CGA-CBA	2.00	129.51	123.08
24	4	608	CHL	C2A-C1A-CHA	-2.00	120.36	123.86
24	N	608	CHL	C11-C12-C13	-2.00	109.45	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	617	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	c	511	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	R	604	CLA	C2A-C1A-CHA	2.00	127.36	123.86
25	a	406	CLA	CHD-C4C-NC	2.00	127.36	124.20
24	7	605	CHL	CGD-CBD-CAD	-2.00	104.25	110.73
24	1	609	CHL	O2D-CGD-O1D	-2.00	119.93	123.84
24	6	609	CHL	CBC-CAC-C3C	-2.00	106.92	112.43
25	B	605	CLA	CAA-C2A-C1A	2.00	118.53	111.97
24	n	608	CHL	CMB-C2B-C3B	2.00	128.42	124.68
24	n	608	CHL	C11-C12-C13	-2.00	109.45	115.92

All (526) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	1	601	CHL	ND
24	1	601	CHL	NA
24	1	601	CHL	NC
24	1	605	CHL	ND
24	1	605	CHL	NA
24	1	605	CHL	NC
24	1	606	CHL	ND
24	1	606	CHL	NA
24	1	606	CHL	NC
24	1	607	CHL	ND
24	1	607	CHL	C8
24	1	607	CHL	NA
24	1	607	CHL	NC
24	1	608	CHL	ND
24	1	608	CHL	NA
24	1	608	CHL	NC
24	1	609	CHL	ND
24	1	609	CHL	C8
24	1	609	CHL	NA
24	1	609	CHL	NC
24	2	601	CHL	ND
24	2	601	CHL	NA
24	2	601	CHL	NC
24	2	605	CHL	ND
24	2	605	CHL	NA
24	2	605	CHL	NC
24	2	606	CHL	ND
24	2	606	CHL	NA

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Mol	Chain	Res	Type	Atom
24	2	606	CHL	NC
24	2	607	CHL	ND
24	2	607	CHL	C8
24	2	607	CHL	NA
24	2	607	CHL	NC
24	2	608	CHL	ND
24	2	608	CHL	NA
24	2	608	CHL	NC
24	2	609	CHL	ND
24	2	609	CHL	C8
24	2	609	CHL	NA
24	2	609	CHL	NC
24	3	601	CHL	ND
24	3	601	CHL	C8
24	3	601	CHL	NA
24	3	601	CHL	NC
24	3	605	CHL	ND
24	3	605	CHL	NA
24	3	605	CHL	NC
24	3	606	CHL	ND
24	3	606	CHL	NA
24	3	606	CHL	NC
24	3	607	CHL	ND
24	3	607	CHL	NA
24	3	607	CHL	NC
24	3	608	CHL	ND
24	3	608	CHL	NA
24	3	608	CHL	NC
24	3	609	CHL	ND
24	3	609	CHL	C8
24	3	609	CHL	NA
24	3	609	CHL	NC
24	4	601	CHL	ND
24	4	601	CHL	NA
24	4	601	CHL	NC
24	4	606	CHL	ND
24	4	606	CHL	NA
24	4	606	CHL	NC
24	4	607	CHL	ND
24	4	607	CHL	NA
24	4	607	CHL	NC
24	4	608	CHL	ND

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Mol	Chain	Res	Type	Atom
24	4	608	CHL	NA
24	4	608	CHL	NC
24	4	609	CHL	ND
24	4	609	CHL	NA
24	4	609	CHL	NC
24	G	601	CHL	ND
24	G	601	CHL	C8
24	G	601	CHL	NA
24	G	601	CHL	NC
24	G	605	CHL	ND
24	G	605	CHL	NA
24	G	605	CHL	NC
24	G	606	CHL	ND
24	G	606	CHL	NA
24	G	606	CHL	NC
24	G	607	CHL	ND
24	G	607	CHL	C8
24	G	607	CHL	NA
24	G	607	CHL	NC
24	G	608	CHL	ND
24	G	608	CHL	C8
24	G	608	CHL	NA
24	G	608	CHL	NC
24	G	609	CHL	ND
24	G	609	CHL	C8
24	G	609	CHL	NA
24	G	609	CHL	NC
24	N	601	CHL	ND
24	N	601	CHL	C8
24	N	601	CHL	NA
24	N	601	CHL	NC
24	N	605	CHL	ND
24	N	605	CHL	NA
24	N	605	CHL	NC
24	N	606	CHL	ND
24	N	606	CHL	NA
24	N	606	CHL	NC
24	N	607	CHL	ND
24	N	607	CHL	C8
24	N	607	CHL	NA
24	N	607	CHL	NC
24	N	608	CHL	ND

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Mol	Chain	Res	Type	Atom
24	N	608	CHL	C8
24	N	608	CHL	NA
24	N	608	CHL	NC
24	N	609	CHL	ND
24	N	609	CHL	C8
24	N	609	CHL	NA
24	N	609	CHL	NC
24	R	606	CHL	ND
24	R	606	CHL	C8
24	R	606	CHL	NA
24	R	606	CHL	NC
24	R	607	CHL	ND
24	R	607	CHL	C8
24	R	607	CHL	NA
24	R	607	CHL	NC
24	R	608	CHL	ND
24	R	608	CHL	C8
24	R	608	CHL	NA
24	R	608	CHL	NC
24	R	614	CHL	ND
24	R	614	CHL	NA
24	R	614	CHL	NC
24	S	601	CHL	ND
24	S	601	CHL	NA
24	S	601	CHL	NC
24	S	606	CHL	ND
24	S	606	CHL	NA
24	S	606	CHL	NC
24	S	607	CHL	ND
24	S	607	CHL	C8
24	S	607	CHL	NA
24	S	607	CHL	NC
24	S	608	CHL	ND
24	S	608	CHL	NA
24	S	608	CHL	NC
24	Y	601	CHL	ND
24	Y	601	CHL	C8
24	Y	601	CHL	NA
24	Y	601	CHL	NC
24	Y	605	CHL	ND
24	Y	605	CHL	NA
24	Y	605	CHL	NC

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Mol	Chain	Res	Type	Atom
24	Y	606	CHL	ND
24	Y	606	CHL	NA
24	Y	606	CHL	NC
24	Y	607	CHL	ND
24	Y	607	CHL	C8
24	Y	607	CHL	NA
24	Y	607	CHL	NC
24	Y	608	CHL	ND
24	Y	608	CHL	C8
24	Y	608	CHL	NA
24	Y	608	CHL	NC
24	Y	609	CHL	ND
24	Y	609	CHL	C8
24	Y	609	CHL	NA
24	Y	609	CHL	NC
24	5	601	CHL	ND
24	5	601	CHL	NA
24	5	601	CHL	NC
24	5	605	CHL	ND
24	5	605	CHL	NA
24	5	605	CHL	NC
24	5	606	CHL	ND
24	5	606	CHL	NA
24	5	606	CHL	NC
24	5	607	CHL	ND
24	5	607	CHL	C8
24	5	607	CHL	NA
24	5	607	CHL	NC
24	5	608	CHL	ND
24	5	608	CHL	NA
24	5	608	CHL	NC
24	5	609	CHL	ND
24	5	609	CHL	C8
24	5	609	CHL	NA
24	5	609	CHL	NC
24	6	601	CHL	ND
24	6	601	CHL	NA
24	6	601	CHL	NC
24	6	605	CHL	ND
24	6	605	CHL	NA
24	6	605	CHL	NC
24	6	606	CHL	ND

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Mol	Chain	Res	Type	Atom
24	6	606	CHL	NA
24	6	606	CHL	NC
24	6	607	CHL	ND
24	6	607	CHL	C8
24	6	607	CHL	NA
24	6	607	CHL	NC
24	6	608	CHL	ND
24	6	608	CHL	NA
24	6	608	CHL	NC
24	6	609	CHL	ND
24	6	609	CHL	C8
24	6	609	CHL	NA
24	6	609	CHL	NC
24	7	601	CHL	ND
24	7	601	CHL	C8
24	7	601	CHL	NA
24	7	601	CHL	NC
24	7	605	CHL	ND
24	7	605	CHL	NA
24	7	605	CHL	NC
24	7	606	CHL	ND
24	7	606	CHL	NA
24	7	606	CHL	NC
24	7	607	CHL	ND
24	7	607	CHL	NA
24	7	607	CHL	NC
24	7	608	CHL	ND
24	7	608	CHL	NA
24	7	608	CHL	NC
24	7	609	CHL	ND
24	7	609	CHL	C8
24	7	609	CHL	NA
24	7	609	CHL	NC
24	8	601	CHL	ND
24	8	601	CHL	NA
24	8	601	CHL	NC
24	8	606	CHL	ND
24	8	606	CHL	NA
24	8	606	CHL	NC
24	8	607	CHL	ND
24	8	607	CHL	NA
24	8	607	CHL	NC

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Mol	Chain	Res	Type	Atom
24	8	608	CHL	ND
24	8	608	CHL	NA
24	8	608	CHL	NC
24	8	609	CHL	ND
24	8	609	CHL	NA
24	8	609	CHL	NC
24	g	601	CHL	ND
24	g	601	CHL	C8
24	g	601	CHL	NA
24	g	601	CHL	NC
24	g	605	CHL	ND
24	g	605	CHL	NA
24	g	605	CHL	NC
24	g	606	CHL	ND
24	g	606	CHL	NA
24	g	606	CHL	NC
24	g	607	CHL	ND
24	g	607	CHL	C8
24	g	607	CHL	NA
24	g	607	CHL	NC
24	g	608	CHL	ND
24	g	608	CHL	C8
24	g	608	CHL	NA
24	g	608	CHL	NC
24	g	609	CHL	ND
24	g	609	CHL	C8
24	g	609	CHL	NA
24	g	609	CHL	NC
24	n	601	CHL	ND
24	n	601	CHL	C8
24	n	601	CHL	NA
24	n	601	CHL	NC
24	n	605	CHL	ND
24	n	605	CHL	NA
24	n	605	CHL	NC
24	n	606	CHL	ND
24	n	606	CHL	NA
24	n	606	CHL	NC
24	n	607	CHL	ND
24	n	607	CHL	C8
24	n	607	CHL	NA
24	n	607	CHL	NC

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Mol	Chain	Res	Type	Atom
24	n	608	CHL	ND
24	n	608	CHL	C8
24	n	608	CHL	NA
24	n	608	CHL	NC
24	n	609	CHL	ND
24	n	609	CHL	C8
24	n	609	CHL	NA
24	n	609	CHL	NC
24	r	606	CHL	ND
24	r	606	CHL	C8
24	r	606	CHL	NA
24	r	606	CHL	NC
24	r	607	CHL	ND
24	r	607	CHL	C8
24	r	607	CHL	NA
24	r	607	CHL	NC
24	r	608	CHL	ND
24	r	608	CHL	C8
24	r	608	CHL	NA
24	r	608	CHL	NC
24	r	614	CHL	ND
24	r	614	CHL	NA
24	r	614	CHL	NC
24	s	601	CHL	ND
24	s	601	CHL	NA
24	s	601	CHL	NC
24	s	606	CHL	ND
24	s	606	CHL	NA
24	s	606	CHL	NC
24	s	607	CHL	ND
24	s	607	CHL	C8
24	s	607	CHL	NA
24	s	607	CHL	NC
24	s	608	CHL	ND
24	s	608	CHL	NA
24	s	608	CHL	NC
24	y	601	CHL	ND
24	y	601	CHL	C8
24	y	601	CHL	NA
24	y	601	CHL	NC
24	y	605	CHL	ND
24	y	605	CHL	NA

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Mol	Chain	Res	Type	Atom
24	y	605	CHL	NC
24	y	606	CHL	ND
24	y	606	CHL	NA
24	y	606	CHL	NC
24	y	607	CHL	ND
24	y	607	CHL	C8
24	y	607	CHL	NA
24	y	607	CHL	NC
24	y	608	CHL	ND
24	y	608	CHL	C8
24	y	608	CHL	NA
24	y	608	CHL	NC
24	y	609	CHL	ND
24	y	609	CHL	C8
24	y	609	CHL	NA
24	y	609	CHL	NC
25	1	602	CLA	ND
25	1	603	CLA	ND
25	1	604	CLA	ND
25	1	610	CLA	ND
25	1	611	CLA	ND
25	1	612	CLA	ND
25	1	614	CLA	ND
25	2	602	CLA	ND
25	2	603	CLA	ND
25	2	610	CLA	ND
25	2	611	CLA	ND
25	2	612	CLA	ND
25	3	602	CLA	ND
25	3	603	CLA	ND
25	3	604	CLA	ND
25	3	610	CLA	ND
25	3	611	CLA	ND
25	3	612	CLA	ND
25	3	613	CLA	ND
25	3	614	CLA	ND
25	4	602	CLA	ND
25	4	603	CLA	ND
25	4	610	CLA	ND
25	4	611	CLA	ND
25	4	612	CLA	ND
25	A	405	CLA	ND

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Mol	Chain	Res	Type	Atom
25	A	406	CLA	ND
25	A	407	CLA	ND
25	A	410	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	B	617	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	512	CLA	ND
25	D	402	CLA	ND
25	G	602	CLA	ND
25	G	603	CLA	ND
25	G	610	CLA	ND
25	G	611	CLA	ND
25	G	612	CLA	ND
25	G	614	CLA	ND
25	N	602	CLA	ND
25	N	603	CLA	ND
25	N	604	CLA	ND
25	N	610	CLA	ND
25	N	611	CLA	ND
25	N	612	CLA	ND
25	N	613	CLA	ND
25	N	614	CLA	ND

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Mol	Chain	Res	Type	Atom
25	R	601	CLA	ND
25	R	602	CLA	ND
25	R	603	CLA	ND
25	R	604	CLA	ND
25	R	609	CLA	ND
25	R	610	CLA	ND
25	R	611	CLA	ND
25	R	612	CLA	ND
25	R	613	CLA	ND
25	S	602	CLA	ND
25	S	603	CLA	ND
25	S	604	CLA	ND
25	S	609	CLA	ND
25	S	610	CLA	ND
25	S	611	CLA	ND
25	S	612	CLA	ND
25	S	613	CLA	ND
25	S	614	CLA	ND
25	Y	602	CLA	ND
25	Y	603	CLA	ND
25	Y	604	CLA	ND
25	Y	610	CLA	ND
25	Y	611	CLA	ND
25	Y	612	CLA	ND
25	Y	613	CLA	ND
25	Y	614	CLA	ND
25	5	602	CLA	ND
25	5	603	CLA	ND
25	5	604	CLA	ND
25	5	610	CLA	ND
25	5	611	CLA	ND
25	5	612	CLA	ND
25	5	614	CLA	ND
25	6	602	CLA	ND
25	6	603	CLA	ND
25	6	610	CLA	ND
25	6	611	CLA	ND
25	6	612	CLA	ND
25	7	602	CLA	ND
25	7	603	CLA	ND
25	7	604	CLA	ND
25	7	610	CLA	ND

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Mol	Chain	Res	Type	Atom
25	7	611	CLA	ND
25	7	612	CLA	ND
25	7	613	CLA	ND
25	7	614	CLA	ND
25	8	602	CLA	ND
25	8	603	CLA	ND
25	8	610	CLA	ND
25	8	611	CLA	ND
25	8	612	CLA	ND
25	a	405	CLA	ND
25	a	406	CLA	ND
25	a	407	CLA	ND
25	a	410	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	b	617	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	512	CLA	ND
25	d	402	CLA	ND
25	g	602	CLA	ND
25	g	603	CLA	ND
25	g	610	CLA	ND
25	g	611	CLA	ND

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Mol	Chain	Res	Type	Atom
25	g	612	CLA	ND
25	g	614	CLA	ND
25	n	602	CLA	ND
25	n	603	CLA	ND
25	n	604	CLA	ND
25	n	610	CLA	ND
25	n	611	CLA	ND
25	n	612	CLA	ND
25	n	613	CLA	ND
25	n	614	CLA	ND
25	r	601	CLA	ND
25	r	602	CLA	ND
25	r	603	CLA	ND
25	r	604	CLA	ND
25	r	609	CLA	ND
25	r	610	CLA	ND
25	r	611	CLA	ND
25	r	612	CLA	ND
25	r	613	CLA	ND
25	s	602	CLA	ND
25	s	603	CLA	ND
25	s	604	CLA	ND
25	s	609	CLA	ND
25	s	610	CLA	ND
25	s	611	CLA	ND
25	s	612	CLA	ND
25	s	613	CLA	ND
25	s	614	CLA	ND
25	y	602	CLA	ND
25	y	603	CLA	ND
25	y	604	CLA	ND
25	y	610	CLA	ND
25	y	611	CLA	ND
25	y	612	CLA	ND
25	y	613	CLA	ND
25	y	614	CLA	ND

All (4767) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	605	CHL	C1C-C2C-CMC-OMC
24	1	605	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	1	606	CHL	C3C-C2C-CMC-OMC
24	1	606	CHL	CBD-CGD-O2D-CED
24	1	607	CHL	C1C-C2C-CMC-OMC
24	1	607	CHL	C3C-C2C-CMC-OMC
24	1	608	CHL	C1A-C2A-CAA-CBA
24	1	609	CHL	C1C-C2C-CMC-OMC
24	1	609	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	C1A-C2A-CAA-CBA
24	2	601	CHL	C3A-C2A-CAA-CBA
24	2	601	CHL	CHA-CBD-CGD-O1D
24	2	601	CHL	CHA-CBD-CGD-O2D
24	2	605	CHL	C1C-C2C-CMC-OMC
24	2	605	CHL	C3C-C2C-CMC-OMC
24	2	606	CHL	C3C-C2C-CMC-OMC
24	2	607	CHL	C1A-C2A-CAA-CBA
24	2	607	CHL	C1C-C2C-CMC-OMC
24	2	607	CHL	C3C-C2C-CMC-OMC
24	2	608	CHL	C1C-C2C-CMC-OMC
24	2	608	CHL	C3C-C2C-CMC-OMC
24	2	609	CHL	C1C-C2C-CMC-OMC
24	2	609	CHL	C3C-C2C-CMC-OMC
24	3	605	CHL	C1C-C2C-CMC-OMC
24	3	605	CHL	C3C-C2C-CMC-OMC
24	3	606	CHL	C1A-C2A-CAA-CBA
24	3	606	CHL	C3A-C2A-CAA-CBA
24	3	607	CHL	C1C-C2C-CMC-OMC
24	3	607	CHL	C3C-C2C-CMC-OMC
24	3	609	CHL	C1C-C2C-CMC-OMC
24	3	609	CHL	C3C-C2C-CMC-OMC
24	4	601	CHL	C1C-C2C-CMC-OMC
24	4	601	CHL	C3C-C2C-CMC-OMC
24	4	606	CHL	C1A-C2A-CAA-CBA
24	4	606	CHL	C3A-C2A-CAA-CBA
24	4	606	CHL	C1C-C2C-CMC-OMC
24	4	607	CHL	C1C-C2C-CMC-OMC
24	4	607	CHL	C3C-C2C-CMC-OMC
24	4	608	CHL	C1A-C2A-CAA-CBA
24	4	608	CHL	C1C-C2C-CMC-OMC
24	4	608	CHL	C3C-C2C-CMC-OMC
24	4	608	CHL	CBD-CGD-O2D-CED
24	4	609	CHL	C1C-C2C-CMC-OMC
24	4	609	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	G	605	CHL	C1C-C2C-CMC-OMC
24	G	605	CHL	C3C-C2C-CMC-OMC
24	G	605	CHL	CHA-CBD-CGD-O1D
24	G	605	CHL	CHA-CBD-CGD-O2D
24	G	605	CHL	CAD-CBD-CGD-O1D
24	G	605	CHL	CAD-CBD-CGD-O2D
24	G	605	CHL	CBD-CGD-O2D-CED
24	G	606	CHL	C1C-C2C-CMC-OMC
24	G	607	CHL	C3C-C2C-CMC-OMC
24	G	608	CHL	C1A-C2A-CAA-CBA
24	G	608	CHL	C3C-C2C-CMC-OMC
24	G	608	CHL	CBD-CGD-O2D-CED
24	G	609	CHL	C1C-C2C-CMC-OMC
24	G	609	CHL	C3C-C2C-CMC-OMC
24	N	605	CHL	C1A-C2A-CAA-CBA
24	N	605	CHL	C1C-C2C-CMC-OMC
24	N	605	CHL	C3C-C2C-CMC-OMC
24	N	605	CHL	CHA-CBD-CGD-O1D
24	N	605	CHL	CAD-CBD-CGD-O1D
24	N	605	CHL	CAD-CBD-CGD-O2D
24	N	606	CHL	C1C-C2C-CMC-OMC
24	N	606	CHL	C3C-C2C-CMC-OMC
24	N	607	CHL	C1C-C2C-CMC-OMC
24	N	607	CHL	C3C-C2C-CMC-OMC
24	N	608	CHL	CBD-CGD-O2D-CED
24	N	609	CHL	C1C-C2C-CMC-OMC
24	N	609	CHL	C3C-C2C-CMC-OMC
24	R	606	CHL	C1A-C2A-CAA-CBA
24	R	608	CHL	C2A-CAA-CBA-CGA
24	R	608	CHL	CBD-CGD-O2D-CED
24	R	614	CHL	CHA-CBD-CGD-O1D
24	R	614	CHL	CHA-CBD-CGD-O2D
24	R	614	CHL	CAD-CBD-CGD-O1D
24	R	614	CHL	CAD-CBD-CGD-O2D
24	R	614	CHL	CBD-CGD-O2D-CED
24	S	601	CHL	C1C-C2C-CMC-OMC
24	S	601	CHL	C3C-C2C-CMC-OMC
24	S	606	CHL	C1C-C2C-CMC-OMC
24	S	606	CHL	C3C-C2C-CMC-OMC
24	S	606	CHL	CHA-CBD-CGD-O1D
24	S	606	CHL	CHA-CBD-CGD-O2D
24	S	606	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	S	607	CHL	C1C-C2C-CMC-OMC
24	S	607	CHL	C3C-C2C-CMC-OMC
24	S	608	CHL	C1A-C2A-CAA-CBA
24	Y	605	CHL	C1A-C2A-CAA-CBA
24	Y	605	CHL	C1C-C2C-CMC-OMC
24	Y	605	CHL	C3C-C2C-CMC-OMC
24	Y	606	CHL	C1C-C2C-CMC-OMC
24	Y	606	CHL	C3C-C2C-CMC-OMC
24	Y	607	CHL	C1C-C2C-CMC-OMC
24	Y	607	CHL	C3C-C2C-CMC-OMC
24	Y	608	CHL	C1A-C2A-CAA-CBA
24	Y	608	CHL	CBD-CGD-O2D-CED
24	Y	609	CHL	C3C-C2C-CMC-OMC
24	5	605	CHL	C1C-C2C-CMC-OMC
24	5	605	CHL	C3C-C2C-CMC-OMC
24	5	606	CHL	C3C-C2C-CMC-OMC
24	5	606	CHL	CBD-CGD-O2D-CED
24	5	607	CHL	C1C-C2C-CMC-OMC
24	5	607	CHL	C3C-C2C-CMC-OMC
24	5	608	CHL	C1A-C2A-CAA-CBA
24	5	609	CHL	C1C-C2C-CMC-OMC
24	5	609	CHL	C3C-C2C-CMC-OMC
24	6	601	CHL	C1A-C2A-CAA-CBA
24	6	601	CHL	C3A-C2A-CAA-CBA
24	6	601	CHL	CHA-CBD-CGD-O1D
24	6	601	CHL	CHA-CBD-CGD-O2D
24	6	605	CHL	C1C-C2C-CMC-OMC
24	6	605	CHL	C3C-C2C-CMC-OMC
24	6	606	CHL	C3C-C2C-CMC-OMC
24	6	607	CHL	C1A-C2A-CAA-CBA
24	6	607	CHL	C1C-C2C-CMC-OMC
24	6	607	CHL	C3C-C2C-CMC-OMC
24	6	608	CHL	C1C-C2C-CMC-OMC
24	6	608	CHL	C3C-C2C-CMC-OMC
24	6	609	CHL	C1C-C2C-CMC-OMC
24	6	609	CHL	C3C-C2C-CMC-OMC
24	7	605	CHL	C1C-C2C-CMC-OMC
24	7	605	CHL	C3C-C2C-CMC-OMC
24	7	606	CHL	C1A-C2A-CAA-CBA
24	7	606	CHL	C3A-C2A-CAA-CBA
24	7	607	CHL	C1C-C2C-CMC-OMC
24	7	607	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	7	609	CHL	C1C-C2C-CMC-OMC
24	7	609	CHL	C3C-C2C-CMC-OMC
24	8	601	CHL	C1C-C2C-CMC-OMC
24	8	601	CHL	C3C-C2C-CMC-OMC
24	8	606	CHL	C1A-C2A-CAA-CBA
24	8	606	CHL	C3A-C2A-CAA-CBA
24	8	606	CHL	C1C-C2C-CMC-OMC
24	8	607	CHL	C1C-C2C-CMC-OMC
24	8	607	CHL	C3C-C2C-CMC-OMC
24	8	608	CHL	C1A-C2A-CAA-CBA
24	8	608	CHL	C1C-C2C-CMC-OMC
24	8	608	CHL	C3C-C2C-CMC-OMC
24	8	608	CHL	CBD-CGD-O2D-CED
24	8	609	CHL	C1C-C2C-CMC-OMC
24	8	609	CHL	C3C-C2C-CMC-OMC
24	g	605	CHL	C1C-C2C-CMC-OMC
24	g	605	CHL	C3C-C2C-CMC-OMC
24	g	605	CHL	CHA-CBD-CGD-O1D
24	g	605	CHL	CHA-CBD-CGD-O2D
24	g	605	CHL	CAD-CBD-CGD-O1D
24	g	605	CHL	CAD-CBD-CGD-O2D
24	g	605	CHL	CBD-CGD-O2D-CED
24	g	606	CHL	C1C-C2C-CMC-OMC
24	g	607	CHL	C3C-C2C-CMC-OMC
24	g	608	CHL	C1A-C2A-CAA-CBA
24	g	608	CHL	C3C-C2C-CMC-OMC
24	g	608	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	C1C-C2C-CMC-OMC
24	g	609	CHL	C3C-C2C-CMC-OMC
24	n	605	CHL	C1A-C2A-CAA-CBA
24	n	605	CHL	C1C-C2C-CMC-OMC
24	n	605	CHL	C3C-C2C-CMC-OMC
24	n	605	CHL	CHA-CBD-CGD-O1D
24	n	605	CHL	CAD-CBD-CGD-O1D
24	n	605	CHL	CAD-CBD-CGD-O2D
24	n	606	CHL	C1C-C2C-CMC-OMC
24	n	606	CHL	C3C-C2C-CMC-OMC
24	n	607	CHL	C1C-C2C-CMC-OMC
24	n	607	CHL	C3C-C2C-CMC-OMC
24	n	608	CHL	CBD-CGD-O2D-CED
24	n	609	CHL	C1C-C2C-CMC-OMC
24	n	609	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	r	606	CHL	C1A-C2A-CAA-CBA
24	r	608	CHL	C2A-CAA-CBA-CGA
24	r	608	CHL	CBD-CGD-O2D-CED
24	r	614	CHL	CHA-CBD-CGD-O1D
24	r	614	CHL	CHA-CBD-CGD-O2D
24	r	614	CHL	CAD-CBD-CGD-O1D
24	r	614	CHL	CAD-CBD-CGD-O2D
24	r	614	CHL	CBD-CGD-O2D-CED
24	s	601	CHL	C1C-C2C-CMC-OMC
24	s	601	CHL	C3C-C2C-CMC-OMC
24	s	606	CHL	C1C-C2C-CMC-OMC
24	s	606	CHL	C3C-C2C-CMC-OMC
24	s	606	CHL	CHA-CBD-CGD-O1D
24	s	606	CHL	CHA-CBD-CGD-O2D
24	s	606	CHL	CAD-CBD-CGD-O1D
24	s	607	CHL	C1C-C2C-CMC-OMC
24	s	607	CHL	C3C-C2C-CMC-OMC
24	s	608	CHL	C1A-C2A-CAA-CBA
24	y	605	CHL	C1A-C2A-CAA-CBA
24	y	605	CHL	C1C-C2C-CMC-OMC
24	y	605	CHL	C3C-C2C-CMC-OMC
24	y	606	CHL	C1C-C2C-CMC-OMC
24	y	606	CHL	C3C-C2C-CMC-OMC
24	y	607	CHL	C1C-C2C-CMC-OMC
24	y	607	CHL	C3C-C2C-CMC-OMC
24	y	608	CHL	C1A-C2A-CAA-CBA
24	y	608	CHL	CBD-CGD-O2D-CED
24	y	609	CHL	C3C-C2C-CMC-OMC
25	1	603	CLA	CBD-CGD-O2D-CED
25	1	604	CLA	CHA-CBD-CGD-O1D
25	1	604	CLA	CHA-CBD-CGD-O2D
25	1	604	CLA	CAD-CBD-CGD-O1D
25	1	604	CLA	CAD-CBD-CGD-O2D
25	1	613	CLA	CBD-CGD-O2D-CED
25	1	614	CLA	CBD-CGD-O2D-CED
25	2	603	CLA	CHA-CBD-CGD-O1D
25	2	603	CLA	CHA-CBD-CGD-O2D
25	2	603	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	C1A-C2A-CAA-CBA
25	2	604	CLA	C3A-C2A-CAA-CBA
25	2	604	CLA	CHA-CBD-CGD-O1D
25	2	604	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	2	604	CLA	CAD-CBD-CGD-O1D
25	2	604	CLA	CBD-CGD-O2D-CED
25	2	613	CLA	CHA-CBD-CGD-O1D
25	2	613	CLA	CHA-CBD-CGD-O2D
25	2	613	CLA	CBD-CGD-O2D-CED
25	2	614	CLA	C1A-C2A-CAA-CBA
25	2	614	CLA	C3A-C2A-CAA-CBA
25	3	603	CLA	O1A-CGA-O2A-C1
25	3	603	CLA	CHA-CBD-CGD-O1D
25	3	603	CLA	CHA-CBD-CGD-O2D
25	3	611	CLA	C1A-C2A-CAA-CBA
25	3	612	CLA	CHA-CBD-CGD-O1D
25	3	612	CLA	CAD-CBD-CGD-O1D
25	3	612	CLA	CAD-CBD-CGD-O2D
25	3	614	CLA	CAD-CBD-CGD-O1D
25	3	614	CLA	CAD-CBD-CGD-O2D
25	3	614	CLA	CBD-CGD-O2D-CED
25	4	602	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	C1A-C2A-CAA-CBA
25	4	604	CLA	CHA-CBD-CGD-O1D
25	4	604	CLA	CHA-CBD-CGD-O2D
25	4	610	CLA	C1A-C2A-CAA-CBA
25	4	610	CLA	CHA-CBD-CGD-O1D
25	4	610	CLA	CHA-CBD-CGD-O2D
25	4	611	CLA	CBD-CGD-O2D-CED
25	A	405	CLA	CBD-CGD-O2D-CED
25	A	405	CLA	O1D-CGD-O2D-CED
25	A	406	CLA	CHA-CBD-CGD-O1D
25	A	406	CLA	CHA-CBD-CGD-O2D
25	A	407	CLA	CHA-CBD-CGD-O1D
25	A	407	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CAD-CBD-CGD-O1D
25	B	603	CLA	C2-C3-C5-C6
25	B	603	CLA	C4-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	B	604	CLA	C4-C3-C5-C6
25	B	607	CLA	C2A-CAA-CBA-CGA
25	B	608	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	C1A-C2A-CAA-CBA
25	B	613	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	613	CLA	C3A-C2A-CAA-CBA
25	B	616	CLA	C11-C10-C8-C9
25	C	502	CLA	C6-C7-C8-C9
25	C	504	CLA	CHA-CBD-CGD-O1D
25	C	504	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	C1A-C2A-CAA-CBA
25	C	507	CLA	C3A-C2A-CAA-CBA
25	C	507	CLA	C11-C10-C8-C9
25	G	610	CLA	C1A-C2A-CAA-CBA
25	G	610	CLA	C3A-C2A-CAA-CBA
25	G	611	CLA	C1A-C2A-CAA-CBA
25	G	611	CLA	C3A-C2A-CAA-CBA
25	N	610	CLA	C1A-C2A-CAA-CBA
25	N	610	CLA	C3A-C2A-CAA-CBA
25	N	612	CLA	CBD-CGD-O2D-CED
25	N	614	CLA	CBD-CGD-O2D-CED
25	R	601	CLA	CHA-CBD-CGD-O1D
25	R	601	CLA	CHA-CBD-CGD-O2D
25	R	601	CLA	CBD-CGD-O2D-CED
25	R	604	CLA	C2A-CAA-CBA-CGA
25	R	604	CLA	CHA-CBD-CGD-O1D
25	R	604	CLA	CHA-CBD-CGD-O2D
25	R	611	CLA	C1A-C2A-CAA-CBA
25	R	611	CLA	C3A-C2A-CAA-CBA
25	R	611	CLA	CBA-CGA-O2A-C1
25	R	612	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	CHA-CBD-CGD-O1D
25	R	613	CLA	CHA-CBD-CGD-O2D
25	R	616	CLA	C1A-C2A-CAA-CBA
25	R	616	CLA	CHA-CBD-CGD-O1D
25	R	616	CLA	CHA-CBD-CGD-O2D
25	S	602	CLA	C1A-C2A-CAA-CBA
25	S	604	CLA	C1A-C2A-CAA-CBA
25	S	610	CLA	C2-C3-C5-C6
25	S	610	CLA	C4-C3-C5-C6
25	S	612	CLA	CBD-CGD-O2D-CED
25	Y	612	CLA	C6-C7-C8-C10
25	5	603	CLA	CBD-CGD-O2D-CED
25	5	604	CLA	CHA-CBD-CGD-O1D
25	5	604	CLA	CHA-CBD-CGD-O2D
25	5	604	CLA	CAD-CBD-CGD-O1D
25	5	604	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	5	613	CLA	CBD-CGD-O2D-CED
25	5	614	CLA	CBD-CGD-O2D-CED
25	6	603	CLA	CHA-CBD-CGD-O1D
25	6	603	CLA	CHA-CBD-CGD-O2D
25	6	603	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	C1A-C2A-CAA-CBA
25	6	604	CLA	C3A-C2A-CAA-CBA
25	6	604	CLA	CHA-CBD-CGD-O1D
25	6	604	CLA	CHA-CBD-CGD-O2D
25	6	604	CLA	CAD-CBD-CGD-O1D
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	613	CLA	CHA-CBD-CGD-O1D
25	6	613	CLA	CHA-CBD-CGD-O2D
25	6	613	CLA	CBD-CGD-O2D-CED
25	6	614	CLA	C1A-C2A-CAA-CBA
25	6	614	CLA	C3A-C2A-CAA-CBA
25	7	603	CLA	O1A-CGA-O2A-C1
25	7	603	CLA	CHA-CBD-CGD-O1D
25	7	603	CLA	CHA-CBD-CGD-O2D
25	7	611	CLA	C1A-C2A-CAA-CBA
25	7	612	CLA	CHA-CBD-CGD-O1D
25	7	612	CLA	CAD-CBD-CGD-O1D
25	7	612	CLA	CAD-CBD-CGD-O2D
25	7	614	CLA	CAD-CBD-CGD-O1D
25	7	614	CLA	CAD-CBD-CGD-O2D
25	7	614	CLA	CBD-CGD-O2D-CED
25	8	602	CLA	CBD-CGD-O2D-CED
25	8	604	CLA	C1A-C2A-CAA-CBA
25	8	604	CLA	CHA-CBD-CGD-O1D
25	8	604	CLA	CHA-CBD-CGD-O2D
25	8	610	CLA	C1A-C2A-CAA-CBA
25	8	610	CLA	CHA-CBD-CGD-O1D
25	8	610	CLA	CHA-CBD-CGD-O2D
25	8	611	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
25	a	406	CLA	CHA-CBD-CGD-O1D
25	a	406	CLA	CHA-CBD-CGD-O2D
25	a	407	CLA	CHA-CBD-CGD-O1D
25	a	407	CLA	CHA-CBD-CGD-O2D
25	b	602	CLA	CHA-CBD-CGD-O1D
25	b	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	CAD-CBD-CGD-O1D
25	b	603	CLA	C2-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	b	607	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C3A-C2A-CAA-CBA
25	b	616	CLA	C11-C10-C8-C9
25	c	502	CLA	C6-C7-C8-C9
25	c	504	CLA	CHA-CBD-CGD-O1D
25	c	504	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	C1A-C2A-CAA-CBA
25	c	507	CLA	C3A-C2A-CAA-CBA
25	c	507	CLA	C11-C10-C8-C9
25	g	610	CLA	C1A-C2A-CAA-CBA
25	g	610	CLA	C3A-C2A-CAA-CBA
25	g	611	CLA	C1A-C2A-CAA-CBA
25	g	611	CLA	C3A-C2A-CAA-CBA
25	n	610	CLA	C1A-C2A-CAA-CBA
25	n	610	CLA	C3A-C2A-CAA-CBA
25	n	612	CLA	CBD-CGD-O2D-CED
25	n	614	CLA	CBD-CGD-O2D-CED
25	r	601	CLA	CHA-CBD-CGD-O1D
25	r	601	CLA	CHA-CBD-CGD-O2D
25	r	601	CLA	CBD-CGD-O2D-CED
25	r	604	CLA	C2A-CAA-CBA-CGA
25	r	604	CLA	CHA-CBD-CGD-O1D
25	r	604	CLA	CHA-CBD-CGD-O2D
25	r	611	CLA	C1A-C2A-CAA-CBA
25	r	611	CLA	C3A-C2A-CAA-CBA
25	r	611	CLA	CBA-CGA-O2A-C1
25	r	612	CLA	CBD-CGD-O2D-CED
25	r	613	CLA	CHA-CBD-CGD-O1D
25	r	613	CLA	CHA-CBD-CGD-O2D
25	r	616	CLA	C1A-C2A-CAA-CBA
25	r	616	CLA	CHA-CBD-CGD-O1D
25	r	616	CLA	CHA-CBD-CGD-O2D
25	s	602	CLA	C1A-C2A-CAA-CBA
25	s	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	s	610	CLA	C2-C3-C5-C6
25	s	610	CLA	C4-C3-C5-C6
25	s	612	CLA	CBD-CGD-O2D-CED
25	y	612	CLA	C6-C7-C8-C10
26	1	1621	LUT	C1-C6-C7-C8
26	4	620	LUT	C11-C12-C13-C14
26	4	620	LUT	C11-C12-C13-C20
26	5	1621	LUT	C1-C6-C7-C8
26	8	620	LUT	C11-C12-C13-C14
26	8	620	LUT	C11-C12-C13-C20
27	1	1622	XAT	C31-C32-C33-C34
27	1	1622	XAT	C31-C32-C33-C40
27	2	1622	XAT	O4-C6-C7-C8
27	2	1622	XAT	C31-C32-C33-C34
27	2	1622	XAT	C31-C32-C33-C40
27	G	1622	XAT	C11-C12-C13-C14
27	G	1622	XAT	C11-C12-C13-C20
27	N	1622	XAT	C11-C12-C13-C14
27	N	1622	XAT	C11-C12-C13-C20
27	Y	1622	XAT	C11-C12-C13-C20
27	5	1622	XAT	C31-C32-C33-C34
27	5	1622	XAT	C31-C32-C33-C40
27	6	1622	XAT	O4-C6-C7-C8
27	6	1622	XAT	C31-C32-C33-C34
27	6	1622	XAT	C31-C32-C33-C40
27	g	1622	XAT	C11-C12-C13-C14
27	g	1622	XAT	C11-C12-C13-C20
27	n	1622	XAT	C11-C12-C13-C14
27	n	1622	XAT	C11-C12-C13-C20
27	y	1622	XAT	C11-C12-C13-C20
28	1	1623	NEX	C11-C12-C13-C14
28	1	1623	NEX	C11-C12-C13-C20
28	N	1623	NEX	C31-C32-C33-C34
28	N	1623	NEX	C31-C32-C33-C40
28	S	1623	NEX	C7-C8-C9-C19
28	5	1623	NEX	C11-C12-C13-C14
28	5	1623	NEX	C11-C12-C13-C20
28	n	1623	NEX	C31-C32-C33-C34
28	n	1623	NEX	C31-C32-C33-C40
28	s	1623	NEX	C7-C8-C9-C19
29	2	2630	LHG	C4-O6-P-O5
29	3	2630	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	3	2630	LHG	C4-O6-P-O5
29	4	2630	LHG	O1-C1-C2-O2
29	4	2630	LHG	C3-O3-P-O5
29	B	2630	LHG	C1-C2-C3-O3
29	B	2630	LHG	C3-O3-P-O5
29	B	2631	LHG	O1-C1-C2-O2
29	B	2631	LHG	O1-C1-C2-C3
29	B	2631	LHG	O2-C2-C3-O3
29	C	2630	LHG	O1-C1-C2-O2
29	C	2630	LHG	O1-C1-C2-C3
29	C	522	LHG	C3-O3-P-O4
29	C	522	LHG	C3-O3-P-O6
29	C	523	LHG	C3-O3-P-O5
29	C	523	LHG	C4-O6-P-O4
29	C	523	LHG	C8-C7-O7-C5
29	D	409	LHG	C4-O6-P-O3
29	D	409	LHG	C4-O6-P-O4
29	D	409	LHG	C4-O6-P-O5
29	G	2630	LHG	C4-O6-P-O5
29	L	101	LHG	C3-O3-P-O5
29	N	2630	LHG	C4-O6-P-O5
29	R	2630	LHG	O1-C1-C2-C3
29	S	2630	LHG	O1-C1-C2-C3
29	S	2630	LHG	C4-O6-P-O5
29	Y	2630	LHG	O1-C1-C2-C3
29	Y	2630	LHG	C4-O6-P-O5
29	6	2630	LHG	C4-O6-P-O5
29	7	2630	LHG	O1-C1-C2-C3
29	7	2630	LHG	C4-O6-P-O5
29	8	2630	LHG	O1-C1-C2-O2
29	8	2630	LHG	C3-O3-P-O5
29	b	2630	LHG	C1-C2-C3-O3
29	b	2630	LHG	C3-O3-P-O5
29	b	2631	LHG	O1-C1-C2-O2
29	b	2631	LHG	O1-C1-C2-C3
29	b	2631	LHG	O2-C2-C3-O3
29	c	2630	LHG	O1-C1-C2-O2
29	c	2630	LHG	O1-C1-C2-C3
29	c	522	LHG	C3-O3-P-O4
29	c	522	LHG	C3-O3-P-O6
29	c	523	LHG	C3-O3-P-O5
29	c	523	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
29	c	523	LHG	C8-C7-O7-C5
29	d	409	LHG	C4-O6-P-O3
29	d	409	LHG	C4-O6-P-O4
29	d	409	LHG	C4-O6-P-O5
29	g	2630	LHG	C4-O6-P-O5
29	l	101	LHG	C3-O3-P-O5
29	n	2630	LHG	C4-O6-P-O5
29	r	2630	LHG	O1-C1-C2-C3
29	s	2630	LHG	O1-C1-C2-C3
29	s	2630	LHG	C4-O6-P-O5
29	y	2630	LHG	O1-C1-C2-C3
29	y	2630	LHG	C4-O6-P-O5
30	4	623	BCR	C1-C6-C7-C8
30	4	623	BCR	C11-C12-C13-C14
30	4	623	BCR	C11-C12-C13-C35
30	4	623	BCR	C21-C22-C23-C24
30	4	623	BCR	C37-C22-C23-C24
30	B	619	BCR	C7-C8-C9-C34
30	B	620	BCR	C7-C8-C9-C10
30	B	620	BCR	C7-C8-C9-C34
30	C	514	BCR	C1-C6-C7-C8
30	C	515	BCR	C23-C24-C25-C30
30	C	516	BCR	C7-C8-C9-C10
30	C	516	BCR	C7-C8-C9-C34
30	C	516	BCR	C21-C22-C23-C24
30	C	516	BCR	C37-C22-C23-C24
30	C	517	BCR	C7-C8-C9-C10
30	C	517	BCR	C7-C8-C9-C34
30	D	404	BCR	C7-C8-C9-C10
30	D	404	BCR	C7-C8-C9-C34
30	H	101	BCR	C7-C8-C9-C10
30	H	101	BCR	C7-C8-C9-C34
30	T	101	BCR	C1-C6-C7-C8
30	T	101	BCR	C5-C6-C7-C8
30	T	101	BCR	C7-C8-C9-C10
30	T	101	BCR	C7-C8-C9-C34
30	T	101	BCR	C17-C18-C19-C20
30	T	101	BCR	C36-C18-C19-C20
30	T	101	BCR	C21-C22-C23-C24
30	T	101	BCR	C37-C22-C23-C24
30	8	623	BCR	C1-C6-C7-C8
30	8	623	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	8	623	BCR	C11-C12-C13-C35
30	8	623	BCR	C21-C22-C23-C24
30	8	623	BCR	C37-C22-C23-C24
30	b	619	BCR	C7-C8-C9-C34
30	b	620	BCR	C7-C8-C9-C10
30	b	620	BCR	C7-C8-C9-C34
30	c	514	BCR	C1-C6-C7-C8
30	c	515	BCR	C23-C24-C25-C30
30	c	516	BCR	C7-C8-C9-C10
30	c	516	BCR	C7-C8-C9-C34
30	c	516	BCR	C21-C22-C23-C24
30	c	516	BCR	C37-C22-C23-C24
30	c	517	BCR	C7-C8-C9-C10
30	c	517	BCR	C7-C8-C9-C34
30	d	404	BCR	C7-C8-C9-C10
30	d	404	BCR	C7-C8-C9-C34
30	h	101	BCR	C7-C8-C9-C10
30	h	101	BCR	C7-C8-C9-C34
30	t	101	BCR	C1-C6-C7-C8
30	t	101	BCR	C5-C6-C7-C8
30	t	101	BCR	C7-C8-C9-C10
30	t	101	BCR	C7-C8-C9-C34
30	t	101	BCR	C17-C18-C19-C20
30	t	101	BCR	C36-C18-C19-C20
30	t	101	BCR	C21-C22-C23-C24
30	t	101	BCR	C37-C22-C23-C24
34	A	412	SQD	O49-C7-O47-C45
34	A	412	SQD	C8-C7-O47-C45
34	A	412	SQD	O5-C5-C6-S
34	A	418	SQD	C2-C1-O6-C44
34	A	418	SQD	O5-C1-O6-C44
34	A	418	SQD	O5-C5-C6-S
34	B	621	SQD	C2-C1-O6-C44
34	B	621	SQD	O5-C1-O6-C44
34	B	621	SQD	C46-C45-O47-C7
34	B	621	SQD	C8-C7-O47-C45
34	B	621	SQD	O5-C5-C6-S
34	B	623	SQD	O47-C45-C46-O48
34	B	623	SQD	C8-C7-O47-C45
34	B	623	SQD	C5-C6-S-O7
34	a	412	SQD	O49-C7-O47-C45
34	a	412	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
34	a	412	SQD	O5-C5-C6-S
34	a	418	SQD	C2-C1-O6-C44
34	a	418	SQD	O5-C1-O6-C44
34	a	418	SQD	O5-C5-C6-S
34	b	621	SQD	C2-C1-O6-C44
34	b	621	SQD	O5-C1-O6-C44
34	b	621	SQD	C46-C45-O47-C7
34	b	621	SQD	C8-C7-O47-C45
34	b	621	SQD	O5-C5-C6-S
34	b	623	SQD	O47-C45-C46-O48
34	b	623	SQD	C8-C7-O47-C45
34	b	623	SQD	C5-C6-S-O7
35	A	413	LMG	C2-C1-O1-C7
35	A	413	LMG	O6-C1-O1-C7
35	B	2633	LMG	O9-C10-O7-C8
35	C	521	LMG	C2-C1-O1-C7
35	C	521	LMG	O6-C1-O1-C7
35	Z	101	LMG	O10-C28-O8-C9
35	a	413	LMG	C2-C1-O1-C7
35	a	413	LMG	O6-C1-O1-C7
35	b	2633	LMG	O9-C10-O7-C8
35	c	521	LMG	C2-C1-O1-C7
35	c	521	LMG	O6-C1-O1-C7
35	z	101	LMG	O10-C28-O8-C9
37	B	626	DGD	O1A-C1A-O1G-C1G
37	B	626	DGD	C2B-C1B-O2G-C2G
37	B	626	DGD	C2D-C1D-O3G-C3G
37	B	626	DGD	O6D-C1D-O3G-C3G
37	C	519	DGD	O1G-C1G-C2G-O2G
37	b	626	DGD	O1A-C1A-O1G-C1G
37	b	626	DGD	C2B-C1B-O2G-C2G
37	b	626	DGD	C2D-C1D-O3G-C3G
37	b	626	DGD	O6D-C1D-O3G-C3G
37	c	519	DGD	O1G-C1G-C2G-O2G
39	F	101	HEM	C3D-CAD-CBD-CGD
39	f	101	HEM	C3D-CAD-CBD-CGD
25	2	612	CLA	O1D-CGD-O2D-CED
25	4	604	CLA	O1D-CGD-O2D-CED
25	6	612	CLA	O1D-CGD-O2D-CED
25	8	604	CLA	O1D-CGD-O2D-CED
25	R	601	CLA	C2C-C3C-CAC-CBC
25	r	601	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	1	608	CHL	O1D-CGD-O2D-CED
24	5	608	CHL	O1D-CGD-O2D-CED
25	2	613	CLA	O1D-CGD-O2D-CED
25	4	611	CLA	O1D-CGD-O2D-CED
25	G	613	CLA	O1D-CGD-O2D-CED
25	R	612	CLA	O1D-CGD-O2D-CED
25	6	613	CLA	O1D-CGD-O2D-CED
25	8	611	CLA	O1D-CGD-O2D-CED
25	g	613	CLA	O1D-CGD-O2D-CED
25	r	612	CLA	O1D-CGD-O2D-CED
29	4	2630	LHG	C24-C23-O8-C6
29	8	2630	LHG	C24-C23-O8-C6
24	1	608	CHL	CBD-CGD-O2D-CED
24	2	606	CHL	CBD-CGD-O2D-CED
24	2	608	CHL	CBD-CGD-O2D-CED
24	3	607	CHL	CBD-CGD-O2D-CED
24	3	608	CHL	CBD-CGD-O2D-CED
24	4	606	CHL	CBD-CGD-O2D-CED
24	G	606	CHL	CBD-CGD-O2D-CED
24	G	609	CHL	CBD-CGD-O2D-CED
24	N	605	CHL	CBD-CGD-O2D-CED
24	S	608	CHL	CBD-CGD-O2D-CED
24	5	608	CHL	CBD-CGD-O2D-CED
24	6	606	CHL	CBD-CGD-O2D-CED
24	6	608	CHL	CBD-CGD-O2D-CED
24	7	607	CHL	CBD-CGD-O2D-CED
24	7	608	CHL	CBD-CGD-O2D-CED
24	8	606	CHL	CBD-CGD-O2D-CED
24	g	606	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	CBD-CGD-O2D-CED
24	n	605	CHL	CBD-CGD-O2D-CED
24	s	608	CHL	CBD-CGD-O2D-CED
25	2	602	CLA	CBD-CGD-O2D-CED
25	2	612	CLA	CBD-CGD-O2D-CED
25	2	614	CLA	CBD-CGD-O2D-CED
25	3	603	CLA	CBD-CGD-O2D-CED
25	3	612	CLA	CBD-CGD-O2D-CED
25	3	613	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	C	508	CLA	CBD-CGD-O2D-CED
25	D	403	CLA	CBD-CGD-O2D-CED
25	G	612	CLA	CBD-CGD-O2D-CED
25	G	613	CLA	CBD-CGD-O2D-CED
25	S	602	CLA	CBD-CGD-O2D-CED
25	S	603	CLA	CBD-CGD-O2D-CED
25	Y	604	CLA	CBD-CGD-O2D-CED
25	6	602	CLA	CBD-CGD-O2D-CED
25	6	612	CLA	CBD-CGD-O2D-CED
25	6	614	CLA	CBD-CGD-O2D-CED
25	7	603	CLA	CBD-CGD-O2D-CED
25	7	604	CLA	CBD-CGD-O2D-CED
25	7	612	CLA	CBD-CGD-O2D-CED
25	7	613	CLA	CBD-CGD-O2D-CED
25	8	604	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	CBD-CGD-O2D-CED
25	d	403	CLA	CBD-CGD-O2D-CED
25	g	612	CLA	CBD-CGD-O2D-CED
25	g	613	CLA	CBD-CGD-O2D-CED
25	s	602	CLA	CBD-CGD-O2D-CED
25	s	603	CLA	CBD-CGD-O2D-CED
25	y	604	CLA	CBD-CGD-O2D-CED
25	N	611	CLA	O1A-CGA-O2A-C1
25	R	611	CLA	O1A-CGA-O2A-C1
25	Y	611	CLA	O1A-CGA-O2A-C1
25	n	611	CLA	O1A-CGA-O2A-C1
25	r	611	CLA	O1A-CGA-O2A-C1
25	y	611	CLA	O1A-CGA-O2A-C1
24	1	606	CHL	O1D-CGD-O2D-CED
24	3	608	CHL	O1D-CGD-O2D-CED
24	4	606	CHL	O1D-CGD-O2D-CED
24	G	606	CHL	O1D-CGD-O2D-CED
24	S	608	CHL	O1D-CGD-O2D-CED
24	5	606	CHL	O1D-CGD-O2D-CED
24	7	608	CHL	O1D-CGD-O2D-CED
24	8	606	CHL	O1D-CGD-O2D-CED
24	g	606	CHL	O1D-CGD-O2D-CED
24	s	608	CHL	O1D-CGD-O2D-CED
25	3	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	C	503	CLA	O1D-CGD-O2D-CED
25	N	612	CLA	O1D-CGD-O2D-CED
25	R	601	CLA	O1D-CGD-O2D-CED
25	7	613	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	n	612	CLA	O1D-CGD-O2D-CED
25	r	601	CLA	O1D-CGD-O2D-CED
24	G	608	CHL	O1D-CGD-O2D-CED
24	R	608	CHL	O1D-CGD-O2D-CED
24	g	608	CHL	O1D-CGD-O2D-CED
24	r	608	CHL	O1D-CGD-O2D-CED
25	1	613	CLA	O1D-CGD-O2D-CED
25	1	614	CLA	O1D-CGD-O2D-CED
25	2	603	CLA	O1D-CGD-O2D-CED
25	4	602	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	O1D-CGD-O2D-CED
25	S	612	CLA	O1D-CGD-O2D-CED
25	5	613	CLA	O1D-CGD-O2D-CED
25	5	614	CLA	O1D-CGD-O2D-CED
25	6	603	CLA	O1D-CGD-O2D-CED
25	8	602	CLA	O1D-CGD-O2D-CED
25	b	608	CLA	O1D-CGD-O2D-CED
25	s	612	CLA	O1D-CGD-O2D-CED
24	Y	608	CHL	C3-C5-C6-C7
24	y	608	CHL	C3-C5-C6-C7
25	3	603	CLA	CBA-CGA-O2A-C1
25	Y	611	CLA	CBA-CGA-O2A-C1
25	7	603	CLA	CBA-CGA-O2A-C1
25	y	611	CLA	CBA-CGA-O2A-C1
35	Z	101	LMG	C29-C28-O8-C9
35	z	101	LMG	C29-C28-O8-C9
37	B	626	DGD	C2A-C1A-O1G-C1G
37	b	626	DGD	C2A-C1A-O1G-C1G
24	2	601	CHL	CBD-CGD-O2D-CED
24	2	605	CHL	CBD-CGD-O2D-CED
24	2	609	CHL	CBD-CGD-O2D-CED
24	3	605	CHL	CBD-CGD-O2D-CED
24	R	607	CHL	CBD-CGD-O2D-CED
24	S	601	CHL	CBD-CGD-O2D-CED
24	S	606	CHL	CBD-CGD-O2D-CED
24	6	601	CHL	CBD-CGD-O2D-CED
24	6	605	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	6	609	CHL	CBD-CGD-O2D-CED
24	7	605	CHL	CBD-CGD-O2D-CED
24	r	607	CHL	CBD-CGD-O2D-CED
24	s	601	CHL	CBD-CGD-O2D-CED
24	s	606	CHL	CBD-CGD-O2D-CED
25	1	604	CLA	CBD-CGD-O2D-CED
25	3	604	CLA	CBD-CGD-O2D-CED
25	4	612	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	N	613	CLA	CBD-CGD-O2D-CED
25	R	602	CLA	CBD-CGD-O2D-CED
25	R	603	CLA	CBD-CGD-O2D-CED
25	R	611	CLA	CBD-CGD-O2D-CED
25	Y	612	CLA	CBD-CGD-O2D-CED
25	5	604	CLA	CBD-CGD-O2D-CED
25	8	612	CLA	CBD-CGD-O2D-CED
25	c	506	CLA	CBD-CGD-O2D-CED
25	c	510	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	n	613	CLA	CBD-CGD-O2D-CED
25	r	602	CLA	CBD-CGD-O2D-CED
25	r	603	CLA	CBD-CGD-O2D-CED
25	r	611	CLA	CBD-CGD-O2D-CED
25	y	612	CLA	CBD-CGD-O2D-CED
25	B	617	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	O1A-CGA-O2A-C1
25	b	617	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
29	S	2630	LHG	O10-C23-O8-C6
29	s	2630	LHG	O10-C23-O8-C6
33	A	408	PHO	O1A-CGA-O2A-C1
33	a	408	PHO	O1A-CGA-O2A-C1
24	4	608	CHL	O1D-CGD-O2D-CED
24	G	605	CHL	O1D-CGD-O2D-CED
24	N	605	CHL	O1D-CGD-O2D-CED
24	Y	608	CHL	O1D-CGD-O2D-CED
24	8	608	CHL	O1D-CGD-O2D-CED
24	g	605	CHL	O1D-CGD-O2D-CED
24	n	605	CHL	O1D-CGD-O2D-CED
24	y	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	604	CLA	O1D-CGD-O2D-CED
25	3	614	CLA	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	7	614	CLA	O1D-CGD-O2D-CED
24	N	608	CHL	O1D-CGD-O2D-CED
24	R	614	CHL	O1D-CGD-O2D-CED
24	n	608	CHL	O1D-CGD-O2D-CED
24	r	614	CHL	O1D-CGD-O2D-CED
25	1	603	CLA	O1D-CGD-O2D-CED
25	N	614	CLA	O1D-CGD-O2D-CED
25	5	603	CLA	O1D-CGD-O2D-CED
25	n	614	CLA	O1D-CGD-O2D-CED
24	g	601	CHL	CBD-CGD-O2D-CED
25	B	612	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	Y	614	CLA	CBD-CGD-O2D-CED
25	b	612	CLA	CBD-CGD-O2D-CED
25	c	502	CLA	CBD-CGD-O2D-CED
25	y	614	CLA	CBD-CGD-O2D-CED
24	2	606	CHL	O1D-CGD-O2D-CED
24	6	606	CHL	O1D-CGD-O2D-CED
25	2	602	CLA	O1D-CGD-O2D-CED
25	3	612	CLA	O1D-CGD-O2D-CED
25	G	612	CLA	O1D-CGD-O2D-CED
25	6	602	CLA	O1D-CGD-O2D-CED
25	7	612	CLA	O1D-CGD-O2D-CED
25	g	612	CLA	O1D-CGD-O2D-CED
29	C	523	LHG	O9-C7-O7-C5
29	c	523	LHG	O9-C7-O7-C5
34	A	418	SQD	O49-C7-O47-C45
34	B	621	SQD	O49-C7-O47-C45
34	B	623	SQD	O49-C7-O47-C45
34	a	418	SQD	O49-C7-O47-C45
34	b	621	SQD	O49-C7-O47-C45
34	b	623	SQD	O49-C7-O47-C45
25	S	611	CLA	O1A-CGA-O2A-C1
25	s	611	CLA	O1A-CGA-O2A-C1
24	1	607	CHL	C3-C5-C6-C7
24	1	609	CHL	C3-C5-C6-C7
24	2	607	CHL	C3-C5-C6-C7
24	3	601	CHL	C3-C5-C6-C7
24	Y	607	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	5	607	CHL	C3-C5-C6-C7
24	5	609	CHL	C3-C5-C6-C7
24	6	607	CHL	C3-C5-C6-C7
24	7	601	CHL	C3-C5-C6-C7
24	y	607	CHL	C3-C5-C6-C7
25	1	603	CLA	C3-C5-C6-C7
25	B	608	CLA	C3-C5-C6-C7
25	B	615	CLA	C3-C5-C6-C7
25	B	617	CLA	C3-C5-C6-C7
25	C	513	CLA	C3-C5-C6-C7
25	R	603	CLA	C3-C5-C6-C7
25	R	613	CLA	C3-C5-C6-C7
25	S	611	CLA	C3-C5-C6-C7
25	S	613	CLA	C3-C5-C6-C7
25	Y	613	CLA	C3-C5-C6-C7
25	5	603	CLA	C3-C5-C6-C7
25	b	608	CLA	C3-C5-C6-C7
25	b	615	CLA	C3-C5-C6-C7
25	b	617	CLA	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
25	r	603	CLA	C3-C5-C6-C7
25	r	613	CLA	C3-C5-C6-C7
25	s	611	CLA	C3-C5-C6-C7
25	s	613	CLA	C3-C5-C6-C7
25	y	613	CLA	C3-C5-C6-C7
25	N	603	CLA	CBA-CGA-O2A-C1
25	N	611	CLA	CBA-CGA-O2A-C1
25	n	603	CLA	CBA-CGA-O2A-C1
25	n	611	CLA	CBA-CGA-O2A-C1
33	A	408	PHO	CBA-CGA-O2A-C1
33	a	408	PHO	CBA-CGA-O2A-C1
35	B	2633	LMG	C11-C10-O7-C8
35	b	2633	LMG	C11-C10-O7-C8
24	G	601	CHL	CBD-CGD-O2D-CED
29	4	2630	LHG	O10-C23-O8-C6
29	8	2630	LHG	O10-C23-O8-C6
24	G	601	CHL	C4-C3-C5-C6
24	g	601	CHL	C4-C3-C5-C6
25	G	610	CLA	C4-C3-C5-C6
25	G	611	CLA	C4-C3-C5-C6
25	Y	602	CLA	C4-C3-C5-C6
25	g	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	g	611	CLA	C4-C3-C5-C6
25	y	602	CLA	C4-C3-C5-C6
25	R	609	CLA	CBD-CGD-O2D-CED
25	r	609	CLA	CBD-CGD-O2D-CED
24	2	605	CHL	C2A-CAA-CBA-CGA
24	3	606	CHL	C2A-CAA-CBA-CGA
24	N	601	CHL	C2A-CAA-CBA-CGA
24	N	607	CHL	C2A-CAA-CBA-CGA
24	S	607	CHL	C2A-CAA-CBA-CGA
24	Y	607	CHL	C2A-CAA-CBA-CGA
24	6	605	CHL	C2A-CAA-CBA-CGA
24	7	606	CHL	C2A-CAA-CBA-CGA
24	n	601	CHL	C2A-CAA-CBA-CGA
24	n	607	CHL	C2A-CAA-CBA-CGA
24	s	607	CHL	C2A-CAA-CBA-CGA
24	y	607	CHL	C2A-CAA-CBA-CGA
25	1	611	CLA	C2A-CAA-CBA-CGA
25	3	603	CLA	C2A-CAA-CBA-CGA
25	4	604	CLA	C2A-CAA-CBA-CGA
25	B	602	CLA	C2A-CAA-CBA-CGA
25	B	605	CLA	C2A-CAA-CBA-CGA
25	C	507	CLA	C2A-CAA-CBA-CGA
25	N	610	CLA	C2A-CAA-CBA-CGA
25	R	611	CLA	C2A-CAA-CBA-CGA
25	5	611	CLA	C2A-CAA-CBA-CGA
25	7	603	CLA	C2A-CAA-CBA-CGA
25	8	604	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
25	b	605	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C2A-CAA-CBA-CGA
25	n	610	CLA	C2A-CAA-CBA-CGA
25	r	611	CLA	C2A-CAA-CBA-CGA
24	G	607	CHL	C3-C5-C6-C7
24	N	607	CHL	C3-C5-C6-C7
24	R	606	CHL	C3-C5-C6-C7
24	g	607	CHL	C3-C5-C6-C7
24	n	607	CHL	C3-C5-C6-C7
24	r	606	CHL	C3-C5-C6-C7
25	1	613	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7
25	N	613	CLA	C3-C5-C6-C7
25	5	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	c	512	CLA	C3-C5-C6-C7
25	n	613	CLA	C3-C5-C6-C7
33	A	408	PHO	C3-C5-C6-C7
33	a	408	PHO	C3-C5-C6-C7
24	G	601	CHL	CBA-CGA-O2A-C1
24	S	607	CHL	CBA-CGA-O2A-C1
24	g	601	CHL	CBA-CGA-O2A-C1
24	s	607	CHL	CBA-CGA-O2A-C1
25	B	617	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	G	603	CLA	CBA-CGA-O2A-C1
25	S	611	CLA	CBA-CGA-O2A-C1
25	Y	612	CLA	CBA-CGA-O2A-C1
25	b	617	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
25	g	603	CLA	CBA-CGA-O2A-C1
25	s	611	CLA	CBA-CGA-O2A-C1
25	y	612	CLA	CBA-CGA-O2A-C1
29	B	2631	LHG	C24-C23-O8-C6
29	S	2630	LHG	C24-C23-O8-C6
29	b	2631	LHG	C24-C23-O8-C6
29	s	2630	LHG	C24-C23-O8-C6
37	C	520	DGD	C2A-C1A-O1G-C1G
37	c	520	DGD	C2A-C1A-O1G-C1G
25	B	606	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	d	403	CLA	O1D-CGD-O2D-CED
36	D	405	PL9	C7-C8-C9-C10
36	d	405	PL9	C7-C8-C9-C10
25	Y	603	CLA	CBD-CGD-O2D-CED
25	y	603	CLA	CBD-CGD-O2D-CED
24	2	608	CHL	O1D-CGD-O2D-CED
24	G	609	CHL	O1D-CGD-O2D-CED
24	6	608	CHL	O1D-CGD-O2D-CED
25	2	614	CLA	O1D-CGD-O2D-CED
25	6	614	CLA	O1D-CGD-O2D-CED
37	B	626	DGD	C4E-C5E-C6E-O5E
37	b	626	DGD	C4E-C5E-C6E-O5E
24	Y	601	CHL	O1A-CGA-O2A-C1
24	y	601	CHL	O1A-CGA-O2A-C1
25	2	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	G	603	CLA	O1A-CGA-O2A-C1
25	6	603	CLA	O1A-CGA-O2A-C1
25	g	603	CLA	O1A-CGA-O2A-C1
29	B	2631	LHG	O10-C23-O8-C6
29	b	2631	LHG	O10-C23-O8-C6
24	g	609	CHL	O1D-CGD-O2D-CED
25	3	603	CLA	O1D-CGD-O2D-CED
25	7	603	CLA	O1D-CGD-O2D-CED
30	4	623	BCR	C19-C20-C21-C22
30	8	623	BCR	C19-C20-C21-C22
37	C	520	DGD	O6E-C5E-C6E-O5E
37	c	520	DGD	O6E-C5E-C6E-O5E
24	1	605	CHL	CBD-CGD-O2D-CED
24	3	601	CHL	CBD-CGD-O2D-CED
24	4	607	CHL	CBD-CGD-O2D-CED
24	N	601	CHL	CBD-CGD-O2D-CED
24	R	606	CHL	CBD-CGD-O2D-CED
24	Y	609	CHL	CBD-CGD-O2D-CED
24	5	605	CHL	CBD-CGD-O2D-CED
24	7	601	CHL	CBD-CGD-O2D-CED
24	8	607	CHL	CBD-CGD-O2D-CED
24	n	601	CHL	CBD-CGD-O2D-CED
24	r	606	CHL	CBD-CGD-O2D-CED
24	y	609	CHL	CBD-CGD-O2D-CED
25	B	611	CLA	CBD-CGD-O2D-CED
25	C	507	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	C	513	CLA	CBD-CGD-O2D-CED
25	N	602	CLA	CBD-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
25	n	602	CLA	CBD-CGD-O2D-CED
25	s	609	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	O1D-CGD-O2D-CED
25	C	508	CLA	O1D-CGD-O2D-CED
25	c	508	CLA	O1D-CGD-O2D-CED
29	2	2630	LHG	O2-C2-C3-O3
29	B	2630	LHG	O2-C2-C3-O3
29	D	410	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
29	6	2630	LHG	O2-C2-C3-O3
29	b	2630	LHG	O2-C2-C3-O3
29	d	410	LHG	O2-C2-C3-O3
25	2	602	CLA	C3-C5-C6-C7
25	2	603	CLA	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	C	510	CLA	C3-C5-C6-C7
25	6	602	CLA	C3-C5-C6-C7
25	6	603	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7
24	Y	601	CHL	CBA-CGA-O2A-C1
24	y	601	CHL	CBA-CGA-O2A-C1
25	S	604	CLA	CBA-CGA-O2A-C1
25	s	604	CLA	CBA-CGA-O2A-C1
24	G	601	CHL	O1A-CGA-O2A-C1
24	g	601	CHL	O1A-CGA-O2A-C1
25	N	603	CLA	O1A-CGA-O2A-C1
25	n	603	CLA	O1A-CGA-O2A-C1
37	C	520	DGD	C4E-C5E-C6E-O5E
37	c	520	DGD	C4E-C5E-C6E-O5E
24	3	607	CHL	O1D-CGD-O2D-CED
24	7	607	CHL	O1D-CGD-O2D-CED
25	b	615	CLA	O1D-CGD-O2D-CED
25	r	601	CLA	C4C-C3C-CAC-CBC
24	N	609	CHL	CBD-CGD-O2D-CED
24	n	609	CHL	CBD-CGD-O2D-CED
25	C	501	CLA	CBD-CGD-O2D-CED
25	G	604	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
25	g	604	CLA	CBD-CGD-O2D-CED
25	R	601	CLA	C4C-C3C-CAC-CBC
25	y	604	CLA	O1D-CGD-O2D-CED
37	C	520	DGD	O1A-C1A-O1G-C1G
37	c	520	DGD	O1A-C1A-O1G-C1G
25	Y	604	CLA	O1D-CGD-O2D-CED
25	A	407	CLA	CBD-CGD-O2D-CED
25	a	407	CLA	CBD-CGD-O2D-CED
24	R	608	CHL	C3-C5-C6-C7
24	r	608	CHL	C3-C5-C6-C7
25	2	603	CLA	CBA-CGA-O2A-C1
25	6	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	H	102	DGD	O6E-C5E-C6E-O5E
37	h	102	DGD	O6E-C5E-C6E-O5E
37	C	520	DGD	O1B-C1B-O2G-C2G
37	c	520	DGD	O1B-C1B-O2G-C2G
24	S	607	CHL	O1A-CGA-O2A-C1
24	s	607	CHL	O1A-CGA-O2A-C1
24	Y	601	CHL	C4-C3-C5-C6
24	y	601	CHL	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
33	A	409	PHO	C4-C3-C5-C6
33	a	409	PHO	C4-C3-C5-C6
24	Y	601	CHL	C2-C3-C5-C6
24	y	601	CHL	C2-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	G	611	CLA	C2-C3-C5-C6
25	b	614	CLA	C2-C3-C5-C6
25	g	611	CLA	C2-C3-C5-C6
33	A	409	PHO	C2-C3-C5-C6
33	a	409	PHO	C2-C3-C5-C6
24	1	607	CHL	C2A-CAA-CBA-CGA
24	2	607	CHL	C2A-CAA-CBA-CGA
24	N	606	CHL	C2A-CAA-CBA-CGA
24	5	607	CHL	C2A-CAA-CBA-CGA
24	6	607	CHL	C2A-CAA-CBA-CGA
24	n	606	CHL	C2A-CAA-CBA-CGA
25	B	611	CLA	C2A-CAA-CBA-CGA
25	b	611	CLA	C2A-CAA-CBA-CGA
24	R	607	CHL	O1D-CGD-O2D-CED
24	r	607	CHL	O1D-CGD-O2D-CED
25	S	602	CLA	O1D-CGD-O2D-CED
25	s	602	CLA	O1D-CGD-O2D-CED
35	D	411	LMG	O6-C5-C6-O5
35	d	411	LMG	O6-C5-C6-O5
37	B	626	DGD	O6E-C5E-C6E-O5E
37	b	626	DGD	O6E-C5E-C6E-O5E
25	S	604	CLA	O1A-CGA-O2A-C1
25	Y	612	CLA	O1A-CGA-O2A-C1
25	s	604	CLA	O1A-CGA-O2A-C1
25	y	612	CLA	O1A-CGA-O2A-C1
35	B	2633	LMG	O6-C1-O1-C7
35	b	2633	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
24	N	608	CHL	C3-C5-C6-C7
24	n	608	CHL	C3-C5-C6-C7
24	R	608	CHL	CBA-CGA-O2A-C1
24	r	608	CHL	CBA-CGA-O2A-C1
25	N	614	CLA	CBA-CGA-O2A-C1
25	R	612	CLA	CBA-CGA-O2A-C1
25	n	614	CLA	CBA-CGA-O2A-C1
25	r	612	CLA	CBA-CGA-O2A-C1
34	B	623	SQD	C24-C23-O48-C46
34	b	623	SQD	C24-C23-O48-C46
25	S	603	CLA	O1D-CGD-O2D-CED
25	s	603	CLA	O1D-CGD-O2D-CED
25	3	604	CLA	O1D-CGD-O2D-CED
25	4	612	CLA	O1D-CGD-O2D-CED
25	7	604	CLA	O1D-CGD-O2D-CED
25	8	612	CLA	O1D-CGD-O2D-CED
24	2	605	CHL	O1D-CGD-O2D-CED
24	3	605	CHL	O1D-CGD-O2D-CED
24	6	605	CHL	O1D-CGD-O2D-CED
24	7	605	CHL	O1D-CGD-O2D-CED
25	N	613	CLA	O1D-CGD-O2D-CED
25	n	613	CLA	O1D-CGD-O2D-CED
29	2	2630	LHG	C1-C2-C3-O3
29	N	2630	LHG	C1-C2-C3-O3
29	6	2630	LHG	C1-C2-C3-O3
29	n	2630	LHG	C1-C2-C3-O3
29	B	2630	LHG	O9-C7-O7-C5
29	C	2630	LHG	O9-C7-O7-C5
29	b	2630	LHG	O9-C7-O7-C5
29	c	2630	LHG	O9-C7-O7-C5
24	R	608	CHL	O1A-CGA-O2A-C1
24	r	608	CHL	O1A-CGA-O2A-C1
25	R	602	CLA	C3-C5-C6-C7
25	r	602	CLA	C3-C5-C6-C7
24	2	601	CHL	O1D-CGD-O2D-CED
24	6	601	CHL	O1D-CGD-O2D-CED
25	D	403	CLA	CBA-CGA-O2A-C1
25	R	601	CLA	CBA-CGA-O2A-C1
25	d	403	CLA	CBA-CGA-O2A-C1
25	r	601	CLA	CBA-CGA-O2A-C1
34	B	621	SQD	C24-C23-O48-C46
34	b	621	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
35	B	622	LMG	C29-C28-O8-C9
35	b	622	LMG	C29-C28-O8-C9
37	C	519	DGD	C2A-C1A-O1G-C1G
37	c	519	DGD	C2A-C1A-O1G-C1G
25	r	613	CLA	CBD-CGD-O2D-CED
35	D	411	LMG	C4-C5-C6-O5
35	d	411	LMG	C4-C5-C6-O5
29	D	408	LHG	C23-C24-C25-C26
29	d	408	LHG	C23-C24-C25-C26
25	N	612	CLA	C5-C6-C7-C8
25	n	612	CLA	C5-C6-C7-C8
35	Z	101	LMG	O6-C5-C6-O5
35	z	101	LMG	O6-C5-C6-O5
25	C	511	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	O1D-CGD-O2D-CED
37	H	102	DGD	C4E-C5E-C6E-O5E
37	h	102	DGD	C4E-C5E-C6E-O5E
24	N	609	CHL	C15-C16-C17-C18
24	n	609	CHL	C15-C16-C17-C18
25	B	603	CLA	C5-C6-C7-C8
25	B	607	CLA	C13-C15-C16-C17
25	B	608	CLA	C13-C15-C16-C17
25	N	602	CLA	C10-C11-C12-C13
25	N	610	CLA	C5-C6-C7-C8
25	b	603	CLA	C5-C6-C7-C8
25	b	607	CLA	C13-C15-C16-C17
25	b	608	CLA	C13-C15-C16-C17
25	n	602	CLA	C10-C11-C12-C13
25	n	610	CLA	C5-C6-C7-C8
37	H	102	DGD	C1A-C2A-C3A-C4A
37	h	102	DGD	C1A-C2A-C3A-C4A
37	C	520	DGD	O1G-C1G-C2G-O2G
37	c	520	DGD	O1G-C1G-C2G-O2G
24	G	601	CHL	C2-C3-C5-C6
24	g	601	CHL	C2-C3-C5-C6
25	G	610	CLA	C2-C3-C5-C6
25	Y	602	CLA	C2-C3-C5-C6
25	g	610	CLA	C2-C3-C5-C6
25	y	602	CLA	C2-C3-C5-C6
24	G	608	CHL	C14-C13-C15-C16
24	N	601	CHL	C11-C10-C8-C9
24	N	608	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	R	606	CHL	C11-C10-C8-C9
24	Y	608	CHL	C14-C13-C15-C16
24	Y	609	CHL	C14-C13-C15-C16
24	g	608	CHL	C14-C13-C15-C16
24	n	601	CHL	C11-C10-C8-C9
24	n	608	CHL	C14-C13-C15-C16
24	r	606	CHL	C11-C10-C8-C9
24	y	608	CHL	C14-C13-C15-C16
24	y	609	CHL	C14-C13-C15-C16
25	B	602	CLA	C14-C13-C15-C16
25	B	606	CLA	C6-C7-C8-C9
25	C	506	CLA	C11-C12-C13-C14
25	C	509	CLA	C6-C7-C8-C9
25	N	612	CLA	C6-C7-C8-C9
25	R	610	CLA	C11-C12-C13-C14
25	Y	611	CLA	C6-C7-C8-C9
25	b	602	CLA	C14-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	509	CLA	C6-C7-C8-C9
25	n	612	CLA	C6-C7-C8-C9
25	r	610	CLA	C11-C12-C13-C14
25	y	611	CLA	C6-C7-C8-C9
33	A	409	PHO	C6-C7-C8-C9
33	a	409	PHO	C6-C7-C8-C9
24	S	601	CHL	O1D-CGD-O2D-CED
24	S	606	CHL	O1D-CGD-O2D-CED
24	s	601	CHL	O1D-CGD-O2D-CED
24	s	606	CHL	O1D-CGD-O2D-CED
25	C	506	CLA	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
25	r	603	CLA	O1D-CGD-O2D-CED
24	3	609	CHL	CBD-CGD-O2D-CED
25	R	613	CLA	CBD-CGD-O2D-CED
29	B	2630	LHG	C32-C33-C34-C35
29	b	2630	LHG	C32-C33-C34-C35
24	3	601	CHL	C5-C6-C7-C8
24	7	601	CHL	C5-C6-C7-C8
25	B	614	CLA	C8-C10-C11-C12
25	B	615	CLA	C15-C16-C17-C18
25	B	617	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	N	612	CLA	C10-C11-C12-C13
25	b	614	CLA	C8-C10-C11-C12
25	b	615	CLA	C15-C16-C17-C18
25	b	617	CLA	C5-C6-C7-C8
25	n	612	CLA	C10-C11-C12-C13
24	4	601	CHL	C2A-CAA-CBA-CGA
24	G	605	CHL	C2A-CAA-CBA-CGA
24	8	601	CHL	C2A-CAA-CBA-CGA
24	g	605	CHL	C2A-CAA-CBA-CGA
27	R	622	XAT	C27-C28-C29-C39
27	r	622	XAT	C27-C28-C29-C39
28	G	1623	NEX	C31-C32-C33-C40
28	g	1623	NEX	C31-C32-C33-C40
30	B	618	BCR	C36-C18-C19-C20
30	B	620	BCR	C37-C22-C23-C24
30	T	101	BCR	C11-C12-C13-C35
30	b	618	BCR	C36-C18-C19-C20
30	b	620	BCR	C37-C22-C23-C24
30	t	101	BCR	C11-C12-C13-C35
30	4	623	BCR	C7-C8-C9-C10
30	T	101	BCR	C11-C12-C13-C14
30	8	623	BCR	C7-C8-C9-C10
30	t	101	BCR	C11-C12-C13-C14
25	R	601	CLA	O1A-CGA-O2A-C1
25	r	601	CLA	O1A-CGA-O2A-C1
24	2	607	CHL	C10-C11-C12-C13
24	6	607	CHL	C10-C11-C12-C13
25	B	609	CLA	C8-C10-C11-C12
25	b	609	CLA	C8-C10-C11-C12
37	H	102	DGD	C4D-C5D-C6D-O5D
37	h	102	DGD	C4D-C5D-C6D-O5D
24	7	609	CHL	CBD-CGD-O2D-CED
25	1	602	CLA	CBD-CGD-O2D-CED
25	2	610	CLA	CBD-CGD-O2D-CED
25	5	602	CLA	CBD-CGD-O2D-CED
25	6	610	CLA	CBD-CGD-O2D-CED
25	y	612	CLA	O1D-CGD-O2D-CED
25	A	410	CLA	C3-C5-C6-C7
25	a	410	CLA	C3-C5-C6-C7
24	1	607	CHL	C13-C15-C16-C17
24	5	607	CHL	C13-C15-C16-C17
24	N	601	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	n	601	CHL	CBA-CGA-O2A-C1
25	B	602	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	CBA-CGA-O2A-C1
25	G	614	CLA	CBA-CGA-O2A-C1
25	b	602	CLA	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1
25	g	614	CLA	CBA-CGA-O2A-C1
29	R	2630	LHG	C24-C23-O8-C6
29	r	2630	LHG	C24-C23-O8-C6
24	Y	601	CHL	C8-C10-C11-C12
24	Y	608	CHL	C15-C16-C17-C18
24	y	601	CHL	C8-C10-C11-C12
24	y	608	CHL	C15-C16-C17-C18
25	1	602	CLA	C10-C11-C12-C13
25	B	604	CLA	C15-C16-C17-C18
25	B	608	CLA	C8-C10-C11-C12
25	C	503	CLA	C5-C6-C7-C8
25	D	403	CLA	C8-C10-C11-C12
25	5	602	CLA	C10-C11-C12-C13
25	b	604	CLA	C15-C16-C17-C18
25	b	608	CLA	C8-C10-C11-C12
25	c	503	CLA	C5-C6-C7-C8
25	d	403	CLA	C8-C10-C11-C12
29	G	2630	LHG	C23-C24-C25-C26
35	Z	101	LMG	C10-C11-C12-C13
35	z	101	LMG	C10-C11-C12-C13
24	2	609	CHL	O1D-CGD-O2D-CED
24	6	609	CHL	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
25	Y	612	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	O1D-CGD-O2D-CED
25	r	611	CLA	O1D-CGD-O2D-CED
25	C	510	CLA	O1D-CGD-O2D-CED
24	2	607	CHL	C8-C10-C11-C12
24	3	601	CHL	C8-C10-C11-C12
24	3	601	CHL	C10-C11-C12-C13
24	3	601	CHL	C13-C15-C16-C17
24	N	601	CHL	C8-C10-C11-C12
24	R	608	CHL	C10-C11-C12-C13
24	S	607	CHL	C5-C6-C7-C8
24	6	607	CHL	C8-C10-C11-C12
24	7	601	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	7	601	CHL	C10-C11-C12-C13
24	7	601	CHL	C13-C15-C16-C17
24	n	601	CHL	C8-C10-C11-C12
24	r	608	CHL	C10-C11-C12-C13
24	s	607	CHL	C5-C6-C7-C8
25	A	410	CLA	C5-C6-C7-C8
25	A	410	CLA	C8-C10-C11-C12
25	B	614	CLA	C10-C11-C12-C13
25	B	616	CLA	C8-C10-C11-C12
25	C	503	CLA	C15-C16-C17-C18
25	G	603	CLA	C15-C16-C17-C18
25	N	611	CLA	C5-C6-C7-C8
25	Y	610	CLA	C5-C6-C7-C8
25	a	410	CLA	C5-C6-C7-C8
25	a	410	CLA	C8-C10-C11-C12
25	b	614	CLA	C10-C11-C12-C13
25	b	616	CLA	C8-C10-C11-C12
25	c	503	CLA	C15-C16-C17-C18
25	g	603	CLA	C15-C16-C17-C18
25	n	611	CLA	C5-C6-C7-C8
25	y	610	CLA	C5-C6-C7-C8
25	1	604	CLA	O1D-CGD-O2D-CED
25	5	604	CLA	O1D-CGD-O2D-CED
29	1	2630	LHG	C23-C24-C25-C26
29	N	2630	LHG	C23-C24-C25-C26
29	5	2630	LHG	C23-C24-C25-C26
29	g	2630	LHG	C23-C24-C25-C26
29	n	2630	LHG	C23-C24-C25-C26
34	A	418	SQD	C23-C24-C25-C26
34	B	621	SQD	C7-C8-C9-C10
34	a	418	SQD	C23-C24-C25-C26
34	b	621	SQD	C7-C8-C9-C10
35	C	521	LMG	C28-C29-C30-C31
35	c	521	LMG	C28-C29-C30-C31
25	3	602	CLA	CBD-CGD-O2D-CED
24	R	606	CHL	C8-C10-C11-C12
24	Y	601	CHL	C13-C15-C16-C17
24	Y	609	CHL	C13-C15-C16-C17
24	r	606	CHL	C8-C10-C11-C12
24	y	601	CHL	C13-C15-C16-C17
24	y	609	CHL	C13-C15-C16-C17
25	2	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	N	611	CLA	C8-C10-C11-C12
25	Y	602	CLA	C10-C11-C12-C13
25	6	602	CLA	C10-C11-C12-C13
25	n	611	CLA	C8-C10-C11-C12
25	y	602	CLA	C10-C11-C12-C13
25	3	613	CLA	C3-C5-C6-C7
25	7	613	CLA	C3-C5-C6-C7
25	B	617	CLA	C13-C15-C16-C17
25	C	512	CLA	C8-C10-C11-C12
25	D	402	CLA	C15-C16-C17-C18
25	G	602	CLA	C10-C11-C12-C13
25	G	603	CLA	C13-C15-C16-C17
25	b	617	CLA	C13-C15-C16-C17
25	c	512	CLA	C8-C10-C11-C12
25	d	402	CLA	C15-C16-C17-C18
25	g	602	CLA	C10-C11-C12-C13
25	g	603	CLA	C13-C15-C16-C17
25	7	602	CLA	CBD-CGD-O2D-CED
24	1	607	CHL	C5-C6-C7-C8
24	N	607	CHL	C5-C6-C7-C8
24	5	607	CHL	C5-C6-C7-C8
24	n	607	CHL	C5-C6-C7-C8
25	B	608	CLA	C5-C6-C7-C8
33	a	408	PHO	C13-C15-C16-C17
24	Y	601	CHL	C6-C7-C8-C10
24	y	601	CHL	C6-C7-C8-C10
25	A	410	CLA	C6-C7-C8-C10
25	B	604	CLA	C6-C7-C8-C10
25	B	612	CLA	C12-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C10
25	N	610	CLA	C11-C12-C13-C15
25	R	610	CLA	C12-C13-C15-C16
25	S	602	CLA	C6-C7-C8-C10
25	a	410	CLA	C6-C7-C8-C10
25	b	604	CLA	C6-C7-C8-C10
25	b	612	CLA	C12-C13-C15-C16
25	c	511	CLA	C6-C7-C8-C10
25	n	610	CLA	C11-C12-C13-C15
25	r	610	CLA	C12-C13-C15-C16
25	s	602	CLA	C6-C7-C8-C10
24	N	601	CHL	O1A-CGA-O2A-C1
24	n	601	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	D	403	CLA	O1A-CGA-O2A-C1
25	d	403	CLA	O1A-CGA-O2A-C1
27	3	1622	XAT	C29-C30-C31-C32
27	7	1622	XAT	C29-C30-C31-C32
25	2	604	CLA	C2A-CAA-CBA-CGA
25	2	613	CLA	C2A-CAA-CBA-CGA
25	3	604	CLA	C2A-CAA-CBA-CGA
25	3	611	CLA	C2A-CAA-CBA-CGA
25	C	501	CLA	C2A-CAA-CBA-CGA
25	6	604	CLA	C2A-CAA-CBA-CGA
25	7	604	CLA	C2A-CAA-CBA-CGA
25	7	611	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
25	C	502	CLA	O1D-CGD-O2D-CED
25	R	602	CLA	O1D-CGD-O2D-CED
25	c	502	CLA	O1D-CGD-O2D-CED
25	r	602	CLA	O1D-CGD-O2D-CED
24	N	601	CHL	C13-C15-C16-C17
24	R	606	CHL	C15-C16-C17-C18
24	Y	601	CHL	C10-C11-C12-C13
24	n	601	CHL	C13-C15-C16-C17
24	r	606	CHL	C15-C16-C17-C18
24	y	601	CHL	C10-C11-C12-C13
25	3	611	CLA	C5-C6-C7-C8
25	B	604	CLA	C5-C6-C7-C8
25	B	605	CLA	C8-C10-C11-C12
25	B	615	CLA	C13-C15-C16-C17
25	C	507	CLA	C15-C16-C17-C18
25	C	508	CLA	C5-C6-C7-C8
25	G	602	CLA	C8-C10-C11-C12
25	G	610	CLA	C5-C6-C7-C8
25	7	611	CLA	C5-C6-C7-C8
25	b	604	CLA	C5-C6-C7-C8
25	b	605	CLA	C8-C10-C11-C12
25	b	608	CLA	C5-C6-C7-C8
25	b	615	CLA	C13-C15-C16-C17
25	c	507	CLA	C15-C16-C17-C18
25	c	508	CLA	C5-C6-C7-C8
25	g	602	CLA	C8-C10-C11-C12
25	g	610	CLA	C5-C6-C7-C8
33	A	408	PHO	C13-C15-C16-C17
37	C	519	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
37	c	519	DGD	O6E-C1E-O5D-C6D
24	3	609	CHL	C10-C11-C12-C13
24	G	601	CHL	C10-C11-C12-C13
24	Y	601	CHL	C5-C6-C7-C8
24	7	609	CHL	C10-C11-C12-C13
24	g	601	CHL	C10-C11-C12-C13
24	y	601	CHL	C5-C6-C7-C8
24	y	607	CHL	C15-C16-C17-C18
25	Y	613	CLA	C8-C10-C11-C12
25	y	613	CLA	C8-C10-C11-C12
24	G	601	CHL	O1D-CGD-O2D-CED
24	g	601	CHL	O1D-CGD-O2D-CED
25	R	609	CLA	O1D-CGD-O2D-CED
25	r	609	CLA	O1D-CGD-O2D-CED
29	B	2630	LHG	C23-C24-C25-C26
29	b	2630	LHG	C23-C24-C25-C26
29	C	2630	LHG	O2-C2-C3-O3
29	D	408	LHG	O2-C2-C3-O3
29	N	2630	LHG	O2-C2-C3-O3
29	c	2630	LHG	O2-C2-C3-O3
29	d	408	LHG	O2-C2-C3-O3
29	n	2630	LHG	O2-C2-C3-O3
24	S	607	CHL	C3-C5-C6-C7
25	G	613	CLA	C3-C5-C6-C7
25	g	613	CLA	C3-C5-C6-C7
24	N	608	CHL	C15-C16-C17-C18
24	Y	607	CHL	C15-C16-C17-C18
24	n	608	CHL	C15-C16-C17-C18
25	3	610	CLA	C10-C11-C12-C13
25	B	611	CLA	C13-C15-C16-C17
25	B	615	CLA	C5-C6-C7-C8
25	C	507	CLA	C13-C15-C16-C17
25	7	610	CLA	C10-C11-C12-C13
25	b	611	CLA	C13-C15-C16-C17
25	b	614	CLA	C13-C15-C16-C17
25	b	615	CLA	C5-C6-C7-C8
25	c	507	CLA	C13-C15-C16-C17
25	B	602	CLA	O1A-CGA-O2A-C1
25	R	612	CLA	O1A-CGA-O2A-C1
25	b	602	CLA	O1A-CGA-O2A-C1
25	r	612	CLA	O1A-CGA-O2A-C1
29	C	523	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
29	D	408	LHG	C7-C8-C9-C10
29	d	408	LHG	C7-C8-C9-C10
34	A	418	SQD	C7-C8-C9-C10
34	a	418	SQD	C7-C8-C9-C10
24	2	609	CHL	C8-C10-C11-C12
24	G	608	CHL	C8-C10-C11-C12
24	N	607	CHL	C15-C16-C17-C18
24	6	609	CHL	C8-C10-C11-C12
24	g	608	CHL	C8-C10-C11-C12
24	n	607	CHL	C15-C16-C17-C18
25	B	610	CLA	C15-C16-C17-C18
25	C	510	CLA	C13-C15-C16-C17
25	R	603	CLA	C10-C11-C12-C13
25	b	610	CLA	C15-C16-C17-C18
25	c	510	CLA	C13-C15-C16-C17
25	r	603	CLA	C10-C11-C12-C13
25	Y	614	CLA	O1D-CGD-O2D-CED
25	y	614	CLA	O1D-CGD-O2D-CED
25	N	614	CLA	O1A-CGA-O2A-C1
25	n	614	CLA	O1A-CGA-O2A-C1
34	A	418	SQD	C8-C7-O47-C45
34	a	418	SQD	C8-C7-O47-C45
24	3	609	CHL	C8-C10-C11-C12
24	G	601	CHL	C13-C15-C16-C17
24	Y	608	CHL	C5-C6-C7-C8
24	7	609	CHL	C8-C10-C11-C12
24	g	601	CHL	C13-C15-C16-C17
24	y	608	CHL	C5-C6-C7-C8
25	B	606	CLA	C15-C16-C17-C18
25	B	607	CLA	C8-C10-C11-C12
25	B	614	CLA	C13-C15-C16-C17
25	C	506	CLA	C13-C15-C16-C17
25	C	506	CLA	C15-C16-C17-C18
25	Y	612	CLA	C10-C11-C12-C13
25	b	606	CLA	C15-C16-C17-C18
25	b	607	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17
25	c	506	CLA	C15-C16-C17-C18
25	y	612	CLA	C10-C11-C12-C13
29	3	2630	LHG	C4-O6-P-O3
29	4	2630	LHG	C3-O3-P-O6
29	B	2630	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
29	D	410	LHG	C4-O6-P-O3
29	G	2630	LHG	C4-O6-P-O3
29	L	101	LHG	C3-O3-P-O6
29	N	2630	LHG	C3-O3-P-O6
29	7	2630	LHG	C4-O6-P-O3
29	8	2630	LHG	C3-O3-P-O6
29	b	2630	LHG	C4-O6-P-O3
29	d	410	LHG	C4-O6-P-O3
29	g	2630	LHG	C4-O6-P-O3
29	l	101	LHG	C3-O3-P-O6
29	n	2630	LHG	C3-O3-P-O6
29	c	523	LHG	C23-C24-C25-C26
24	s	607	CHL	C3-C5-C6-C7
25	3	611	CLA	C3-C5-C6-C7
25	7	611	CLA	C3-C5-C6-C7
24	Y	609	CHL	CBA-CGA-O2A-C1
25	C	501	CLA	CBA-CGA-O2A-C1
25	C	505	CLA	CBA-CGA-O2A-C1
25	c	501	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
29	C	522	LHG	C24-C23-O8-C6
29	c	522	LHG	C24-C23-O8-C6
25	b	612	CLA	O1D-CGD-O2D-CED
29	C	2630	LHG	C23-C24-C25-C26
29	c	2630	LHG	C23-C24-C25-C26
37	h	102	DGD	C1B-C2B-C3B-C4B
25	B	612	CLA	O1D-CGD-O2D-CED
25	y	603	CLA	O1D-CGD-O2D-CED
29	B	2631	LHG	C1-C2-C3-O3
29	C	2630	LHG	C1-C2-C3-O3
29	D	408	LHG	C1-C2-C3-O3
29	b	2631	LHG	C1-C2-C3-O3
29	c	2630	LHG	C1-C2-C3-O3
29	d	408	LHG	C1-C2-C3-O3
37	C	519	DGD	O6E-C5E-C6E-O5E
29	S	2630	LHG	O9-C7-O7-C5
29	s	2630	LHG	O9-C7-O7-C5
25	C	507	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
24	N	608	CHL	C13-C15-C16-C17
24	n	608	CHL	C13-C15-C16-C17
25	C	508	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	C15-C16-C17-C18
25	Y	603	CLA	O1D-CGD-O2D-CED
25	G	614	CLA	O1A-CGA-O2A-C1
24	3	607	CHL	C2A-CAA-CBA-CGA
24	G	607	CHL	C2A-CAA-CBA-CGA
24	R	607	CHL	C2A-CAA-CBA-CGA
24	7	607	CHL	C2A-CAA-CBA-CGA
24	g	607	CHL	C2A-CAA-CBA-CGA
24	r	607	CHL	C2A-CAA-CBA-CGA
25	G	610	CLA	C2A-CAA-CBA-CGA
25	S	602	CLA	C2A-CAA-CBA-CGA
25	6	613	CLA	C2A-CAA-CBA-CGA
25	g	610	CLA	C2A-CAA-CBA-CGA
25	s	602	CLA	C2A-CAA-CBA-CGA
24	Y	607	CHL	C16-C17-C18-C19
24	y	607	CHL	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C20
25	C	508	CLA	C16-C17-C18-C19
25	R	613	CLA	C11-C12-C13-C14
25	c	502	CLA	C16-C17-C18-C20
25	c	508	CLA	C16-C17-C18-C19
25	r	613	CLA	C11-C12-C13-C14
37	c	519	DGD	O6E-C5E-C6E-O5E
24	y	609	CHL	CBA-CGA-O2A-C1
25	3	611	CLA	CBA-CGA-O2A-C1
25	B	611	CLA	CBA-CGA-O2A-C1
25	S	614	CLA	CBA-CGA-O2A-C1
25	Y	603	CLA	CBA-CGA-O2A-C1
25	7	611	CLA	CBA-CGA-O2A-C1
25	b	611	CLA	CBA-CGA-O2A-C1
25	s	614	CLA	CBA-CGA-O2A-C1
25	y	603	CLA	CBA-CGA-O2A-C1
24	Y	609	CHL	C10-C11-C12-C13
24	y	609	CHL	C10-C11-C12-C13
37	H	102	DGD	C1B-C2B-C3B-C4B
25	g	614	CLA	O1A-CGA-O2A-C1
25	A	410	CLA	C10-C11-C12-C13
25	a	410	CLA	C10-C11-C12-C13
29	G	2630	LHG	C25-C26-C27-C28
29	g	2630	LHG	C25-C26-C27-C28
34	A	412	SQD	C18-C19-C20-C21
34	a	412	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C15-C16-C17-C18
25	C	510	CLA	C15-C16-C17-C18
25	b	607	CLA	C15-C16-C17-C18
25	c	510	CLA	C15-C16-C17-C18
29	1	2630	LHG	C12-C13-C14-C15
29	B	2630	LHG	C27-C28-C29-C30
29	b	2630	LHG	C27-C28-C29-C30
29	c	2630	LHG	C31-C32-C33-C34
35	B	2633	LMG	C30-C31-C32-C33
35	Z	101	LMG	C18-C19-C20-C21
35	b	2633	LMG	C30-C31-C32-C33
37	C	519	DGD	C4A-C5A-C6A-C7A
37	c	519	DGD	C4A-C5A-C6A-C7A
35	Z	101	LMG	C4-C5-C6-O5
35	z	101	LMG	C4-C5-C6-O5
25	R	603	CLA	CBA-CGA-O2A-C1
25	r	603	CLA	CBA-CGA-O2A-C1
29	C	2630	LHG	C31-C32-C33-C34
29	Y	2630	LHG	C26-C27-C28-C29
29	5	2630	LHG	C12-C13-C14-C15
29	y	2630	LHG	C26-C27-C28-C29
35	A	415	LMG	C35-C36-C37-C38
35	C	521	LMG	C32-C33-C34-C35
35	a	415	LMG	C35-C36-C37-C38
35	c	521	LMG	C32-C33-C34-C35
35	z	101	LMG	C18-C19-C20-C21
34	A	418	SQD	C44-C45-O47-C7
34	a	418	SQD	C44-C45-O47-C7
24	R	606	CHL	O1D-CGD-O2D-CED
24	r	606	CHL	O1D-CGD-O2D-CED
29	3	2630	LHG	C23-C24-C25-C26
29	7	2630	LHG	C23-C24-C25-C26
29	L	101	LHG	C25-C26-C27-C28
29	l	101	LHG	C25-C26-C27-C28
35	B	622	LMG	C37-C38-C39-C40
35	B	2633	LMG	C32-C33-C34-C35
35	b	622	LMG	C37-C38-C39-C40
35	b	2633	LMG	C32-C33-C34-C35
37	C	520	DGD	C4B-C5B-C6B-C7B
37	c	520	DGD	C4B-C5B-C6B-C7B
29	C	522	LHG	C11-C10-C9-C8
29	D	410	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	Y	2630	LHG	C16-C17-C18-C19
29	c	522	LHG	C11-C10-C9-C8
29	d	410	LHG	C13-C14-C15-C16
29	y	2630	LHG	C16-C17-C18-C19
35	B	622	LMG	C19-C20-C21-C22
35	C	521	LMG	C11-C12-C13-C14
35	C	521	LMG	C12-C13-C14-C15
35	b	622	LMG	C19-C20-C21-C22
35	c	521	LMG	C11-C12-C13-C14
35	c	521	LMG	C12-C13-C14-C15
24	3	601	CHL	O1D-CGD-O2D-CED
24	7	601	CHL	O1D-CGD-O2D-CED
25	B	602	CLA	C5-C6-C7-C8
25	b	602	CLA	C5-C6-C7-C8
29	3	2630	LHG	C28-C29-C30-C31
29	D	409	LHG	C30-C31-C32-C33
29	7	2630	LHG	C28-C29-C30-C31
29	b	2630	LHG	C29-C30-C31-C32
29	d	409	LHG	C30-C31-C32-C33
37	C	520	DGD	C6A-C7A-C8A-C9A
37	b	626	DGD	C5B-C6B-C7B-C8B
37	c	520	DGD	C6A-C7A-C8A-C9A
29	Y	2630	LHG	C23-C24-C25-C26
29	y	2630	LHG	C23-C24-C25-C26
24	1	605	CHL	O1D-CGD-O2D-CED
24	5	605	CHL	O1D-CGD-O2D-CED
35	B	2633	LMG	C2-C1-O1-C7
35	b	2633	LMG	C2-C1-O1-C7
37	C	519	DGD	C2E-C1E-O5D-C6D
37	c	519	DGD	C2E-C1E-O5D-C6D
29	S	2630	LHG	O7-C5-C6-O8
29	s	2630	LHG	O7-C5-C6-O8
34	A	412	SQD	O6-C44-C45-O47
34	a	412	SQD	O6-C44-C45-O47
24	G	609	CHL	CBA-CGA-O2A-C1
24	N	609	CHL	CBA-CGA-O2A-C1
24	Y	605	CHL	CBA-CGA-O2A-C1
24	g	609	CHL	CBA-CGA-O2A-C1
24	n	609	CHL	CBA-CGA-O2A-C1
24	y	605	CHL	CBA-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	B	2630	LHG	C29-C30-C31-C32
29	C	523	LHG	C15-C16-C17-C18
29	G	2630	LHG	C18-C19-C20-C21
29	L	101	LHG	C30-C31-C32-C33
29	N	2630	LHG	C25-C26-C27-C28
29	c	523	LHG	C15-C16-C17-C18
29	g	2630	LHG	C18-C19-C20-C21
29	l	101	LHG	C30-C31-C32-C33
29	n	2630	LHG	C25-C26-C27-C28
35	B	2633	LMG	C16-C17-C18-C19
35	C	521	LMG	C17-C18-C19-C20
35	b	2633	LMG	C16-C17-C18-C19
37	B	626	DGD	C5B-C6B-C7B-C8B
24	G	608	CHL	C13-C15-C16-C17
24	g	608	CHL	C13-C15-C16-C17
25	B	613	CLA	C10-C11-C12-C13
25	b	613	CLA	C10-C11-C12-C13
25	C	501	CLA	O1A-CGA-O2A-C1
25	c	501	CLA	O1A-CGA-O2A-C1
24	2	609	CHL	C11-C12-C13-C15
24	N	608	CHL	C16-C17-C18-C20
24	N	609	CHL	C16-C17-C18-C20
24	6	609	CHL	C11-C12-C13-C15
24	n	608	CHL	C16-C17-C18-C20
24	n	609	CHL	C16-C17-C18-C20
24	4	607	CHL	O1D-CGD-O2D-CED
24	Y	609	CHL	O1D-CGD-O2D-CED
24	8	607	CHL	O1D-CGD-O2D-CED
24	y	609	CHL	O1D-CGD-O2D-CED
24	2	607	CHL	C4-C3-C5-C6
24	6	607	CHL	C4-C3-C5-C6
29	c	2630	LHG	C32-C33-C34-C35
34	A	412	SQD	C10-C11-C12-C13
34	a	412	SQD	C10-C11-C12-C13
35	A	413	LMG	C37-C38-C39-C40
35	A	415	LMG	C30-C31-C32-C33
35	a	413	LMG	C37-C38-C39-C40
35	a	415	LMG	C30-C31-C32-C33
35	c	521	LMG	C17-C18-C19-C20
37	B	626	DGD	C4B-C5B-C6B-C7B
37	b	626	DGD	C4B-C5B-C6B-C7B
24	1	609	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	604	CLA	C6-C7-C8-C9
25	B	617	CLA	C14-C13-C15-C16
25	C	505	CLA	C14-C13-C15-C16
25	D	403	CLA	C14-C13-C15-C16
25	G	602	CLA	C6-C7-C8-C9
25	N	603	CLA	C11-C10-C8-C9
25	S	602	CLA	C11-C12-C13-C14
25	Y	603	CLA	C6-C7-C8-C9
25	b	604	CLA	C6-C7-C8-C9
25	b	617	CLA	C14-C13-C15-C16
25	c	505	CLA	C14-C13-C15-C16
25	d	403	CLA	C14-C13-C15-C16
25	g	602	CLA	C6-C7-C8-C9
25	n	603	CLA	C11-C10-C8-C9
25	s	602	CLA	C11-C12-C13-C14
25	y	603	CLA	C6-C7-C8-C9
33	A	408	PHO	C14-C13-C15-C16
33	a	408	PHO	C14-C13-C15-C16
25	C	513	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
29	C	2630	LHG	C32-C33-C34-C35
29	C	522	LHG	C27-C28-C29-C30
29	C	522	LHG	C28-C29-C30-C31
29	D	408	LHG	C26-C27-C28-C29
29	L	101	LHG	C13-C14-C15-C16
29	S	2630	LHG	C32-C33-C34-C35
29	c	522	LHG	C27-C28-C29-C30
29	c	522	LHG	C28-C29-C30-C31
29	d	408	LHG	C28-C29-C30-C31
29	l	101	LHG	C13-C14-C15-C16
29	s	2630	LHG	C32-C33-C34-C35
34	A	412	SQD	C29-C30-C31-C32
34	a	412	SQD	C29-C30-C31-C32
35	A	413	LMG	C17-C18-C19-C20
35	a	413	LMG	C17-C18-C19-C20
37	B	626	DGD	C2A-C3A-C4A-C5A
37	C	518	DGD	C4A-C5A-C6A-C7A
37	C	520	DGD	C2A-C3A-C4A-C5A
37	c	518	DGD	C4A-C5A-C6A-C7A
25	B	613	CLA	C13-C15-C16-C17
25	N	603	CLA	C5-C6-C7-C8
25	b	613	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	n	603	CLA	C5-C6-C7-C8
24	3	605	CHL	C2A-CAA-CBA-CGA
24	Y	601	CHL	C2A-CAA-CBA-CGA
24	7	605	CHL	C2A-CAA-CBA-CGA
24	y	601	CHL	C2A-CAA-CBA-CGA
25	B	608	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	C2A-CAA-CBA-CGA
25	C	503	CLA	C2A-CAA-CBA-CGA
25	S	611	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	C2A-CAA-CBA-CGA
25	b	613	CLA	C2A-CAA-CBA-CGA
25	c	503	CLA	C2A-CAA-CBA-CGA
25	s	611	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	O1A-CGA-O2A-C1
25	C	505	CLA	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
30	4	623	BCR	C7-C8-C9-C34
30	8	623	BCR	C7-C8-C9-C34
24	1	607	CHL	C2C-C3C-CAC-CBC
24	5	607	CHL	C2C-C3C-CAC-CBC
29	B	2630	LHG	C12-C13-C14-C15
29	D	408	LHG	C28-C29-C30-C31
29	b	2630	LHG	C12-C13-C14-C15
29	d	408	LHG	C26-C27-C28-C29
29	r	2630	LHG	C12-C13-C14-C15
34	B	621	SQD	C34-C35-C36-C37
34	a	412	SQD	C12-C13-C14-C15
34	b	621	SQD	C34-C35-C36-C37
35	C	521	LMG	C35-C36-C37-C38
35	c	521	LMG	C35-C36-C37-C38
37	B	626	DGD	CCB-CDB-CEB-CFB
37	b	626	DGD	C2A-C3A-C4A-C5A
37	b	626	DGD	CCB-CDB-CEB-CFB
37	c	520	DGD	C2A-C3A-C4A-C5A
29	2	2630	LHG	O1-C1-C2-C3
29	4	2630	LHG	O1-C1-C2-C3
29	B	2630	LHG	O1-C1-C2-C3
29	D	410	LHG	O1-C1-C2-C3
29	6	2630	LHG	O1-C1-C2-C3
29	8	2630	LHG	O1-C1-C2-C3
29	b	2630	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	d	410	LHG	O1-C1-C2-C3
37	B	626	DGD	O1B-C1B-O2G-C2G
37	b	626	DGD	O1B-C1B-O2G-C2G
29	3	2630	LHG	C10-C11-C12-C13
29	B	2630	LHG	C11-C10-C9-C8
29	C	2630	LHG	C14-C15-C16-C17
29	R	2630	LHG	C12-C13-C14-C15
29	7	2630	LHG	C10-C11-C12-C13
29	b	2630	LHG	C11-C10-C9-C8
29	c	2630	LHG	C14-C15-C16-C17
29	l	101	LHG	C11-C10-C9-C8
34	A	412	SQD	C12-C13-C14-C15
35	Z	101	LMG	C30-C31-C32-C33
35	z	101	LMG	C30-C31-C32-C33
29	2	2630	LHG	C23-C24-C25-C26
29	B	2631	LHG	C23-C24-C25-C26
29	L	101	LHG	C7-C8-C9-C10
29	6	2630	LHG	C23-C24-C25-C26
29	b	2631	LHG	C23-C24-C25-C26
29	l	101	LHG	C7-C8-C9-C10
37	C	520	DGD	C1A-C2A-C3A-C4A
37	c	520	DGD	C1A-C2A-C3A-C4A
29	C	522	LHG	C32-C33-C34-C35
29	G	2630	LHG	C27-C28-C29-C30
29	L	101	LHG	C11-C10-C9-C8
29	N	2630	LHG	C11-C10-C9-C8
29	N	2630	LHG	C27-C28-C29-C30
29	c	522	LHG	C32-C33-C34-C35
29	g	2630	LHG	C27-C28-C29-C30
29	n	2630	LHG	C11-C10-C9-C8
29	n	2630	LHG	C27-C28-C29-C30
34	A	412	SQD	C13-C14-C15-C16
34	B	621	SQD	C9-C10-C11-C12
34	B	623	SQD	C9-C10-C11-C12
34	a	412	SQD	C13-C14-C15-C16
34	b	621	SQD	C9-C10-C11-C12
34	b	623	SQD	C9-C10-C11-C12
35	A	415	LMG	C36-C37-C38-C39
35	C	521	LMG	C16-C17-C18-C19
35	a	415	LMG	C36-C37-C38-C39
35	c	521	LMG	C16-C17-C18-C19
37	C	519	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
37	c	519	DGD	C5B-C6B-C7B-C8B
24	R	606	CHL	C16-C17-C18-C19
24	r	606	CHL	C16-C17-C18-C19
25	B	605	CLA	C16-C17-C18-C20
25	C	502	CLA	C16-C17-C18-C19
25	b	605	CLA	C16-C17-C18-C20
25	c	502	CLA	C16-C17-C18-C19
25	r	603	CLA	C11-C12-C13-C14
29	1	2630	LHG	C9-C10-C11-C12
29	3	2630	LHG	C14-C15-C16-C17
29	C	2630	LHG	C24-C25-C26-C27
29	L	101	LHG	C16-C17-C18-C19
29	S	2630	LHG	C24-C25-C26-C27
29	5	2630	LHG	C9-C10-C11-C12
29	7	2630	LHG	C14-C15-C16-C17
29	c	2630	LHG	C24-C25-C26-C27
29	l	101	LHG	C16-C17-C18-C19
29	s	2630	LHG	C24-C25-C26-C27
29	y	2630	LHG	C32-C33-C34-C35
35	B	622	LMG	C13-C14-C15-C16
35	B	2633	LMG	C15-C16-C17-C18
35	b	622	LMG	C13-C14-C15-C16
35	b	2633	LMG	C15-C16-C17-C18
37	C	519	DGD	C4B-C5B-C6B-C7B
37	C	520	DGD	C7A-C8A-C9A-CAA
37	c	519	DGD	C4B-C5B-C6B-C7B
37	c	520	DGD	C7A-C8A-C9A-CAA
25	G	602	CLA	CBD-CGD-O2D-CED
25	g	602	CLA	CBD-CGD-O2D-CED
25	n	611	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	O1D-CGD-O2D-CED
25	s	609	CLA	O1D-CGD-O2D-CED
29	B	2631	LHG	C27-C28-C29-C30
29	C	523	LHG	C33-C34-C35-C36
29	D	410	LHG	C15-C16-C17-C18
29	Y	2630	LHG	C12-C13-C14-C15
29	Y	2630	LHG	C32-C33-C34-C35
29	b	2631	LHG	C27-C28-C29-C30
29	c	523	LHG	C33-C34-C35-C36
29	y	2630	LHG	C12-C13-C14-C15
34	B	621	SQD	C11-C12-C13-C14
34	b	621	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	B	622	LMG	C35-C36-C37-C38
35	C	521	LMG	C31-C32-C33-C34
35	b	622	LMG	C35-C36-C37-C38
35	c	521	LMG	C31-C32-C33-C34
34	B	623	SQD	C23-C24-C25-C26
34	b	623	SQD	C23-C24-C25-C26
24	G	601	CHL	C8-C10-C11-C12
24	G	607	CHL	C8-C10-C11-C12
24	g	601	CHL	C8-C10-C11-C12
24	g	607	CHL	C8-C10-C11-C12
25	B	606	CLA	C8-C10-C11-C12
25	b	606	CLA	C8-C10-C11-C12
25	y	602	CLA	C8-C10-C11-C12
34	B	623	SQD	O10-C23-O48-C46
34	b	623	SQD	O10-C23-O48-C46
29	D	410	LHG	C27-C28-C29-C30
29	d	410	LHG	C15-C16-C17-C18
29	d	410	LHG	C27-C28-C29-C30
35	D	411	LMG	C32-C33-C34-C35
35	d	411	LMG	C32-C33-C34-C35
37	C	518	DGD	C4B-C5B-C6B-C7B
37	C	520	DGD	CCA-CDA-CEA-CFA
37	c	518	DGD	C4B-C5B-C6B-C7B
37	c	520	DGD	CCA-CDA-CEA-CFA
25	B	611	CLA	O1D-CGD-O2D-CED
35	B	622	LMG	C18-C19-C20-C21
35	B	2633	LMG	C31-C32-C33-C34
35	b	622	LMG	C18-C19-C20-C21
35	b	2633	LMG	C31-C32-C33-C34
25	c	512	CLA	O1D-CGD-O2D-CED
24	1	605	CHL	C3A-C2A-CAA-CBA
24	1	607	CHL	C3A-C2A-CAA-CBA
24	2	605	CHL	C3A-C2A-CAA-CBA
24	2	607	CHL	C3A-C2A-CAA-CBA
24	3	605	CHL	C3A-C2A-CAA-CBA
24	4	608	CHL	C3A-C2A-CAA-CBA
24	R	606	CHL	C3A-C2A-CAA-CBA
24	5	605	CHL	C3A-C2A-CAA-CBA
24	5	607	CHL	C3A-C2A-CAA-CBA
24	6	605	CHL	C3A-C2A-CAA-CBA
24	6	607	CHL	C3A-C2A-CAA-CBA
24	7	605	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	8	608	CHL	C3A-C2A-CAA-CBA
24	r	606	CHL	C3A-C2A-CAA-CBA
24	y	605	CHL	C3A-C2A-CAA-CBA
25	1	611	CLA	C3A-C2A-CAA-CBA
25	R	616	CLA	C3A-C2A-CAA-CBA
25	S	602	CLA	C3A-C2A-CAA-CBA
25	S	609	CLA	C3A-C2A-CAA-CBA
25	5	611	CLA	C3A-C2A-CAA-CBA
25	r	616	CLA	C3A-C2A-CAA-CBA
25	s	602	CLA	C3A-C2A-CAA-CBA
25	s	609	CLA	C3A-C2A-CAA-CBA
24	Y	607	CHL	C13-C15-C16-C17
24	y	607	CHL	C13-C15-C16-C17
25	B	606	CLA	C5-C6-C7-C8
25	Y	602	CLA	C8-C10-C11-C12
25	b	606	CLA	C5-C6-C7-C8
29	2	2630	LHG	C11-C12-C13-C14
29	6	2630	LHG	C11-C12-C13-C14
25	S	609	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
25	B	611	CLA	O1A-CGA-O2A-C1
25	b	611	CLA	O1A-CGA-O2A-C1
25	B	605	CLA	C16-C17-C18-C19
25	R	603	CLA	C11-C12-C13-C14
25	b	605	CLA	C16-C17-C18-C19
29	2	2630	LHG	C12-C13-C14-C15
29	D	408	LHG	C27-C28-C29-C30
29	6	2630	LHG	C12-C13-C14-C15
29	d	408	LHG	C27-C28-C29-C30
29	l	101	LHG	C32-C33-C34-C35
24	N	601	CHL	O1D-CGD-O2D-CED
24	n	601	CHL	O1D-CGD-O2D-CED
25	N	602	CLA	O1D-CGD-O2D-CED
25	N	611	CLA	CBD-CGD-O2D-CED
29	D	409	LHG	C34-C35-C36-C37
29	L	101	LHG	C32-C33-C34-C35
29	d	409	LHG	C34-C35-C36-C37
37	H	102	DGD	C9A-CAA-CBA-CCA
37	h	102	DGD	C9A-CAA-CBA-CCA
25	n	602	CLA	O1D-CGD-O2D-CED
29	D	408	LHG	C30-C31-C32-C33
29	D	409	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	d	408	LHG	C30-C31-C32-C33
29	d	409	LHG	C33-C34-C35-C36
24	3	607	CHL	C4-C3-C5-C6
24	7	607	CHL	C4-C3-C5-C6
24	1	609	CHL	CBA-CGA-O2A-C1
24	5	609	CHL	CBA-CGA-O2A-C1
37	C	519	DGD	C4E-C5E-C6E-O5E
37	c	519	DGD	C4E-C5E-C6E-O5E
24	2	607	CHL	C2-C3-C5-C6
24	3	607	CHL	C2-C3-C5-C6
24	6	607	CHL	C2-C3-C5-C6
24	7	607	CHL	C2-C3-C5-C6
25	B	616	CLA	C2-C3-C5-C6
25	Y	603	CLA	C2-C3-C5-C6
25	b	616	CLA	C2-C3-C5-C6
25	y	603	CLA	C2-C3-C5-C6
36	D	405	PL9	C13-C14-C16-C17
36	D	405	PL9	C43-C44-C46-C47
36	d	405	PL9	C13-C14-C16-C17
36	d	405	PL9	C43-C44-C46-C47
29	D	408	LHG	C25-C26-C27-C28
29	L	101	LHG	C29-C30-C31-C32
29	d	408	LHG	C25-C26-C27-C28
35	Z	101	LMG	C32-C33-C34-C35
35	z	101	LMG	C32-C33-C34-C35
37	B	626	DGD	C5A-C6A-C7A-C8A
37	b	626	DGD	C5A-C6A-C7A-C8A
24	3	608	CHL	C2A-CAA-CBA-CGA
24	7	608	CHL	C2A-CAA-CBA-CGA
29	R	2630	LHG	O1-C1-C2-O2
29	Y	2630	LHG	O1-C1-C2-O2
29	r	2630	LHG	O1-C1-C2-O2
29	y	2630	LHG	O1-C1-C2-O2
24	n	601	CHL	C5-C6-C7-C8
25	b	612	CLA	C15-C16-C17-C18
29	2	2630	LHG	C24-C25-C26-C27
29	C	523	LHG	C24-C25-C26-C27
29	L	101	LHG	C28-C29-C30-C31
29	6	2630	LHG	C24-C25-C26-C27
29	c	523	LHG	C24-C25-C26-C27
29	l	101	LHG	C28-C29-C30-C31
29	l	101	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
34	A	412	SQD	C9-C10-C11-C12
34	A	418	SQD	C11-C10-C9-C8
34	a	412	SQD	C9-C10-C11-C12
34	a	418	SQD	C11-C10-C9-C8
35	B	622	LMG	C21-C22-C23-C24
35	B	622	LMG	C29-C30-C31-C32
35	B	2633	LMG	C34-C35-C36-C37
35	b	622	LMG	C21-C22-C23-C24
35	b	622	LMG	C29-C30-C31-C32
35	b	2633	LMG	C34-C35-C36-C37
37	C	519	DGD	C6B-C7B-C8B-C9B
37	c	519	DGD	C6B-C7B-C8B-C9B
25	3	611	CLA	O1A-CGA-O2A-C1
25	S	614	CLA	O1A-CGA-O2A-C1
25	7	611	CLA	O1A-CGA-O2A-C1
25	s	614	CLA	O1A-CGA-O2A-C1
24	2	609	CHL	C11-C12-C13-C14
24	6	609	CHL	C11-C12-C13-C14
29	D	409	LHG	C12-C13-C14-C15
29	S	2630	LHG	C34-C35-C36-C37
29	d	409	LHG	C12-C13-C14-C15
29	s	2630	LHG	C34-C35-C36-C37
34	A	412	SQD	C17-C18-C19-C20
29	S	2630	LHG	O2-C2-C3-O3
29	s	2630	LHG	O2-C2-C3-O3
24	N	601	CHL	C5-C6-C7-C8
25	B	612	CLA	C15-C16-C17-C18
25	C	504	CLA	C13-C15-C16-C17
25	D	402	CLA	C10-C11-C12-C13
25	c	504	CLA	C13-C15-C16-C17
25	d	402	CLA	C10-C11-C12-C13
29	l	101	LHG	C10-C11-C12-C13
34	A	418	SQD	C32-C33-C34-C35
34	a	412	SQD	C17-C18-C19-C20
29	L	101	LHG	C10-C11-C12-C13
29	S	2630	LHG	C11-C12-C13-C14
29	s	2630	LHG	C11-C12-C13-C14
34	a	418	SQD	C32-C33-C34-C35
37	H	102	DGD	C7A-C8A-C9A-CAA
24	Y	609	CHL	O1A-CGA-O2A-C1
24	y	609	CHL	O1A-CGA-O2A-C1
25	R	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	r	603	CLA	O1A-CGA-O2A-C1
25	G	613	CLA	C8-C10-C11-C12
25	g	613	CLA	C8-C10-C11-C12
29	D	410	LHG	C1-C2-C3-O3
29	d	410	LHG	C1-C2-C3-O3
29	3	2630	LHG	C33-C34-C35-C36
29	B	2630	LHG	C25-C26-C27-C28
29	D	409	LHG	C24-C25-C26-C27
29	L	101	LHG	C24-C25-C26-C27
29	N	2630	LHG	C30-C31-C32-C33
29	7	2630	LHG	C33-C34-C35-C36
29	b	2630	LHG	C25-C26-C27-C28
29	d	409	LHG	C24-C25-C26-C27
29	l	101	LHG	C24-C25-C26-C27
29	n	2630	LHG	C30-C31-C32-C33
34	A	418	SQD	C13-C14-C15-C16
34	a	418	SQD	C13-C14-C15-C16
37	h	102	DGD	C7A-C8A-C9A-CAA
24	R	608	CHL	C2-C1-O2A-CGA
24	r	608	CHL	C2-C1-O2A-CGA
29	B	2631	LHG	C28-C29-C30-C31
29	b	2630	LHG	C11-C12-C13-C14
29	b	2631	LHG	C28-C29-C30-C31
37	C	519	DGD	C3B-C4B-C5B-C6B
37	c	519	DGD	C3B-C4B-C5B-C6B
24	1	607	CHL	C8-C10-C11-C12
24	Y	609	CHL	C15-C16-C17-C18
24	5	607	CHL	C8-C10-C11-C12
24	y	609	CHL	C15-C16-C17-C18
25	C	505	CLA	C5-C6-C7-C8
25	c	505	CLA	C5-C6-C7-C8
25	Y	603	CLA	O1A-CGA-O2A-C1
25	y	603	CLA	O1A-CGA-O2A-C1
29	B	2630	LHG	C11-C12-C13-C14
29	B	2631	LHG	C14-C15-C16-C17
29	b	2631	LHG	C14-C15-C16-C17
34	A	412	SQD	C11-C10-C9-C8
24	N	607	CHL	C16-C17-C18-C19
24	Y	607	CHL	C16-C17-C18-C20
24	n	607	CHL	C16-C17-C18-C19
24	y	607	CHL	C16-C17-C18-C20
26	1	1620	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	1	1620	LUT	C5-C6-C7-C8
26	1	1621	LUT	C5-C6-C7-C8
26	2	1620	LUT	C1-C6-C7-C8
26	2	1620	LUT	C5-C6-C7-C8
26	N	1620	LUT	C1-C6-C7-C8
26	N	1620	LUT	C5-C6-C7-C8
26	R	620	LUT	C1-C6-C7-C8
26	R	620	LUT	C5-C6-C7-C8
26	Y	1620	LUT	C1-C6-C7-C8
26	Y	1620	LUT	C5-C6-C7-C8
26	5	1620	LUT	C1-C6-C7-C8
26	5	1620	LUT	C5-C6-C7-C8
26	5	1621	LUT	C5-C6-C7-C8
26	6	1620	LUT	C1-C6-C7-C8
26	6	1620	LUT	C5-C6-C7-C8
26	n	1620	LUT	C1-C6-C7-C8
26	n	1620	LUT	C5-C6-C7-C8
26	r	620	LUT	C1-C6-C7-C8
26	r	620	LUT	C5-C6-C7-C8
26	y	1620	LUT	C1-C6-C7-C8
26	y	1620	LUT	C5-C6-C7-C8
30	4	623	BCR	C5-C6-C7-C8
30	A	411	BCR	C23-C24-C25-C26
30	A	411	BCR	C23-C24-C25-C30
30	B	618	BCR	C1-C6-C7-C8
30	B	618	BCR	C5-C6-C7-C8
30	B	620	BCR	C23-C24-C25-C26
30	B	620	BCR	C23-C24-C25-C30
30	C	514	BCR	C5-C6-C7-C8
30	C	515	BCR	C23-C24-C25-C26
30	D	404	BCR	C1-C6-C7-C8
30	D	404	BCR	C5-C6-C7-C8
30	T	101	BCR	C23-C24-C25-C26
30	8	623	BCR	C5-C6-C7-C8
30	a	411	BCR	C23-C24-C25-C26
30	a	411	BCR	C23-C24-C25-C30
30	b	618	BCR	C1-C6-C7-C8
30	b	618	BCR	C5-C6-C7-C8
30	b	620	BCR	C23-C24-C25-C26
30	b	620	BCR	C23-C24-C25-C30
30	c	514	BCR	C5-C6-C7-C8
30	c	515	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	d	404	BCR	C1-C6-C7-C8
30	d	404	BCR	C5-C6-C7-C8
30	t	101	BCR	C23-C24-C25-C26
29	B	2631	LHG	C32-C33-C34-C35
29	b	2631	LHG	C32-C33-C34-C35
34	a	412	SQD	C11-C10-C9-C8
35	B	622	LMG	C17-C18-C19-C20
37	H	102	DGD	CCA-CDA-CEA-CFA
37	h	102	DGD	CCA-CDA-CEA-CFA
24	2	609	CHL	CBA-CGA-O2A-C1
24	G	606	CHL	CBA-CGA-O2A-C1
24	6	609	CHL	CBA-CGA-O2A-C1
24	g	606	CHL	CBA-CGA-O2A-C1
25	B	605	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	CBA-CGA-O2A-C1
24	R	608	CHL	C8-C10-C11-C12
24	r	608	CHL	C8-C10-C11-C12
25	A	406	CLA	C10-C11-C12-C13
25	B	617	CLA	C10-C11-C12-C13
25	B	617	CLA	C15-C16-C17-C18
25	a	406	CLA	C10-C11-C12-C13
25	b	617	CLA	C10-C11-C12-C13
25	b	617	CLA	C15-C16-C17-C18
35	b	622	LMG	C17-C18-C19-C20
37	C	519	DGD	C3A-C4A-C5A-C6A
37	C	519	DGD	C9A-CAA-CBA-CCA
37	c	519	DGD	C3A-C4A-C5A-C6A
24	N	609	CHL	O1A-CGA-O2A-C1
24	Y	605	CHL	O1A-CGA-O2A-C1
24	n	609	CHL	O1A-CGA-O2A-C1
24	y	605	CHL	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
37	c	519	DGD	C9A-CAA-CBA-CCA
29	C	523	LHG	C12-C13-C14-C15
29	c	523	LHG	C12-C13-C14-C15
34	A	418	SQD	C25-C26-C27-C28
34	a	418	SQD	C25-C26-C27-C28
35	d	411	LMG	C18-C19-C20-C21
24	1	607	CHL	C4-C3-C5-C6
24	R	608	CHL	C4-C3-C5-C6
24	5	607	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	r	608	CHL	C4-C3-C5-C6
25	C	501	CLA	C4-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	Y	603	CLA	C4-C3-C5-C6
25	c	501	CLA	C4-C3-C5-C6
25	c	504	CLA	C4-C3-C5-C6
25	y	603	CLA	C4-C3-C5-C6
36	D	405	PL9	C30-C29-C31-C32
36	d	405	PL9	C30-C29-C31-C32
24	1	607	CHL	C2-C3-C5-C6
24	N	608	CHL	C12-C13-C15-C16
24	R	606	CHL	C11-C10-C8-C7
24	R	608	CHL	C2-C3-C5-C6
24	Y	608	CHL	C12-C13-C15-C16
24	5	607	CHL	C2-C3-C5-C6
24	n	608	CHL	C12-C13-C15-C16
24	r	606	CHL	C11-C10-C8-C7
24	r	608	CHL	C2-C3-C5-C6
24	y	608	CHL	C12-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C10
25	B	613	CLA	C6-C7-C8-C10
25	B	617	CLA	C12-C13-C15-C16
25	C	505	CLA	C12-C13-C15-C16
25	C	513	CLA	C11-C12-C13-C15
25	D	403	CLA	C12-C13-C15-C16
25	G	602	CLA	C6-C7-C8-C10
25	N	603	CLA	C11-C10-C8-C7
25	S	602	CLA	C11-C12-C13-C15
25	Y	612	CLA	C11-C10-C8-C7
25	b	603	CLA	C6-C7-C8-C10
25	b	613	CLA	C6-C7-C8-C10
25	b	617	CLA	C12-C13-C15-C16
25	c	505	CLA	C12-C13-C15-C16
25	c	513	CLA	C11-C12-C13-C15
25	d	403	CLA	C12-C13-C15-C16
25	g	602	CLA	C6-C7-C8-C10
25	n	603	CLA	C11-C10-C8-C7
25	s	602	CLA	C11-C12-C13-C15
25	y	612	CLA	C11-C10-C8-C7
24	G	609	CHL	O1A-CGA-O2A-C1
24	g	609	CHL	O1A-CGA-O2A-C1
35	B	2633	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
35	b	2633	LMG	O10-C28-O8-C9
29	R	2630	LHG	C13-C14-C15-C16
29	r	2630	LHG	C13-C14-C15-C16
35	D	411	LMG	C18-C19-C20-C21
25	B	602	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C20
24	N	609	CHL	O1D-CGD-O2D-CED
24	n	609	CHL	O1D-CGD-O2D-CED
25	C	507	CLA	O1D-CGD-O2D-CED
25	c	507	CLA	O1D-CGD-O2D-CED
35	D	411	LMG	O9-C10-O7-C8
35	d	411	LMG	O9-C10-O7-C8
35	Z	101	LMG	C28-C29-C30-C31
35	z	101	LMG	C28-C29-C30-C31
24	R	607	CHL	CBA-CGA-O2A-C1
24	r	607	CHL	CBA-CGA-O2A-C1
25	B	606	CLA	CBA-CGA-O2A-C1
25	B	608	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	CBA-CGA-O2A-C1
25	b	606	CLA	CBA-CGA-O2A-C1
25	b	608	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
34	A	418	SQD	C10-C11-C12-C13
34	a	418	SQD	C10-C11-C12-C13
35	C	521	LMG	C29-C30-C31-C32
35	c	521	LMG	C29-C30-C31-C32
25	C	505	CLA	C2A-CAA-CBA-CGA
25	G	602	CLA	C2A-CAA-CBA-CGA
25	Y	602	CLA	C2A-CAA-CBA-CGA
25	c	505	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C2A-CAA-CBA-CGA
25	y	602	CLA	C2A-CAA-CBA-CGA
25	G	602	CLA	C15-C16-C17-C18
25	N	603	CLA	C10-C11-C12-C13
25	g	602	CLA	C15-C16-C17-C18
25	n	603	CLA	C10-C11-C12-C13
24	3	609	CHL	C2C-C3C-CAC-CBC
29	d	408	LHG	C29-C30-C31-C32
35	A	415	LMG	C37-C38-C39-C40
35	B	2633	LMG	C17-C18-C19-C20
35	a	415	LMG	C37-C38-C39-C40
35	b	2633	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	R	602	CLA	C8-C10-C11-C12
25	r	602	CLA	C8-C10-C11-C12
24	7	609	CHL	C2C-C3C-CAC-CBC
29	D	408	LHG	C29-C30-C31-C32
37	C	520	DGD	C5A-C6A-C7A-C8A
37	c	520	DGD	C5A-C6A-C7A-C8A
29	S	2630	LHG	C26-C27-C28-C29
29	s	2630	LHG	C26-C27-C28-C29
35	A	415	LMG	C32-C33-C34-C35
35	a	415	LMG	C32-C33-C34-C35
25	3	602	CLA	C11-C12-C13-C15
25	7	602	CLA	C11-C12-C13-C15
37	C	520	DGD	O6D-C1D-O3G-C3G
37	C	520	DGD	O6E-C1E-O5D-C6D
37	H	102	DGD	O6E-C1E-O5D-C6D
37	c	520	DGD	O6D-C1D-O3G-C3G
37	c	520	DGD	O6E-C1E-O5D-C6D
37	h	102	DGD	O6E-C1E-O5D-C6D
24	N	607	CHL	C13-C15-C16-C17
24	n	607	CHL	C13-C15-C16-C17
25	G	604	CLA	O1D-CGD-O2D-CED
25	g	604	CLA	O1D-CGD-O2D-CED
29	B	2630	LHG	C10-C11-C12-C13
29	B	2630	LHG	C26-C27-C28-C29
29	C	523	LHG	C11-C10-C9-C8
29	D	410	LHG	C25-C26-C27-C28
29	b	2630	LHG	C10-C11-C12-C13
29	b	2630	LHG	C26-C27-C28-C29
29	c	523	LHG	C11-C10-C9-C8
29	d	410	LHG	C25-C26-C27-C28
34	A	412	SQD	C14-C15-C16-C17
34	a	412	SQD	C14-C15-C16-C17
29	B	2630	LHG	C8-C7-O7-C5
29	C	2630	LHG	C8-C7-O7-C5
29	S	2630	LHG	C8-C7-O7-C5
29	b	2630	LHG	C8-C7-O7-C5
29	c	2630	LHG	C8-C7-O7-C5
29	s	2630	LHG	C8-C7-O7-C5
35	C	521	LMG	C11-C10-O7-C8
35	c	521	LMG	C11-C10-O7-C8
37	C	520	DGD	C2B-C1B-O2G-C2G
37	c	520	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
24	1	609	CHL	C2C-C3C-CAC-CBC
24	5	609	CHL	C2C-C3C-CAC-CBC
29	N	2630	LHG	C24-C25-C26-C27
29	n	2630	LHG	C24-C25-C26-C27
37	H	102	DGD	C5B-C6B-C7B-C8B
37	c	519	DGD	C2B-C3B-C4B-C5B
37	h	102	DGD	C5B-C6B-C7B-C8B
25	N	602	CLA	C8-C10-C11-C12
25	n	602	CLA	C8-C10-C11-C12
25	B	605	CLA	CBD-CGD-O2D-CED
25	R	610	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	r	610	CLA	CBD-CGD-O2D-CED
37	C	519	DGD	C2B-C3B-C4B-C5B
37	C	520	DGD	C2E-C1E-O5D-C6D
37	H	102	DGD	C2E-C1E-O5D-C6D
37	c	520	DGD	C2E-C1E-O5D-C6D
37	h	102	DGD	C2E-C1E-O5D-C6D
29	3	2630	LHG	O7-C5-C6-O8
29	4	2630	LHG	O7-C5-C6-O8
29	B	2631	LHG	O7-C5-C6-O8
29	7	2630	LHG	O7-C5-C6-O8
29	8	2630	LHG	O7-C5-C6-O8
29	b	2631	LHG	O7-C5-C6-O8
35	A	415	LMG	O7-C8-C9-O8
35	a	415	LMG	O7-C8-C9-O8
37	C	518	DGD	C5B-C6B-C7B-C8B
37	c	518	DGD	C5B-C6B-C7B-C8B
25	4	603	CLA	CBD-CGD-O2D-CED
25	8	603	CLA	CBD-CGD-O2D-CED
24	N	608	CHL	C16-C17-C18-C19
25	C	505	CLA	C16-C17-C18-C20
25	C	508	CLA	C16-C17-C18-C20
25	c	505	CLA	C16-C17-C18-C20
25	c	508	CLA	C16-C17-C18-C20
29	G	2630	LHG	C28-C29-C30-C31
29	g	2630	LHG	C28-C29-C30-C31
25	B	612	CLA	C4-C3-C5-C6
25	B	616	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
25	b	616	CLA	C4-C3-C5-C6
36	D	405	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
36	d	405	PL9	C15-C14-C16-C17
29	R	2630	LHG	C23-C24-C25-C26
25	C	504	CLA	C2-C3-C5-C6
25	C	507	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
29	C	2630	LHG	C26-C27-C28-C29
29	c	2630	LHG	C26-C27-C28-C29
24	5	609	CHL	C11-C10-C8-C9
25	A	410	CLA	C6-C7-C8-C9
25	B	615	CLA	C6-C7-C8-C9
25	C	502	CLA	C14-C13-C15-C16
25	C	513	CLA	C11-C12-C13-C14
25	G	610	CLA	C14-C13-C15-C16
25	N	610	CLA	C11-C12-C13-C14
25	S	602	CLA	C6-C7-C8-C9
25	a	410	CLA	C6-C7-C8-C9
25	b	615	CLA	C6-C7-C8-C9
25	c	502	CLA	C14-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C9
25	c	513	CLA	C11-C12-C13-C14
25	g	610	CLA	C14-C13-C15-C16
25	n	610	CLA	C11-C12-C13-C14
25	s	602	CLA	C6-C7-C8-C9
37	c	519	DGD	O1A-C1A-O1G-C1G
35	A	413	LMG	C32-C33-C34-C35
35	a	413	LMG	C32-C33-C34-C35
25	A	405	CLA	C3-C5-C6-C7
25	a	405	CLA	C3-C5-C6-C7
25	c	501	CLA	O1D-CGD-O2D-CED
24	Y	606	CHL	C2A-CAA-CBA-CGA
24	y	606	CHL	C2A-CAA-CBA-CGA
25	3	602	CLA	C2A-CAA-CBA-CGA
25	G	611	CLA	C2A-CAA-CBA-CGA
25	N	602	CLA	C2A-CAA-CBA-CGA
25	7	602	CLA	C2A-CAA-CBA-CGA
25	g	611	CLA	C2A-CAA-CBA-CGA
25	n	602	CLA	C2A-CAA-CBA-CGA
29	R	2630	LHG	C18-C19-C20-C21
34	B	623	SQD	C25-C26-C27-C28
34	b	623	SQD	C25-C26-C27-C28
37	C	520	DGD	C3B-C4B-C5B-C6B
37	c	520	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
25	G	604	CLA	CBA-CGA-O2A-C1
25	g	604	CLA	CBA-CGA-O2A-C1
29	r	2630	LHG	C23-C24-C25-C26
25	A	407	CLA	O1D-CGD-O2D-CED
25	C	501	CLA	O1D-CGD-O2D-CED
25	a	407	CLA	O1D-CGD-O2D-CED
24	1	609	CHL	C8-C10-C11-C12
24	5	609	CHL	C8-C10-C11-C12
29	L	101	LHG	C27-C28-C29-C30
29	l	101	LHG	C27-C28-C29-C30
29	r	2630	LHG	C18-C19-C20-C21
24	1	609	CHL	O1A-CGA-O2A-C1
24	5	609	CHL	O1A-CGA-O2A-C1
37	C	519	DGD	O1A-C1A-O1G-C1G
24	1	605	CHL	C1A-C2A-CAA-CBA
24	1	609	CHL	C1A-C2A-CAA-CBA
24	2	605	CHL	C1A-C2A-CAA-CBA
24	2	608	CHL	C1A-C2A-CAA-CBA
24	3	605	CHL	C1A-C2A-CAA-CBA
24	3	608	CHL	C1A-C2A-CAA-CBA
24	4	607	CHL	C1A-C2A-CAA-CBA
24	N	608	CHL	C1A-C2A-CAA-CBA
24	R	608	CHL	C1A-C2A-CAA-CBA
24	5	605	CHL	C1A-C2A-CAA-CBA
24	5	609	CHL	C1A-C2A-CAA-CBA
24	6	605	CHL	C1A-C2A-CAA-CBA
24	6	608	CHL	C1A-C2A-CAA-CBA
24	7	605	CHL	C1A-C2A-CAA-CBA
24	7	608	CHL	C1A-C2A-CAA-CBA
24	8	607	CHL	C1A-C2A-CAA-CBA
24	n	608	CHL	C1A-C2A-CAA-CBA
24	r	608	CHL	C1A-C2A-CAA-CBA
25	1	604	CLA	C1A-C2A-CAA-CBA
25	1	610	CLA	C1A-C2A-CAA-CBA
25	1	611	CLA	C1A-C2A-CAA-CBA
25	2	602	CLA	C1A-C2A-CAA-CBA
25	2	610	CLA	C1A-C2A-CAA-CBA
25	3	604	CLA	C1A-C2A-CAA-CBA
25	3	610	CLA	C1A-C2A-CAA-CBA
25	4	611	CLA	C1A-C2A-CAA-CBA
25	A	406	CLA	C1A-C2A-CAA-CBA
25	A	407	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	B	612	CLA	C1A-C2A-CAA-CBA
25	C	501	CLA	C1A-C2A-CAA-CBA
25	C	506	CLA	C1A-C2A-CAA-CBA
25	G	602	CLA	C1A-C2A-CAA-CBA
25	G	614	CLA	C1A-C2A-CAA-CBA
25	N	602	CLA	C1A-C2A-CAA-CBA
25	N	604	CLA	C1A-C2A-CAA-CBA
25	N	614	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	C1A-C2A-CAA-CBA
25	Y	602	CLA	C1A-C2A-CAA-CBA
25	Y	604	CLA	C1A-C2A-CAA-CBA
25	Y	610	CLA	C1A-C2A-CAA-CBA
25	5	604	CLA	C1A-C2A-CAA-CBA
25	5	610	CLA	C1A-C2A-CAA-CBA
25	5	611	CLA	C1A-C2A-CAA-CBA
25	6	602	CLA	C1A-C2A-CAA-CBA
25	6	610	CLA	C1A-C2A-CAA-CBA
25	7	604	CLA	C1A-C2A-CAA-CBA
25	7	610	CLA	C1A-C2A-CAA-CBA
25	8	611	CLA	C1A-C2A-CAA-CBA
25	a	406	CLA	C1A-C2A-CAA-CBA
25	a	407	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	c	501	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C1A-C2A-CAA-CBA
25	g	602	CLA	C1A-C2A-CAA-CBA
25	g	614	CLA	C1A-C2A-CAA-CBA
25	n	602	CLA	C1A-C2A-CAA-CBA
25	n	604	CLA	C1A-C2A-CAA-CBA
25	n	614	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	C1A-C2A-CAA-CBA
25	y	602	CLA	C1A-C2A-CAA-CBA
25	y	604	CLA	C1A-C2A-CAA-CBA
25	y	610	CLA	C1A-C2A-CAA-CBA
24	R	606	CHL	C16-C17-C18-C20
24	n	608	CHL	C16-C17-C18-C19
24	r	606	CHL	C16-C17-C18-C20
25	3	602	CLA	C11-C12-C13-C14
25	B	602	CLA	C16-C17-C18-C19
25	N	603	CLA	C16-C17-C18-C19
25	R	603	CLA	C11-C12-C13-C15
25	7	602	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	C16-C17-C18-C19
25	n	603	CLA	C16-C17-C18-C19
25	r	603	CLA	C11-C12-C13-C15
35	C	521	LMG	C37-C38-C39-C40
35	c	521	LMG	C37-C38-C39-C40
26	1	1621	LUT	C29-C30-C31-C32
26	N	1621	LUT	C29-C30-C31-C32
26	5	1621	LUT	C29-C30-C31-C32
26	n	1621	LUT	C29-C30-C31-C32
27	R	622	XAT	C29-C30-C31-C32
27	r	622	XAT	C29-C30-C31-C32
28	G	1623	NEX	C33-C34-C35-C15
28	g	1623	NEX	C33-C34-C35-C15
25	C	505	CLA	C15-C16-C17-C18
25	c	505	CLA	C15-C16-C17-C18
29	S	2630	LHG	C27-C28-C29-C30
29	s	2630	LHG	C27-C28-C29-C30
37	H	102	DGD	CBA-CCA-CDA-CEA
24	Y	601	CHL	C15-C16-C17-C18
24	y	601	CHL	C15-C16-C17-C18
25	C	504	CLA	C10-C11-C12-C13
25	b	614	CLA	C5-C6-C7-C8
25	c	504	CLA	C10-C11-C12-C13
29	S	2630	LHG	C13-C14-C15-C16
29	s	2630	LHG	C13-C14-C15-C16
37	B	626	DGD	C6A-C7A-C8A-C9A
37	h	102	DGD	CBA-CCA-CDA-CEA
25	1	602	CLA	O1D-CGD-O2D-CED
25	5	602	CLA	O1D-CGD-O2D-CED
29	G	2630	LHG	C13-C14-C15-C16
29	g	2630	LHG	C13-C14-C15-C16
37	b	626	DGD	C6A-C7A-C8A-C9A
35	A	413	LMG	O6-C5-C6-O5
35	a	413	LMG	O6-C5-C6-O5
25	B	614	CLA	C5-C6-C7-C8
24	R	607	CHL	C6-C7-C8-C9
24	r	607	CHL	C6-C7-C8-C9
25	R	613	CLA	C11-C12-C13-C15
25	r	613	CLA	C11-C12-C13-C15
29	L	101	LHG	C34-C35-C36-C37
29	N	2630	LHG	C13-C14-C15-C16
29	l	101	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	n	2630	LHG	C13-C14-C15-C16
35	C	521	LMG	C36-C37-C38-C39
35	c	521	LMG	C36-C37-C38-C39
25	D	402	CLA	C13-C15-C16-C17
25	d	402	CLA	C13-C15-C16-C17
25	1	604	CLA	CBA-CGA-O2A-C1
25	R	613	CLA	CBA-CGA-O2A-C1
25	5	604	CLA	CBA-CGA-O2A-C1
25	r	613	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	C2-C3-C5-C6
29	S	2630	LHG	C9-C10-C11-C12
29	S	2630	LHG	C29-C30-C31-C32
29	s	2630	LHG	C9-C10-C11-C12
29	s	2630	LHG	C29-C30-C31-C32
37	C	520	DGD	C6B-C7B-C8B-C9B
37	c	520	DGD	C6B-C7B-C8B-C9B
24	2	609	CHL	O1A-CGA-O2A-C1
24	G	606	CHL	O1A-CGA-O2A-C1
24	R	607	CHL	O1A-CGA-O2A-C1
24	6	609	CHL	O1A-CGA-O2A-C1
24	g	606	CHL	O1A-CGA-O2A-C1
24	r	607	CHL	O1A-CGA-O2A-C1
25	B	605	CLA	O1A-CGA-O2A-C1
25	B	606	CLA	O1A-CGA-O2A-C1
25	B	608	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	O1A-CGA-O2A-C1
25	b	606	CLA	O1A-CGA-O2A-C1
25	b	608	CLA	O1A-CGA-O2A-C1
34	B	621	SQD	O10-C23-O48-C46
34	b	621	SQD	O10-C23-O48-C46
29	1	2630	LHG	C26-C27-C28-C29
29	C	2630	LHG	C27-C28-C29-C30
29	D	409	LHG	C32-C33-C34-C35
29	5	2630	LHG	C26-C27-C28-C29
29	c	2630	LHG	C27-C28-C29-C30
29	d	409	LHG	C32-C33-C34-C35
25	6	610	CLA	O1D-CGD-O2D-CED
29	2	2630	LHG	C4-C5-C6-O8
29	3	2630	LHG	C4-C5-C6-O8
29	3	2630	LHG	C16-C17-C18-C19
29	B	2630	LHG	C13-C14-C15-C16
29	C	522	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
29	C	523	LHG	C13-C14-C15-C16
29	Y	2630	LHG	C4-C5-C6-O8
29	Y	2630	LHG	C18-C19-C20-C21
29	6	2630	LHG	C4-C5-C6-O8
29	7	2630	LHG	C4-C5-C6-O8
29	7	2630	LHG	C16-C17-C18-C19
29	b	2630	LHG	C13-C14-C15-C16
29	c	522	LHG	C4-C5-C6-O8
29	c	523	LHG	C13-C14-C15-C16
29	y	2630	LHG	C4-C5-C6-O8
29	y	2630	LHG	C18-C19-C20-C21
34	A	412	SQD	O6-C44-C45-C46
34	A	418	SQD	C44-C45-C46-O48
34	B	623	SQD	C44-C45-C46-O48
34	a	412	SQD	O6-C44-C45-C46
34	a	418	SQD	C44-C45-C46-O48
34	b	623	SQD	C44-C45-C46-O48
35	B	2633	LMG	C7-C8-C9-O8
35	D	411	LMG	O1-C7-C8-C9
35	Z	101	LMG	O1-C7-C8-C9
35	b	2633	LMG	C7-C8-C9-O8
35	d	411	LMG	O1-C7-C8-C9
35	z	101	LMG	O1-C7-C8-C9
37	C	519	DGD	O1G-C1G-C2G-C3G
37	c	519	DGD	C2A-C3A-C4A-C5A
37	c	519	DGD	O1G-C1G-C2G-C3G
24	R	606	CHL	C13-C15-C16-C17
24	Y	607	CHL	C5-C6-C7-C8
24	r	606	CHL	C13-C15-C16-C17
24	y	607	CHL	C5-C6-C7-C8
29	1	2630	LHG	C27-C28-C29-C30
29	Y	2630	LHG	C34-C35-C36-C37
29	5	2630	LHG	C27-C28-C29-C30
29	y	2630	LHG	C34-C35-C36-C37
35	A	413	LMG	C19-C20-C21-C22
35	a	413	LMG	C19-C20-C21-C22
37	C	519	DGD	C2A-C3A-C4A-C5A
25	C	513	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
35	Z	101	LMG	C8-C7-O1-C1
35	z	101	LMG	C8-C7-O1-C1
25	2	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	C	2630	LHG	C28-C29-C30-C31
24	G	607	CHL	C10-C11-C12-C13
24	g	607	CHL	C10-C11-C12-C13
25	S	602	CLA	C14-C13-C15-C16
25	s	602	CLA	C14-C13-C15-C16
29	3	2630	LHG	C35-C36-C37-C38
29	B	2630	LHG	C19-C20-C21-C22
29	b	2630	LHG	C19-C20-C21-C22
29	c	2630	LHG	C28-C29-C30-C31
34	B	623	SQD	C27-C28-C29-C30
34	b	623	SQD	C27-C28-C29-C30
35	B	622	LMG	C28-C29-C30-C31
35	b	622	LMG	C28-C29-C30-C31
29	C	522	LHG	C33-C34-C35-C36
29	7	2630	LHG	C35-C36-C37-C38
35	b	622	LMG	C30-C31-C32-C33
25	G	611	CLA	C5-C6-C7-C8
25	g	611	CLA	C5-C6-C7-C8
29	c	522	LHG	C33-C34-C35-C36
35	B	622	LMG	C30-C31-C32-C33
29	2	2630	LHG	O1-C1-C2-O2
29	3	2630	LHG	O1-C1-C2-O2
29	S	2630	LHG	O1-C1-C2-O2
29	6	2630	LHG	O1-C1-C2-O2
29	7	2630	LHG	O1-C1-C2-O2
29	s	2630	LHG	O1-C1-C2-O2
29	D	408	LHG	C16-C17-C18-C19
29	G	2630	LHG	C12-C13-C14-C15
29	d	408	LHG	C16-C17-C18-C19
29	g	2630	LHG	C12-C13-C14-C15
37	C	518	DGD	O6E-C5E-C6E-O5E
37	c	518	DGD	O6E-C5E-C6E-O5E
37	B	626	DGD	CDB-CEB-CFB-CGB
37	C	518	DGD	CAB-CBB-CCB-CDB
37	b	626	DGD	CDB-CEB-CFB-CGB
37	c	518	DGD	CAB-CBB-CCB-CDB
24	Y	608	CHL	C13-C15-C16-C17
24	y	608	CHL	C13-C15-C16-C17
25	C	510	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
36	D	405	PL9	C45-C44-C46-C47
36	d	405	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
34	B	623	SQD	C11-C10-C9-C8
34	b	623	SQD	C11-C10-C9-C8
29	C	522	LHG	C24-C25-C26-C27
29	c	522	LHG	C24-C25-C26-C27
37	C	520	DGD	C3A-C4A-C5A-C6A
24	G	607	CHL	C15-C16-C17-C18
24	Y	608	CHL	C8-C10-C11-C12
24	g	607	CHL	C15-C16-C17-C18
24	y	608	CHL	C8-C10-C11-C12
25	G	612	CLA	C8-C10-C11-C12
29	D	408	LHG	C11-C12-C13-C14
29	G	2630	LHG	C29-C30-C31-C32
29	d	408	LHG	C11-C12-C13-C14
29	g	2630	LHG	C17-C18-C19-C20
29	g	2630	LHG	C29-C30-C31-C32
37	c	520	DGD	C3A-C4A-C5A-C6A
25	R	613	CLA	O1D-CGD-O2D-CED
25	r	613	CLA	O1D-CGD-O2D-CED
35	B	2633	LMG	O6-C5-C6-O5
35	b	2633	LMG	O6-C5-C6-O5
25	A	405	CLA	C2A-CAA-CBA-CGA
25	a	405	CLA	C2A-CAA-CBA-CGA
25	D	402	CLA	C8-C10-C11-C12
25	d	402	CLA	C8-C10-C11-C12
25	g	612	CLA	C8-C10-C11-C12
29	G	2630	LHG	C17-C18-C19-C20
35	D	411	LMG	C11-C12-C13-C14
35	d	411	LMG	C11-C12-C13-C14
29	L	101	LHG	C33-C34-C35-C36
29	l	101	LHG	C33-C34-C35-C36
34	A	418	SQD	C18-C19-C20-C21
34	a	418	SQD	C18-C19-C20-C21
25	3	602	CLA	O1D-CGD-O2D-CED
25	7	602	CLA	O1D-CGD-O2D-CED
29	D	409	LHG	C28-C29-C30-C31
29	d	409	LHG	C28-C29-C30-C31
25	N	604	CLA	CBA-CGA-O2A-C1
25	n	604	CLA	CBA-CGA-O2A-C1
29	D	410	LHG	O6-C4-C5-O7
29	d	410	LHG	O6-C4-C5-O7
35	Z	101	LMG	C15-C16-C17-C18
35	z	101	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	2	607	CHL	C5-C6-C7-C8
24	6	607	CHL	C5-C6-C7-C8
29	c	522	LHG	O2-C2-C3-O3
35	C	521	LMG	C4-C5-C6-O5
35	c	521	LMG	C4-C5-C6-O5
35	B	622	LMG	C16-C17-C18-C19
35	b	622	LMG	C16-C17-C18-C19
35	d	411	LMG	C16-C17-C18-C19
24	G	608	CHL	C15-C16-C17-C18
24	g	608	CHL	C15-C16-C17-C18
24	2	607	CHL	C2C-C3C-CAC-CBC
24	6	607	CHL	C2C-C3C-CAC-CBC
35	D	411	LMG	C16-C17-C18-C19
29	Y	2630	LHG	O7-C5-C6-O8
29	y	2630	LHG	O7-C5-C6-O8
24	N	601	CHL	C10-C11-C12-C13
24	n	601	CHL	C10-C11-C12-C13
29	Y	2630	LHG	C14-C15-C16-C17
29	y	2630	LHG	C14-C15-C16-C17
24	G	608	CHL	C12-C13-C15-C16
24	g	608	CHL	C12-C13-C15-C16
25	3	602	CLA	C6-C7-C8-C10
25	B	616	CLA	C12-C13-C15-C16
25	C	502	CLA	C12-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C7
25	C	509	CLA	C6-C7-C8-C10
25	C	510	CLA	C2-C3-C5-C6
25	C	510	CLA	C12-C13-C15-C16
25	D	403	CLA	C11-C12-C13-C15
25	G	603	CLA	C11-C10-C8-C7
25	G	610	CLA	C11-C12-C13-C15
25	G	610	CLA	C12-C13-C15-C16
25	N	602	CLA	C6-C7-C8-C10
25	N	612	CLA	C6-C7-C8-C10
25	R	610	CLA	C11-C12-C13-C15
25	Y	613	CLA	C11-C12-C13-C15
25	7	602	CLA	C6-C7-C8-C10
25	b	616	CLA	C12-C13-C15-C16
25	c	502	CLA	C12-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C7
25	c	509	CLA	C6-C7-C8-C10
25	c	510	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c	510	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
25	g	603	CLA	C11-C10-C8-C7
25	g	610	CLA	C11-C12-C13-C15
25	g	610	CLA	C12-C13-C15-C16
25	n	602	CLA	C6-C7-C8-C10
25	n	612	CLA	C6-C7-C8-C10
25	r	610	CLA	C11-C12-C13-C15
25	y	613	CLA	C11-C12-C13-C15
29	3	2630	LHG	O8-C23-C24-C25
29	7	2630	LHG	O8-C23-C24-C25
25	G	604	CLA	O1A-CGA-O2A-C1
24	3	601	CHL	C14-C13-C15-C16
24	G	607	CHL	C14-C13-C15-C16
24	7	601	CHL	C14-C13-C15-C16
24	g	607	CHL	C14-C13-C15-C16
25	3	602	CLA	C6-C7-C8-C9
25	B	603	CLA	C6-C7-C8-C9
25	B	612	CLA	C14-C13-C15-C16
25	B	613	CLA	C6-C7-C8-C9
25	B	616	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	510	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
25	C	512	CLA	C14-C13-C15-C16
25	G	603	CLA	C11-C10-C8-C9
25	G	612	CLA	C11-C10-C8-C9
25	G	613	CLA	C11-C12-C13-C14
25	R	610	CLA	C11-C10-C8-C9
25	R	610	CLA	C14-C13-C15-C16
25	Y	602	CLA	C6-C7-C8-C9
25	Y	611	CLA	C11-C10-C8-C9
25	Y	612	CLA	C11-C10-C8-C9
25	Y	613	CLA	C11-C12-C13-C14
25	Y	613	CLA	C14-C13-C15-C16
25	7	602	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	612	CLA	C14-C13-C15-C16
25	b	613	CLA	C6-C7-C8-C9
25	b	616	CLA	C14-C13-C15-C16
25	c	510	CLA	C14-C13-C15-C16
25	c	511	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	512	CLA	C14-C13-C15-C16
25	g	603	CLA	C11-C10-C8-C9
25	g	612	CLA	C11-C10-C8-C9
25	g	613	CLA	C11-C12-C13-C14
25	r	610	CLA	C11-C10-C8-C9
25	r	610	CLA	C14-C13-C15-C16
25	y	602	CLA	C6-C7-C8-C9
25	y	611	CLA	C11-C10-C8-C9
25	y	612	CLA	C11-C10-C8-C9
25	y	613	CLA	C11-C12-C13-C14
25	y	613	CLA	C14-C13-C15-C16
28	2	1623	NEX	C9-C10-C11-C12
28	6	1623	NEX	C9-C10-C11-C12
29	y	2630	LHG	C25-C26-C27-C28
37	H	102	DGD	C6A-C7A-C8A-C9A
37	h	102	DGD	C6A-C7A-C8A-C9A
25	1	603	CLA	CBA-CGA-O2A-C1
25	B	615	CLA	CBA-CGA-O2A-C1
25	5	603	CLA	CBA-CGA-O2A-C1
25	b	615	CLA	CBA-CGA-O2A-C1
24	3	609	CHL	O1D-CGD-O2D-CED
24	7	609	CHL	O1D-CGD-O2D-CED
25	R	602	CLA	C2A-CAA-CBA-CGA
25	r	602	CLA	C2A-CAA-CBA-CGA
29	Y	2630	LHG	C25-C26-C27-C28
25	1	604	CLA	O1A-CGA-O2A-C1
25	g	604	CLA	O1A-CGA-O2A-C1
37	C	518	DGD	C4D-C5D-C6D-O5D
37	c	518	DGD	C4D-C5D-C6D-O5D
30	B	619	BCR	C7-C8-C9-C10
30	b	619	BCR	C7-C8-C9-C10
29	N	2630	LHG	C34-C35-C36-C37
29	n	2630	LHG	C34-C35-C36-C37
34	A	418	SQD	C17-C18-C19-C20
35	B	622	LMG	C11-C10-O7-C8
35	b	622	LMG	C11-C10-O7-C8
29	1	2630	LHG	C11-C12-C13-C14
29	5	2630	LHG	C11-C12-C13-C14
34	a	418	SQD	C17-C18-C19-C20
25	5	604	CLA	O1A-CGA-O2A-C1
25	C	503	CLA	CBA-CGA-O2A-C1
25	G	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	c	503	CLA	CBA-CGA-O2A-C1
25	g	613	CLA	CBA-CGA-O2A-C1
29	B	2631	LHG	C31-C32-C33-C34
29	D	409	LHG	C15-C16-C17-C18
29	b	2631	LHG	C31-C32-C33-C34
29	d	409	LHG	C15-C16-C17-C18
37	C	518	DGD	O6D-C5D-C6D-O5D
37	c	518	DGD	O6D-C5D-C6D-O5D
24	R	608	CHL	C5-C6-C7-C8
24	r	608	CHL	C5-C6-C7-C8
25	3	602	CLA	C8-C10-C11-C12
25	N	603	CLA	C15-C16-C17-C18
25	7	602	CLA	C8-C10-C11-C12
29	D	409	LHG	O6-C4-C5-C6
29	d	409	LHG	O6-C4-C5-C6
34	b	623	SQD	C13-C14-C15-C16
29	C	2630	LHG	C30-C31-C32-C33
29	c	2630	LHG	C30-C31-C32-C33
34	B	623	SQD	C13-C14-C15-C16
25	B	602	CLA	C13-C15-C16-C17
25	b	602	CLA	C13-C15-C16-C17
25	n	603	CLA	C15-C16-C17-C18
25	1	603	CLA	C4-C3-C5-C6
25	5	603	CLA	C4-C3-C5-C6
25	B	612	CLA	C2-C3-C5-C6
25	C	501	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
25	c	501	CLA	C2-C3-C5-C6
35	B	622	LMG	C40-C41-C42-C43
35	b	622	LMG	C40-C41-C42-C43
24	G	601	CHL	C15-C16-C17-C18
24	g	601	CHL	C15-C16-C17-C18
29	C	522	LHG	O2-C2-C3-O3
29	C	523	LHG	C27-C28-C29-C30
29	c	523	LHG	C27-C28-C29-C30
25	1	613	CLA	C6-C7-C8-C10
25	5	613	CLA	C6-C7-C8-C10
24	S	607	CHL	C8-C10-C11-C12
24	s	607	CHL	C8-C10-C11-C12
29	Y	2630	LHG	C11-C12-C13-C14
29	y	2630	LHG	C11-C12-C13-C14
25	3	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	C	502	CLA	CBA-CGA-O2A-C1
25	7	610	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
25	g	602	CLA	O1D-CGD-O2D-CED
24	R	608	CHL	C3A-C2A-CAA-CBA
24	Y	605	CHL	C3A-C2A-CAA-CBA
24	r	608	CHL	C3A-C2A-CAA-CBA
25	B	610	CLA	C3A-C2A-CAA-CBA
25	S	604	CLA	C3A-C2A-CAA-CBA
25	b	610	CLA	C3A-C2A-CAA-CBA
25	s	604	CLA	C3A-C2A-CAA-CBA
24	R	607	CHL	C5-C6-C7-C8
24	r	607	CHL	C5-C6-C7-C8
29	C	2630	LHG	C34-C35-C36-C37
25	G	602	CLA	O1D-CGD-O2D-CED
30	T	101	BCR	C19-C20-C21-C22
30	t	101	BCR	C19-C20-C21-C22
29	c	2630	LHG	C34-C35-C36-C37
37	c	520	DGD	C5B-C6B-C7B-C8B
25	R	603	CLA	C5-C6-C7-C8
25	r	603	CLA	C5-C6-C7-C8
29	Y	2630	LHG	C28-C29-C30-C31
29	y	2630	LHG	C28-C29-C30-C31
37	C	520	DGD	C5B-C6B-C7B-C8B
24	N	609	CHL	C16-C17-C18-C19
24	n	609	CHL	C16-C17-C18-C19
24	3	609	CHL	CBA-CGA-O2A-C1
24	7	609	CHL	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	G	612	CLA	CBA-CGA-O2A-C1
25	Y	613	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	g	612	CLA	CBA-CGA-O2A-C1
25	y	613	CLA	CBA-CGA-O2A-C1
29	Y	2630	LHG	C35-C36-C37-C38
29	B	2631	LHG	C4-C5-C6-O8
29	C	2630	LHG	C4-C5-C6-O8
29	G	2630	LHG	C4-C5-C6-O8
29	R	2630	LHG	C4-C5-C6-O8
29	S	2630	LHG	C4-C5-C6-O8
29	b	2631	LHG	C4-C5-C6-O8
29	c	2630	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
29	g	2630	LHG	C4-C5-C6-O8
29	r	2630	LHG	C4-C5-C6-O8
29	s	2630	LHG	C4-C5-C6-O8
34	B	621	SQD	C44-C45-C46-O48
34	b	621	SQD	C44-C45-C46-O48
35	A	415	LMG	C7-C8-C9-O8
35	C	521	LMG	C7-C8-C9-O8
35	a	415	LMG	C7-C8-C9-O8
35	c	521	LMG	C7-C8-C9-O8
37	C	520	DGD	O1G-C1G-C2G-C3G
37	c	520	DGD	O1G-C1G-C2G-C3G
29	y	2630	LHG	C35-C36-C37-C38
24	G	609	CHL	C10-C11-C12-C13
24	g	609	CHL	C10-C11-C12-C13
29	C	523	LHG	C30-C31-C32-C33
29	c	523	LHG	C30-C31-C32-C33
29	C	523	LHG	C16-C17-C18-C19
29	c	523	LHG	C16-C17-C18-C19
25	5	603	CLA	C2-C3-C5-C6
25	N	611	CLA	O1D-CGD-O2D-CED
25	n	611	CLA	O1D-CGD-O2D-CED
25	Y	611	CLA	C5-C6-C7-C8
25	y	611	CLA	C5-C6-C7-C8
24	1	601	CHL	C3C-C2C-CMC-OMC
24	3	606	CHL	C3C-C2C-CMC-OMC
24	4	606	CHL	C3C-C2C-CMC-OMC
24	G	606	CHL	C3C-C2C-CMC-OMC
24	Y	608	CHL	C3C-C2C-CMC-OMC
24	5	601	CHL	C3C-C2C-CMC-OMC
24	7	606	CHL	C3C-C2C-CMC-OMC
24	8	606	CHL	C3C-C2C-CMC-OMC
24	g	606	CHL	C3C-C2C-CMC-OMC
24	y	608	CHL	C3C-C2C-CMC-OMC
29	3	2630	LHG	C24-C25-C26-C27
29	7	2630	LHG	C24-C25-C26-C27
29	D	410	LHG	O1-C1-C2-O2
29	d	410	LHG	O1-C1-C2-O2
37	C	520	DGD	C4D-C5D-C6D-O5D
37	c	520	DGD	C4D-C5D-C6D-O5D
29	y	2630	LHG	C27-C28-C29-C30
25	N	604	CLA	O1A-CGA-O2A-C1
25	n	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	C16-C17-C18-C19
25	C	505	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C19
29	Y	2630	LHG	C27-C28-C29-C30
29	R	2630	LHG	O10-C23-O8-C6
29	r	2630	LHG	O10-C23-O8-C6
29	2	2630	LHG	O7-C5-C6-O8
29	G	2630	LHG	O7-C5-C6-O8
29	R	2630	LHG	O7-C5-C6-O8
29	6	2630	LHG	O7-C5-C6-O8
29	g	2630	LHG	O7-C5-C6-O8
29	r	2630	LHG	O7-C5-C6-O8
34	B	621	SQD	O6-C44-C45-O47
34	B	623	SQD	O6-C44-C45-O47
34	b	621	SQD	O6-C44-C45-O47
34	b	623	SQD	O6-C44-C45-O47
35	A	413	LMG	O1-C7-C8-O7
35	a	413	LMG	O1-C7-C8-O7
25	Y	603	CLA	C5-C6-C7-C8
24	3	601	CHL	C15-C16-C17-C18
24	7	601	CHL	C15-C16-C17-C18
29	l	101	LHG	C31-C32-C33-C34
25	B	616	CLA	C16-C17-C18-C20
25	N	602	CLA	C16-C17-C18-C19
25	b	616	CLA	C16-C17-C18-C20
25	n	602	CLA	C16-C17-C18-C19
29	L	101	LHG	C31-C32-C33-C34
35	A	413	LMG	C11-C12-C13-C14
35	a	413	LMG	C11-C12-C13-C14
24	y	609	CHL	C8-C10-C11-C12
25	y	603	CLA	C5-C6-C7-C8
36	D	405	PL9	C39-C41-C42-C43
36	d	405	PL9	C39-C41-C42-C43
29	D	410	LHG	C32-C33-C34-C35
29	N	2630	LHG	C11-C12-C13-C14
29	d	410	LHG	C32-C33-C34-C35
29	n	2630	LHG	C11-C12-C13-C14
24	G	606	CHL	C2-C1-O2A-CGA
24	R	606	CHL	C2-C1-O2A-CGA
24	Y	608	CHL	C2-C1-O2A-CGA
24	g	606	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	r	606	CHL	C2-C1-O2A-CGA
24	y	608	CHL	C2-C1-O2A-CGA
25	B	603	CLA	C2-C1-O2A-CGA
25	D	402	CLA	C2-C1-O2A-CGA
25	G	603	CLA	C2-C1-O2A-CGA
25	b	603	CLA	C2-C1-O2A-CGA
25	d	402	CLA	C2-C1-O2A-CGA
25	g	603	CLA	C2-C1-O2A-CGA
25	1	603	CLA	C2-C3-C5-C6
35	b	622	LMG	O10-C28-O8-C9
24	Y	609	CHL	C8-C10-C11-C12
25	B	611	CLA	C15-C16-C17-C18
25	b	611	CLA	C15-C16-C17-C18
24	1	607	CHL	C6-C7-C8-C9
24	5	607	CHL	C6-C7-C8-C9
25	B	602	CLA	C6-C7-C8-C9
25	B	609	CLA	C14-C13-C15-C16
25	C	502	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C12-C13-C14
25	C	507	CLA	C14-C13-C15-C16
25	G	610	CLA	C11-C12-C13-C14
25	G	611	CLA	C6-C7-C8-C9
25	N	602	CLA	C6-C7-C8-C9
25	b	602	CLA	C6-C7-C8-C9
25	b	609	CLA	C14-C13-C15-C16
25	c	502	CLA	C11-C10-C8-C9
25	c	507	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
25	g	610	CLA	C11-C12-C13-C14
25	g	611	CLA	C6-C7-C8-C9
25	n	602	CLA	C6-C7-C8-C9
29	R	2630	LHG	C15-C16-C17-C18
29	r	2630	LHG	C15-C16-C17-C18
25	1	610	CLA	C5-C6-C7-C8
25	C	505	CLA	C10-C11-C12-C13
25	C	513	CLA	C15-C16-C17-C18
25	5	610	CLA	C5-C6-C7-C8
25	c	505	CLA	C10-C11-C12-C13
25	c	513	CLA	C15-C16-C17-C18
35	B	622	LMG	O10-C28-O8-C9
29	B	2630	LHG	C28-C29-C30-C31
29	D	410	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	b	2630	LHG	C28-C29-C30-C31
29	d	410	LHG	C28-C29-C30-C31
35	D	411	LMG	C17-C18-C19-C20
35	d	411	LMG	C17-C18-C19-C20
25	2	602	CLA	C2A-CAA-CBA-CGA
25	G	603	CLA	C2A-CAA-CBA-CGA
25	S	614	CLA	C2A-CAA-CBA-CGA
25	6	602	CLA	C2A-CAA-CBA-CGA
25	g	603	CLA	C2A-CAA-CBA-CGA
25	s	614	CLA	C2A-CAA-CBA-CGA
24	N	607	CHL	C16-C17-C18-C20
24	n	607	CHL	C16-C17-C18-C20
25	N	610	CLA	C16-C17-C18-C19
25	n	610	CLA	C16-C17-C18-C19
25	C	506	CLA	C3-C5-C6-C7
25	c	506	CLA	C3-C5-C6-C7
26	3	1620	LUT	C5-C6-C7-C8
26	3	1621	LUT	C1-C6-C7-C8
26	3	1621	LUT	C5-C6-C7-C8
26	G	1620	LUT	C5-C6-C7-C8
26	S	1620	LUT	C5-C6-C7-C8
26	S	1621	LUT	C1-C6-C7-C8
26	S	1621	LUT	C5-C6-C7-C8
26	7	1620	LUT	C5-C6-C7-C8
26	7	1621	LUT	C1-C6-C7-C8
26	7	1621	LUT	C5-C6-C7-C8
26	g	1620	LUT	C5-C6-C7-C8
26	s	1620	LUT	C5-C6-C7-C8
26	s	1621	LUT	C1-C6-C7-C8
26	s	1621	LUT	C5-C6-C7-C8
30	C	516	BCR	C1-C6-C7-C8
30	C	516	BCR	C5-C6-C7-C8
30	T	101	BCR	C23-C24-C25-C30
30	c	516	BCR	C1-C6-C7-C8
30	c	516	BCR	C5-C6-C7-C8
30	t	101	BCR	C23-C24-C25-C30
25	N	613	CLA	C8-C10-C11-C12
25	a	405	CLA	C5-C6-C7-C8
25	n	613	CLA	C8-C10-C11-C12
26	4	620	LUT	C27-C28-C29-C30
26	8	620	LUT	C27-C28-C29-C30
27	Y	1622	XAT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	y	1622	XAT	C11-C12-C13-C14
30	B	620	BCR	C21-C22-C23-C24
30	b	620	BCR	C21-C22-C23-C24
24	G	609	CHL	C8-C10-C11-C12
24	R	606	CHL	C5-C6-C7-C8
24	r	606	CHL	C5-C6-C7-C8
25	A	405	CLA	C5-C6-C7-C8
29	g	2630	LHG	C24-C25-C26-C27
37	C	520	DGD	O6D-C5D-C6D-O5D
37	c	520	DGD	O6D-C5D-C6D-O5D
24	1	607	CHL	C4C-C3C-CAC-CBC
24	5	607	CHL	C4C-C3C-CAC-CBC
29	G	2630	LHG	C24-C25-C26-C27
29	S	2630	LHG	C35-C36-C37-C38
29	s	2630	LHG	C35-C36-C37-C38
24	R	607	CHL	C6-C7-C8-C10
24	r	607	CHL	C6-C7-C8-C10
25	B	604	CLA	C16-C17-C18-C19
25	N	603	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C19
25	n	603	CLA	C16-C17-C18-C20
24	N	601	CHL	C3-C5-C6-C7
24	n	601	CHL	C3-C5-C6-C7
25	C	502	CLA	C3-C5-C6-C7
25	c	502	CLA	C3-C5-C6-C7
24	g	609	CHL	C8-C10-C11-C12
25	B	612	CLA	C8-C10-C11-C12
25	y	610	CLA	C10-C11-C12-C13
25	1	603	CLA	O1A-CGA-O2A-C1
25	B	615	CLA	O1A-CGA-O2A-C1
25	5	603	CLA	O1A-CGA-O2A-C1
25	b	615	CLA	O1A-CGA-O2A-C1
35	d	411	LMG	C33-C34-C35-C36
37	h	102	DGD	CCB-CDB-CEB-CFB
25	B	614	CLA	C15-C16-C17-C18
25	Y	610	CLA	C10-C11-C12-C13
25	b	612	CLA	C8-C10-C11-C12
25	b	614	CLA	C15-C16-C17-C18
29	C	523	LHG	O6-C4-C5-C6
29	c	523	LHG	O6-C4-C5-C6
29	C	523	LHG	O2-C2-C3-O3
29	c	523	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
35	D	411	LMG	C33-C34-C35-C36
37	C	519	DGD	C8B-C9B-CAB-CBB
37	H	102	DGD	CCB-CDB-CEB-CFB
37	c	519	DGD	C8B-C9B-CAB-CBB
24	1	607	CHL	C6-C7-C8-C10
24	2	607	CHL	C6-C7-C8-C10
24	3	601	CHL	C11-C10-C8-C7
24	G	607	CHL	C12-C13-C15-C16
24	N	601	CHL	C11-C10-C8-C7
24	N	607	CHL	C12-C13-C15-C16
24	R	606	CHL	C12-C13-C15-C16
24	Y	607	CHL	C12-C13-C15-C16
24	Y	609	CHL	C12-C13-C15-C16
24	5	607	CHL	C6-C7-C8-C10
24	6	607	CHL	C6-C7-C8-C10
24	7	601	CHL	C11-C10-C8-C7
24	g	607	CHL	C12-C13-C15-C16
24	n	601	CHL	C11-C10-C8-C7
24	n	607	CHL	C12-C13-C15-C16
24	r	606	CHL	C12-C13-C15-C16
24	y	607	CHL	C12-C13-C15-C16
24	y	609	CHL	C12-C13-C15-C16
25	1	602	CLA	C6-C7-C8-C10
25	B	609	CLA	C12-C13-C15-C16
25	B	613	CLA	C11-C10-C8-C7
25	B	616	CLA	C11-C10-C8-C7
25	B	616	CLA	C11-C12-C13-C15
25	C	502	CLA	C6-C7-C8-C10
25	C	502	CLA	C11-C10-C8-C7
25	C	506	CLA	C11-C12-C13-C15
25	C	507	CLA	C6-C7-C8-C10
25	C	507	CLA	C11-C10-C8-C7
25	C	507	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C10-C8-C7
25	C	512	CLA	C12-C13-C15-C16
25	G	612	CLA	C11-C10-C8-C7
25	G	613	CLA	C11-C12-C13-C15
25	N	603	CLA	C12-C13-C15-C16
25	R	610	CLA	C11-C10-C8-C7
25	S	611	CLA	C6-C7-C8-C10
25	Y	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	Y	603	CLA	C12-C13-C15-C16
25	Y	613	CLA	C12-C13-C15-C16
25	5	602	CLA	C6-C7-C8-C10
25	b	609	CLA	C12-C13-C15-C16
25	b	613	CLA	C11-C10-C8-C7
25	b	616	CLA	C11-C10-C8-C7
25	b	616	CLA	C11-C12-C13-C15
25	c	502	CLA	C6-C7-C8-C10
25	c	502	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	507	CLA	C6-C7-C8-C10
25	c	507	CLA	C11-C10-C8-C7
25	c	507	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C7
25	c	510	CLA	C11-C10-C8-C7
25	c	512	CLA	C12-C13-C15-C16
25	g	612	CLA	C11-C10-C8-C7
25	g	613	CLA	C11-C12-C13-C15
25	n	603	CLA	C12-C13-C15-C16
25	r	610	CLA	C11-C10-C8-C7
25	s	611	CLA	C6-C7-C8-C10
25	y	602	CLA	C6-C7-C8-C10
25	y	603	CLA	C12-C13-C15-C16
25	y	613	CLA	C12-C13-C15-C16
29	1	2630	LHG	C15-C16-C17-C18
29	C	2630	LHG	C13-C14-C15-C16
29	5	2630	LHG	C15-C16-C17-C18
37	H	102	DGD	C8A-C9A-CAA-CBA
37	h	102	DGD	C8A-C9A-CAA-CBA
25	b	613	CLA	C15-C16-C17-C18
25	c	501	CLA	C15-C16-C17-C18
26	G	1621	LUT	C29-C30-C31-C32
26	Y	1621	LUT	C29-C30-C31-C32
26	g	1621	LUT	C29-C30-C31-C32
26	y	1621	LUT	C29-C30-C31-C32
30	H	101	BCR	C9-C10-C11-C12
30	h	101	BCR	C9-C10-C11-C12
37	h	102	DGD	O6D-C5D-C6D-O5D
29	c	2630	LHG	C13-C14-C15-C16
25	G	610	CLA	C15-C16-C17-C18
25	r	610	CLA	O1D-CGD-O2D-CED
24	N	607	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	n	607	CHL	C10-C11-C12-C13
25	B	613	CLA	C15-C16-C17-C18
25	C	501	CLA	C15-C16-C17-C18
25	C	503	CLA	O1A-CGA-O2A-C1
25	c	503	CLA	O1A-CGA-O2A-C1
25	g	610	CLA	C15-C16-C17-C18
29	C	2630	LHG	C7-C8-C9-C10
29	c	2630	LHG	C7-C8-C9-C10
25	1	613	CLA	C6-C7-C8-C9
25	5	613	CLA	C6-C7-C8-C9
24	n	609	CHL	C8-C10-C11-C12
25	c	511	CLA	C8-C10-C11-C12
35	A	415	LMG	C29-C30-C31-C32
25	S	602	CLA	C12-C13-C15-C16
25	s	602	CLA	C12-C13-C15-C16
35	a	415	LMG	C29-C30-C31-C32
24	N	609	CHL	C8-C10-C11-C12
25	C	511	CLA	C8-C10-C11-C12
37	H	102	DGD	O6D-C5D-C6D-O5D
35	C	521	LMG	C40-C41-C42-C43
24	2	608	CHL	CAD-CBD-CGD-O2D
24	R	606	CHL	CAD-CBD-CGD-O2D
24	S	606	CHL	CAD-CBD-CGD-O2D
24	6	608	CHL	CAD-CBD-CGD-O2D
24	r	606	CHL	CAD-CBD-CGD-O2D
24	s	606	CHL	CAD-CBD-CGD-O2D
25	1	602	CLA	CAD-CBD-CGD-O2D
25	2	602	CLA	CAD-CBD-CGD-O2D
25	2	604	CLA	CAD-CBD-CGD-O2D
25	4	611	CLA	CAD-CBD-CGD-O2D
25	B	602	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
25	C	508	CLA	CAD-CBD-CGD-O2D
25	D	403	CLA	CAD-CBD-CGD-O2D
25	G	614	CLA	CAD-CBD-CGD-O2D
25	N	602	CLA	CAD-CBD-CGD-O2D
25	N	610	CLA	CAD-CBD-CGD-O2D
25	N	614	CLA	CAD-CBD-CGD-O2D
25	R	603	CLA	CAD-CBD-CGD-O2D
25	S	614	CLA	CAD-CBD-CGD-O2D
25	Y	603	CLA	CAD-CBD-CGD-O2D
25	5	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	6	602	CLA	CAD-CBD-CGD-O2D
25	6	604	CLA	CAD-CBD-CGD-O2D
25	8	611	CLA	CAD-CBD-CGD-O2D
25	b	602	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	c	508	CLA	CAD-CBD-CGD-O2D
25	d	403	CLA	CAD-CBD-CGD-O2D
25	g	614	CLA	CAD-CBD-CGD-O2D
25	n	602	CLA	CAD-CBD-CGD-O2D
25	n	610	CLA	CAD-CBD-CGD-O2D
25	n	614	CLA	CAD-CBD-CGD-O2D
25	r	603	CLA	CAD-CBD-CGD-O2D
25	s	614	CLA	CAD-CBD-CGD-O2D
25	y	603	CLA	CAD-CBD-CGD-O2D
35	c	521	LMG	C40-C41-C42-C43
24	G	607	CHL	C13-C15-C16-C17
25	R	610	CLA	O1D-CGD-O2D-CED
29	D	410	LHG	C16-C17-C18-C19
29	D	410	LHG	C29-C30-C31-C32
29	d	410	LHG	C16-C17-C18-C19
29	d	410	LHG	C29-C30-C31-C32
35	A	413	LMG	C29-C28-O8-C9
35	a	413	LMG	C29-C28-O8-C9
25	4	603	CLA	O1D-CGD-O2D-CED
25	8	603	CLA	O1D-CGD-O2D-CED
25	N	612	CLA	C4-C3-C5-C6
25	n	612	CLA	C4-C3-C5-C6
24	r	608	CHL	C11-C12-C13-C15
25	N	610	CLA	C16-C17-C18-C20
25	Y	610	CLA	C11-C12-C13-C15
25	n	610	CLA	C16-C17-C18-C20
25	y	610	CLA	C11-C12-C13-C15
24	g	607	CHL	C13-C15-C16-C17
25	D	403	CLA	C10-C11-C12-C13
25	d	403	CLA	C10-C11-C12-C13
25	n	612	CLA	C2-C3-C5-C6
29	4	2630	LHG	C4-C5-C6-O8
29	B	2630	LHG	C4-C5-C6-O8
29	8	2630	LHG	C4-C5-C6-O8
29	b	2630	LHG	C4-C5-C6-O8
34	B	621	SQD	O6-C44-C45-C46
34	b	621	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
25	G	613	CLA	O1A-CGA-O2A-C1
25	R	613	CLA	O1A-CGA-O2A-C1
25	g	613	CLA	O1A-CGA-O2A-C1
25	r	613	CLA	O1A-CGA-O2A-C1
29	Y	2630	LHG	O10-C23-O8-C6
29	y	2630	LHG	O10-C23-O8-C6
29	D	409	LHG	O6-C4-C5-O7
29	d	409	LHG	O6-C4-C5-O7
24	N	607	CHL	C8-C10-C11-C12
24	n	607	CHL	C8-C10-C11-C12
25	R	612	CLA	O2A-C1-C2-C3
25	r	612	CLA	O2A-C1-C2-C3
29	N	2630	LHG	C14-C15-C16-C17
25	G	603	CLA	C5-C6-C7-C8
25	g	603	CLA	C5-C6-C7-C8
29	n	2630	LHG	C14-C15-C16-C17
24	R	608	CHL	C11-C12-C13-C15
29	L	101	LHG	C9-C10-C11-C12
29	l	101	LHG	C9-C10-C11-C12
24	s	601	CHL	CHA-CBD-CGD-O1D
25	1	603	CLA	CHA-CBD-CGD-O1D
25	1	612	CLA	CHA-CBD-CGD-O1D
25	1	612	CLA	CHA-CBD-CGD-O2D
25	2	612	CLA	CHA-CBD-CGD-O1D
25	3	604	CLA	CHA-CBD-CGD-O1D
25	3	604	CLA	CHA-CBD-CGD-O2D
25	3	611	CLA	CHA-CBD-CGD-O1D
25	3	611	CLA	CHA-CBD-CGD-O2D
25	3	612	CLA	CHA-CBD-CGD-O2D
25	B	605	CLA	CHA-CBD-CGD-O1D
25	B	605	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	613	CLA	CHA-CBD-CGD-O1D
25	B	615	CLA	CHA-CBD-CGD-O1D
25	B	615	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O2D
25	C	505	CLA	CHA-CBD-CGD-O1D
25	C	505	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	Y	603	CLA	CHA-CBD-CGD-O1D
25	5	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	5	612	CLA	CHA-CBD-CGD-O1D
25	5	612	CLA	CHA-CBD-CGD-O2D
25	6	612	CLA	CHA-CBD-CGD-O1D
25	7	604	CLA	CHA-CBD-CGD-O1D
25	7	604	CLA	CHA-CBD-CGD-O2D
25	7	611	CLA	CHA-CBD-CGD-O1D
25	7	611	CLA	CHA-CBD-CGD-O2D
25	7	612	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CHA-CBD-CGD-O1D
25	b	605	CLA	CHA-CBD-CGD-O2D
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	613	CLA	CHA-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	505	CLA	CHA-CBD-CGD-O1D
25	c	505	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	y	603	CLA	CHA-CBD-CGD-O1D
24	3	609	CHL	O1A-CGA-O2A-C1
24	7	609	CHL	O1A-CGA-O2A-C1
25	3	610	CLA	O1A-CGA-O2A-C1
25	C	512	CLA	O1A-CGA-O2A-C1
25	7	610	CLA	O1A-CGA-O2A-C1
25	c	502	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
25	G	614	CLA	O2A-C1-C2-C3
25	g	614	CLA	O2A-C1-C2-C3
36	A	414	PL9	C2-C3-C7-C8
36	a	414	PL9	C2-C3-C7-C8
35	z	101	LMG	C11-C12-C13-C14
29	C	522	LHG	O7-C5-C6-O8
29	c	522	LHG	O7-C5-C6-O8
34	A	418	SQD	O47-C45-C46-O48
34	a	418	SQD	O47-C45-C46-O48
35	B	2633	LMG	O7-C8-C9-O8
35	C	521	LMG	O7-C8-C9-O8
35	D	411	LMG	O1-C7-C8-O7
35	b	2633	LMG	O7-C8-C9-O8
35	c	521	LMG	O7-C8-C9-O8
35	d	411	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
35	Z	101	LMG	C11-C12-C13-C14
25	C	502	CLA	O1A-CGA-O2A-C1
25	Y	613	CLA	O1A-CGA-O2A-C1
25	y	613	CLA	O1A-CGA-O2A-C1
29	c	522	LHG	O10-C23-O8-C6
29	B	2631	LHG	C12-C13-C14-C15
29	b	2631	LHG	C12-C13-C14-C15
34	A	418	SQD	C28-C29-C30-C31
24	R	608	CHL	C11-C12-C13-C14
24	r	608	CHL	C11-C12-C13-C14
29	d	409	LHG	C25-C26-C27-C28
34	a	418	SQD	C28-C29-C30-C31
25	Y	612	CLA	C4-C3-C5-C6
25	y	612	CLA	C4-C3-C5-C6
29	D	409	LHG	C25-C26-C27-C28
25	G	612	CLA	O1A-CGA-O2A-C1
25	g	612	CLA	O1A-CGA-O2A-C1
29	C	522	LHG	O10-C23-O8-C6
25	N	612	CLA	C2-C3-C5-C6
25	Y	612	CLA	C2-C3-C5-C6
25	y	612	CLA	C2-C3-C5-C6
24	2	607	CHL	C6-C7-C8-C9
24	R	606	CHL	C14-C13-C15-C16
24	6	607	CHL	C6-C7-C8-C9
24	r	606	CHL	C14-C13-C15-C16
25	B	613	CLA	C11-C10-C8-C9
25	B	616	CLA	C11-C12-C13-C14
25	Y	612	CLA	C6-C7-C8-C9
25	b	613	CLA	C11-C10-C8-C9
25	b	616	CLA	C11-C12-C13-C14
25	y	612	CLA	C6-C7-C8-C9
29	G	2630	LHG	C9-C10-C11-C12
29	g	2630	LHG	C9-C10-C11-C12
34	B	621	SQD	C4-C5-C6-S
34	B	623	SQD	C5-C6-S-O8
34	b	621	SQD	C4-C5-C6-S
34	b	623	SQD	C5-C6-S-O8
25	B	606	CLA	C2A-CAA-CBA-CGA
25	G	613	CLA	C2A-CAA-CBA-CGA
25	N	603	CLA	C2A-CAA-CBA-CGA
25	Y	613	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	g	613	CLA	C2A-CAA-CBA-CGA
25	n	603	CLA	C2A-CAA-CBA-CGA
25	y	613	CLA	C2A-CAA-CBA-CGA
37	H	102	DGD	C3A-C4A-C5A-C6A
37	h	102	DGD	C3A-C4A-C5A-C6A
26	4	620	LUT	C27-C28-C29-C39
26	8	620	LUT	C27-C28-C29-C39
30	4	623	BCR	C36-C18-C19-C20
30	C	515	BCR	C36-C18-C19-C20
30	8	623	BCR	C36-C18-C19-C20
30	c	515	BCR	C36-C18-C19-C20
28	G	1623	NEX	C31-C32-C33-C34
28	g	1623	NEX	C31-C32-C33-C34
24	1	607	CHL	C1A-C2A-CAA-CBA
24	N	609	CHL	C1A-C2A-CAA-CBA
24	5	607	CHL	C1A-C2A-CAA-CBA
24	n	609	CHL	C1A-C2A-CAA-CBA
25	1	614	CLA	C1A-C2A-CAA-CBA
25	3	602	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
25	Y	614	CLA	C1A-C2A-CAA-CBA
25	5	614	CLA	C1A-C2A-CAA-CBA
25	7	602	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	y	614	CLA	C1A-C2A-CAA-CBA
29	g	2630	LHG	O9-C7-O7-C5
25	N	610	CLA	C13-C15-C16-C17
25	n	610	CLA	C13-C15-C16-C17
25	C	506	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
35	B	622	LMG	C33-C34-C35-C36
35	b	622	LMG	C33-C34-C35-C36
28	N	1623	NEX	C33-C34-C35-C15
28	n	1623	NEX	C33-C34-C35-C15
24	N	601	CHL	C15-C16-C17-C18
29	C	523	LHG	C4-O6-P-O3
29	c	523	LHG	C4-O6-P-O3
35	A	413	LMG	C12-C13-C14-C15
35	a	413	LMG	C12-C13-C14-C15
37	H	102	DGD	CAB-CBB-CCB-CDB
37	h	102	DGD	CAB-CBB-CCB-CDB
29	N	2630	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	n	2630	LHG	C29-C30-C31-C32
34	A	412	SQD	C16-C17-C18-C19
34	a	412	SQD	C16-C17-C18-C19
25	G	612	CLA	C3-C5-C6-C7
25	g	612	CLA	C3-C5-C6-C7
29	G	2630	LHG	C5-C4-O6-P
29	g	2630	LHG	C5-C4-O6-P
29	3	2630	LHG	O10-C23-O8-C6
29	7	2630	LHG	O10-C23-O8-C6
29	3	2630	LHG	C4-O6-P-O4
29	B	2630	LHG	C4-O6-P-O5
29	D	410	LHG	C4-O6-P-O5
29	G	2630	LHG	C4-O6-P-O4
29	N	2630	LHG	C3-O3-P-O5
29	7	2630	LHG	C4-O6-P-O4
29	b	2630	LHG	C4-O6-P-O5
29	d	410	LHG	C4-O6-P-O5
29	g	2630	LHG	C4-O6-P-O4
29	n	2630	LHG	C3-O3-P-O5
24	G	608	CHL	C16-C17-C18-C20
24	g	608	CHL	C16-C17-C18-C20
29	S	2630	LHG	C19-C20-C21-C22
29	s	2630	LHG	C19-C20-C21-C22
34	a	412	SQD	C28-C29-C30-C31
37	c	520	DGD	C2B-C3B-C4B-C5B
24	1	607	CHL	C10-C11-C12-C13
24	5	607	CHL	C10-C11-C12-C13
24	n	601	CHL	C15-C16-C17-C18
29	D	408	LHG	C24-C23-O8-C6
29	d	408	LHG	C24-C23-O8-C6
29	B	2630	LHG	O6-C4-C5-C6
29	b	2630	LHG	O6-C4-C5-C6
34	A	412	SQD	C28-C29-C30-C31
37	C	520	DGD	C2B-C3B-C4B-C5B
29	G	2630	LHG	O9-C7-O7-C5
37	C	518	DGD	CBB-CCB-CDB-CEB
37	c	518	DGD	CBB-CCB-CDB-CEB
24	4	609	CHL	C2C-C3C-CAC-CBC
25	N	602	CLA	C16-C17-C18-C20
25	n	602	CLA	C16-C17-C18-C20
25	1	603	CLA	CAD-CBD-CGD-O1D
25	2	603	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	3	603	CLA	CAD-CBD-CGD-O1D
25	3	604	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	606	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	615	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	513	CLA	CAD-CBD-CGD-O1D
25	5	603	CLA	CAD-CBD-CGD-O1D
25	6	603	CLA	CAD-CBD-CGD-O1D
25	7	603	CLA	CAD-CBD-CGD-O1D
25	7	604	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	606	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	615	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	513	CLA	CAD-CBD-CGD-O1D
28	S	1623	NEX	C7-C8-C9-C10
28	s	1623	NEX	C7-C8-C9-C10
24	N	608	CHL	C10-C11-C12-C13
24	n	608	CHL	C10-C11-C12-C13
24	n	609	CHL	C10-C11-C12-C13
29	C	523	LHG	C19-C20-C21-C22
29	c	523	LHG	C19-C20-C21-C22
35	B	2633	LMG	C21-C22-C23-C24
29	2	2630	LHG	O10-C23-O8-C6
29	6	2630	LHG	O10-C23-O8-C6
35	b	2633	LMG	C21-C22-C23-C24
24	N	609	CHL	C10-C11-C12-C13
29	B	2631	LHG	C33-C34-C35-C36
29	b	2631	LHG	C33-C34-C35-C36
24	8	609	CHL	C2C-C3C-CAC-CBC
24	G	601	CHL	C12-C13-C15-C16
24	G	608	CHL	C11-C10-C8-C7
24	N	601	CHL	C12-C13-C15-C16
24	R	606	CHL	C6-C7-C8-C10
24	g	601	CHL	C12-C13-C15-C16
24	g	608	CHL	C11-C10-C8-C7
24	n	601	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	r	606	CHL	C6-C7-C8-C10
25	2	602	CLA	C11-C12-C13-C15
25	B	606	CLA	C6-C7-C8-C10
25	B	607	CLA	C11-C10-C8-C7
25	B	617	CLA	C6-C7-C8-C10
25	C	513	CLA	C3A-C2A-CAA-CBA
25	G	613	CLA	C12-C13-C15-C16
25	6	602	CLA	C11-C12-C13-C15
25	b	606	CLA	C6-C7-C8-C10
25	b	607	CLA	C11-C10-C8-C7
25	b	617	CLA	C6-C7-C8-C10
25	c	513	CLA	C3A-C2A-CAA-CBA
25	g	613	CLA	C12-C13-C15-C16
29	B	2630	LHG	O6-C4-C5-O7
29	C	522	LHG	O6-C4-C5-O7
29	C	523	LHG	O6-C4-C5-O7
29	b	2630	LHG	O6-C4-C5-O7
29	c	522	LHG	O6-C4-C5-O7
29	c	523	LHG	O6-C4-C5-O7
33	A	409	PHO	C5-C6-C7-C8
33	a	409	PHO	C5-C6-C7-C8
29	b	2631	LHG	C13-C14-C15-C16
29	B	2631	LHG	C13-C14-C15-C16
37	h	102	DGD	CAA-CBA-CCA-CDA
37	H	102	DGD	CAA-CBA-CCA-CDA
25	1	602	CLA	C2A-CAA-CBA-CGA
25	4	602	CLA	C2A-CAA-CBA-CGA
25	5	602	CLA	C2A-CAA-CBA-CGA
25	8	602	CLA	C2A-CAA-CBA-CGA
25	B	617	CLA	C16-C17-C18-C20
25	b	617	CLA	C16-C17-C18-C20
37	H	102	DGD	C3B-C4B-C5B-C6B
25	Y	602	CLA	C3-C5-C6-C7
25	y	602	CLA	C3-C5-C6-C7
34	A	418	SQD	O47-C7-C8-C9
34	a	418	SQD	O47-C7-C8-C9
24	1	601	CHL	C1C-C2C-CMC-OMC
24	1	606	CHL	C1C-C2C-CMC-OMC
24	3	606	CHL	C1C-C2C-CMC-OMC
24	G	607	CHL	C1C-C2C-CMC-OMC
24	G	608	CHL	C1C-C2C-CMC-OMC
24	Y	608	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	Y	609	CHL	C1C-C2C-CMC-OMC
24	5	601	CHL	C1C-C2C-CMC-OMC
24	5	606	CHL	C1C-C2C-CMC-OMC
24	7	606	CHL	C1C-C2C-CMC-OMC
24	g	607	CHL	C1C-C2C-CMC-OMC
24	g	608	CHL	C1C-C2C-CMC-OMC
24	y	608	CHL	C1C-C2C-CMC-OMC
24	y	609	CHL	C1C-C2C-CMC-OMC
34	B	623	SQD	O6-C44-C45-C46
34	b	623	SQD	O6-C44-C45-C46
37	h	102	DGD	C3B-C4B-C5B-C6B
34	B	621	SQD	O47-C45-C46-O48
34	b	621	SQD	O47-C45-C46-O48
35	Z	101	LMG	O1-C7-C8-O7
35	z	101	LMG	O1-C7-C8-O7
29	3	2630	LHG	C27-C28-C29-C30
35	B	622	LMG	C38-C39-C40-C41
35	b	622	LMG	C38-C39-C40-C41
24	2	608	CHL	C2C-C3C-CAC-CBC
29	7	2630	LHG	C27-C28-C29-C30
25	c	506	CLA	O1A-CGA-O2A-C1
25	N	602	CLA	C3-C5-C6-C7
25	c	511	CLA	C3-C5-C6-C7
25	n	602	CLA	C3-C5-C6-C7
29	G	2630	LHG	C14-C15-C16-C17
25	C	506	CLA	O1A-CGA-O2A-C1
24	Y	607	CHL	C8-C10-C11-C12
24	y	607	CHL	C8-C10-C11-C12
24	G	608	CHL	C4-C3-C5-C6
24	g	608	CHL	C4-C3-C5-C6
25	2	603	CLA	C4-C3-C5-C6
25	6	603	CLA	C4-C3-C5-C6
29	g	2630	LHG	C14-C15-C16-C17
25	S	614	CLA	O2A-C1-C2-C3
25	s	614	CLA	O2A-C1-C2-C3
25	C	502	CLA	C8-C10-C11-C12
25	G	612	CLA	C10-C11-C12-C13
25	c	502	CLA	C8-C10-C11-C12
25	g	612	CLA	C10-C11-C12-C13
24	3	601	CHL	C11-C10-C8-C9
24	N	607	CHL	C14-C13-C15-C16
24	R	606	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	Y	607	CHL	C11-C12-C13-C14
24	Y	607	CHL	C14-C13-C15-C16
24	7	601	CHL	C11-C10-C8-C9
24	n	607	CHL	C14-C13-C15-C16
24	r	606	CHL	C6-C7-C8-C9
24	y	607	CHL	C11-C12-C13-C14
24	y	607	CHL	C14-C13-C15-C16
25	1	602	CLA	C6-C7-C8-C9
25	3	602	CLA	C11-C10-C8-C9
25	B	606	CLA	C14-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C9
25	N	603	CLA	C14-C13-C15-C16
25	S	611	CLA	C6-C7-C8-C9
25	Y	603	CLA	C14-C13-C15-C16
25	5	602	CLA	C6-C7-C8-C9
25	7	602	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	c	507	CLA	C6-C7-C8-C9
25	n	603	CLA	C14-C13-C15-C16
25	s	611	CLA	C6-C7-C8-C9
25	y	603	CLA	C14-C13-C15-C16
24	6	608	CHL	C2C-C3C-CAC-CBC
29	1	2630	LHG	C14-C15-C16-C17
29	5	2630	LHG	C14-C15-C16-C17
25	C	511	CLA	C3-C5-C6-C7
25	B	603	CLA	C16-C17-C18-C19
25	b	603	CLA	C16-C17-C18-C19
24	1	609	CHL	C4C-C3C-CAC-CBC
24	5	609	CHL	C4C-C3C-CAC-CBC
29	C	522	LHG	C17-C18-C19-C20
29	c	522	LHG	C17-C18-C19-C20
28	1	1623	NEX	C31-C32-C33-C40
28	5	1623	NEX	C31-C32-C33-C40
29	C	2630	LHG	C17-C18-C19-C20
29	S	2630	LHG	C33-C34-C35-C36
29	c	2630	LHG	C17-C18-C19-C20
29	s	2630	LHG	C33-C34-C35-C36
29	D	409	LHG	O2-C2-C3-O3
29	d	409	LHG	O2-C2-C3-O3
37	H	102	DGD	CDB-CEB-CFB-CGB
37	h	102	DGD	CDB-CEB-CFB-CGB
25	R	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	r	610	CLA	C5-C6-C7-C8
37	H	102	DGD	O2G-C1B-C2B-C3B
37	h	102	DGD	O2G-C1B-C2B-C3B
37	C	519	DGD	C1B-C2B-C3B-C4B
37	c	519	DGD	C1B-C2B-C3B-C4B
35	B	2633	LMG	C35-C36-C37-C38
37	c	518	DGD	CCB-CDB-CEB-CFB
35	b	2633	LMG	C35-C36-C37-C38
37	C	518	DGD	CCB-CDB-CEB-CFB
24	G	606	CHL	C1-C2-C3-C4
24	N	606	CHL	C1-C2-C3-C4
24	Y	606	CHL	C1-C2-C3-C4
24	g	606	CHL	C1-C2-C3-C4
24	n	606	CHL	C1-C2-C3-C4
24	y	606	CHL	C1-C2-C3-C4
25	R	601	CLA	C1-C2-C3-C4
25	R	611	CLA	C1-C2-C3-C4
25	R	612	CLA	C1-C2-C3-C4
25	S	612	CLA	C1-C2-C3-C4
25	r	601	CLA	C1-C2-C3-C4
25	r	611	CLA	C1-C2-C3-C4
25	r	612	CLA	C1-C2-C3-C4
25	s	612	CLA	C1-C2-C3-C4
25	G	611	CLA	O1A-CGA-O2A-C1
37	c	519	DGD	CBA-CCA-CDA-CEA
24	1	606	CHL	C2A-CAA-CBA-CGA
24	G	601	CHL	C2A-CAA-CBA-CGA
24	5	606	CHL	C2A-CAA-CBA-CGA
24	g	601	CHL	C2A-CAA-CBA-CGA
25	B	604	CLA	C2A-CAA-CBA-CGA
25	b	604	CLA	C2A-CAA-CBA-CGA
29	C	522	LHG	O9-C7-O7-C5
29	c	522	LHG	O9-C7-O7-C5
35	C	521	LMG	O9-C10-O7-C8
35	c	521	LMG	O9-C10-O7-C8
25	g	611	CLA	O1A-CGA-O2A-C1
29	G	2630	LHG	O10-C23-O8-C6
29	g	2630	LHG	O10-C23-O8-C6
24	N	608	CHL	C2-C1-O2A-CGA
24	N	609	CHL	C2-C1-O2A-CGA
24	n	608	CHL	C2-C1-O2A-CGA
24	n	609	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	1	604	CLA	C2-C1-O2A-CGA
25	C	506	CLA	C2-C1-O2A-CGA
25	C	511	CLA	C2-C1-O2A-CGA
25	S	602	CLA	C2-C1-O2A-CGA
25	5	604	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
25	c	511	CLA	C2-C1-O2A-CGA
25	s	602	CLA	C2-C1-O2A-CGA
37	C	519	DGD	CBA-CCA-CDA-CEA
24	3	609	CHL	C4C-C3C-CAC-CBC
24	7	609	CHL	C4C-C3C-CAC-CBC
29	D	408	LHG	C33-C34-C35-C36
29	d	408	LHG	C33-C34-C35-C36
35	D	411	LMG	C14-C15-C16-C17
24	y	601	CHL	O1D-CGD-O2D-CED
30	C	517	BCR	C9-C10-C11-C12
30	c	517	BCR	C9-C10-C11-C12
35	d	411	LMG	C14-C15-C16-C17
25	B	615	CLA	C16-C17-C18-C20
25	Y	602	CLA	C16-C17-C18-C19
25	y	602	CLA	C16-C17-C18-C19
24	Y	601	CHL	O1D-CGD-O2D-CED
26	G	1620	LUT	C1-C6-C7-C8
26	S	1620	LUT	C1-C6-C7-C8
26	g	1620	LUT	C1-C6-C7-C8
26	s	1620	LUT	C1-C6-C7-C8
29	C	522	LHG	C29-C30-C31-C32
25	B	604	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
29	c	522	LHG	C29-C30-C31-C32
25	R	613	CLA	C2A-CAA-CBA-CGA
25	S	613	CLA	C2A-CAA-CBA-CGA
25	r	613	CLA	C2A-CAA-CBA-CGA
25	s	613	CLA	C2A-CAA-CBA-CGA
25	N	614	CLA	O2A-C1-C2-C3
25	n	614	CLA	O2A-C1-C2-C3
37	C	520	DGD	C2D-C1D-O3G-C3G
37	c	520	DGD	C2D-C1D-O3G-C3G
29	3	2630	LHG	C3-O3-P-O6
29	B	2630	LHG	C3-O3-P-O6
29	B	2631	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
29	C	523	LHG	C3-O3-P-O6
29	D	409	LHG	C3-O3-P-O6
29	R	2630	LHG	C3-O3-P-O6
29	7	2630	LHG	C3-O3-P-O6
29	b	2630	LHG	C3-O3-P-O6
29	b	2631	LHG	C4-O6-P-O3
29	c	523	LHG	C3-O3-P-O6
29	d	409	LHG	C3-O3-P-O6
29	r	2630	LHG	C3-O3-P-O6
25	3	603	CLA	C5-C6-C7-C8
25	7	603	CLA	C5-C6-C7-C8
33	A	409	PHO	CHA-CBD-CGD-O2D
33	a	409	PHO	CHA-CBD-CGD-O2D
29	D	410	LHG	C10-C11-C12-C13
29	d	410	LHG	C10-C11-C12-C13
25	3	602	CLA	C10-C11-C12-C13
24	3	601	CHL	C12-C13-C15-C16
24	G	601	CHL	C6-C7-C8-C10
24	7	601	CHL	C12-C13-C15-C16
24	g	601	CHL	C6-C7-C8-C10
24	G	601	CHL	C14-C13-C15-C16
24	G	608	CHL	C11-C10-C8-C9
24	g	601	CHL	C14-C13-C15-C16
24	g	608	CHL	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	c	509	CLA	C11-C10-C8-C9
25	d	403	CLA	C11-C12-C13-C14
28	1	1623	NEX	C33-C34-C35-C15
28	5	1623	NEX	C33-C34-C35-C15
30	D	404	BCR	C9-C10-C11-C12
30	d	404	BCR	C9-C10-C11-C12
25	B	615	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
35	A	413	LMG	C36-C37-C38-C39
35	a	413	LMG	C36-C37-C38-C39
25	7	602	CLA	C10-C11-C12-C13
35	b	622	LMG	C32-C33-C34-C35
35	B	622	LMG	C32-C33-C34-C35
29	D	408	LHG	O1-C1-C2-C3
29	d	408	LHG	O1-C1-C2-C3
29	3	2630	LHG	C5-C4-O6-P

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Mol	Chain	Res	Type	Atoms
29	7	2630	LHG	C5-C4-O6-P
25	b	617	CLA	O1D-CGD-O2D-CED
29	D	408	LHG	O1-C1-C2-O2
29	d	408	LHG	O1-C1-C2-O2
25	G	611	CLA	CBA-CGA-O2A-C1
25	g	611	CLA	CBA-CGA-O2A-C1
35	B	2633	LMG	C29-C28-O8-C9
35	b	2633	LMG	C29-C28-O8-C9
25	B	617	CLA	O1D-CGD-O2D-CED
29	3	2630	LHG	C15-C16-C17-C18
29	7	2630	LHG	C15-C16-C17-C18
24	G	608	CHL	C16-C17-C18-C19
24	g	608	CHL	C16-C17-C18-C19
25	c	509	CLA	C13-C15-C16-C17
28	3	1623	NEX	C9-C10-C11-C12
28	7	1623	NEX	C9-C10-C11-C12
30	C	515	BCR	C9-C10-C11-C12
30	C	516	BCR	C19-C20-C21-C22
30	C	517	BCR	C19-C20-C21-C22
30	c	515	BCR	C9-C10-C11-C12
30	c	516	BCR	C19-C20-C21-C22
30	c	517	BCR	C19-C20-C21-C22
37	B	626	DGD	C7A-C8A-C9A-CAA
29	N	2630	LHG	C26-C27-C28-C29
29	7	2630	LHG	C29-C30-C31-C32
37	b	626	DGD	C7A-C8A-C9A-CAA
29	r	2630	LHG	C7-C8-C9-C10
25	C	509	CLA	C13-C15-C16-C17
24	2	607	CHL	C4C-C3C-CAC-CBC
24	6	607	CHL	C4C-C3C-CAC-CBC
29	3	2630	LHG	C29-C30-C31-C32
29	D	410	LHG	C9-C10-C11-C12
29	d	410	LHG	C9-C10-C11-C12
29	n	2630	LHG	C26-C27-C28-C29
24	2	609	CHL	C5-C6-C7-C8
24	6	609	CHL	C5-C6-C7-C8
34	A	418	SQD	C14-C15-C16-C17
34	a	418	SQD	C14-C15-C16-C17
29	R	2630	LHG	C7-C8-C9-C10
25	b	603	CLA	C16-C17-C18-C20
29	N	2630	LHG	C35-C36-C37-C38
37	H	102	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
37	h	102	DGD	O1B-C1B-C2B-C3B
29	n	2630	LHG	C35-C36-C37-C38
35	z	101	LMG	C33-C34-C35-C36
29	D	410	LHG	C14-C15-C16-C17
29	d	410	LHG	C14-C15-C16-C17
35	Z	101	LMG	C33-C34-C35-C36
25	A	405	CLA	C2-C1-O2A-CGA
25	B	605	CLA	C2-C1-O2A-CGA
25	D	403	CLA	C2-C1-O2A-CGA
25	a	405	CLA	C2-C1-O2A-CGA
25	b	605	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
24	N	608	CHL	C5-C6-C7-C8
24	n	608	CHL	C5-C6-C7-C8
25	B	603	CLA	C16-C17-C18-C20
34	A	418	SQD	C11-C12-C13-C14
35	b	622	LMG	C31-C32-C33-C34
35	B	622	LMG	C31-C32-C33-C34
25	3	604	CLA	CAA-CBA-CGA-O2A
25	7	604	CLA	CAA-CBA-CGA-O2A
25	1	613	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C2A-CAA-CBA-CGA
25	B	617	CLA	C2A-CAA-CBA-CGA
25	5	613	CLA	C2A-CAA-CBA-CGA
25	b	615	CLA	C2A-CAA-CBA-CGA
25	b	617	CLA	C2A-CAA-CBA-CGA
29	D	410	LHG	C2-C3-O3-P
29	d	410	LHG	C2-C3-O3-P
25	4	610	CLA	C3A-C2A-CAA-CBA
25	R	604	CLA	C3A-C2A-CAA-CBA
25	8	610	CLA	C3A-C2A-CAA-CBA
25	r	604	CLA	C3A-C2A-CAA-CBA
25	2	614	CLA	CAA-CBA-CGA-O1A
25	2	614	CLA	CAA-CBA-CGA-O2A
25	6	614	CLA	CAA-CBA-CGA-O1A
25	6	614	CLA	CAA-CBA-CGA-O2A
29	g	2630	LHG	C11-C12-C13-C14
34	a	418	SQD	C11-C12-C13-C14
34	b	621	SQD	C12-C13-C14-C15
24	G	609	CHL	C2C-C3C-CAC-CBC
29	G	2630	LHG	C11-C12-C13-C14
37	H	102	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
26	4	620	LUT	C29-C30-C31-C32
26	8	620	LUT	C29-C30-C31-C32
24	g	609	CHL	C2C-C3C-CAC-CBC
34	B	621	SQD	C12-C13-C14-C15
37	h	102	DGD	CBB-CCB-CDB-CEB
25	R	616	CLA	CAA-CBA-CGA-O1A
25	r	616	CLA	CAA-CBA-CGA-O1A
25	2	602	CLA	C4-C3-C5-C6
25	6	602	CLA	C4-C3-C5-C6
25	2	603	CLA	C2-C3-C5-C6
25	6	603	CLA	C2-C3-C5-C6
37	C	518	DGD	C5A-C6A-C7A-C8A
37	c	518	DGD	C5A-C6A-C7A-C8A
24	2	609	CHL	C6-C7-C8-C9
24	N	601	CHL	C14-C13-C15-C16
24	N	609	CHL	C14-C13-C15-C16
24	6	609	CHL	C6-C7-C8-C9
24	n	601	CHL	C14-C13-C15-C16
24	n	609	CHL	C14-C13-C15-C16
25	B	603	CLA	C11-C10-C8-C9
25	B	608	CLA	C6-C7-C8-C9
25	N	603	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C10-C8-C9
25	b	608	CLA	C6-C7-C8-C9
25	n	603	CLA	C6-C7-C8-C9
37	C	520	DGD	C9B-CAB-CBB-CCB
37	c	520	DGD	C9B-CAB-CBB-CCB
28	1	1623	NEX	C39-C29-C30-C31
28	2	1623	NEX	C39-C29-C30-C31
28	3	1623	NEX	C39-C29-C30-C31
28	G	1623	NEX	C39-C29-C30-C31
28	N	1623	NEX	C39-C29-C30-C31
28	R	623	NEX	C39-C29-C30-C31
28	S	1623	NEX	C39-C29-C30-C31
28	Y	1623	NEX	C39-C29-C30-C31
28	5	1623	NEX	C39-C29-C30-C31
28	6	1623	NEX	C39-C29-C30-C31
28	7	1623	NEX	C39-C29-C30-C31
28	g	1623	NEX	C39-C29-C30-C31
28	n	1623	NEX	C39-C29-C30-C31
28	r	623	NEX	C39-C29-C30-C31
28	s	1623	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	y	1623	NEX	C39-C29-C30-C31
25	C	501	CLA	C16-C17-C18-C20
25	c	501	CLA	C16-C17-C18-C20
37	C	518	DGD	O6E-C1E-O5D-C6D
37	c	518	DGD	O6E-C1E-O5D-C6D
24	4	609	CHL	CAA-CBA-CGA-O1A
27	4	622	XAT	C27-C28-C29-C39
27	8	622	XAT	C27-C28-C29-C39
30	C	516	BCR	C36-C18-C19-C20
30	c	516	BCR	C36-C18-C19-C20
37	c	518	DGD	C6A-C7A-C8A-C9A
24	8	609	CHL	CAA-CBA-CGA-O1A
25	B	616	CLA	C15-C16-C17-C18
25	b	616	CLA	C15-C16-C17-C18
24	3	609	CHL	C4-C3-C5-C6
24	7	609	CHL	C4-C3-C5-C6
24	3	607	CHL	C1A-C2A-CAA-CBA
24	7	607	CHL	C1A-C2A-CAA-CBA
25	C	508	CLA	C1A-C2A-CAA-CBA
25	C	511	CLA	C1A-C2A-CAA-CBA
25	G	604	CLA	C1A-C2A-CAA-CBA
25	R	602	CLA	C1A-C2A-CAA-CBA
25	S	609	CLA	C1A-C2A-CAA-CBA
25	S	610	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	g	604	CLA	C1A-C2A-CAA-CBA
25	r	602	CLA	C1A-C2A-CAA-CBA
25	s	609	CLA	C1A-C2A-CAA-CBA
25	s	610	CLA	C1A-C2A-CAA-CBA
37	C	518	DGD	C6A-C7A-C8A-C9A
37	C	518	DGD	C6B-C7B-C8B-C9B
25	B	614	CLA	C11-C12-C13-C15
25	b	614	CLA	C11-C12-C13-C15
25	1	612	CLA	CAA-CBA-CGA-O1A
25	5	612	CLA	CAA-CBA-CGA-O1A
37	c	518	DGD	C6B-C7B-C8B-C9B
26	3	1621	LUT	C29-C30-C31-C32
30	4	623	BCR	C9-C10-C11-C12
30	8	623	BCR	C9-C10-C11-C12
35	B	2633	LMG	C39-C40-C41-C42
37	h	102	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
25	Y	611	CLA	C8-C10-C11-C12
25	y	611	CLA	C8-C10-C11-C12
29	N	2630	LHG	C4-O6-P-O3
29	n	2630	LHG	C4-O6-P-O3
37	H	102	DGD	CDA-CEA-CFA-CGA
24	4	609	CHL	CAA-CBA-CGA-O2A
24	N	607	CHL	C2C-C3C-CAC-CBC
35	b	2633	LMG	C39-C40-C41-C42
24	6	608	CHL	C4C-C3C-CAC-CBC
24	n	607	CHL	C2C-C3C-CAC-CBC
29	R	2630	LHG	C14-C15-C16-C17
29	r	2630	LHG	C14-C15-C16-C17
25	N	613	CLA	C2A-CAA-CBA-CGA
25	n	613	CLA	C2A-CAA-CBA-CGA
25	Y	610	CLA	C8-C10-C11-C12
25	y	610	CLA	C8-C10-C11-C12
29	D	410	LHG	C31-C32-C33-C34
35	C	521	LMG	O6-C5-C6-O5
24	4	607	CHL	CAA-CBA-CGA-O1A
24	8	607	CHL	CAA-CBA-CGA-O1A
24	8	609	CHL	CAA-CBA-CGA-O2A
25	3	604	CLA	CAA-CBA-CGA-O1A
25	7	604	CLA	CAA-CBA-CGA-O1A
29	d	410	LHG	C31-C32-C33-C34
24	2	608	CHL	C4C-C3C-CAC-CBC
29	D	408	LHG	C14-C15-C16-C17
29	d	408	LHG	C14-C15-C16-C17
35	c	521	LMG	O6-C5-C6-O5
25	R	616	CLA	CAA-CBA-CGA-O2A
25	5	612	CLA	CAA-CBA-CGA-O2A
25	8	612	CLA	CAA-CBA-CGA-O2A
25	r	616	CLA	CAA-CBA-CGA-O2A
29	S	2630	LHG	C12-C13-C14-C15
35	B	622	LMG	C22-C23-C24-C25
35	b	622	LMG	C22-C23-C24-C25
25	C	509	CLA	C10-C11-C12-C13
25	c	509	CLA	C10-C11-C12-C13
29	b	2630	LHG	C18-C19-C20-C21
29	s	2630	LHG	C12-C13-C14-C15
35	A	415	LMG	C29-C28-O8-C9
35	a	415	LMG	C29-C28-O8-C9
25	4	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	8	603	CLA	CAA-CBA-CGA-O1A
29	B	2630	LHG	C18-C19-C20-C21
25	B	612	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
35	B	622	LMG	O9-C10-O7-C8
35	b	622	LMG	O9-C10-O7-C8
28	1	1623	NEX	C28-C29-C30-C31
28	2	1623	NEX	C28-C29-C30-C31
28	3	1623	NEX	C28-C29-C30-C31
28	G	1623	NEX	C28-C29-C30-C31
28	N	1623	NEX	C28-C29-C30-C31
28	R	623	NEX	C28-C29-C30-C31
28	S	1623	NEX	C28-C29-C30-C31
28	Y	1623	NEX	C28-C29-C30-C31
28	5	1623	NEX	C28-C29-C30-C31
28	6	1623	NEX	C28-C29-C30-C31
28	7	1623	NEX	C28-C29-C30-C31
28	g	1623	NEX	C28-C29-C30-C31
28	n	1623	NEX	C28-C29-C30-C31
28	r	623	NEX	C28-C29-C30-C31
28	s	1623	NEX	C28-C29-C30-C31
28	y	1623	NEX	C28-C29-C30-C31
24	s	601	CHL	CAA-CBA-CGA-O1A
25	4	603	CLA	CAA-CBA-CGA-O1A
29	B	2630	LHG	O7-C5-C6-O8
29	C	2630	LHG	O7-C5-C6-O8
29	b	2630	LHG	O7-C5-C6-O8
29	c	2630	LHG	O7-C5-C6-O8
29	B	2630	LHG	C17-C18-C19-C20
29	b	2630	LHG	C17-C18-C19-C20
35	a	413	LMG	C33-C34-C35-C36
35	B	2633	LMG	C8-C9-O8-C28
35	b	2633	LMG	C8-C9-O8-C28
24	R	606	CHL	C2A-CAA-CBA-CGA
24	r	606	CHL	C2A-CAA-CBA-CGA
26	7	1621	LUT	C29-C30-C31-C32
27	N	1622	XAT	C29-C30-C31-C32
27	n	1622	XAT	C29-C30-C31-C32
28	1	1623	NEX	C29-C30-C31-C32
28	5	1623	NEX	C29-C30-C31-C32
30	C	515	BCR	C19-C20-C21-C22
30	c	515	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
24	S	601	CHL	CAA-CBA-CGA-O1A
24	S	601	CHL	CAA-CBA-CGA-O2A
24	s	601	CHL	CAA-CBA-CGA-O2A
25	1	612	CLA	CAA-CBA-CGA-O2A
25	C	509	CLA	C8-C10-C11-C12
25	c	509	CLA	C8-C10-C11-C12
35	A	413	LMG	C33-C34-C35-C36
29	s	2630	LHG	C31-C32-C33-C34
25	C	503	CLA	C13-C15-C16-C17
25	c	503	CLA	C13-C15-C16-C17
29	S	2630	LHG	C31-C32-C33-C34
25	b	609	CLA	C15-C16-C17-C18
24	N	609	CHL	C4-C3-C5-C6
24	S	607	CHL	C4-C3-C5-C6
24	n	609	CHL	C4-C3-C5-C6
24	s	607	CHL	C4-C3-C5-C6
24	2	609	CHL	C2-C1-O2A-CGA
24	G	608	CHL	C2-C1-O2A-CGA
24	Y	609	CHL	C2-C1-O2A-CGA
24	6	609	CHL	C2-C1-O2A-CGA
24	g	608	CHL	C2-C1-O2A-CGA
24	y	609	CHL	C2-C1-O2A-CGA
25	B	609	CLA	C2-C1-O2A-CGA
25	C	502	CLA	C2-C1-O2A-CGA
25	Y	603	CLA	C2-C1-O2A-CGA
25	b	609	CLA	C2-C1-O2A-CGA
25	c	502	CLA	C2-C1-O2A-CGA
25	y	603	CLA	C2-C1-O2A-CGA
33	A	409	PHO	O1A-CGA-O2A-C1
33	a	409	PHO	O1A-CGA-O2A-C1
25	B	607	CLA	C10-C11-C12-C13
25	B	609	CLA	C15-C16-C17-C18
25	b	607	CLA	C10-C11-C12-C13
25	4	612	CLA	CAA-CBA-CGA-O1A
25	8	612	CLA	CAA-CBA-CGA-O1A
24	Y	601	CHL	C6-C7-C8-C9
24	y	601	CHL	C6-C7-C8-C9
25	C	504	CLA	C11-C12-C13-C14
25	c	504	CLA	C11-C12-C13-C14
25	3	614	CLA	O2A-C1-C2-C3
24	8	607	CHL	CAA-CBA-CGA-O2A
29	d	409	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	B	614	CLA	O1A-CGA-O2A-C1
25	b	614	CLA	O1A-CGA-O2A-C1
29	D	409	LHG	C13-C14-C15-C16
25	G	610	CLA	C10-C11-C12-C13
24	4	607	CHL	C2A-CAA-CBA-CGA
24	8	607	CHL	C2A-CAA-CBA-CGA
24	4	607	CHL	CAA-CBA-CGA-O2A
25	4	603	CLA	CAA-CBA-CGA-O2A
25	8	603	CLA	CAA-CBA-CGA-O2A
24	R	606	CHL	O1A-CGA-O2A-C1
24	r	606	CHL	O1A-CGA-O2A-C1
26	2	1621	LUT	C1-C6-C7-C8
26	3	1620	LUT	C1-C6-C7-C8
26	Y	1621	LUT	C1-C6-C7-C8
26	6	1621	LUT	C1-C6-C7-C8
26	7	1620	LUT	C1-C6-C7-C8
26	y	1621	LUT	C1-C6-C7-C8
30	C	517	BCR	C23-C24-C25-C26
30	C	517	BCR	C23-C24-C25-C30
30	H	101	BCR	C23-C24-C25-C26
30	H	101	BCR	C23-C24-C25-C30
30	c	517	BCR	C23-C24-C25-C26
30	c	517	BCR	C23-C24-C25-C30
30	h	101	BCR	C23-C24-C25-C26
30	h	101	BCR	C23-C24-C25-C30
25	B	602	CLA	CAA-CBA-CGA-O2A
25	b	602	CLA	CAA-CBA-CGA-O2A
35	A	413	LMG	O1-C7-C8-C9
35	a	413	LMG	O1-C7-C8-C9
25	g	610	CLA	C10-C11-C12-C13
24	N	606	CHL	CBA-CGA-O2A-C1
24	n	606	CHL	CBA-CGA-O2A-C1
27	R	622	XAT	C27-C28-C29-C30
27	r	622	XAT	C27-C28-C29-C30
24	G	608	CHL	C2-C3-C5-C6
24	g	608	CHL	C2-C3-C5-C6
24	3	605	CHL	CAA-CBA-CGA-O2A
24	S	606	CHL	CAA-CBA-CGA-O2A
24	7	605	CHL	CAA-CBA-CGA-O2A
24	s	606	CHL	CAA-CBA-CGA-O2A
37	c	518	DGD	O1A-C1A-O1G-C1G
25	g	603	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
37	C	518	DGD	C5D-C6D-O5D-C1E
37	c	518	DGD	C5D-C6D-O5D-C1E
25	A	405	CLA	C4C-C3C-CAC-CBC
25	a	405	CLA	C4C-C3C-CAC-CBC
35	a	413	LMG	C31-C32-C33-C34
25	7	614	CLA	O2A-C1-C2-C3
35	A	413	LMG	C31-C32-C33-C34
24	3	608	CHL	CAA-CBA-CGA-O2A
24	7	608	CHL	CAA-CBA-CGA-O2A
25	4	611	CLA	CAA-CBA-CGA-O2A
25	8	604	CLA	CAA-CBA-CGA-O2A
25	8	611	CLA	CAA-CBA-CGA-O2A
29	n	2630	LHG	C12-C13-C14-C15
25	G	603	CLA	C10-C11-C12-C13
29	N	2630	LHG	C12-C13-C14-C15
25	4	604	CLA	CAA-CBA-CGA-O2A
25	S	609	CLA	C2A-CAA-CBA-CGA
25	s	609	CLA	C2A-CAA-CBA-CGA
29	N	2630	LHG	C28-C29-C30-C31
29	n	2630	LHG	C28-C29-C30-C31
25	b	605	CLA	O1D-CGD-O2D-CED
24	R	606	CHL	CBA-CGA-O2A-C1
24	r	606	CHL	CBA-CGA-O2A-C1
37	C	518	DGD	O1A-C1A-O1G-C1G
24	2	601	CHL	CAA-CBA-CGA-O1A
29	c	523	LHG	C11-C12-C13-C14
29	D	410	LHG	O6-C4-C5-C6
29	d	410	LHG	O6-C4-C5-C6
24	G	609	CHL	C4-C3-C5-C6
24	g	609	CHL	C4-C3-C5-C6
25	A	405	CLA	C4-C3-C5-C6
25	C	506	CLA	C4-C3-C5-C6
25	Y	611	CLA	C4-C3-C5-C6
25	a	405	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
25	y	611	CLA	C4-C3-C5-C6
37	B	626	DGD	O6D-C5D-C6D-O5D
37	b	626	DGD	O6D-C5D-C6D-O5D
29	C	523	LHG	C11-C12-C13-C14
24	Y	608	CHL	C11-C10-C8-C7
24	y	608	CHL	C11-C10-C8-C7
24	1	605	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	5	605	CHL	CAA-CBA-CGA-O2A
24	6	601	CHL	CAA-CBA-CGA-O1A
29	B	2630	LHG	C31-C32-C33-C34
29	C	2630	LHG	C25-C26-C27-C28
29	b	2630	LHG	C31-C32-C33-C34
29	c	2630	LHG	C25-C26-C27-C28
37	C	519	DGD	CBB-CCB-CDB-CEB
27	R	622	XAT	C9-C10-C11-C12
27	Y	1622	XAT	C29-C30-C31-C32
27	r	622	XAT	C9-C10-C11-C12
27	y	1622	XAT	C29-C30-C31-C32
25	b	617	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C19
37	c	519	DGD	CBB-CCB-CDB-CEB
25	C	504	CLA	CBA-CGA-O2A-C1
25	c	504	CLA	CBA-CGA-O2A-C1
33	A	409	PHO	CBA-CGA-O2A-C1
33	a	409	PHO	CBA-CGA-O2A-C1
24	4	609	CHL	C4C-C3C-CAC-CBC
24	Y	607	CHL	C2C-C3C-CAC-CBC
29	B	2630	LHG	C33-C34-C35-C36
29	5	2630	LHG	C18-C19-C20-C21
25	B	617	CLA	CBD-CGD-O2D-CED
24	y	607	CHL	C2C-C3C-CAC-CBC
29	1	2630	LHG	C18-C19-C20-C21
24	1	601	CHL	CAA-CBA-CGA-O2A
24	5	601	CHL	CAA-CBA-CGA-O2A
25	S	609	CLA	CAA-CBA-CGA-O2A
24	Y	606	CHL	O2A-C1-C2-C3
24	y	606	CHL	O2A-C1-C2-C3
24	8	609	CHL	C4C-C3C-CAC-CBC
29	b	2630	LHG	C33-C34-C35-C36
35	Z	101	LMG	C17-C18-C19-C20
35	z	101	LMG	C17-C18-C19-C20
25	B	605	CLA	O1D-CGD-O2D-CED
35	C	521	LMG	C14-C15-C16-C17
37	B	626	DGD	C8B-C9B-CAB-CBB
37	C	519	DGD	C6A-C7A-C8A-C9A
25	s	609	CLA	CAA-CBA-CGA-O2A
35	c	521	LMG	C14-C15-C16-C17
37	b	626	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
25	S	604	CLA	CAA-CBA-CGA-O2A
25	s	604	CLA	CAA-CBA-CGA-O2A
37	c	519	DGD	C6A-C7A-C8A-C9A
24	N	608	CHL	C4-C3-C5-C6
24	n	608	CHL	C4-C3-C5-C6
25	B	607	CLA	C4-C3-C5-C6
25	D	403	CLA	C4-C3-C5-C6
25	b	607	CLA	C4-C3-C5-C6
25	d	403	CLA	C4-C3-C5-C6
24	1	605	CHL	CAA-CBA-CGA-O1A
24	1	606	CHL	CAA-CBA-CGA-O2A
24	5	605	CHL	CAA-CBA-CGA-O1A
24	5	606	CHL	CAA-CBA-CGA-O2A
24	3	609	CHL	C2-C3-C5-C6
24	S	607	CHL	C2-C3-C5-C6
24	7	609	CHL	C2-C3-C5-C6
24	s	607	CHL	C2-C3-C5-C6
25	s	613	CLA	C2-C3-C5-C6
35	A	413	LMG	C15-C16-C17-C18
35	a	413	LMG	C15-C16-C17-C18
25	2	603	CLA	CAA-CBA-CGA-O2A
25	3	611	CLA	CAA-CBA-CGA-O2A
25	6	603	CLA	CAA-CBA-CGA-O2A
25	7	611	CLA	CAA-CBA-CGA-O2A
35	A	415	LMG	O7-C10-C11-C12
24	Y	608	CHL	C11-C10-C8-C9
24	y	608	CHL	C11-C10-C8-C9
25	2	602	CLA	C11-C12-C13-C14
25	B	607	CLA	C11-C10-C8-C9
25	B	614	CLA	C11-C12-C13-C14
25	B	617	CLA	C6-C7-C8-C9
25	C	510	CLA	C11-C10-C8-C9
25	G	613	CLA	C14-C13-C15-C16
25	6	602	CLA	C11-C12-C13-C14
25	b	607	CLA	C11-C10-C8-C9
25	b	614	CLA	C11-C12-C13-C14
25	b	617	CLA	C6-C7-C8-C9
25	c	510	CLA	C11-C10-C8-C9
25	g	613	CLA	C14-C13-C15-C16
24	3	607	CHL	C3A-C2A-CAA-CBA
24	N	605	CHL	C3A-C2A-CAA-CBA
24	Y	608	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	7	607	CHL	C3A-C2A-CAA-CBA
24	n	605	CHL	C3A-C2A-CAA-CBA
24	y	608	CHL	C3A-C2A-CAA-CBA
35	a	415	LMG	O7-C10-C11-C12
37	c	518	DGD	O2G-C1B-C2B-C3B
25	B	610	CLA	CBD-CGD-O2D-CED
24	3	605	CHL	CAD-CBD-CGD-O2D
24	G	609	CHL	CAD-CBD-CGD-O2D
24	7	605	CHL	CAD-CBD-CGD-O2D
24	g	609	CHL	CAD-CBD-CGD-O2D
25	1	610	CLA	CAD-CBD-CGD-O2D
25	1	614	CLA	CAD-CBD-CGD-O2D
25	2	611	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	CAD-CBD-CGD-O2D
25	B	608	CLA	CAD-CBD-CGD-O2D
25	B	611	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	509	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	CAD-CBD-CGD-O2D
25	G	603	CLA	CAD-CBD-CGD-O2D
25	N	603	CLA	CAD-CBD-CGD-O2D
25	N	604	CLA	CAD-CBD-CGD-O2D
25	S	602	CLA	CAD-CBD-CGD-O2D
25	Y	604	CLA	CAD-CBD-CGD-O2D
25	5	610	CLA	CAD-CBD-CGD-O2D
25	5	614	CLA	CAD-CBD-CGD-O2D
25	6	611	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	b	608	CLA	CAD-CBD-CGD-O2D
25	b	611	CLA	CAD-CBD-CGD-O2D
25	c	501	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
25	g	603	CLA	CAD-CBD-CGD-O2D
25	n	603	CLA	CAD-CBD-CGD-O2D
25	n	604	CLA	CAD-CBD-CGD-O2D
25	s	602	CLA	CAD-CBD-CGD-O2D
25	y	604	CLA	CAD-CBD-CGD-O2D
25	n	613	CLA	C5-C6-C7-C8
35	Z	101	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
35	z	101	LMG	O9-C10-O7-C8
25	b	610	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	C10-C11-C12-C13
25	b	605	CLA	C10-C11-C12-C13
24	3	609	CHL	C2-C1-O2A-CGA
24	7	609	CHL	C2-C1-O2A-CGA
24	4	608	CHL	CAA-CBA-CGA-O2A
24	8	608	CHL	CAA-CBA-CGA-O2A
25	1	611	CLA	CAA-CBA-CGA-O2A
25	Y	612	CLA	CAA-CBA-CGA-O2A
25	y	612	CLA	CAA-CBA-CGA-O2A
29	C	2630	LHG	O8-C23-C24-C25
29	c	2630	LHG	O8-C23-C24-C25
35	Z	101	LMG	O8-C28-C29-C30
35	z	101	LMG	O8-C28-C29-C30
37	C	518	DGD	O2G-C1B-C2B-C3B
35	Z	101	LMG	C19-C20-C21-C22
25	C	504	CLA	O1A-CGA-O2A-C1
25	N	613	CLA	C5-C6-C7-C8
24	7	605	CHL	CAA-CBA-CGA-O1A
25	5	611	CLA	CAA-CBA-CGA-O2A
35	z	101	LMG	C19-C20-C21-C22
24	G	607	CHL	C5-C6-C7-C8
24	g	607	CHL	C5-C6-C7-C8
25	S	613	CLA	C2-C3-C5-C6
25	Y	611	CLA	C2-C3-C5-C6
25	y	611	CLA	C2-C3-C5-C6
37	C	519	DGD	O1G-C1A-C2A-C3A
37	c	519	DGD	O1G-C1A-C2A-C3A
29	C	522	LHG	C30-C31-C32-C33
29	c	522	LHG	C30-C31-C32-C33
25	c	504	CLA	O1A-CGA-O2A-C1
26	1	1621	LUT	C7-C8-C9-C10
26	5	1621	LUT	C7-C8-C9-C10
30	B	618	BCR	C17-C18-C19-C20
30	C	516	BCR	C17-C18-C19-C20
30	b	618	BCR	C17-C18-C19-C20
30	c	516	BCR	C17-C18-C19-C20
37	B	626	DGD	C7B-C8B-C9B-CAB
37	b	626	DGD	C7B-C8B-C9B-CAB
27	4	622	XAT	O4-C6-C7-C8
27	8	622	XAT	O4-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	1	1623	NEX	O24-C26-C27-C28
28	2	1623	NEX	O24-C26-C27-C28
28	3	1623	NEX	O24-C26-C27-C28
28	R	623	NEX	O24-C26-C27-C28
28	S	1623	NEX	O24-C26-C27-C28
28	Y	1623	NEX	O24-C26-C27-C28
28	5	1623	NEX	O24-C26-C27-C28
28	6	1623	NEX	O24-C26-C27-C28
28	7	1623	NEX	O24-C26-C27-C28
28	g	1623	NEX	O24-C26-C27-C28
28	r	623	NEX	O24-C26-C27-C28
28	s	1623	NEX	O24-C26-C27-C28
28	y	1623	NEX	O24-C26-C27-C28
33	A	408	PHO	C2C-C3C-CAC-CBC
33	a	408	PHO	C2C-C3C-CAC-CBC
35	Z	101	LMG	C7-C8-C9-O8
35	z	101	LMG	C7-C8-C9-O8
24	5	606	CHL	CAA-CBA-CGA-O1A
24	s	606	CHL	CAA-CBA-CGA-O1A
25	4	604	CLA	CAA-CBA-CGA-O1A
25	4	611	CLA	CAA-CBA-CGA-O1A
25	8	604	CLA	CAA-CBA-CGA-O1A
25	8	611	CLA	CAA-CBA-CGA-O1A
25	C	501	CLA	CAA-CBA-CGA-O2A
25	c	501	CLA	CAA-CBA-CGA-O2A
24	1	606	CHL	CAA-CBA-CGA-O1A
24	3	605	CHL	CAA-CBA-CGA-O1A
25	4	610	CLA	CAA-CBA-CGA-O1A
24	G	607	CHL	O2A-C1-C2-C3
24	N	607	CHL	O2A-C1-C2-C3
24	Y	607	CHL	O2A-C1-C2-C3
24	g	607	CHL	O2A-C1-C2-C3
24	n	607	CHL	O2A-C1-C2-C3
24	y	607	CHL	O2A-C1-C2-C3
29	r	2630	LHG	C24-C25-C26-C27
24	1	601	CHL	C2A-CAA-CBA-CGA
24	5	601	CHL	C2A-CAA-CBA-CGA
25	Y	604	CLA	C2A-CAA-CBA-CGA
29	R	2630	LHG	C24-C25-C26-C27
24	3	608	CHL	CAA-CBA-CGA-O1A
24	S	606	CHL	CAA-CBA-CGA-O1A
24	7	608	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	1	611	CLA	CAA-CBA-CGA-O1A
25	4	610	CLA	CAA-CBA-CGA-O2A
25	5	611	CLA	CAA-CBA-CGA-O1A
25	8	610	CLA	CAA-CBA-CGA-O1A
25	8	610	CLA	CAA-CBA-CGA-O2A
25	Y	610	CLA	C11-C12-C13-C14
25	y	610	CLA	C11-C12-C13-C14
24	2	609	CHL	CHA-CBD-CGD-O1D
24	2	609	CHL	CHA-CBD-CGD-O2D
24	N	605	CHL	CHA-CBD-CGD-O2D
24	S	601	CHL	CHA-CBD-CGD-O1D
24	S	601	CHL	CHA-CBD-CGD-O2D
24	6	609	CHL	CHA-CBD-CGD-O1D
24	6	609	CHL	CHA-CBD-CGD-O2D
24	n	605	CHL	CHA-CBD-CGD-O2D
24	s	601	CHL	CHA-CBD-CGD-O2D
25	1	603	CLA	CHA-CBD-CGD-O2D
25	2	612	CLA	CHA-CBD-CGD-O2D
25	3	602	CLA	CHA-CBD-CGD-O1D
25	3	613	CLA	CHA-CBD-CGD-O1D
25	3	613	CLA	CHA-CBD-CGD-O2D
25	4	612	CLA	CHA-CBD-CGD-O1D
25	4	612	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	612	CLA	CHA-CBD-CGD-O1D
25	B	612	CLA	CHA-CBD-CGD-O2D
25	B	613	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	511	CLA	CHA-CBD-CGD-O1D
25	C	511	CLA	CHA-CBD-CGD-O2D
25	S	603	CLA	CHA-CBD-CGD-O1D
25	S	611	CLA	CHA-CBD-CGD-O2D
25	S	613	CLA	CHA-CBD-CGD-O1D
25	S	613	CLA	CHA-CBD-CGD-O2D
25	Y	602	CLA	CHA-CBD-CGD-O1D
25	Y	602	CLA	CHA-CBD-CGD-O2D
25	5	603	CLA	CHA-CBD-CGD-O2D
25	6	612	CLA	CHA-CBD-CGD-O2D
25	7	613	CLA	CHA-CBD-CGD-O1D
25	7	613	CLA	CHA-CBD-CGD-O2D
25	8	612	CLA	CHA-CBD-CGD-O1D
25	8	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	b	606	CLA	CHA-CBD-CGD-O2D
25	b	612	CLA	CHA-CBD-CGD-O1D
25	b	612	CLA	CHA-CBD-CGD-O2D
25	b	613	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	511	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CHA-CBD-CGD-O2D
25	s	603	CLA	CHA-CBD-CGD-O1D
25	s	611	CLA	CHA-CBD-CGD-O2D
25	s	613	CLA	CHA-CBD-CGD-O1D
25	s	613	CLA	CHA-CBD-CGD-O2D
25	y	602	CLA	CHA-CBD-CGD-O1D
25	y	602	CLA	CHA-CBD-CGD-O2D
26	S	1621	LUT	C29-C30-C31-C32
26	s	1621	LUT	C29-C30-C31-C32
25	2	611	CLA	CAA-CBA-CGA-O2A
25	6	611	CLA	CAA-CBA-CGA-O2A
24	2	609	CHL	C4-C3-C5-C6
24	6	609	CHL	C4-C3-C5-C6
35	Z	101	LMG	C20-C21-C22-C23
35	z	101	LMG	C20-C21-C22-C23
37	B	626	DGD	C6B-C7B-C8B-C9B
37	b	626	DGD	C6B-C7B-C8B-C9B
24	4	608	CHL	CAA-CBA-CGA-O1A
25	B	607	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C20
24	1	607	CHL	CAA-CBA-CGA-O2A
24	N	601	CHL	CAA-CBA-CGA-O2A
24	5	607	CHL	CAA-CBA-CGA-O2A
24	n	601	CHL	CAA-CBA-CGA-O2A
25	1	602	CLA	CAA-CBA-CGA-O2A
25	B	617	CLA	CAA-CBA-CGA-O2A
25	C	507	CLA	CAA-CBA-CGA-O2A
25	G	612	CLA	CAA-CBA-CGA-O2A
25	5	602	CLA	CAA-CBA-CGA-O2A
25	6	602	CLA	CAA-CBA-CGA-O2A
25	7	602	CLA	CAA-CBA-CGA-O2A
25	b	617	CLA	CAA-CBA-CGA-O2A
25	c	507	CLA	CAA-CBA-CGA-O2A
25	g	612	CLA	CAA-CBA-CGA-O2A
29	d	409	LHG	C29-C30-C31-C32
25	A	405	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	b	610	CLA	O1D-CGD-O2D-CED
29	2	2630	LHG	C13-C14-C15-C16
29	D	409	LHG	C29-C30-C31-C32
25	B	605	CLA	C13-C15-C16-C17
25	b	605	CLA	C13-C15-C16-C17
24	8	608	CHL	CAA-CBA-CGA-O1A
29	6	2630	LHG	C13-C14-C15-C16
24	2	607	CHL	CAA-CBA-CGA-O2A
24	3	607	CHL	CAA-CBA-CGA-O2A
24	6	607	CHL	CAA-CBA-CGA-O2A
25	2	602	CLA	CAA-CBA-CGA-O2A
29	D	410	LHG	O8-C23-C24-C25
29	d	410	LHG	O8-C23-C24-C25
25	B	610	CLA	O1D-CGD-O2D-CED
25	y	604	CLA	C2A-CAA-CBA-CGA
25	A	405	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	O1A-CGA-O2A-C1
25	3	602	CLA	CAA-CBA-CGA-O2A
25	G	611	CLA	CAA-CBA-CGA-O2A
25	R	603	CLA	CAA-CBA-CGA-O2A
34	A	412	SQD	O47-C7-C8-C9
34	a	412	SQD	O47-C7-C8-C9
24	N	606	CHL	O1A-CGA-O2A-C1
24	3	601	CHL	C11-C12-C13-C15
24	7	601	CHL	C11-C12-C13-C15
25	3	613	CLA	C6-C7-C8-C10
25	C	501	CLA	C11-C10-C8-C7
25	C	506	CLA	C6-C7-C8-C10
25	7	613	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C10-C8-C7
25	c	506	CLA	C6-C7-C8-C10
25	g	611	CLA	CAA-CBA-CGA-O2A
25	r	603	CLA	CAA-CBA-CGA-O2A
29	C	2630	LHG	O10-C23-O8-C6
35	B	622	LMG	C39-C40-C41-C42
25	3	613	CLA	C6-C7-C8-C9
25	B	608	CLA	C14-C13-C15-C16
25	C	501	CLA	C11-C10-C8-C9
25	C	506	CLA	C6-C7-C8-C9
25	G	602	CLA	C11-C12-C13-C14
25	7	613	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C14-C13-C15-C16
25	c	501	CLA	C11-C10-C8-C9
25	c	506	CLA	C6-C7-C8-C9
25	g	602	CLA	C11-C12-C13-C14
37	B	626	DGD	C4D-C5D-C6D-O5D
37	b	626	DGD	C4D-C5D-C6D-O5D
26	1	1621	LUT	C9-C10-C11-C12
26	5	1621	LUT	C9-C10-C11-C12
24	n	606	CHL	O1A-CGA-O2A-C1
29	c	2630	LHG	O10-C23-O8-C6
24	5	601	CHL	CAA-CBA-CGA-O1A
35	D	411	LMG	C15-C16-C17-C18
35	b	622	LMG	C39-C40-C41-C42
35	d	411	LMG	C15-C16-C17-C18
25	B	614	CLA	CBA-CGA-O2A-C1
25	b	614	CLA	CBA-CGA-O2A-C1
24	7	607	CHL	CAA-CBA-CGA-O2A
29	G	2630	LHG	O8-C23-C24-C25
29	g	2630	LHG	O8-C23-C24-C25
34	A	412	SQD	C4-C5-C6-S
34	a	412	SQD	C4-C5-C6-S
24	1	601	CHL	CAA-CBA-CGA-O1A
25	S	609	CLA	CAA-CBA-CGA-O1A
25	s	609	CLA	CAA-CBA-CGA-O1A
25	3	613	CLA	C2A-CAA-CBA-CGA
25	7	613	CLA	C2A-CAA-CBA-CGA
36	D	405	PL9	C46-C47-C48-C49
36	d	405	PL9	C46-C47-C48-C49
24	N	607	CHL	C4C-C3C-CAC-CBC
24	n	607	CHL	C4C-C3C-CAC-CBC
25	C	510	CLA	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
29	L	101	LHG	O7-C7-C8-C9
29	l	101	LHG	O7-C7-C8-C9
25	C	502	CLA	C13-C15-C16-C17
25	c	502	CLA	C13-C15-C16-C17
29	G	2630	LHG	C30-C31-C32-C33
29	g	2630	LHG	C30-C31-C32-C33
25	6	603	CLA	CAA-CBA-CGA-O1A
25	R	602	CLA	C4-C3-C5-C6
25	r	602	CLA	C4-C3-C5-C6
25	B	607	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	607	CLA	C2-C3-C5-C6
35	A	415	LMG	O8-C28-C29-C30
35	a	415	LMG	O8-C28-C29-C30
24	2	601	CHL	CAA-CBA-CGA-O2A
24	6	601	CHL	CAA-CBA-CGA-O2A
25	2	603	CLA	CAA-CBA-CGA-O1A
29	C	2630	LHG	O9-C7-C8-C9
29	C	522	LHG	O9-C7-C8-C9
29	L	101	LHG	O9-C7-C8-C9
29	c	2630	LHG	O9-C7-C8-C9
29	c	522	LHG	O9-C7-C8-C9
29	l	101	LHG	O9-C7-C8-C9
27	R	622	XAT	C11-C12-C13-C14
27	r	622	XAT	C11-C12-C13-C14
28	R	623	NEX	C11-C12-C13-C14
28	r	623	NEX	C11-C12-C13-C14
30	C	515	BCR	C17-C18-C19-C20
30	c	515	BCR	C17-C18-C19-C20
25	S	611	CLA	C5-C6-C7-C8
25	s	611	CLA	C5-C6-C7-C8
24	3	609	CHL	C1A-C2A-CAA-CBA
24	4	601	CHL	C1A-C2A-CAA-CBA
24	4	609	CHL	C1A-C2A-CAA-CBA
24	7	609	CHL	C1A-C2A-CAA-CBA
24	8	601	CHL	C1A-C2A-CAA-CBA
24	8	609	CHL	C1A-C2A-CAA-CBA
25	2	612	CLA	C1A-C2A-CAA-CBA
25	4	612	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	6	612	CLA	C1A-C2A-CAA-CBA
25	8	612	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	S	604	CLA	CAA-CBA-CGA-O1A
25	s	604	CLA	CAA-CBA-CGA-O1A
29	G	2630	LHG	O10-C23-C24-C25
35	d	411	LMG	C11-C10-O7-C8
24	3	607	CHL	C2-C1-O2A-CGA
24	7	607	CHL	C2-C1-O2A-CGA
29	D	409	LHG	C10-C11-C12-C13
29	d	409	LHG	C10-C11-C12-C13
35	D	411	LMG	C13-C14-C15-C16
25	3	611	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	y	612	CLA	CAA-CBA-CGA-O1A
29	g	2630	LHG	O10-C23-C24-C25
34	B	623	SQD	O49-C7-C8-C9
29	c	2630	LHG	C12-C13-C14-C15
35	d	411	LMG	C13-C14-C15-C16
29	C	2630	LHG	C12-C13-C14-C15
25	C	513	CLA	C2A-CAA-CBA-CGA
25	R	610	CLA	C2A-CAA-CBA-CGA
25	c	513	CLA	C2A-CAA-CBA-CGA
25	r	610	CLA	C2A-CAA-CBA-CGA
25	B	611	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C19
25	Y	612	CLA	CAA-CBA-CGA-O1A
25	7	611	CLA	CAA-CBA-CGA-O1A
34	b	623	SQD	O49-C7-C8-C9
25	B	606	CLA	C13-C15-C16-C17
25	b	606	CLA	C13-C15-C16-C17
24	3	607	CHL	CAA-CBA-CGA-O1A
24	7	607	CHL	CAA-CBA-CGA-O1A
25	G	612	CLA	CAA-CBA-CGA-O1A
25	R	603	CLA	CAA-CBA-CGA-O1A
25	g	612	CLA	CAA-CBA-CGA-O1A
25	r	603	CLA	CAA-CBA-CGA-O1A
29	C	2630	LHG	O10-C23-C24-C25
29	N	2630	LHG	O10-C23-C24-C25
29	c	2630	LHG	O10-C23-C24-C25
25	2	603	CLA	C5-C6-C7-C8
25	C	507	CLA	C5-C6-C7-C8
25	6	603	CLA	C5-C6-C7-C8
25	c	507	CLA	C5-C6-C7-C8
29	3	2630	LHG	C3-O3-P-O5
29	B	2631	LHG	C4-O6-P-O5
29	D	409	LHG	C3-O3-P-O5
29	R	2630	LHG	C3-O3-P-O5
29	7	2630	LHG	C3-O3-P-O5
29	b	2631	LHG	C4-O6-P-O5
29	d	409	LHG	C3-O3-P-O5
29	r	2630	LHG	C3-O3-P-O5
35	D	411	LMG	C11-C10-O7-C8
25	C	501	CLA	CAA-CBA-CGA-O1A
25	C	507	CLA	CAA-CBA-CGA-O1A
25	C	510	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	c	507	CLA	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
29	D	410	LHG	O10-C23-C24-C25
29	d	410	LHG	O10-C23-C24-C25
29	n	2630	LHG	O10-C23-C24-C25
37	C	520	DGD	O1B-C1B-C2B-C3B
37	c	520	DGD	O1B-C1B-C2B-C3B
25	R	611	CLA	O2A-C1-C2-C3
25	r	611	CLA	O2A-C1-C2-C3
26	G	1621	LUT	C1-C6-C7-C8
26	g	1621	LUT	C1-C6-C7-C8
24	1	609	CHL	C5-C6-C7-C8
24	5	609	CHL	C5-C6-C7-C8
25	c	501	CLA	CAA-CBA-CGA-O1A
37	c	519	DGD	O1B-C1B-C2B-C3B
29	3	2630	LHG	C9-C10-C11-C12
29	7	2630	LHG	C9-C10-C11-C12
37	b	626	DGD	C3B-C4B-C5B-C6B
25	Y	610	CLA	C2A-CAA-CBA-CGA
25	y	610	CLA	C2A-CAA-CBA-CGA
25	b	617	CLA	CAA-CBA-CGA-O1A
37	C	519	DGD	O1B-C1B-C2B-C3B
25	s	602	CLA	O1A-CGA-O2A-C1
37	B	626	DGD	C3B-C4B-C5B-C6B
24	S	607	CHL	CAA-CBA-CGA-O2A
24	s	607	CHL	CAA-CBA-CGA-O2A
29	C	522	LHG	O7-C7-C8-C9
29	c	522	LHG	O7-C7-C8-C9
25	B	617	CLA	CAA-CBA-CGA-O1A
25	S	613	CLA	C4-C3-C5-C6
25	s	613	CLA	C4-C3-C5-C6
24	1	607	CHL	CAD-CBD-CGD-O1D
24	G	601	CHL	CAD-CBD-CGD-O1D
24	5	607	CHL	CAD-CBD-CGD-O1D
24	g	601	CHL	CAD-CBD-CGD-O1D
25	B	610	CLA	CAD-CBD-CGD-O1D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	C	511	CLA	CAD-CBD-CGD-O1D
25	S	611	CLA	CAD-CBD-CGD-O1D
25	b	610	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	c	511	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	s	611	CLA	CAD-CBD-CGD-O1D
35	B	2633	LMG	C7-C8-O7-C10
35	b	2633	LMG	C7-C8-O7-C10
25	S	602	CLA	O1A-CGA-O2A-C1
24	2	607	CHL	CAA-CBA-CGA-O1A
25	2	602	CLA	CAA-CBA-CGA-O1A
25	3	602	CLA	CAA-CBA-CGA-O1A
25	6	602	CLA	CAA-CBA-CGA-O1A
25	7	602	CLA	CAA-CBA-CGA-O1A
25	C	506	CLA	C5-C6-C7-C8
25	c	506	CLA	C5-C6-C7-C8
24	N	607	CHL	C11-C12-C13-C14
24	n	607	CHL	C11-C12-C13-C14
25	2	602	CLA	C6-C7-C8-C9
25	R	603	CLA	C11-C10-C8-C9
25	6	602	CLA	C6-C7-C8-C9
25	r	603	CLA	C11-C10-C8-C9
25	2	611	CLA	CAA-CBA-CGA-O1A
25	6	611	CLA	CAA-CBA-CGA-O1A
29	D	410	LHG	C23-C24-C25-C26
29	d	410	LHG	C23-C24-C25-C26
24	6	607	CHL	CAA-CBA-CGA-O1A
29	B	2631	LHG	C11-C12-C13-C14
29	b	2631	LHG	C11-C12-C13-C14
24	N	606	CHL	CAA-CBA-CGA-O2A
24	Y	601	CHL	CAA-CBA-CGA-O2A
24	n	606	CHL	CAA-CBA-CGA-O2A
24	y	601	CHL	CAA-CBA-CGA-O2A
35	a	413	LMG	O10-C28-C29-C30
29	2	2630	LHG	C10-C11-C12-C13
29	6	2630	LHG	C10-C11-C12-C13
25	Y	603	CLA	C2A-CAA-CBA-CGA
25	y	603	CLA	C2A-CAA-CBA-CGA
25	1	613	CLA	CAA-CBA-CGA-O2A
25	Y	602	CLA	CAA-CBA-CGA-O2A
25	5	613	CLA	CAA-CBA-CGA-O2A
25	n	602	CLA	CAA-CBA-CGA-O2A
25	y	602	CLA	CAA-CBA-CGA-O2A
25	g	610	CLA	C16-C17-C18-C19
24	N	601	CHL	CAA-CBA-CGA-O1A
24	n	601	CHL	CAA-CBA-CGA-O1A
25	5	602	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
37	C	519	DGD	C7A-C8A-C9A-CAA
29	N	2630	LHG	C5-C4-O6-P
29	n	2630	LHG	C5-C4-O6-P
25	R	613	CLA	C4-C3-C5-C6
25	r	613	CLA	C4-C3-C5-C6
25	G	610	CLA	C16-C17-C18-C19
37	c	519	DGD	C7A-C8A-C9A-CAA
24	2	607	CHL	C11-C10-C8-C7
24	G	607	CHL	C11-C10-C8-C7
24	G	608	CHL	C3A-C2A-CAA-CBA
24	Y	609	CHL	C11-C12-C13-C15
24	6	607	CHL	C11-C10-C8-C7
24	g	607	CHL	C11-C10-C8-C7
24	g	608	CHL	C3A-C2A-CAA-CBA
24	y	609	CHL	C11-C12-C13-C15
25	2	602	CLA	C2-C3-C5-C6
25	2	602	CLA	C6-C7-C8-C10
25	2	612	CLA	C3A-C2A-CAA-CBA
25	3	602	CLA	C11-C10-C8-C7
25	4	604	CLA	C3A-C2A-CAA-CBA
25	4	612	CLA	C3A-C2A-CAA-CBA
25	B	602	CLA	C12-C13-C15-C16
25	B	608	CLA	C12-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C10
25	C	502	CLA	C11-C12-C13-C15
25	G	602	CLA	C11-C12-C13-C15
25	6	602	CLA	C2-C3-C5-C6
25	6	602	CLA	C6-C7-C8-C10
25	6	612	CLA	C3A-C2A-CAA-CBA
25	7	602	CLA	C11-C10-C8-C7
25	8	604	CLA	C3A-C2A-CAA-CBA
25	8	612	CLA	C3A-C2A-CAA-CBA
25	b	602	CLA	C12-C13-C15-C16
25	b	608	CLA	C12-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C10
25	c	502	CLA	C11-C12-C13-C15
25	g	602	CLA	C11-C12-C13-C15
24	1	607	CHL	CAA-CBA-CGA-O1A
24	5	607	CHL	CAA-CBA-CGA-O1A
25	1	602	CLA	CAA-CBA-CGA-O1A
25	G	611	CLA	CAA-CBA-CGA-O1A
25	b	614	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	g	611	CLA	CAA-CBA-CGA-O1A
35	A	413	LMG	O10-C28-C29-C30
35	Z	101	LMG	O10-C28-C29-C30
24	G	601	CHL	CAA-CBA-CGA-O2A
24	g	601	CHL	CAA-CBA-CGA-O2A
25	B	614	CLA	CAA-CBA-CGA-O2A
25	N	602	CLA	CAA-CBA-CGA-O2A
25	N	612	CLA	CAA-CBA-CGA-O2A
25	n	612	CLA	CAA-CBA-CGA-O2A
29	l	101	LHG	C23-C24-C25-C26
26	S	1621	LUT	C7-C8-C9-C10
26	s	1621	LUT	C7-C8-C9-C10
27	4	622	XAT	C27-C28-C29-C30
27	8	622	XAT	C27-C28-C29-C30
28	1	1623	NEX	C31-C32-C33-C34
28	5	1623	NEX	C31-C32-C33-C34
30	4	623	BCR	C17-C18-C19-C20
30	8	623	BCR	C17-C18-C19-C20
24	G	601	CHL	CAA-CBA-CGA-O1A
24	g	601	CHL	CAA-CBA-CGA-O1A
25	B	614	CLA	CAA-CBA-CGA-O1A
25	Y	602	CLA	CAA-CBA-CGA-O1A
25	n	602	CLA	CAA-CBA-CGA-O1A
25	y	602	CLA	CAA-CBA-CGA-O1A
35	z	101	LMG	O10-C28-C29-C30
27	2	1622	XAT	C13-C14-C15-C35
27	6	1622	XAT	C13-C14-C15-C35
29	3	2630	LHG	C17-C18-C19-C20
29	7	2630	LHG	C17-C18-C19-C20
25	B	610	CLA	C16-C17-C18-C19
25	b	614	CLA	CAA-CBA-CGA-O2A
25	R	610	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
25	r	610	CLA	C10-C11-C12-C13
24	Y	601	CHL	CAA-CBA-CGA-O1A
24	y	601	CHL	CAA-CBA-CGA-O1A
25	N	602	CLA	CAA-CBA-CGA-O1A
24	2	605	CHL	CAA-CBA-CGA-O2A
24	6	605	CHL	CAA-CBA-CGA-O2A
25	N	610	CLA	C8-C10-C11-C12
25	S	610	CLA	C5-C6-C7-C8
25	n	610	CLA	C8-C10-C11-C12

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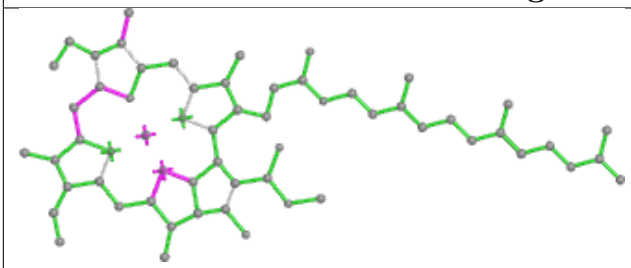
Mol	Chain	Res	Type	Atoms
25	s	610	CLA	C5-C6-C7-C8
29	Y	2630	LHG	C11-C10-C9-C8
29	y	2630	LHG	C11-C10-C9-C8
34	A	418	SQD	C15-C16-C17-C18
25	C	510	CLA	C10-C11-C12-C13
25	N	611	CLA	C10-C11-C12-C13
25	n	611	CLA	C10-C11-C12-C13
24	N	606	CHL	CAA-CBA-CGA-O1A
24	4	606	CHL	C2A-CAA-CBA-CGA
24	8	606	CHL	C2A-CAA-CBA-CGA
25	b	610	CLA	C16-C17-C18-C19
25	B	603	CLA	C8-C10-C11-C12
25	b	603	CLA	C8-C10-C11-C12
33	A	409	PHO	C8-C10-C11-C12
33	a	409	PHO	C8-C10-C11-C12
34	a	418	SQD	C15-C16-C17-C18
29	L	101	LHG	C23-C24-C25-C26
24	n	606	CHL	CAA-CBA-CGA-O1A
24	g	605	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

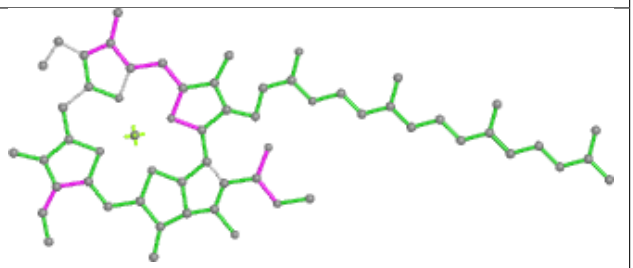
No monomer is involved in short contacts.

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

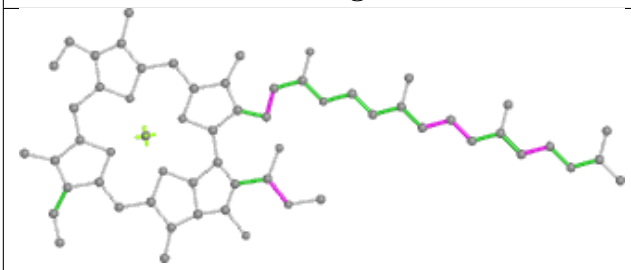
Ligand CLA n 613



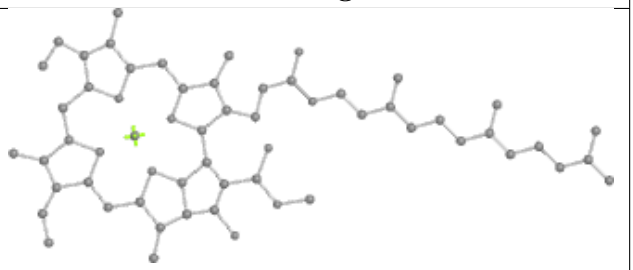
Bond lengths



Bond angles

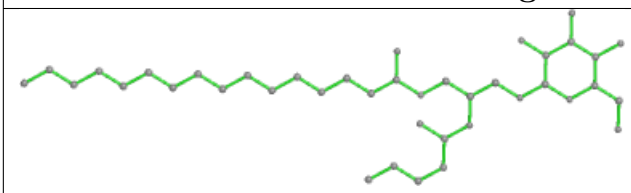


Torsions



Rings

Ligand LMG A 415



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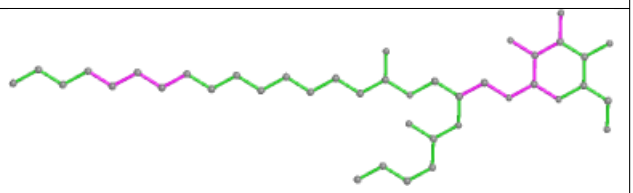
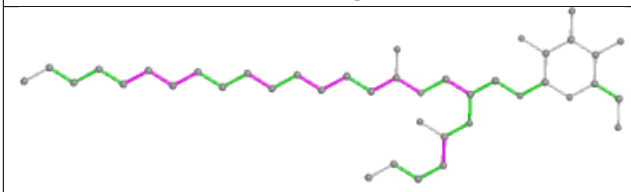


Bond angles



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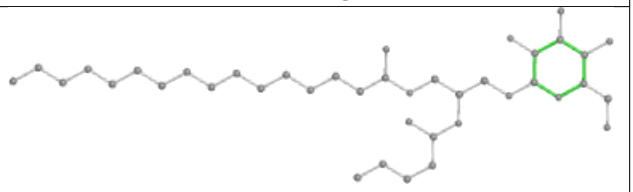
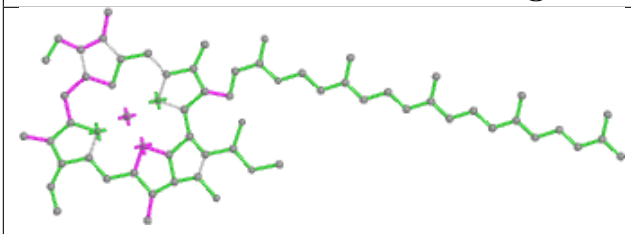
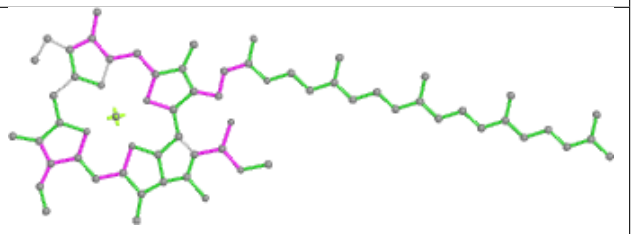


Rings

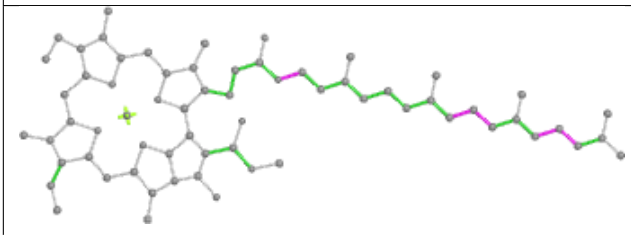
Ligand CLA d 402



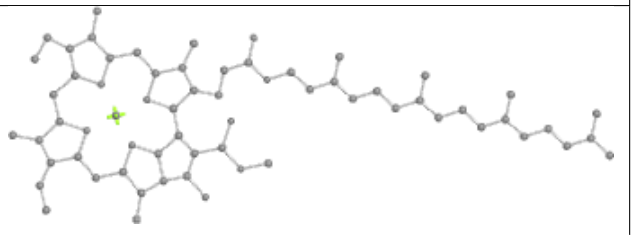
Bond lengths



Bond angles

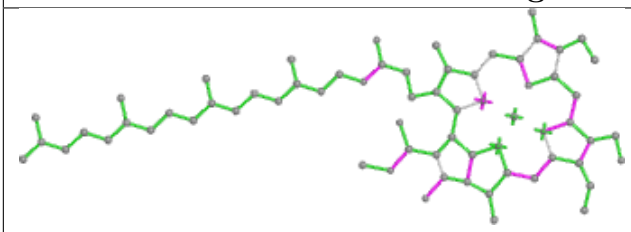


Torsions

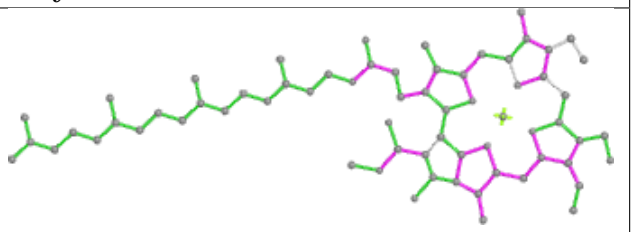


Rings

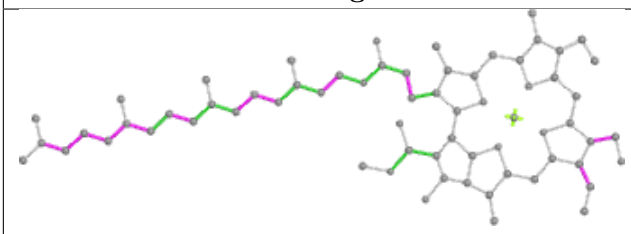
Ligand CHL y 607



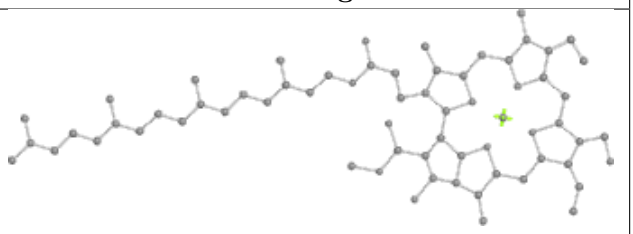
Bond lengths



Bond angles

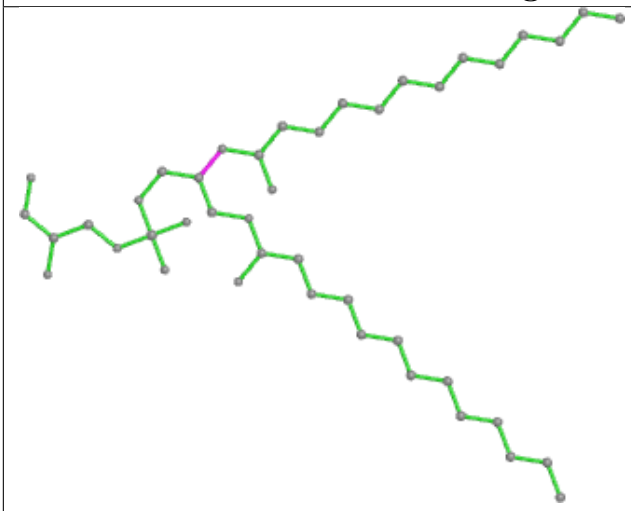


Torsions

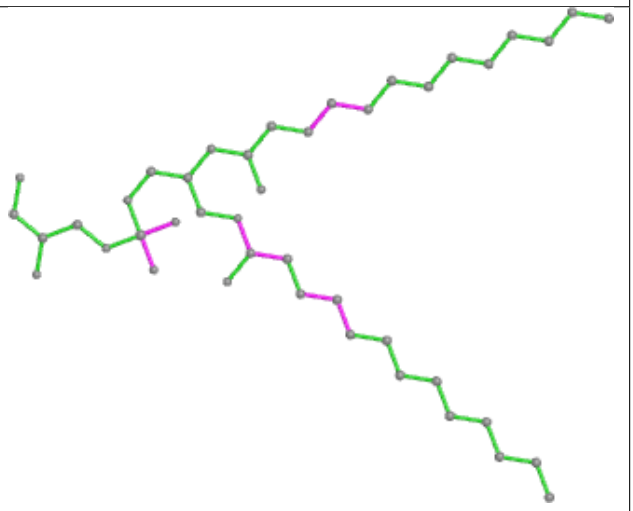


Rings

Ligand LHG D 410



Bond lengths



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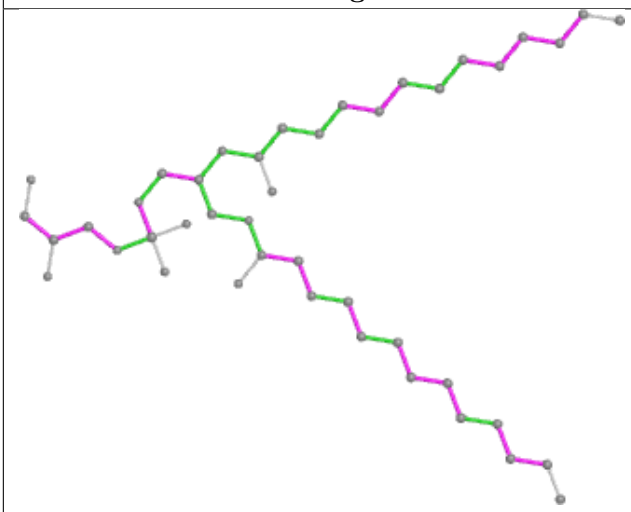
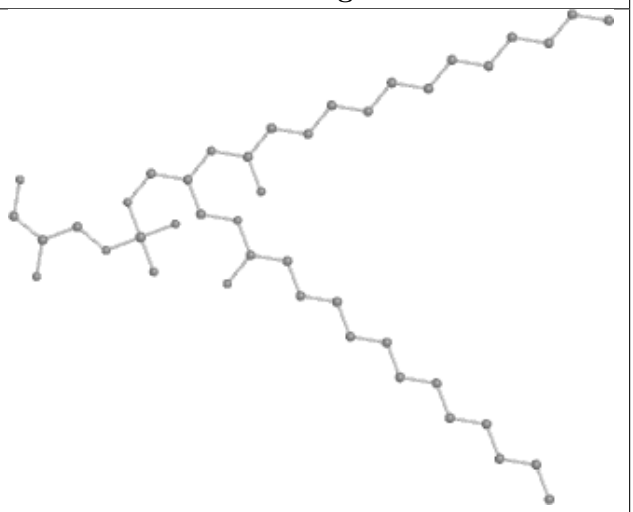
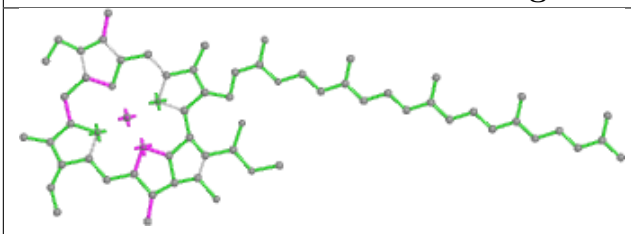
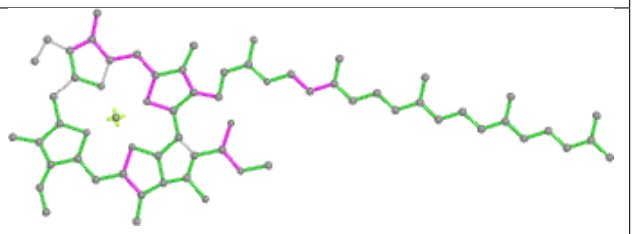
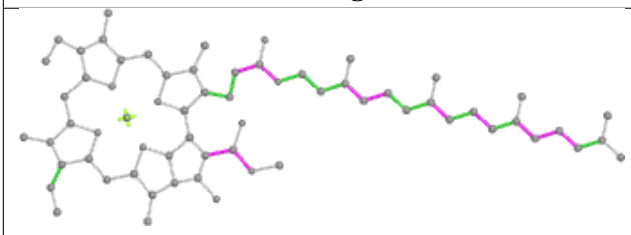
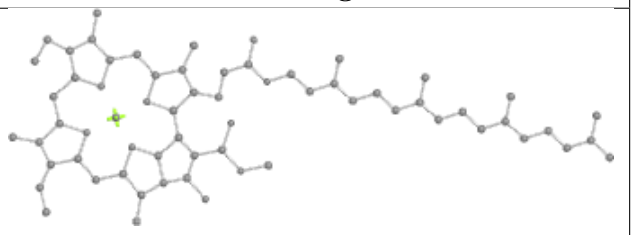
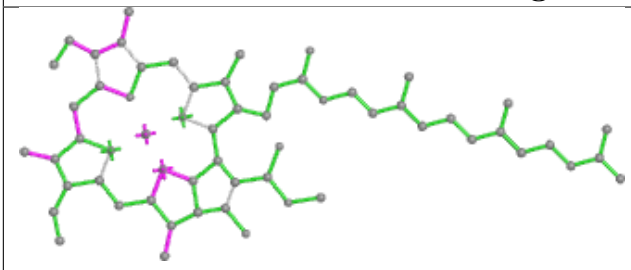
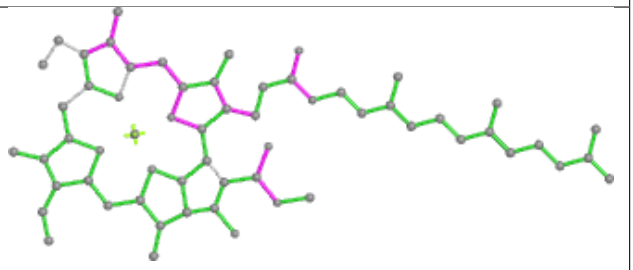
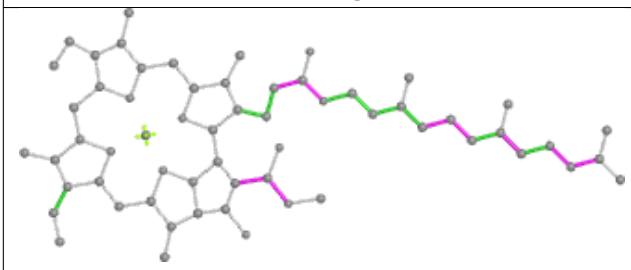
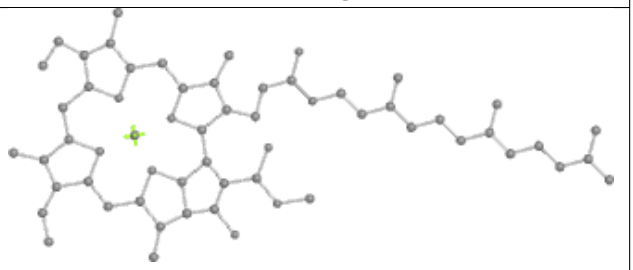


Torsions

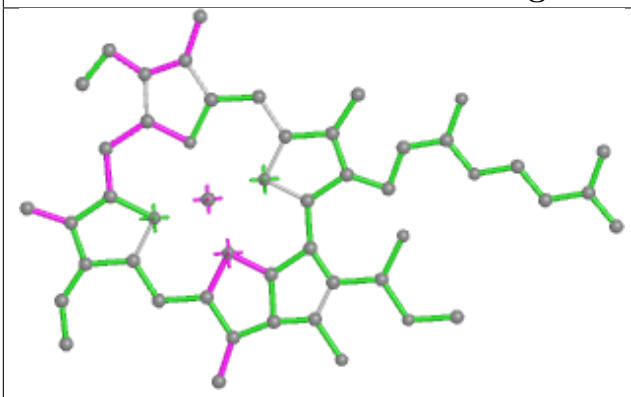


Rings

Ligand CLA c 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 604



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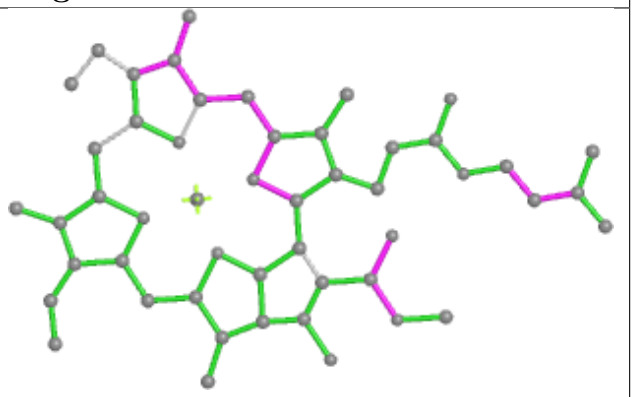
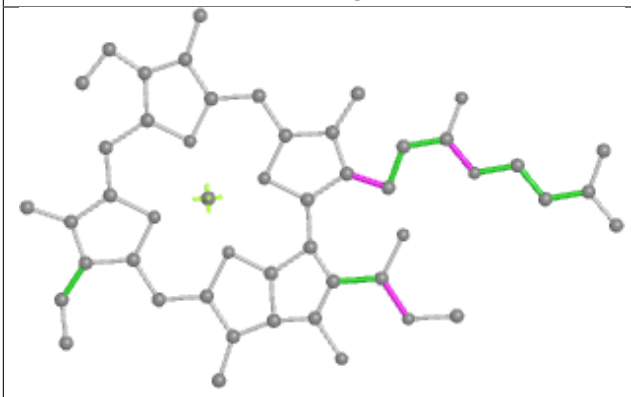


Bond angles



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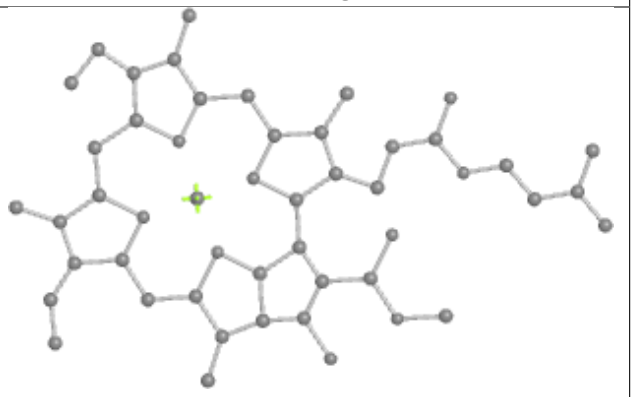
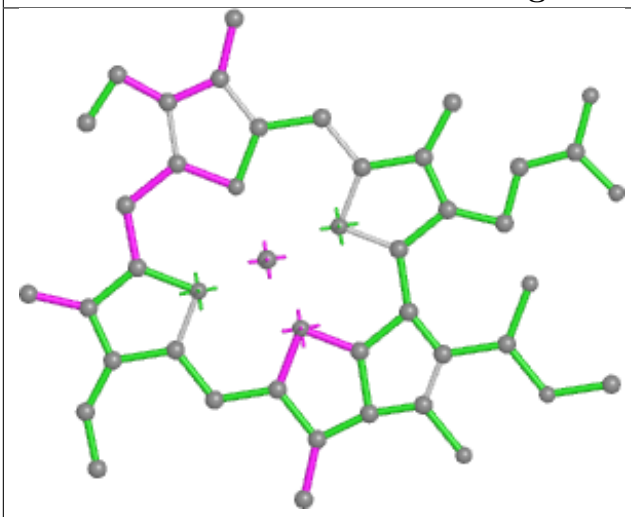


Rings

Ligand CLA 1 612



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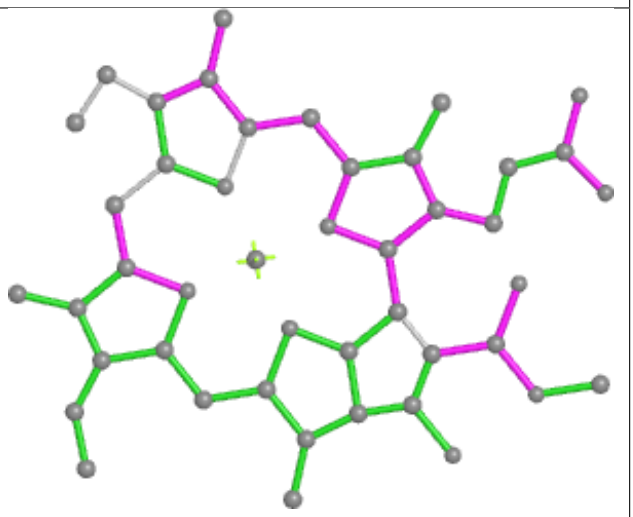

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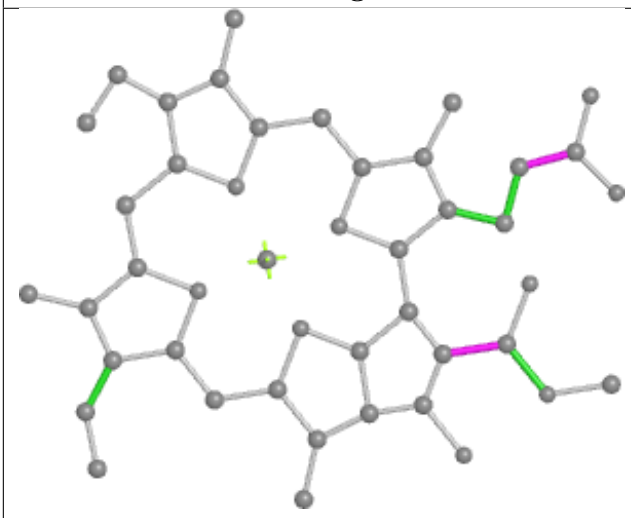

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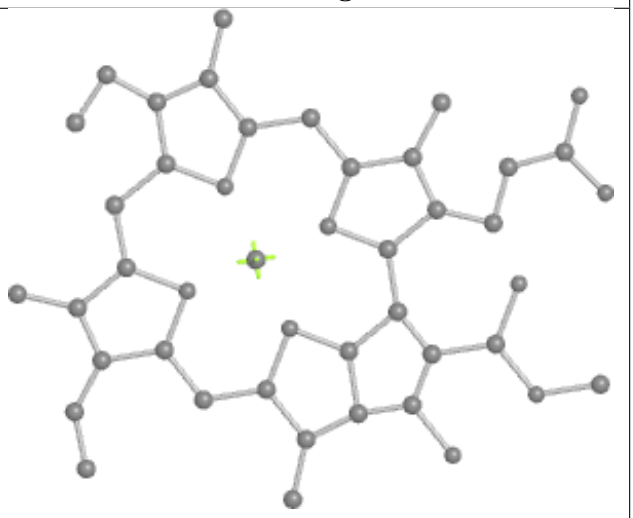
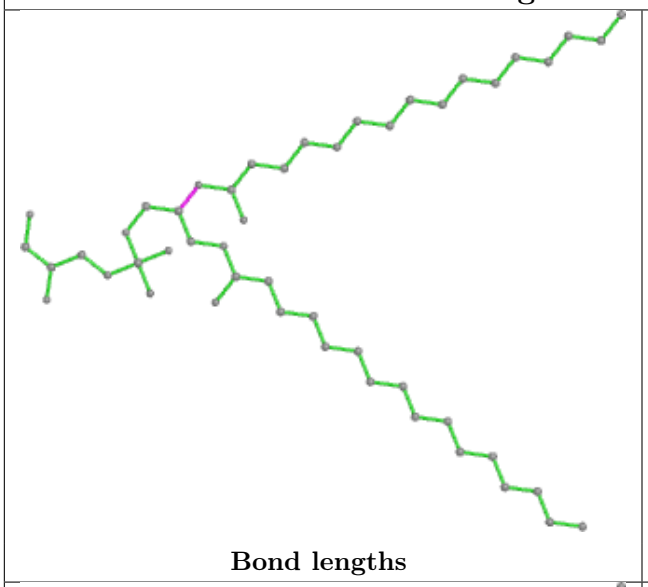
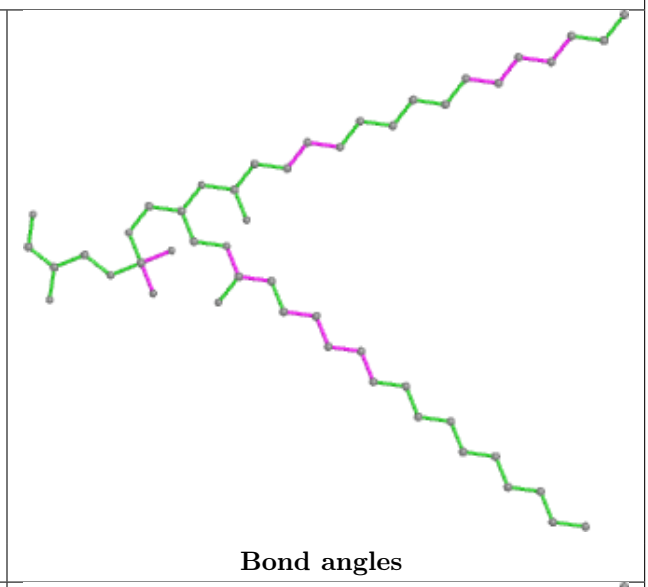


Rings

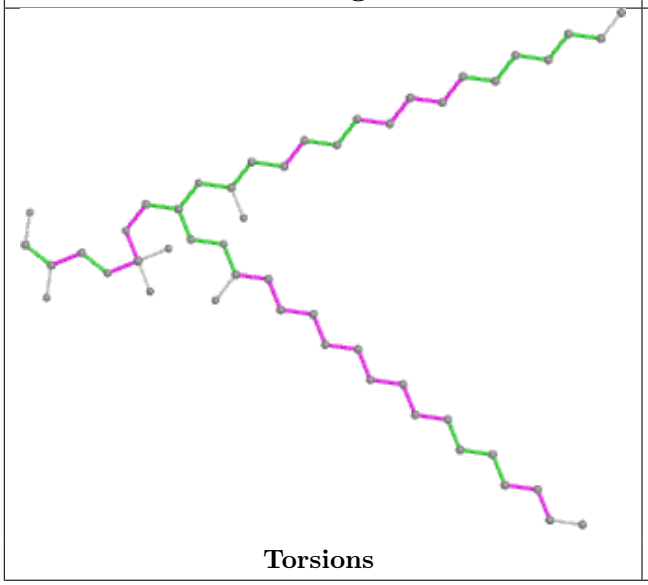
Ligand LHG n 2630



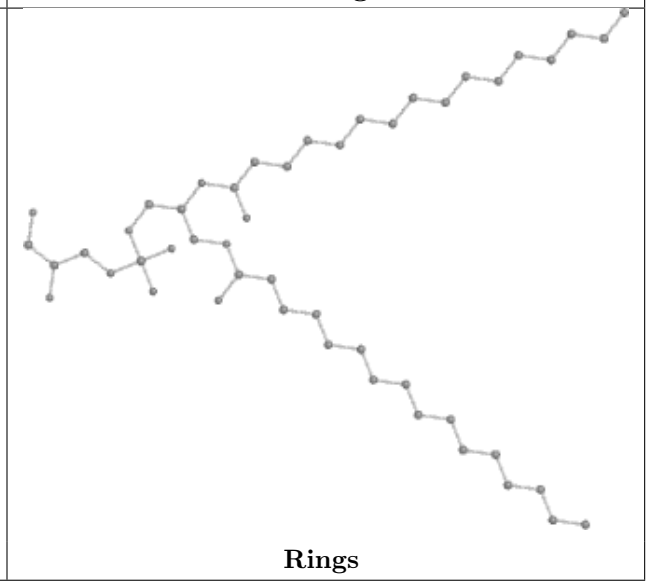
Bond lengths



Bond angles

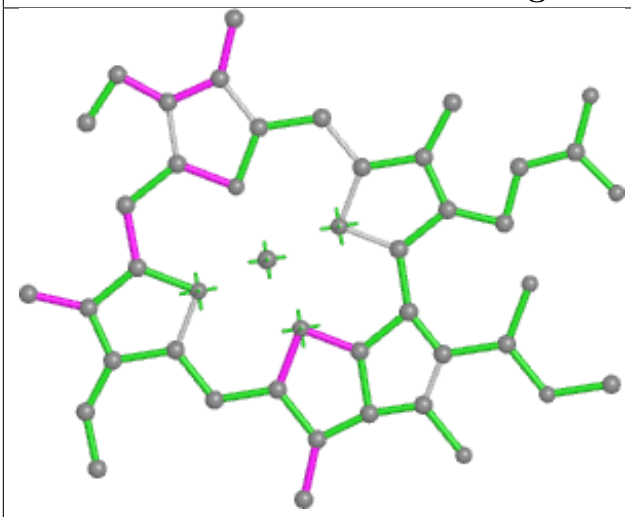


Torsions



Rings

Ligand CLA 4 611



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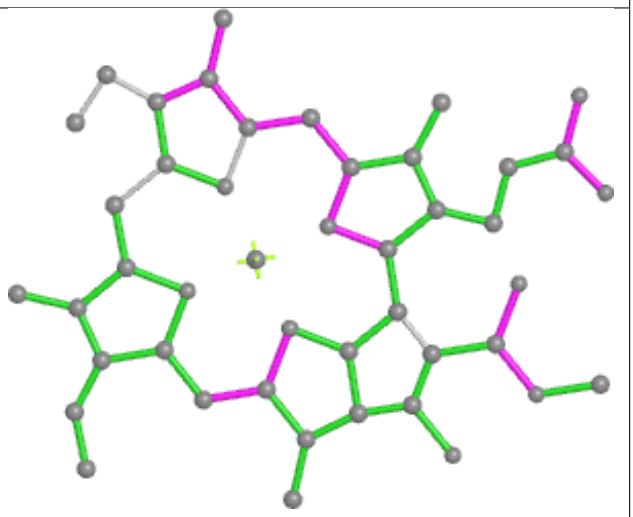

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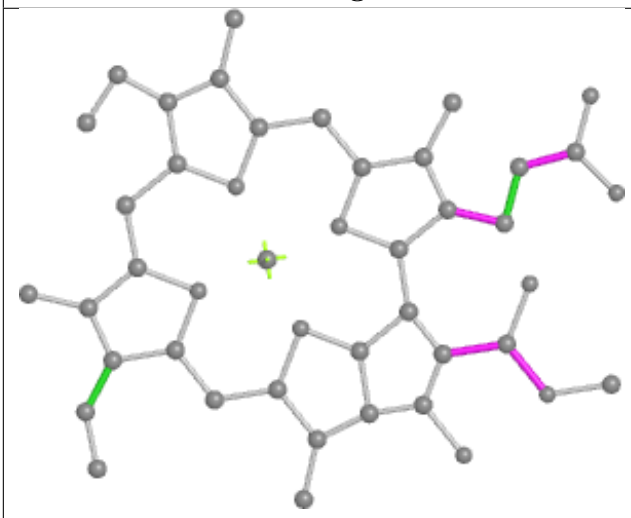

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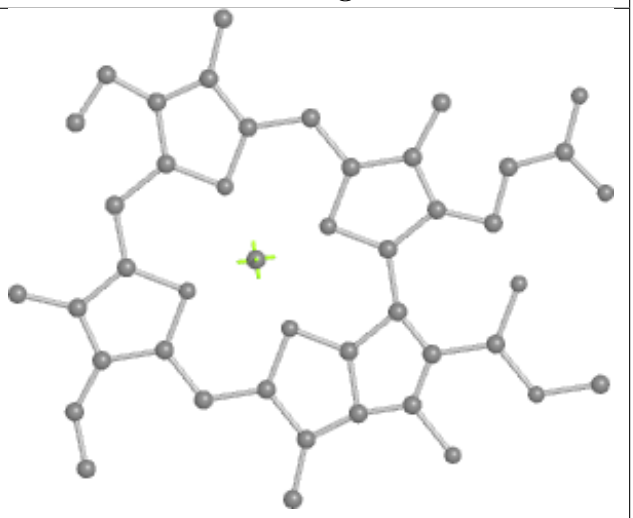
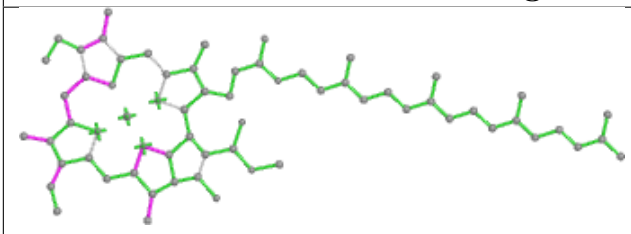


Rings

Ligand CLA A 406



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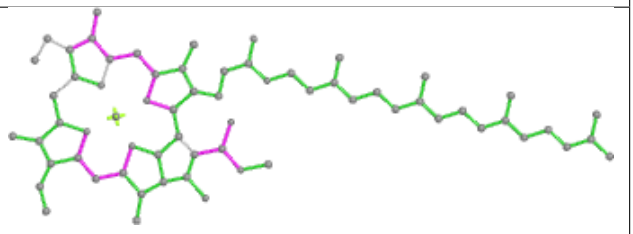

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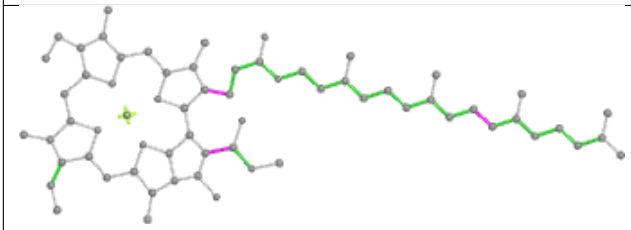

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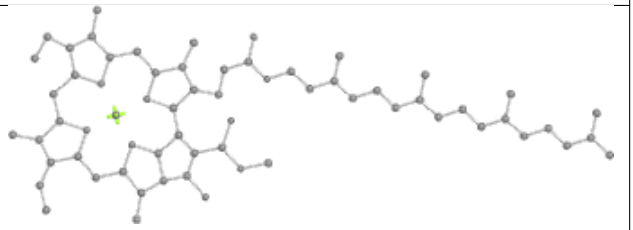
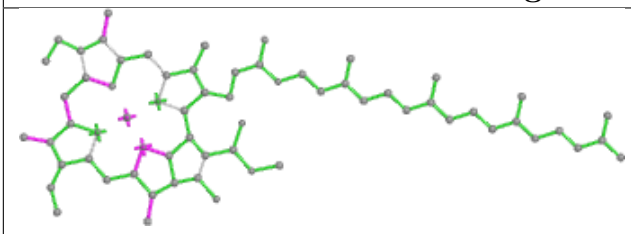


Rings

Ligand CLA C 509



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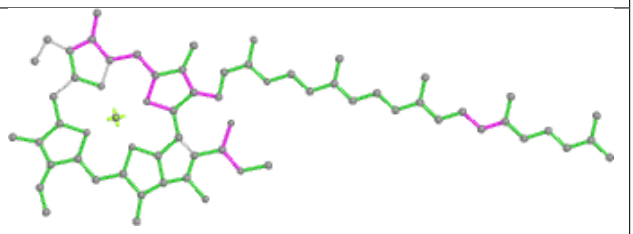
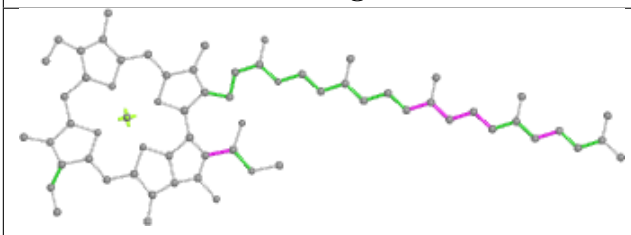


Bond angles



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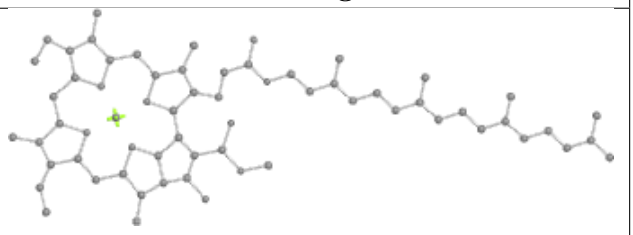
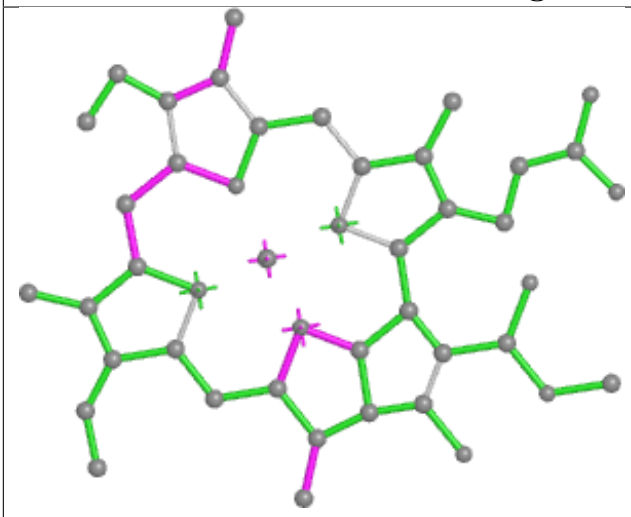


Rings

Ligand CLA 6 612



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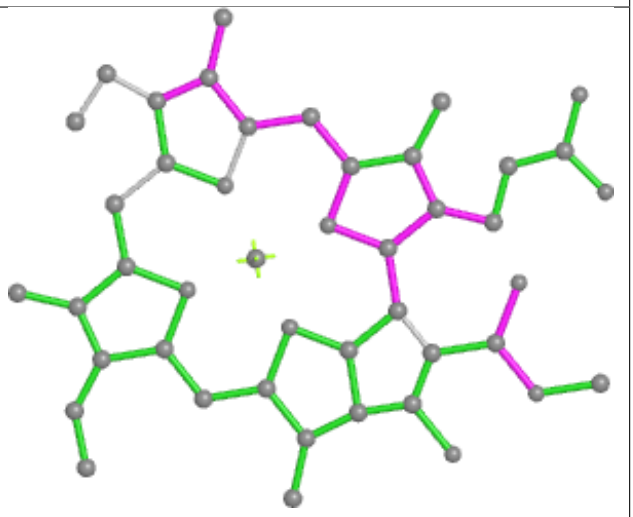

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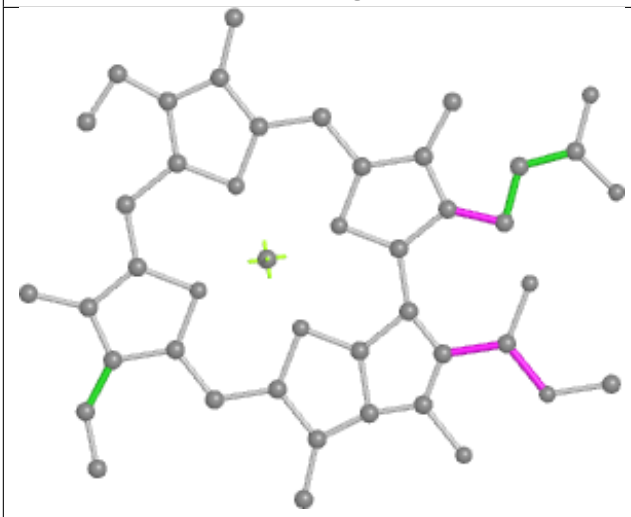

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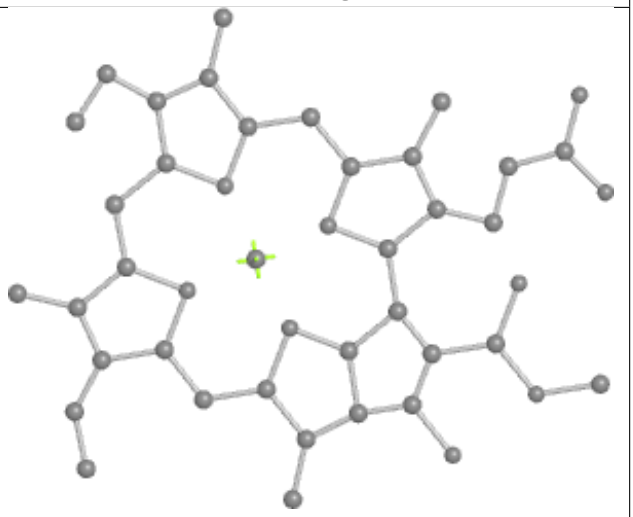
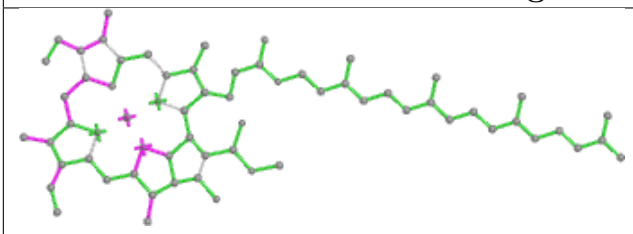


Rings

Ligand CLA b 606



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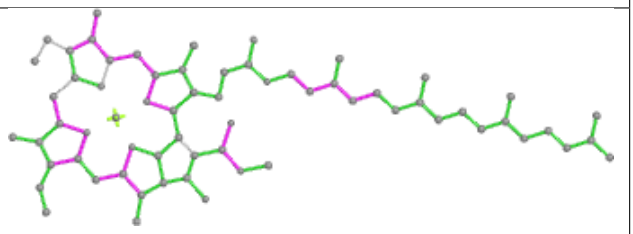

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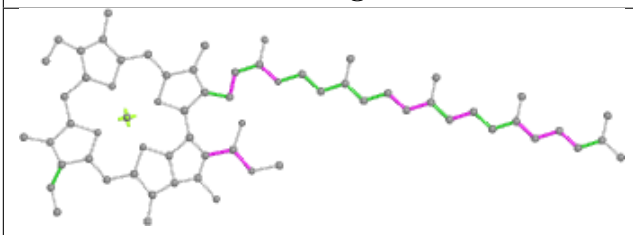

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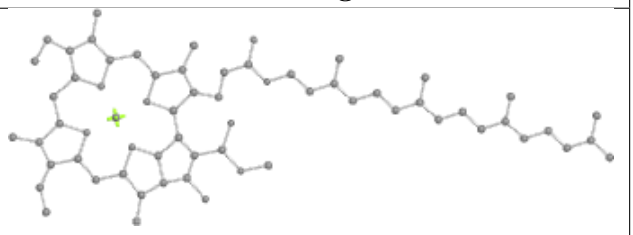
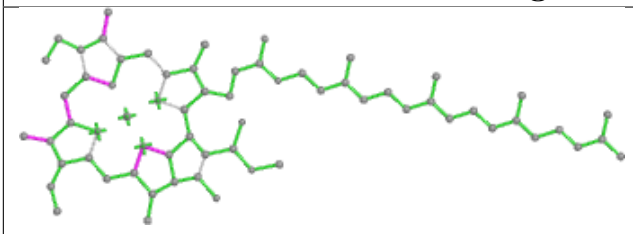


Rings

Ligand CLA c 502



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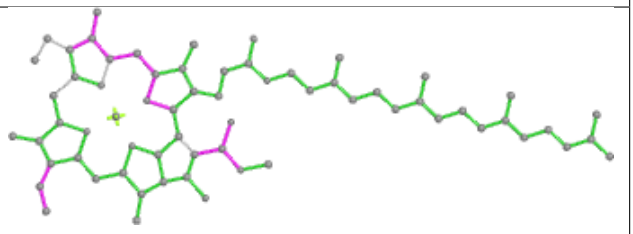
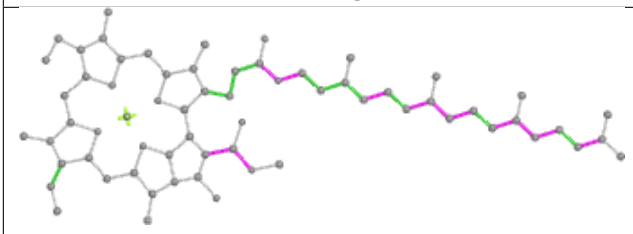


Bond angles



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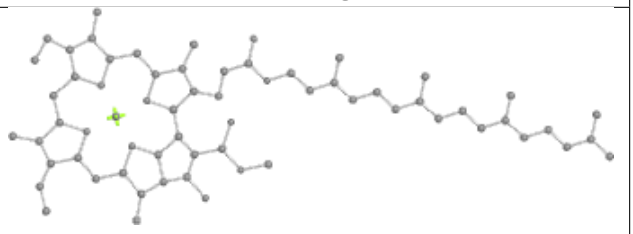
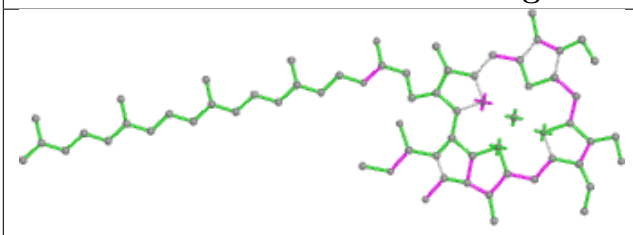


Rings

Ligand CHL N 601



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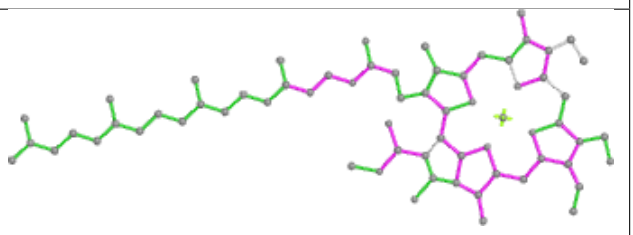

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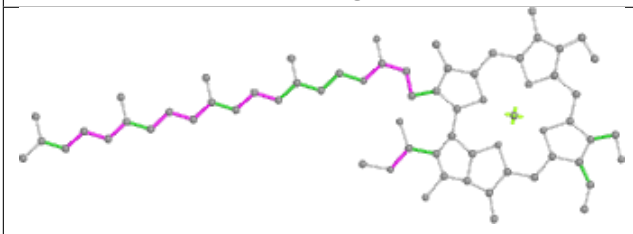

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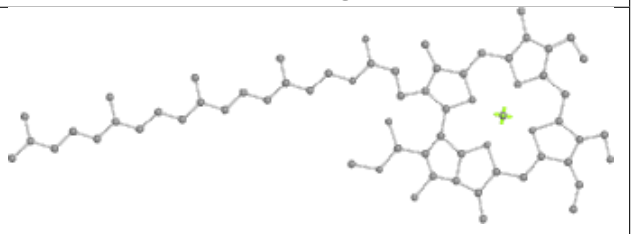
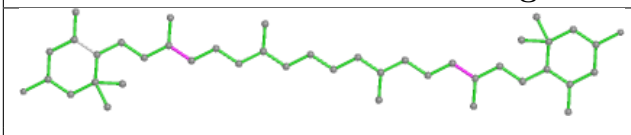


Rings

Ligand LUT 1 1620



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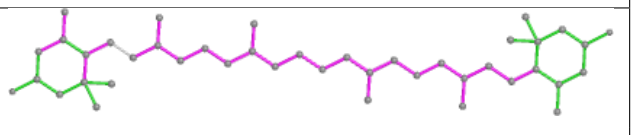
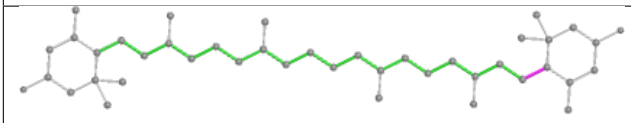


Bond angles



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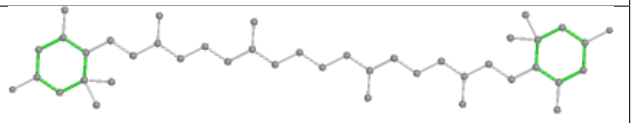
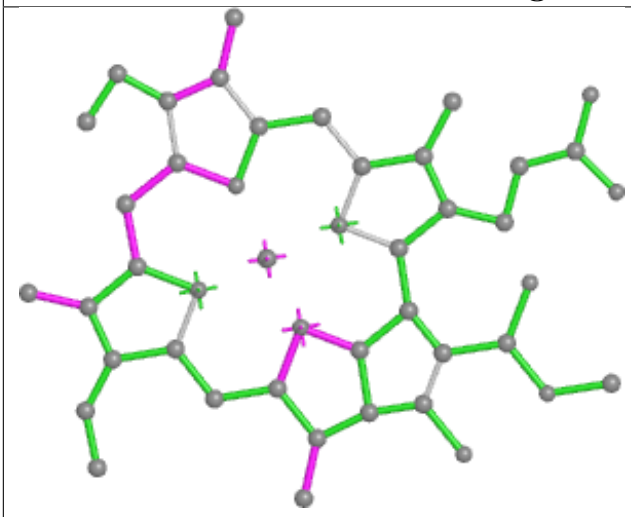


Rings

Ligand CLA 2 604



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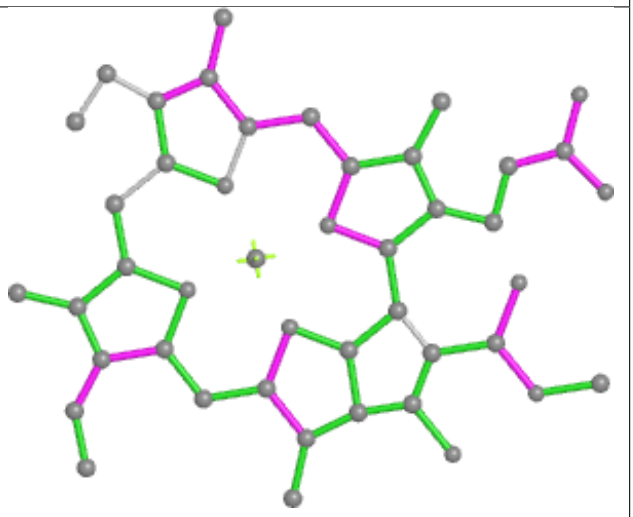

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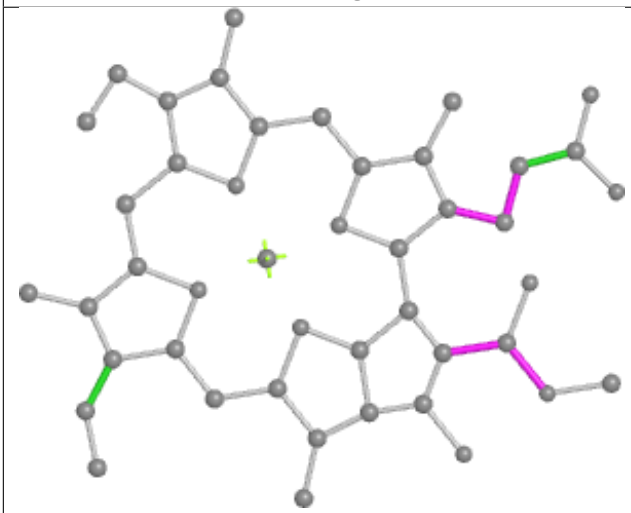

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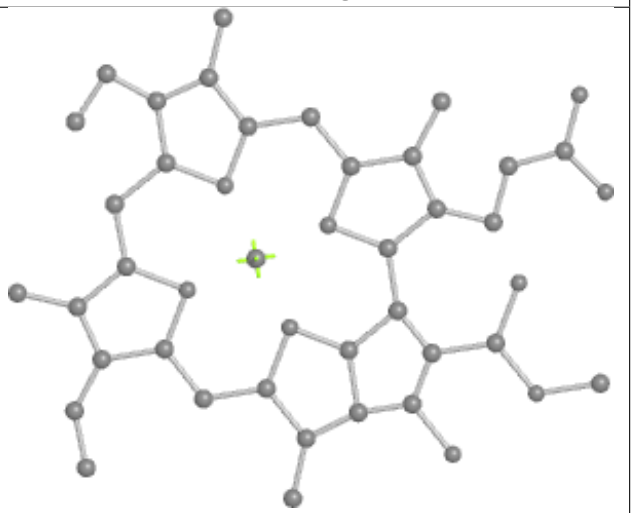
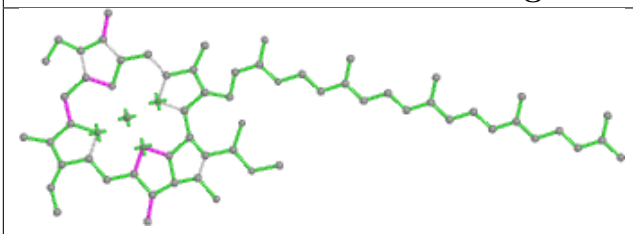


Rings

Ligand CLA C 503



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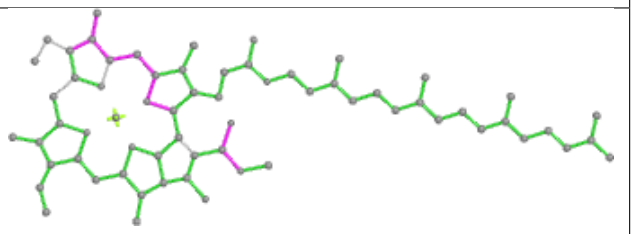
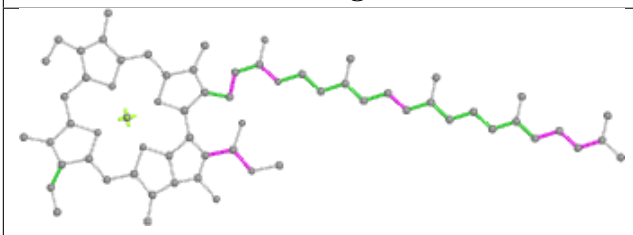


Bond angles



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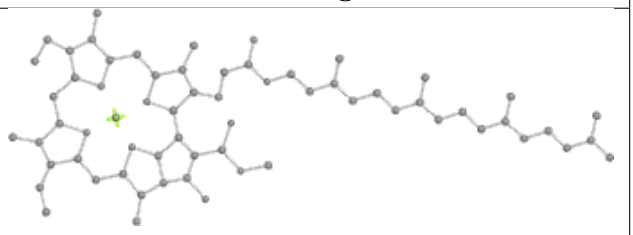
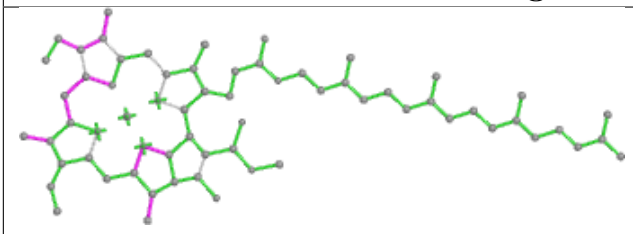


Rings

Ligand CLA n 610



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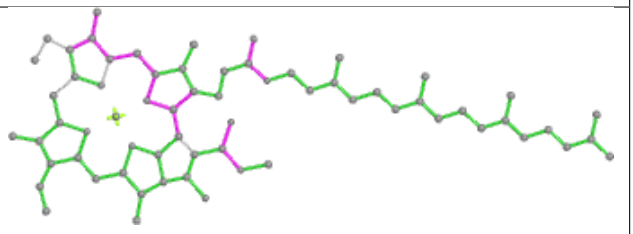
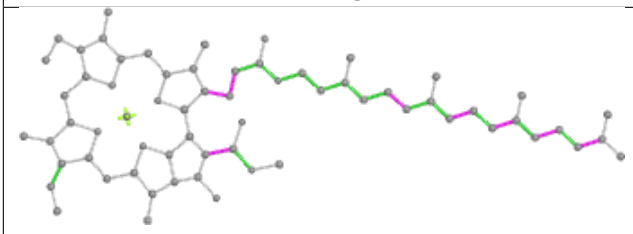


Bond angles



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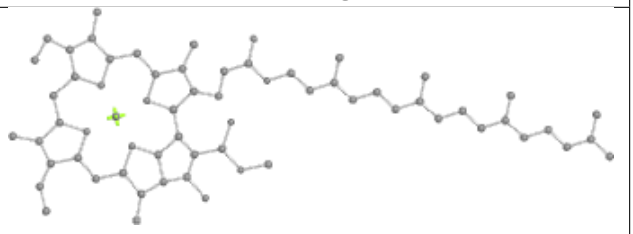
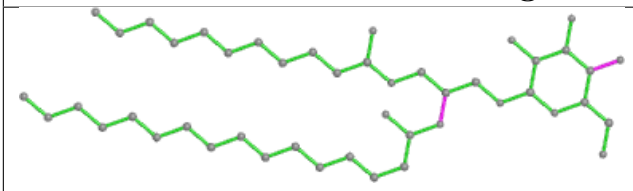


Rings

Ligand LMG D 411



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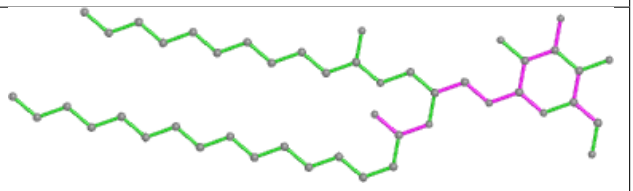
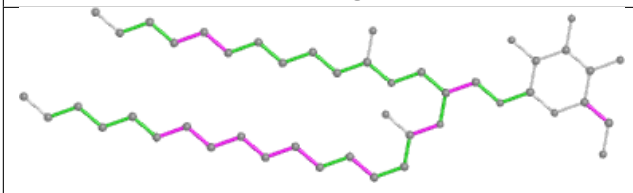


Bond angles



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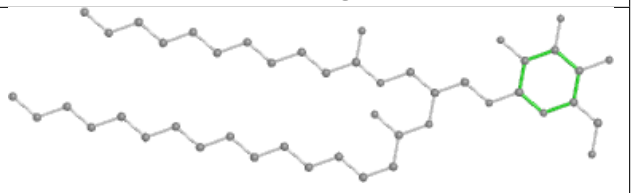
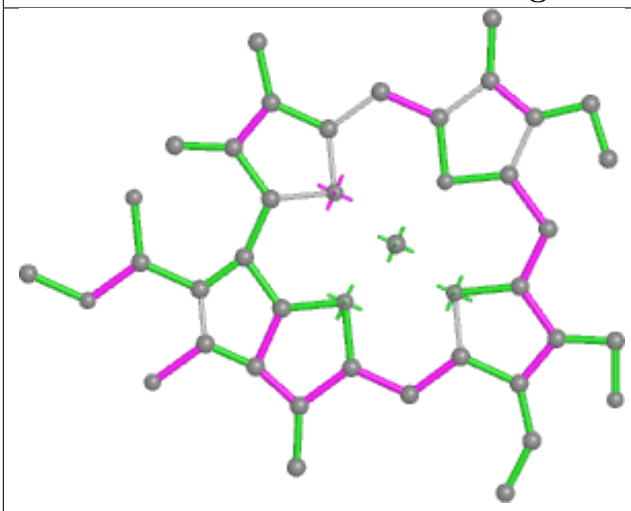
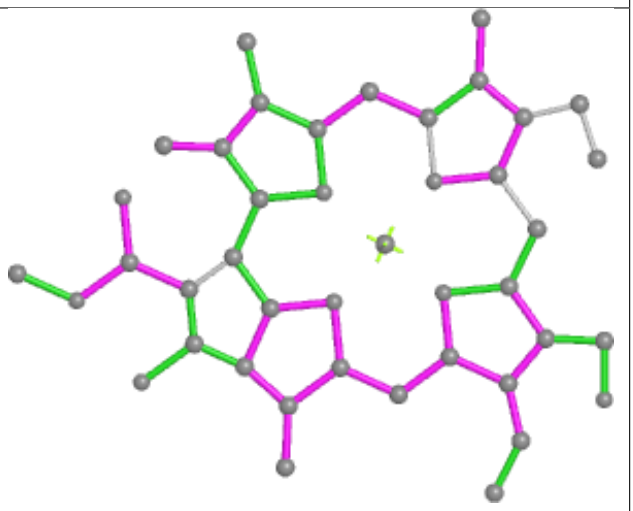


Rings

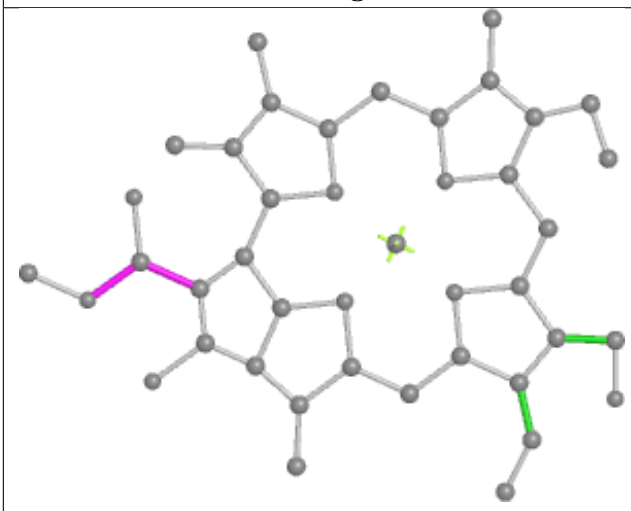
Ligand CHL r 614



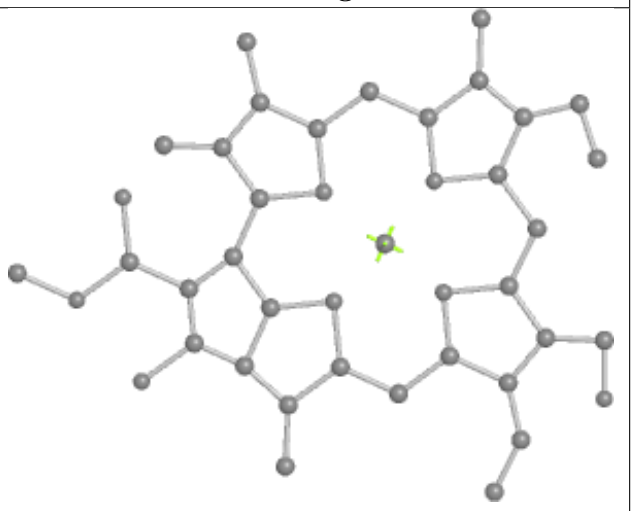
Bond lengths



Bond angles

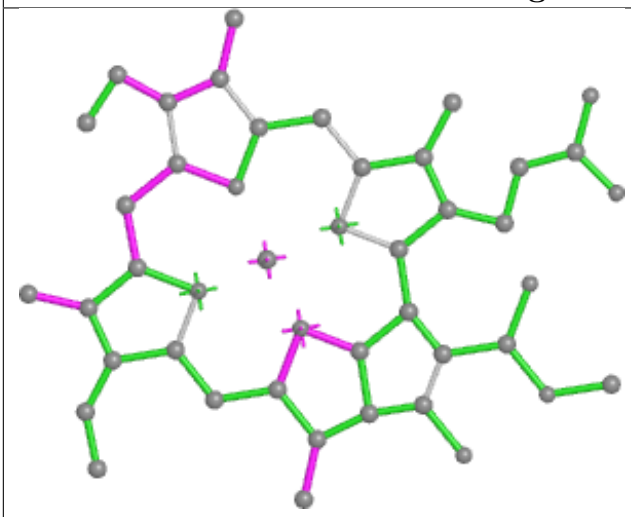


Torsions

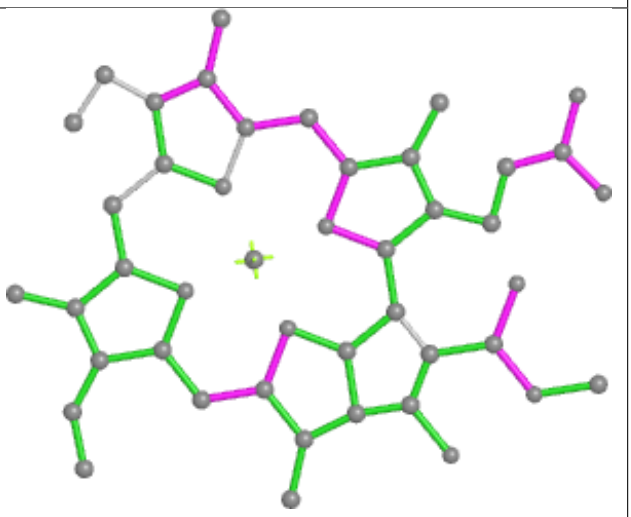


Rings

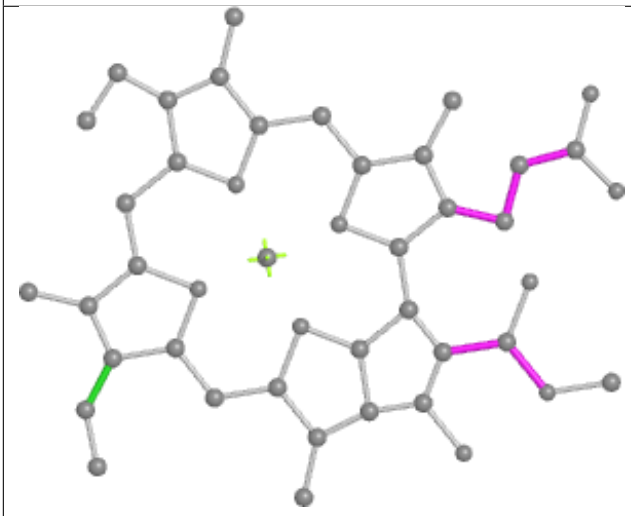
Ligand CLA 8 604



Bond lengths



Bond angles



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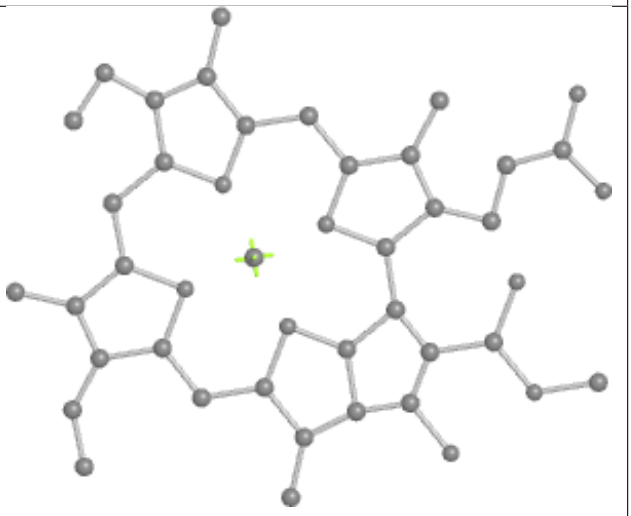
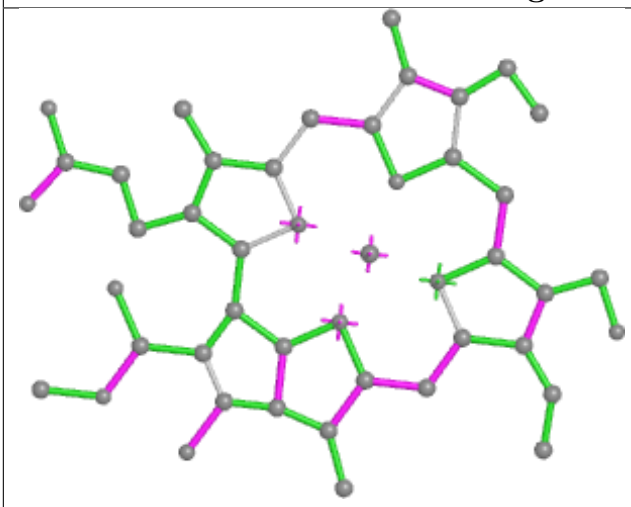


Rings

Ligand CHL 5 601



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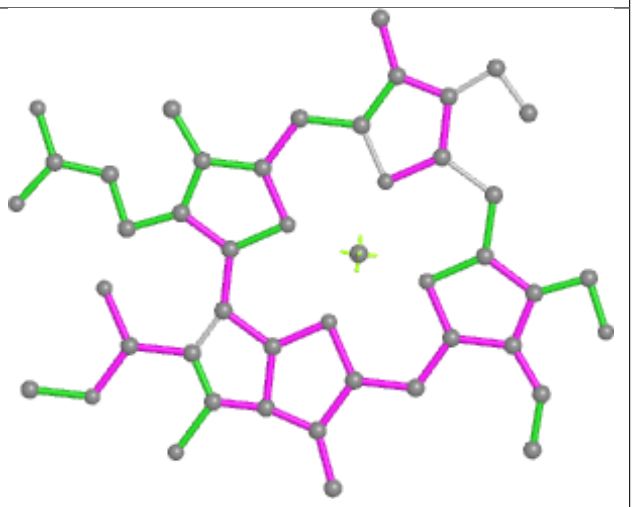
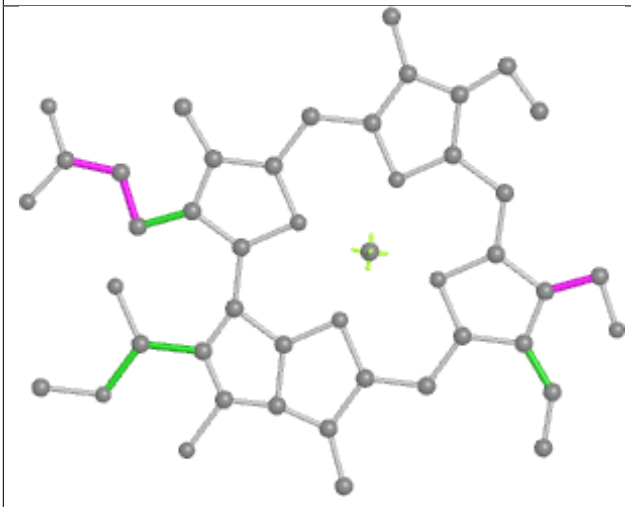


Bond angles



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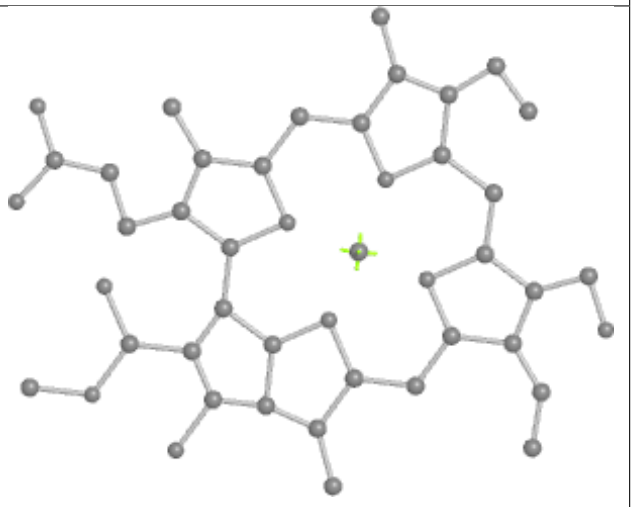
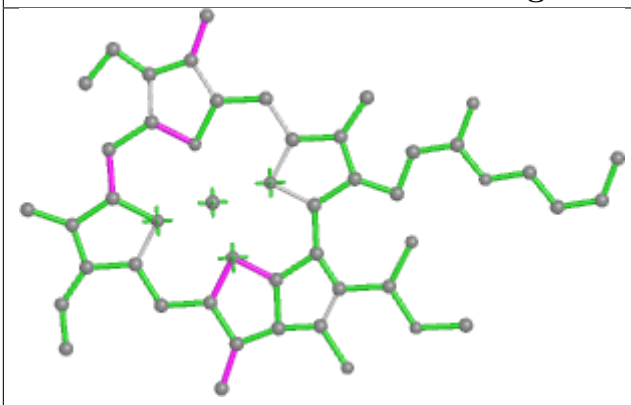


Rings

Ligand CLA S 614



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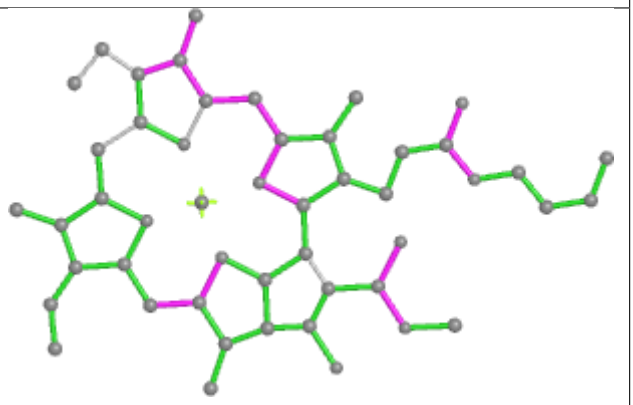
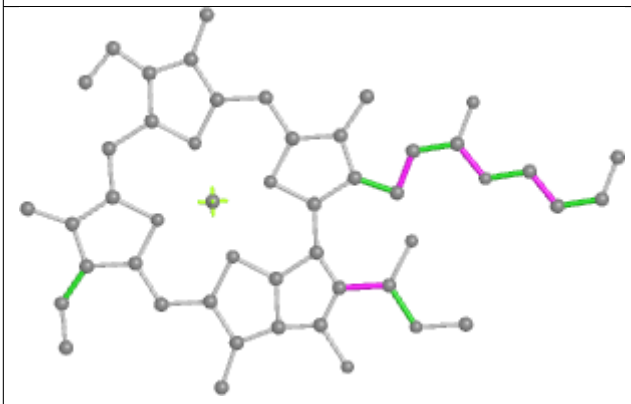


Bond angles



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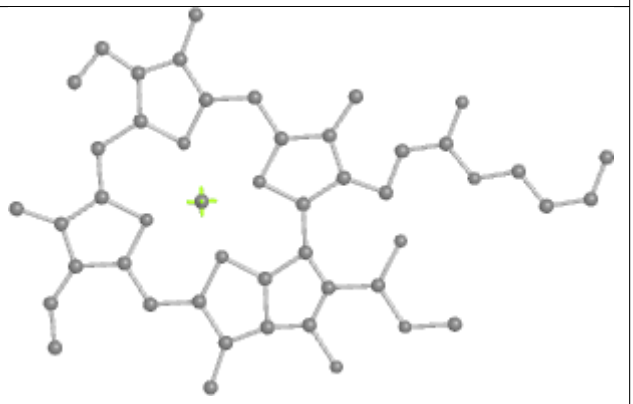
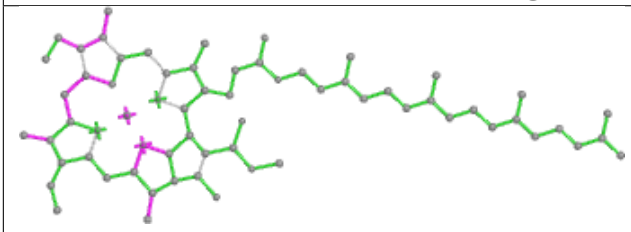


Rings

Ligand CLA B 612



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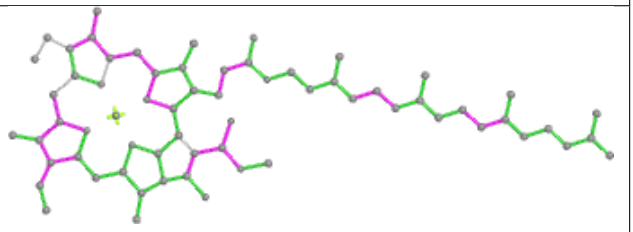
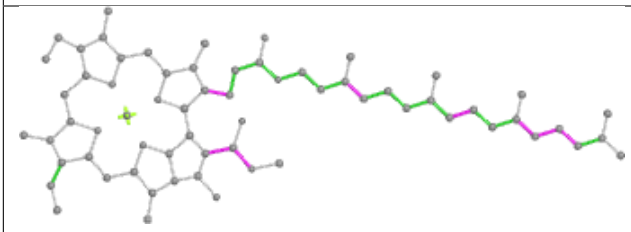
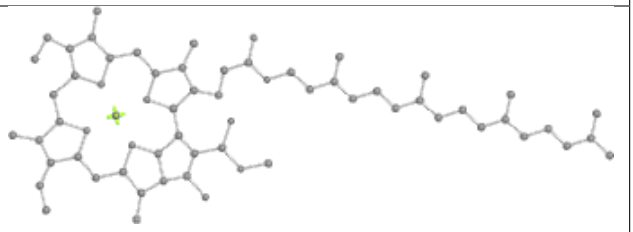


Bond angles

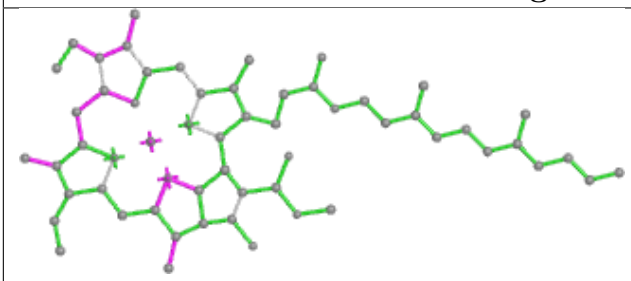


Torsions



Rings

Ligand CLA r 609



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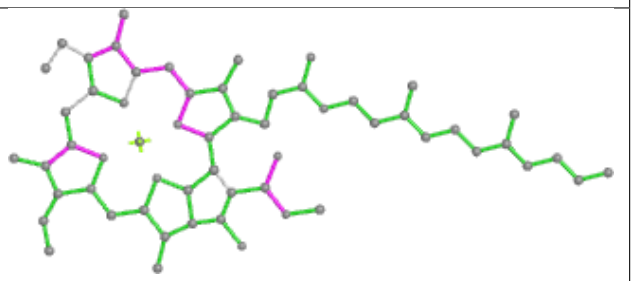
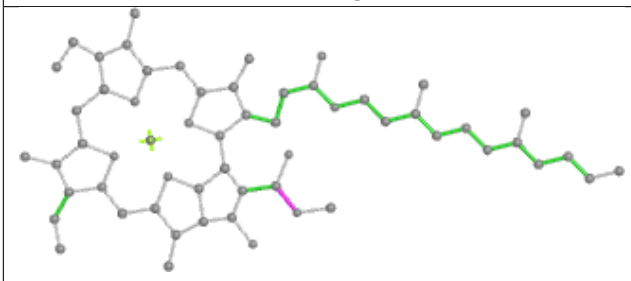


Bond angles



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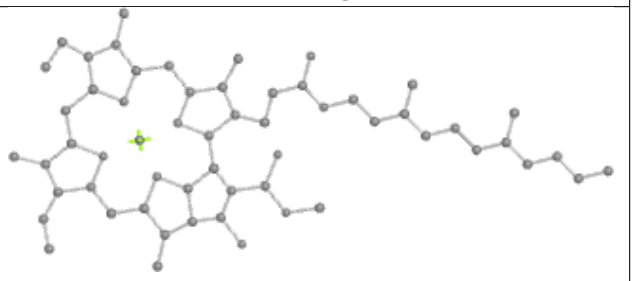
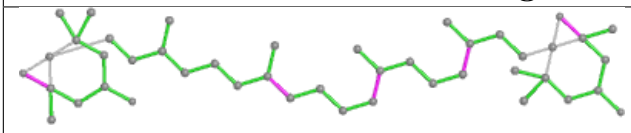


Rings

Ligand XAT 7 1622



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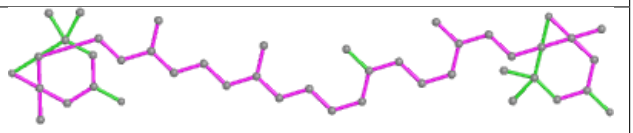
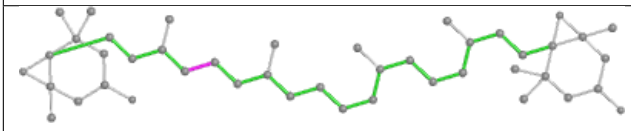


Bond angles



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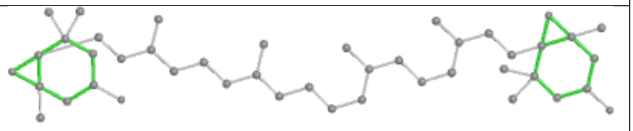
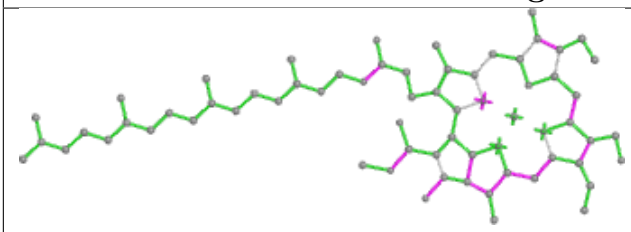


Rings

Ligand CHL g 607



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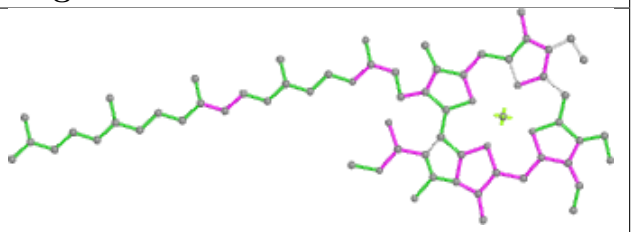
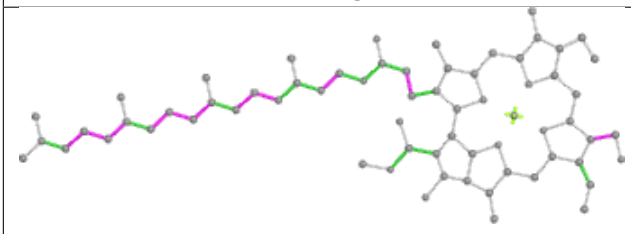


Bond angles



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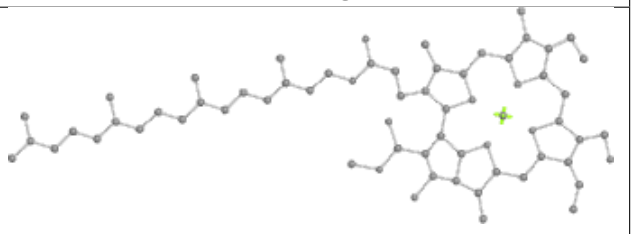
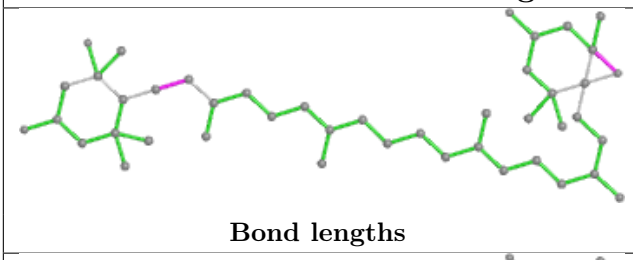


Rings

Ligand NEX g 1623



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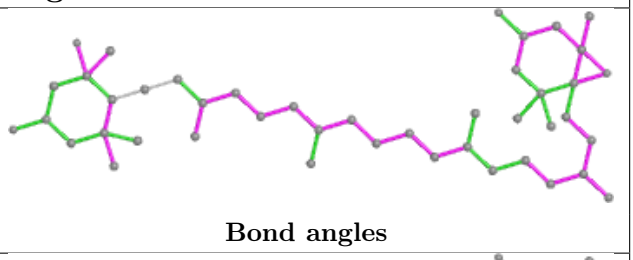
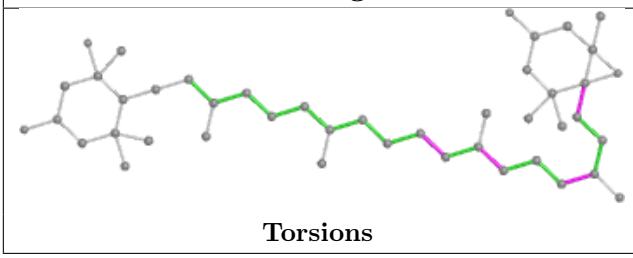


Bond angles



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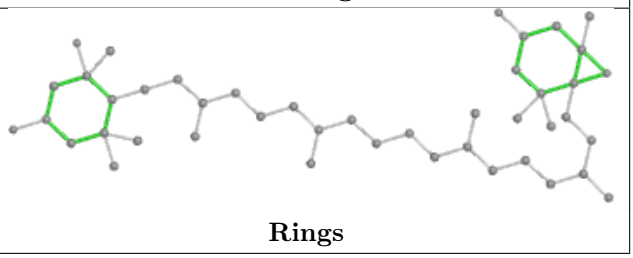
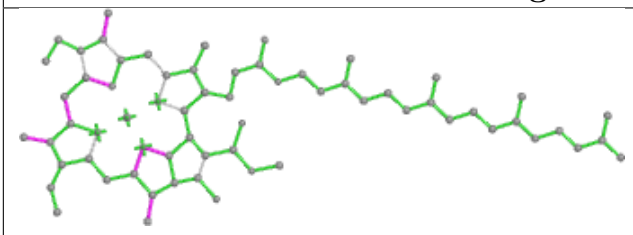


Rings

Ligand CLA c 513



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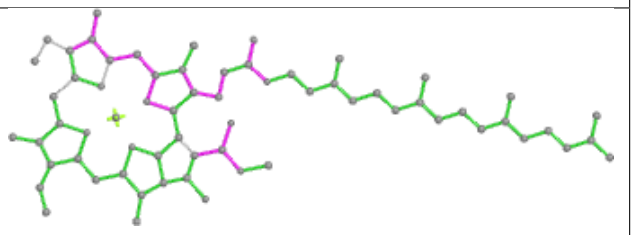
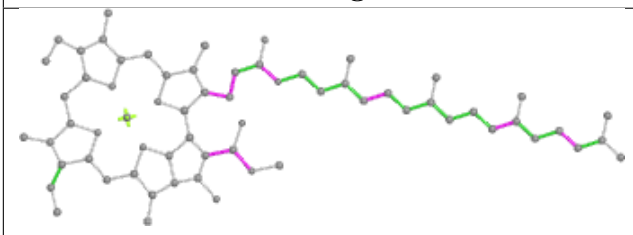


Bond angles



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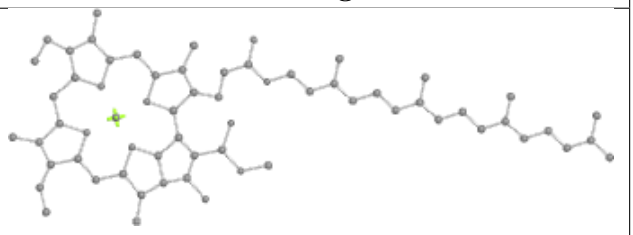
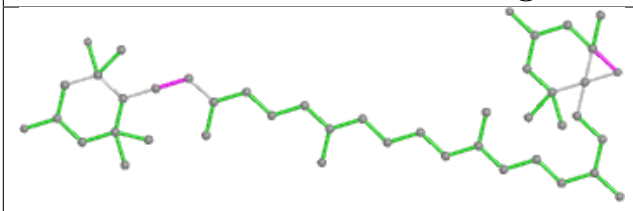


Rings

Ligand NEX 3 1623



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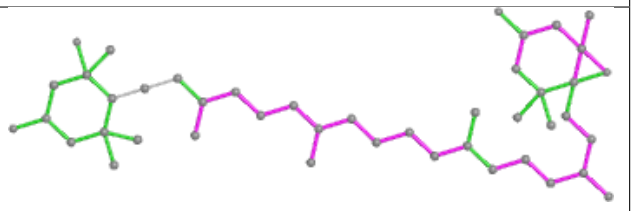
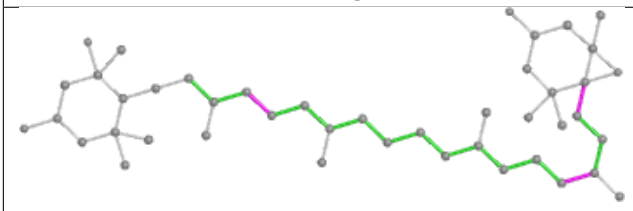


Bond angles



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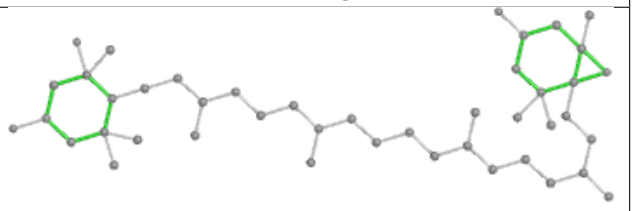
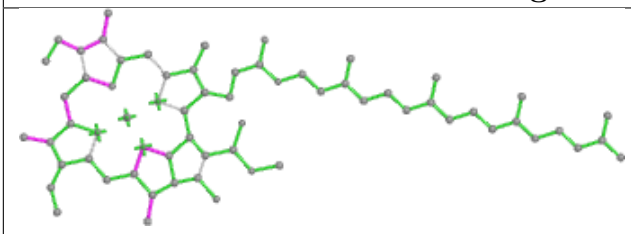


Rings

Ligand CLA r 610



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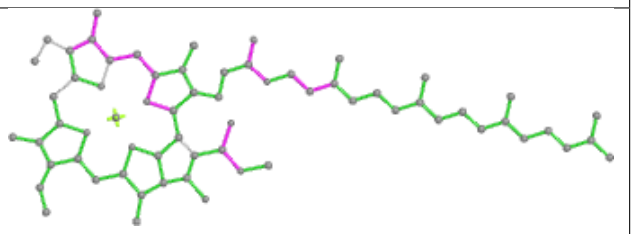
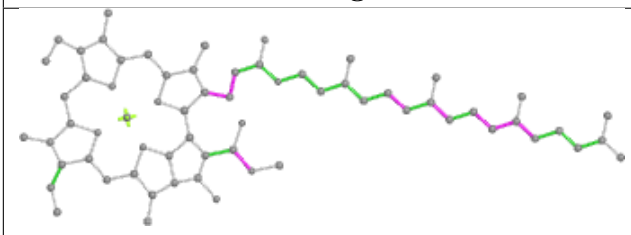


Bond angles



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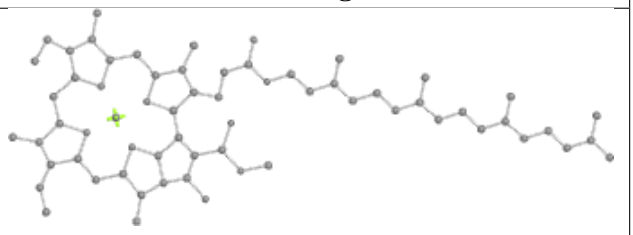
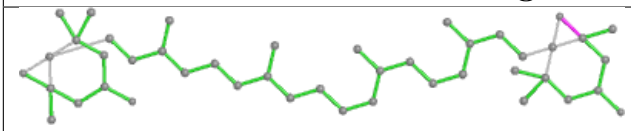


Rings

Ligand XAT n 1622



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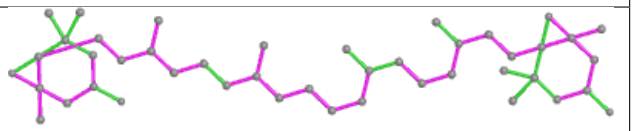
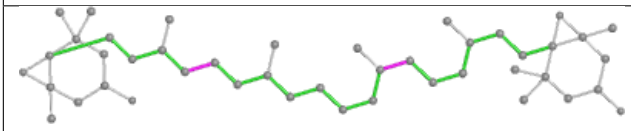


Bond angles



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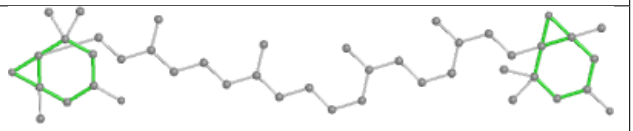
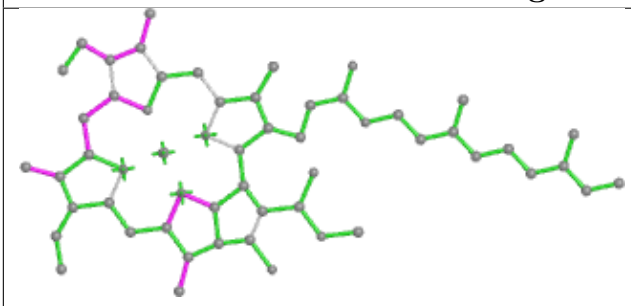


Rings

Ligand CLA 5 610



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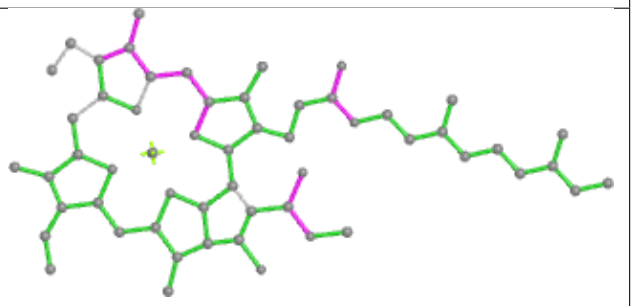
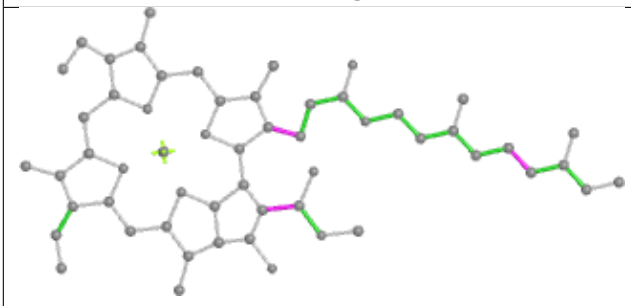


Bond angles



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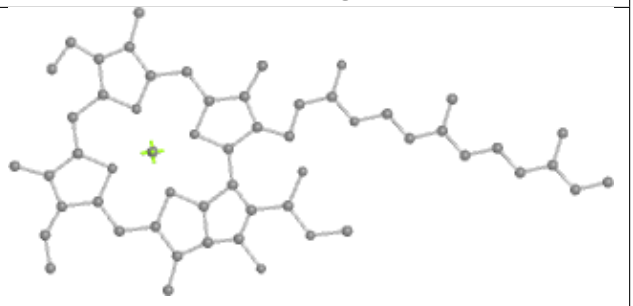
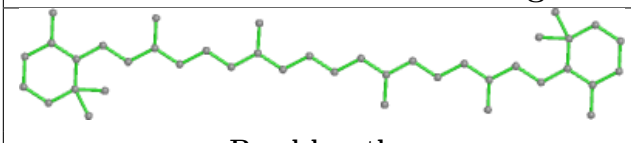
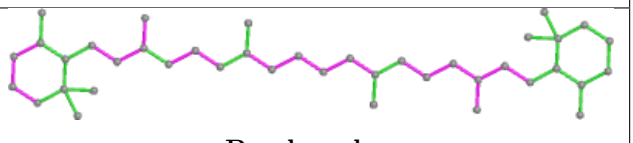


Rings

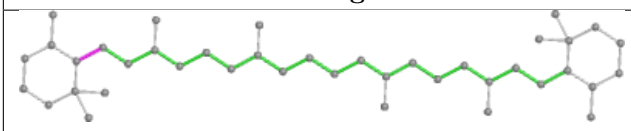
Ligand BCR c 514



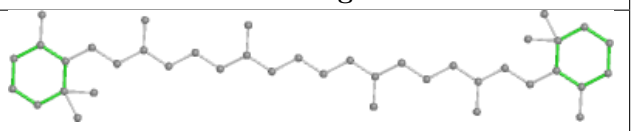
Bond lengths



Bond angles

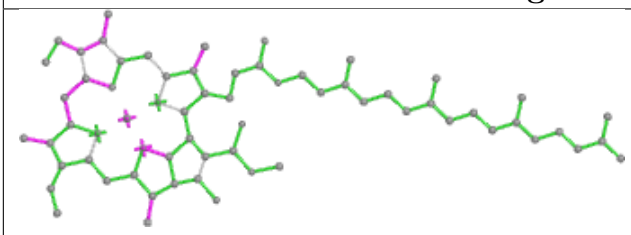


Torsions

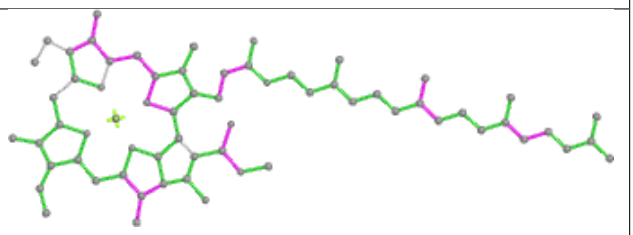


Rings

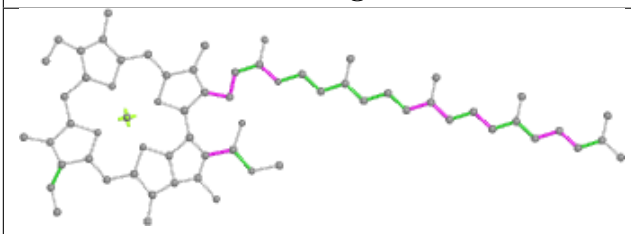
Ligand CLA b 613



Bond lengths



Bond angles



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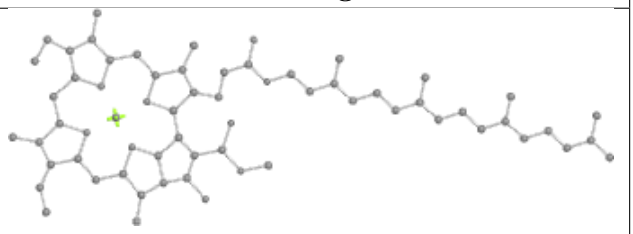
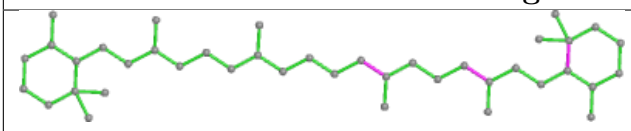
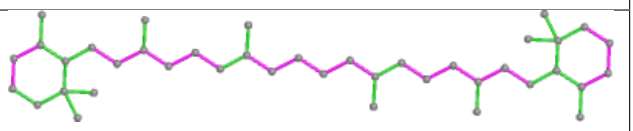


Rings

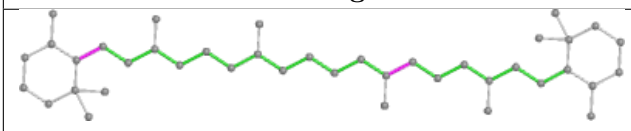
Ligand BCR B 618



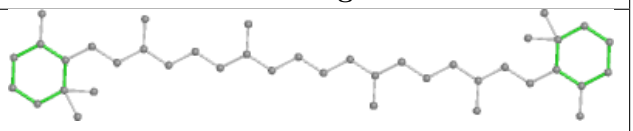
Bond lengths



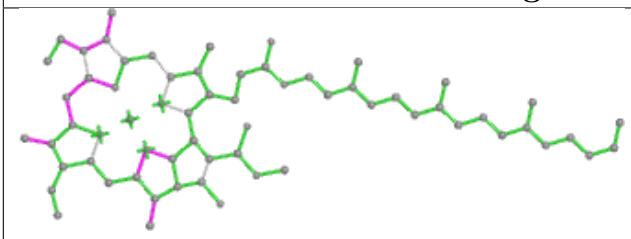
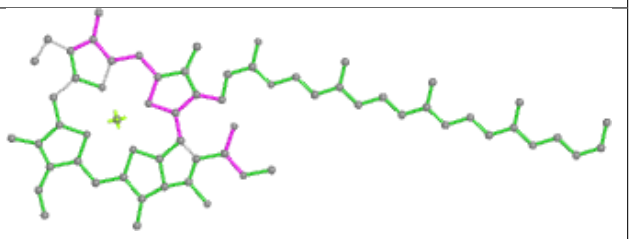
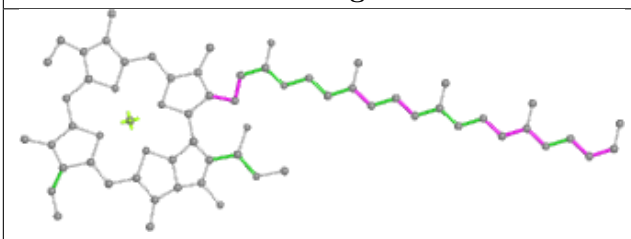
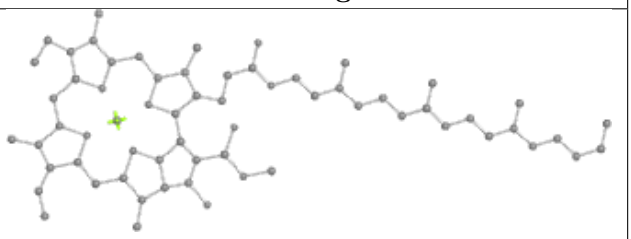
Bond angles

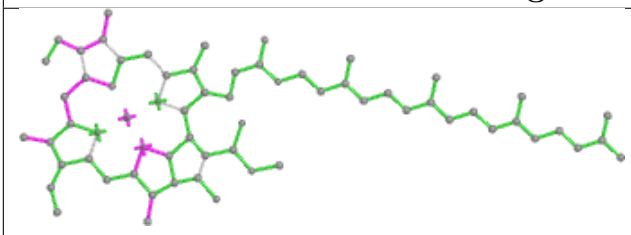
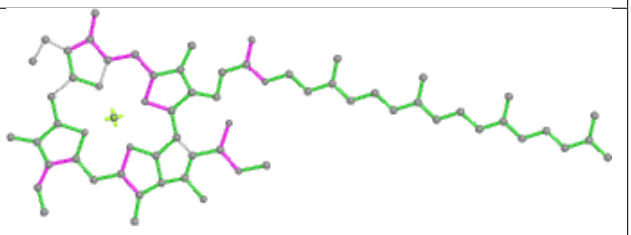
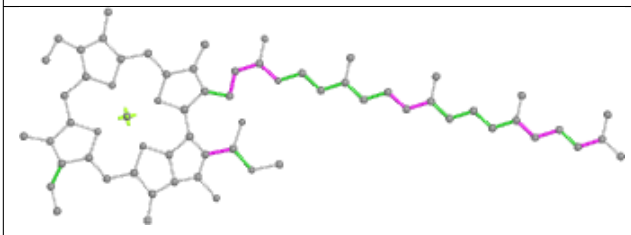
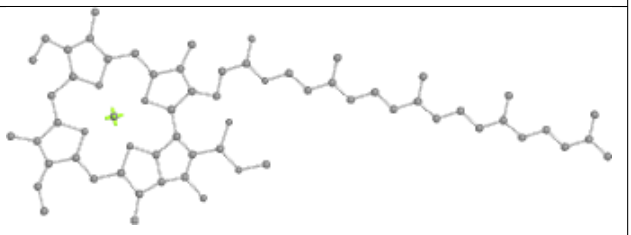


Torsions

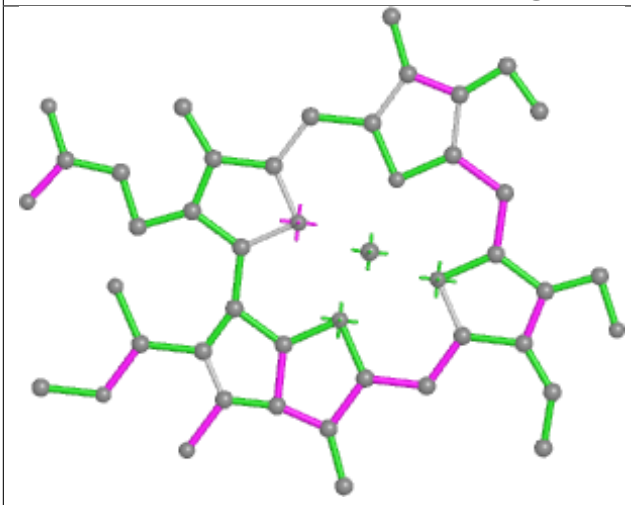


Rings

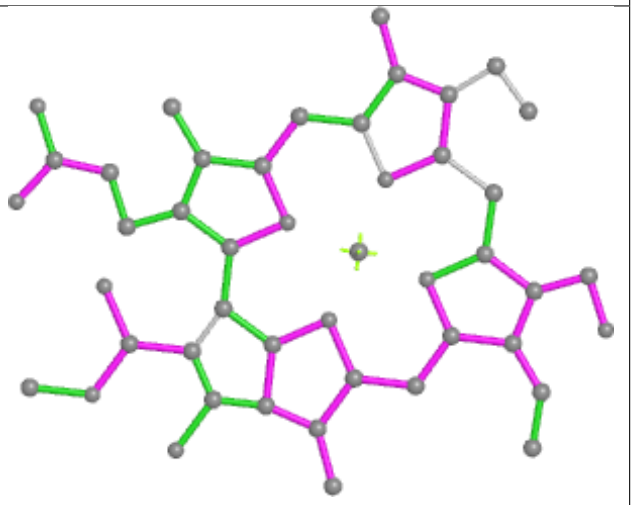
Ligand CLA G 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

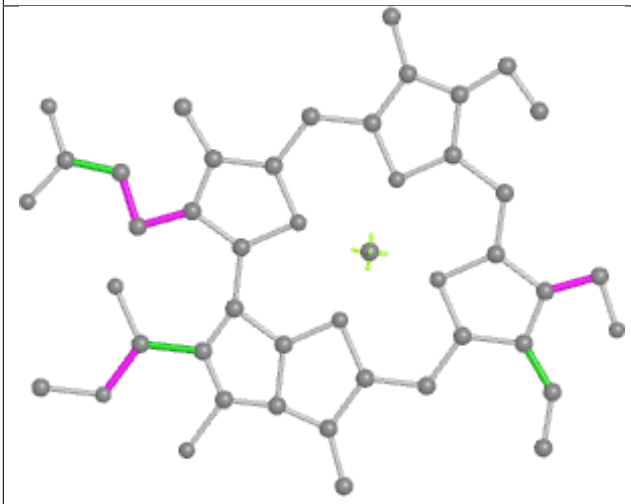
Ligand CHL 8 606



Bond lengths



Bond angles



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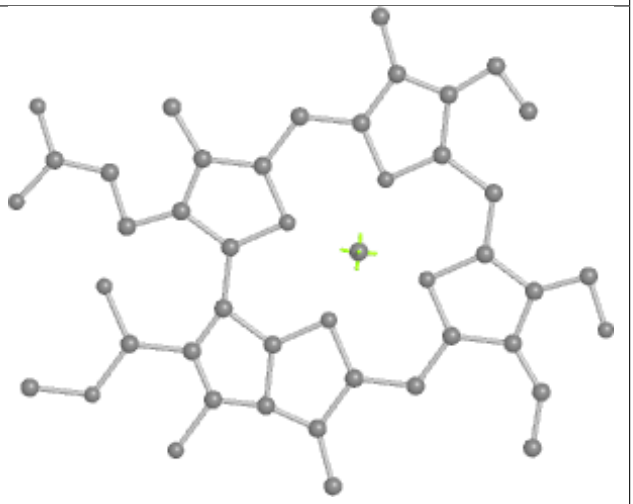
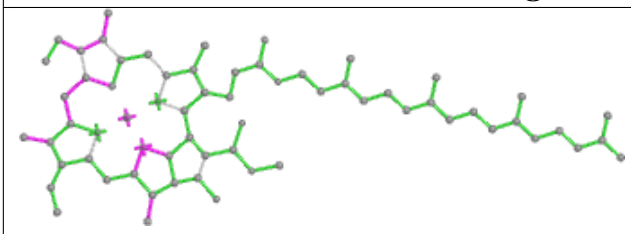


Rings

Ligand CLA B 608



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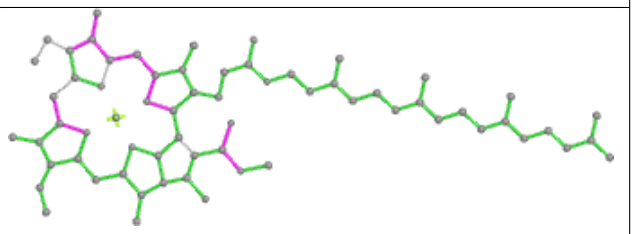
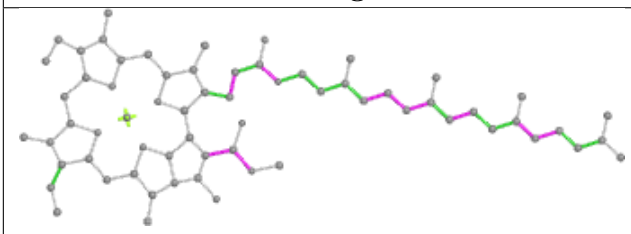


Bond angles



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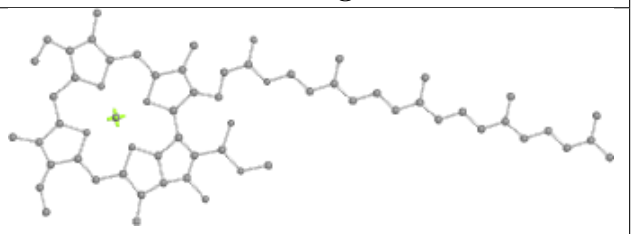
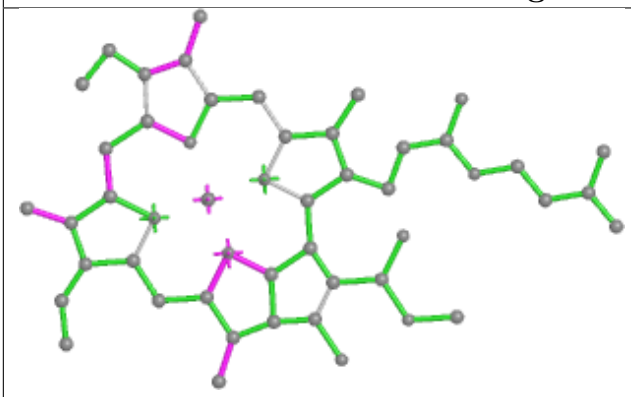
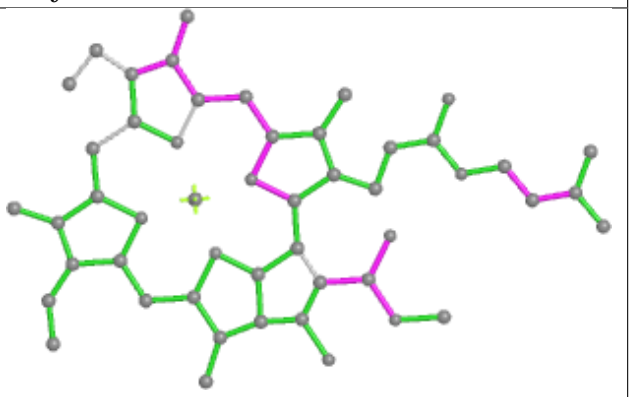
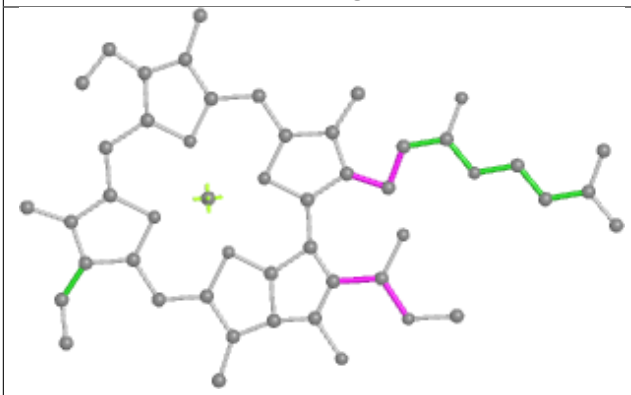
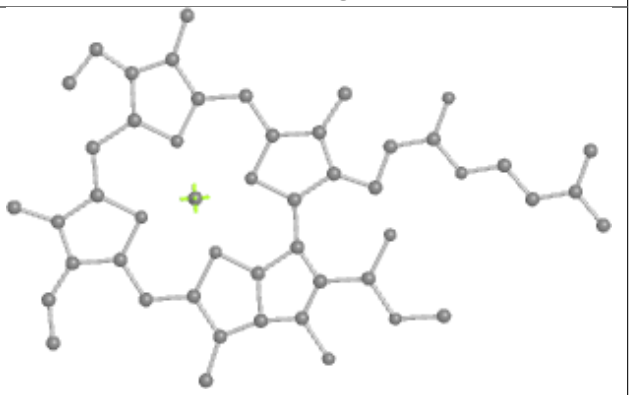
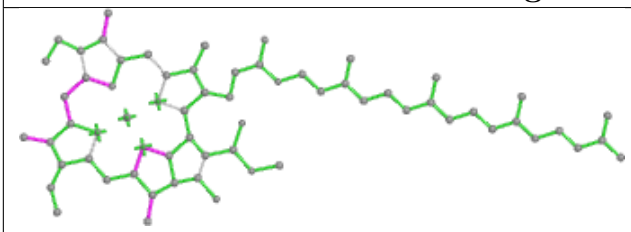
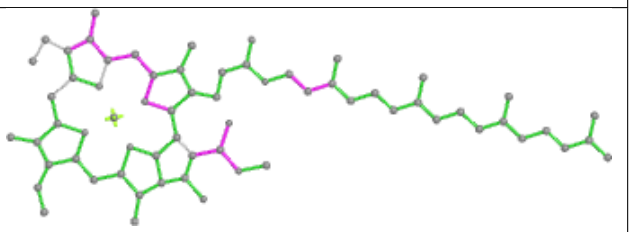
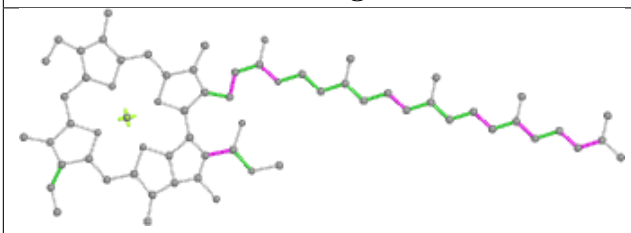
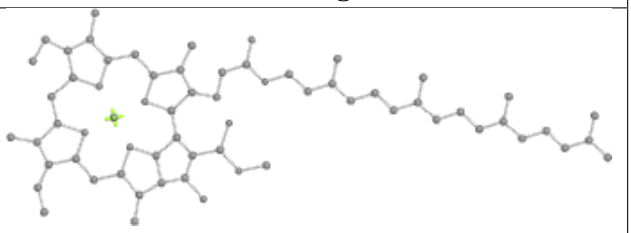
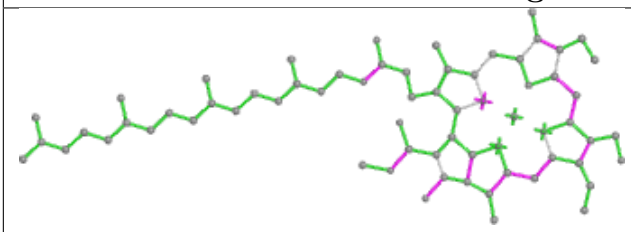


Rings

Ligand CLA y 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL n 608



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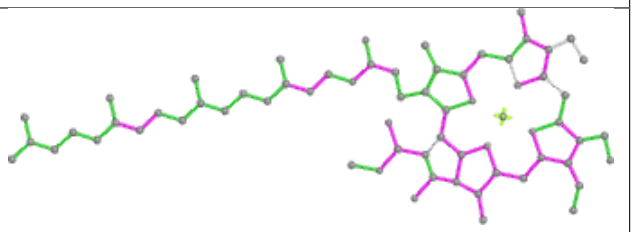
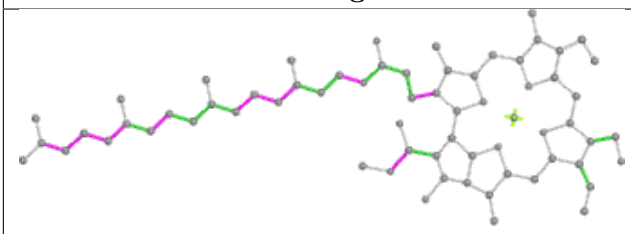
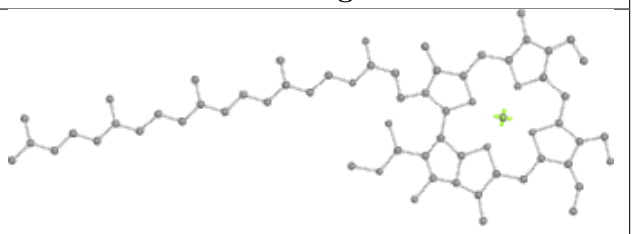


Bond angles

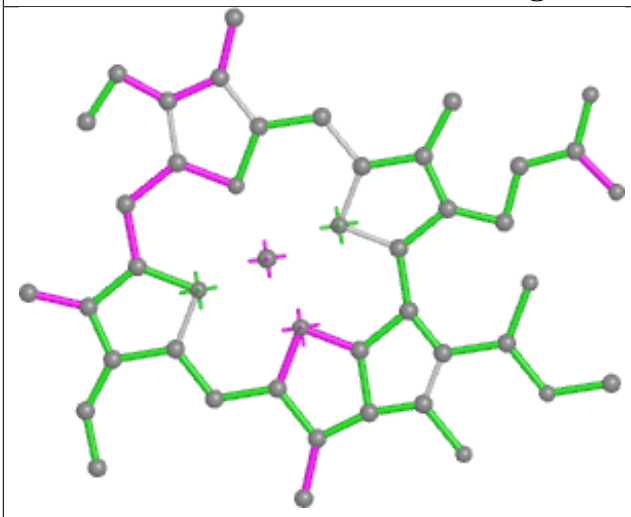


Torsions



Rings

Ligand CLA 1 611



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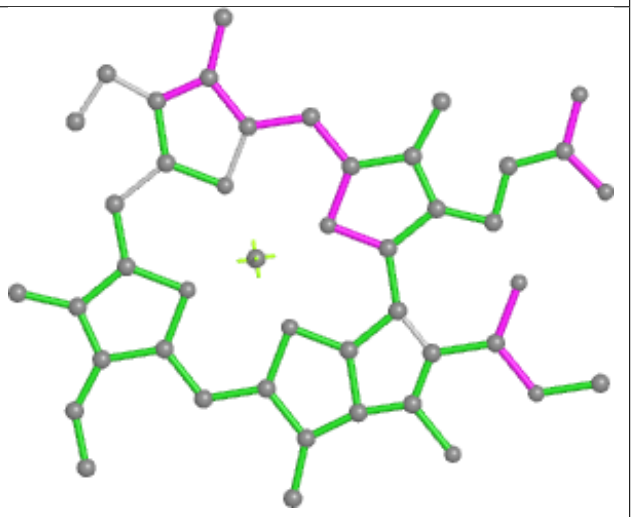
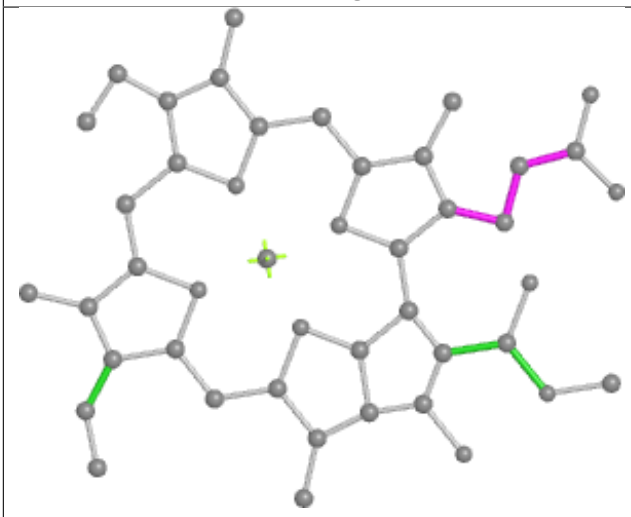


Bond angles



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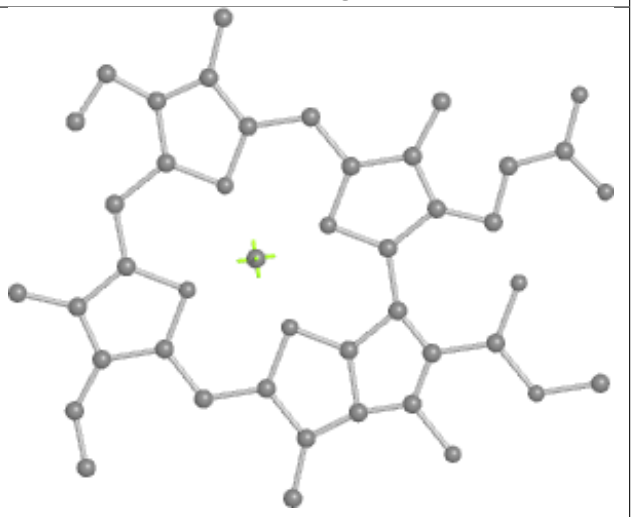
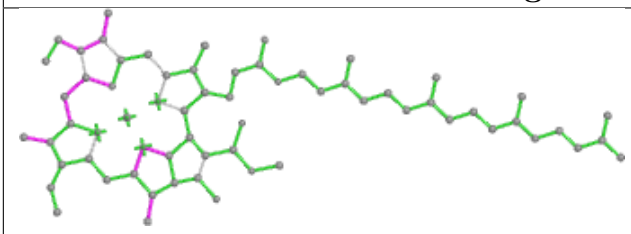


Rings

Ligand CLA B 616



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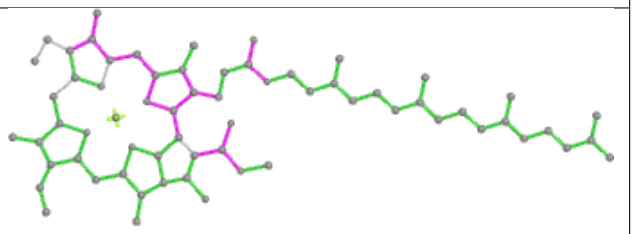
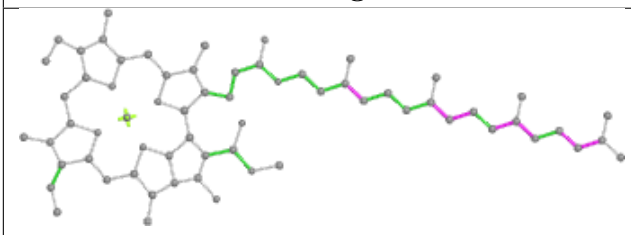


Bond angles



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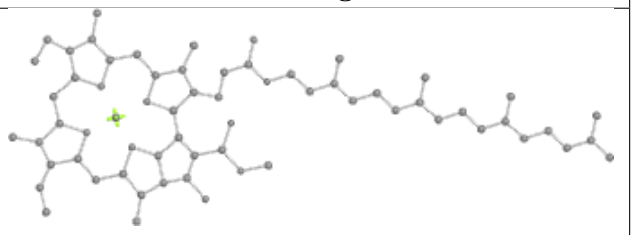
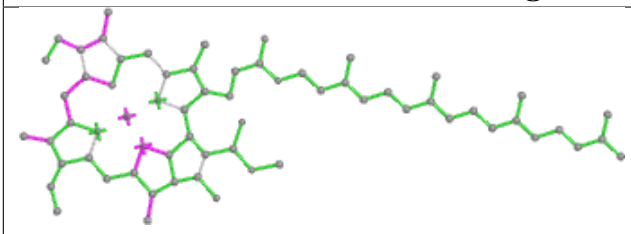
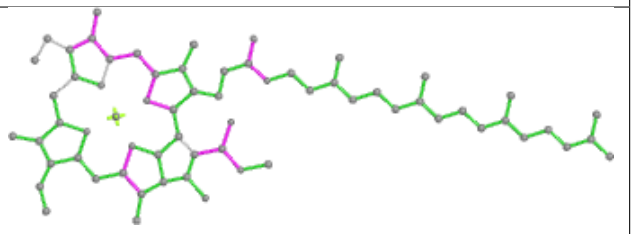


Rings

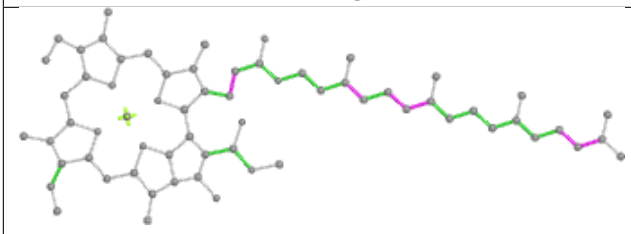
Ligand CLA B 604



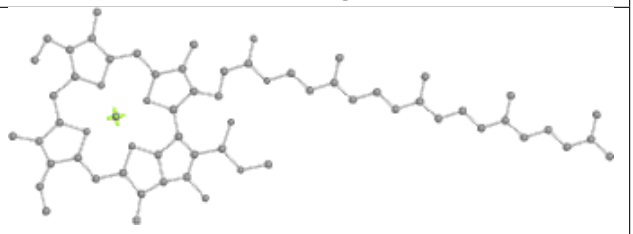
Bond lengths



Bond angles

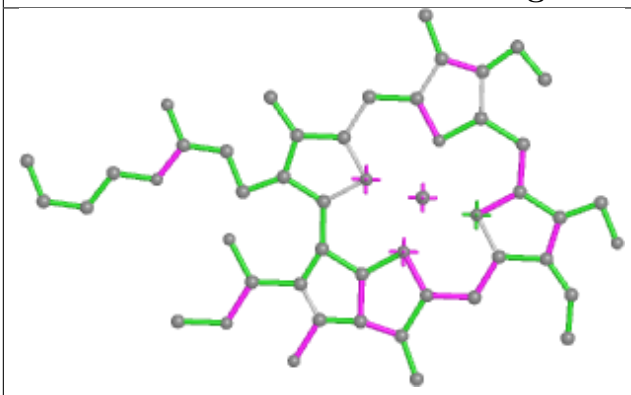


Torsions



Rings

Ligand CHL y 606



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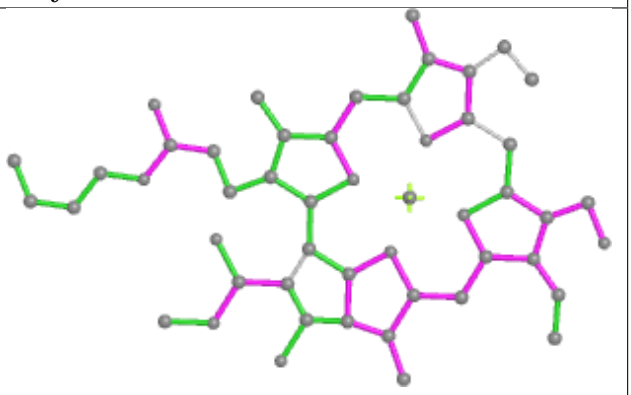
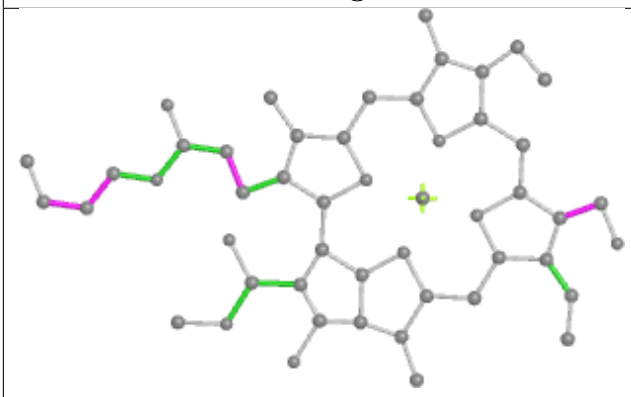
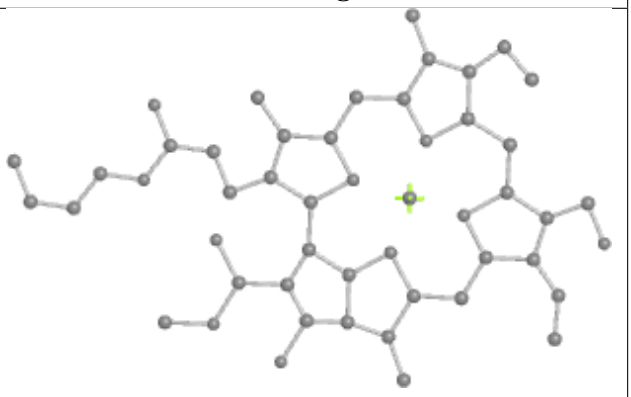


Bond angles

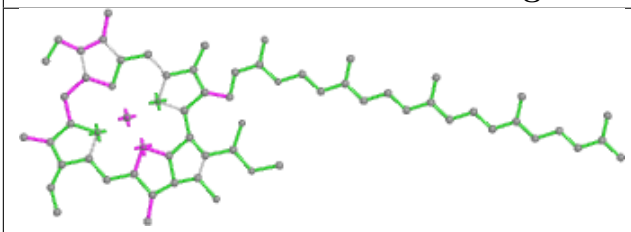


Torsions



Rings

Ligand CLA D 402



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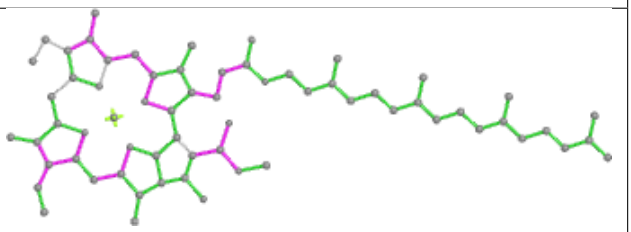
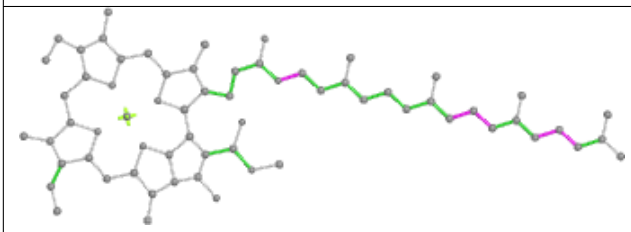


Bond angles



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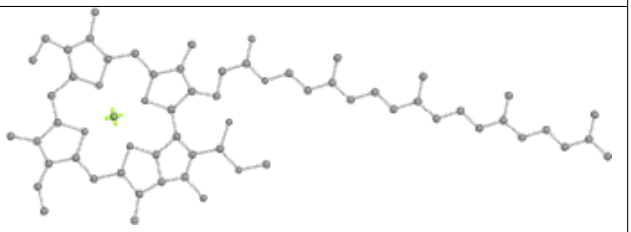
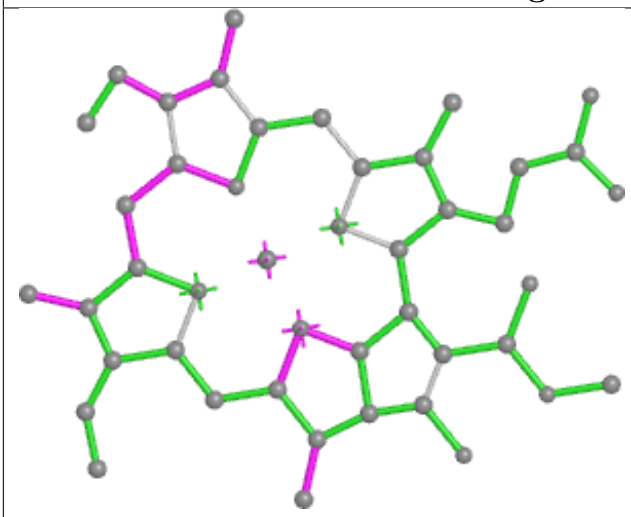


Rings

Ligand CLA 5 612



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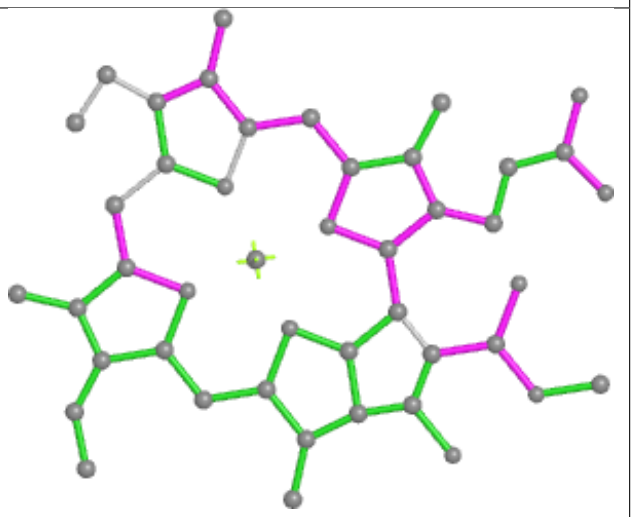

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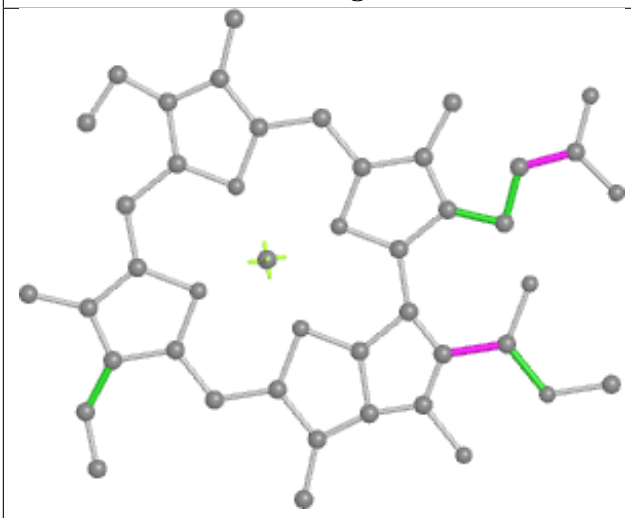

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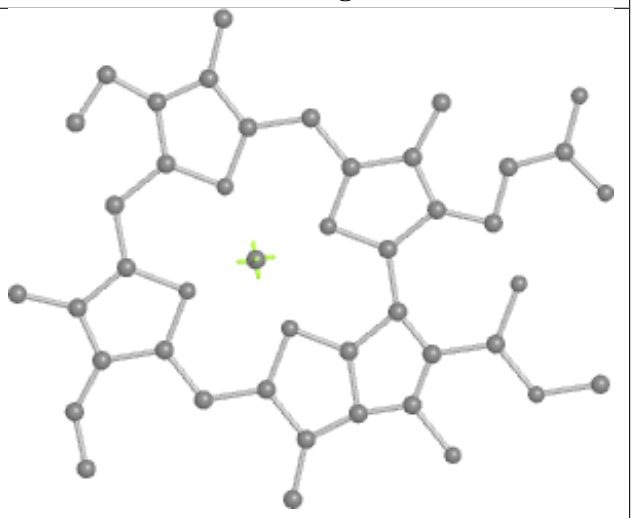
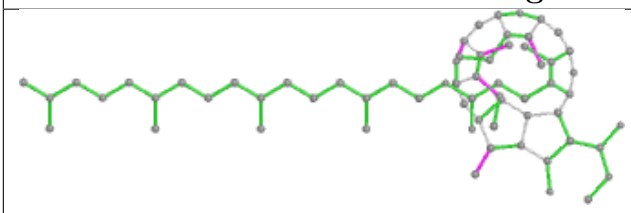


Rings

Ligand PHO a 409



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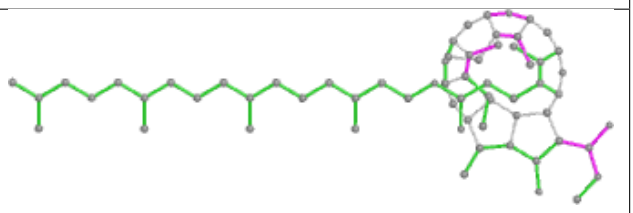
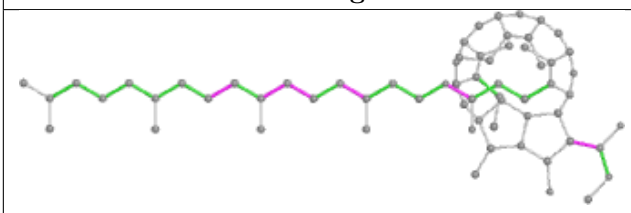


Bond angles



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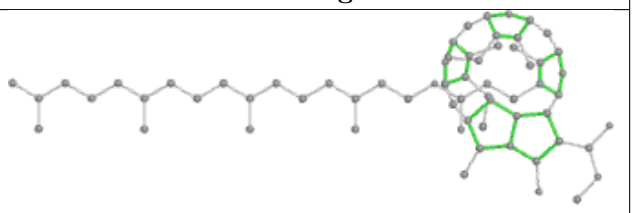
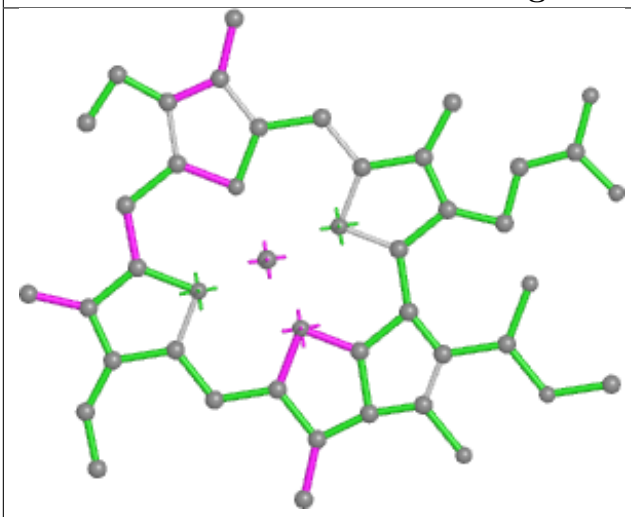


Rings

Ligand CLA 1 614



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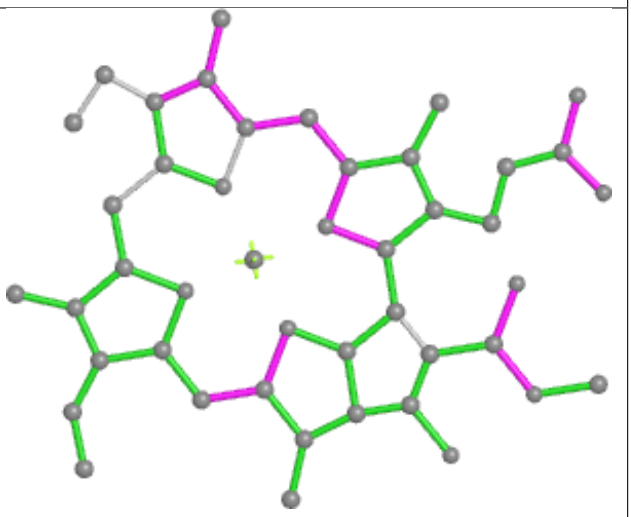
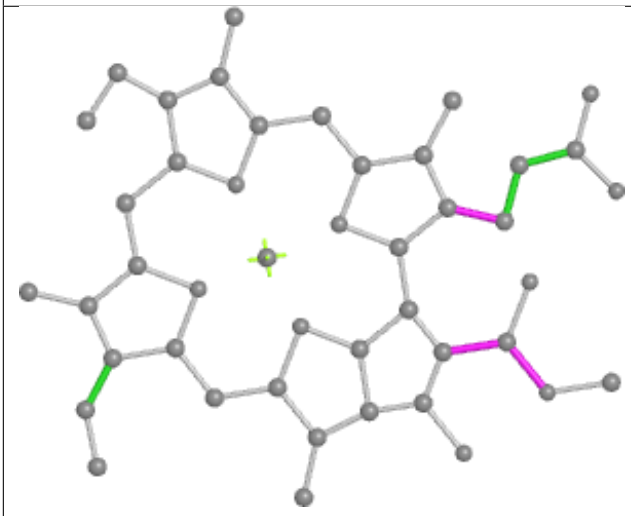


Bond angles



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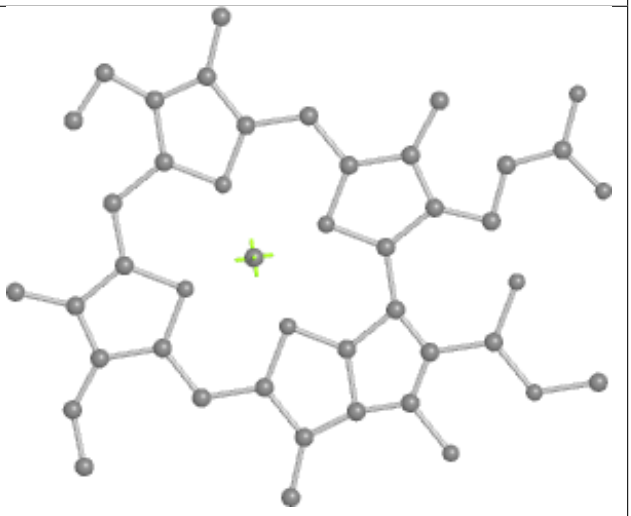
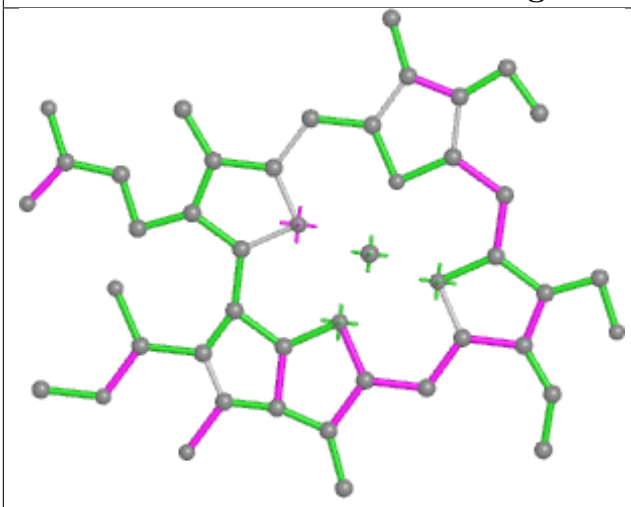


Rings

Ligand CHL 7 606



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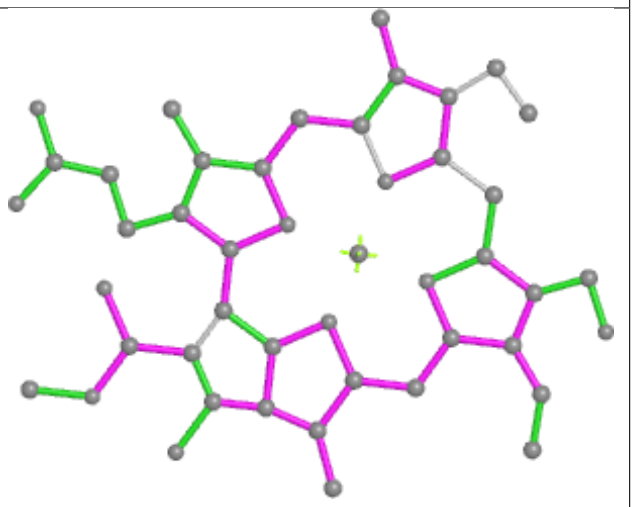

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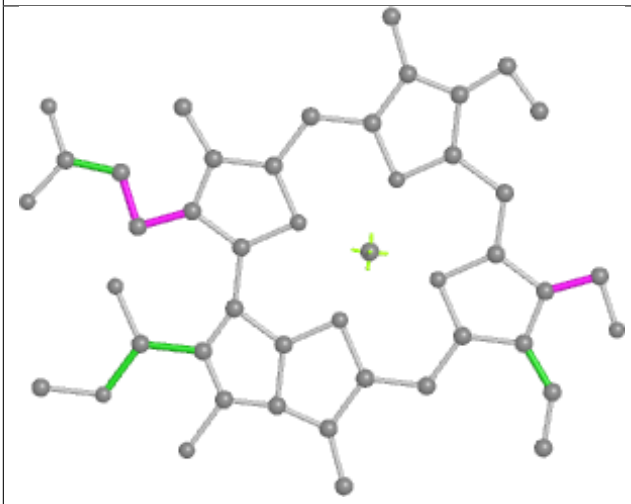

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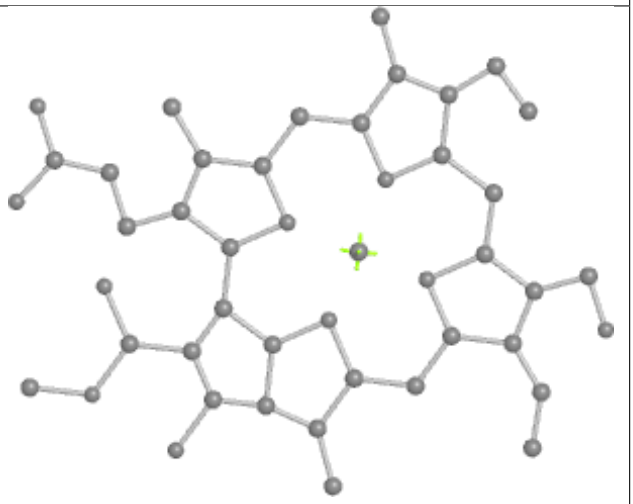

Rings

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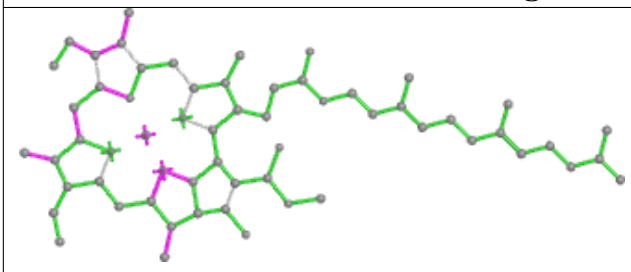

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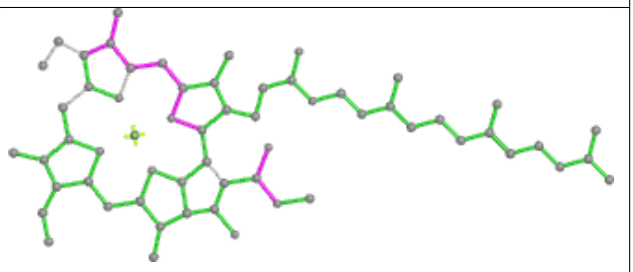

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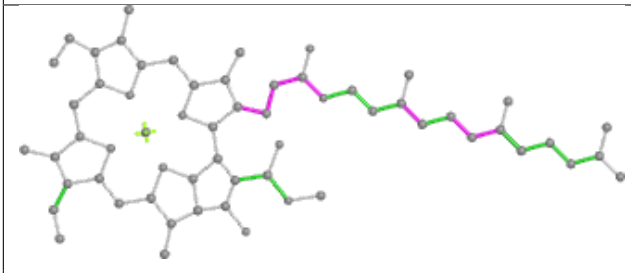

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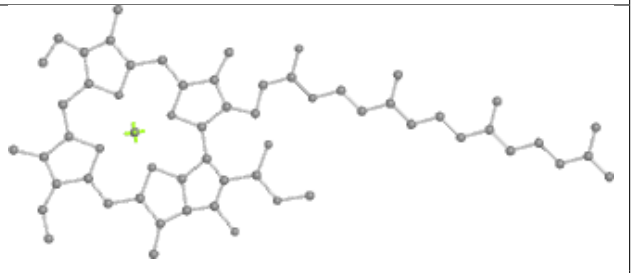

Rings

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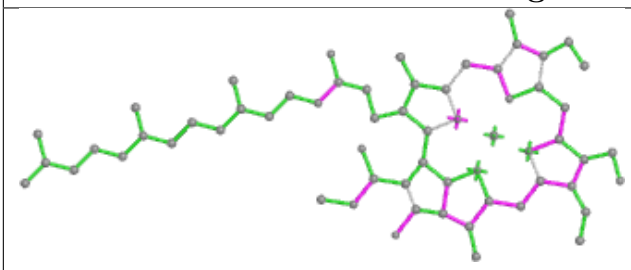

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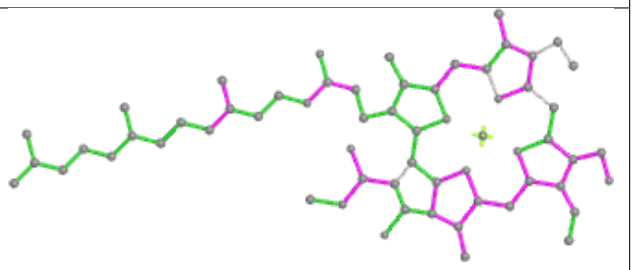

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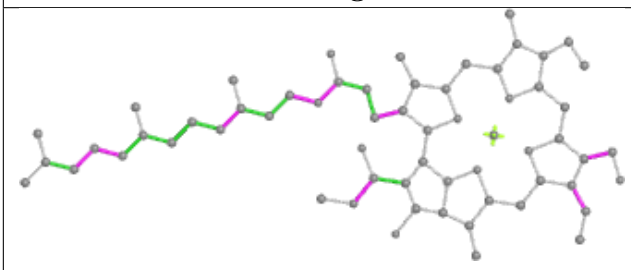

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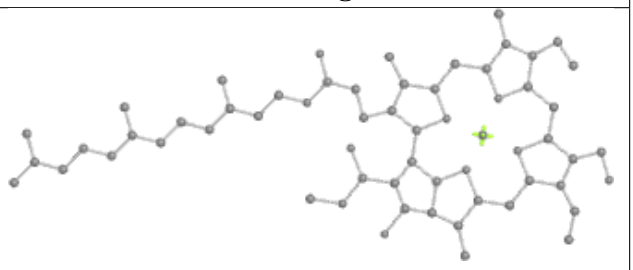

Rings

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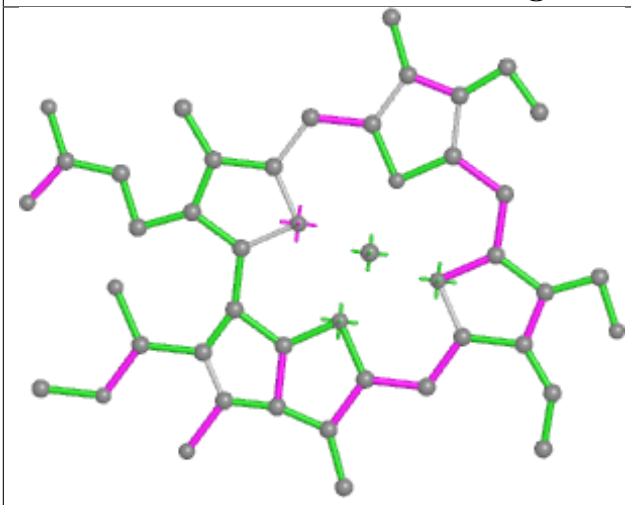

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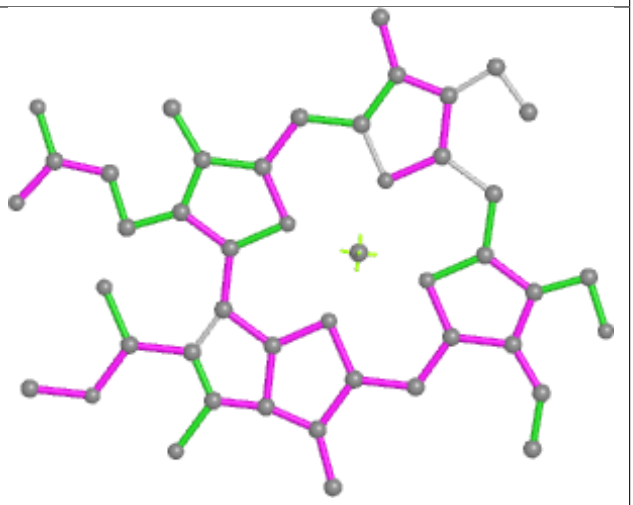

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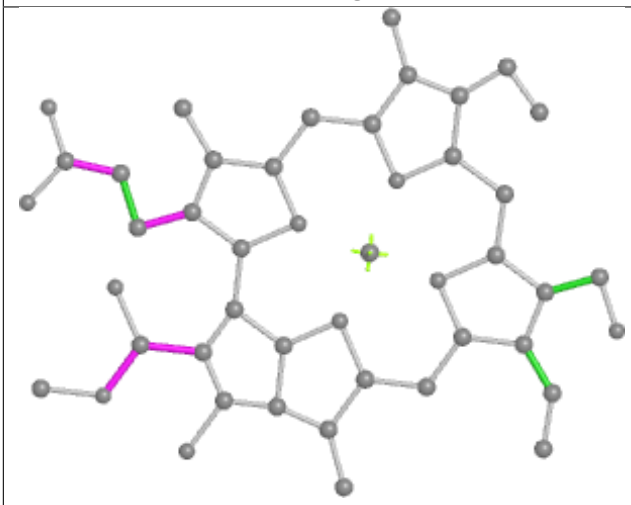

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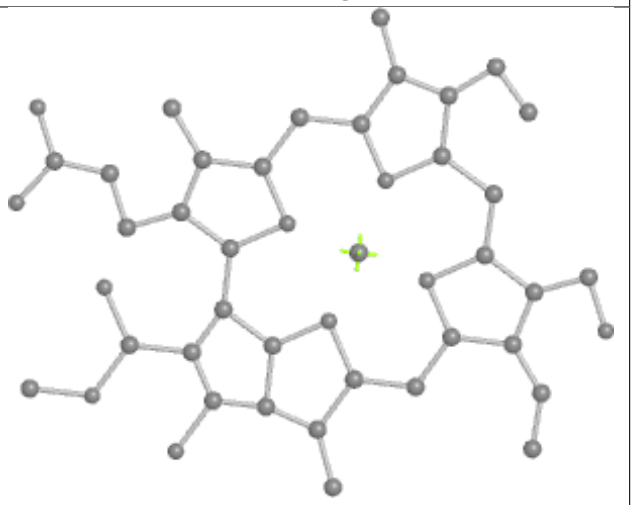
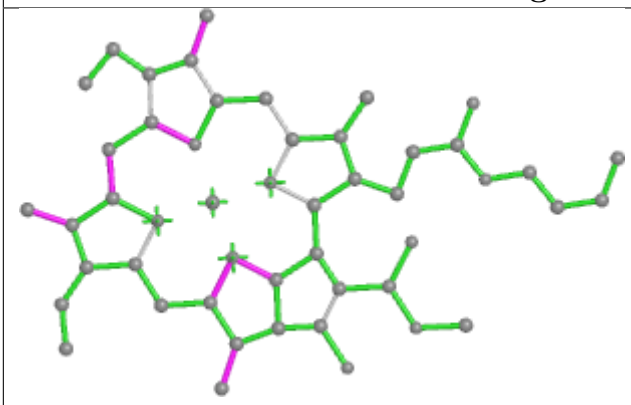


Rings

Ligand CLA s 612



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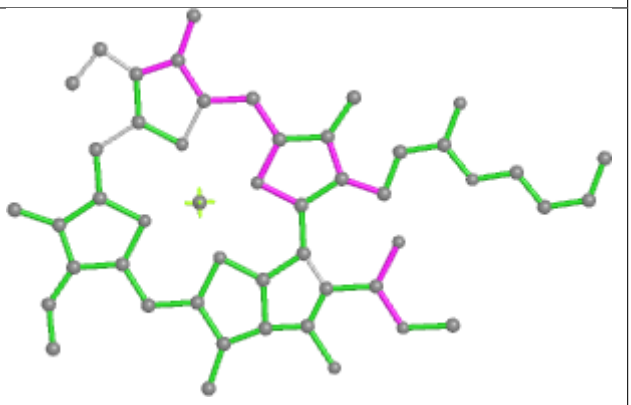
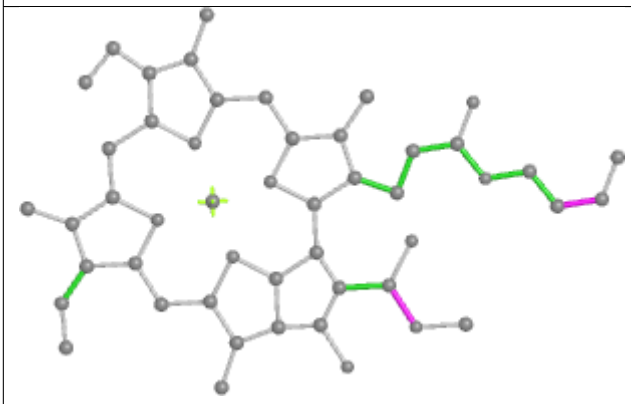


Bond angles



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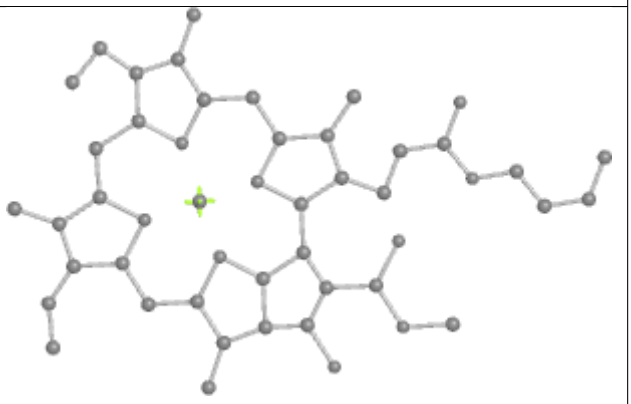

Rings

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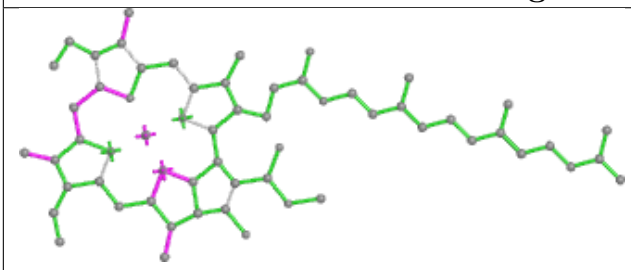

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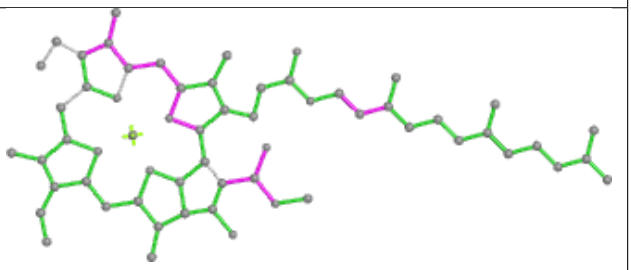

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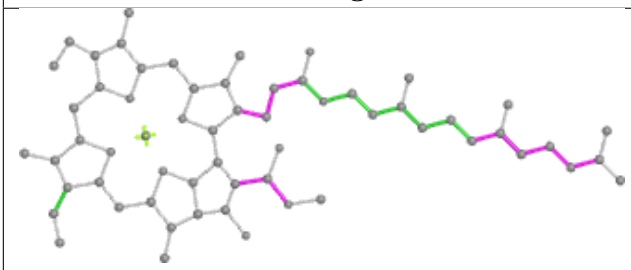

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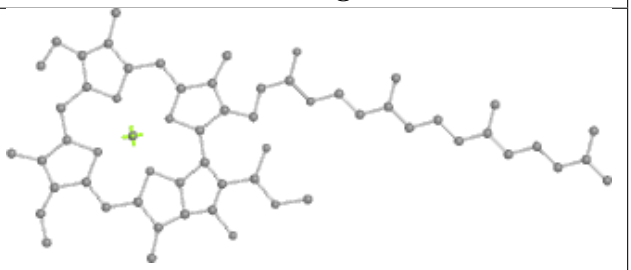
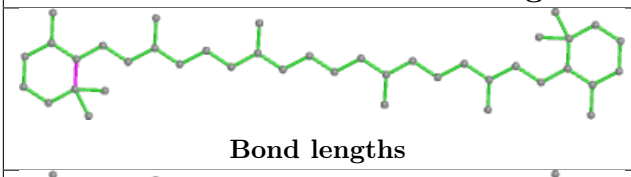


Rings

Ligand BCR b 620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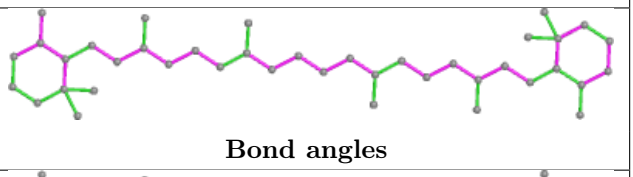
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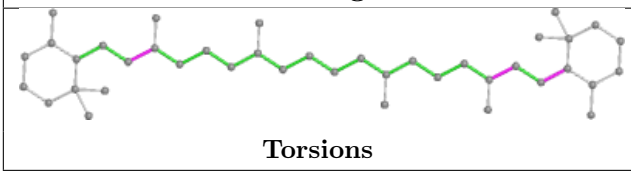
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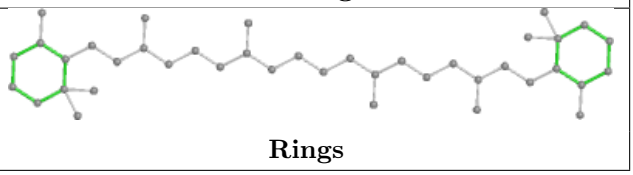
Rings

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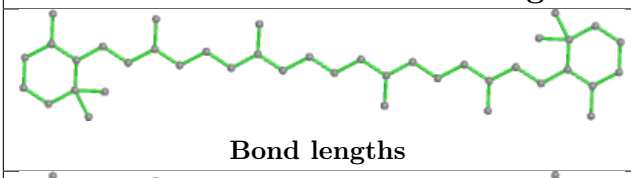
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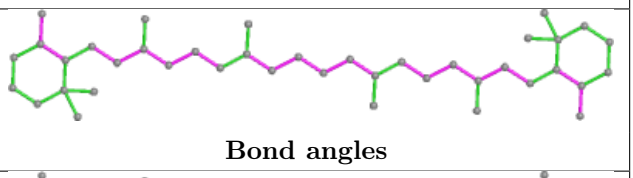
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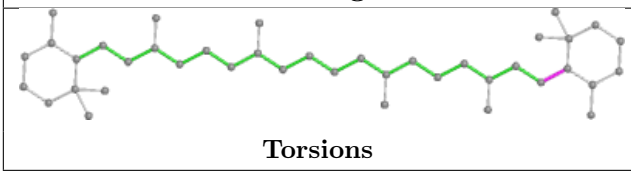
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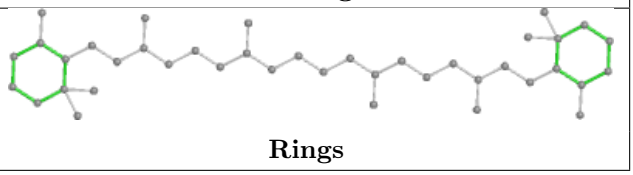
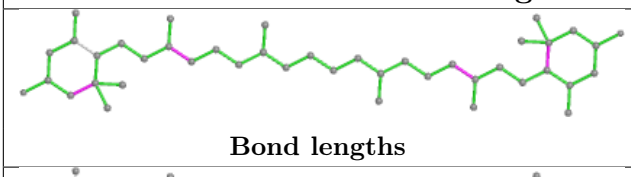

Rings

Ligand LUT Y 1621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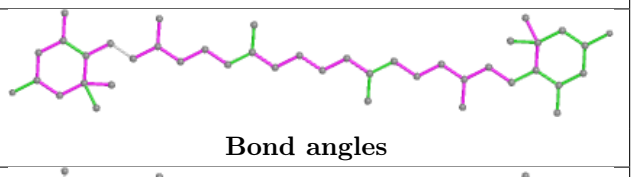
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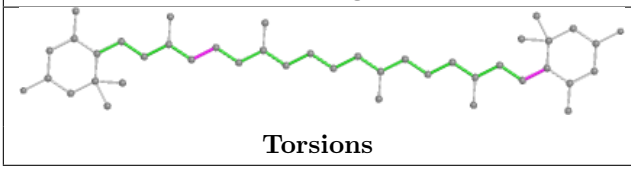
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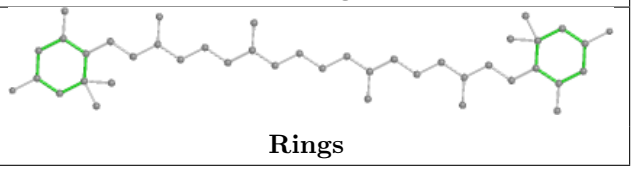
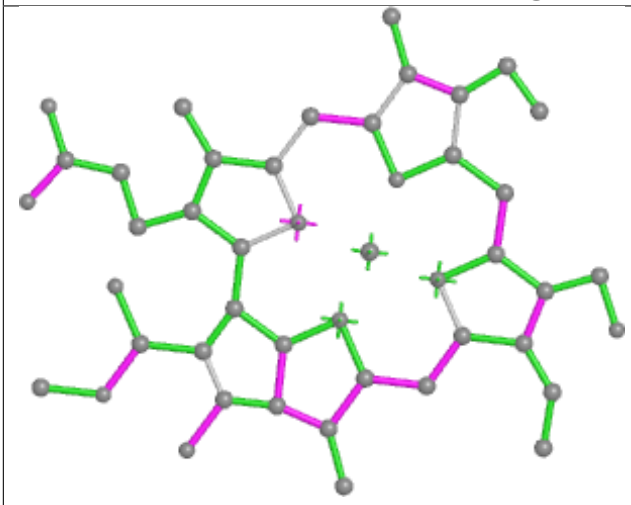
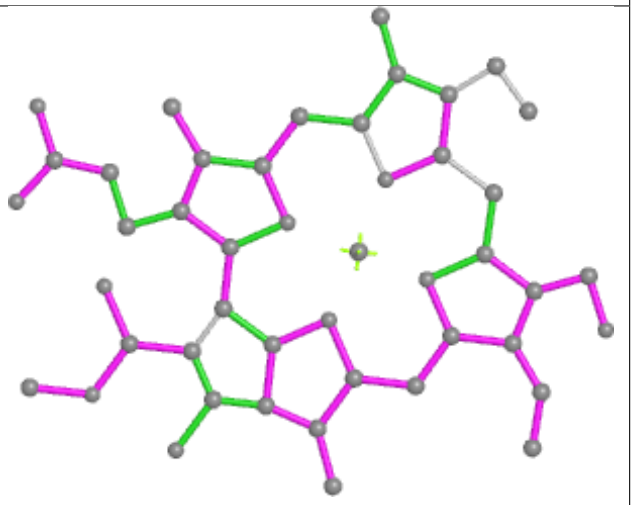

Rings

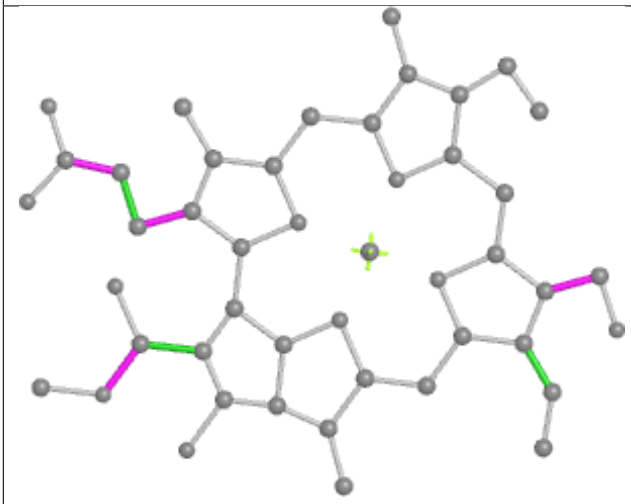
Ligand CHL 4 608



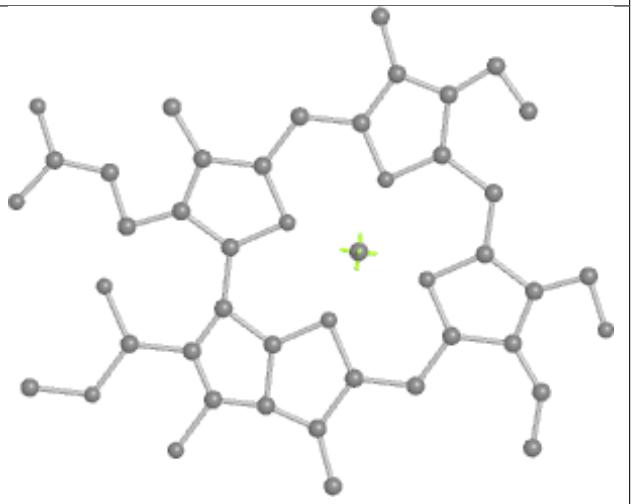
Bond lengths



Bond angles

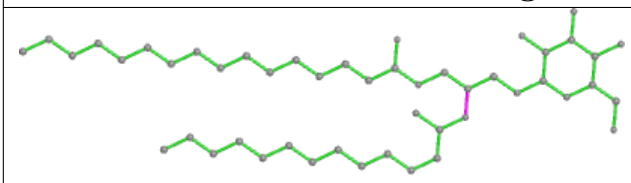


Torsions



Rings

Ligand LMG A 413



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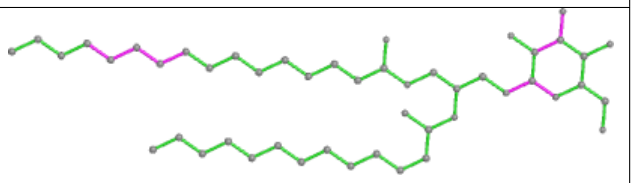

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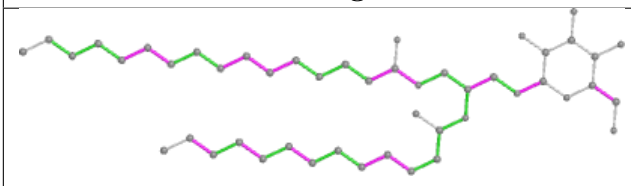

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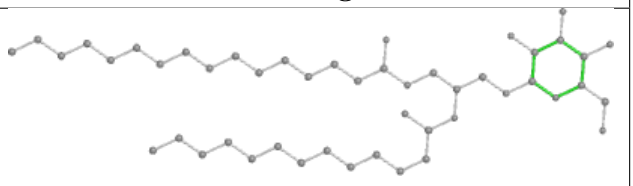
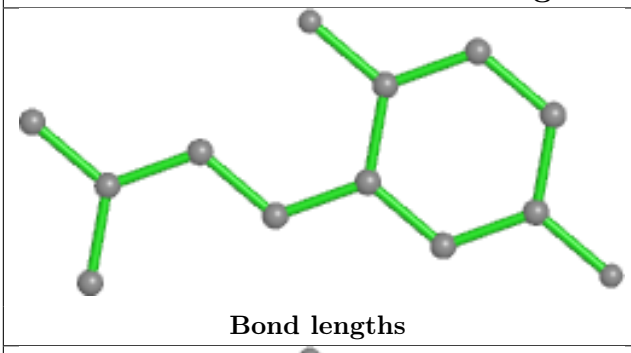


Rings

Ligand PL9 a 414



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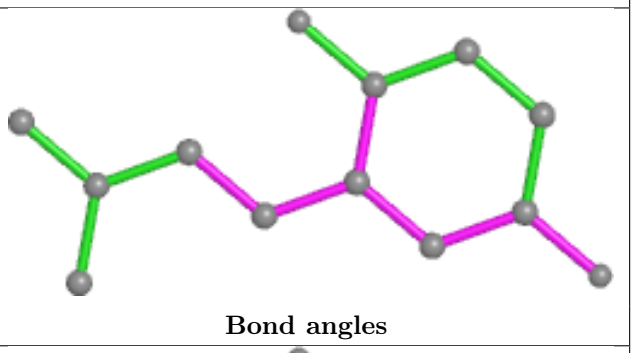

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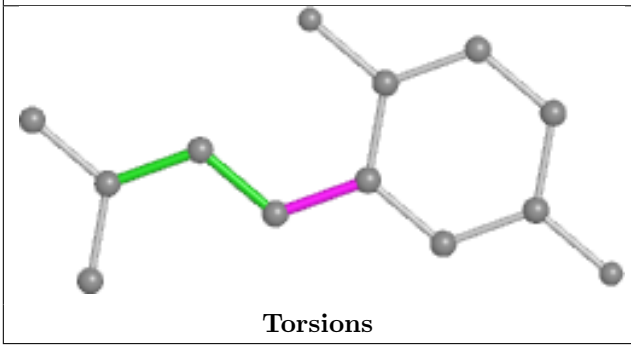

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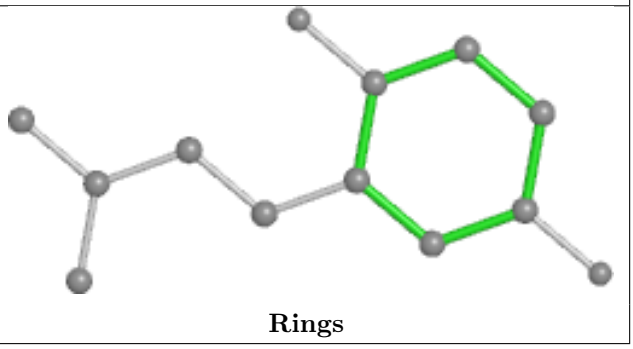
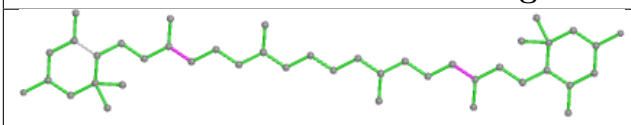


Rings

Ligand LUT 5 1620



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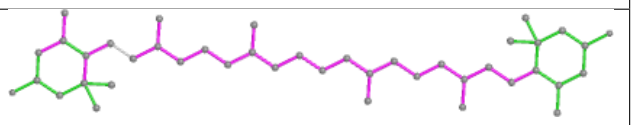

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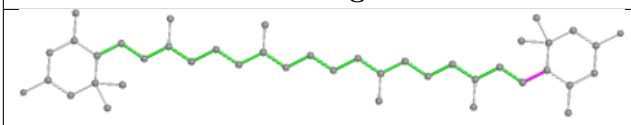
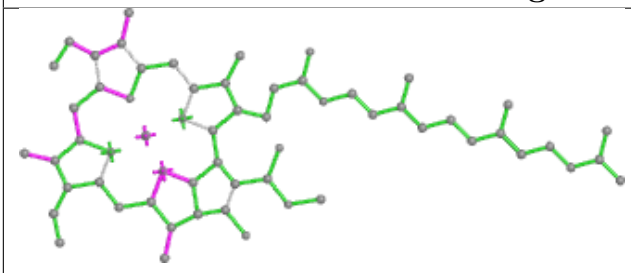


Torsions

Rings

Ligand CLA g 611



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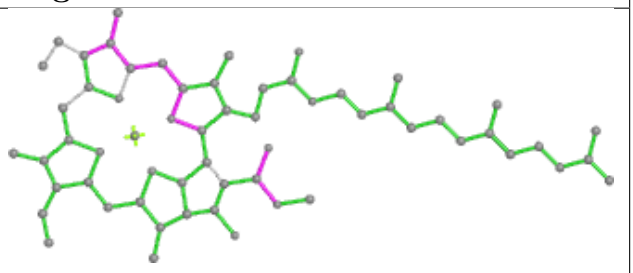

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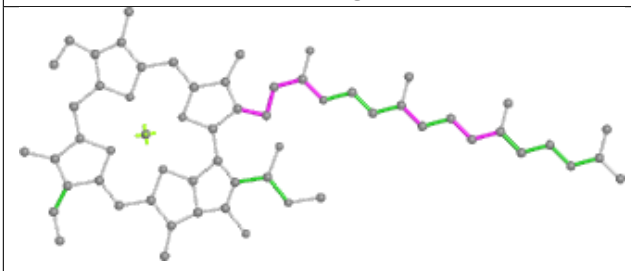

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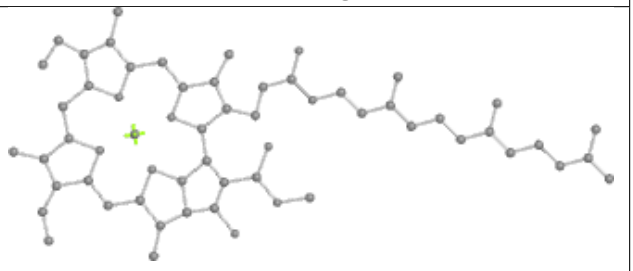
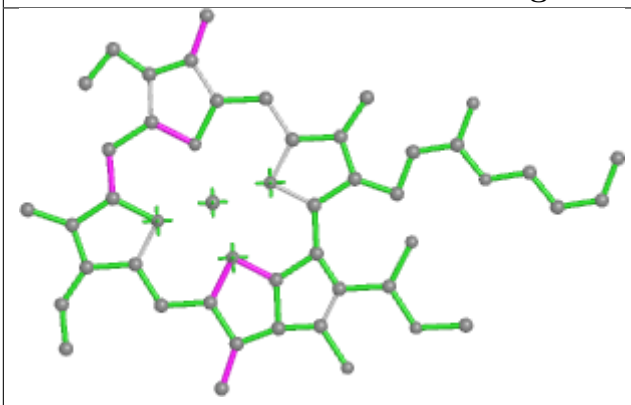


Rings

Ligand CLA s 614



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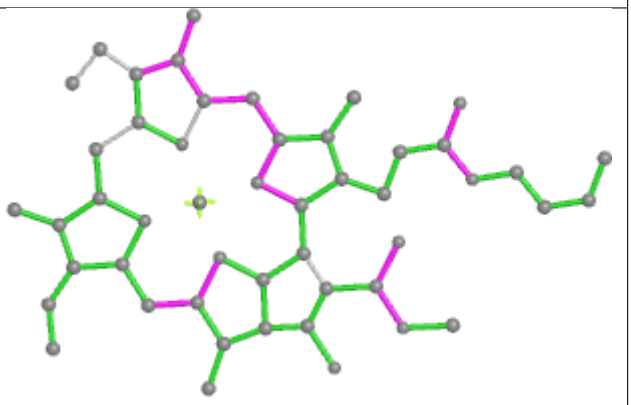

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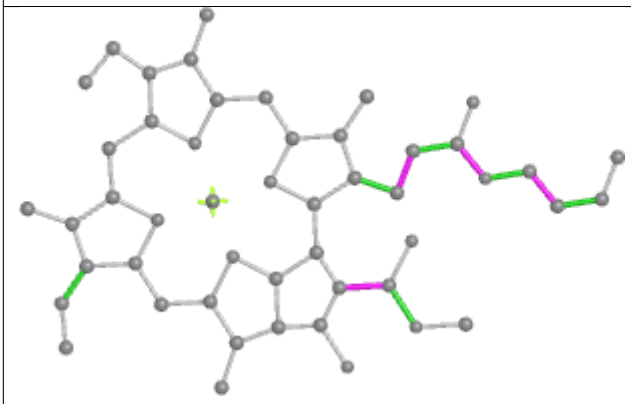

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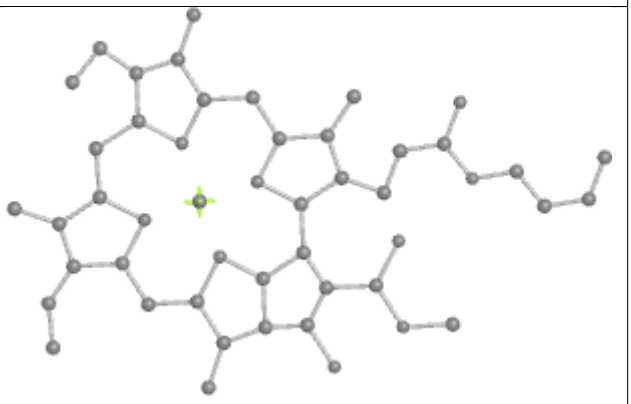
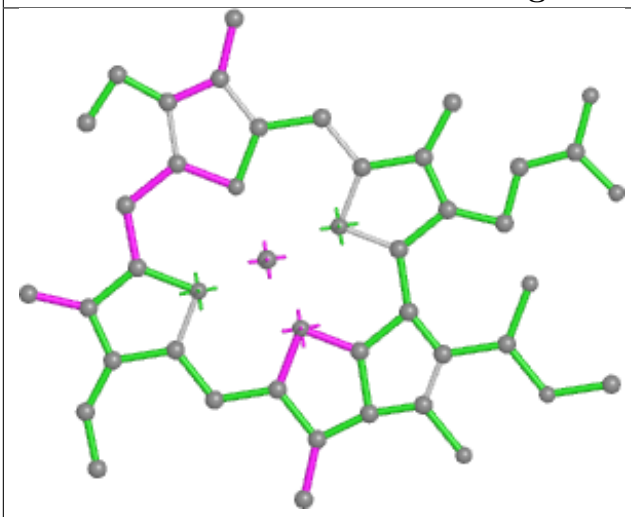


Rings

Ligand CLA 2 612



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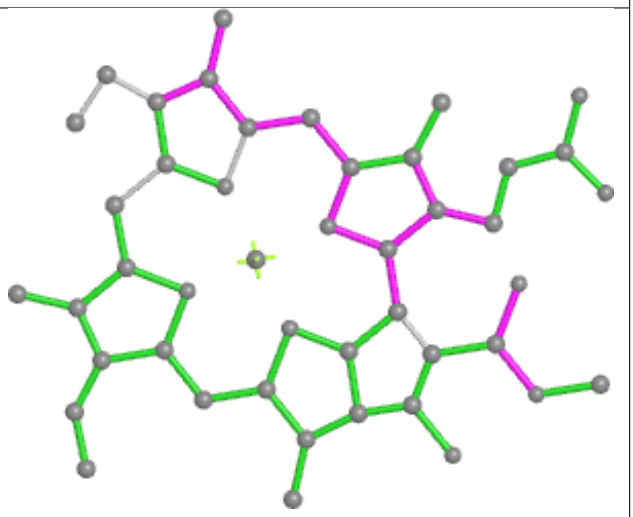
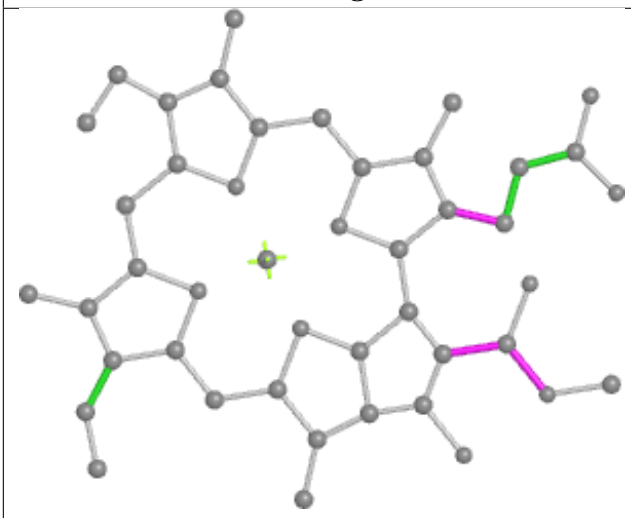


Bond angles



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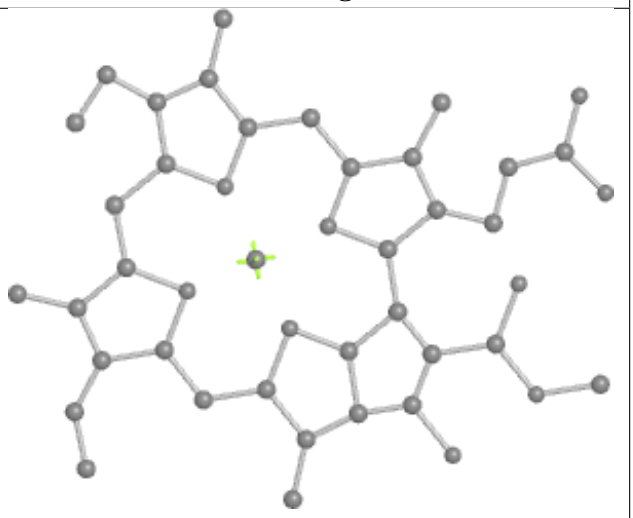
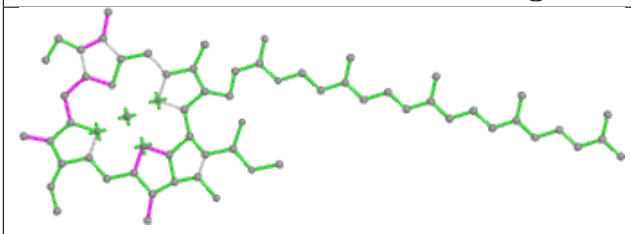


Rings

Ligand CLA b 617



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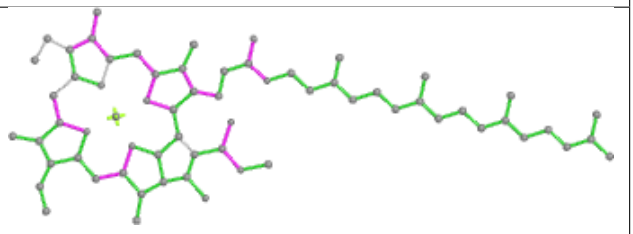
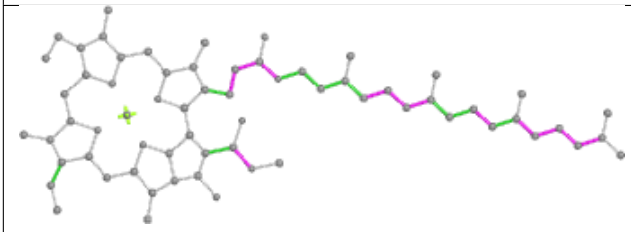


Bond angles



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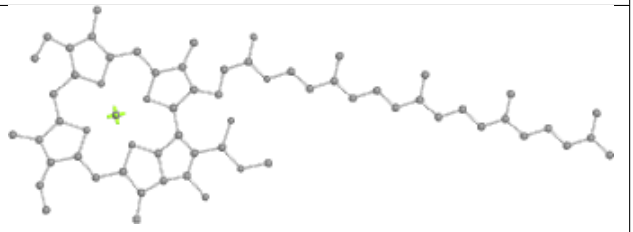
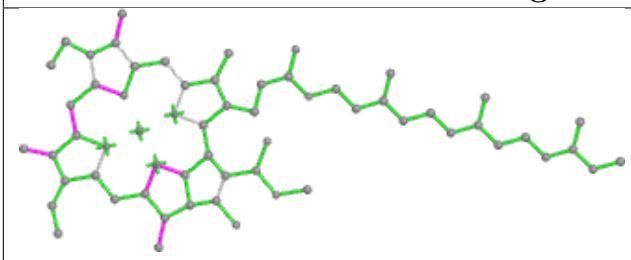


Rings

Ligand CLA s 602



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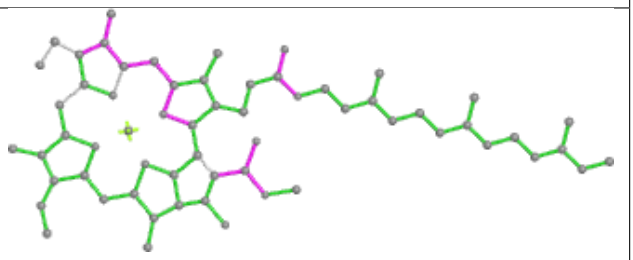
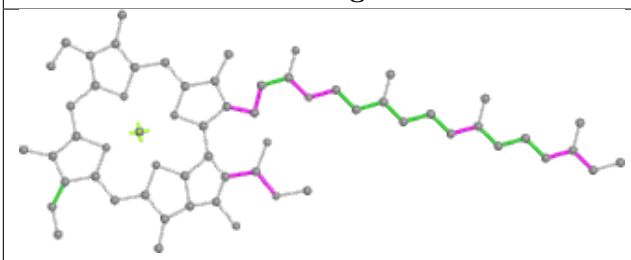


Bond angles



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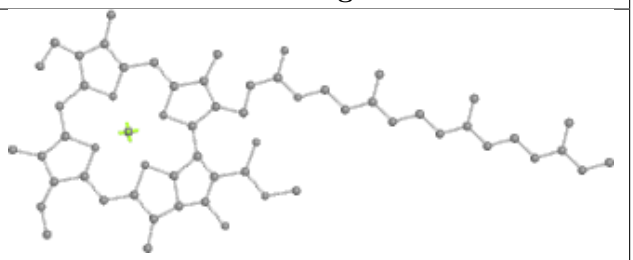
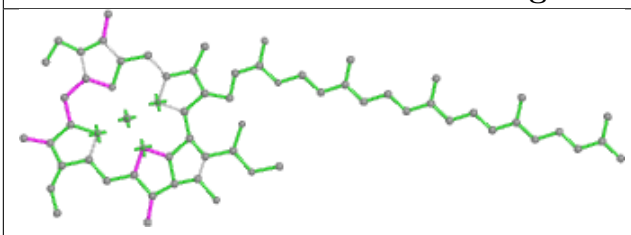


Rings

Ligand CLA c 507



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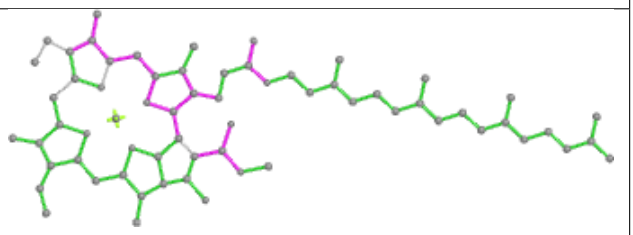
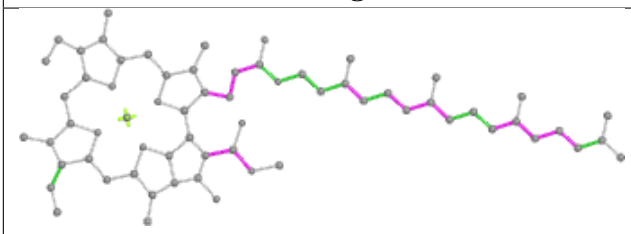


Bond angles



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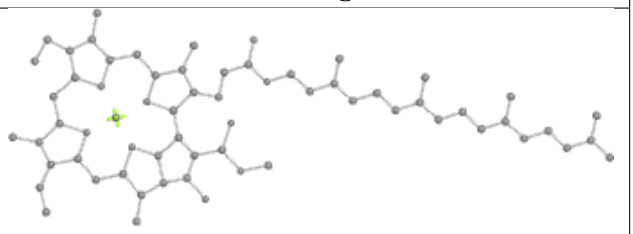
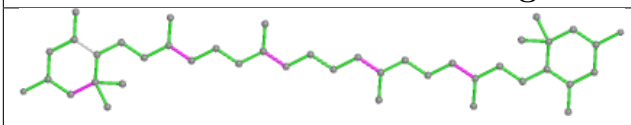


Rings

Ligand LUT y 1620



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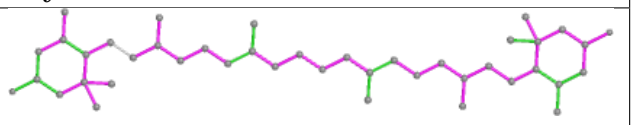
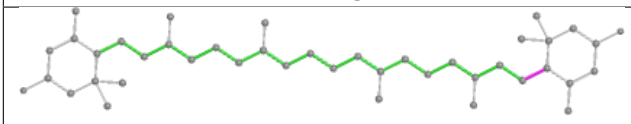


Bond angles



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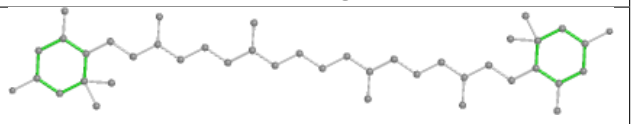
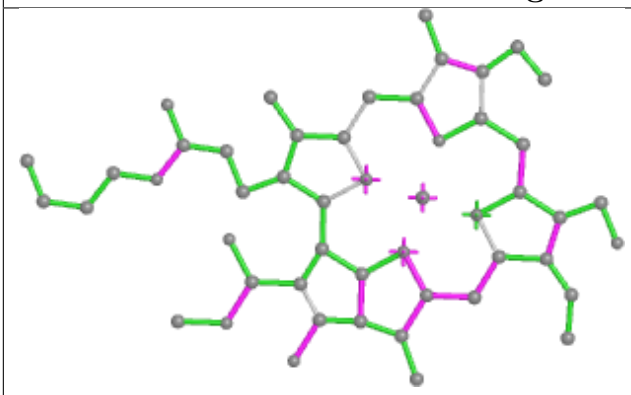


Rings

Ligand CHL n 606



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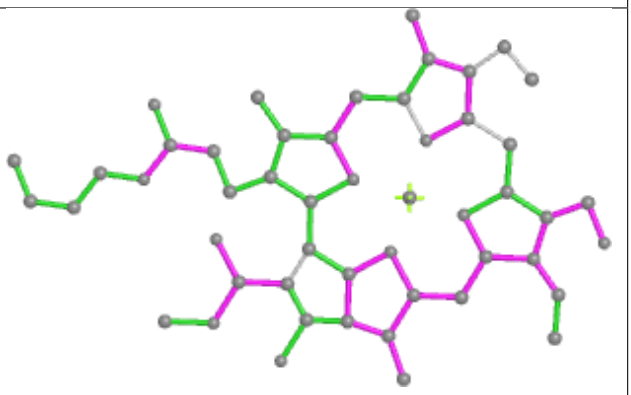
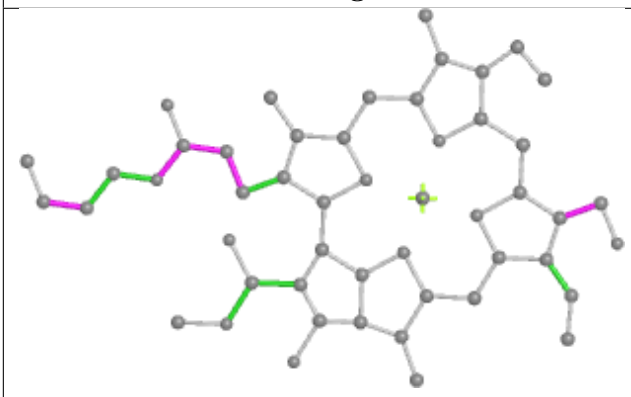
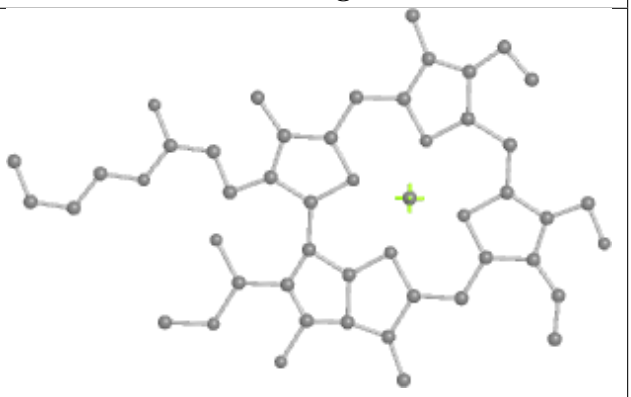


Bond angles

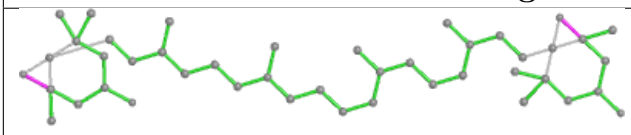


Torsions



Rings

Ligand XAT 1 1622



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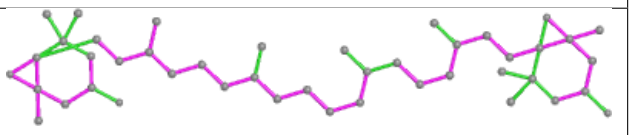
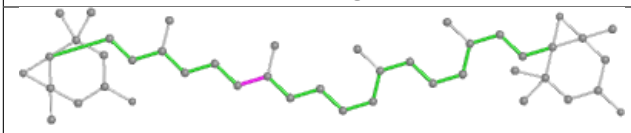


Bond angles



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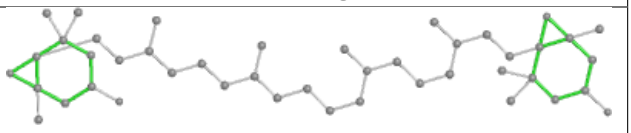
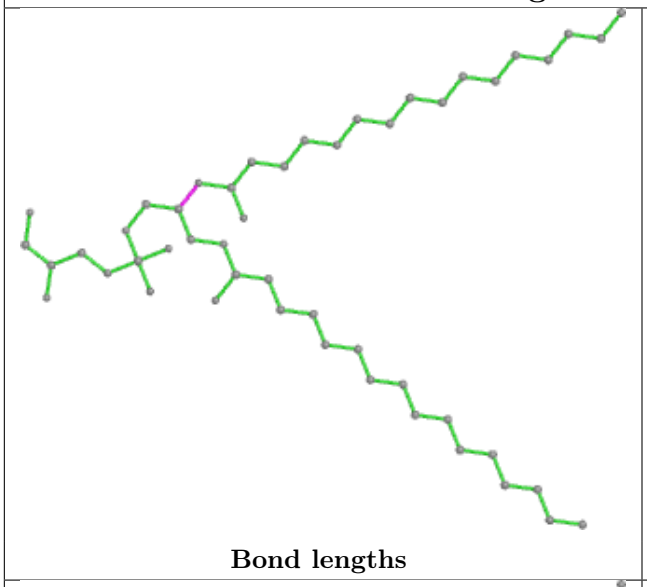


Rings

Ligand LHG c 522



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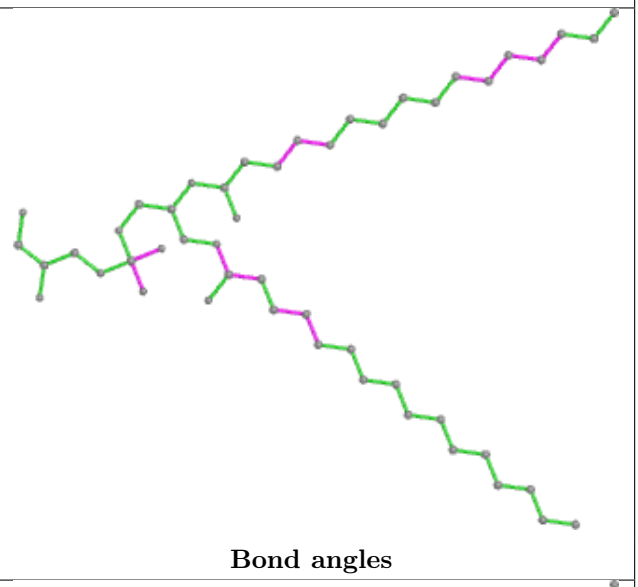
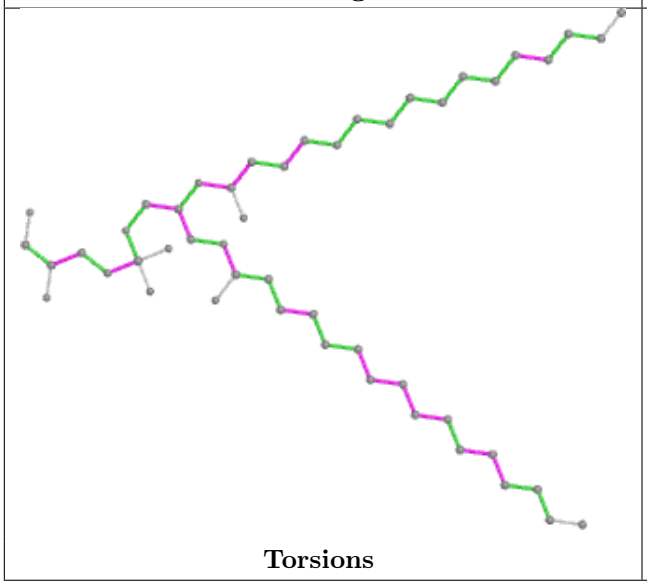


Bond angles



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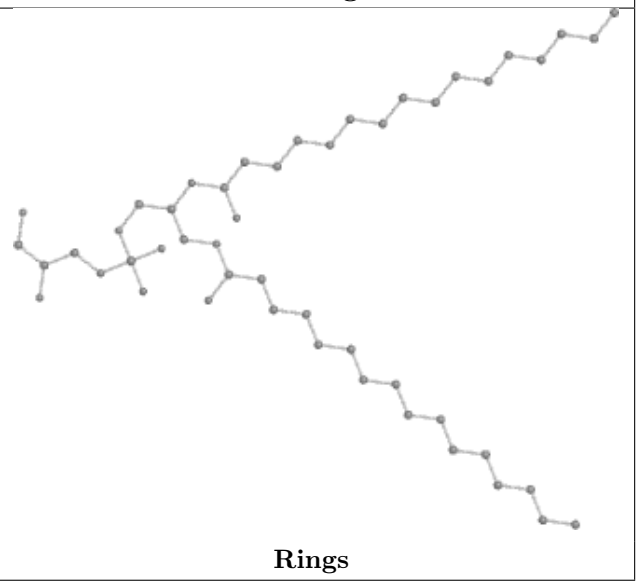
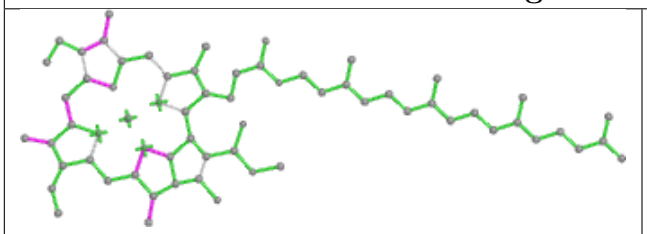
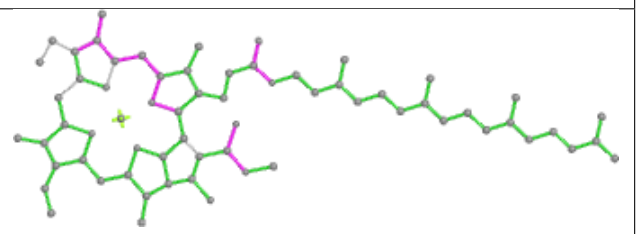


Rings

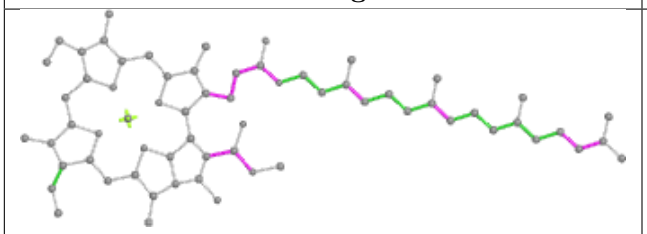
Ligand CLA C 501



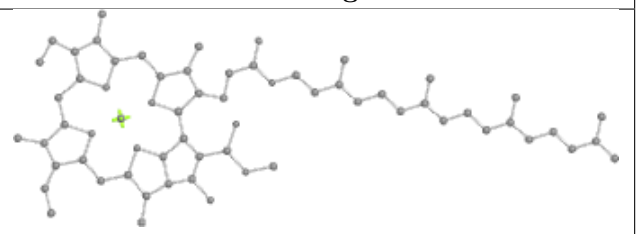
Bond lengths



Bond angles

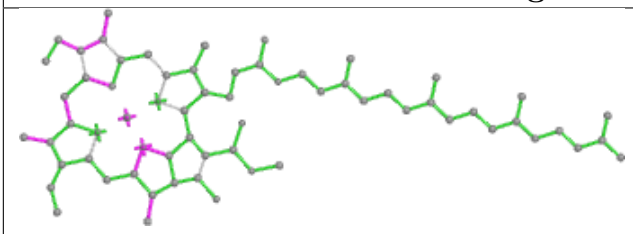


Torsions



Rings

Ligand CLA b 603



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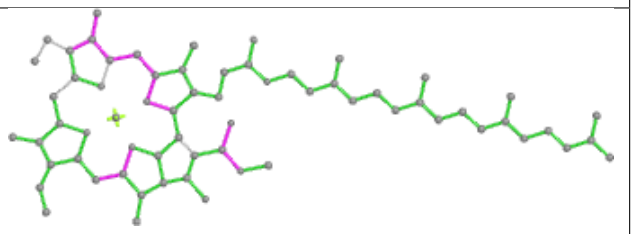

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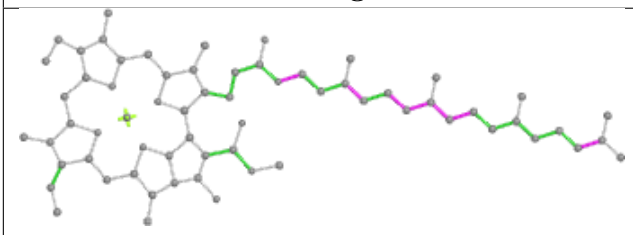

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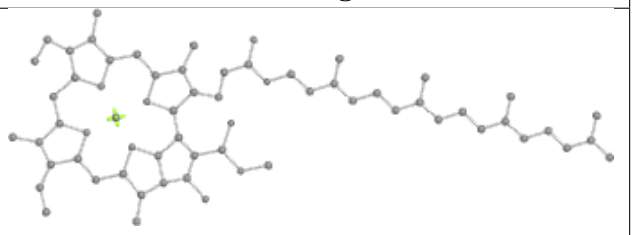
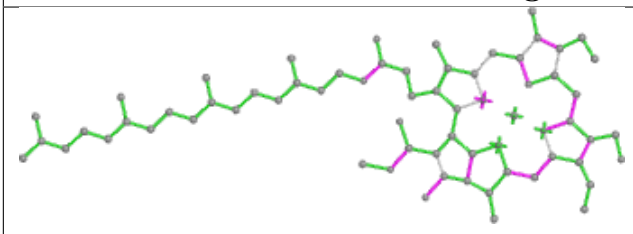


Rings

Ligand CHL Y 607



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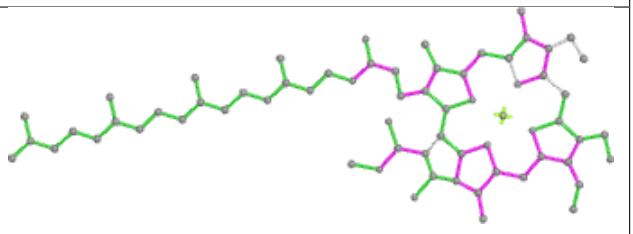
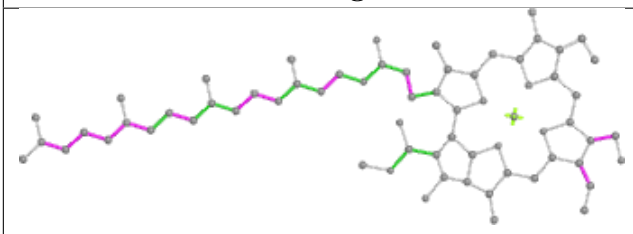


Bond angles



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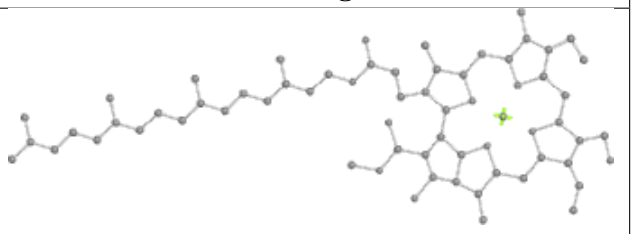
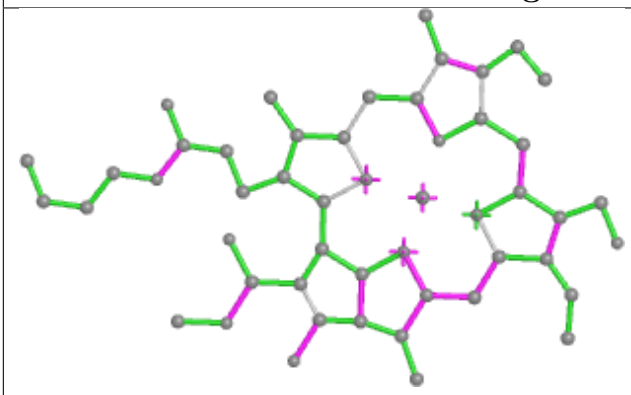


Rings

Ligand CHL N 606



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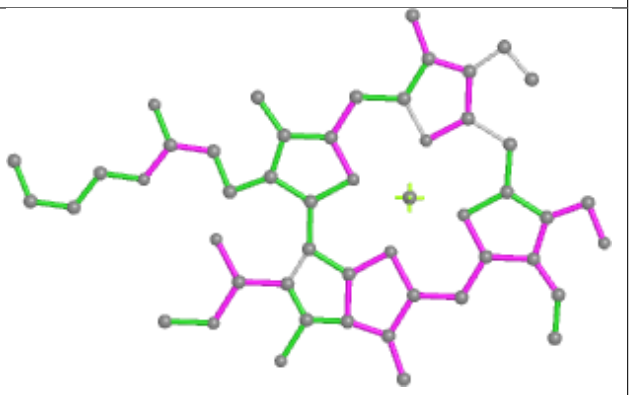

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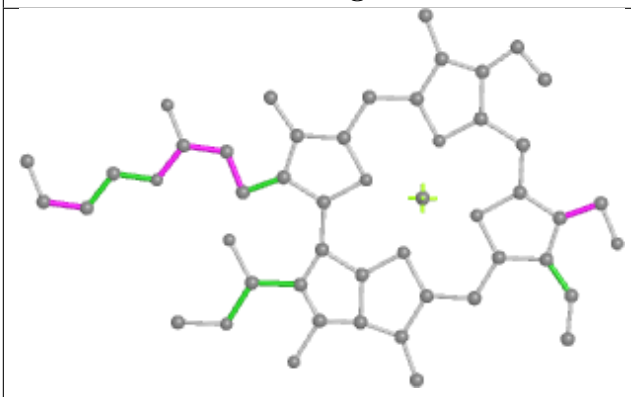

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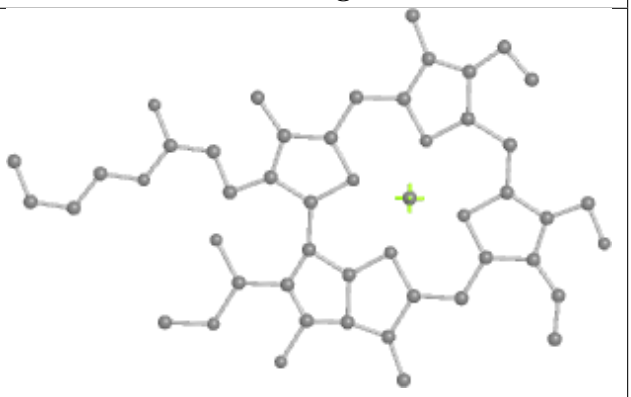
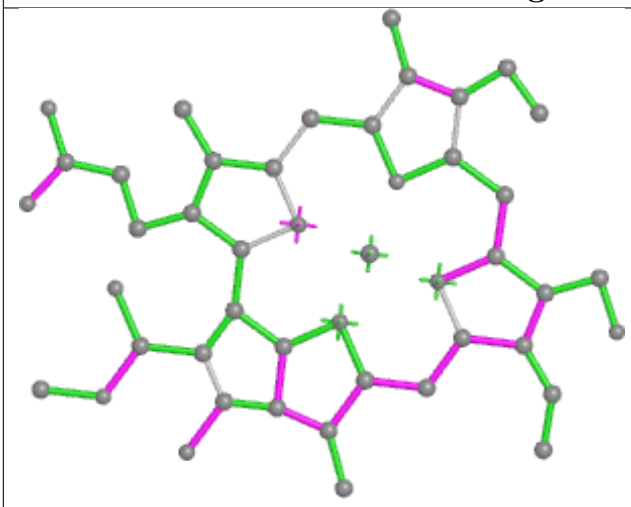


Rings

Ligand CHL 4 609



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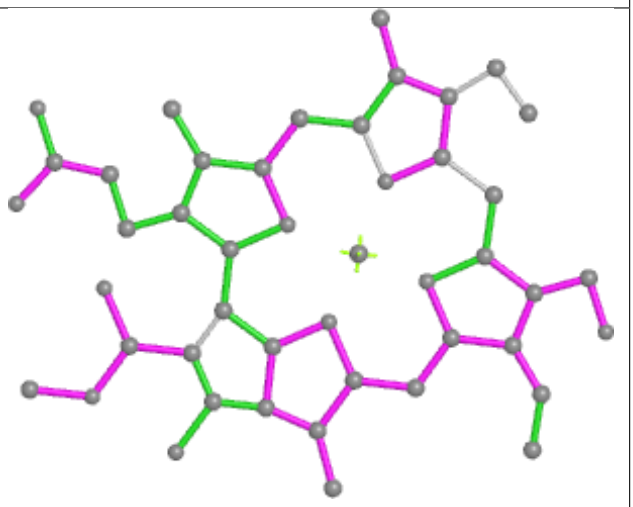

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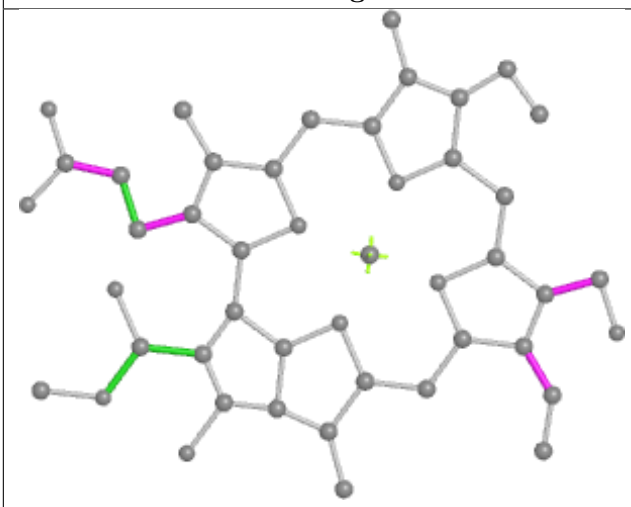

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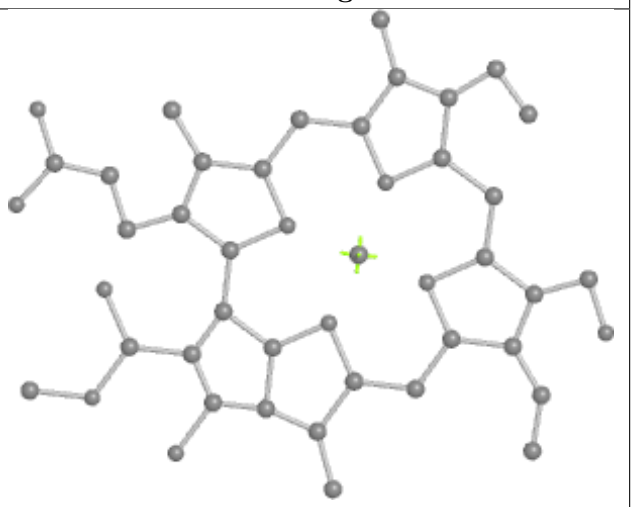

Rings

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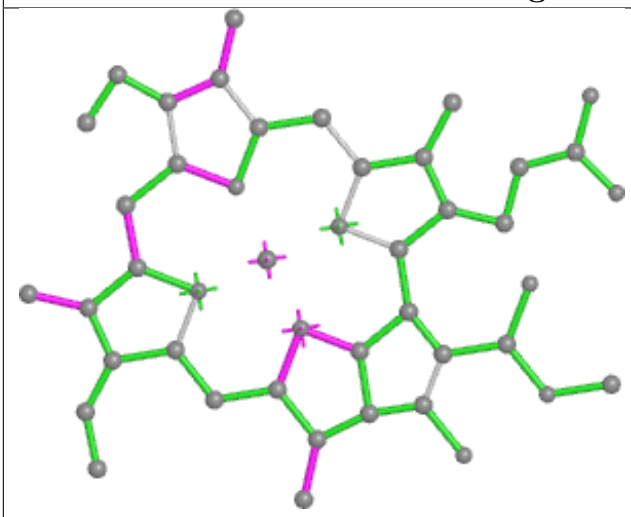

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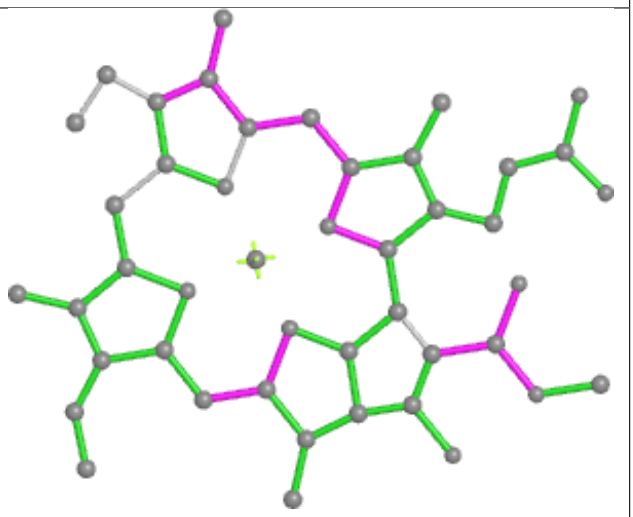

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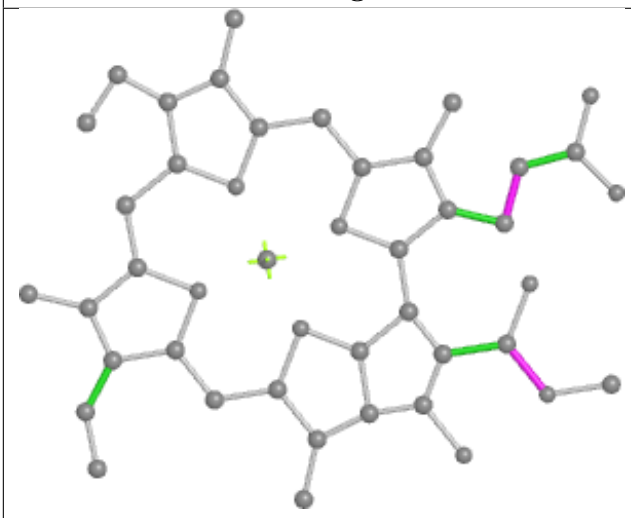

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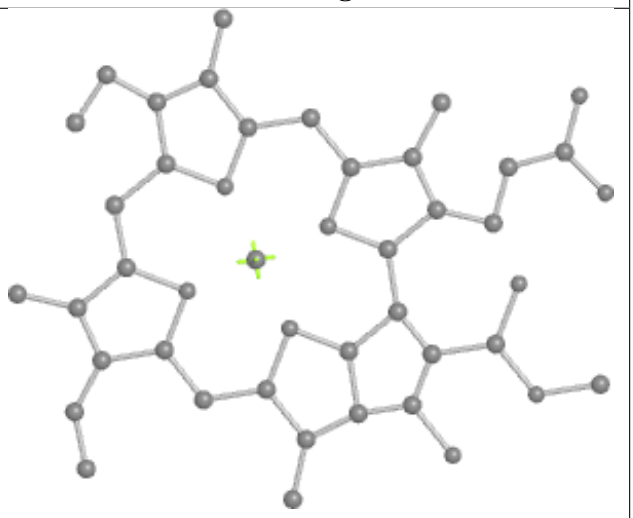

Rings

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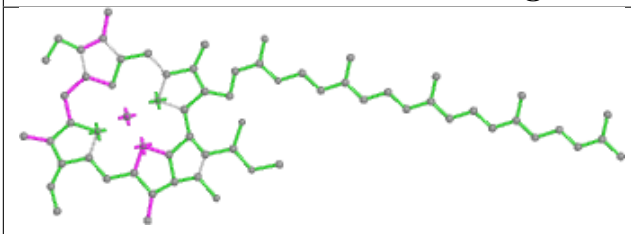

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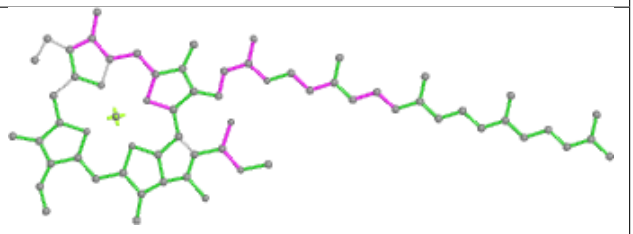

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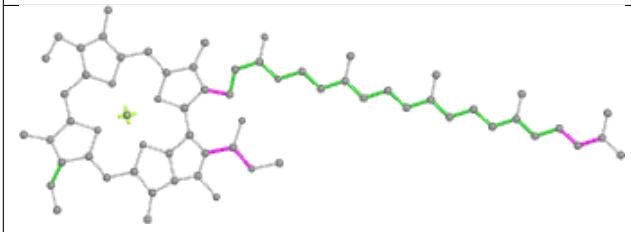

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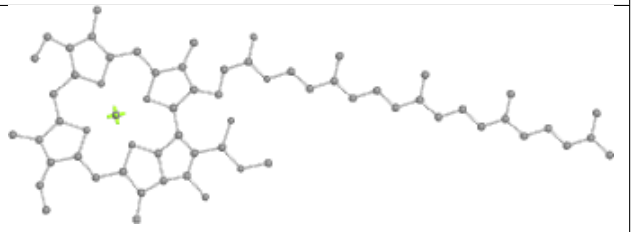
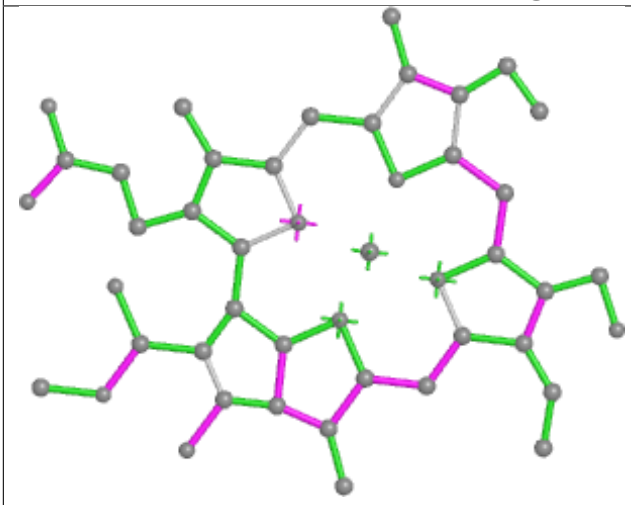


Rings

Ligand CHL 7 605



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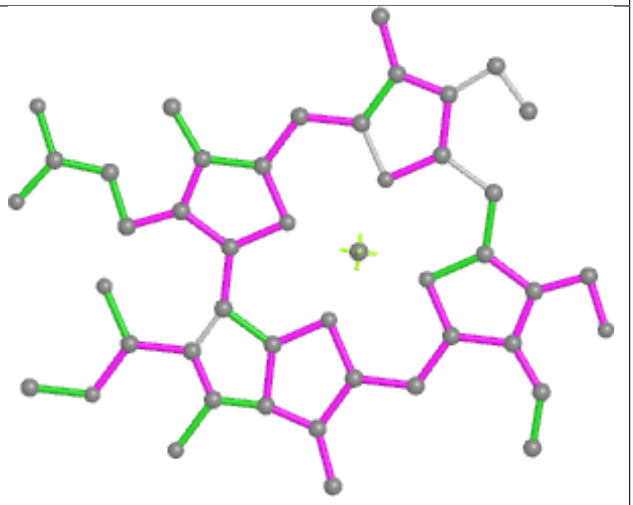

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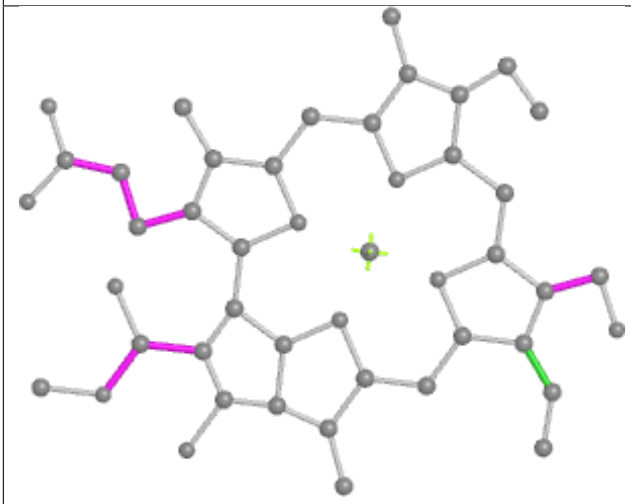

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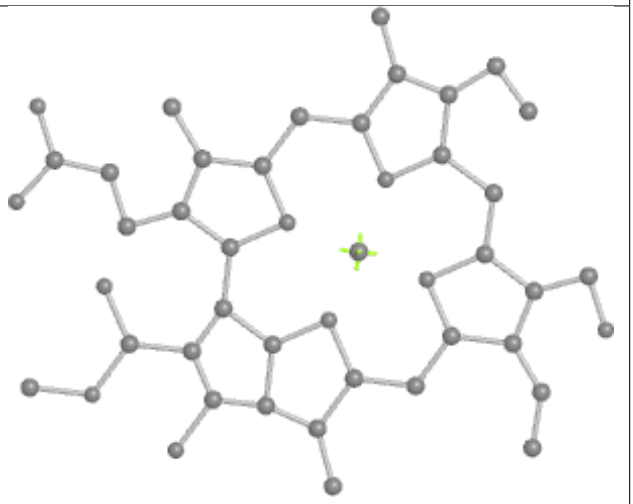
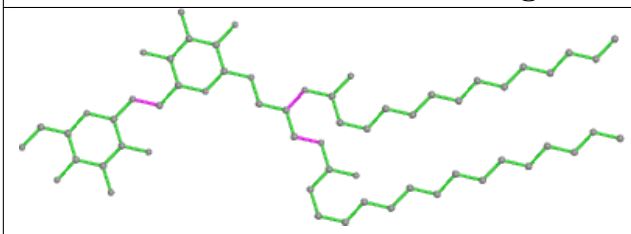


Rings

Ligand DGD C 520



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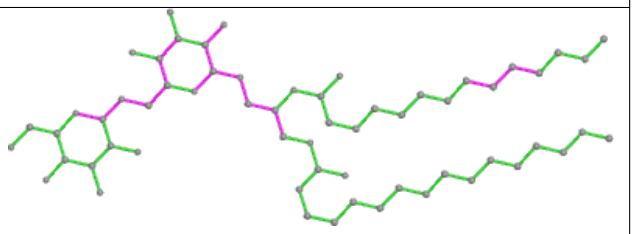
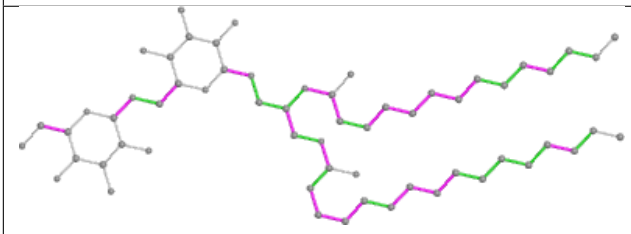


Bond angles



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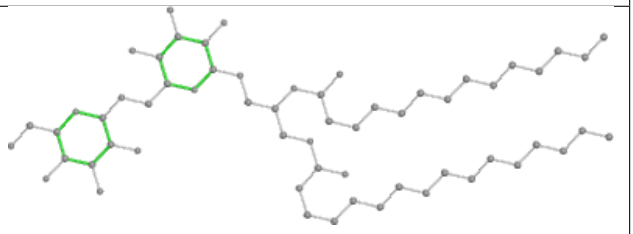
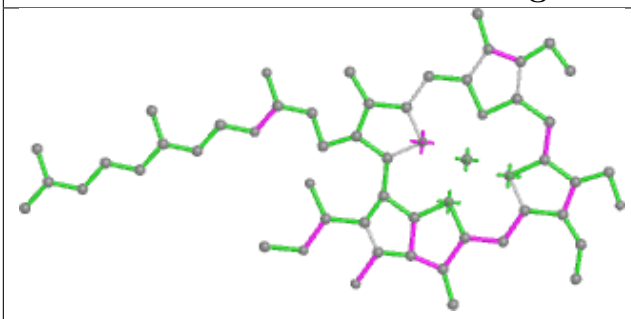


Rings

Ligand CHL r 607



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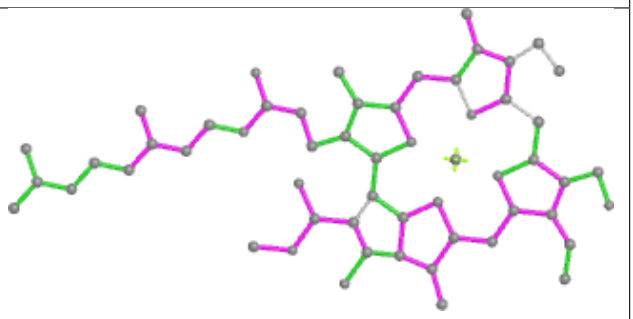

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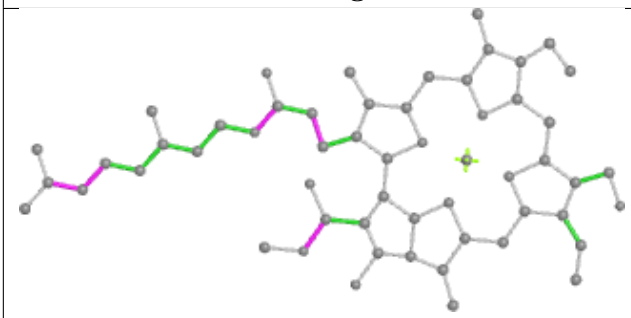

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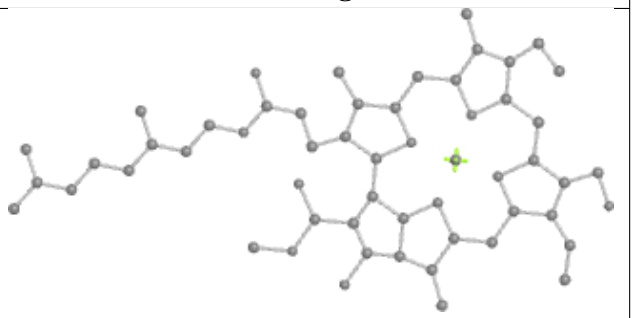
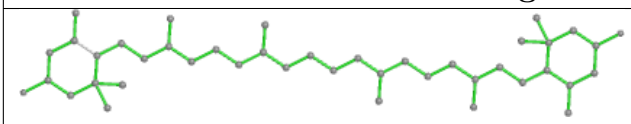


Rings

Ligand LUT S 1621



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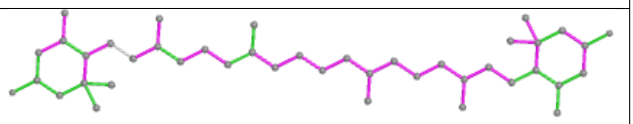

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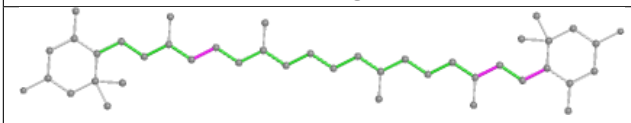

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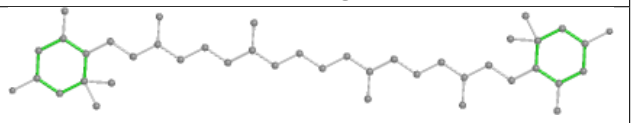
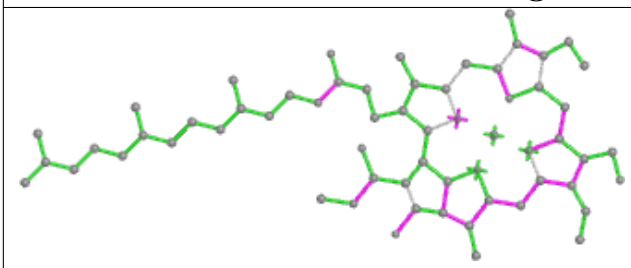


Rings

Ligand CHL g 609



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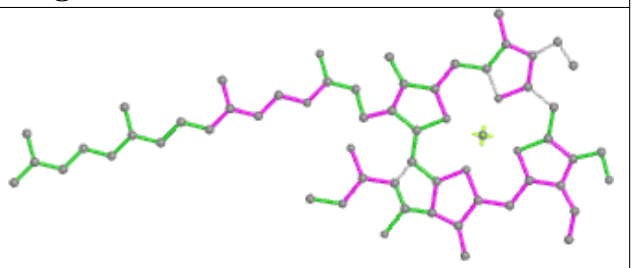
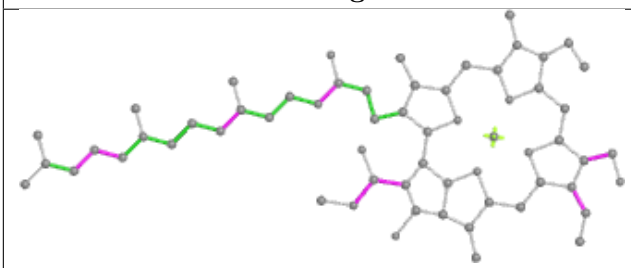
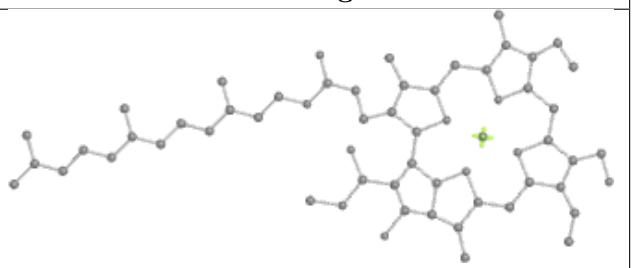


Bond angles

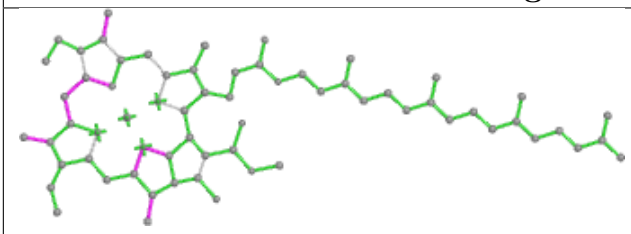


Torsions



Rings

Ligand CLA C 508



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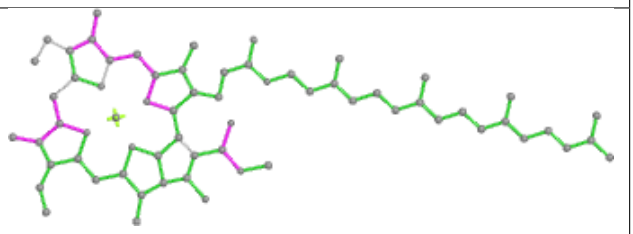
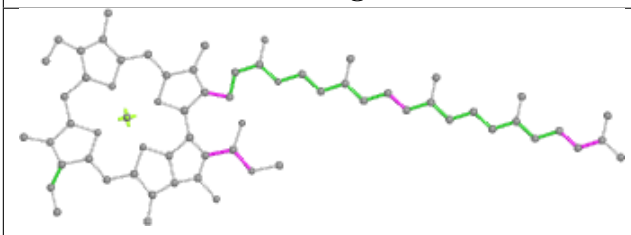


Bond angles



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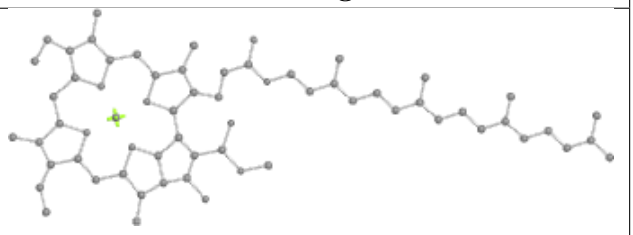
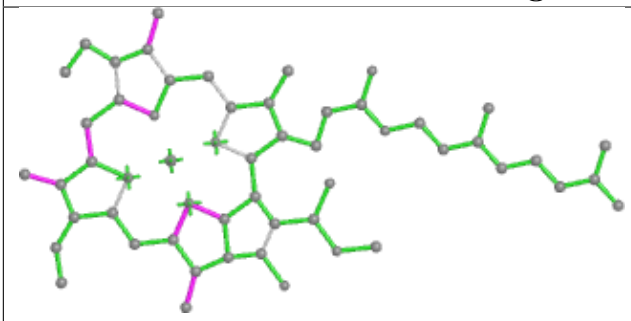


Rings

Ligand CLA S 613



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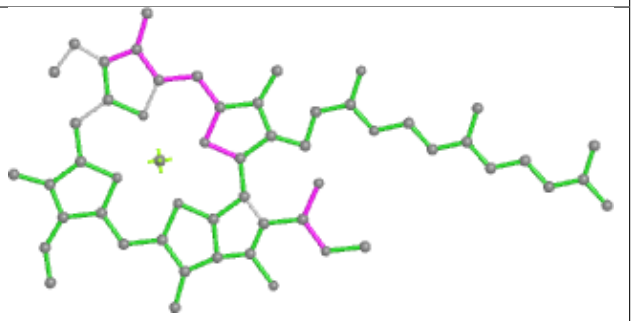
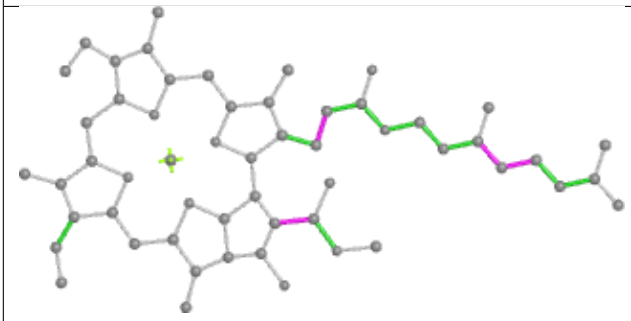
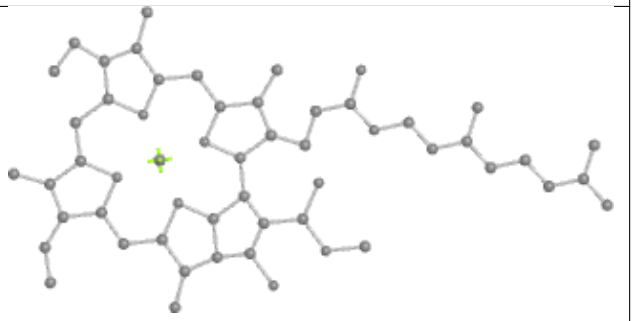


Bond angles

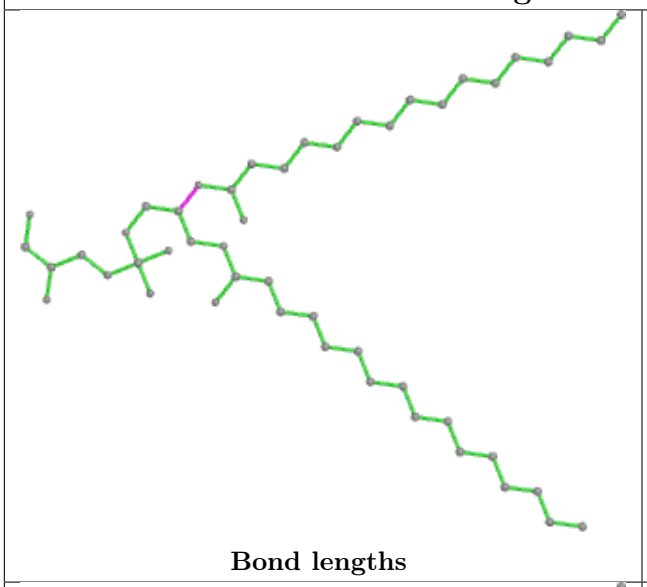


Torsions

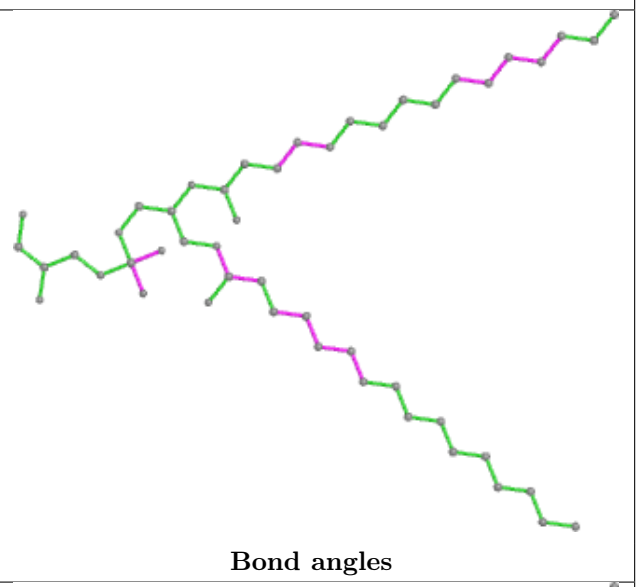


Rings

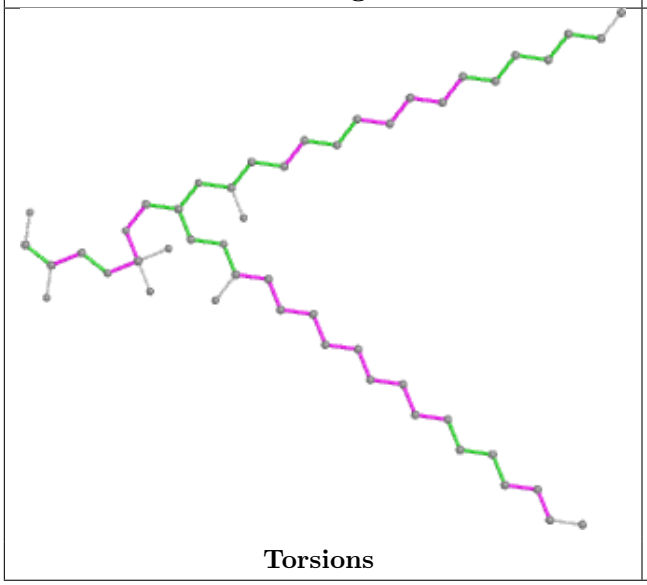
Ligand LHG N 2630



Bond lengths



Bond angles



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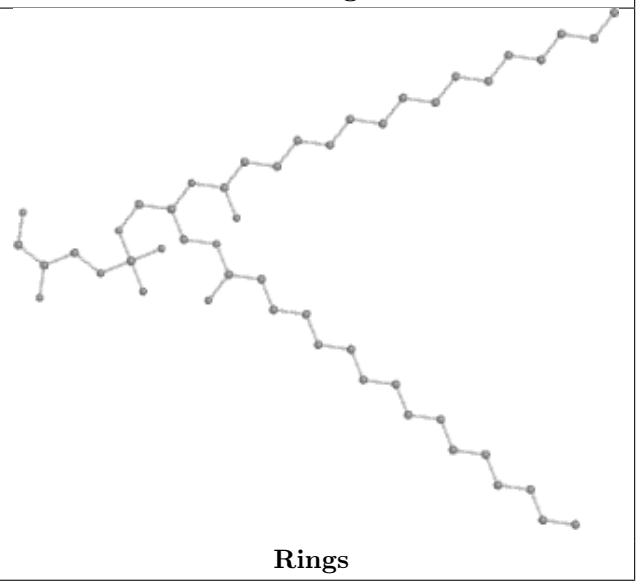
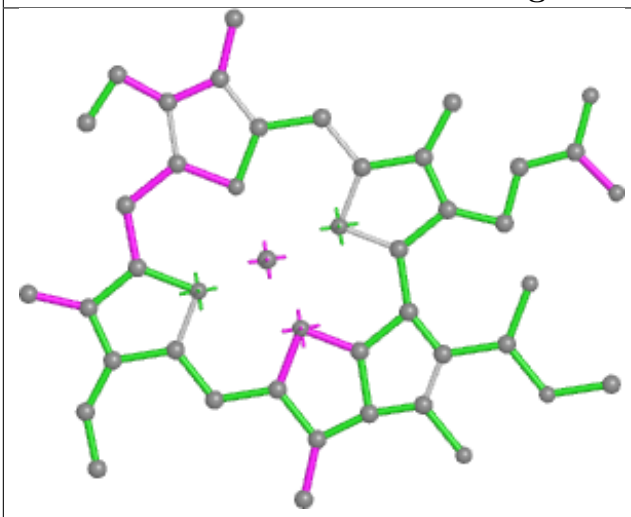


Rings

Ligand CLA 5 611



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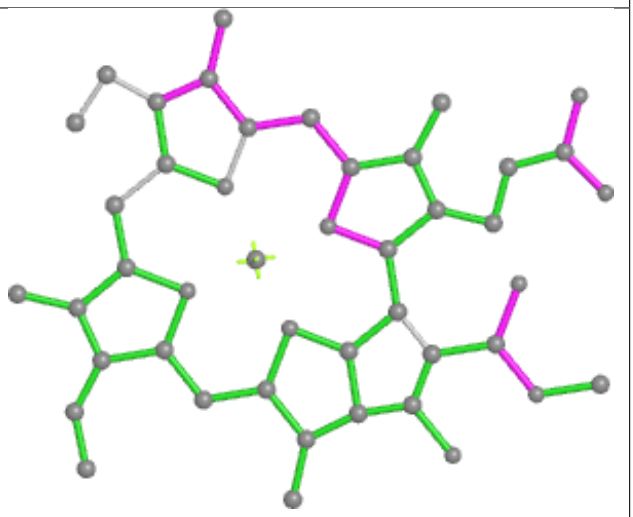

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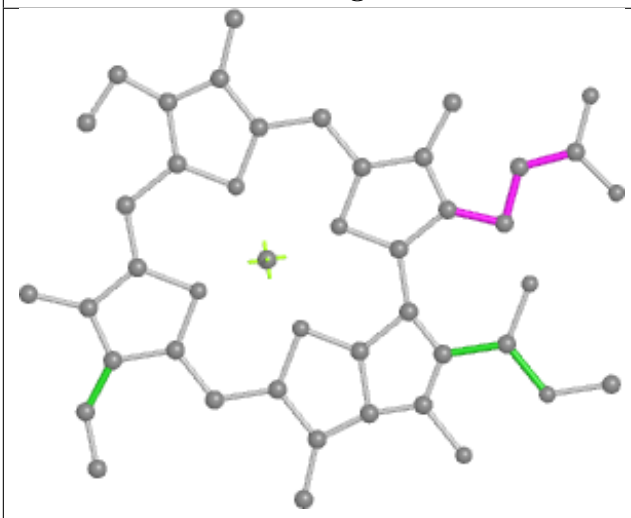

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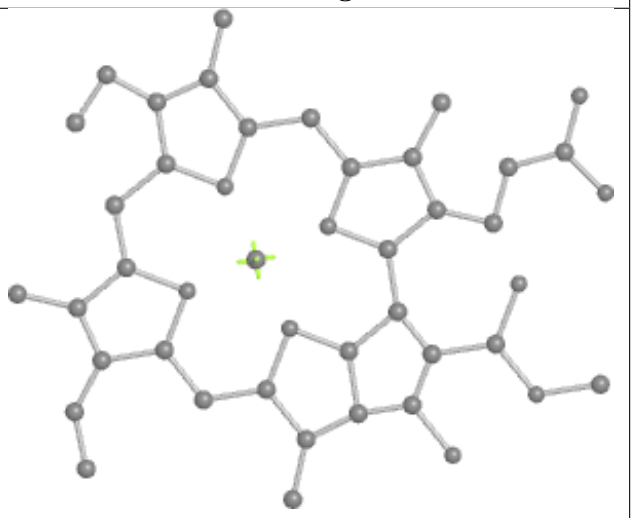
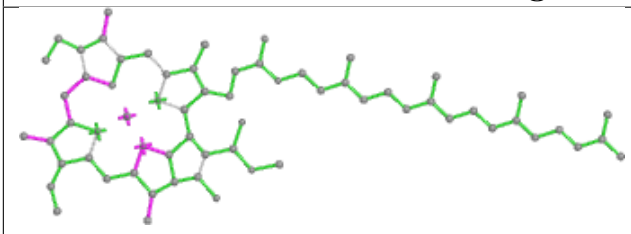


Rings

Ligand CLA a 405



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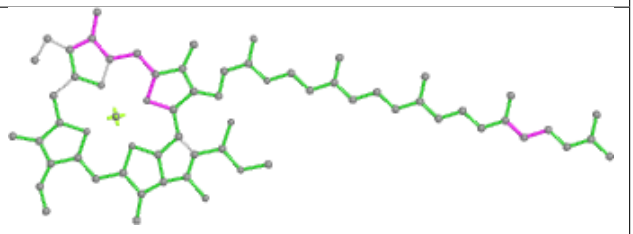
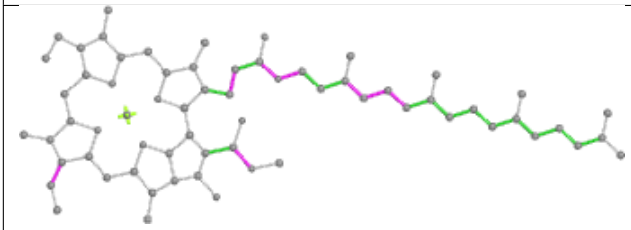


Bond angles



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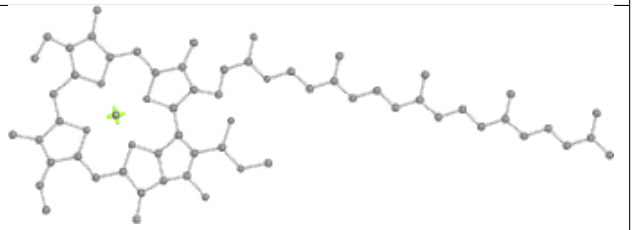
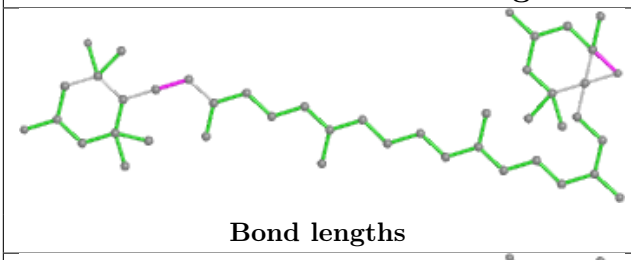


Rings

Ligand NEX Y 1623



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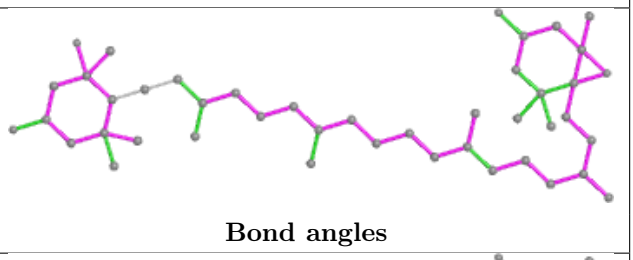

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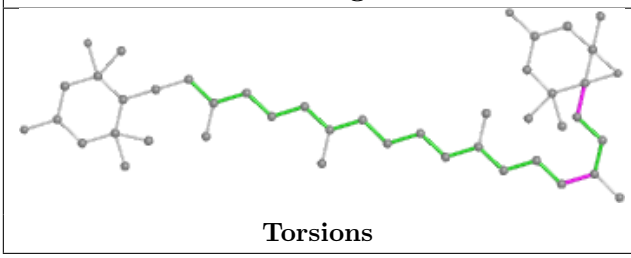

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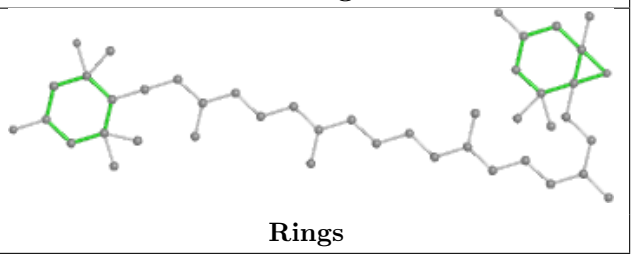
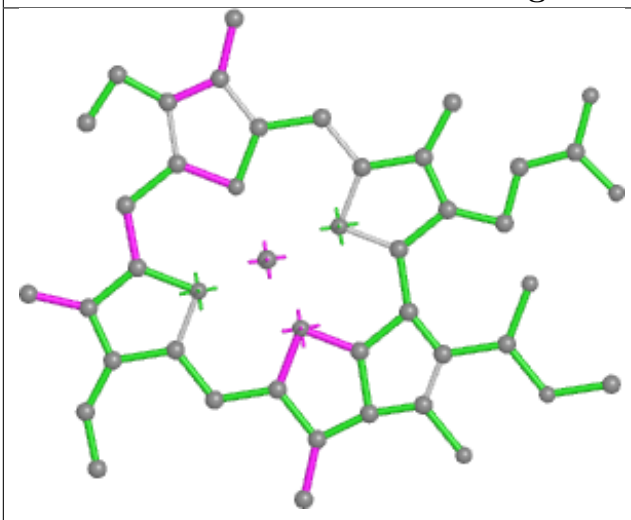


Rings

Ligand CLA 5 614



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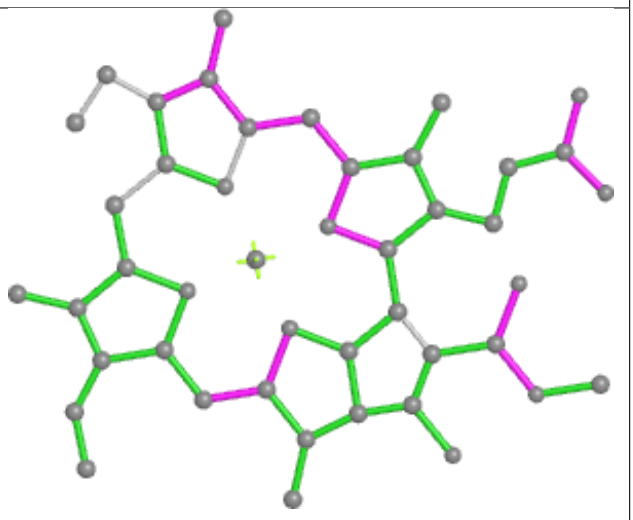
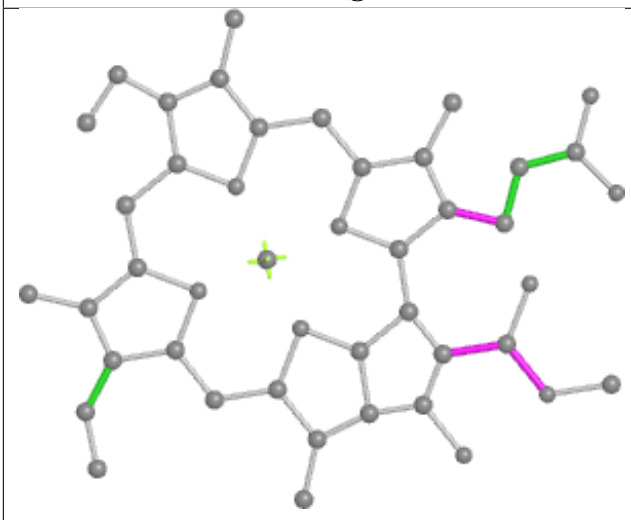


Bond angles



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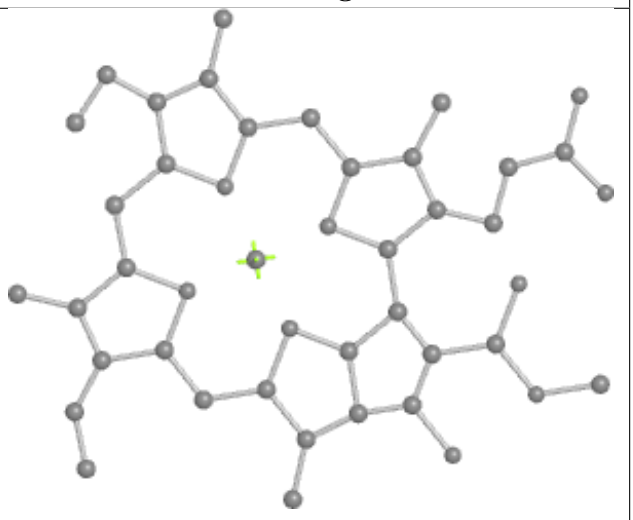

Rings

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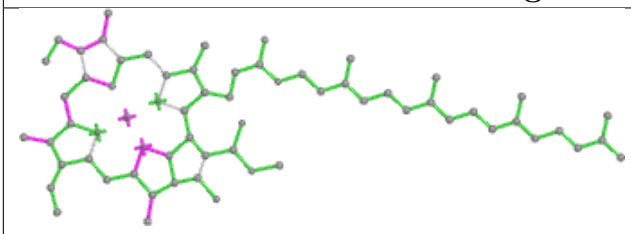

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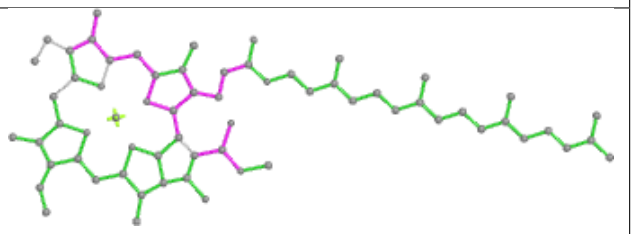

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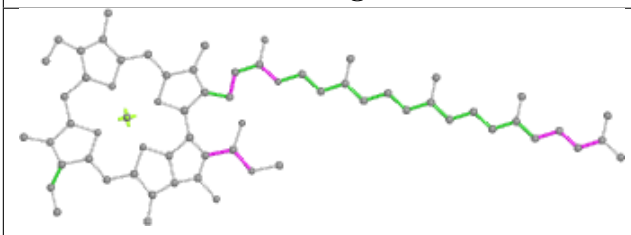

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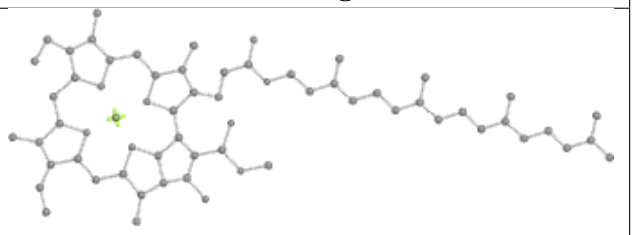
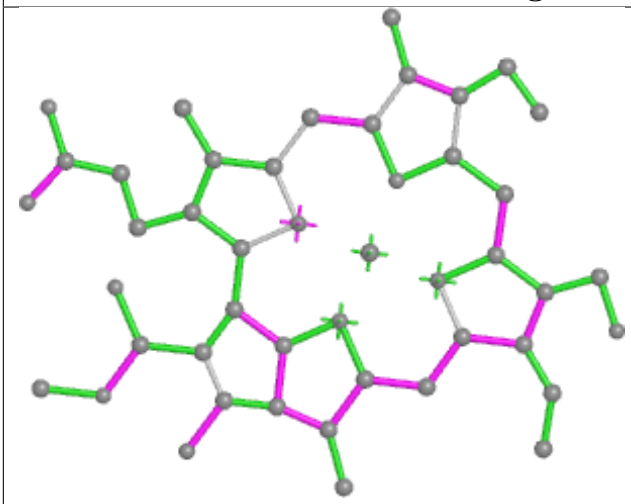


Rings

Ligand CHL S 608



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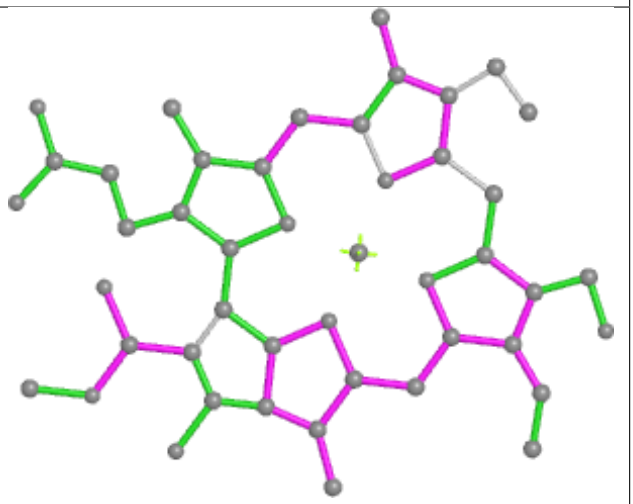

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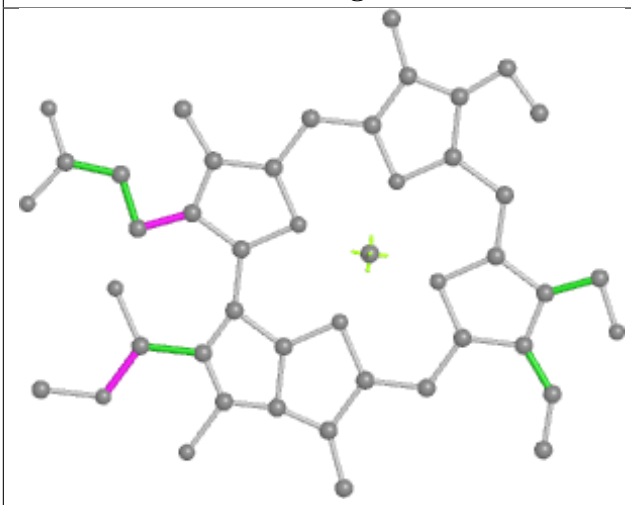

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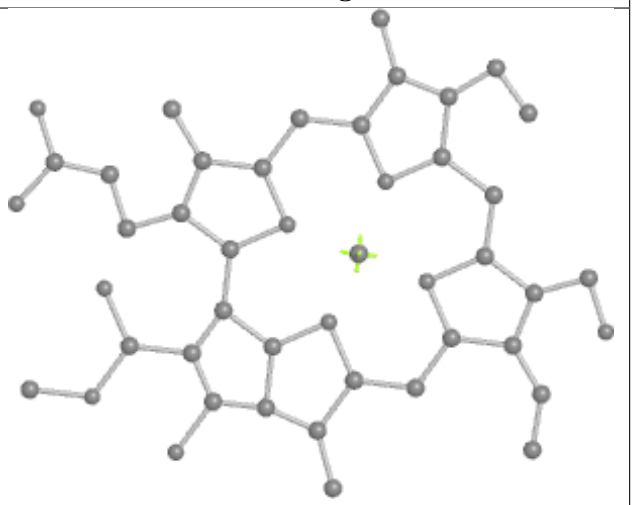
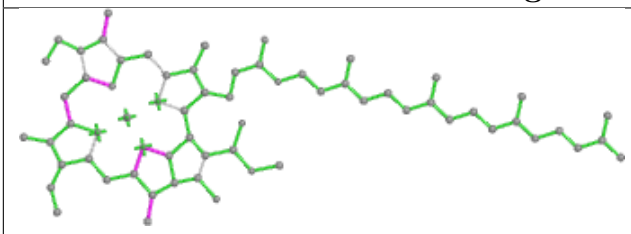


Rings

Ligand CLA C 511



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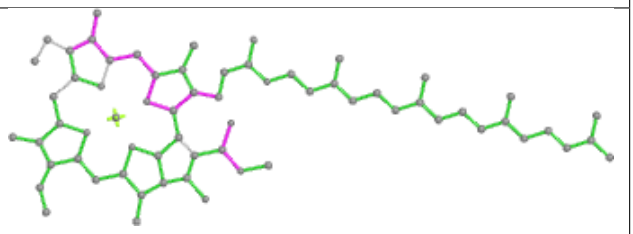
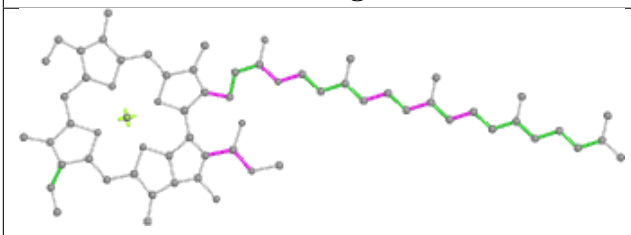


Bond angles



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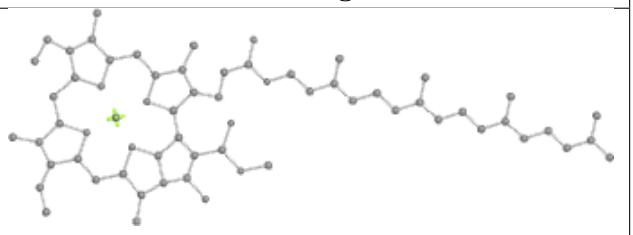
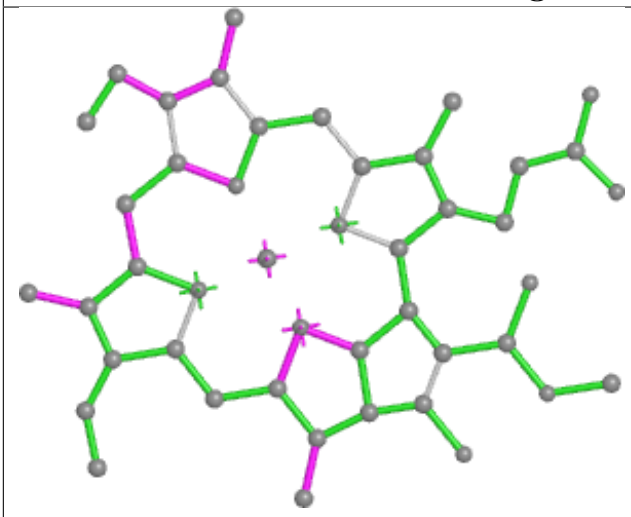


Rings

Ligand CLA 8 610



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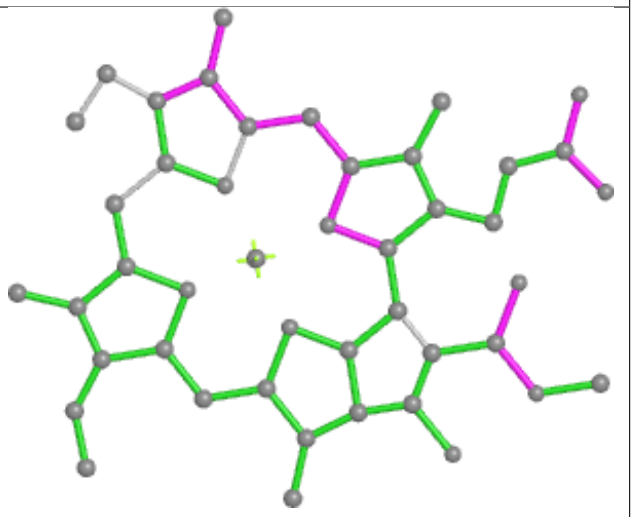

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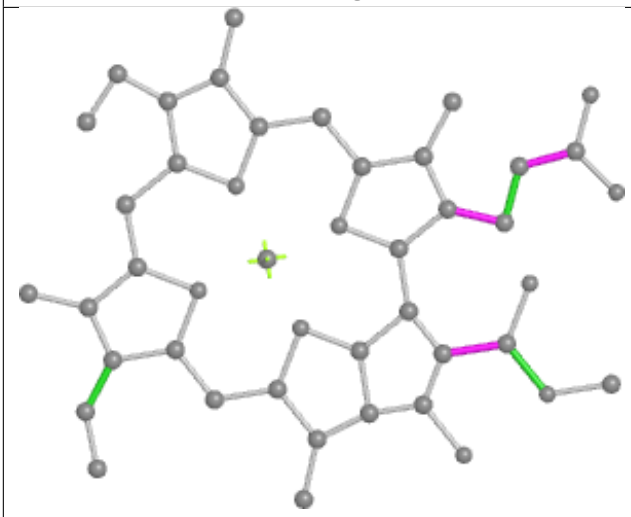

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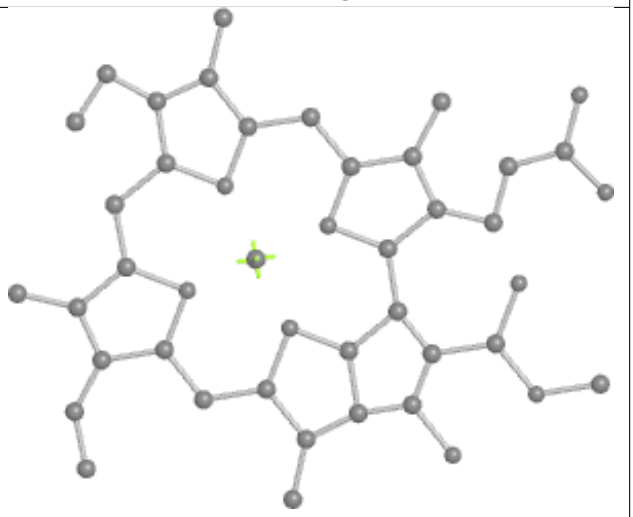
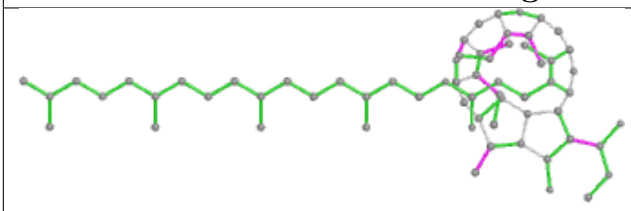


Rings

Ligand PHO A 408



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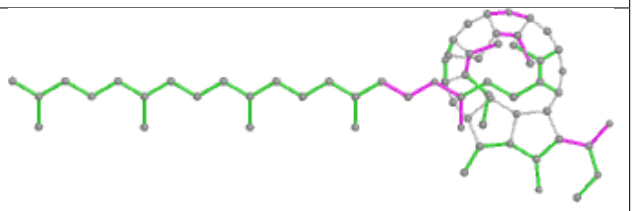
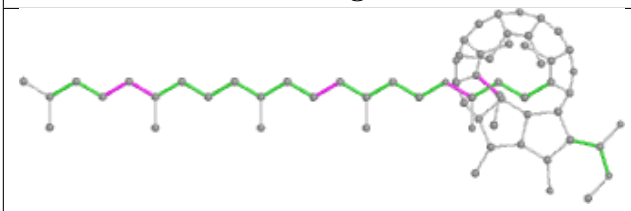


Bond angles



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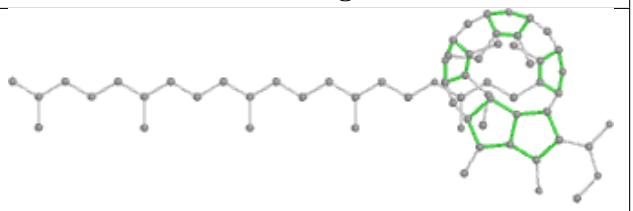
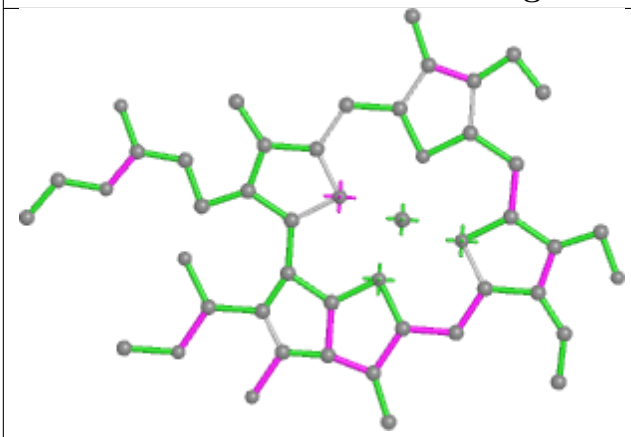


Rings

Ligand CHL Y 605



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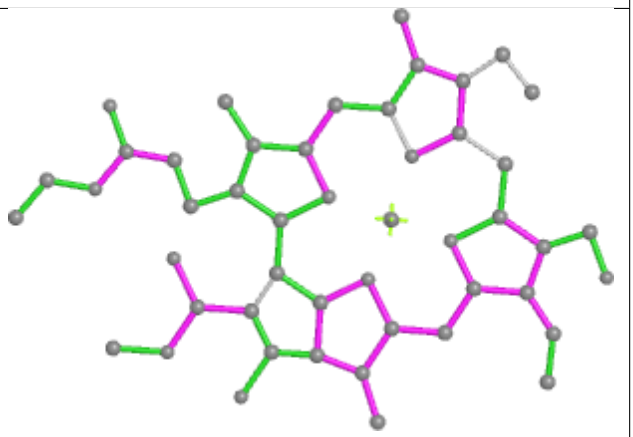
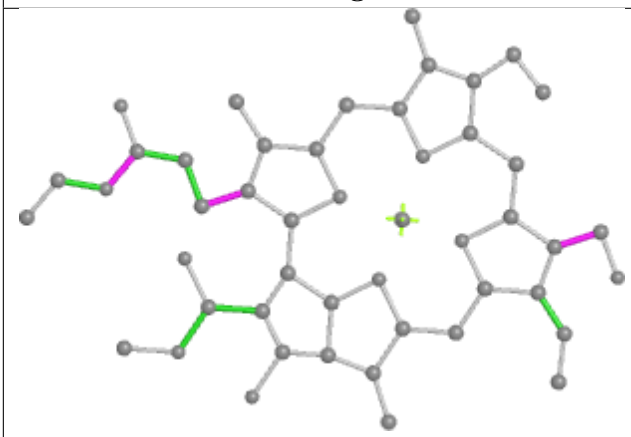


Bond angles



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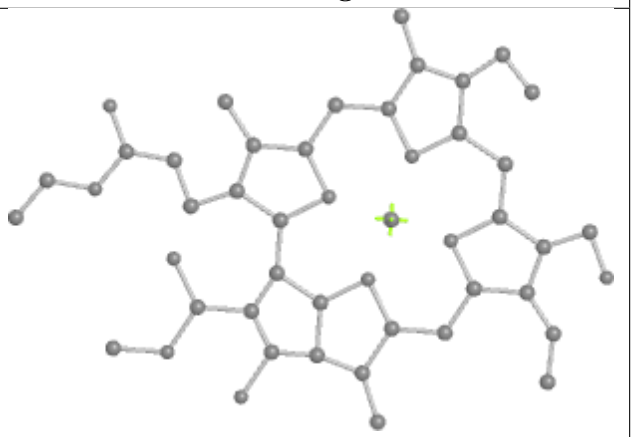
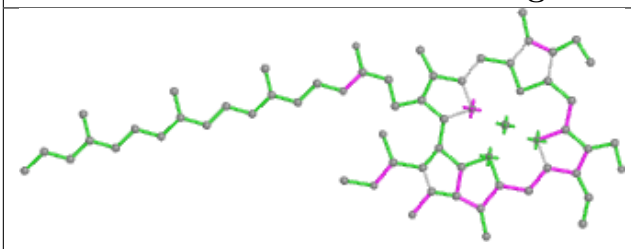


Rings

Ligand CHL 1 607



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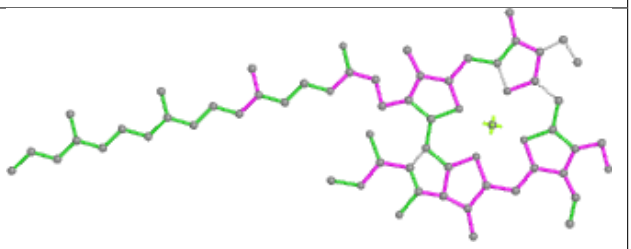
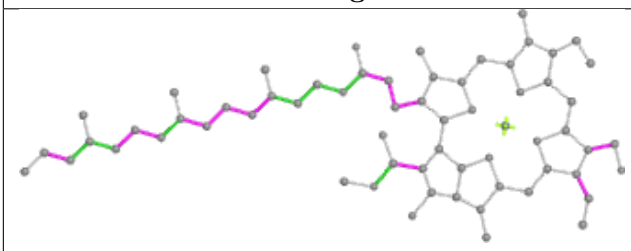


Bond angles



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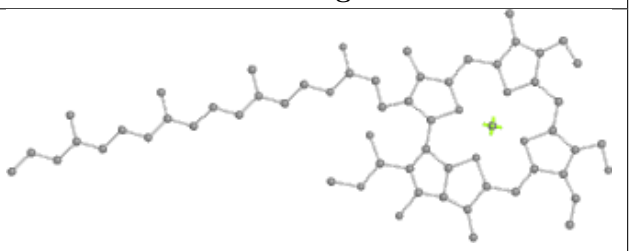
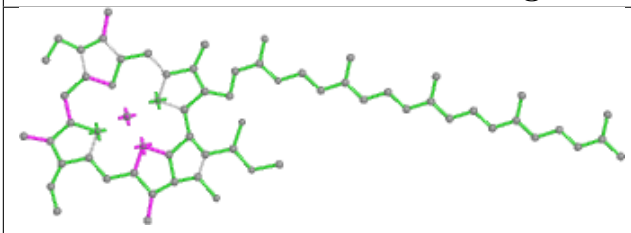


Rings

Ligand CLA G 602



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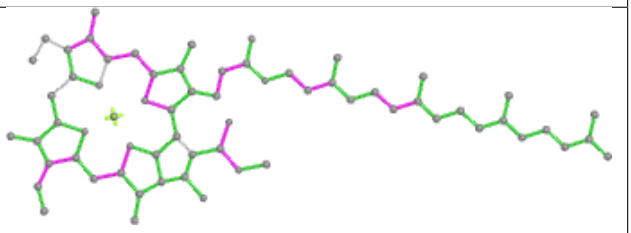
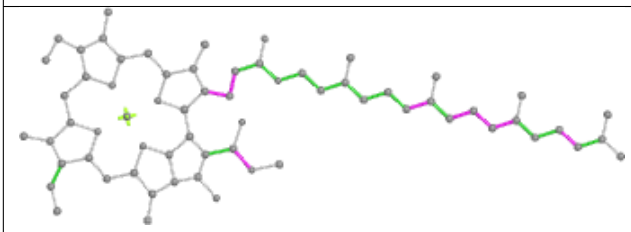


Bond angles



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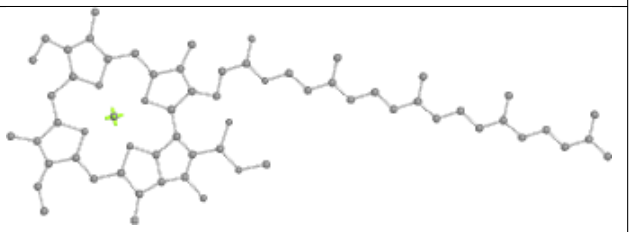
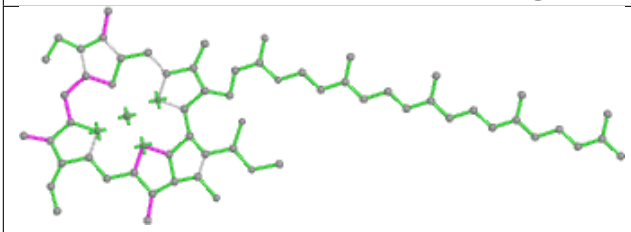
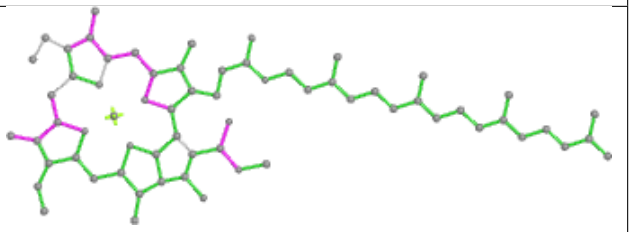


Rings

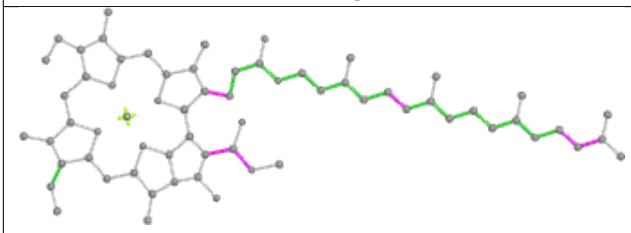
Ligand CLA c 508



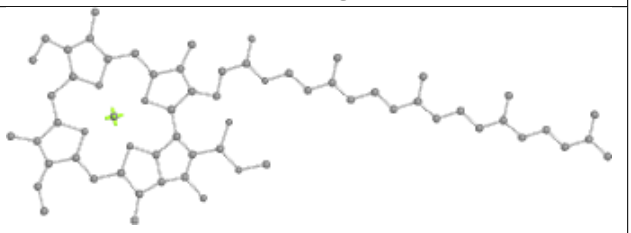
Bond lengths



Bond angles

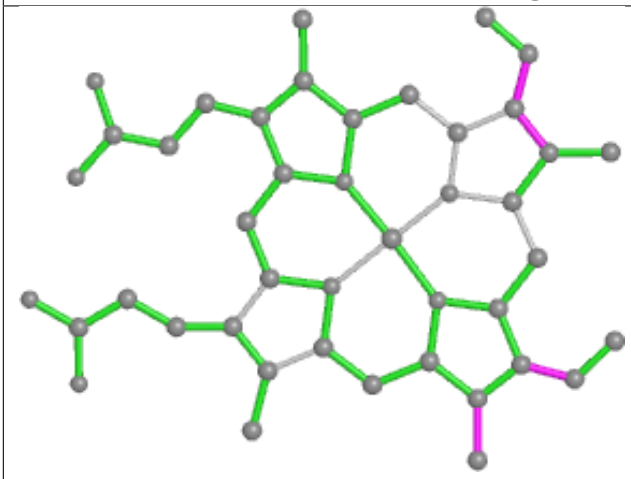


Torsions



Rings

Ligand HEM f 101



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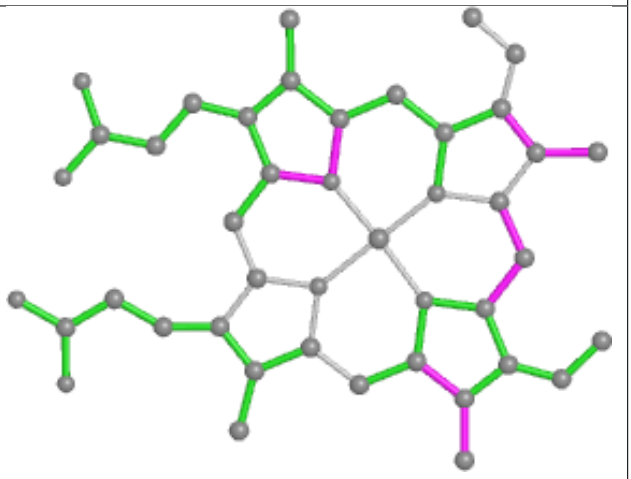
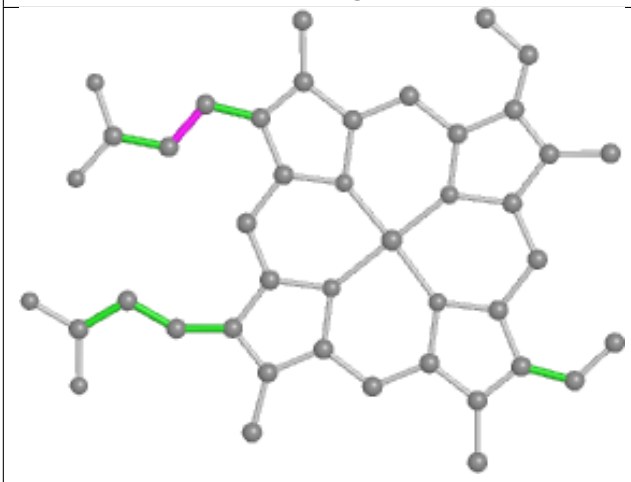


Bond angles



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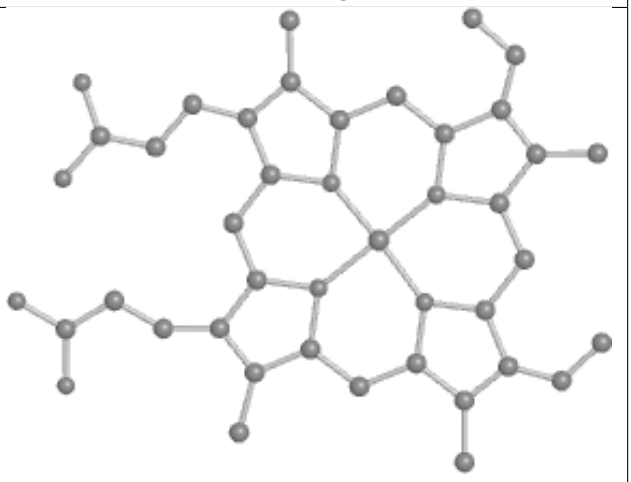
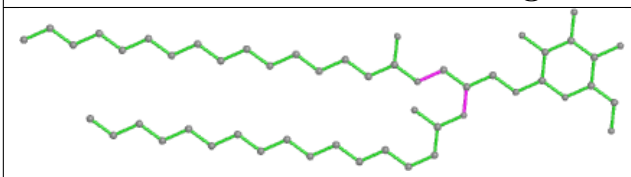


Rings

Ligand LMG b 622



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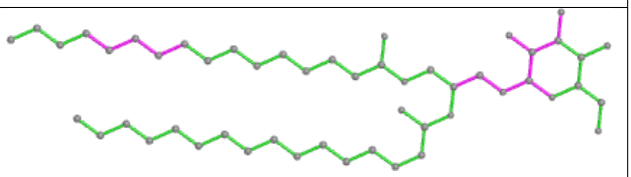

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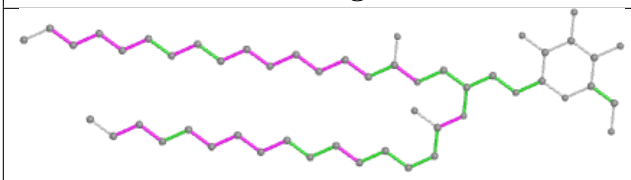

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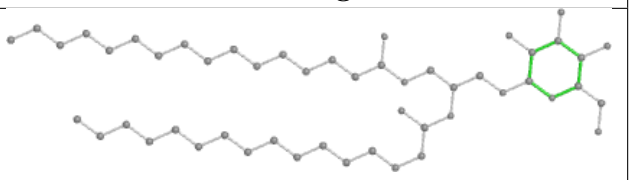
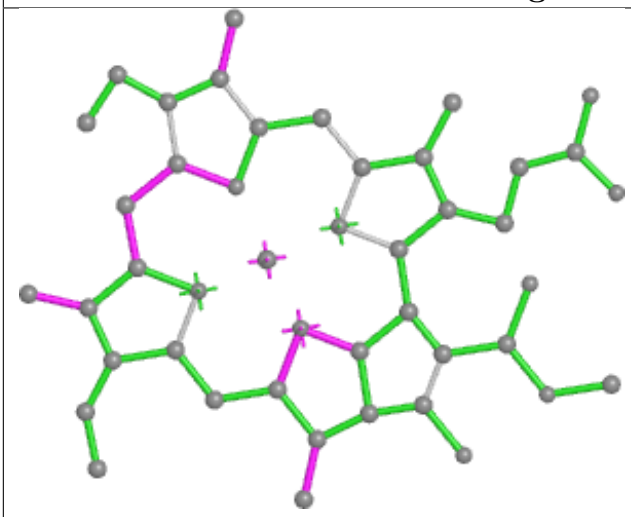


Rings

Ligand CLA 2 611



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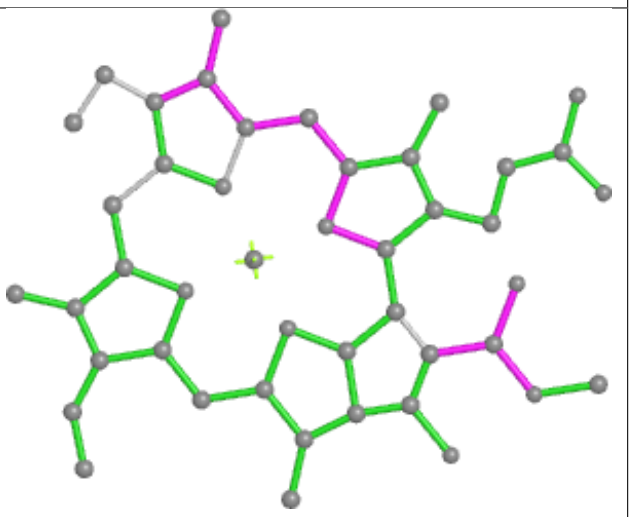

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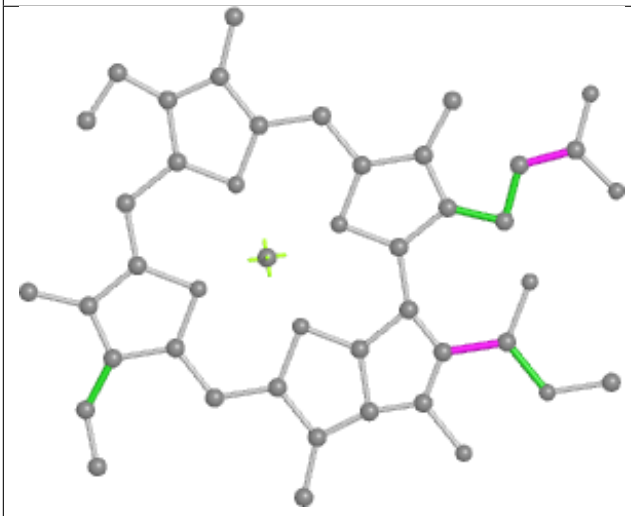

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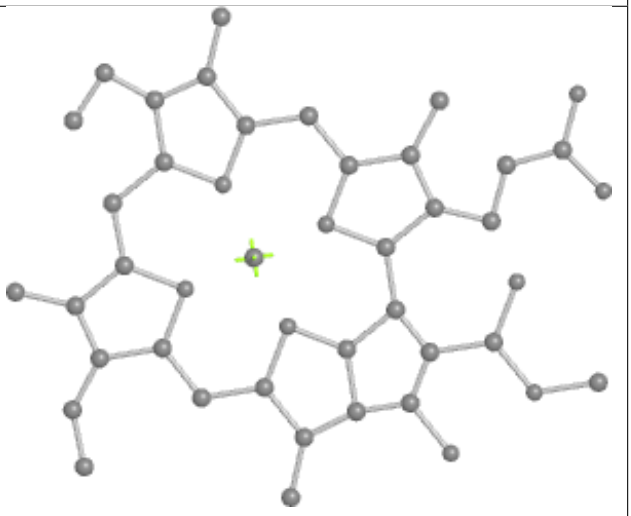
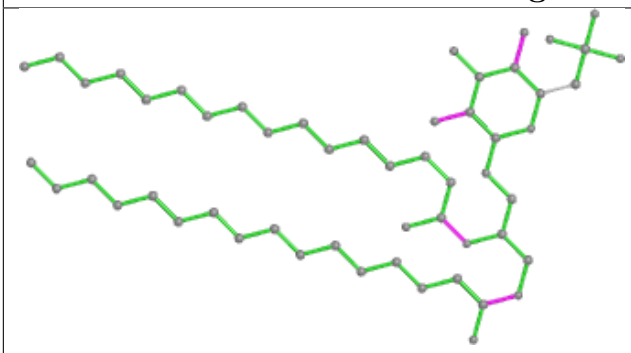


Rings

Ligand SQD a 418



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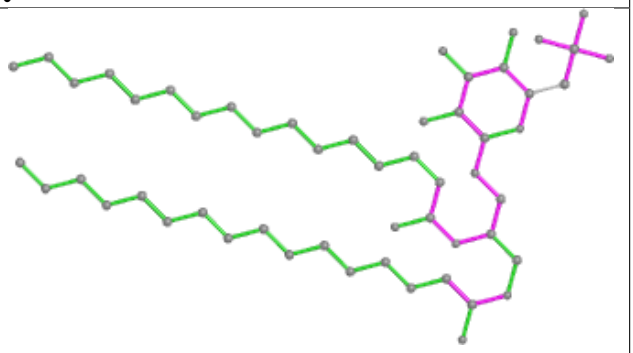
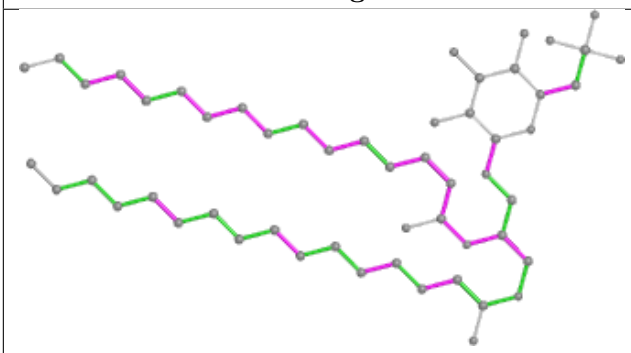


Bond angles



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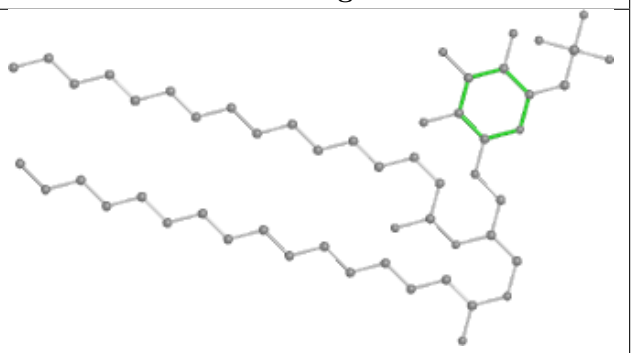
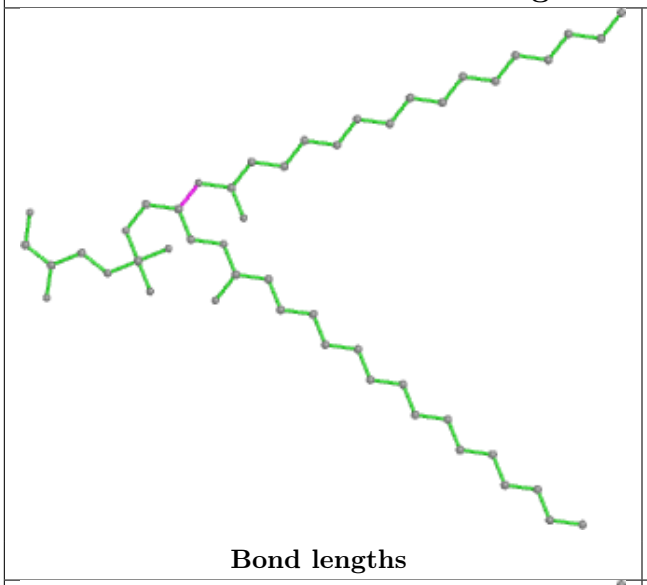


Rings

Ligand LHG l 101



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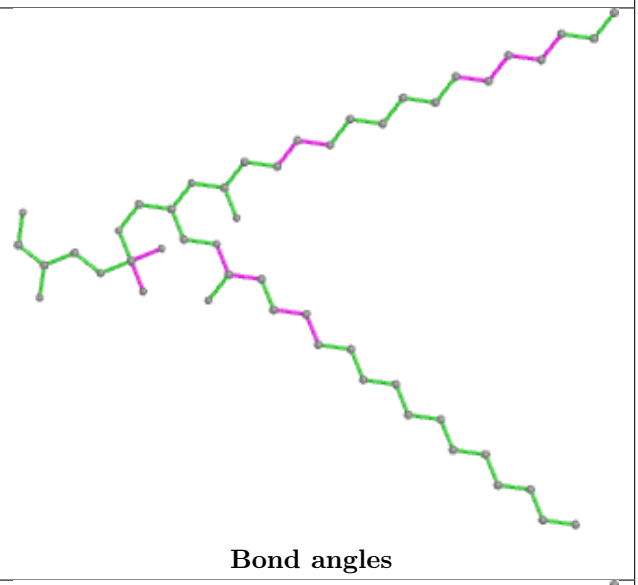
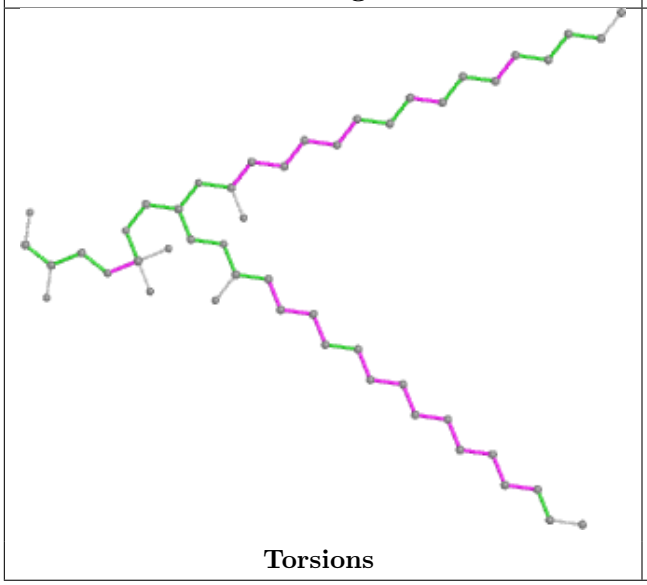


Bond angles



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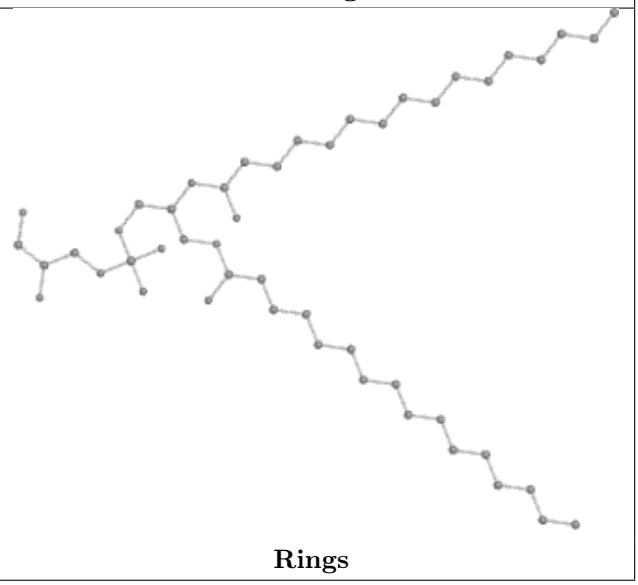
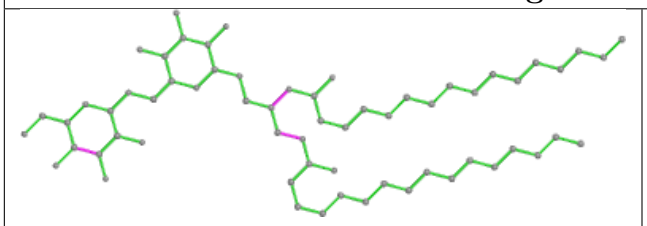


Rings

Ligand DGD c 519



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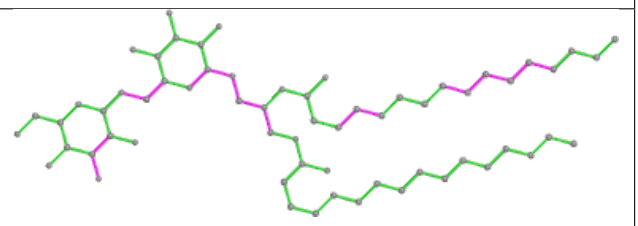
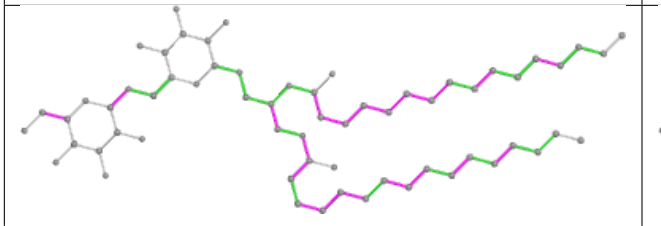
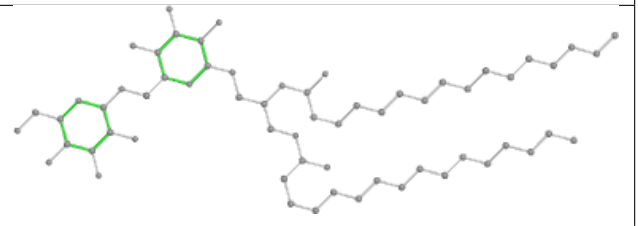


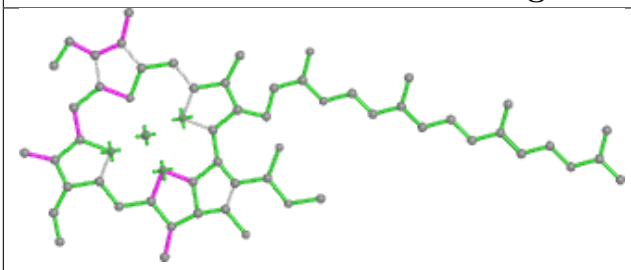
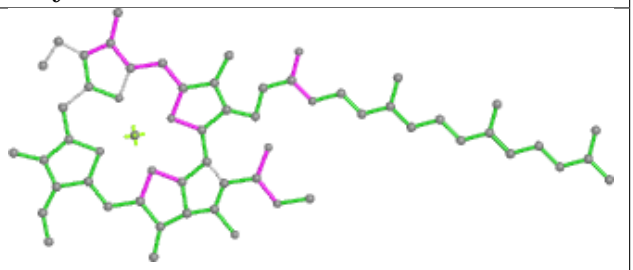
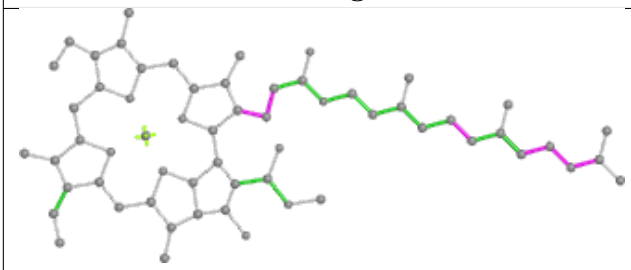
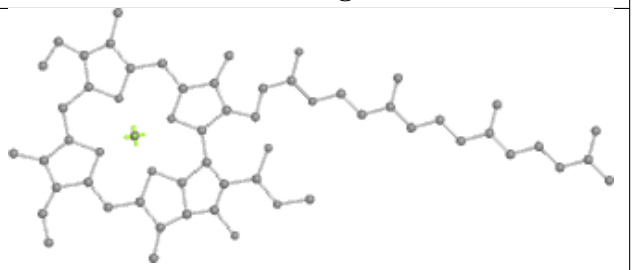
Bond angles

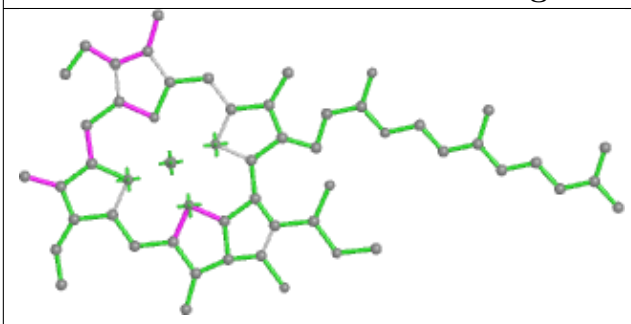
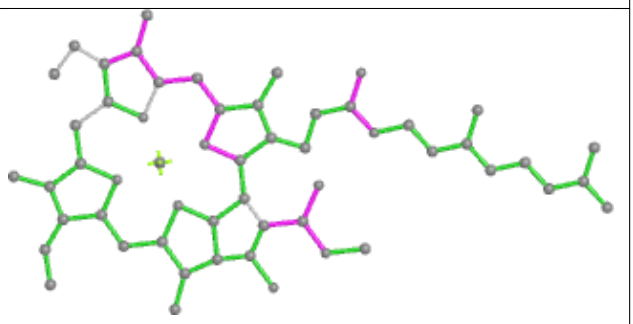
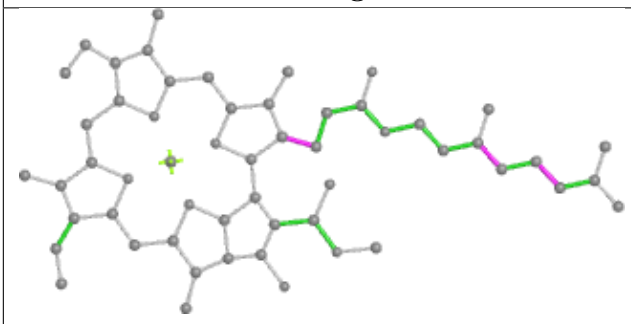
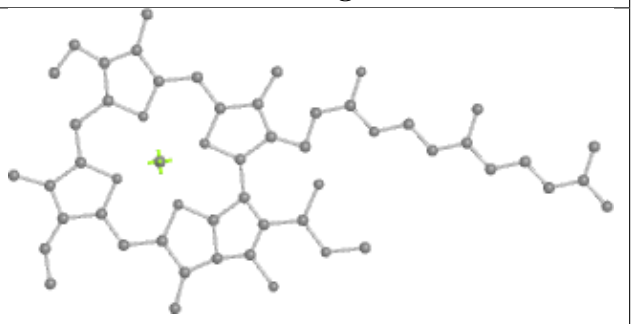


Torsions

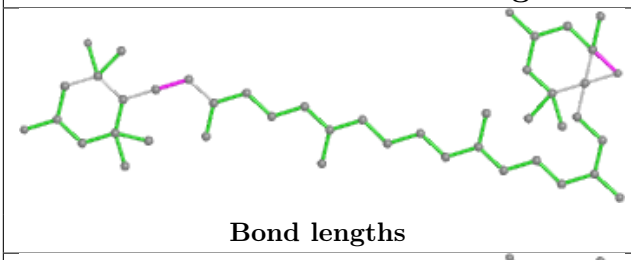


Rings

Ligand CLA y 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NEX G 1623



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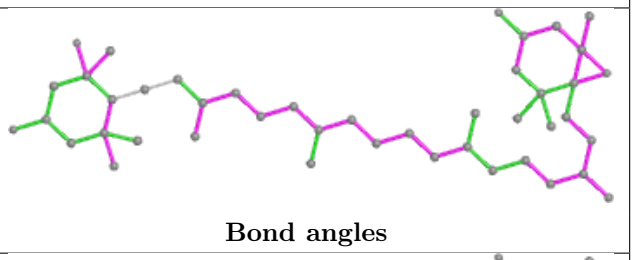
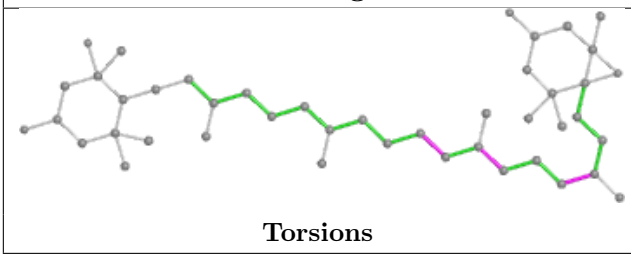


Bond angles



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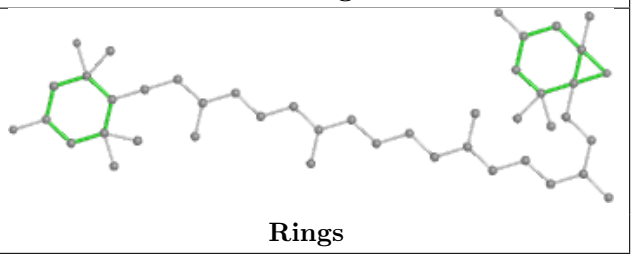
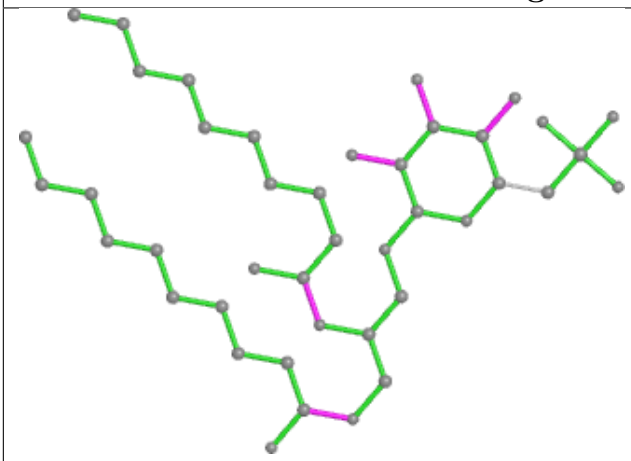


Rings

Ligand SQD b 623



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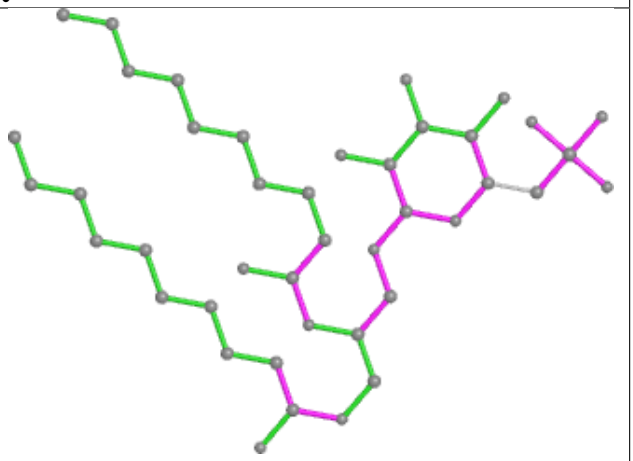
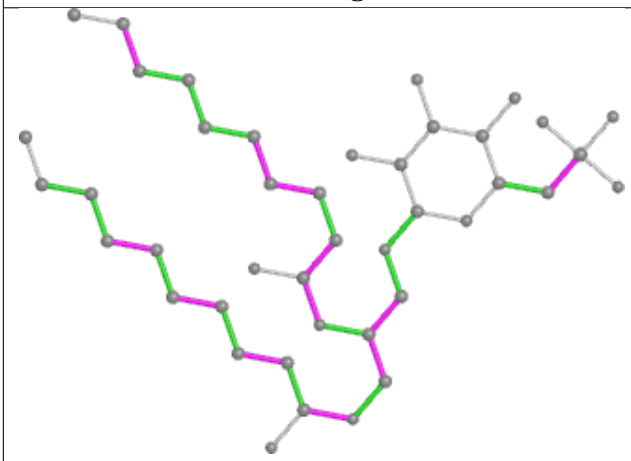


Bond angles



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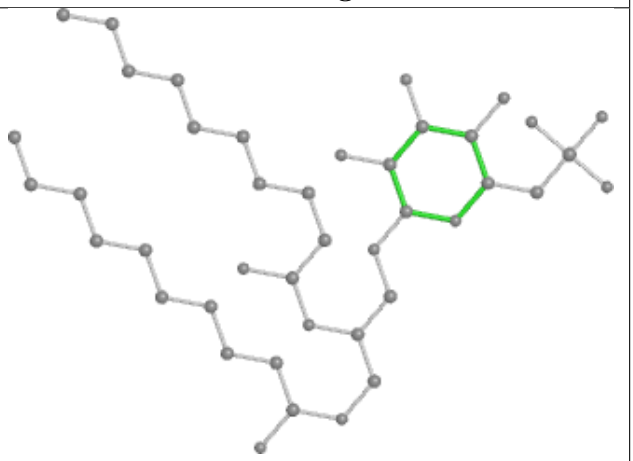
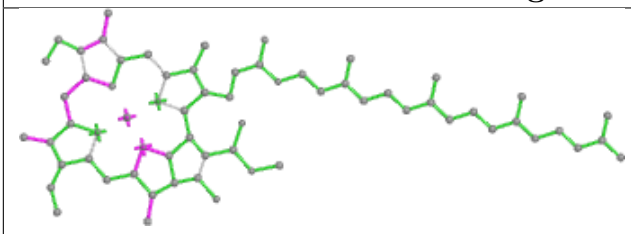


Rings

Ligand CLA b 610



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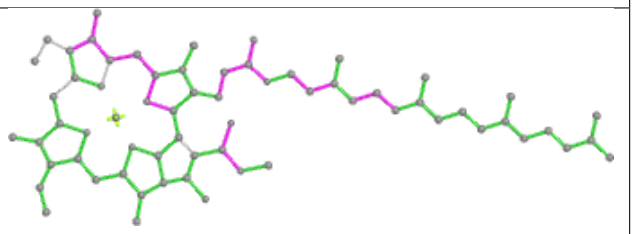
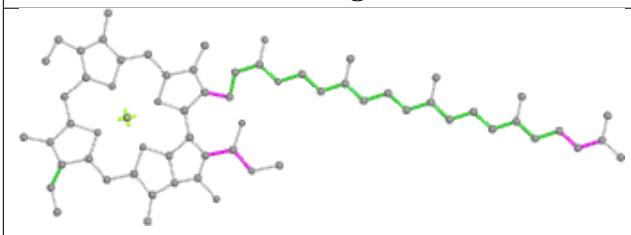


Bond angles



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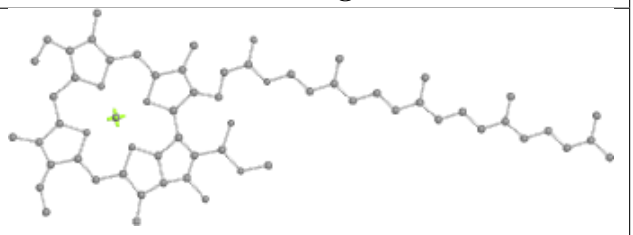
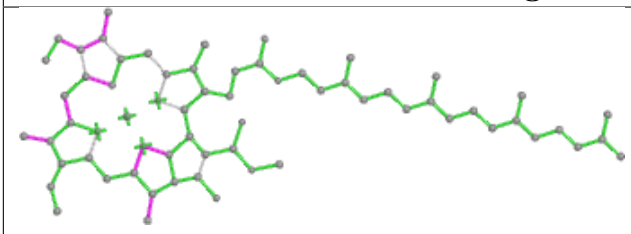


Rings

Ligand CLA R 610



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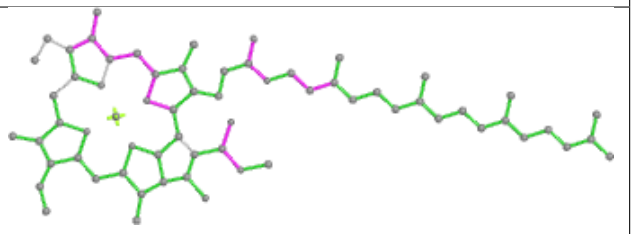
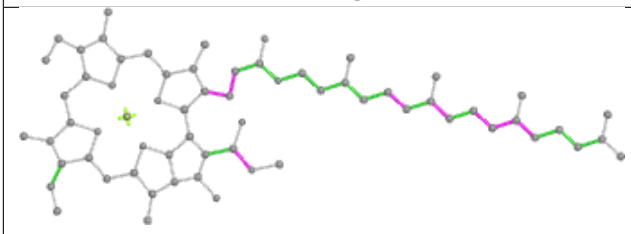


Bond angles



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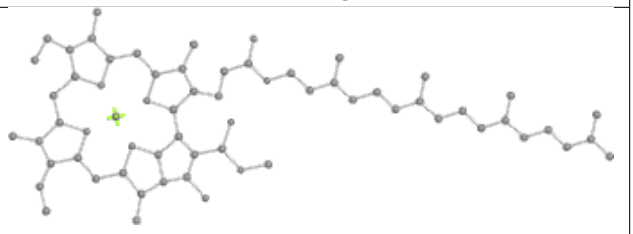
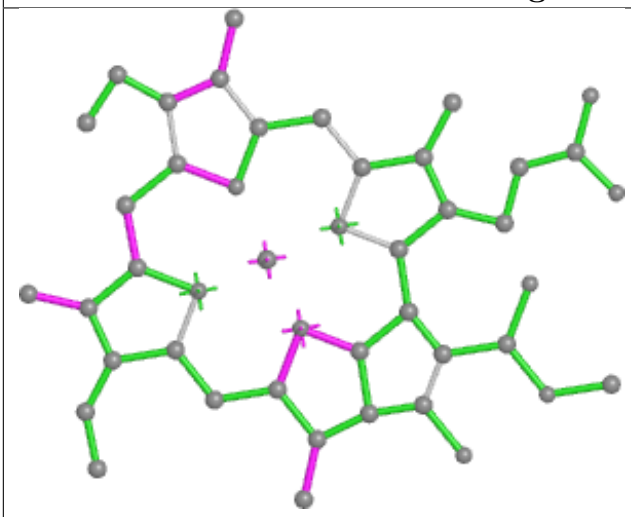


Rings

Ligand CLA 2 614



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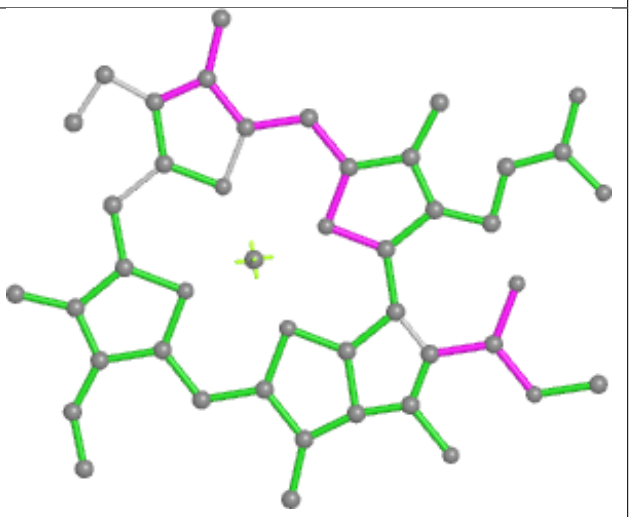
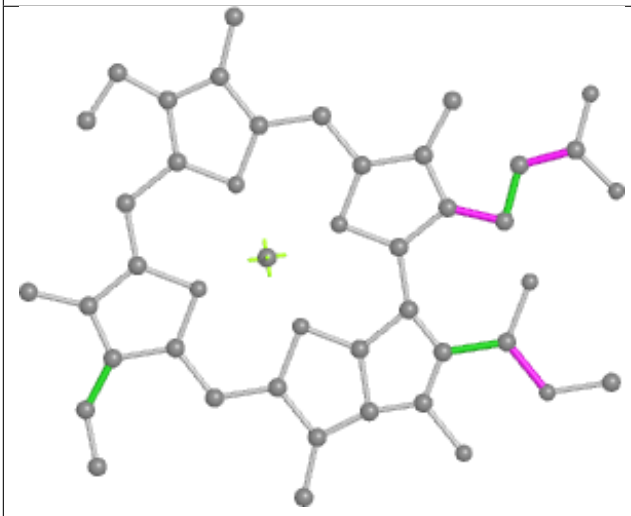
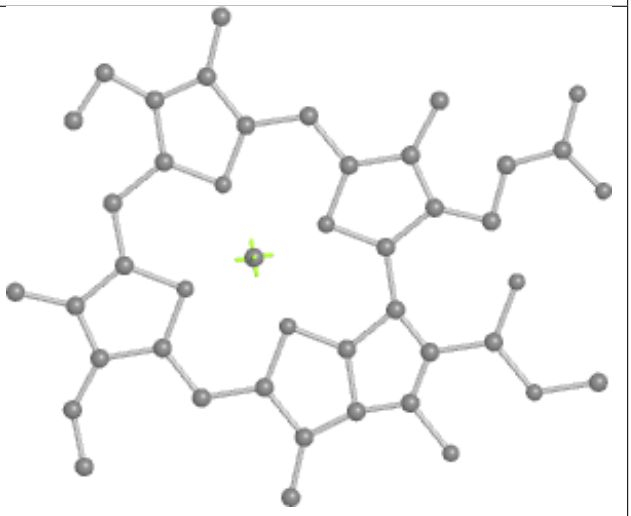


Bond angles

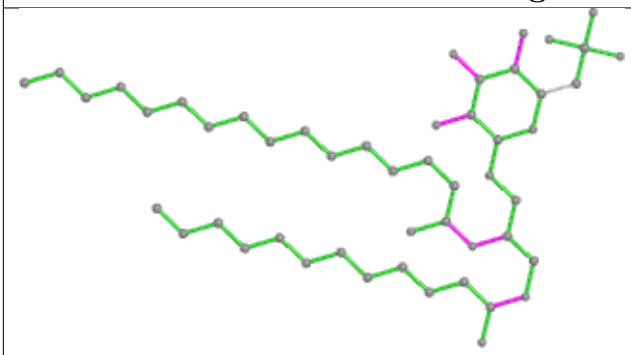


Torsions

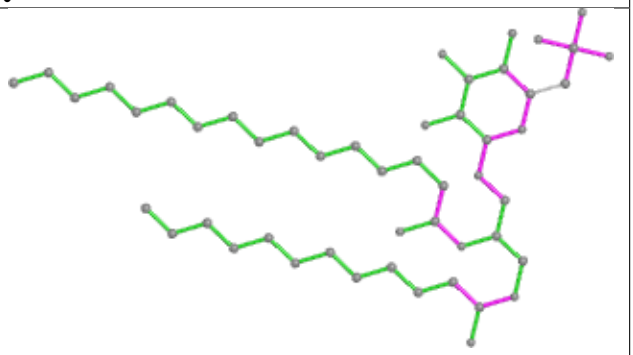


Rings

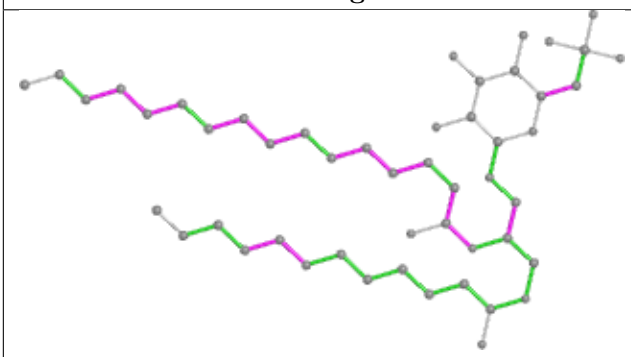
Ligand SQD a 412



Bond lengths



Bond angles



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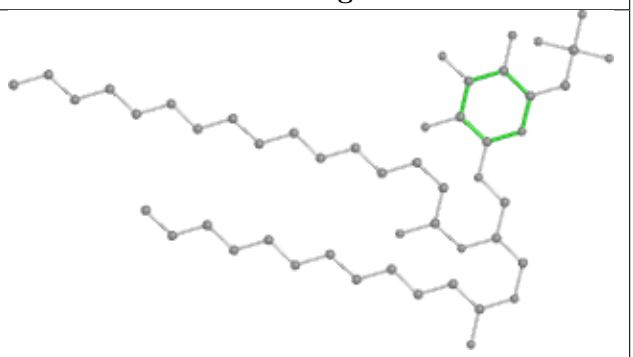
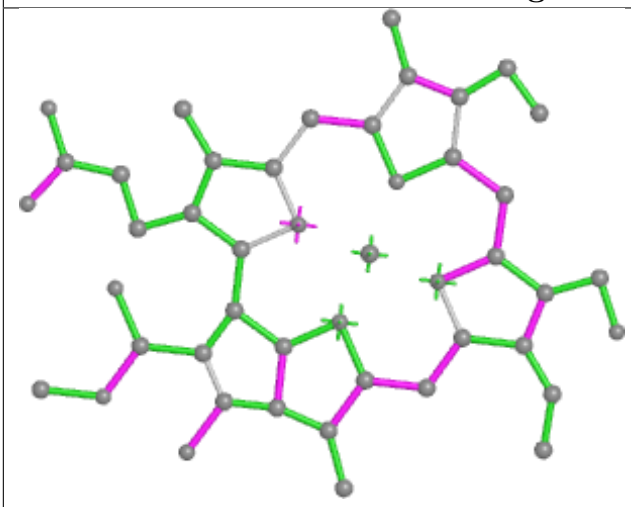


Rings

Ligand CHL 2 601



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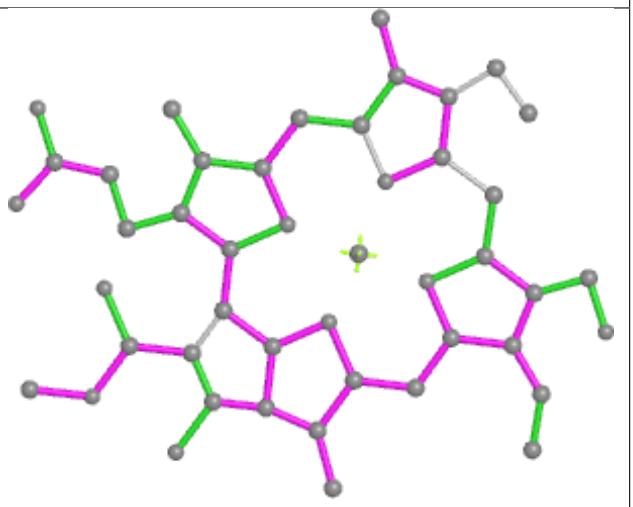

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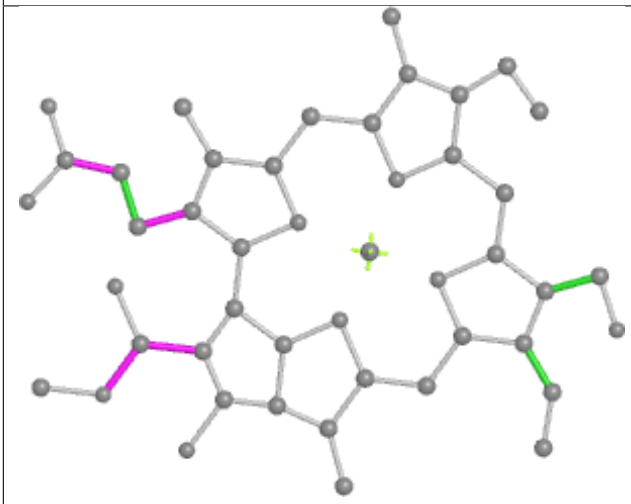

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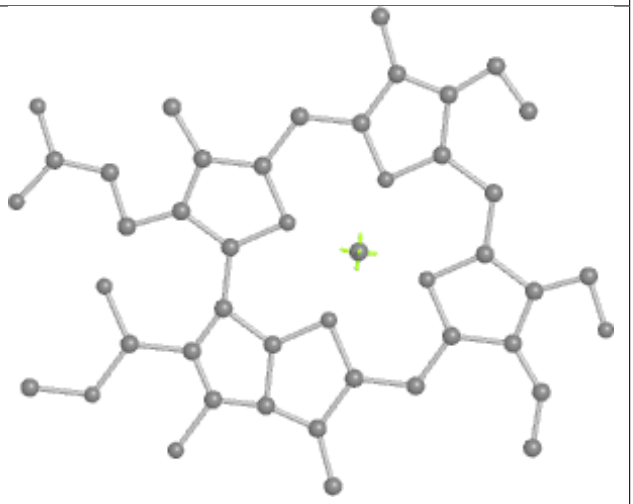
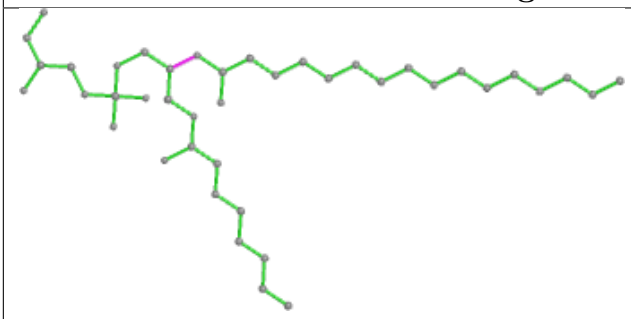


Rings

Ligand LHG 1 2630



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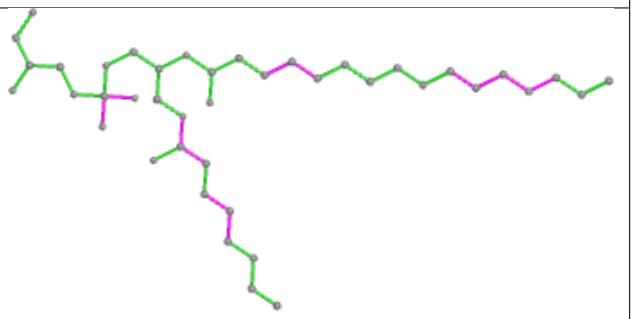
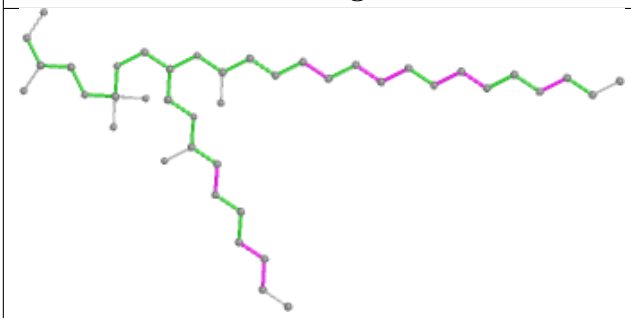


Bond angles



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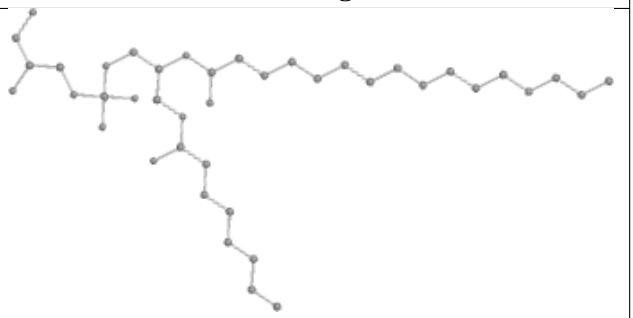
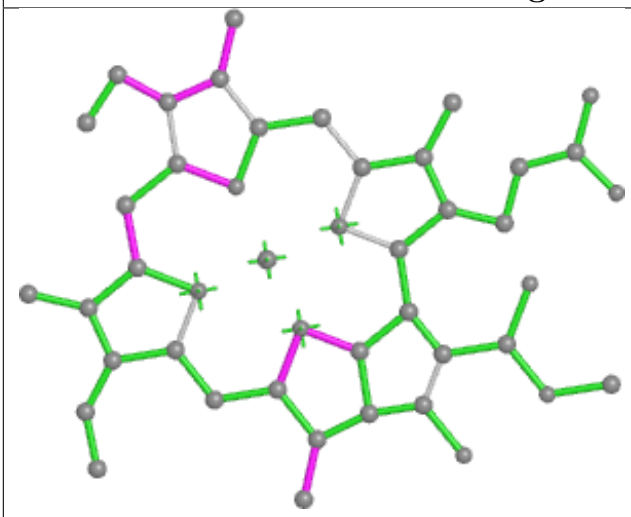


Rings

Ligand CLA 8 611



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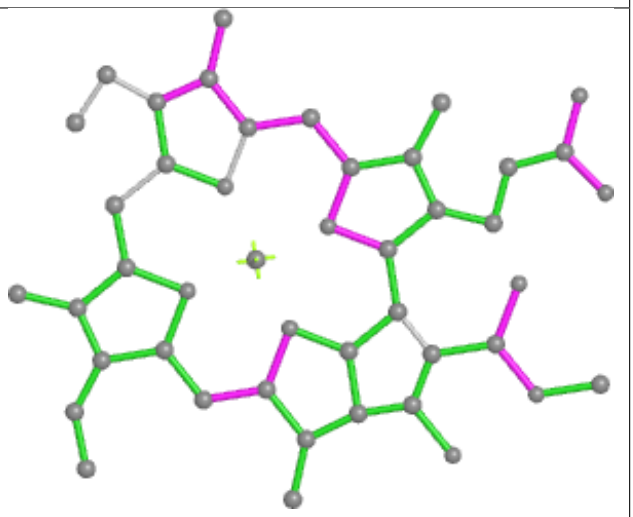

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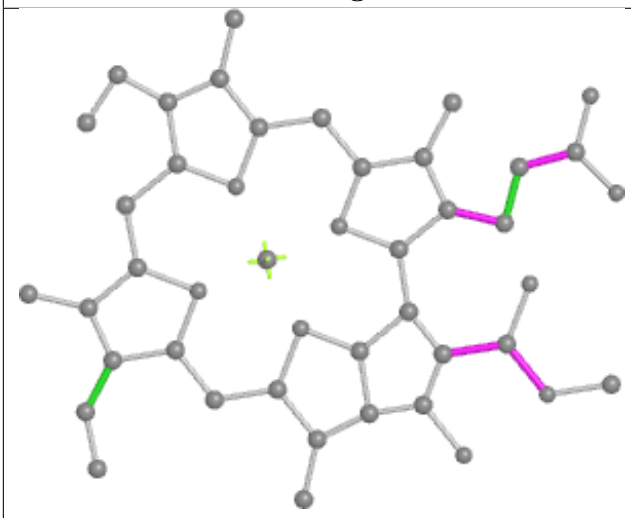

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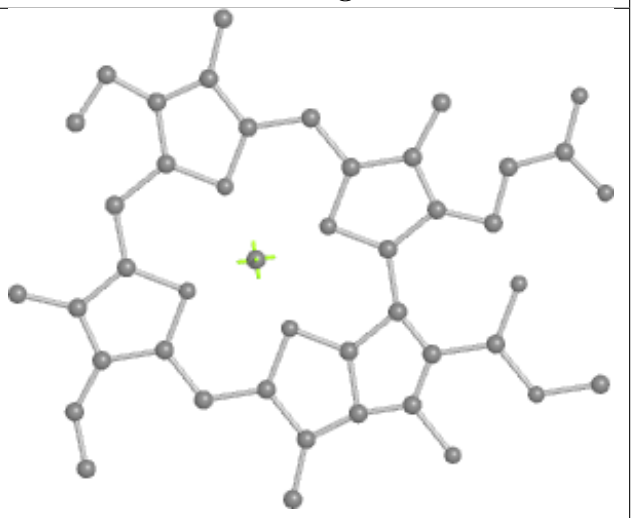
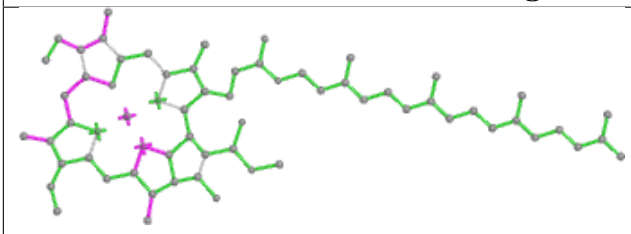


Rings

Ligand CLA Y 602



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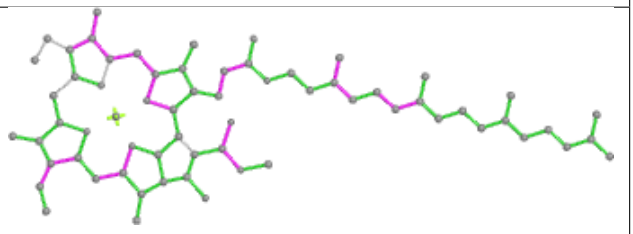
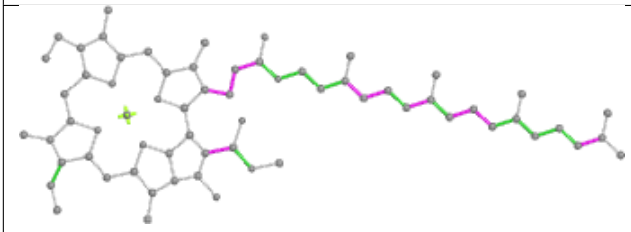


Bond angles



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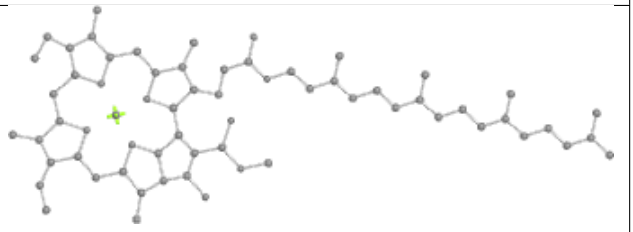
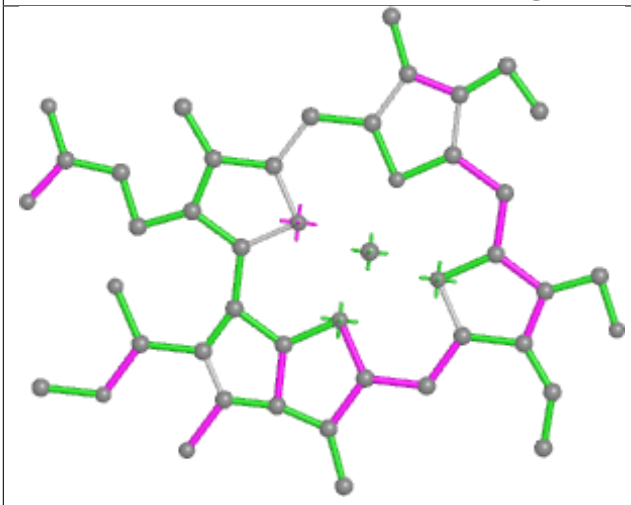


Rings

Ligand CHL 3 608



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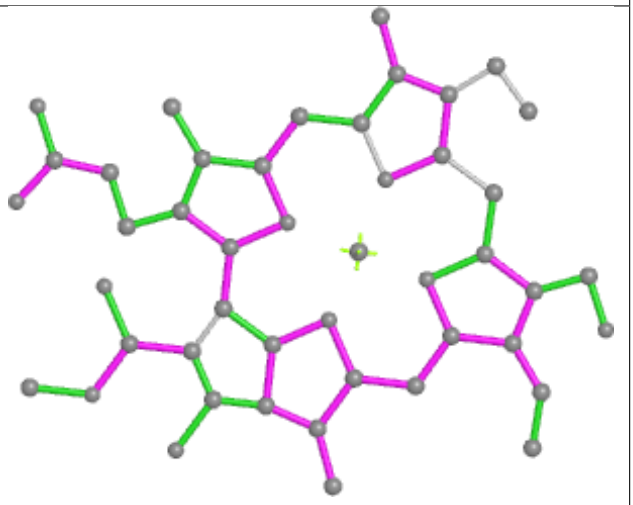
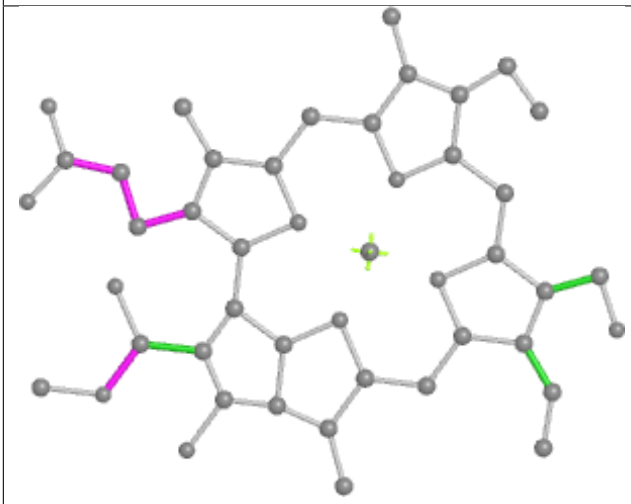


Bond angles



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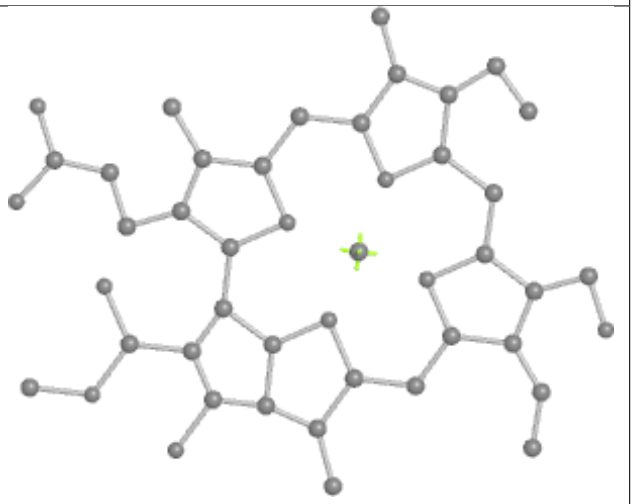
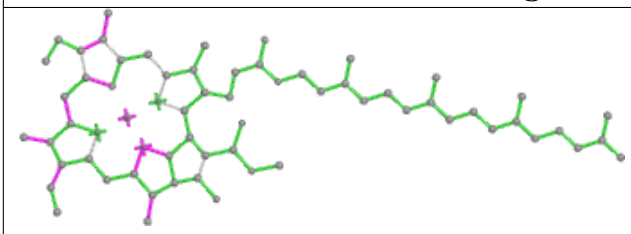


Rings

Ligand CLA G 603



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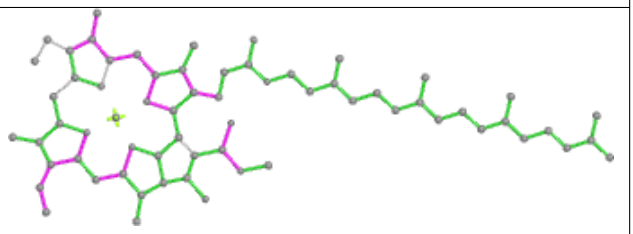

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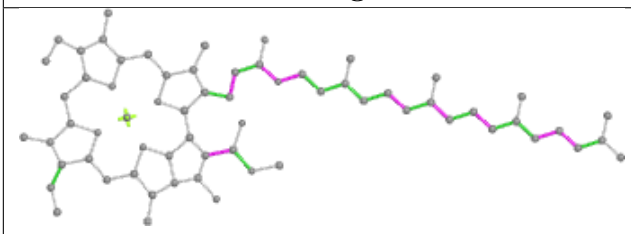

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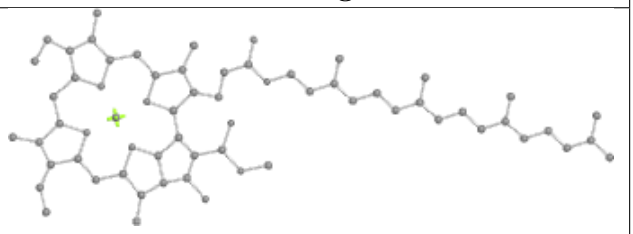
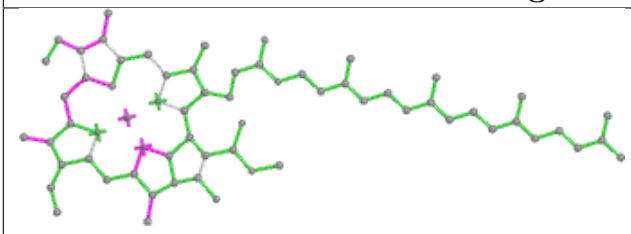


Rings

Ligand CLA g 613



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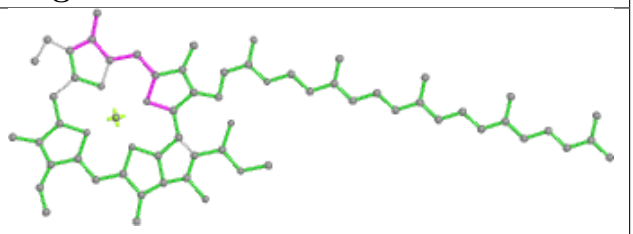
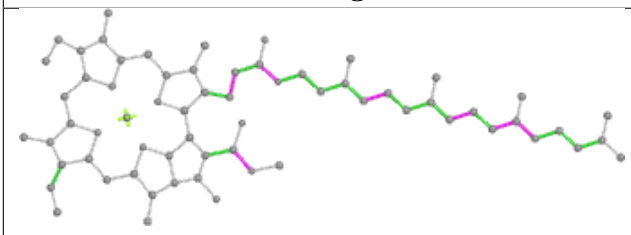


Bond angles



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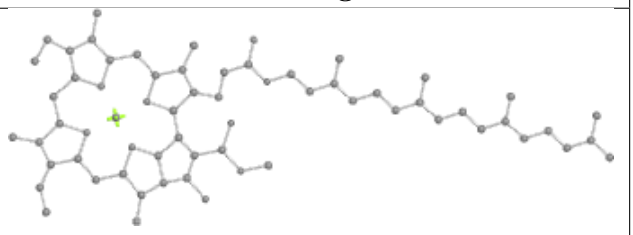
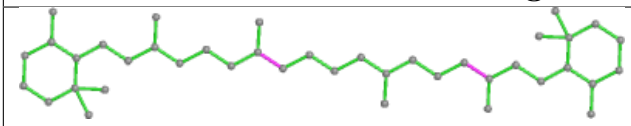


Rings

Ligand BCR b 619



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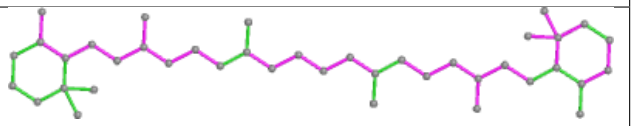
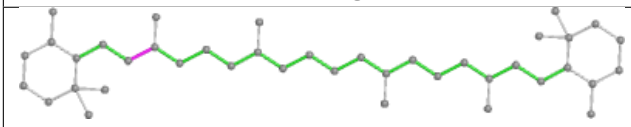


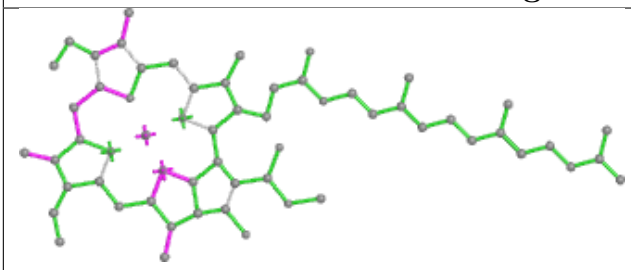
Bond angles



Torsions

Rings

Ligand CLA N 612



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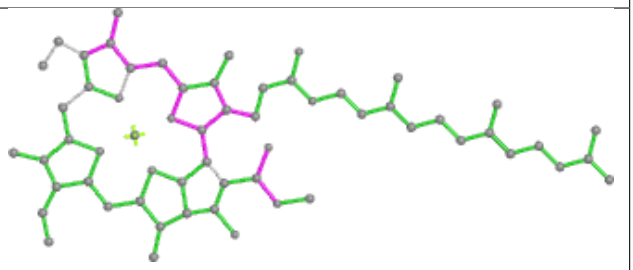
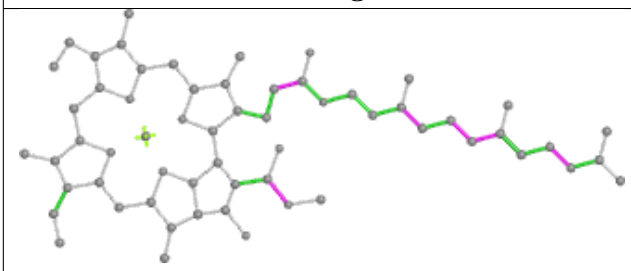


Bond angles



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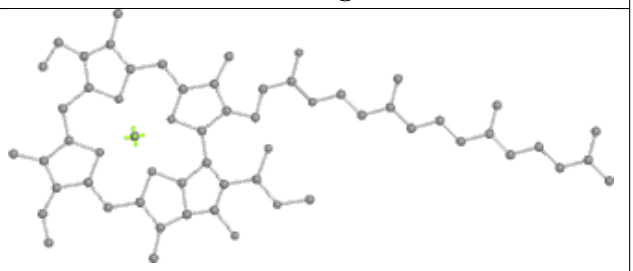
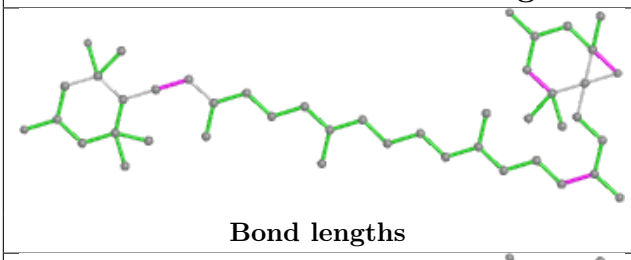


Rings

Ligand NEX 1 1623



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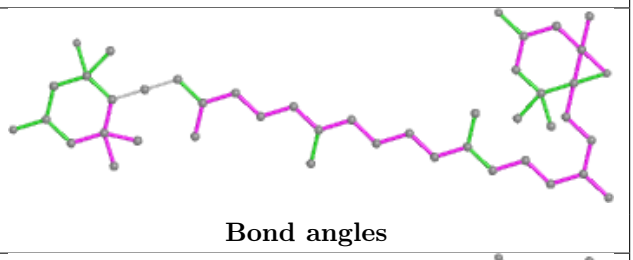

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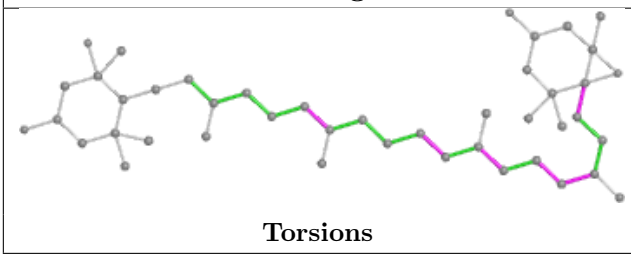

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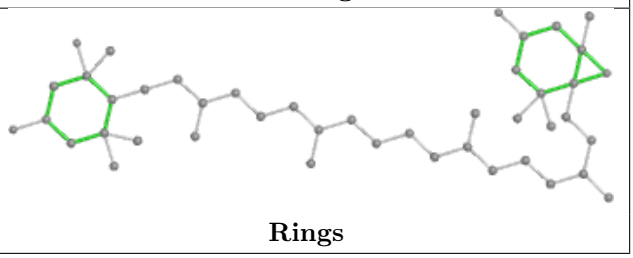
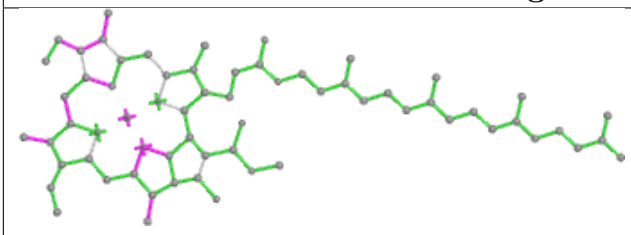


Rings

Ligand CLA b 611



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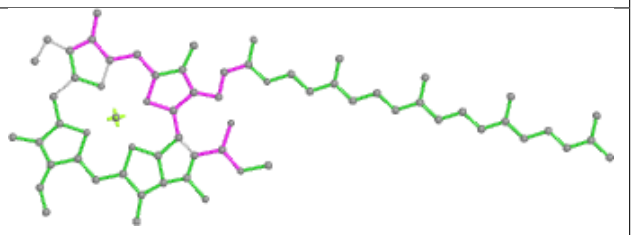
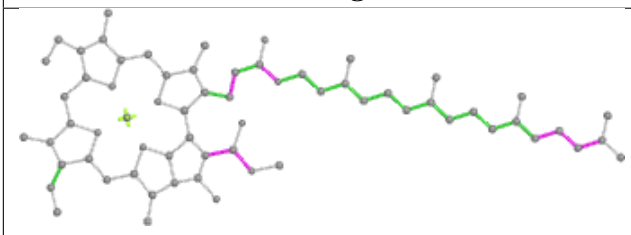


Bond angles



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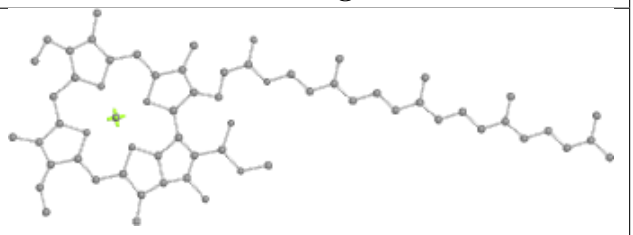
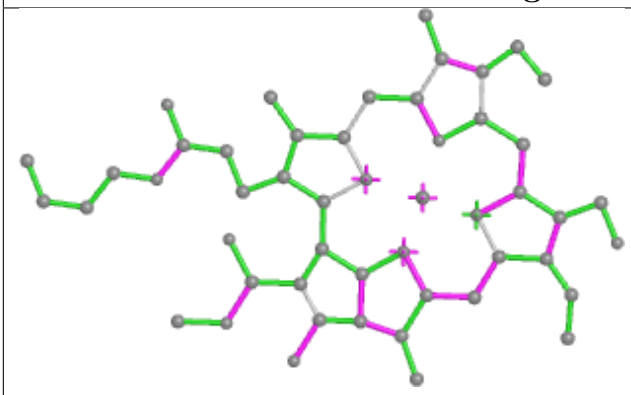


Rings

Ligand CHL Y 606



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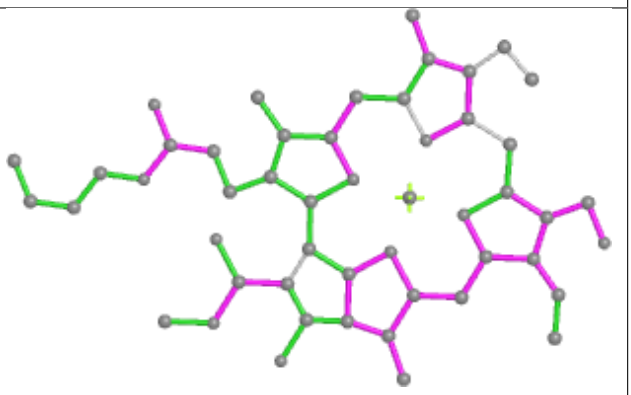
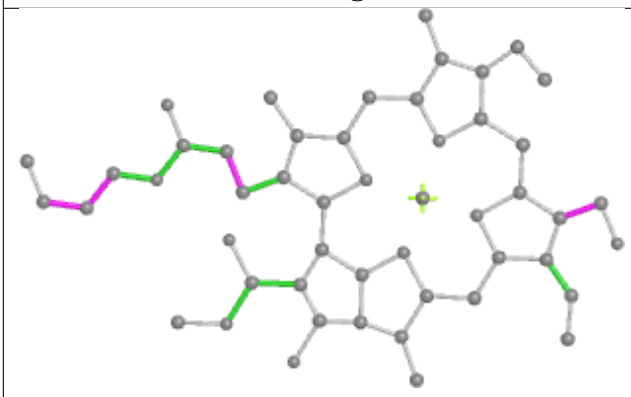


Bond angles



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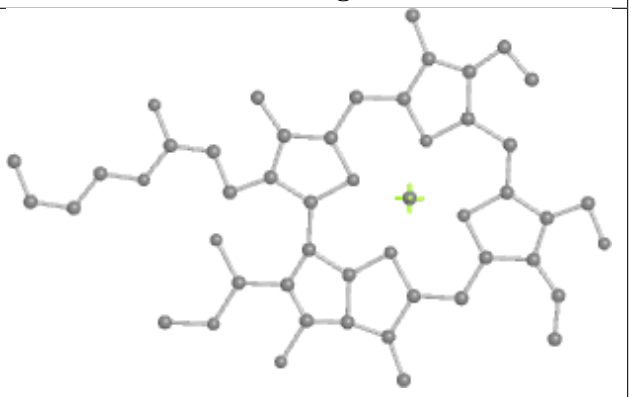

Rings

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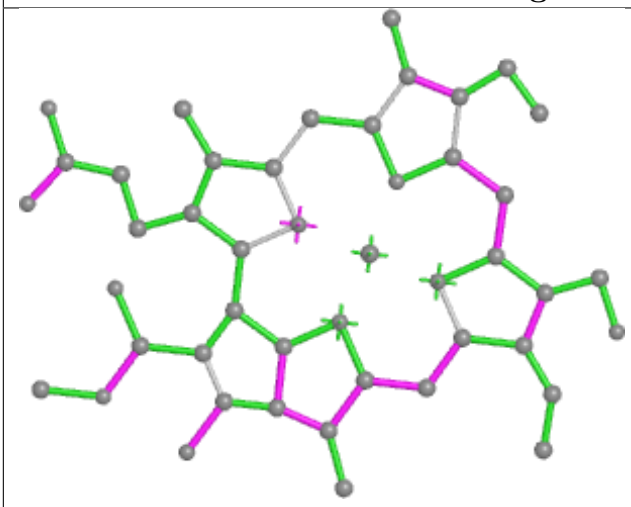

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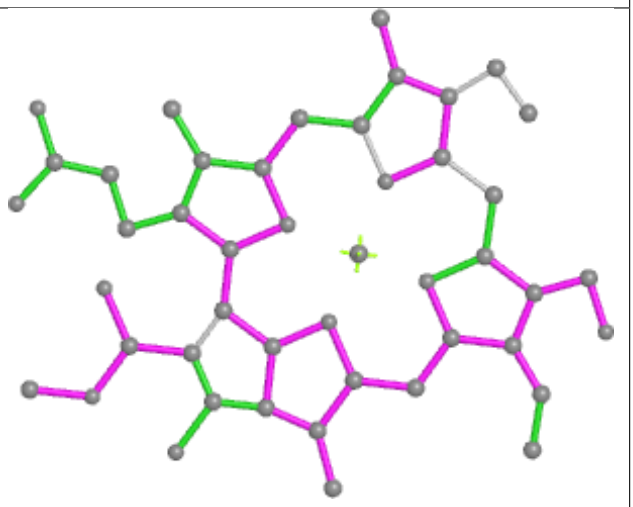
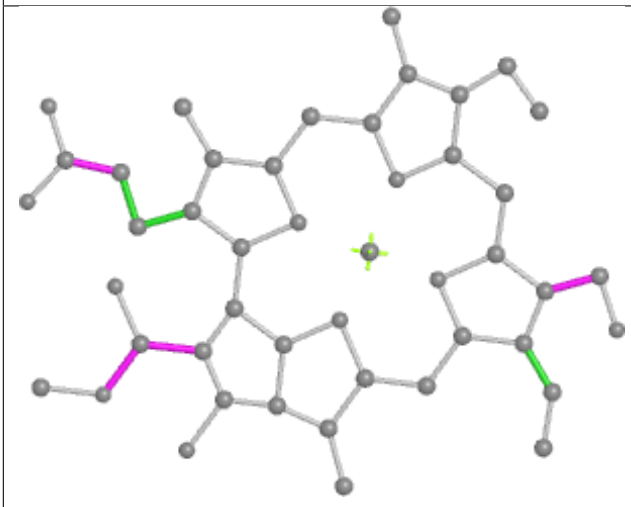
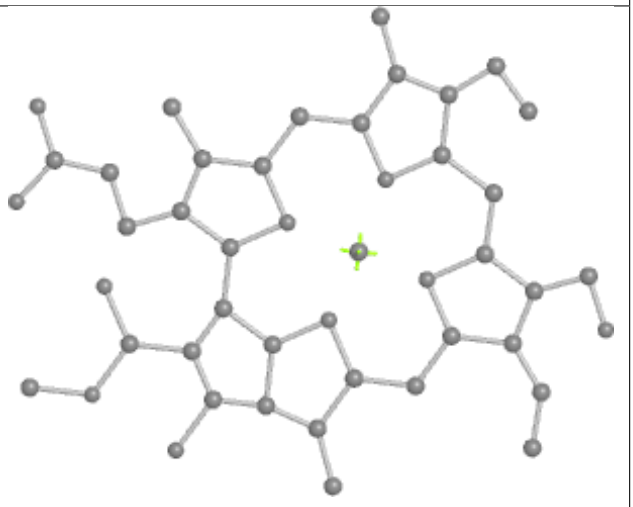


Bond angles

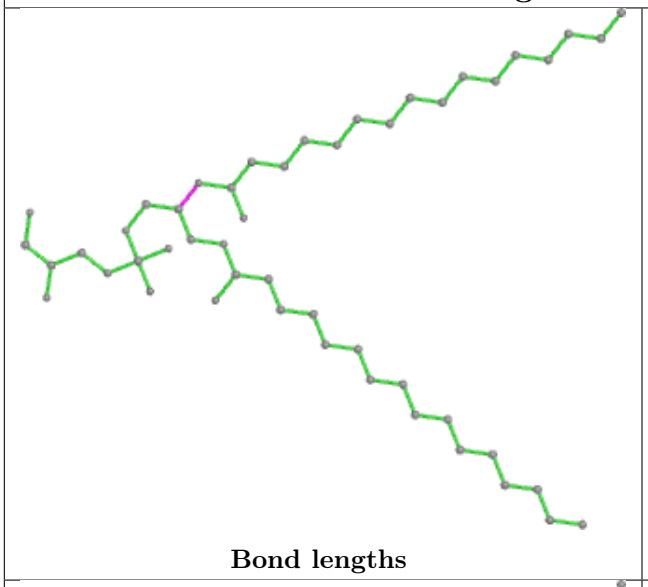


Torsions

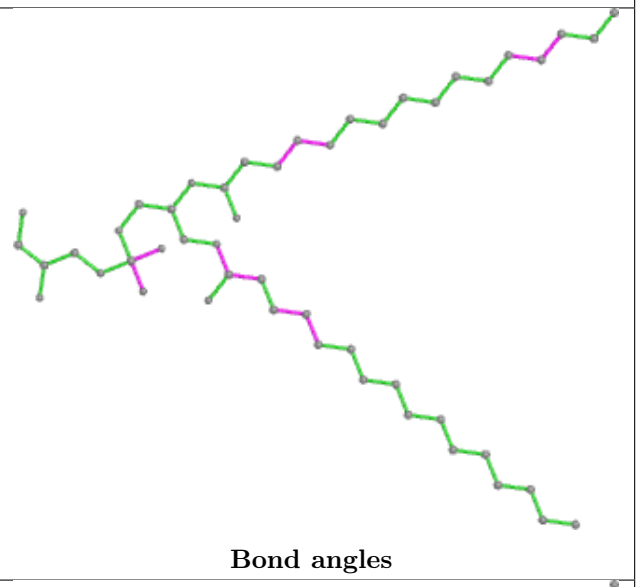


Rings

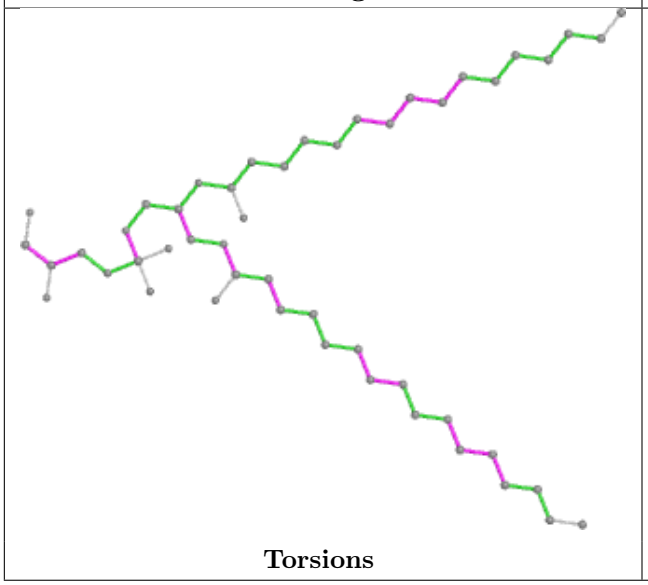
Ligand LHG B 2631



Bond lengths



Bond angles



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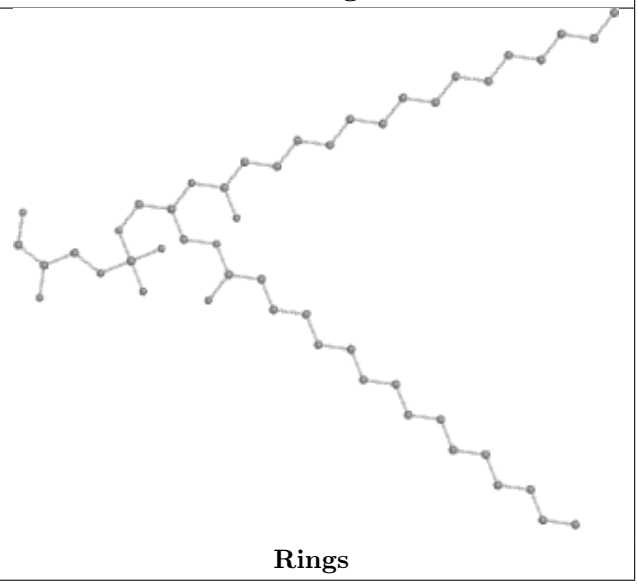
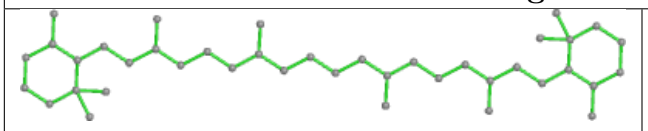


Rings

Ligand BCR 4 623



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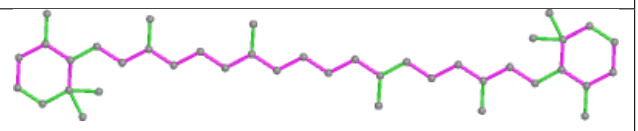
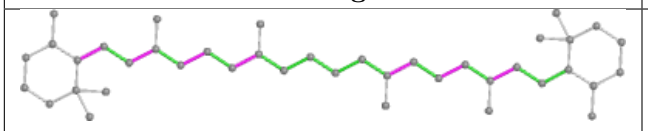
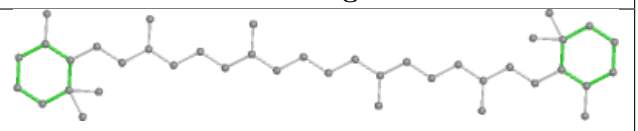


Bond angles

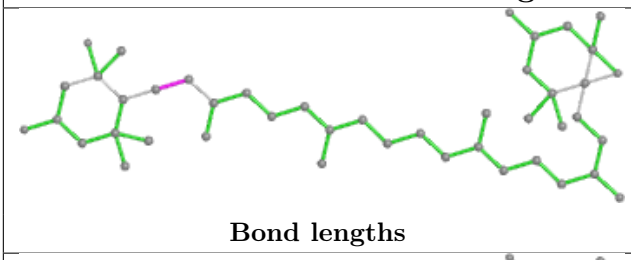


Torsions



Rings

Ligand NEX 6 1623



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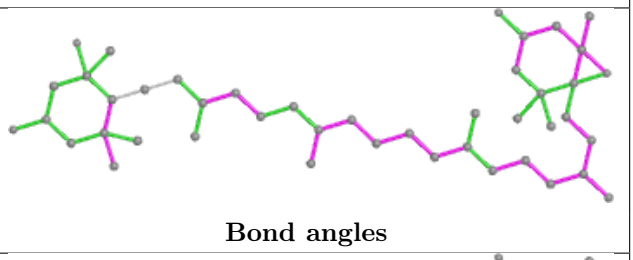
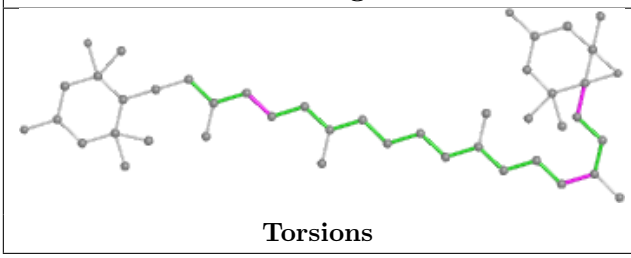


Bond angles



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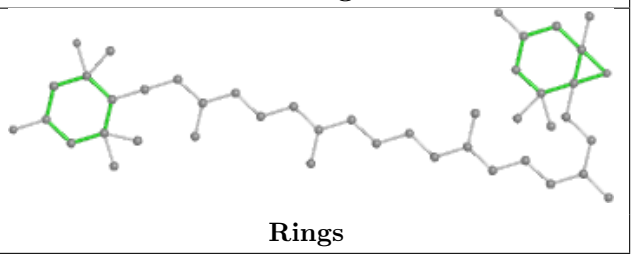
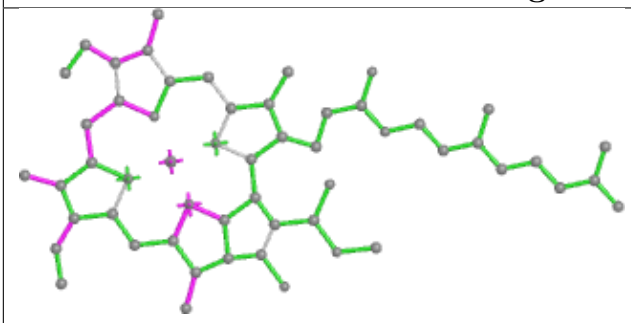


Rings

Ligand CLA 7 603



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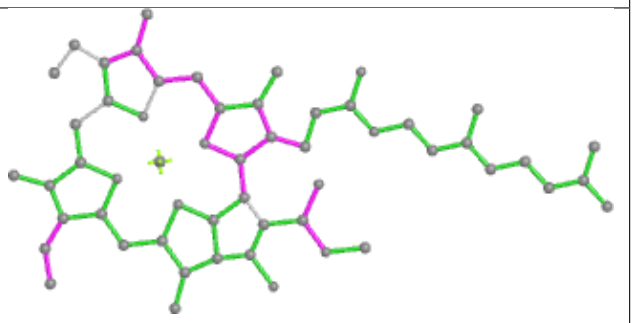
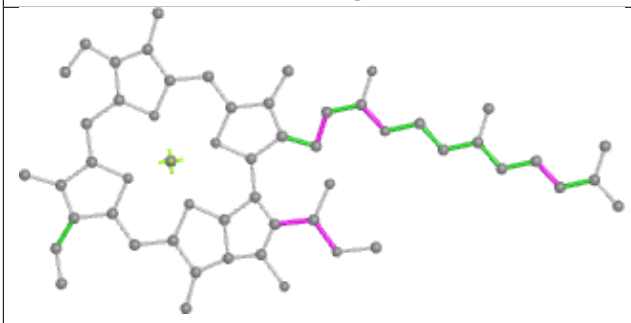


Bond angles



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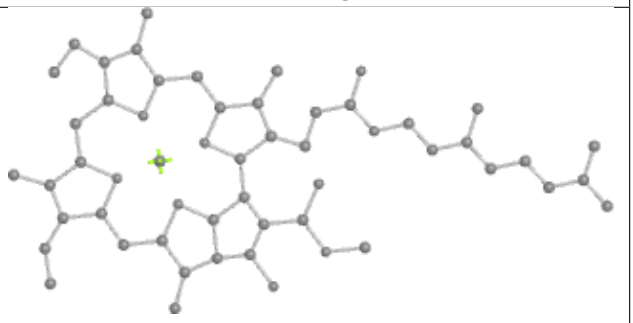
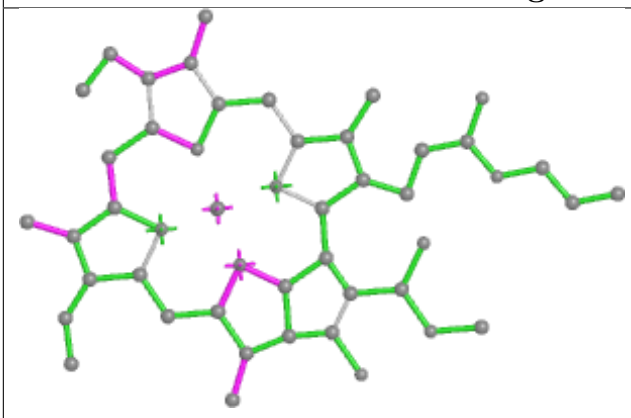


Rings

Ligand CLA y 614



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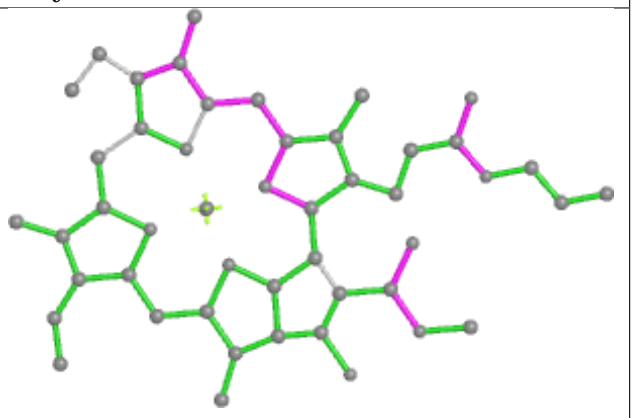
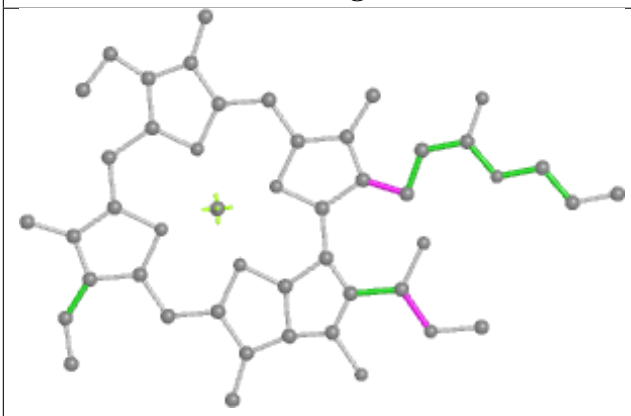


Bond angles



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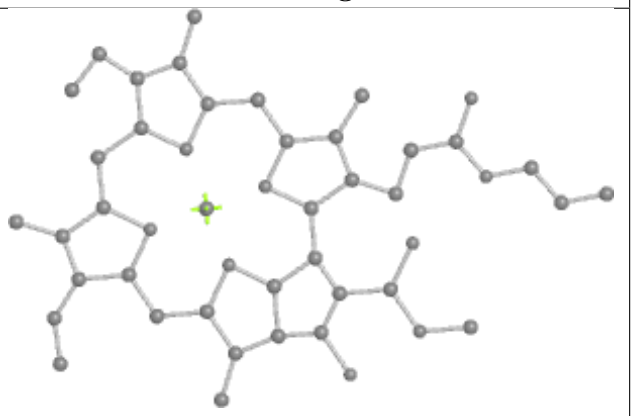
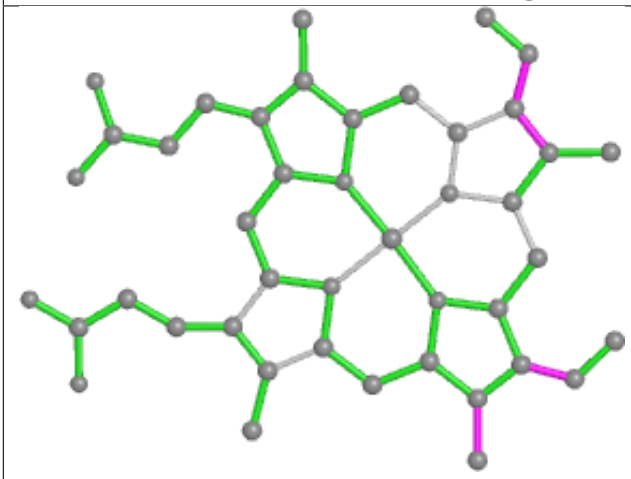


Rings

Ligand HEM F 101



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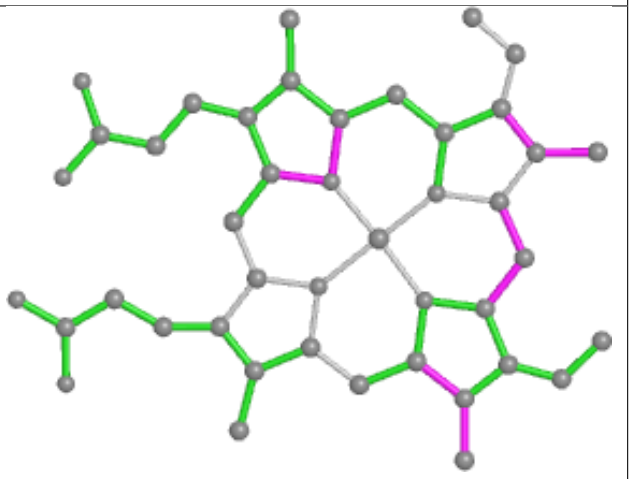
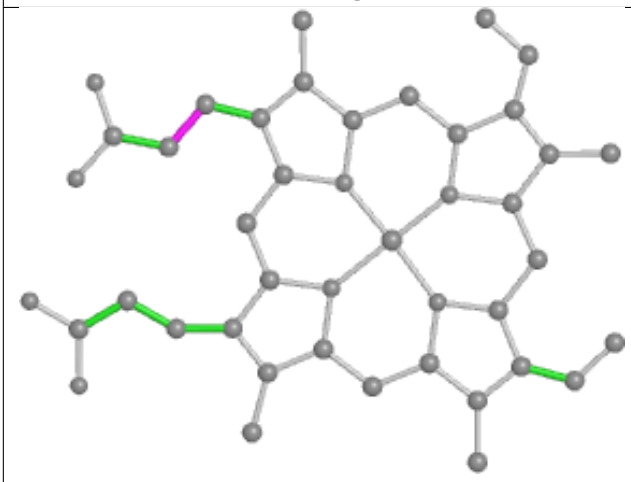


Bond angles



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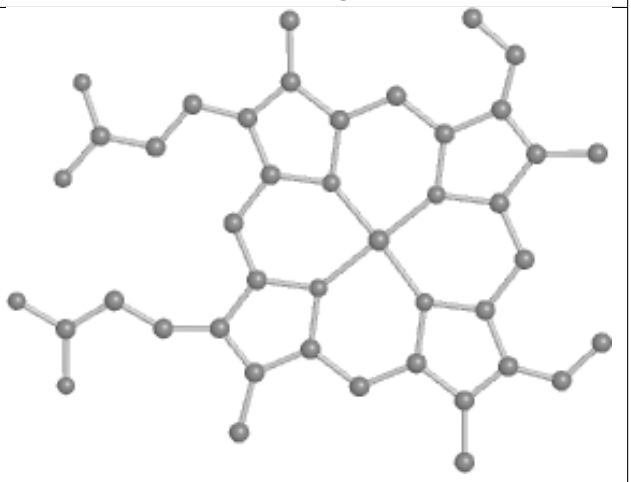
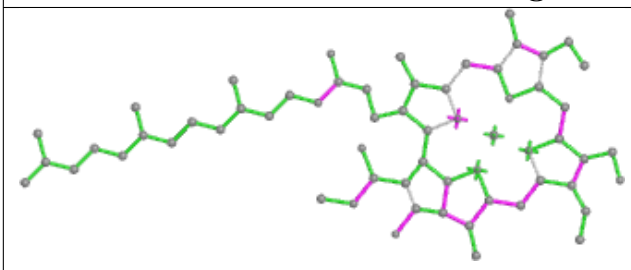


Rings

Ligand CHL 2 609



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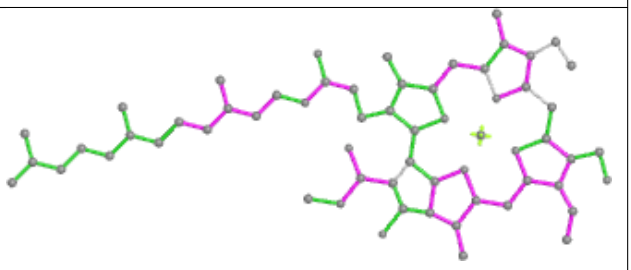

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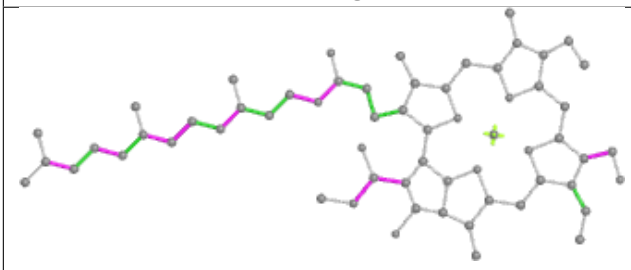

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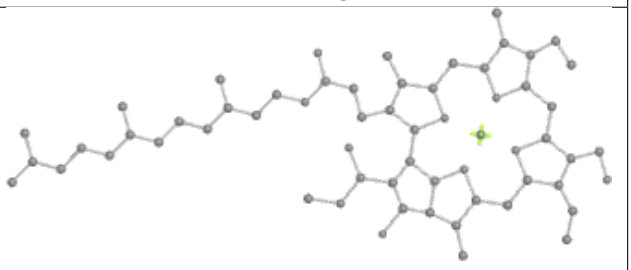
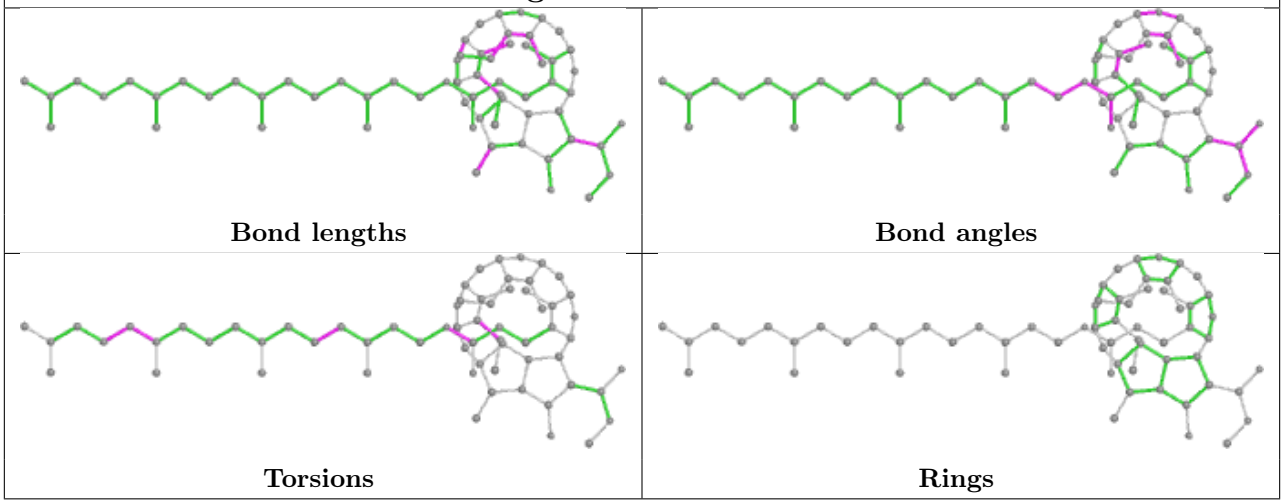


Rings

Ligand PHO a 408



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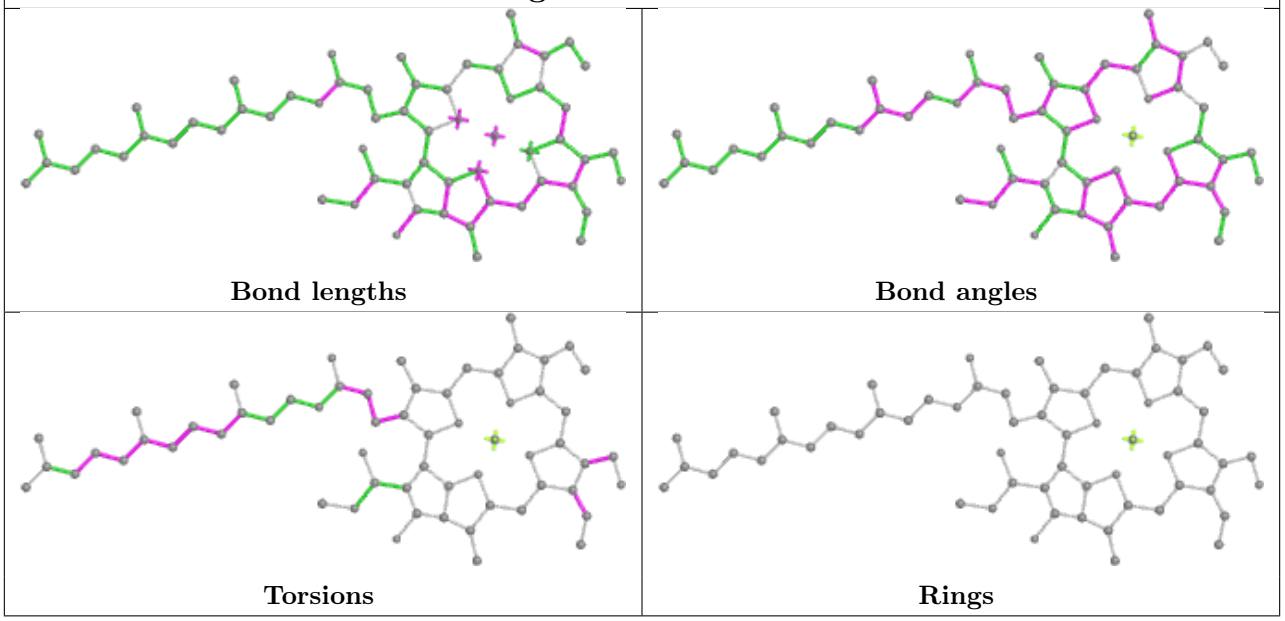
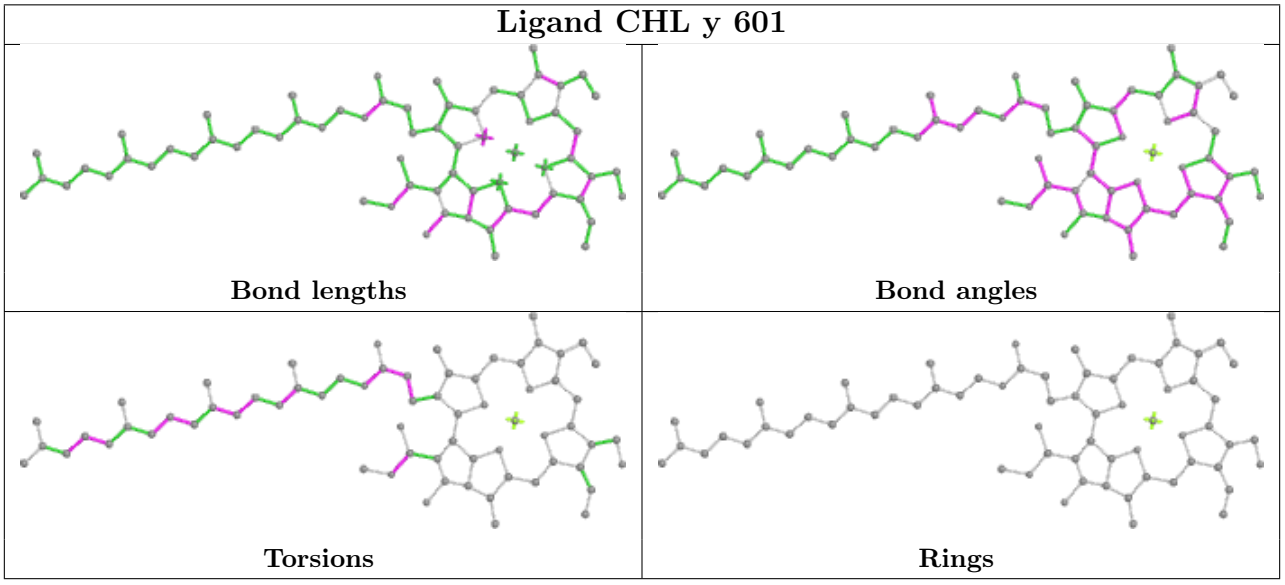
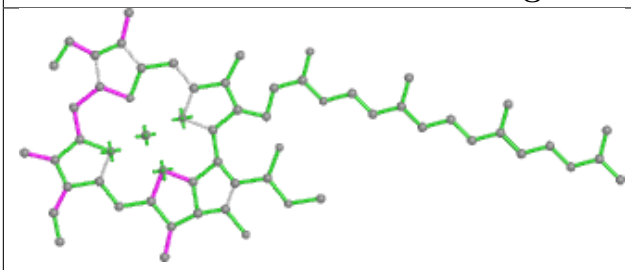


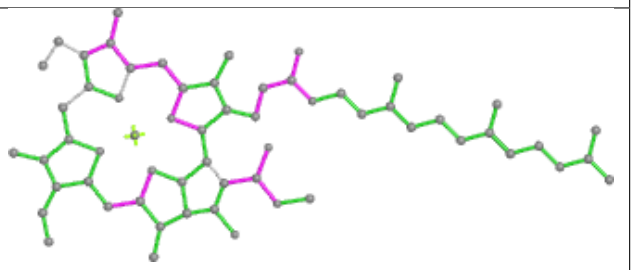
Ligand CHL y 601



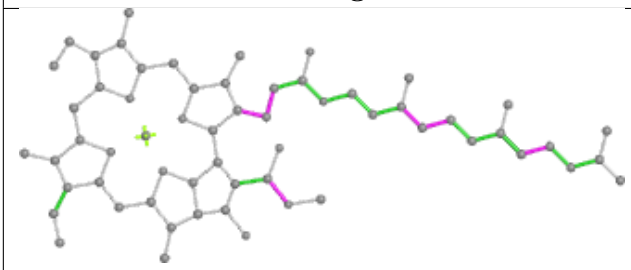
Ligand CLA R 602



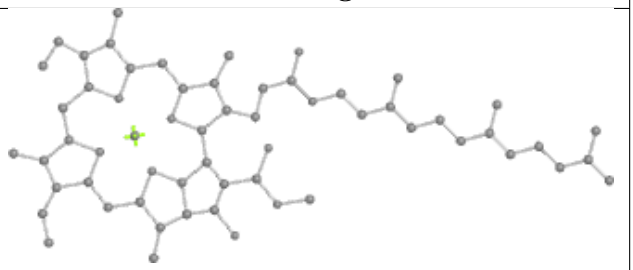
Bond lengths



Bond angles

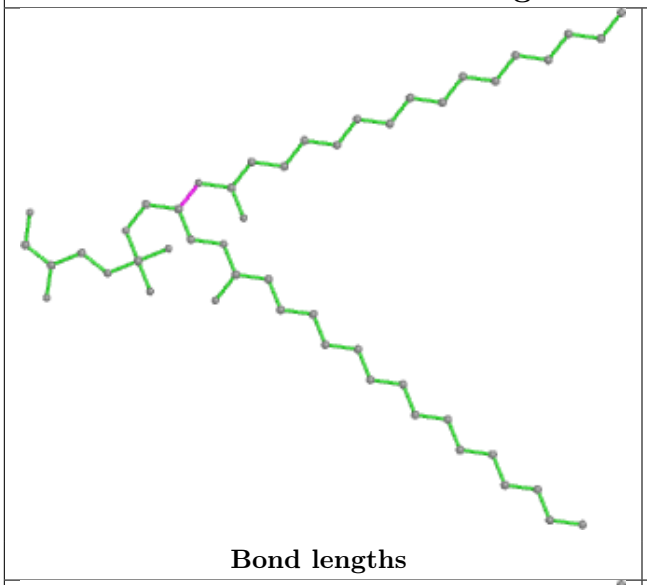


Torsions



Rings

Ligand LHG G 2630



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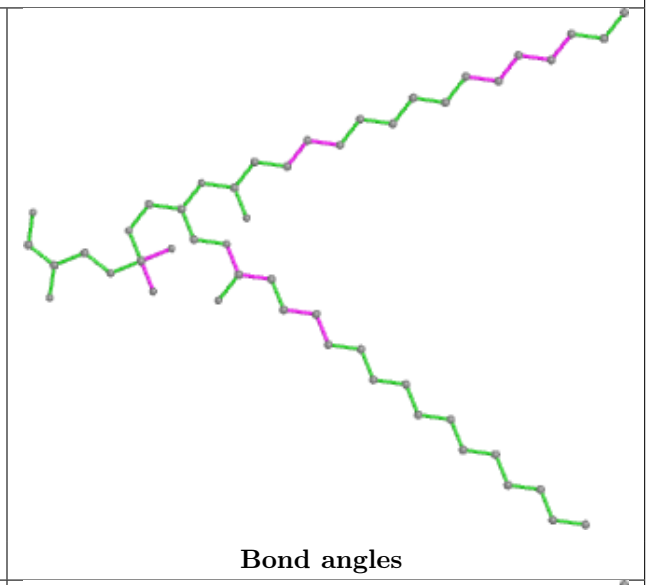
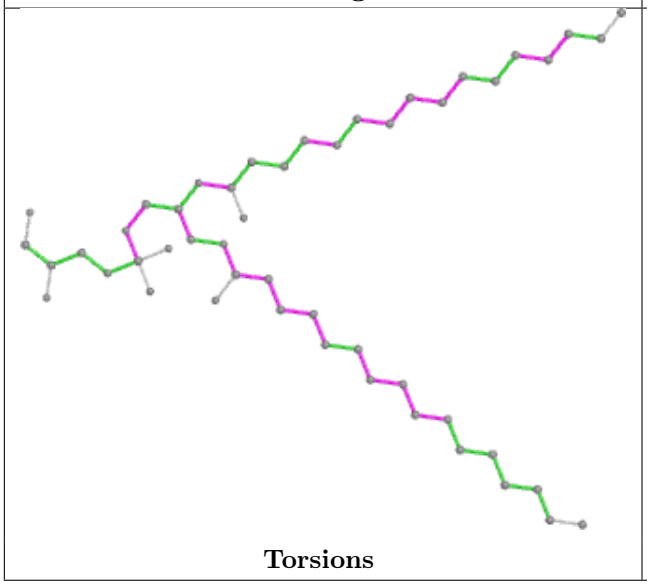


Bond angles



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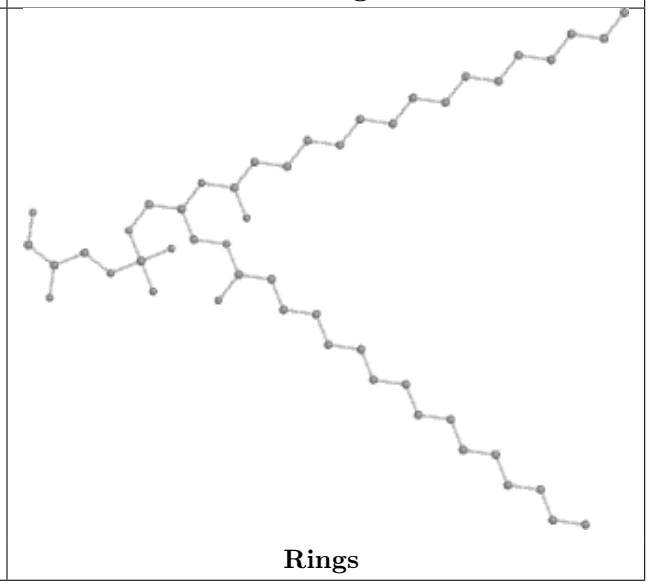
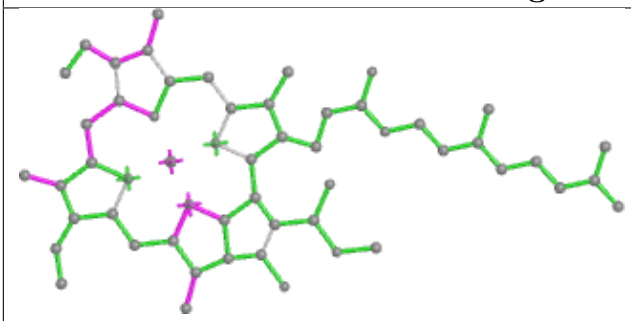


Rings

Ligand CLA 2 603



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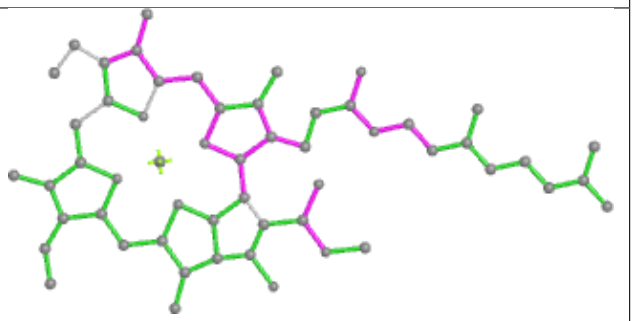
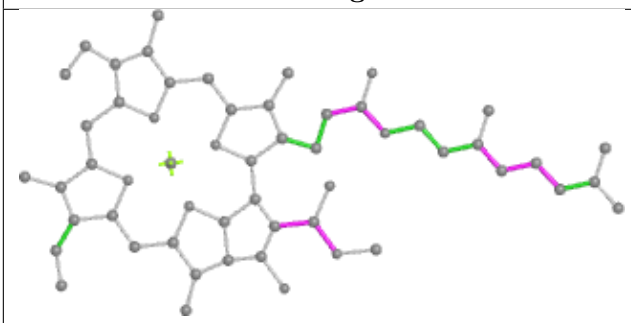


Bond angles



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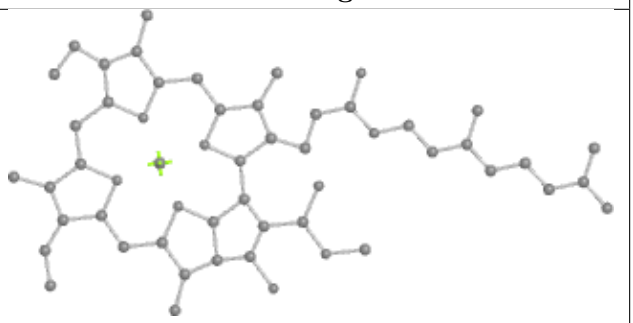
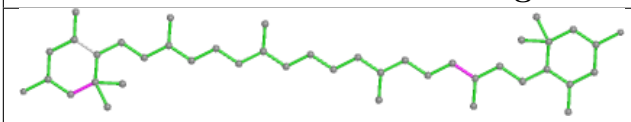


Rings

Ligand LUT N 1621



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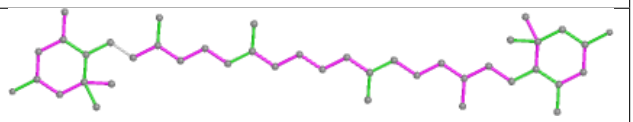
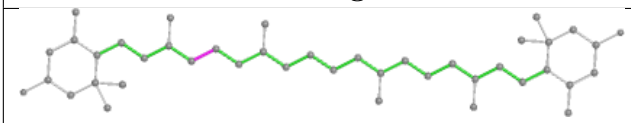


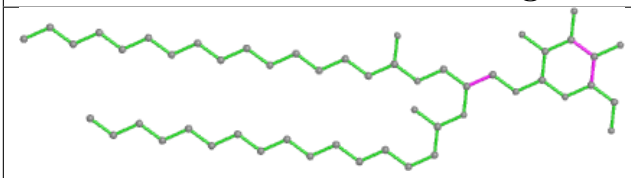
Bond angles



Torsions

Rings

Ligand LMG Z 101



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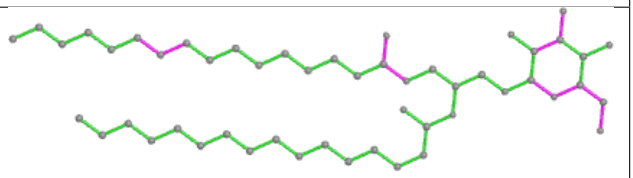
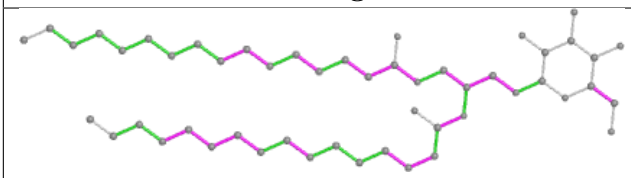
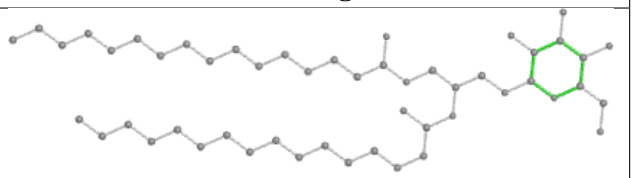


Bond angles

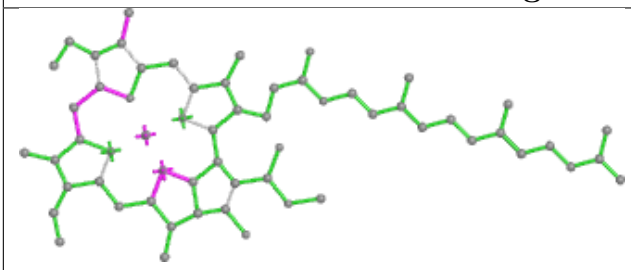


Torsions



Rings

Ligand CLA N 613



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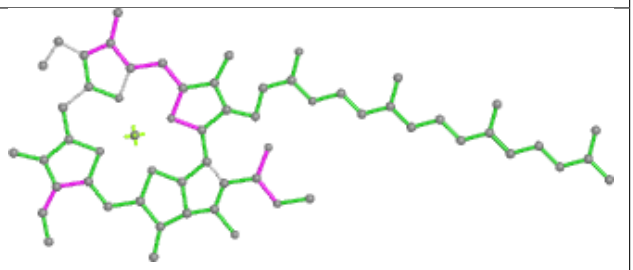
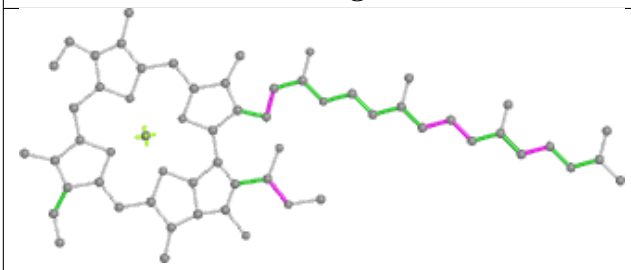
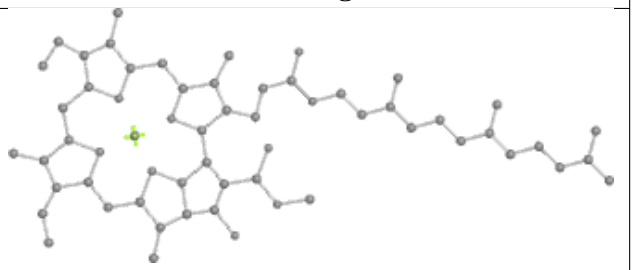


Bond angles

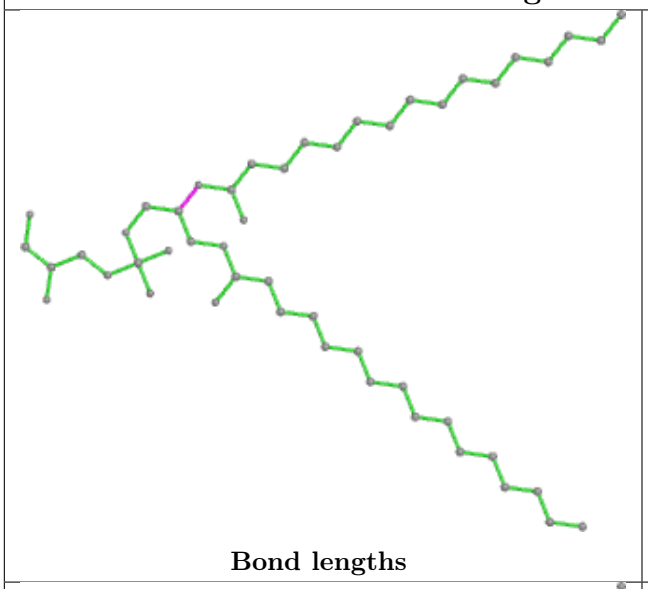


Torsions



Rings

Ligand LHG C 522



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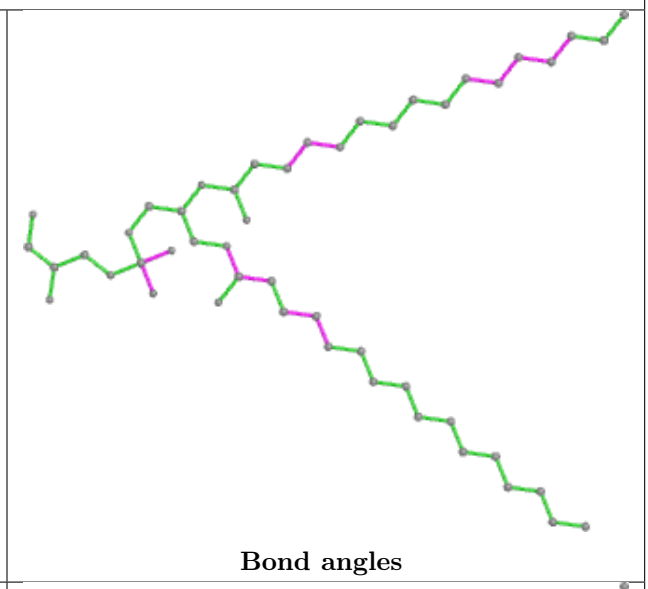

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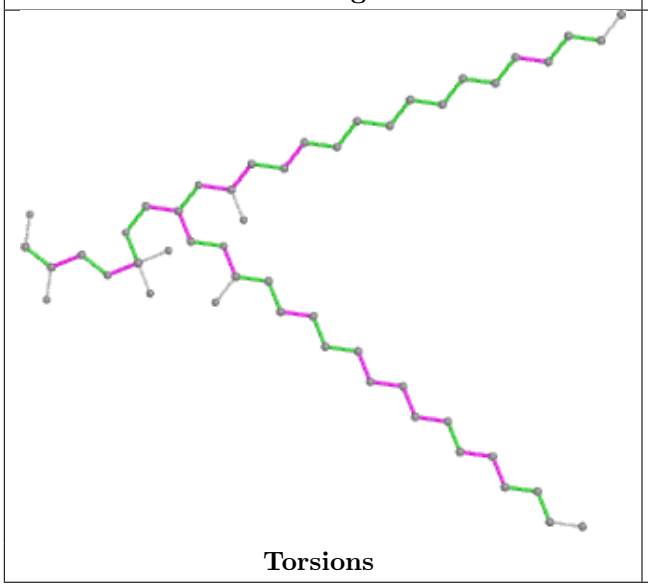

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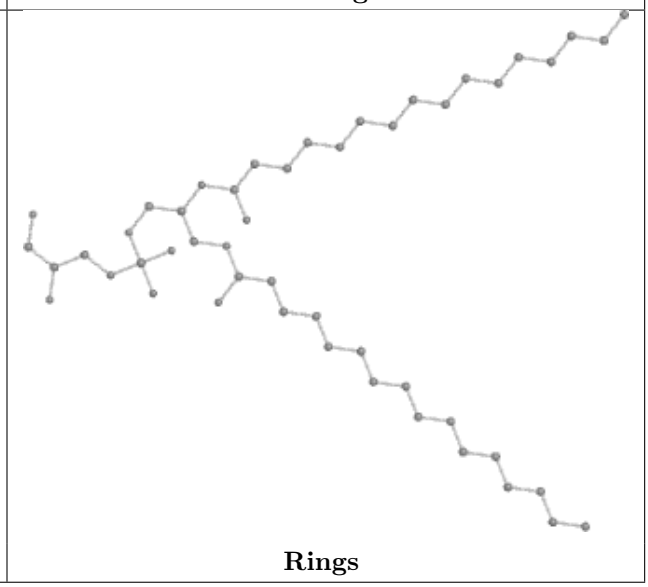
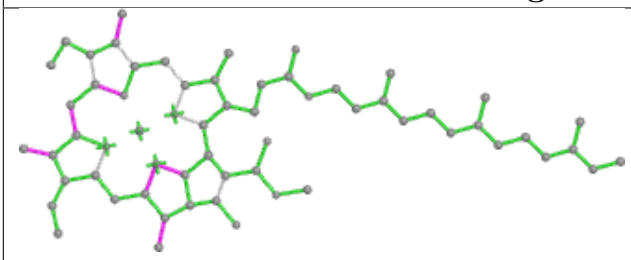


Rings

Ligand CLA S 602



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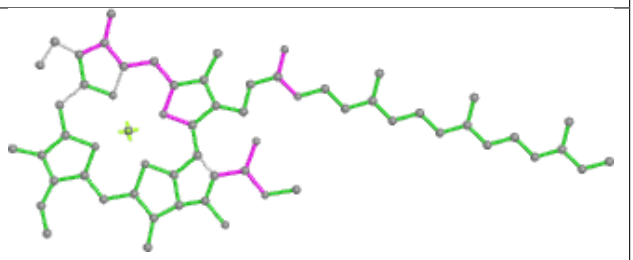

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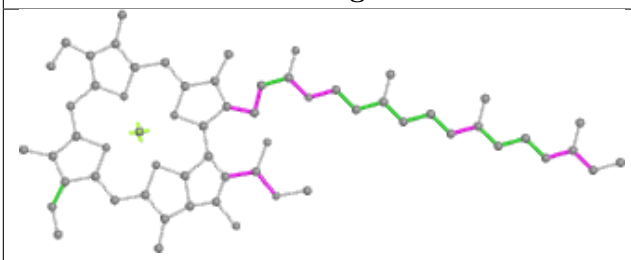

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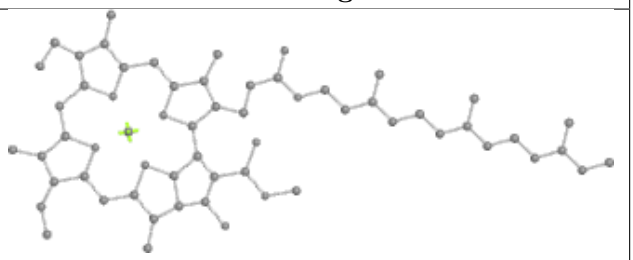
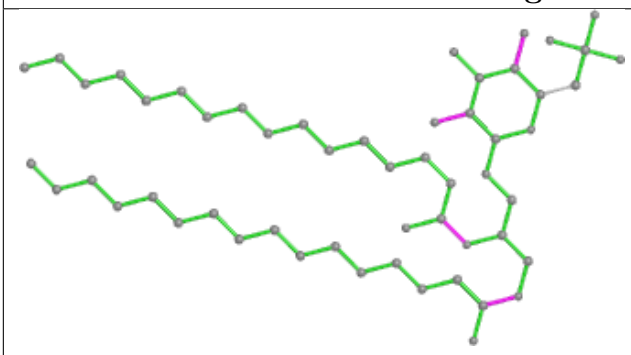


Rings

Ligand SQD B 621



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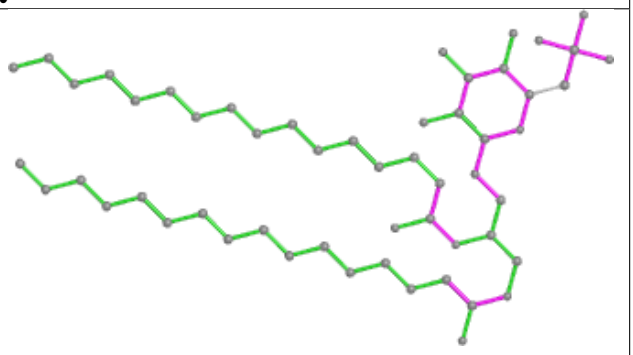

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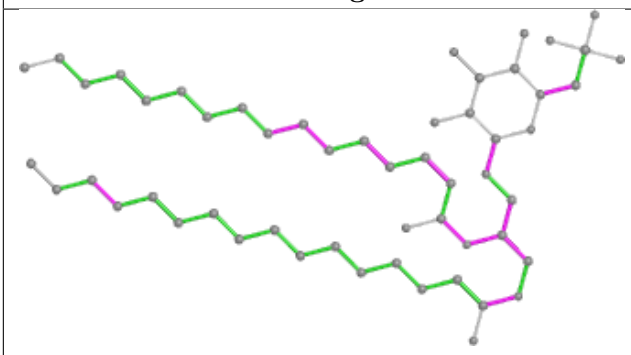

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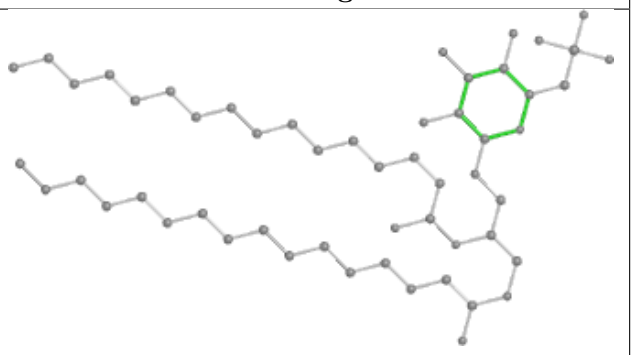
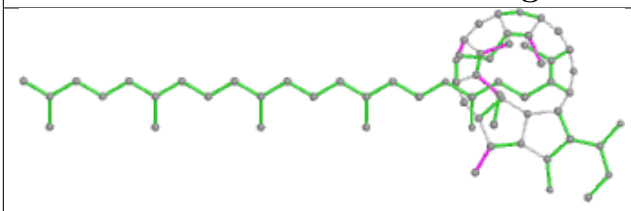


Rings

Ligand PHO A 409



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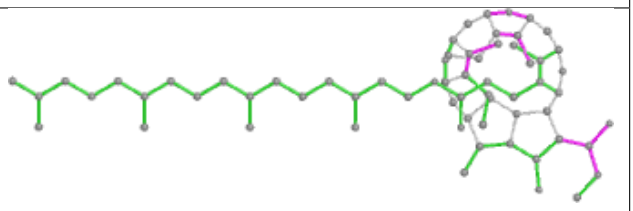

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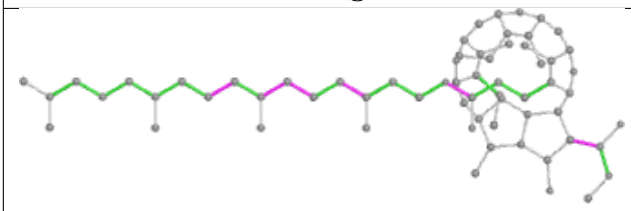

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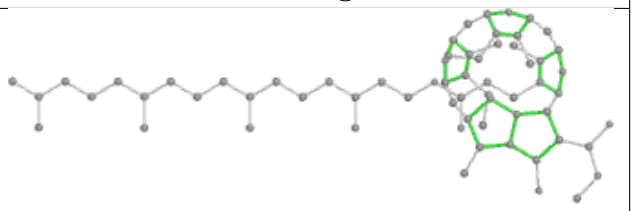
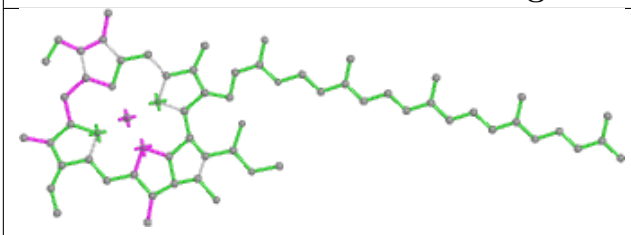


Rings

Ligand CLA b 612



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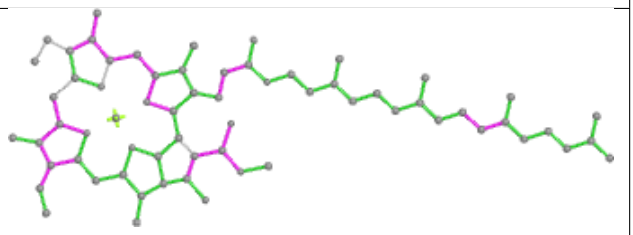

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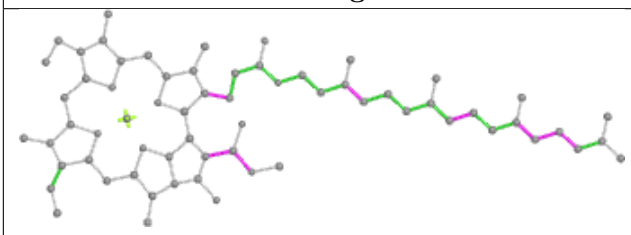

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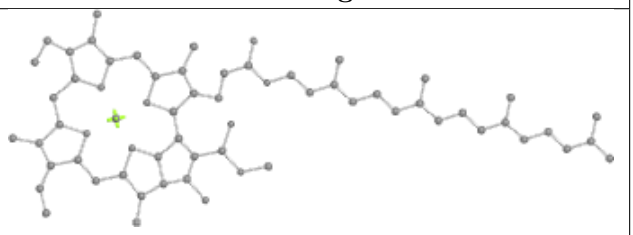

Rings

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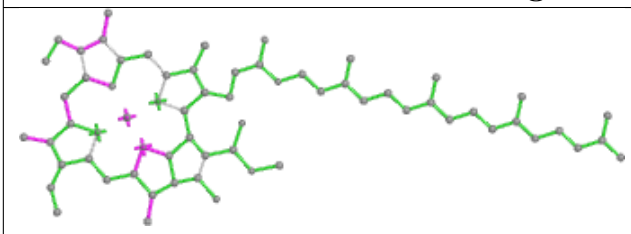

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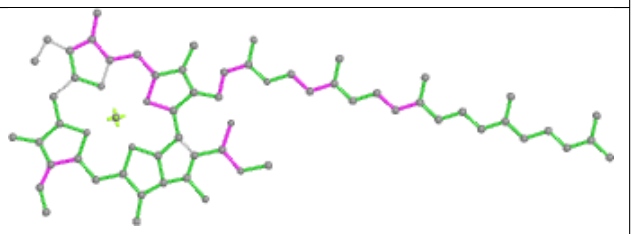

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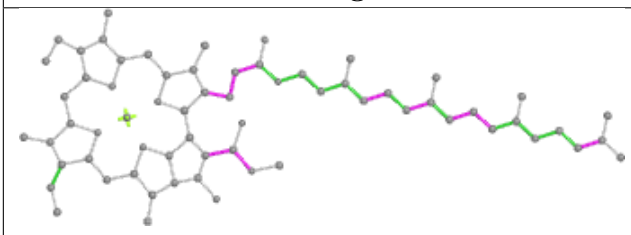

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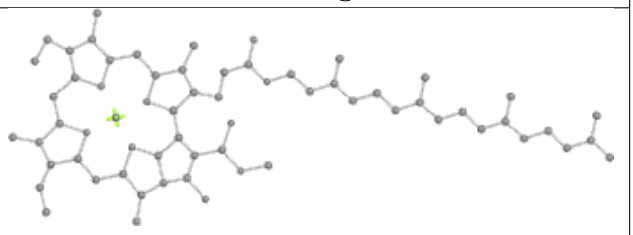
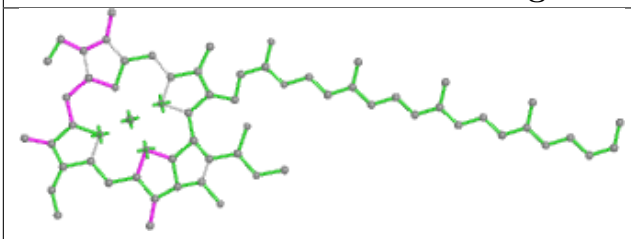


Rings

Ligand CLA g 610



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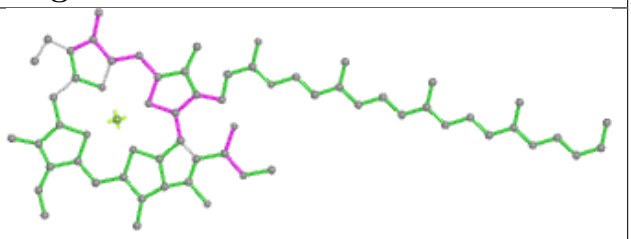

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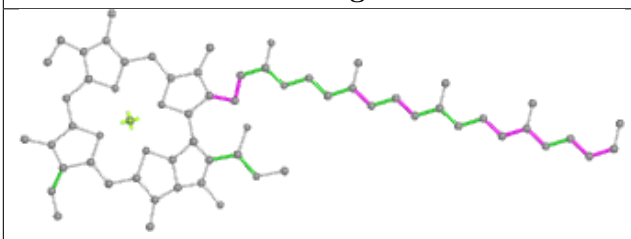

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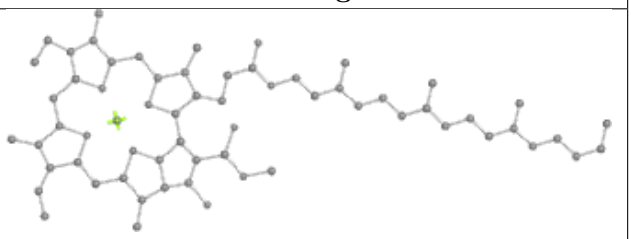
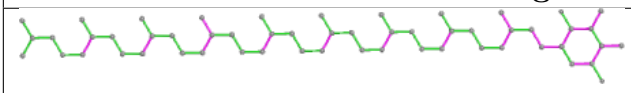


Rings

Ligand PL9 d 405



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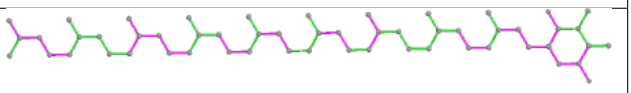

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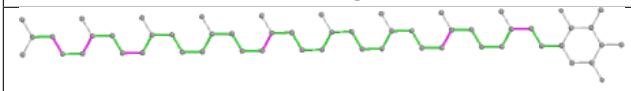

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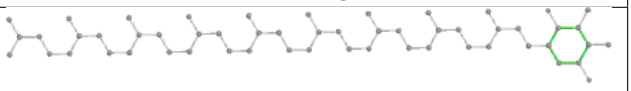
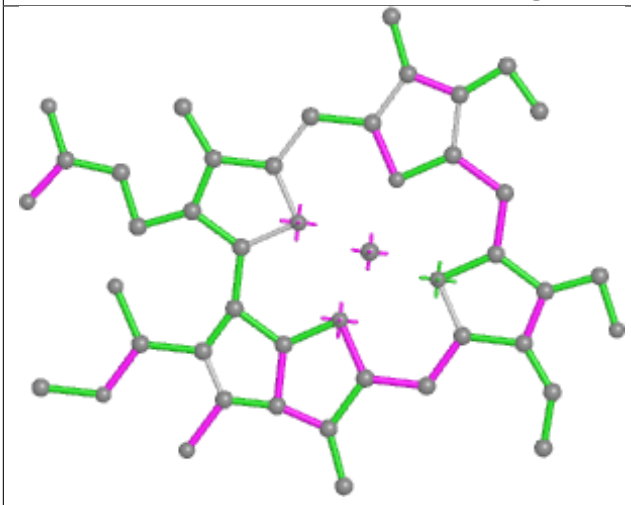


Rings

Ligand CHL 1 606



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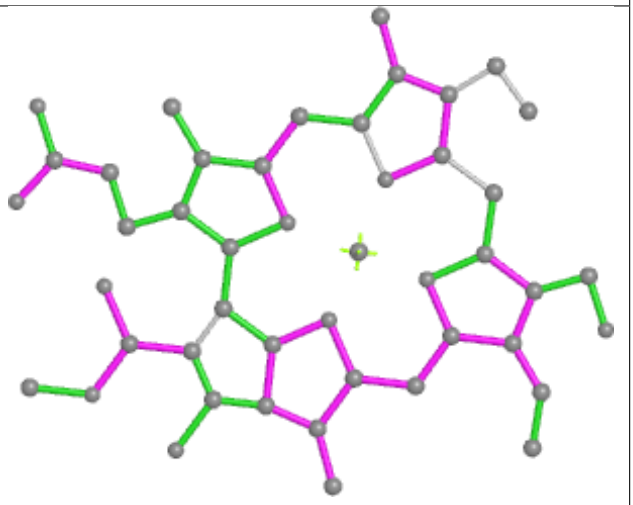

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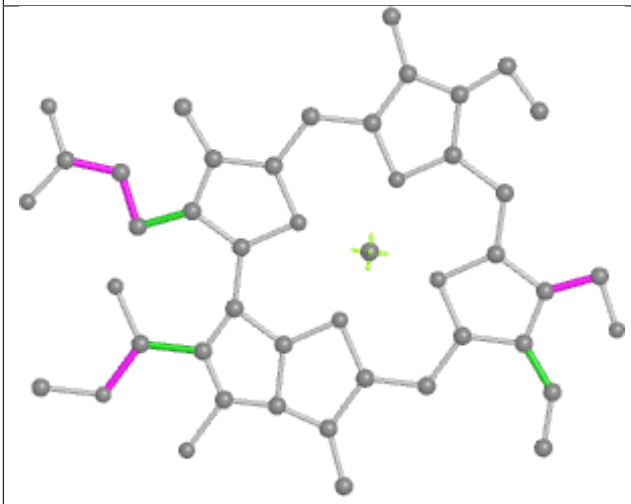

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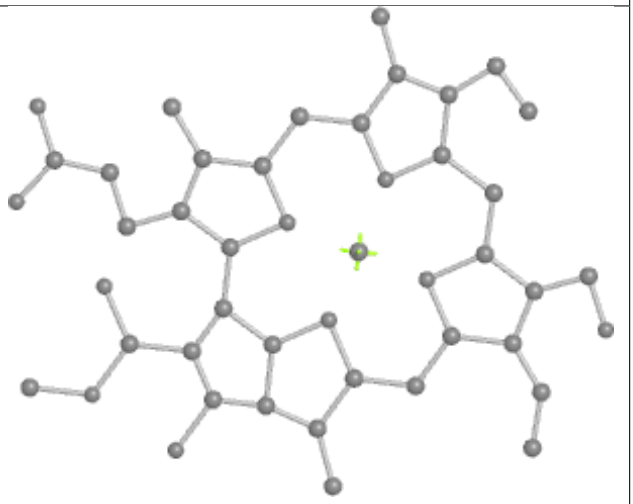
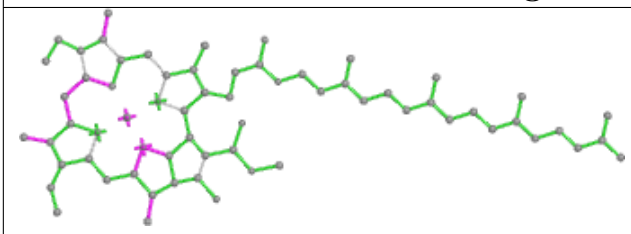


Rings

Ligand CLA A 405



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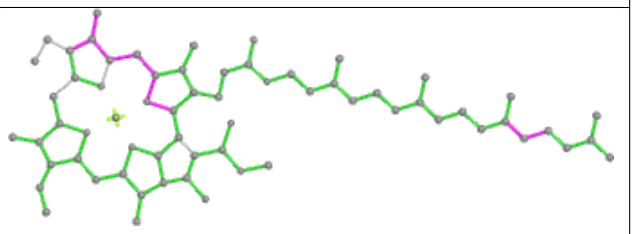
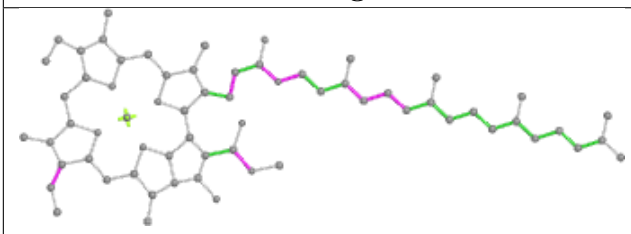


Bond angles



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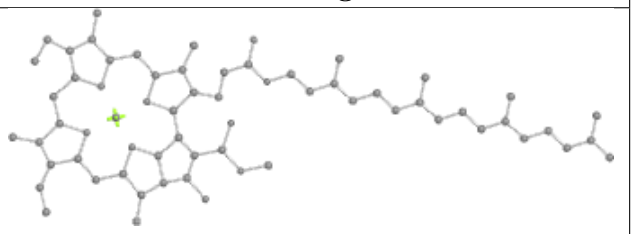
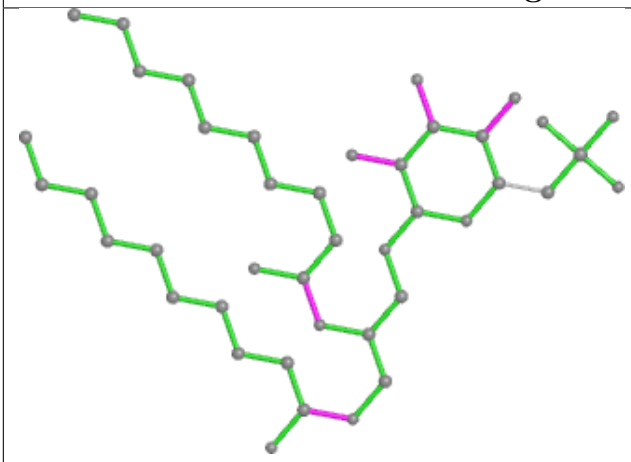


Rings

Ligand SQD B 623



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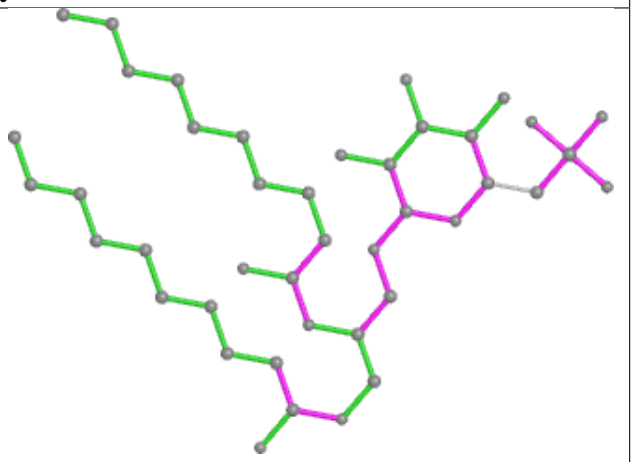
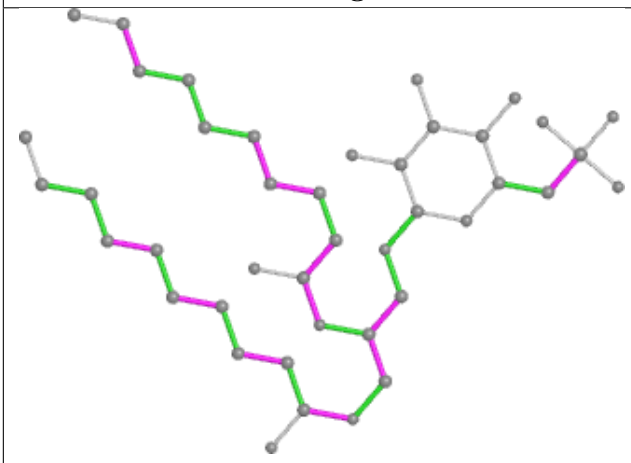


Bond angles



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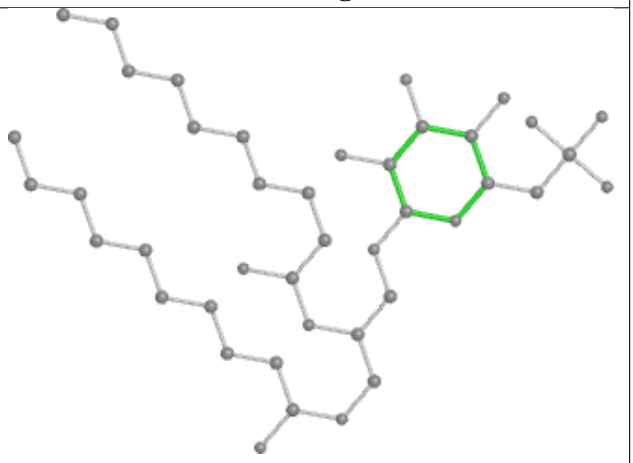
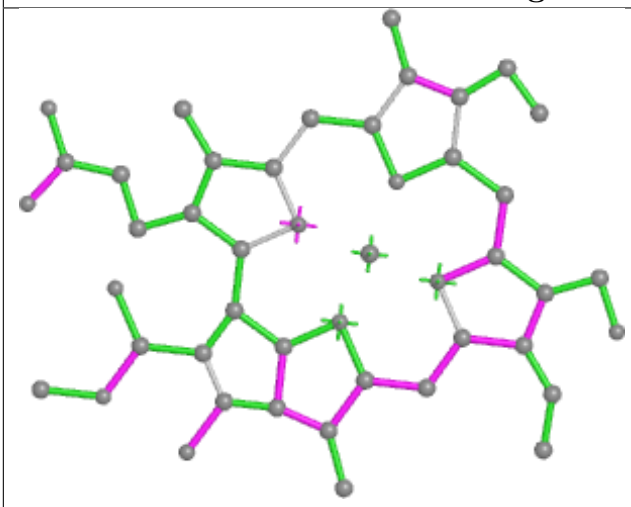


Rings

Ligand CHL 6 606



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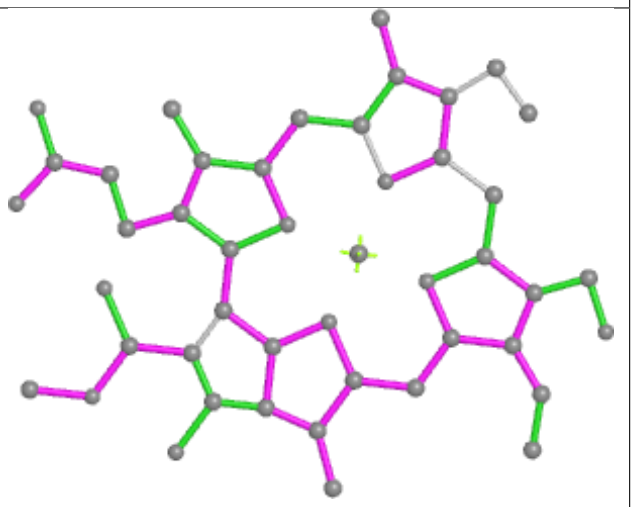
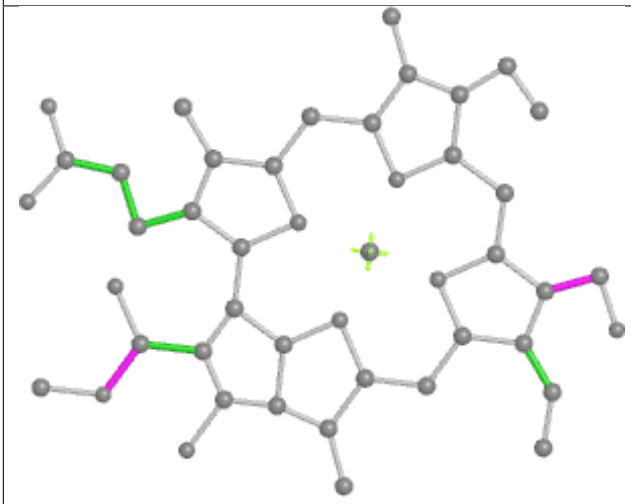


Bond angles



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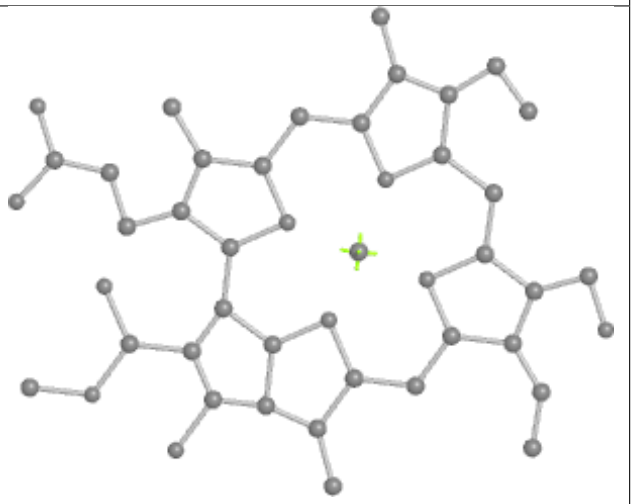

Rings

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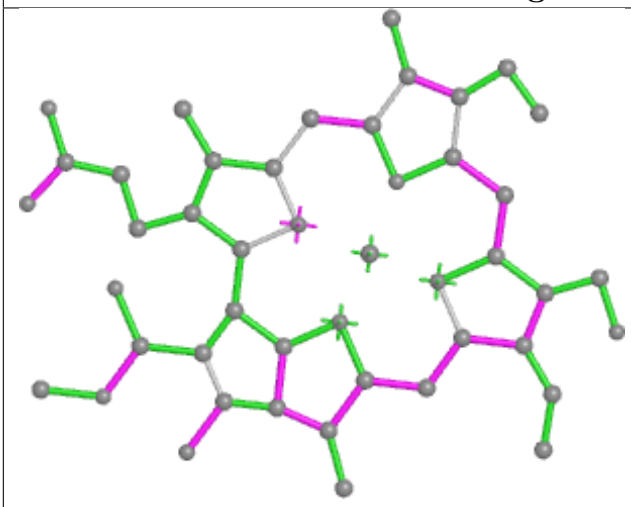

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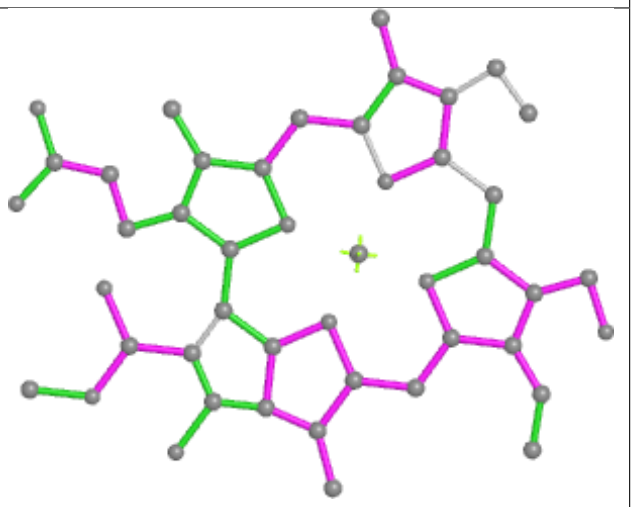
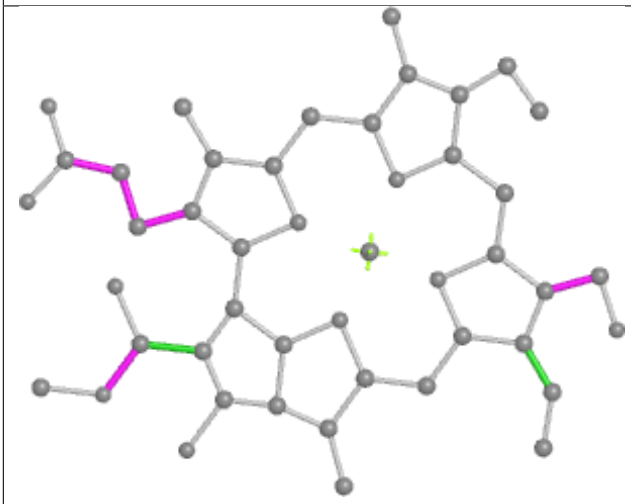


Bond angles



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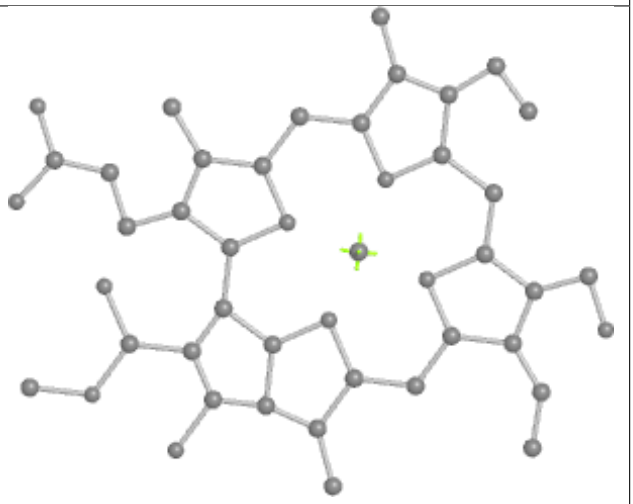
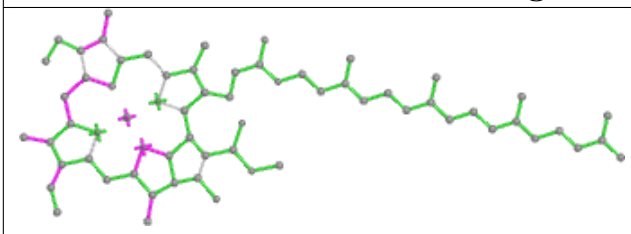


Rings

Ligand CLA y 603



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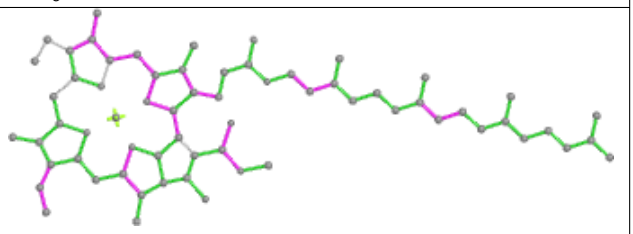
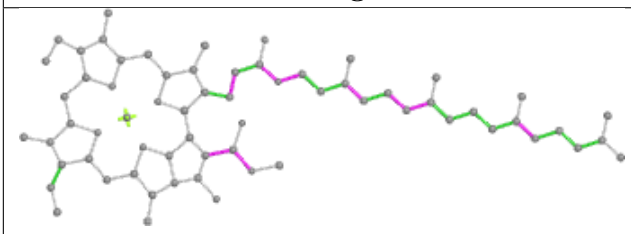
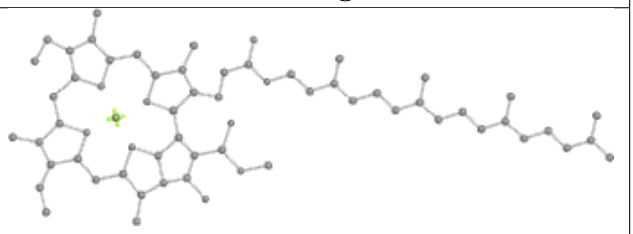


Bond angles

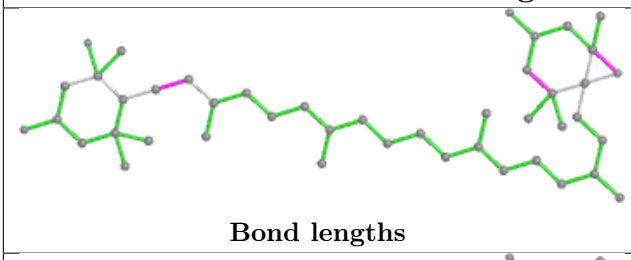


Torsions



Rings

Ligand NEX 5 1623



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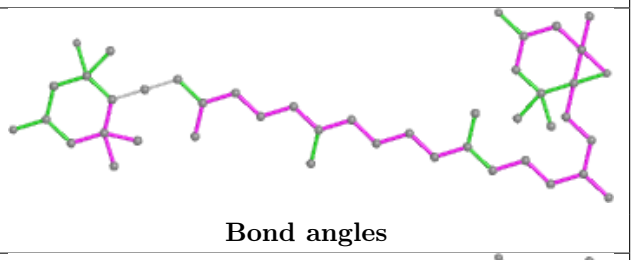

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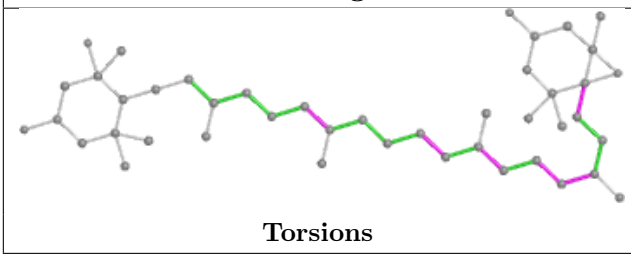

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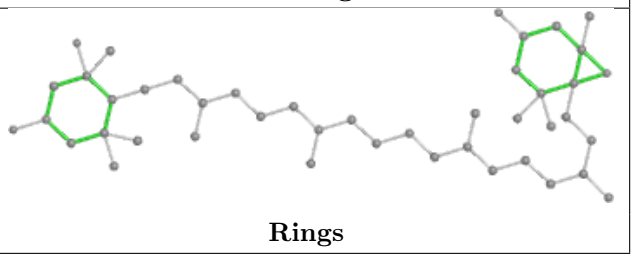
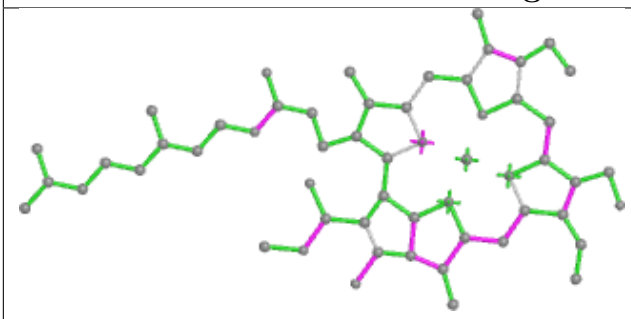


Rings

Ligand CHL R 607



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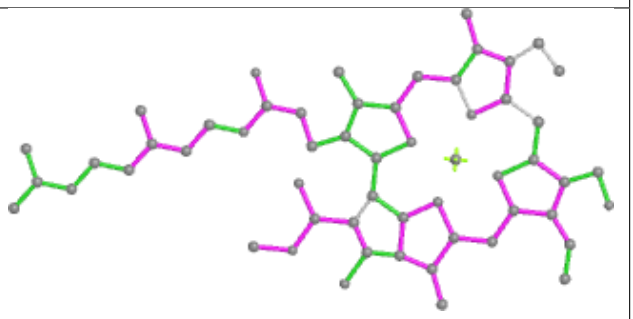
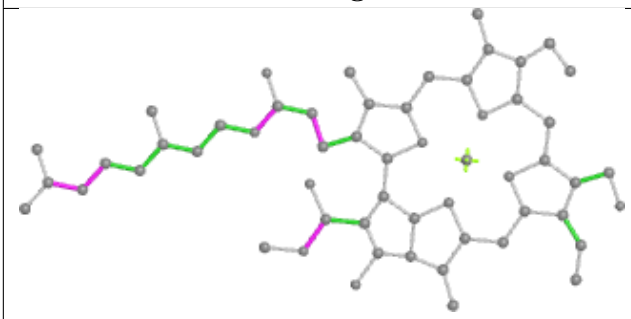


Bond angles



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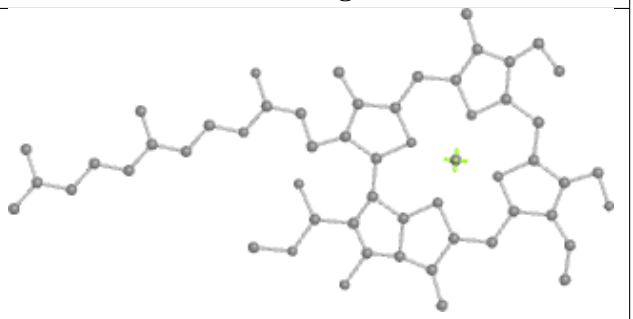
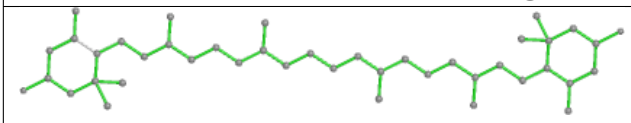


Rings

Ligand LUT s 1620



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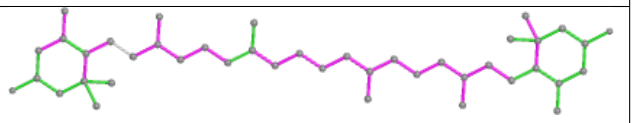

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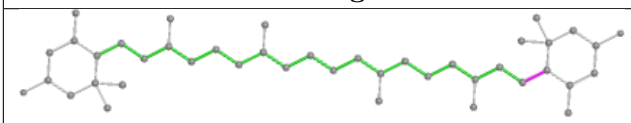

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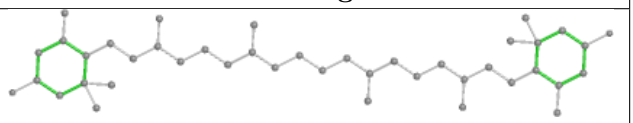
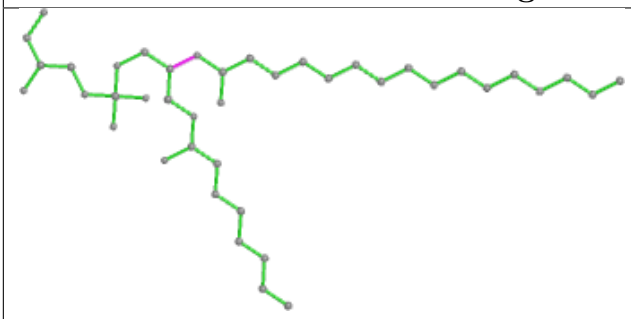


Rings

Ligand LHG 5 2630



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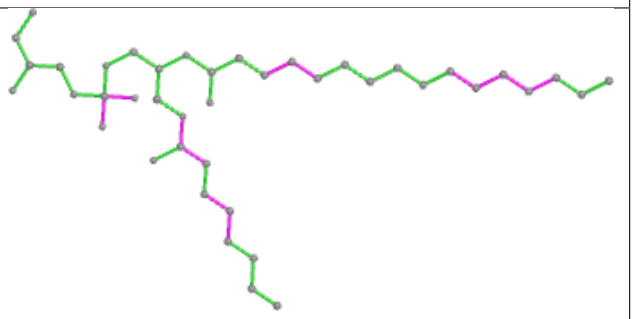

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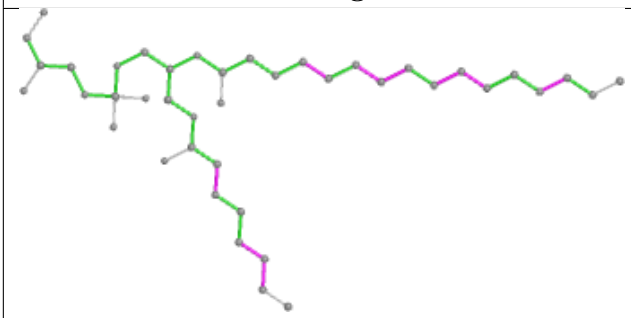

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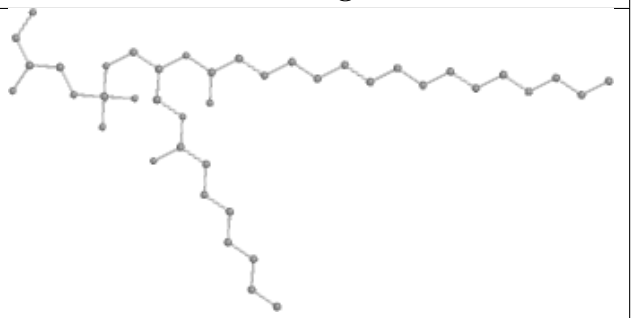
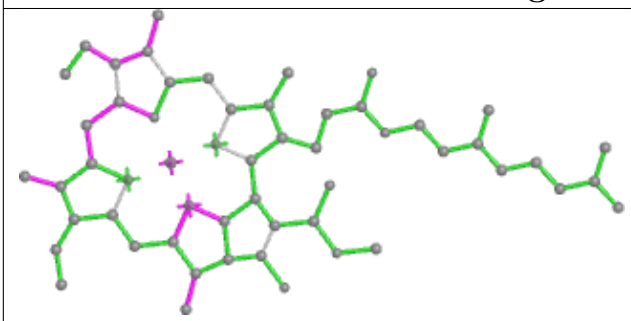


Rings

Ligand CLA 7 611



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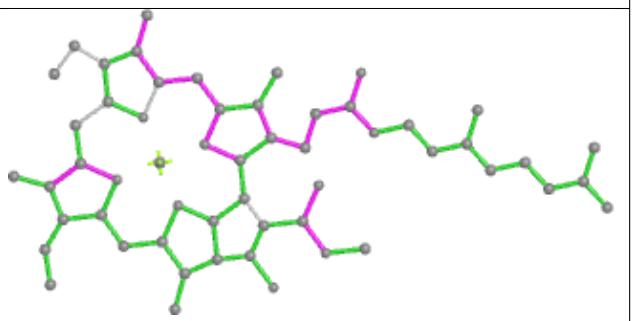

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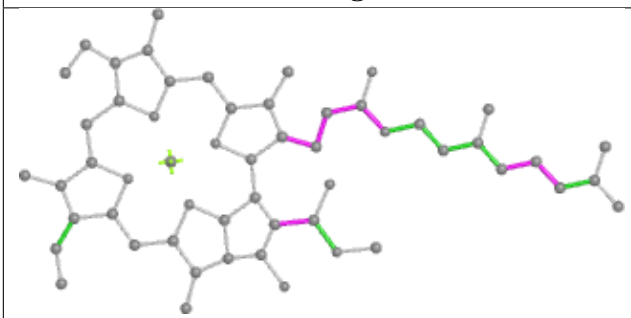

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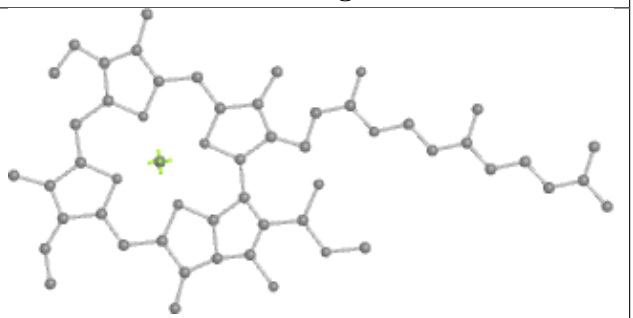
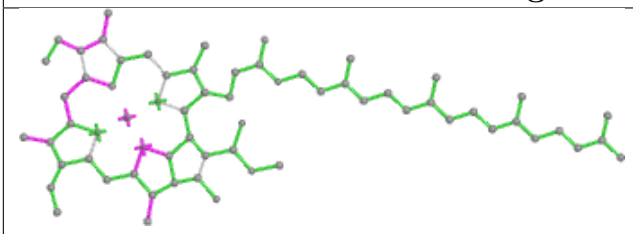


Rings

Ligand CLA b 608



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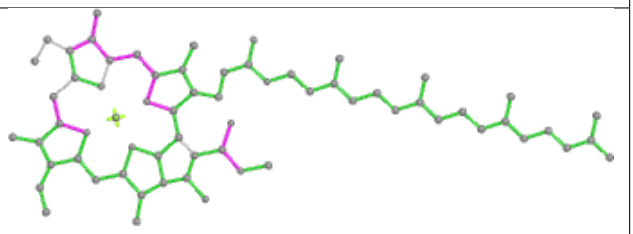
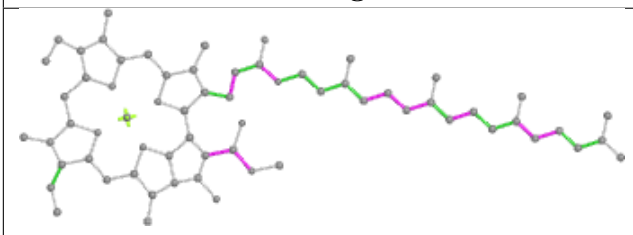


Bond angles



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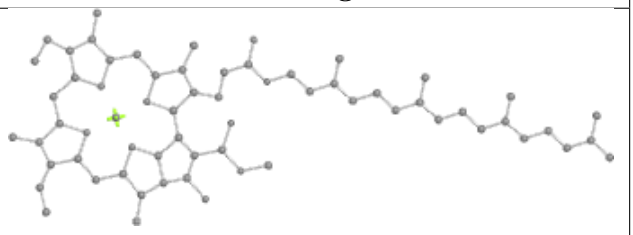
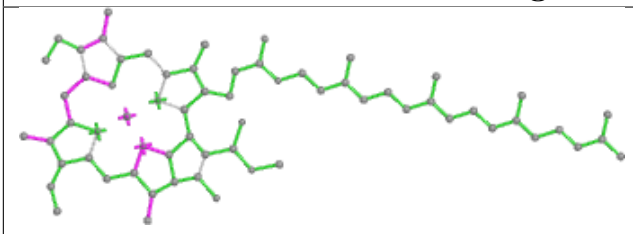


Rings

Ligand CLA c 506



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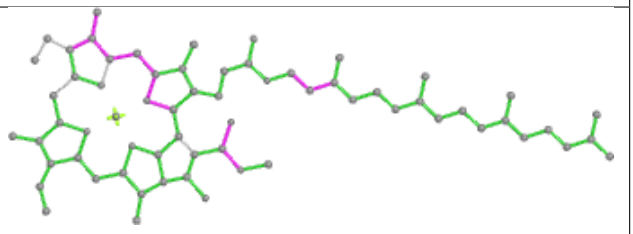

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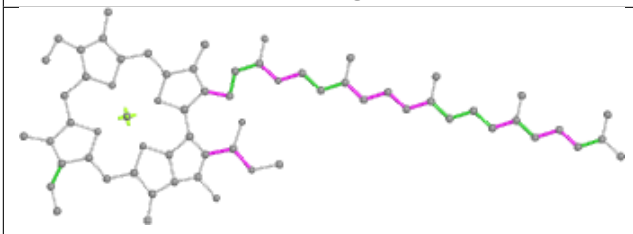

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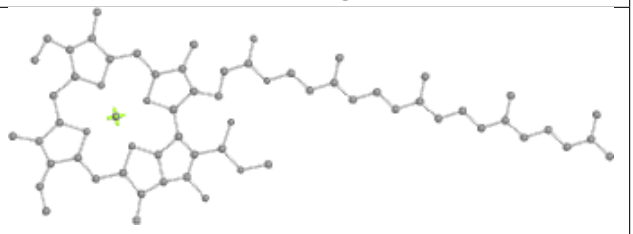
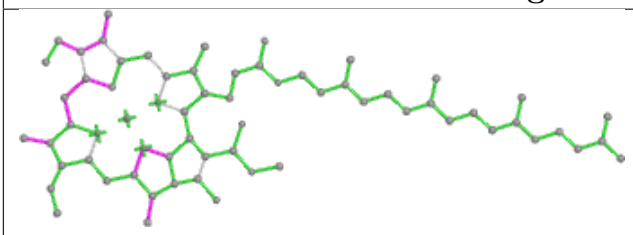


Rings

Ligand CLA b 616



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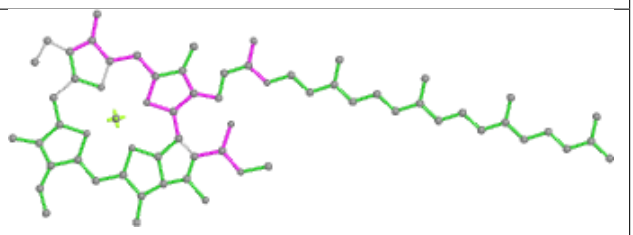
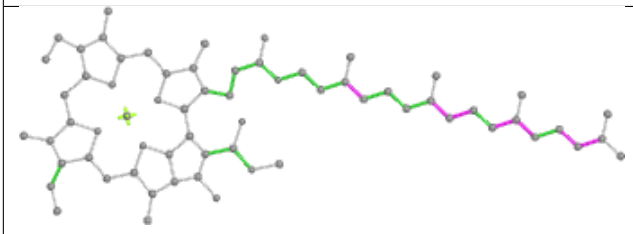


Bond angles



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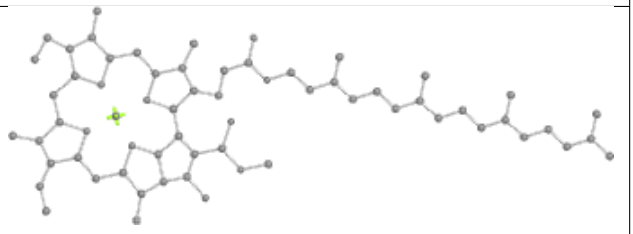
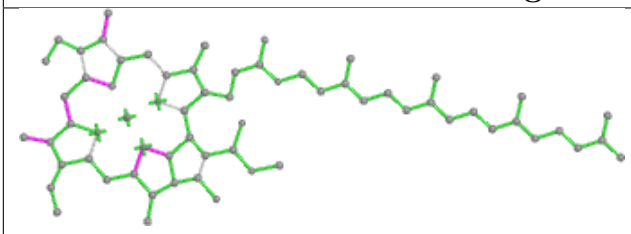


Rings

Ligand CLA C 502



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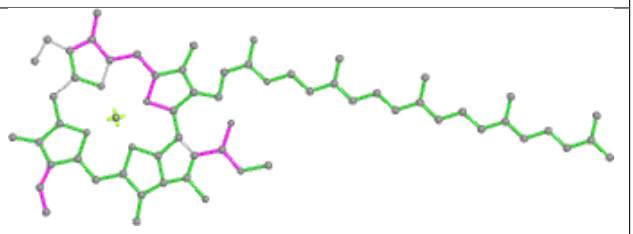

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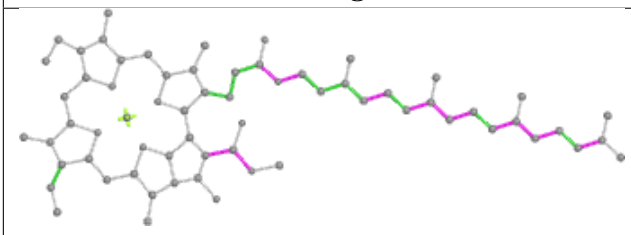

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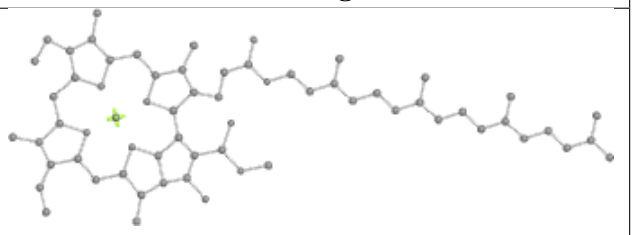
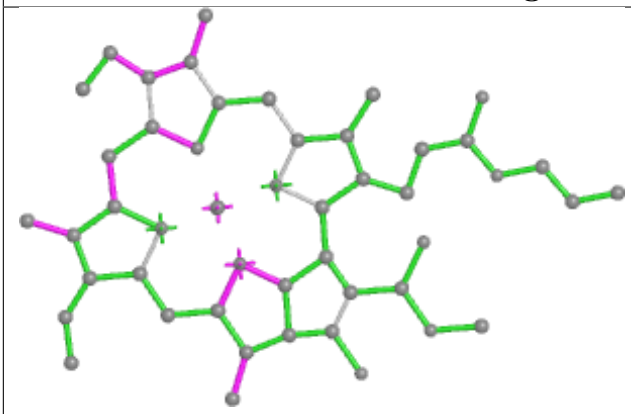


Rings

Ligand CLA G 614



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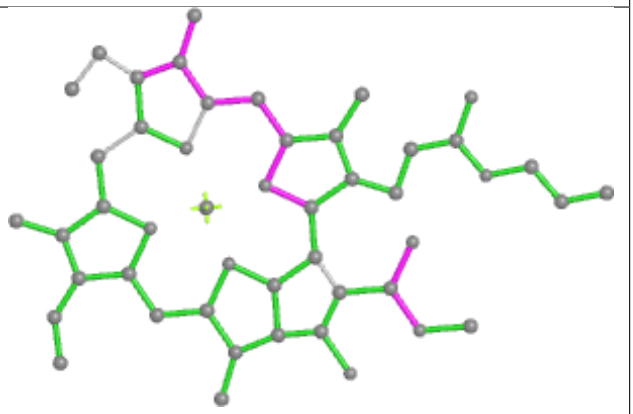
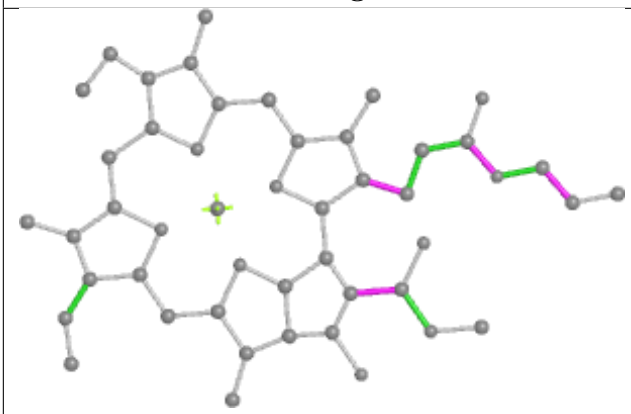


Bond angles



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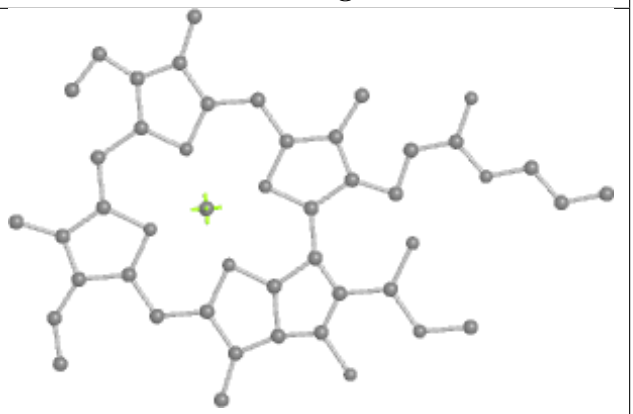
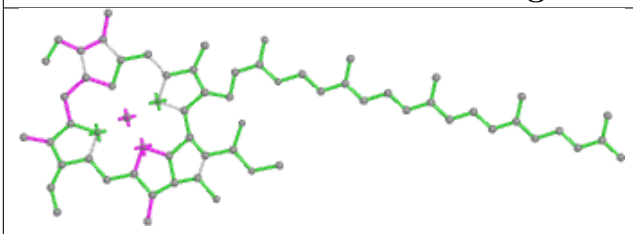


Rings

Ligand CLA b 604



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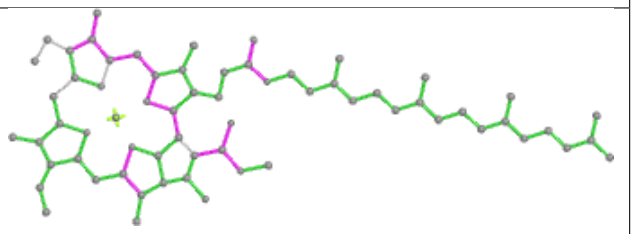
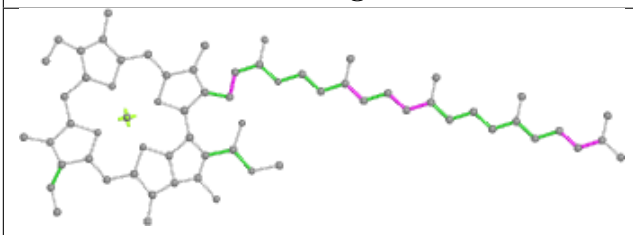


Bond angles



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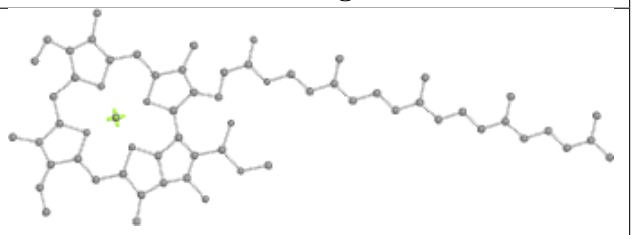
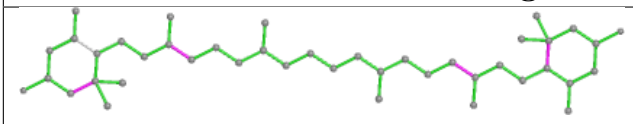


Rings

Ligand LUT g 1621



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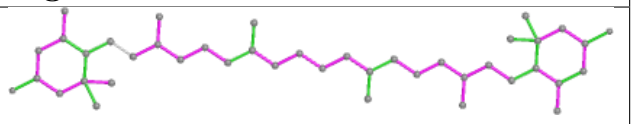
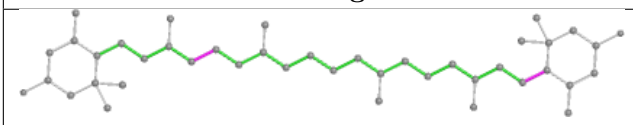


Bond angles



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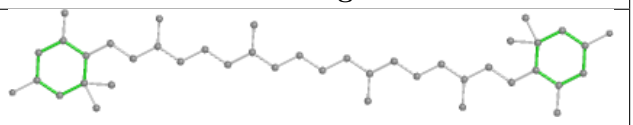
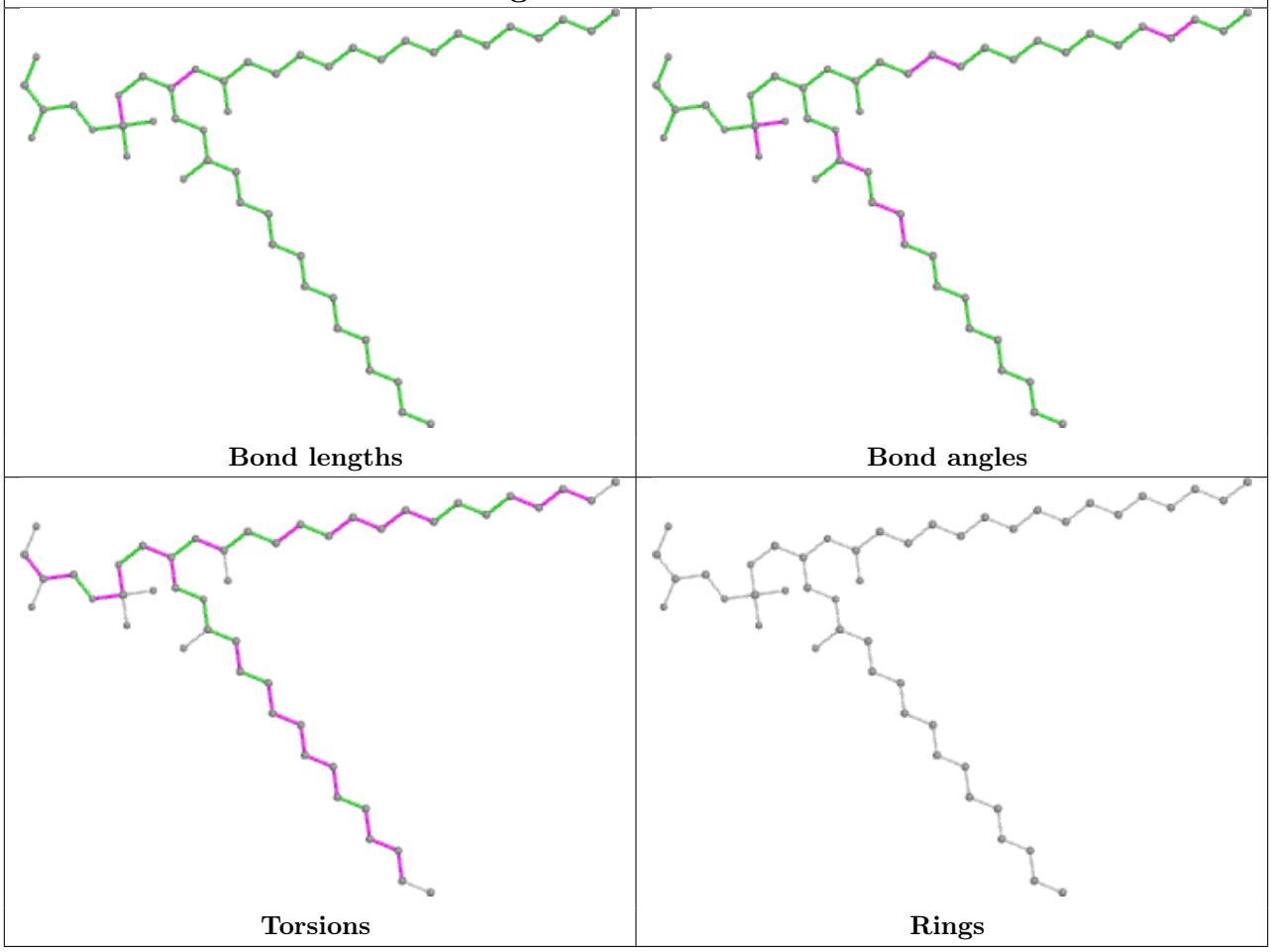
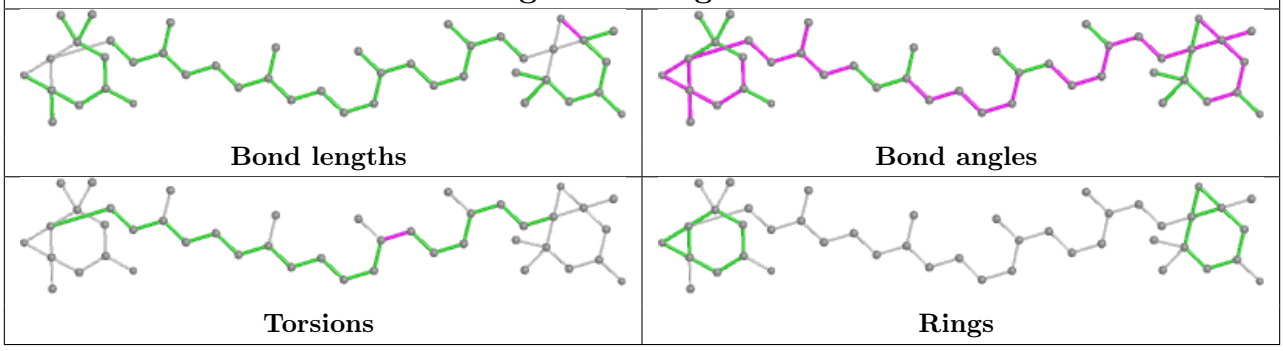


Rings

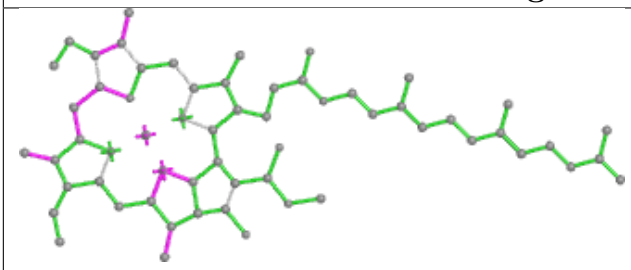
Ligand LHG B 2630



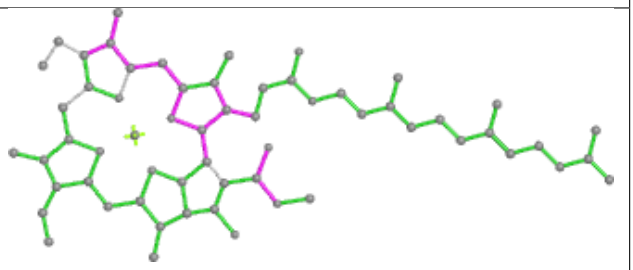
Ligand XAT g 1622



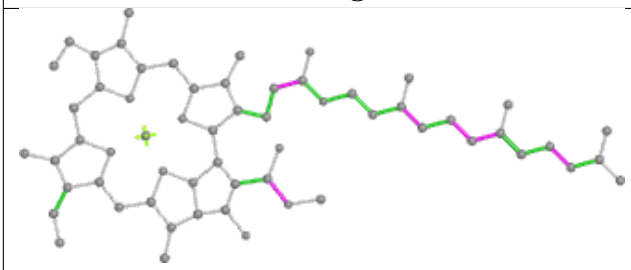
Ligand CLA n 612



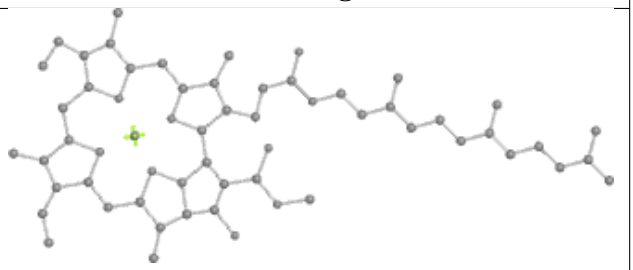
Bond lengths



Bond angles

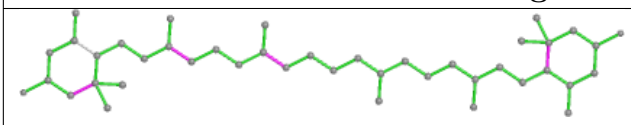


Torsions



Rings

Ligand LUT r 620



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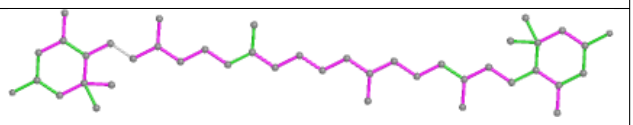

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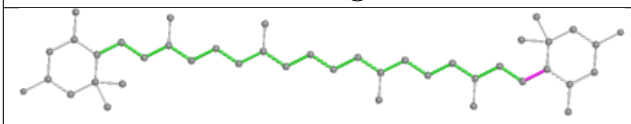

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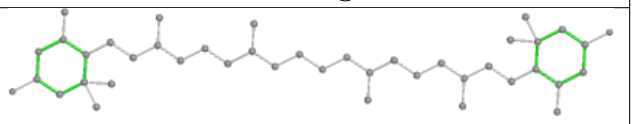
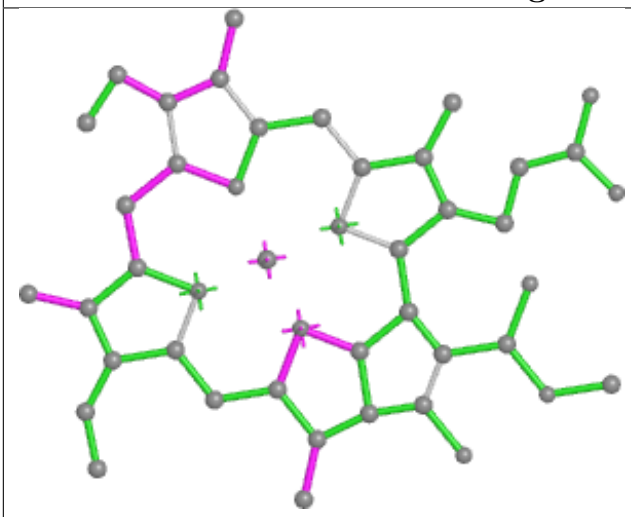


Rings

Ligand CLA 6 604



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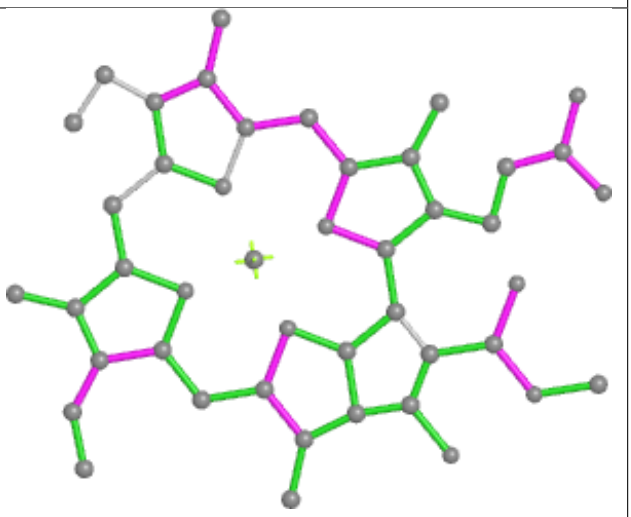

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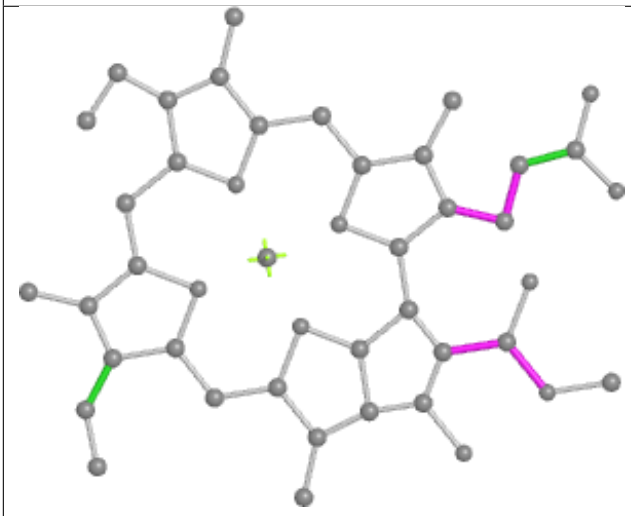

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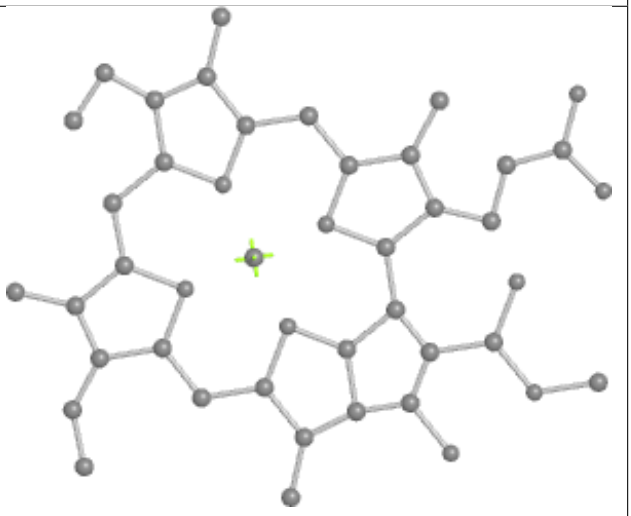

Rings

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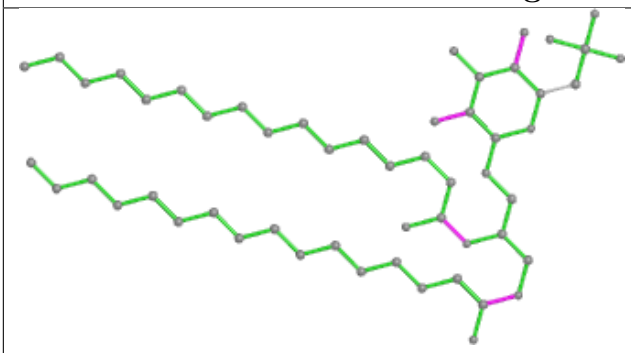

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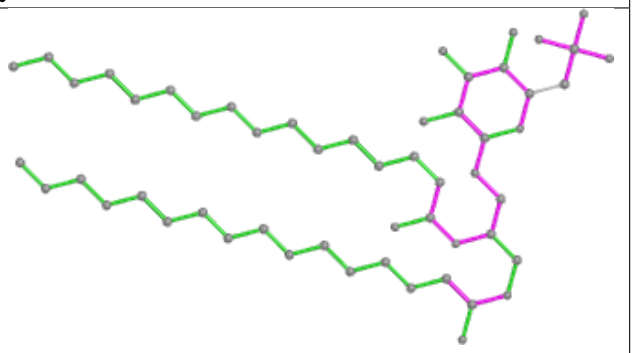
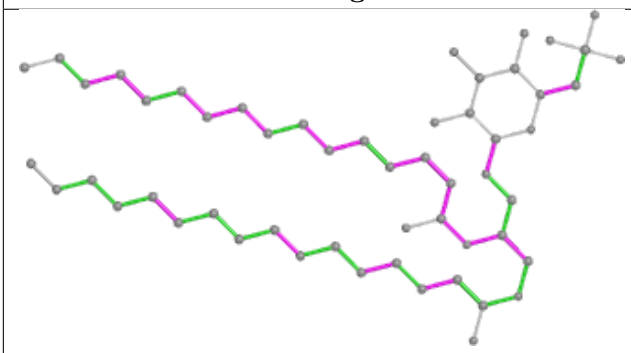


Bond angles



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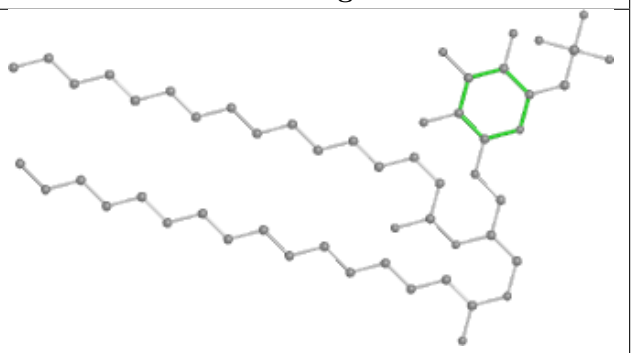
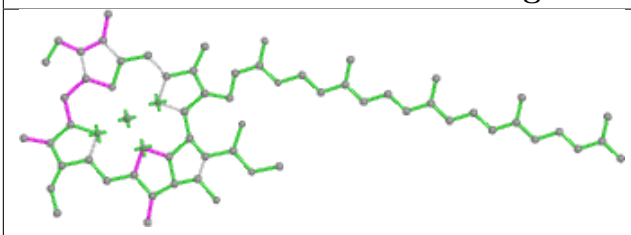


Rings

Ligand CLA N 610



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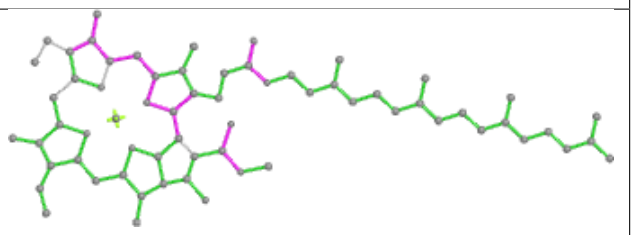

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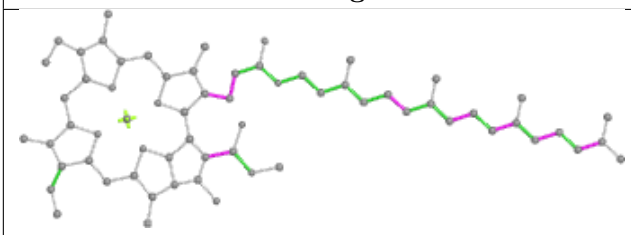

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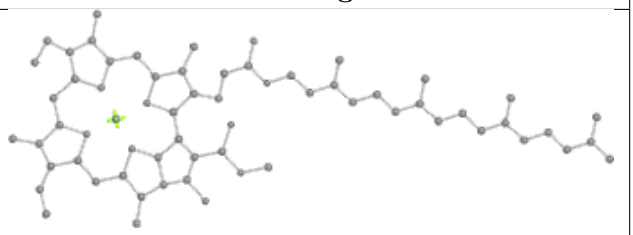

Rings

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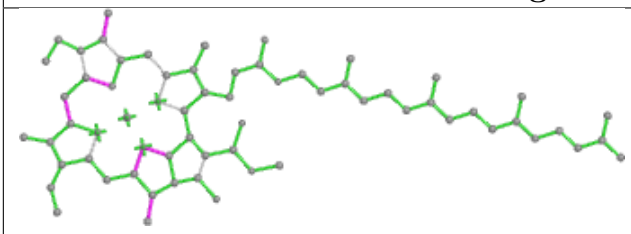

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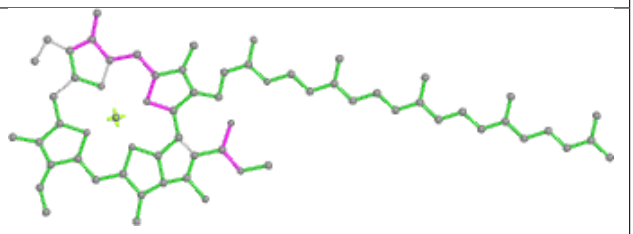

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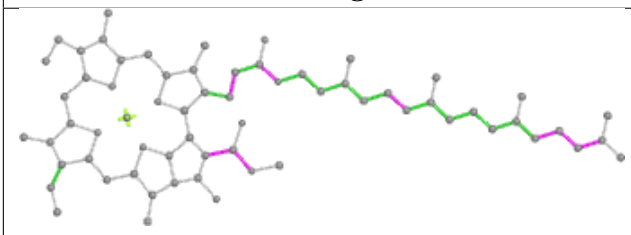

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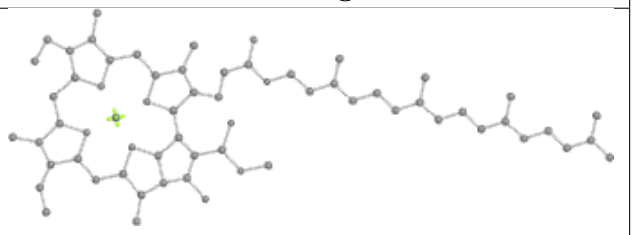

Rings

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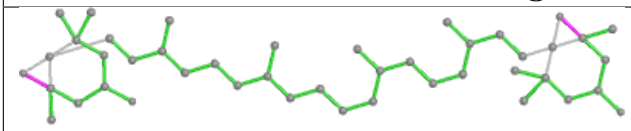

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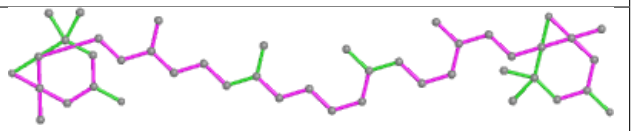

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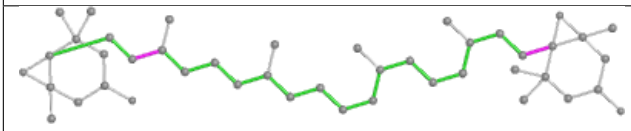

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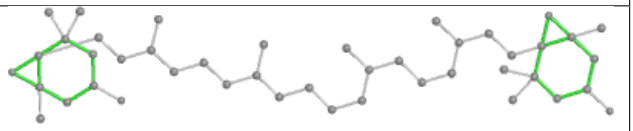

Rings

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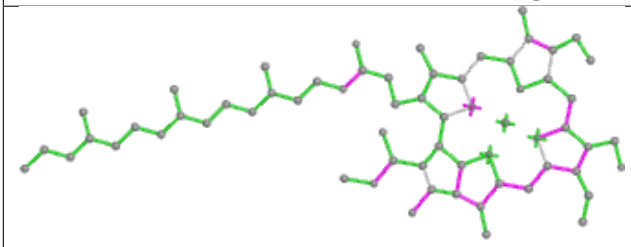

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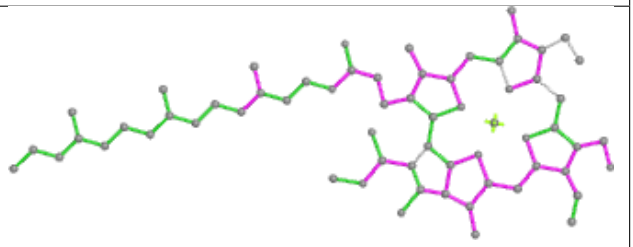

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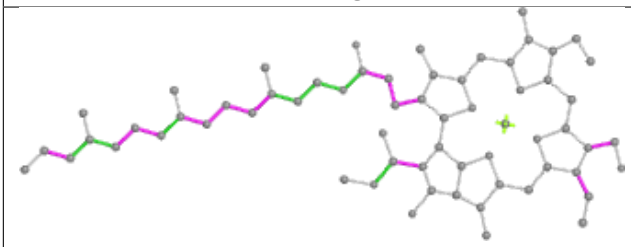

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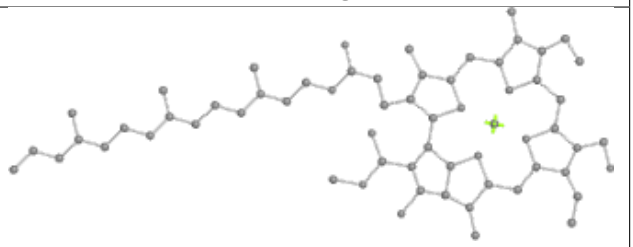

Rings

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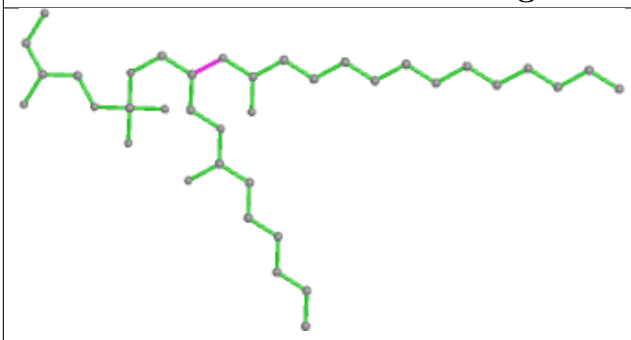

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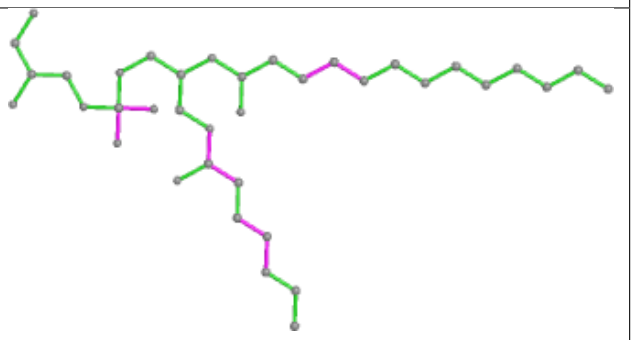
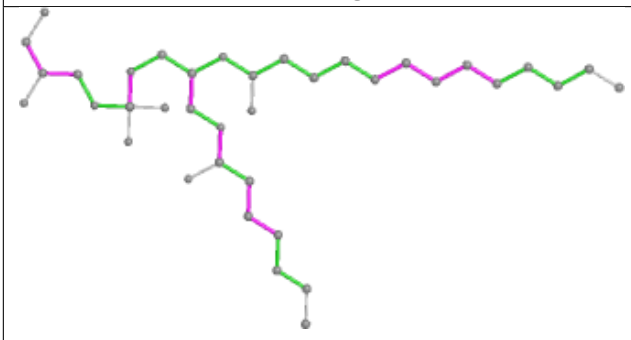


Bond angles



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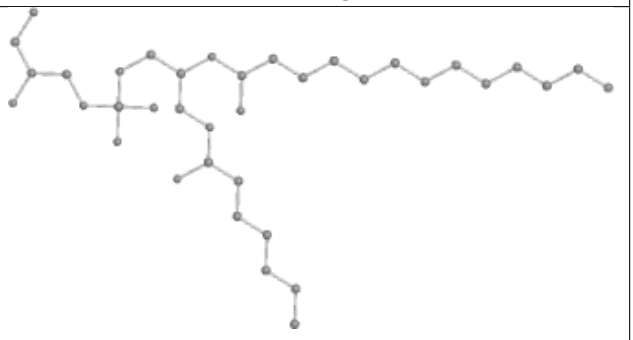
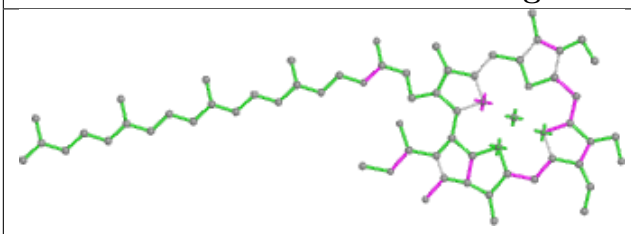


Rings

Ligand CHL Y 608



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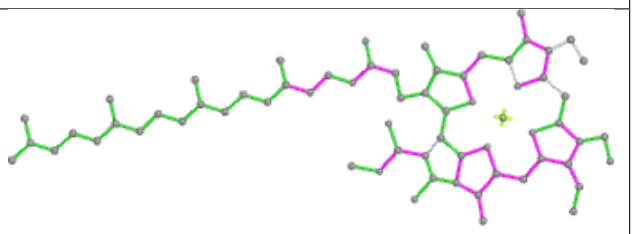

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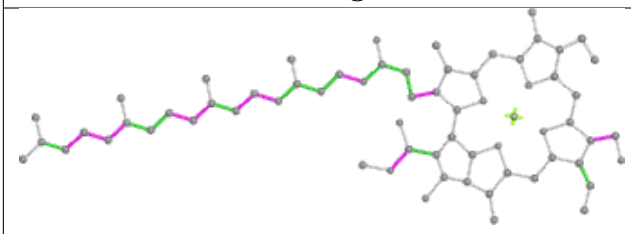

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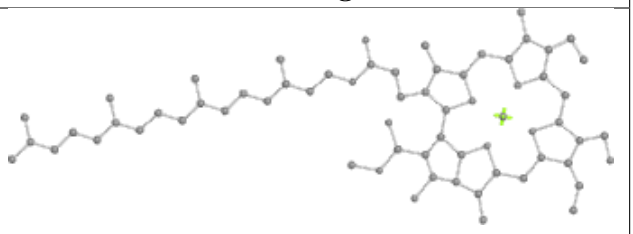

Rings

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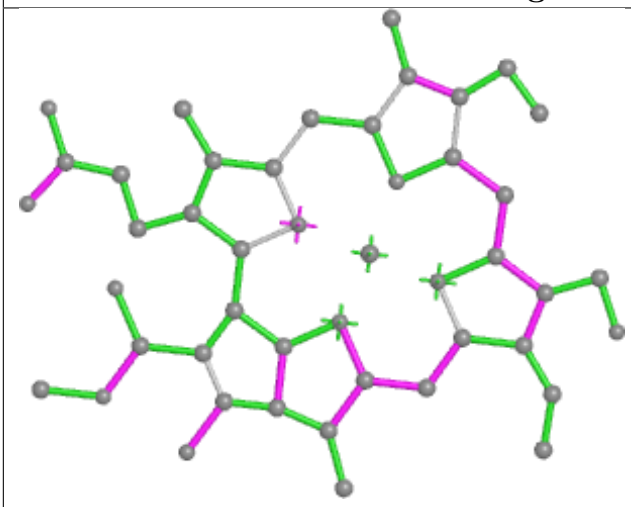

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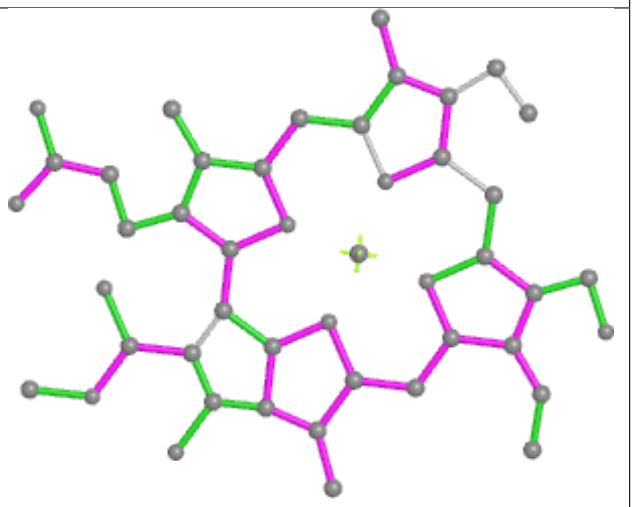

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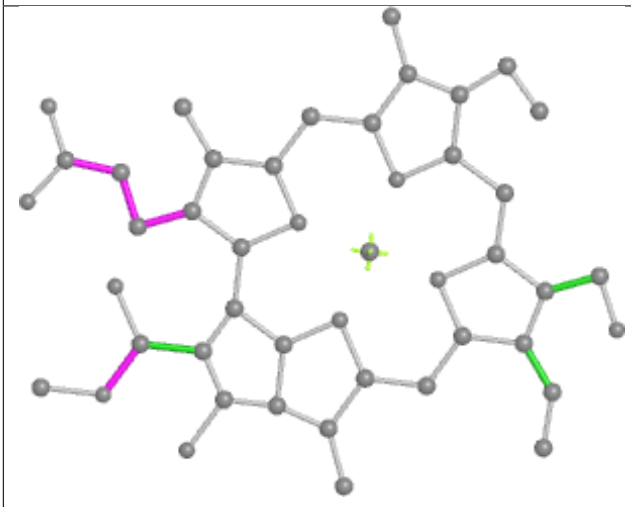

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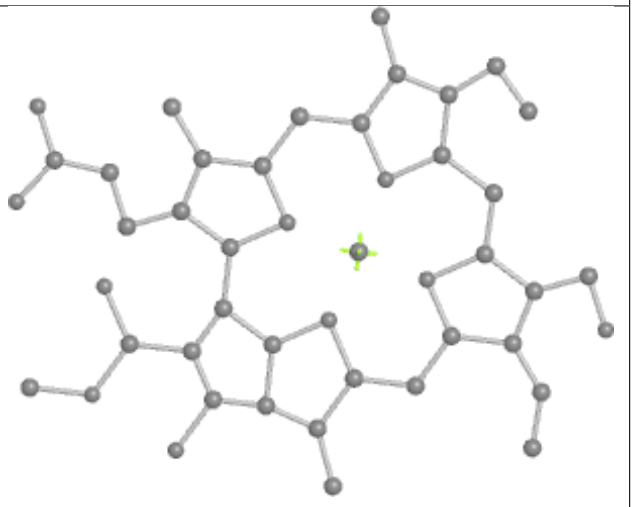

Rings

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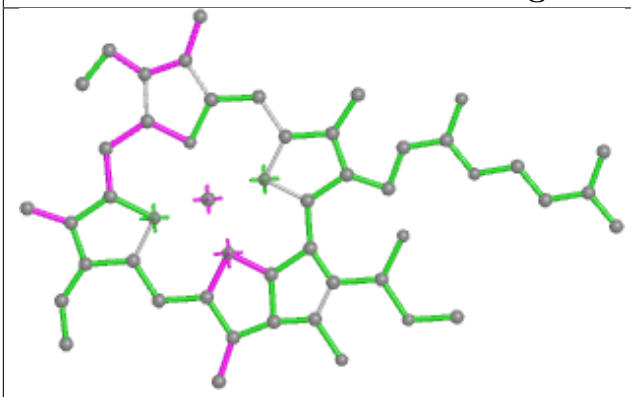

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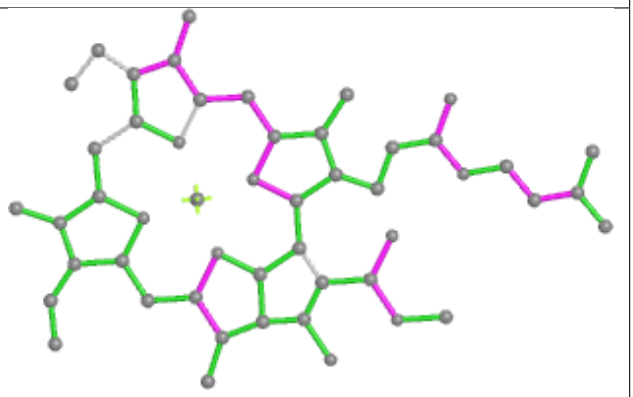
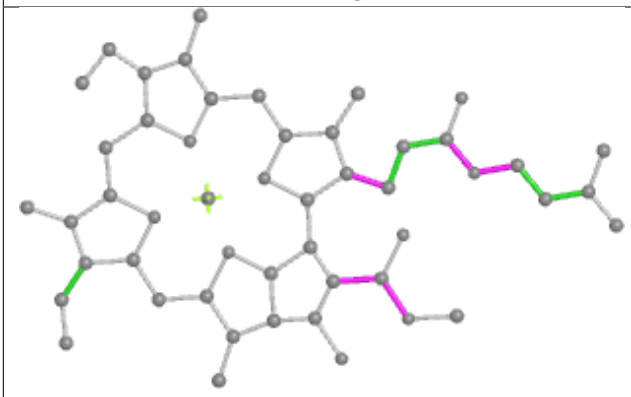


Bond angles



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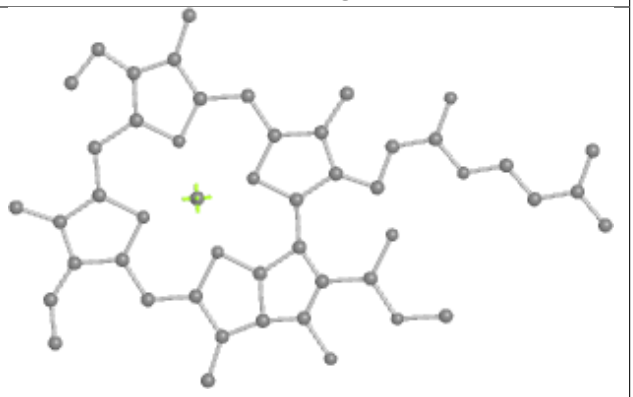

Rings

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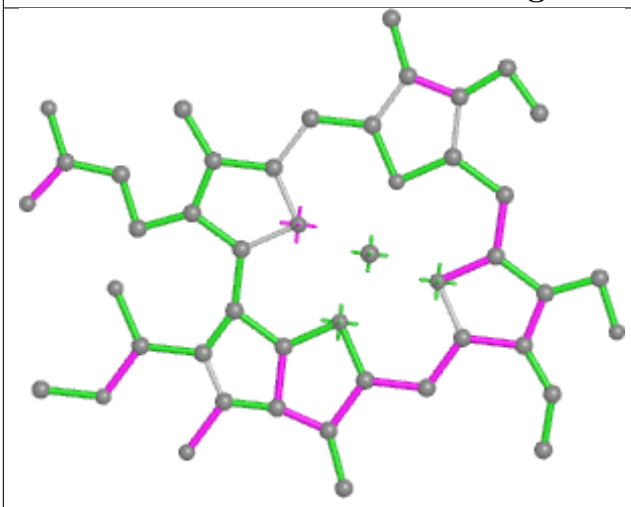

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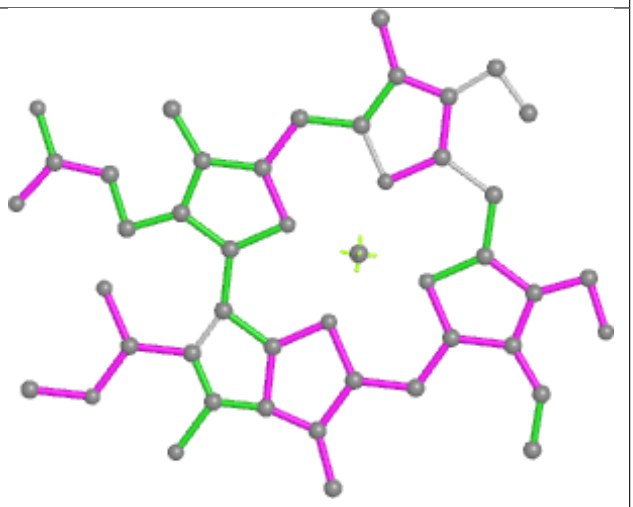
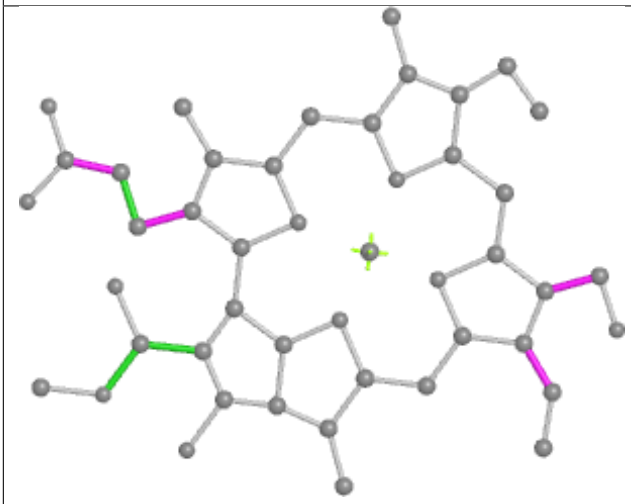


Bond angles



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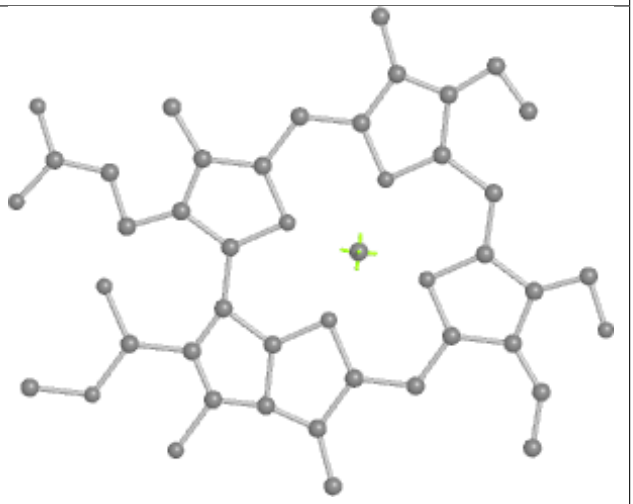

Rings

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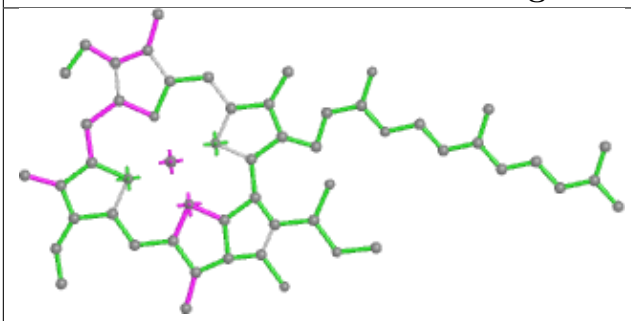

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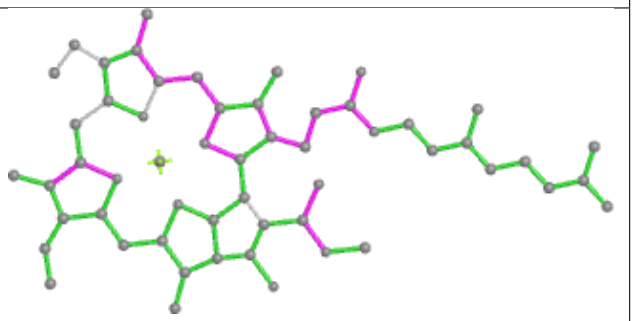
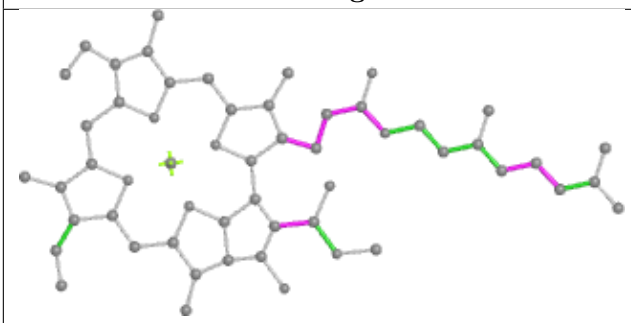
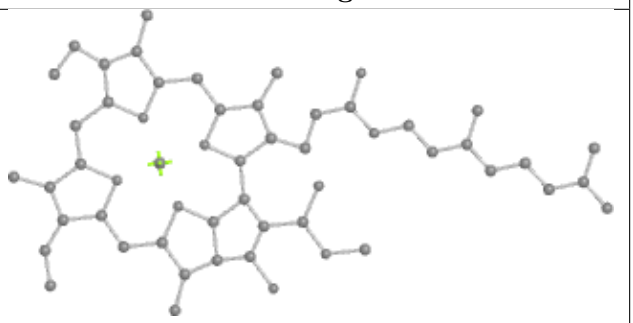


Bond angles

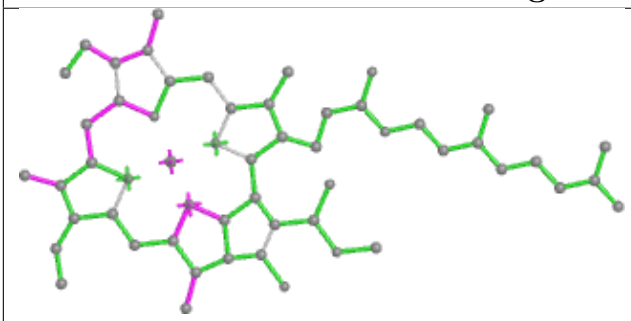


Torsions



Rings

Ligand CLA 6 603



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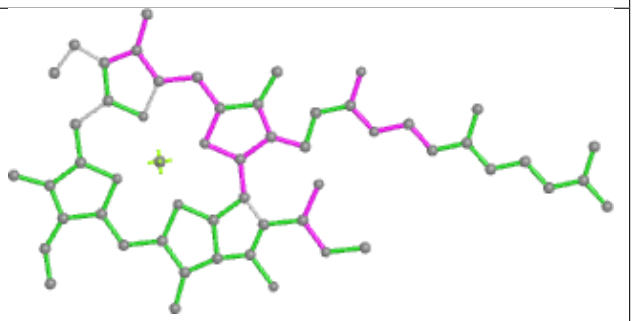

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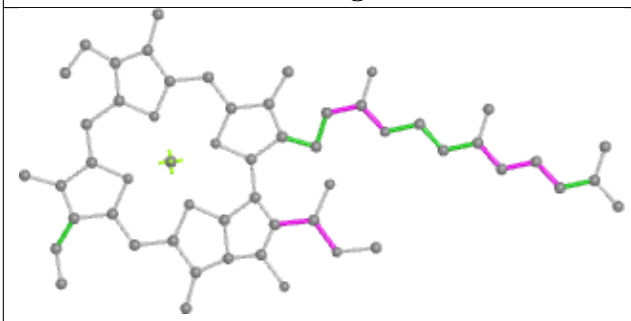

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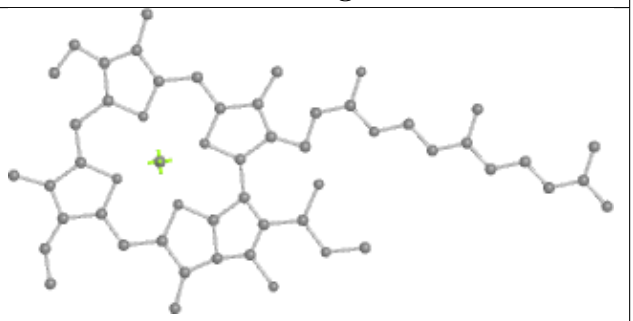
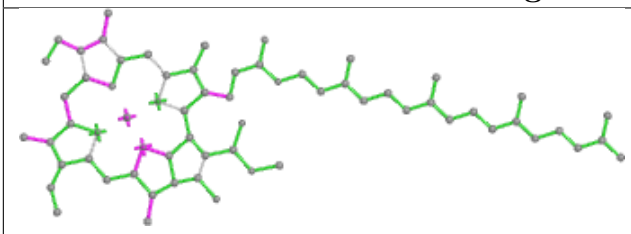


Rings

Ligand CLA B 614



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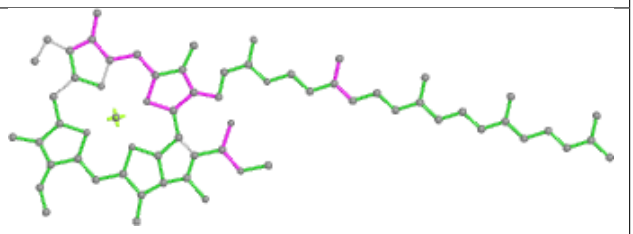

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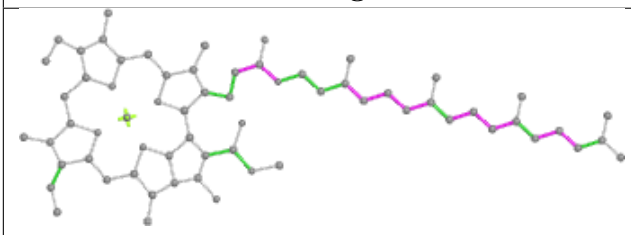

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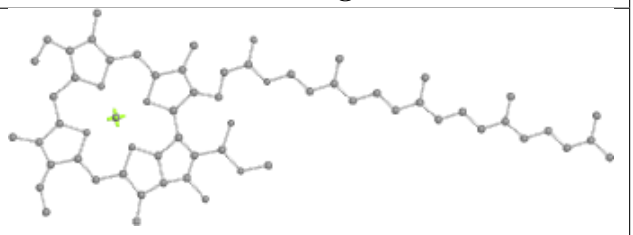
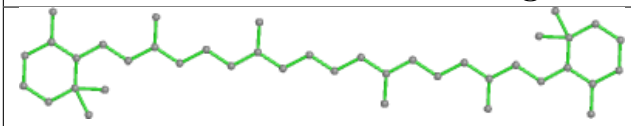


Rings

Ligand BCR D 404



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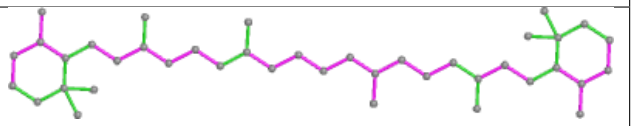

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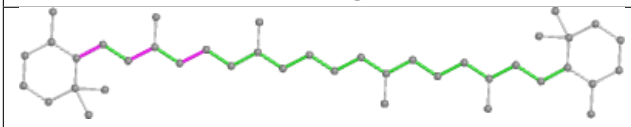
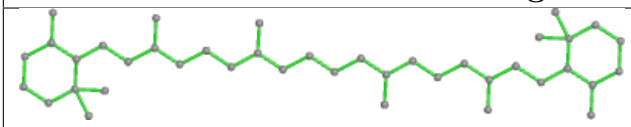


Torsions

Rings

Ligand BCR c 516



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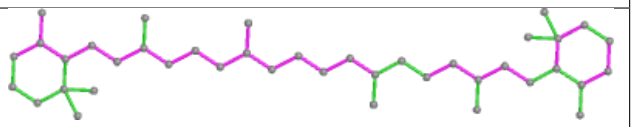

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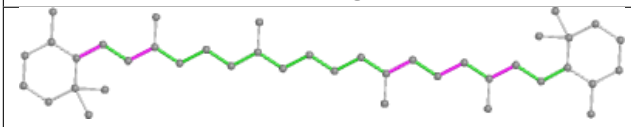
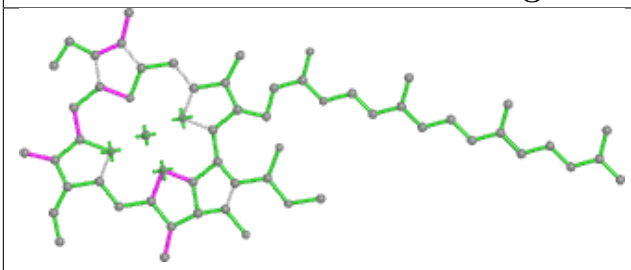


Torsions

Rings

Ligand CLA N 611



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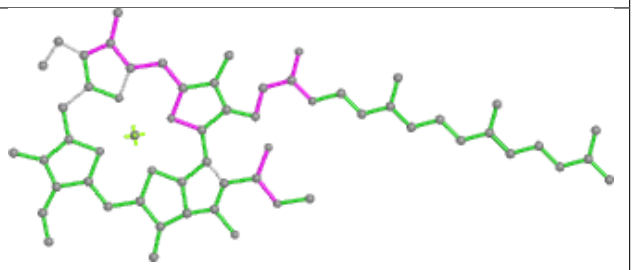

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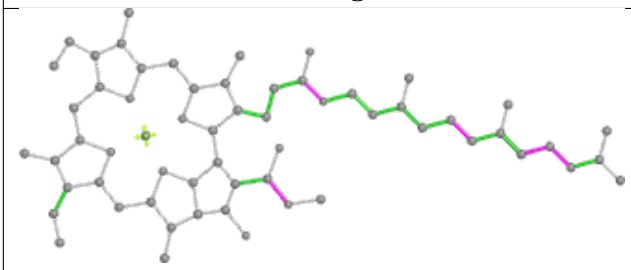

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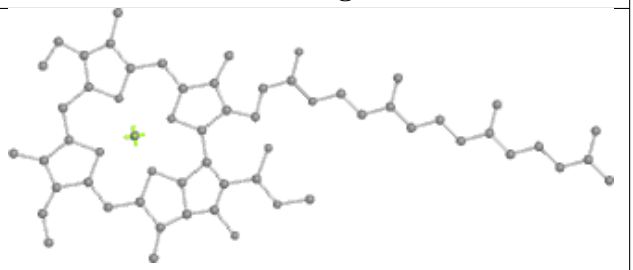
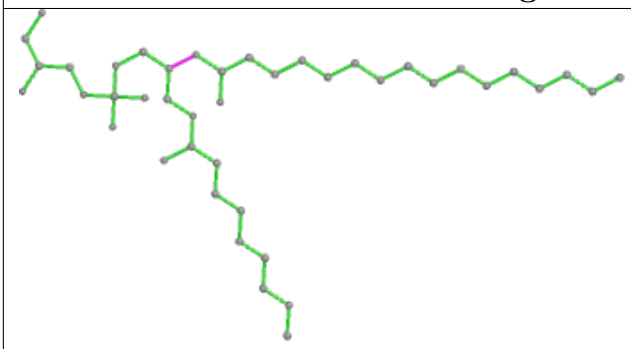


Rings

Ligand LHG r 2630



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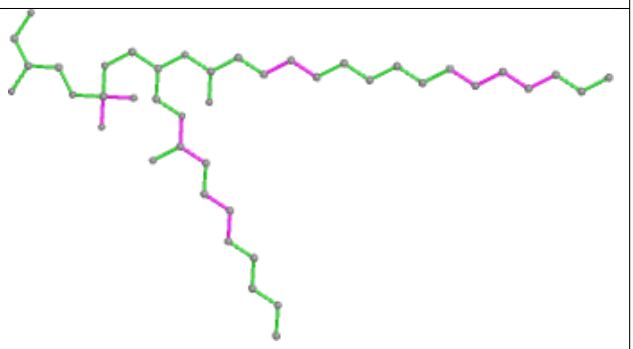

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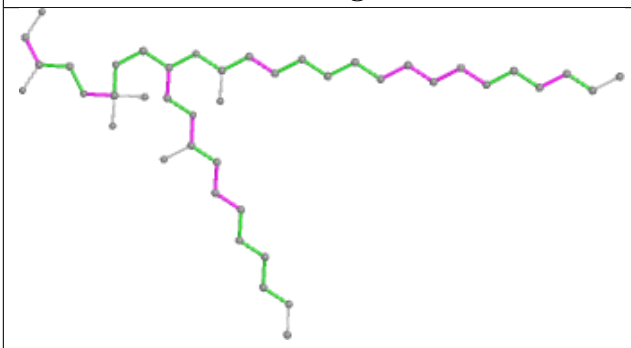

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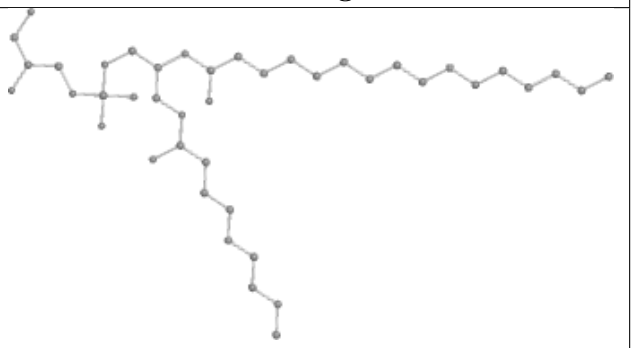

Rings

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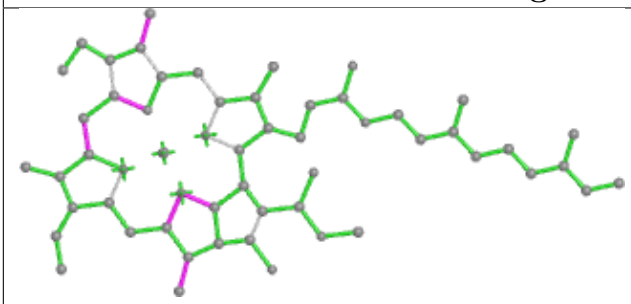

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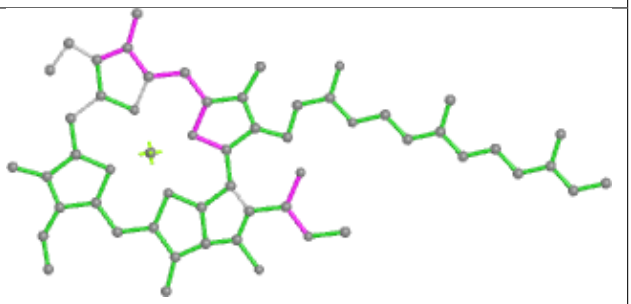

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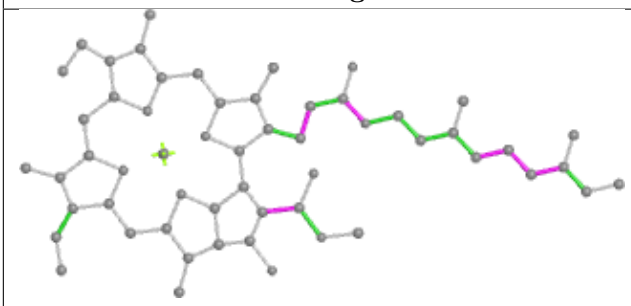

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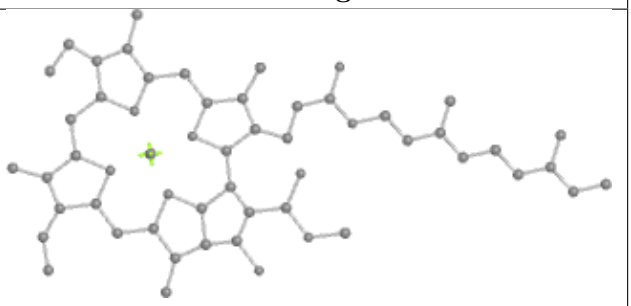
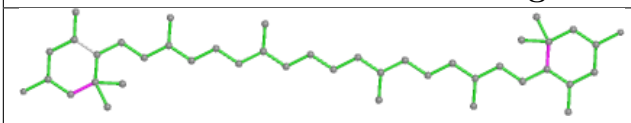


Rings

Ligand LUT 4 620



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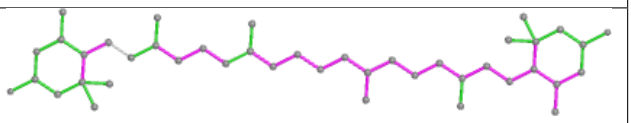

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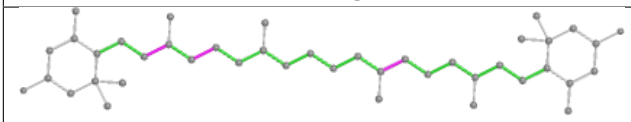

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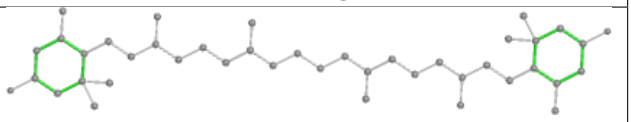

Rings

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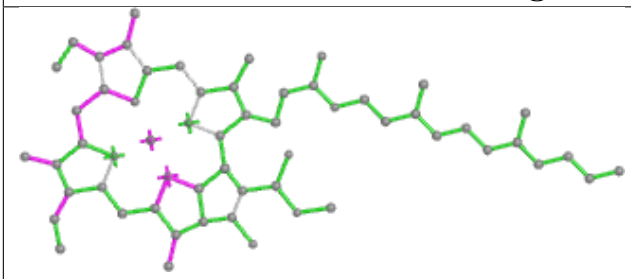

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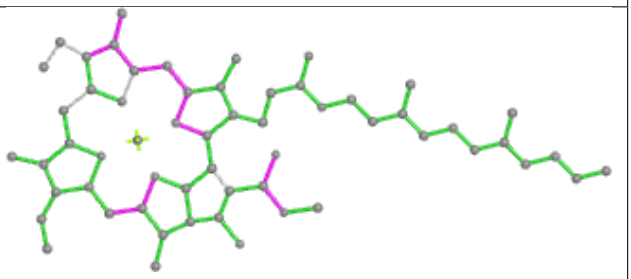

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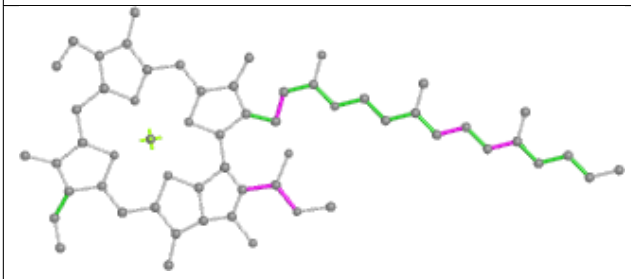

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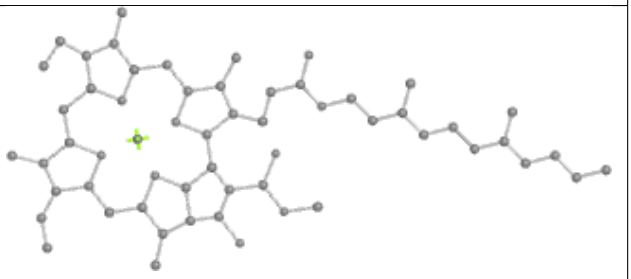
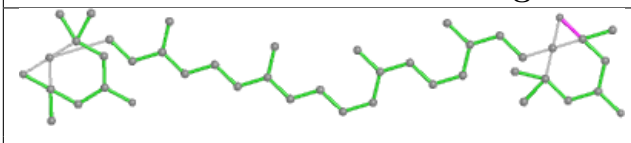


Rings

Ligand XAT N 1622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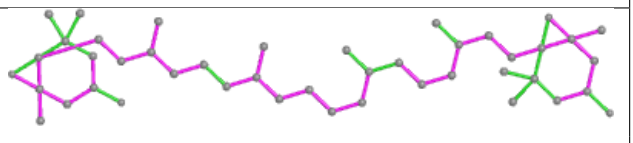
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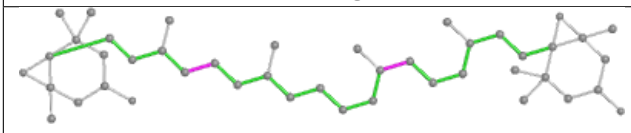
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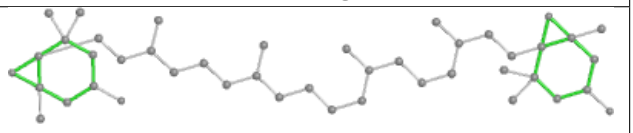
Rings

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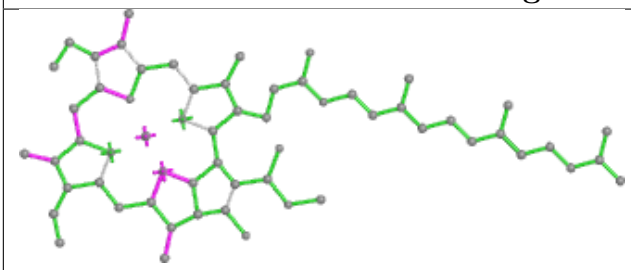
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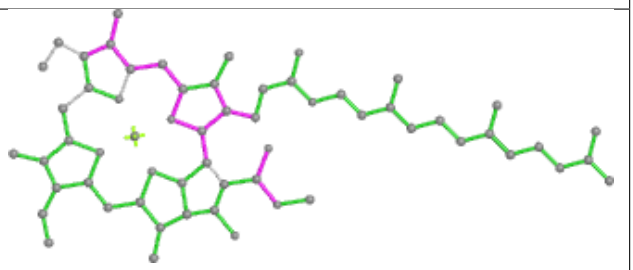
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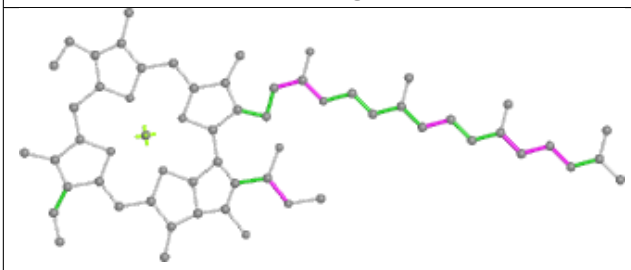
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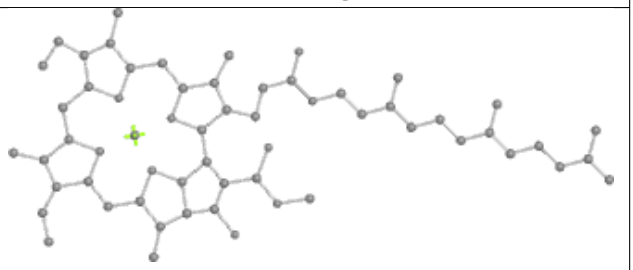
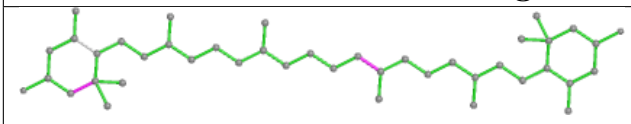

Rings

Ligand LUT N 1620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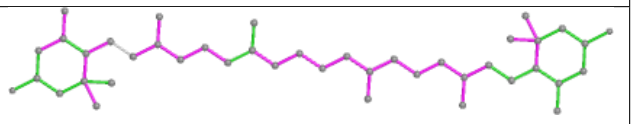
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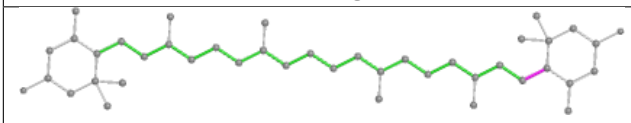
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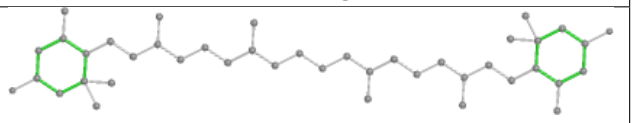
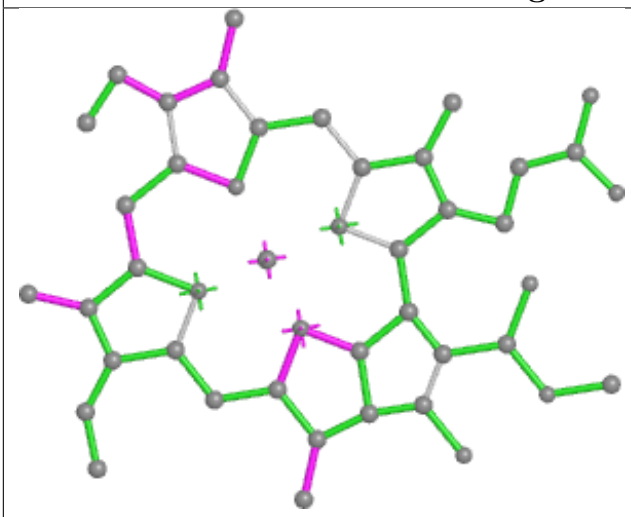

Rings

Ligand CLA 2 613



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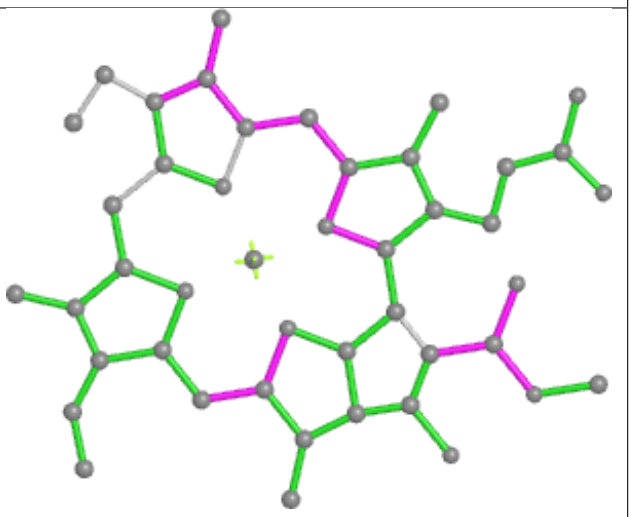

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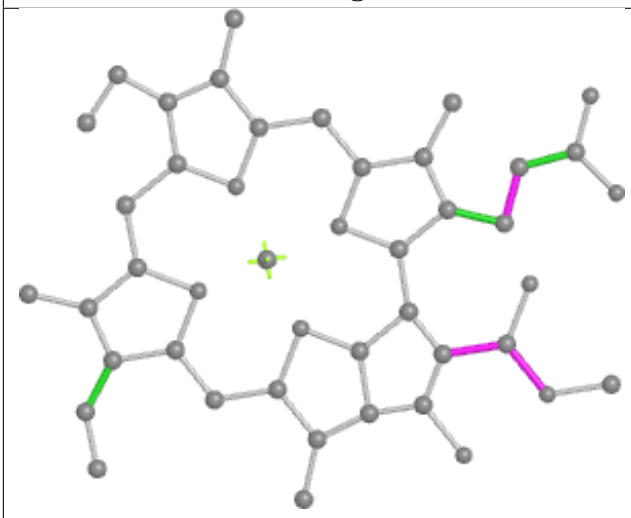

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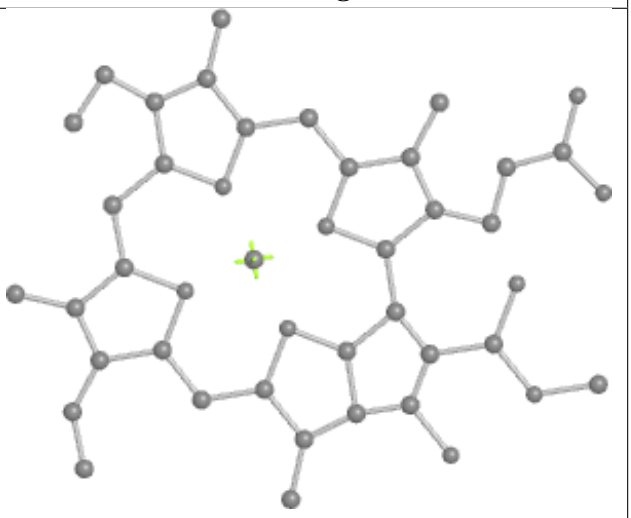

Rings

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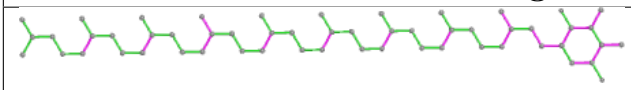

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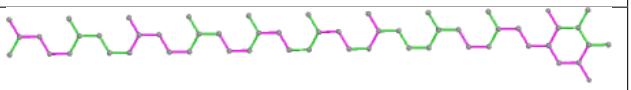

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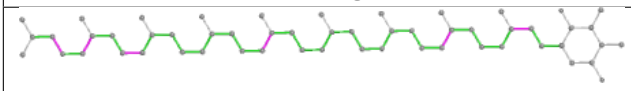
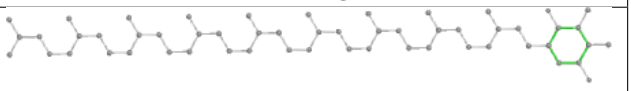
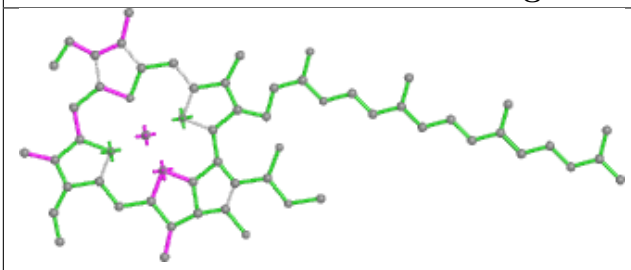


Torsions



Rings

Ligand CLA R 603



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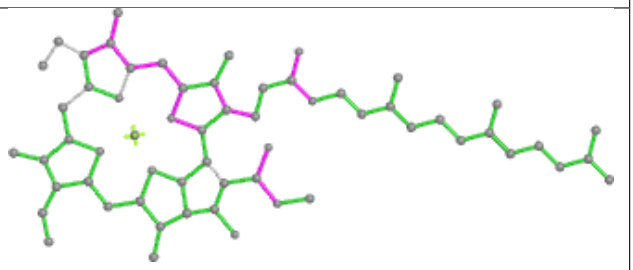
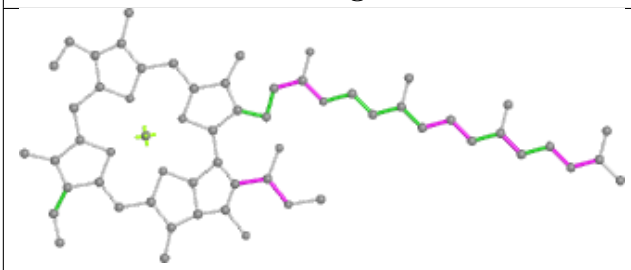
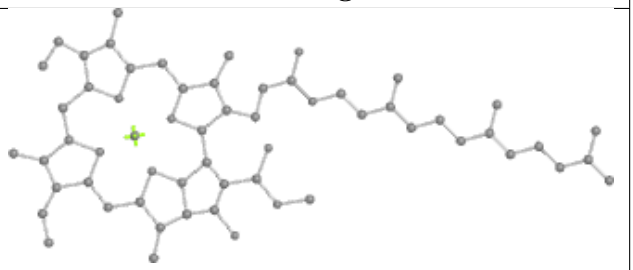


Bond angles

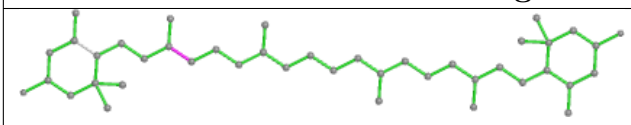


Torsions



Rings

Ligand LUT G 1620



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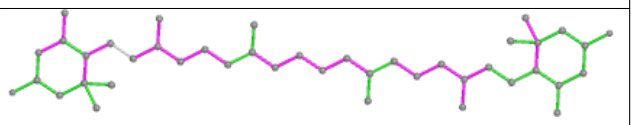

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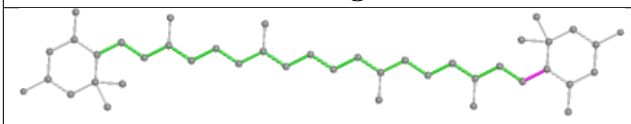

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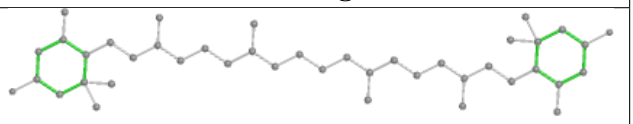
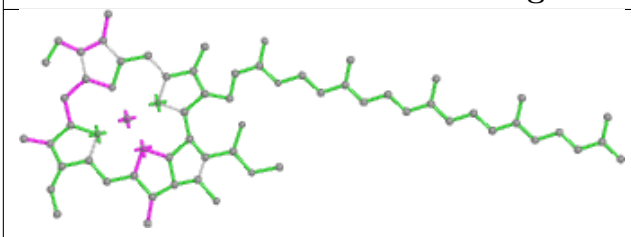


Rings

Ligand CLA b 607



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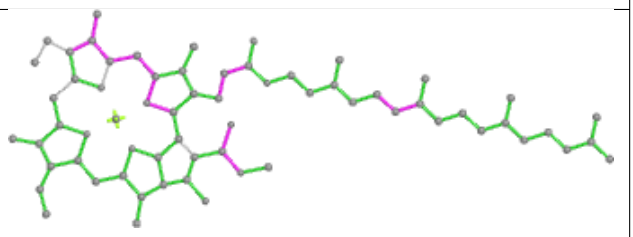

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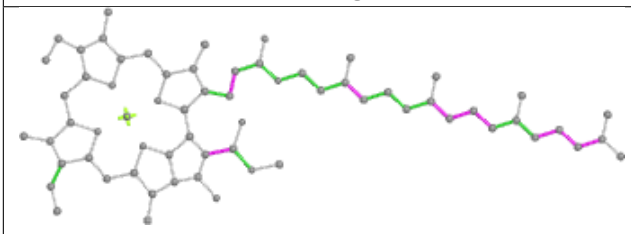

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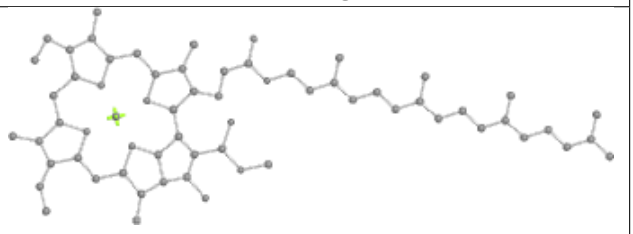
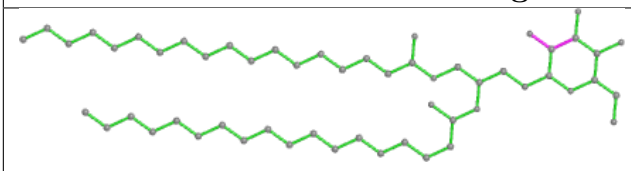


Rings

Ligand LMG B 2633



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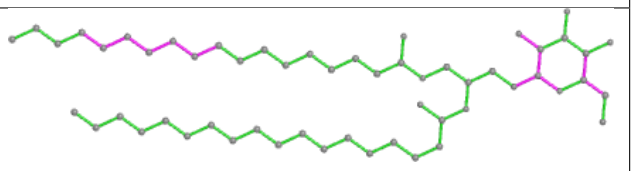
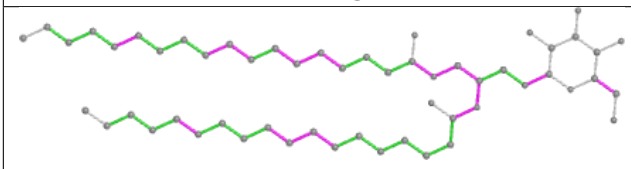


Bond angles



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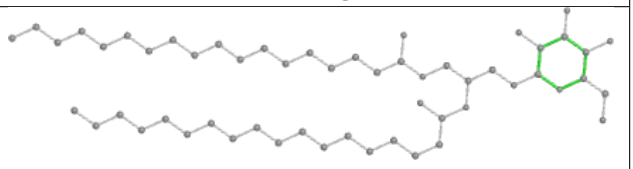
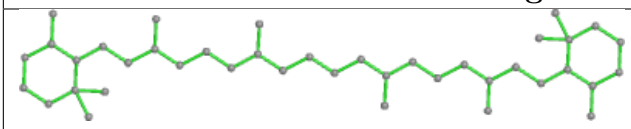


Rings

Ligand BCR d 404



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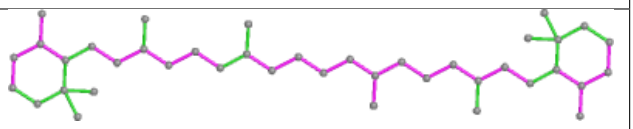

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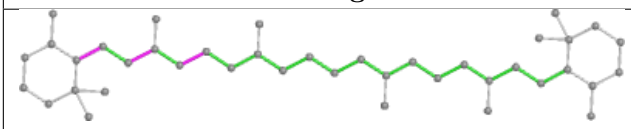

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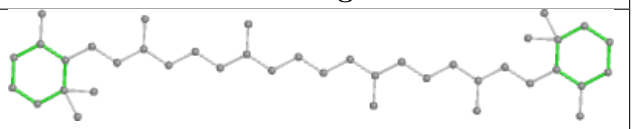
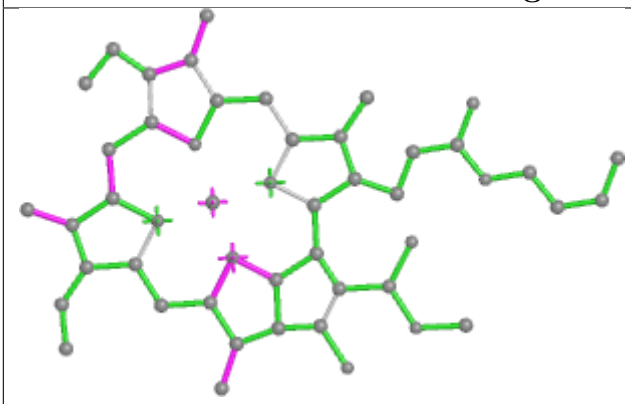


Rings

Ligand CLA R 612



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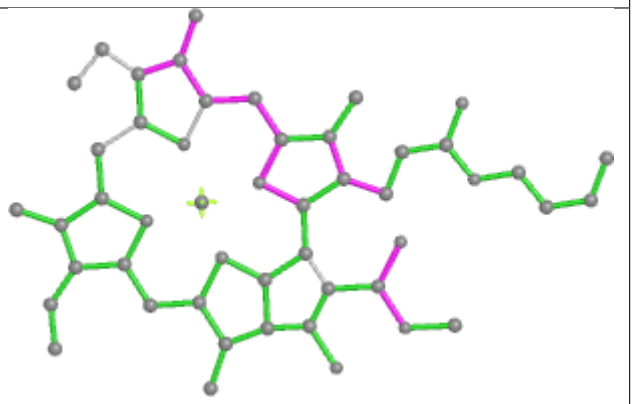
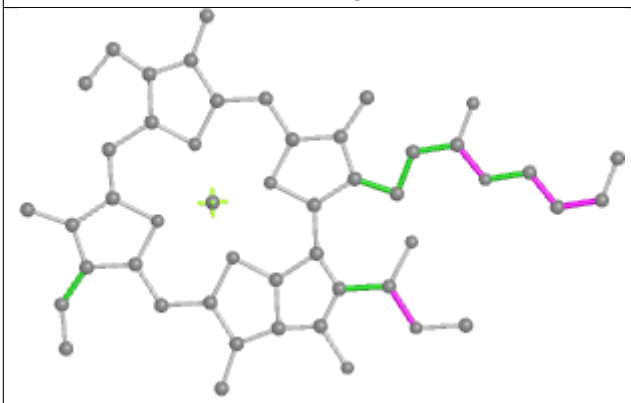


Bond angles



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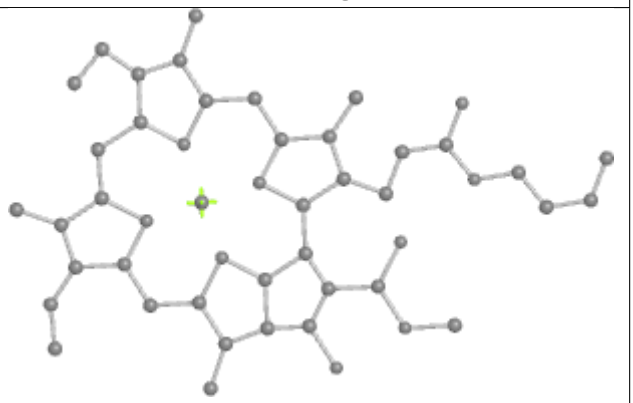
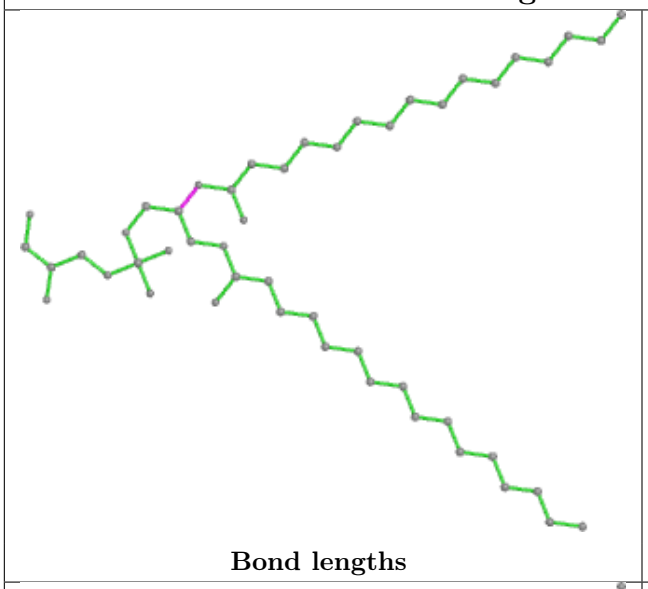


Rings

Ligand LHG g 2630



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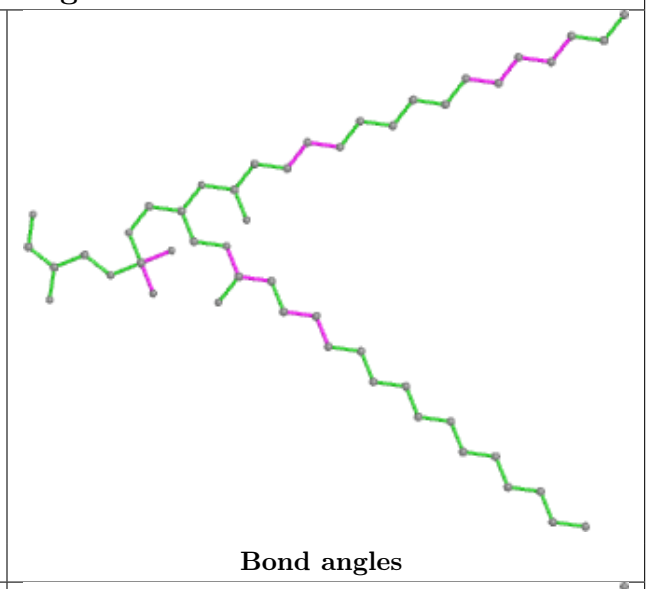

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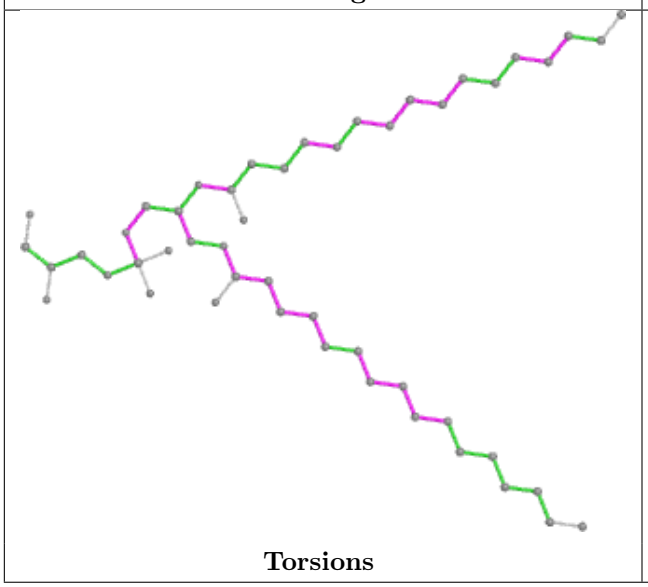

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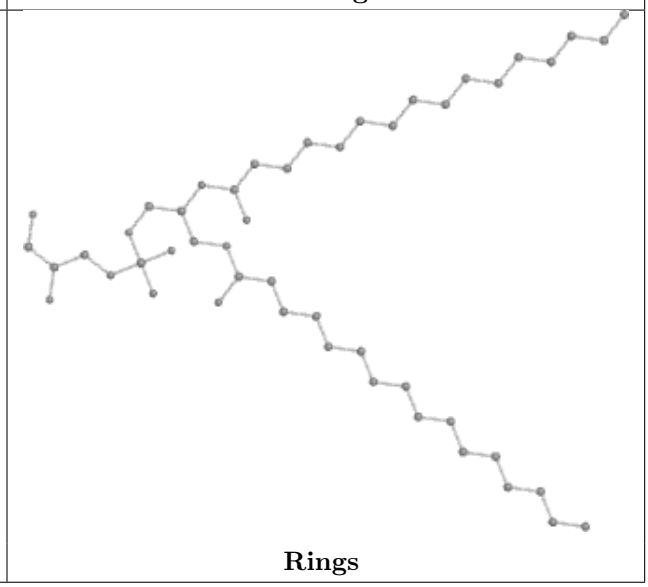
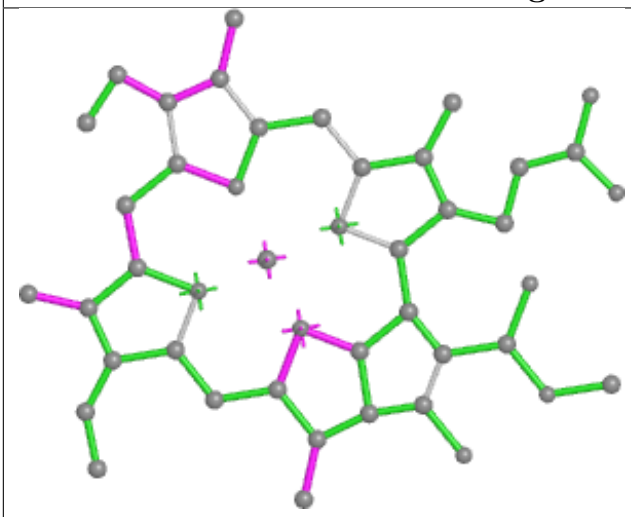


Rings

Ligand CLA 6 613



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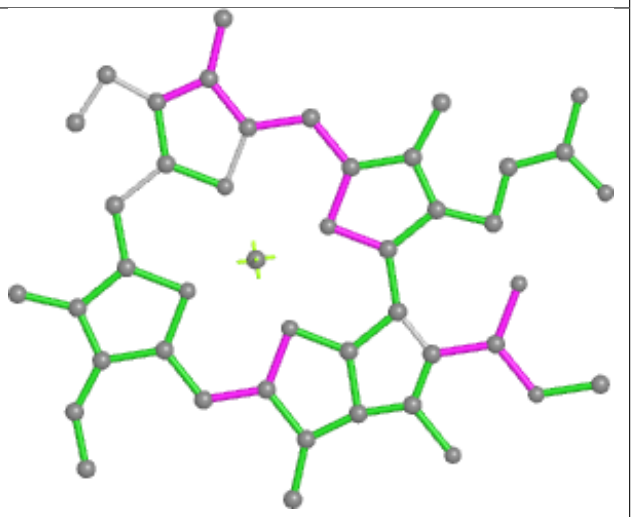
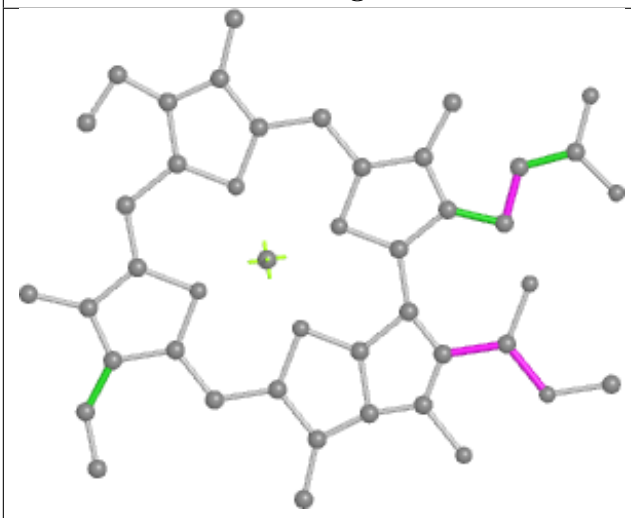


Bond angles



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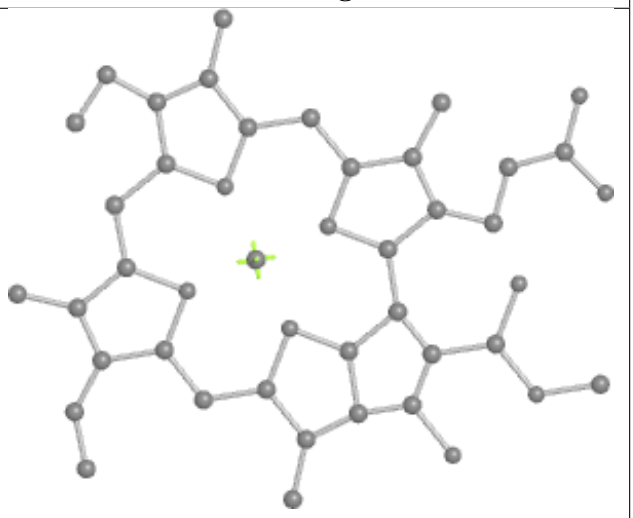
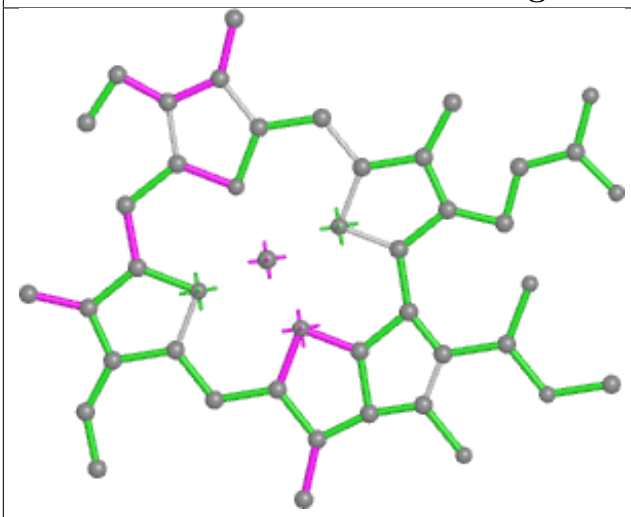


Rings

Ligand CLA 4 610



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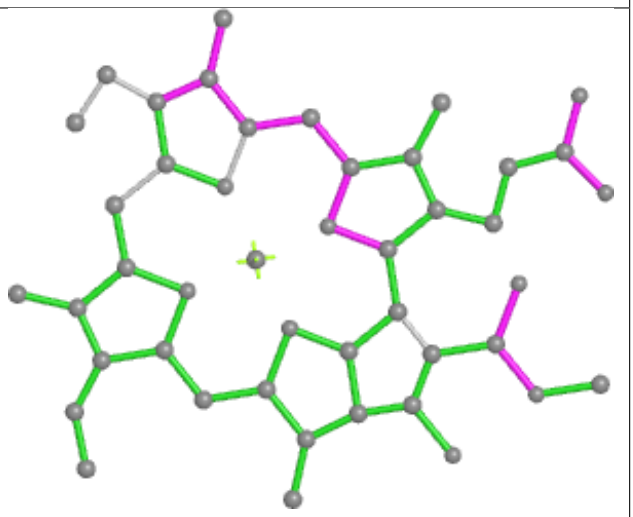

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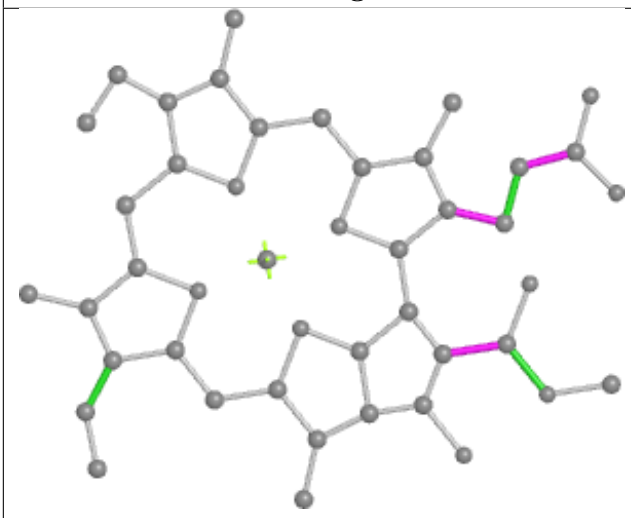

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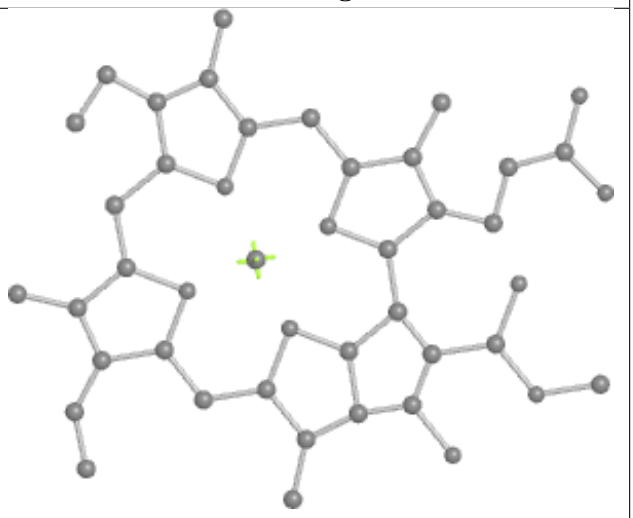
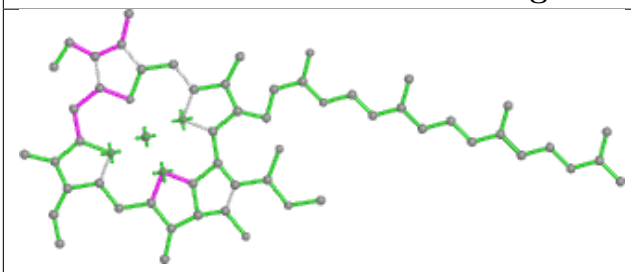


Rings

Ligand CLA r 613



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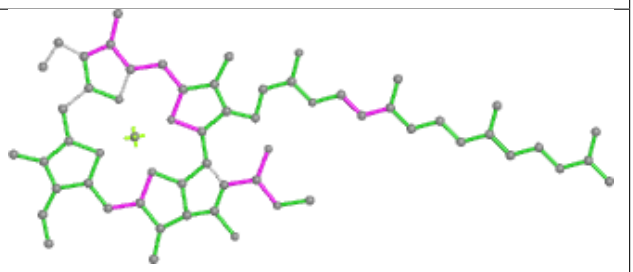

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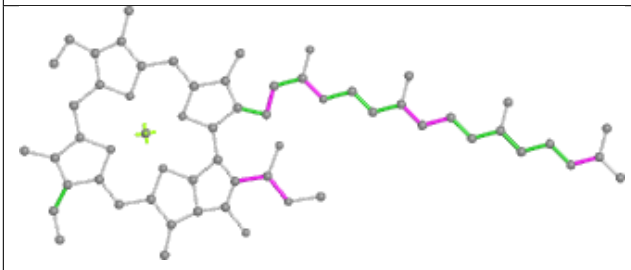

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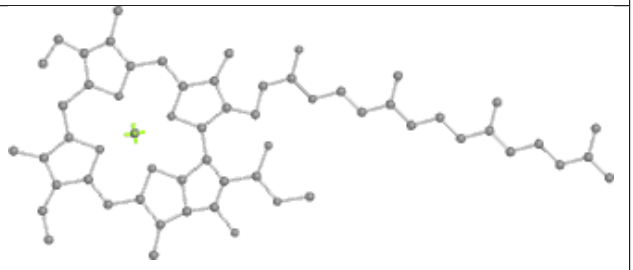
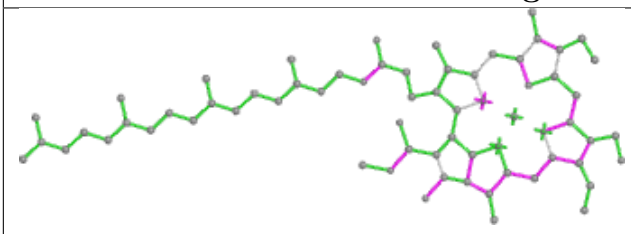


Rings

Ligand CHL N 609



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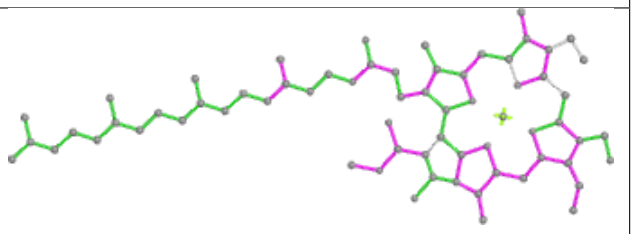

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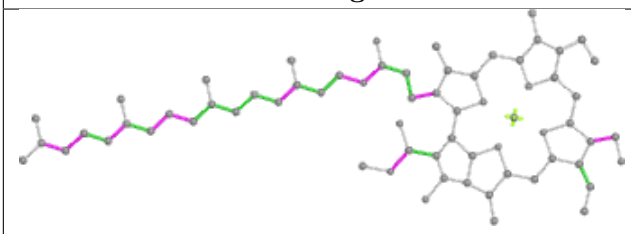

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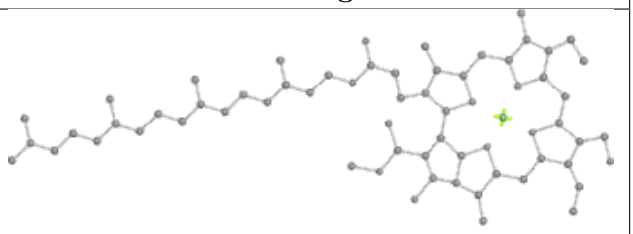
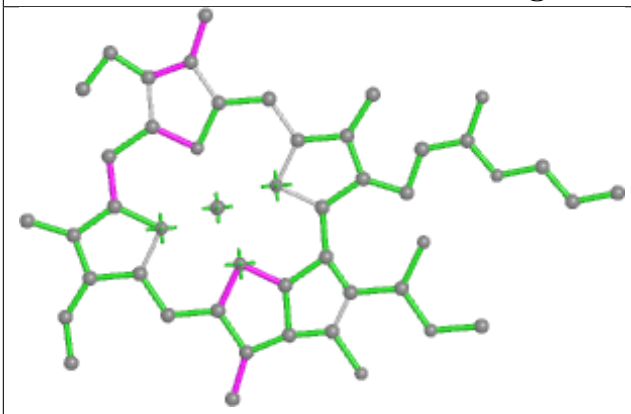


Rings

Ligand CLA 3 614



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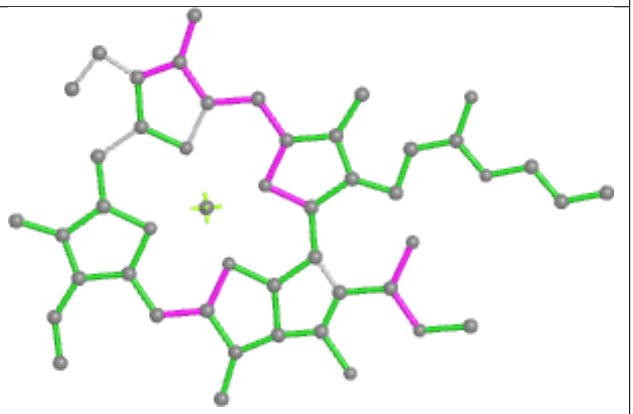
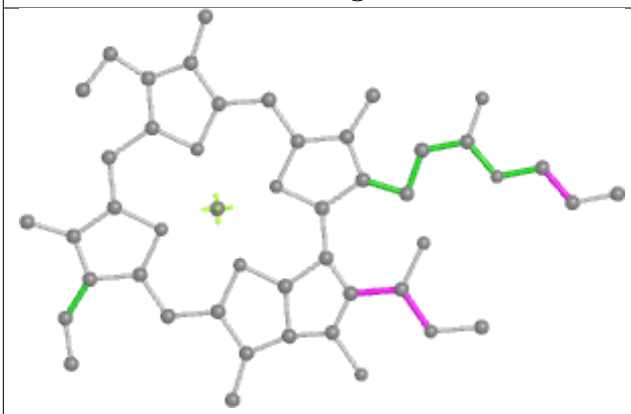


Bond angles



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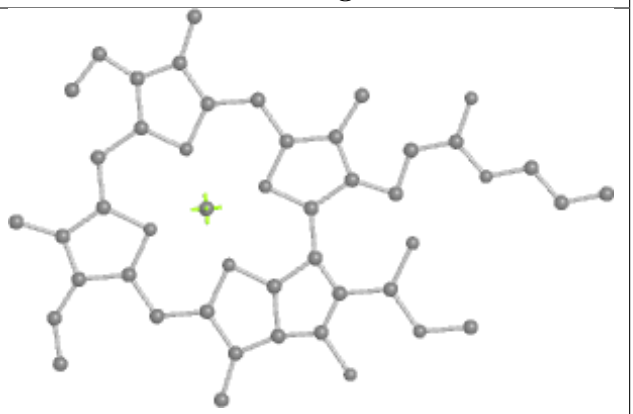
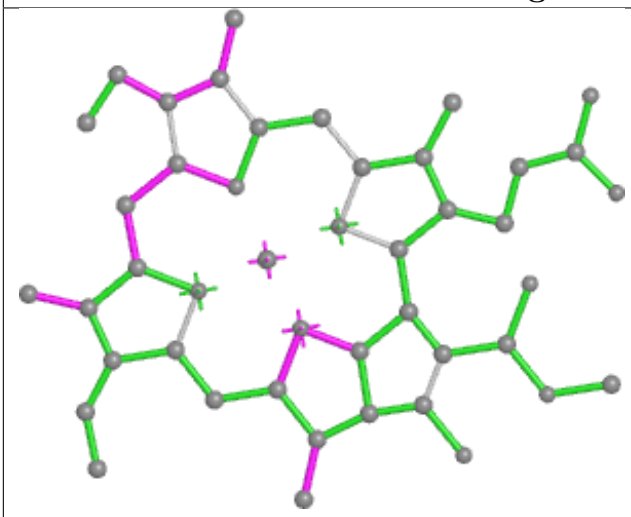


Rings

Ligand CLA 4 604



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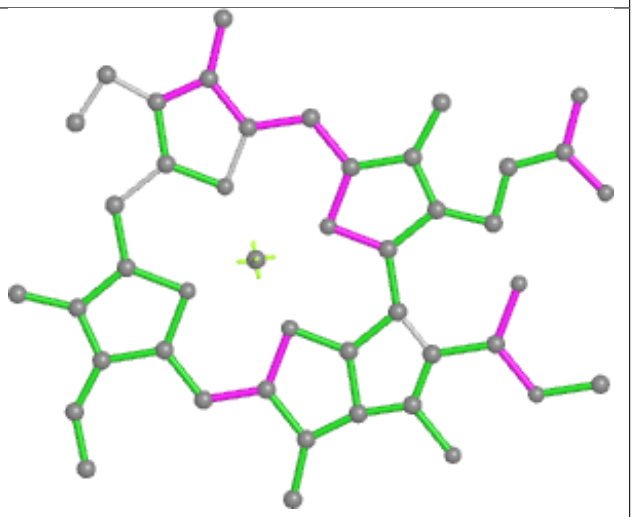
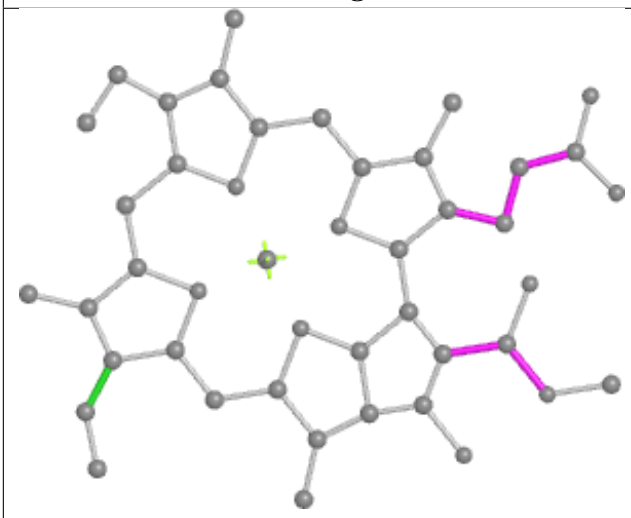


Bond angles



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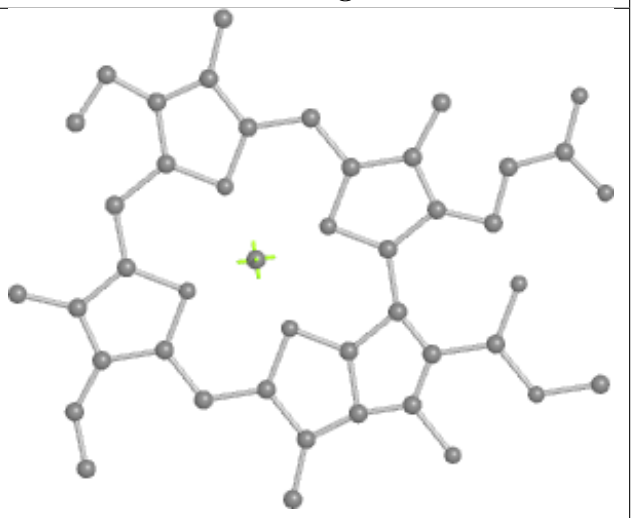
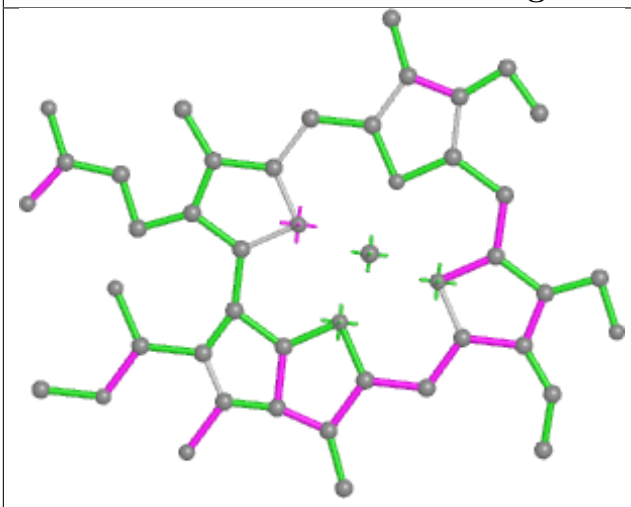
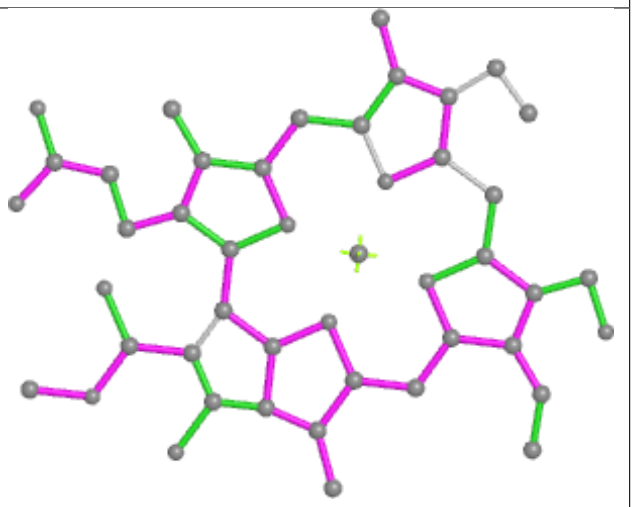


Rings

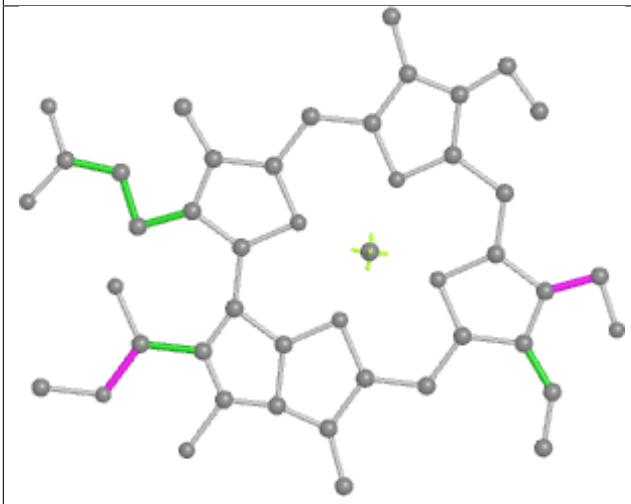
Ligand CHL 2 606



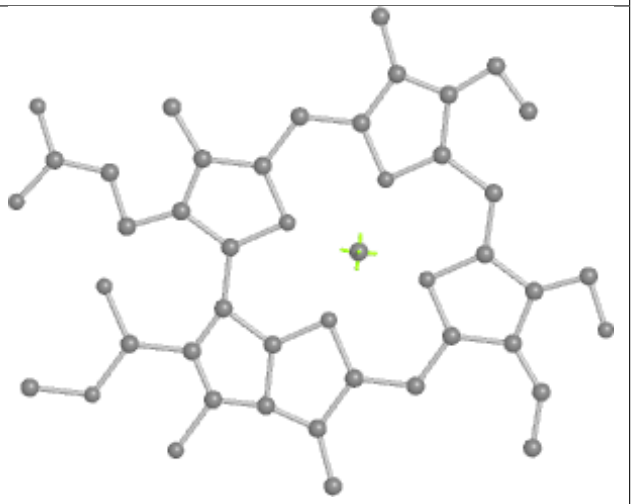
Bond lengths



Bond angles

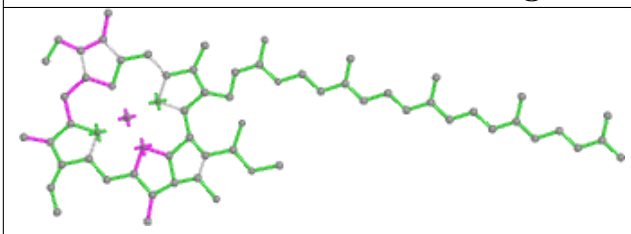


Torsions



Rings

Ligand CLA G 613



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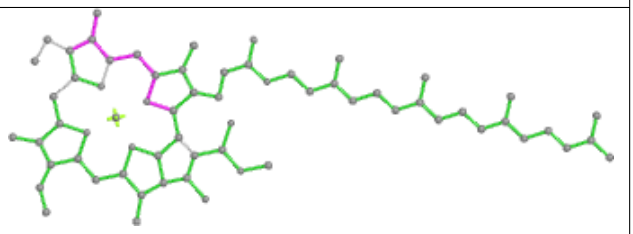

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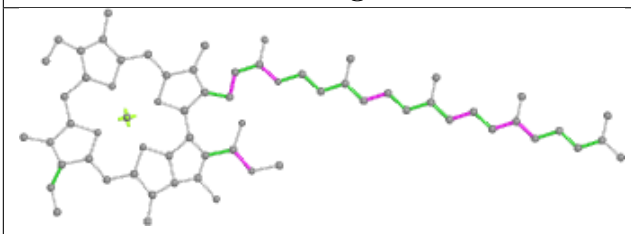

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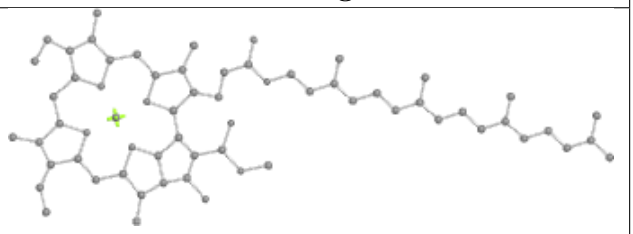
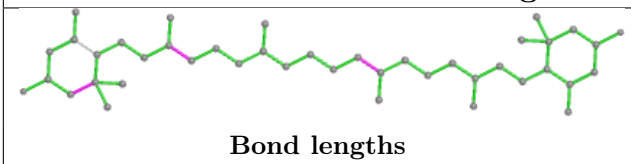


Rings

Ligand LUT 3 1620



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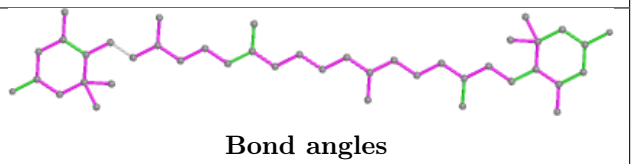

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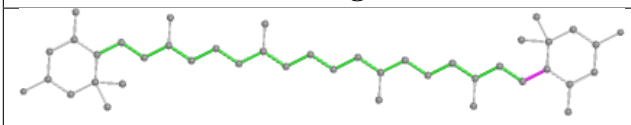

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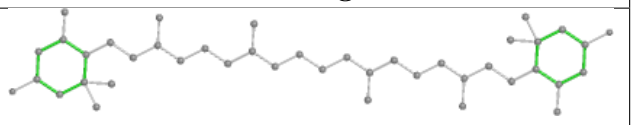
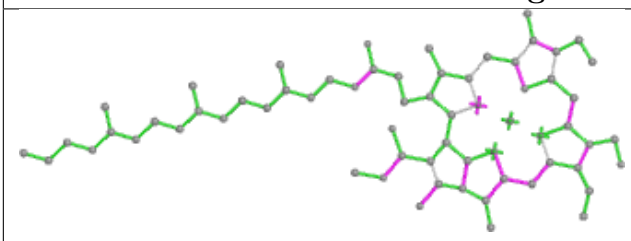


Rings

Ligand CHL 3 601



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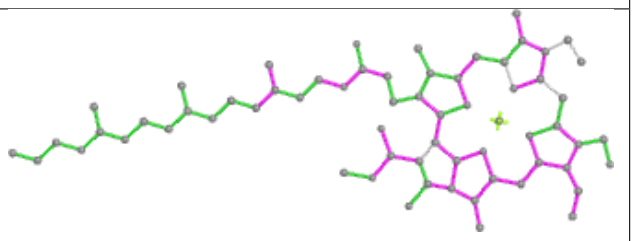
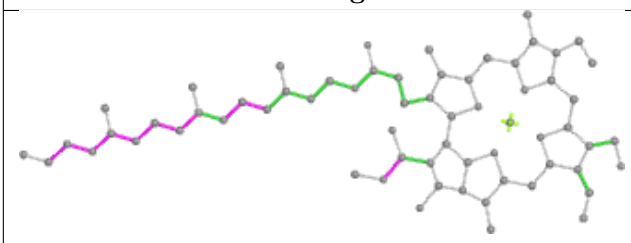


Bond angles



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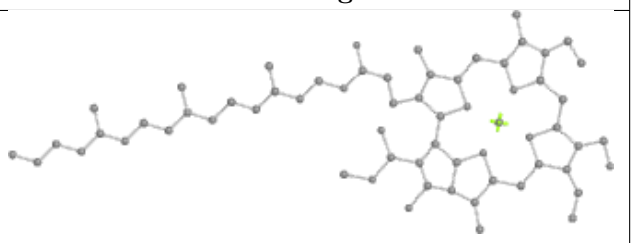
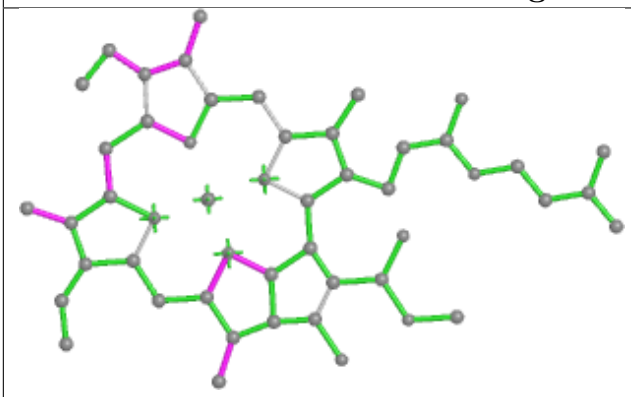


Rings

Ligand CLA 6 610



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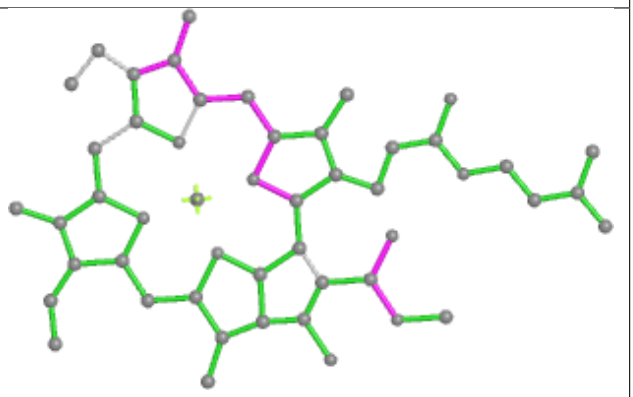

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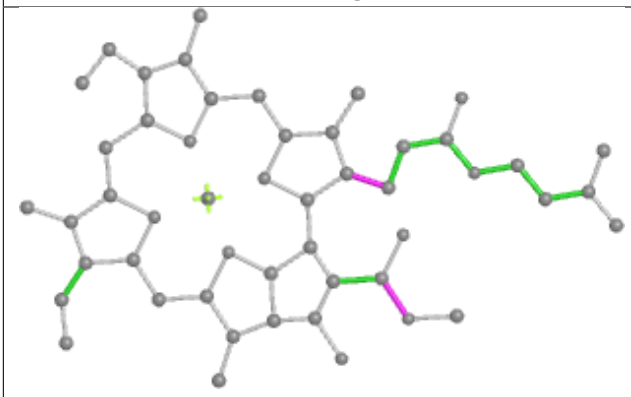

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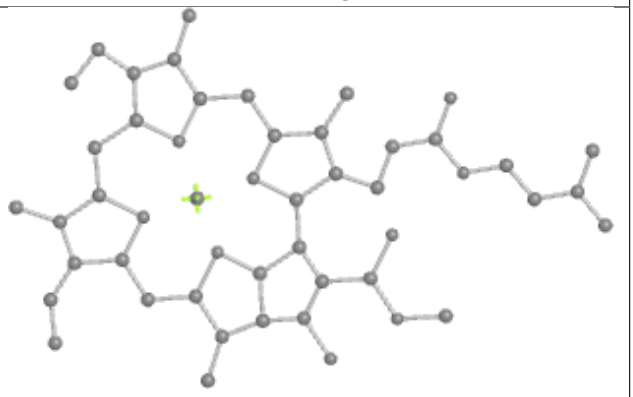

Rings

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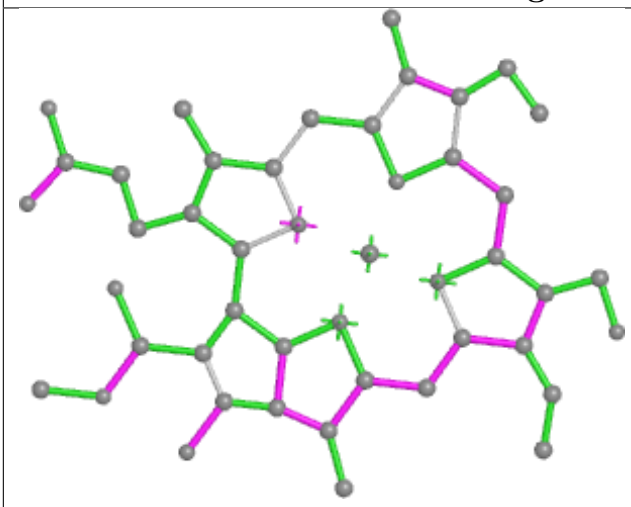

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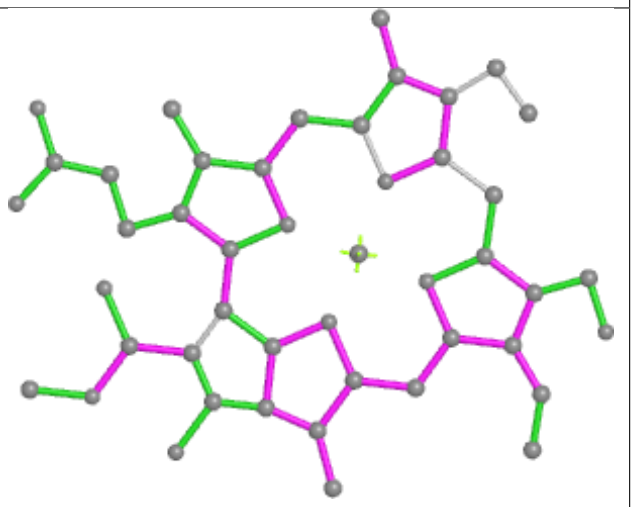
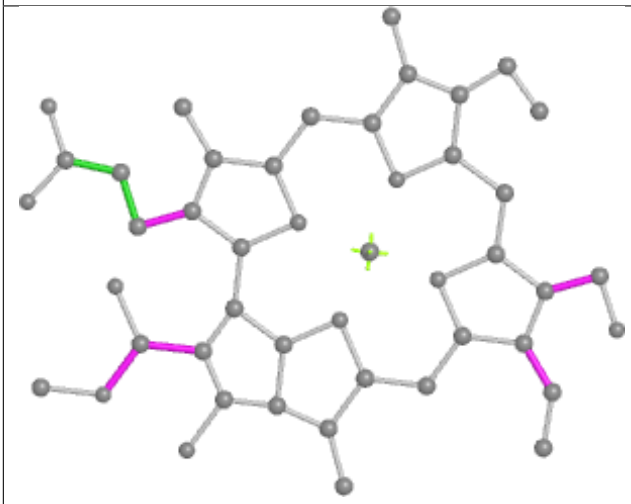


Bond angles



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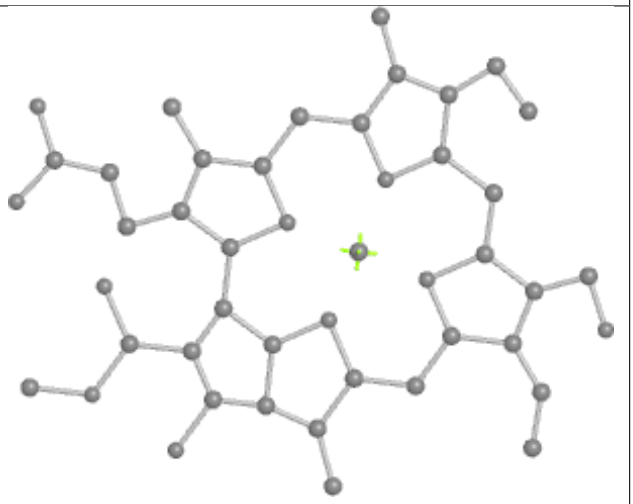
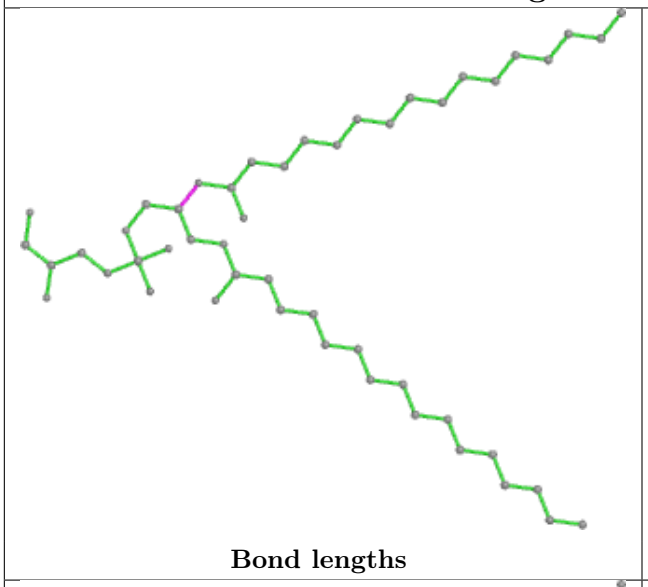


Rings

Ligand LHG c 523



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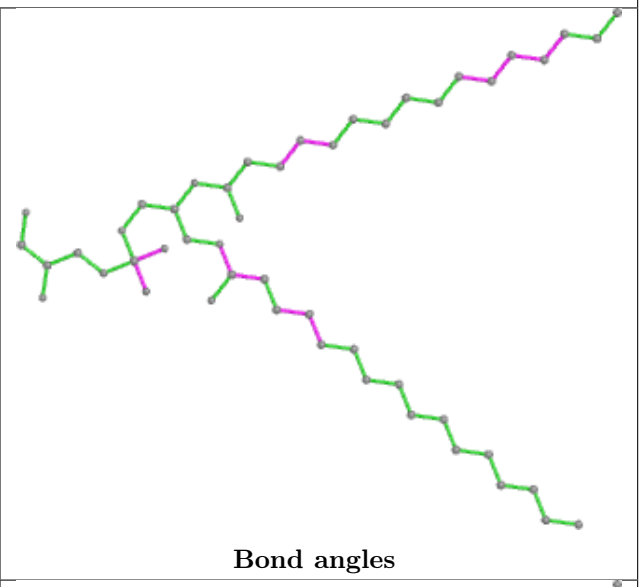

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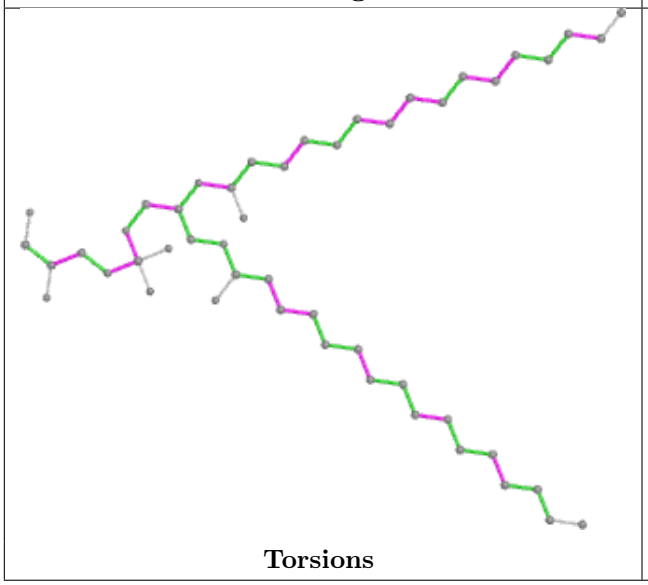

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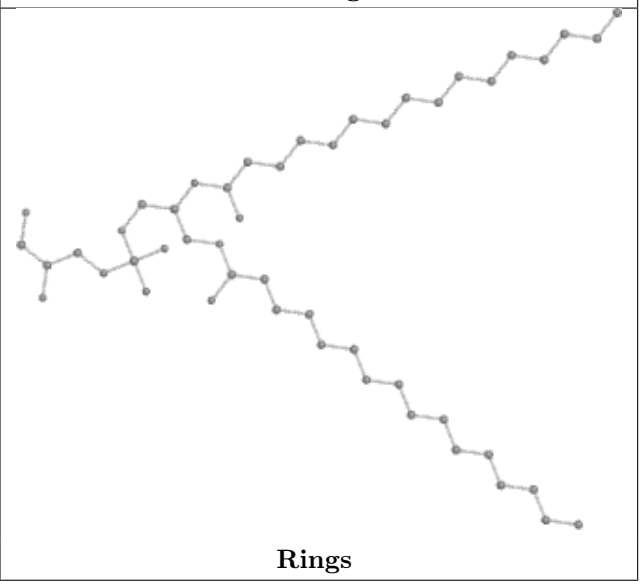

Rings

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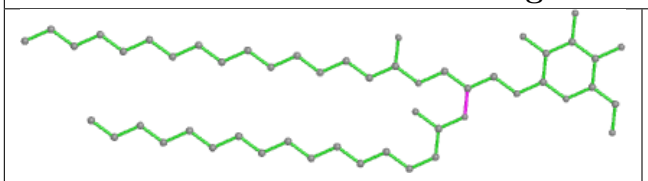

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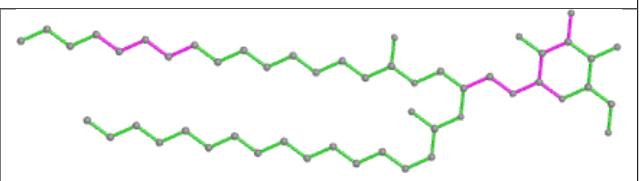

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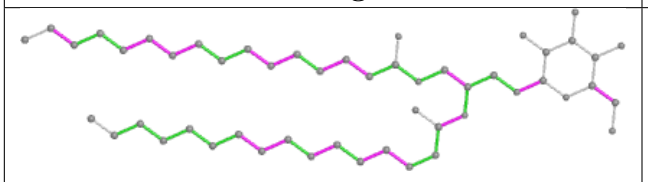

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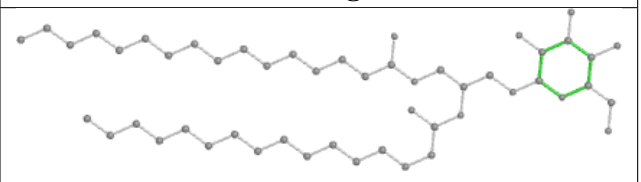
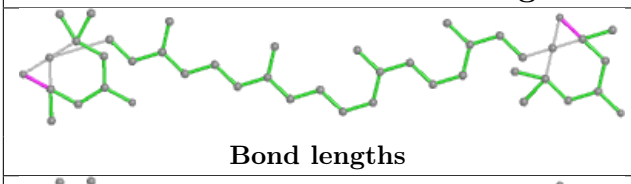


Rings

Ligand XAT 5 1622



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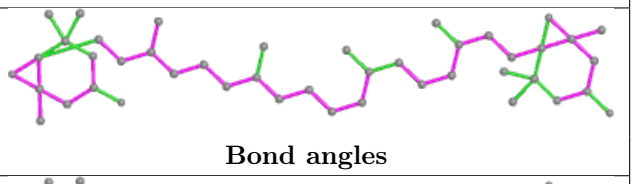
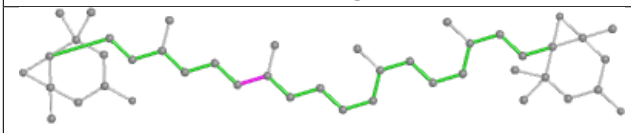


Bond angles



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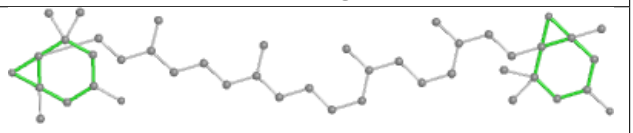
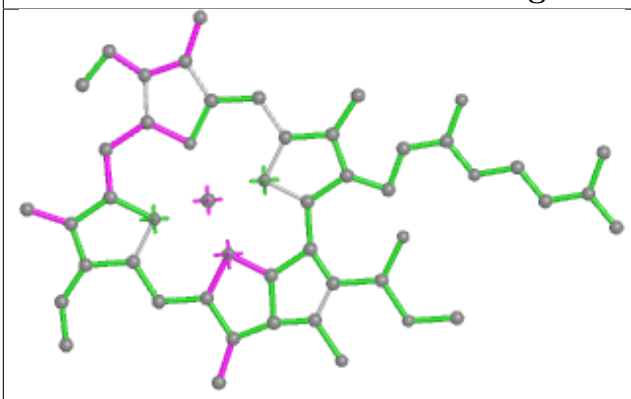


Rings

Ligand CLA 5 604



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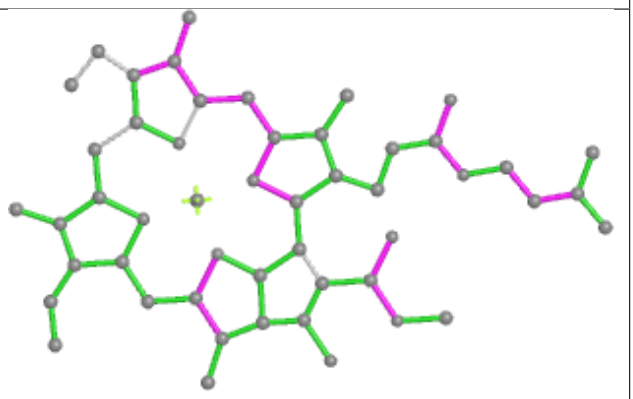

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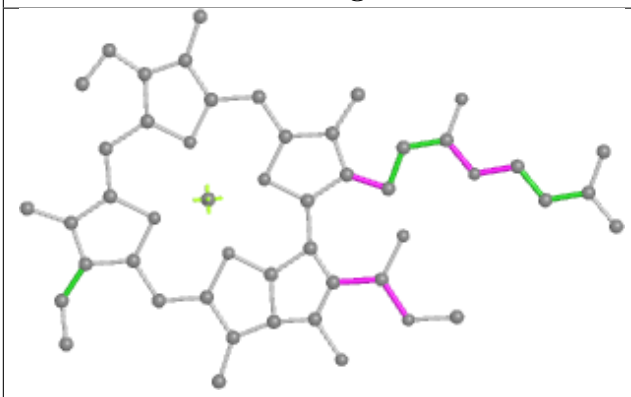

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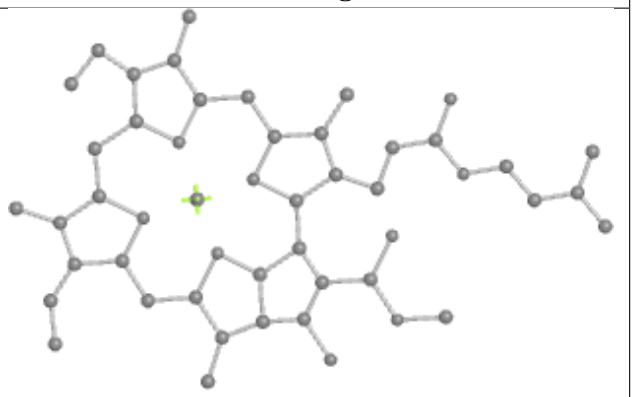
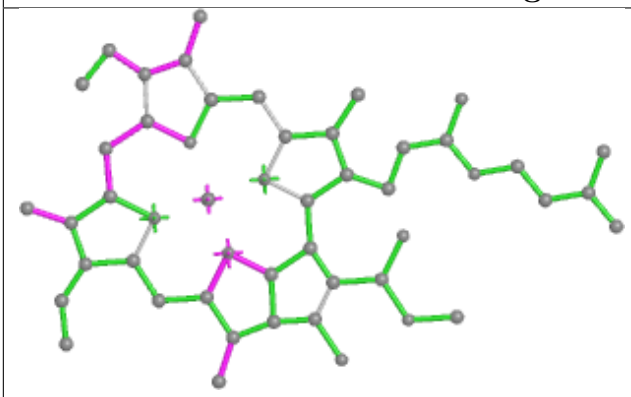


Rings

Ligand CLA A 407



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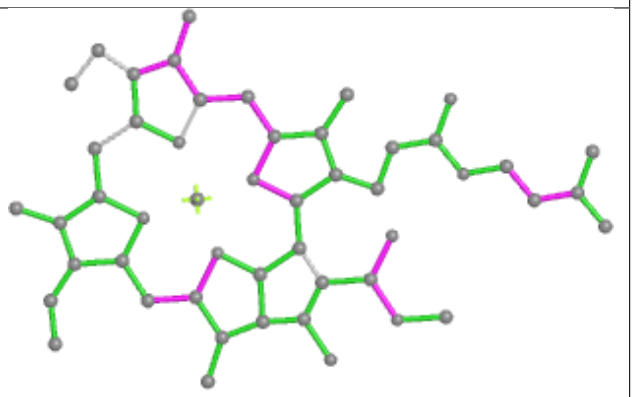
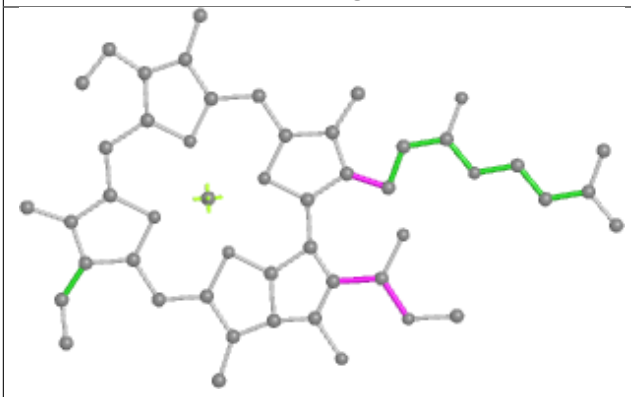


Bond angles



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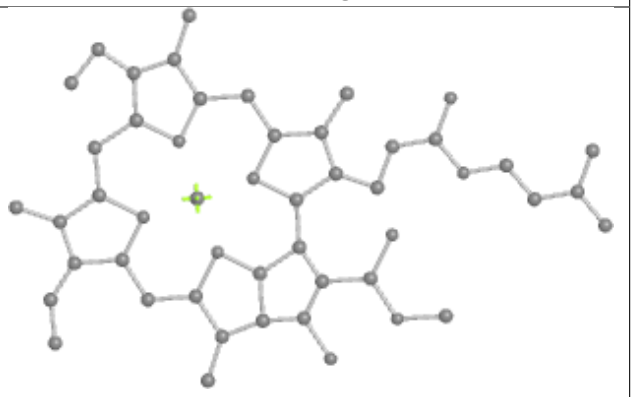
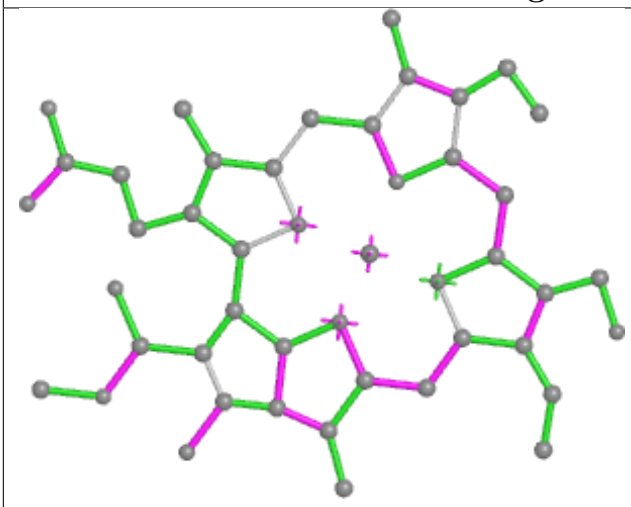


Rings

Ligand CHL 5 606



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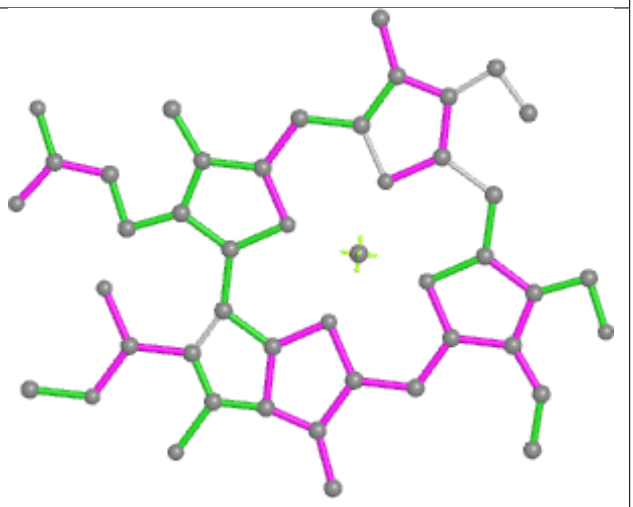
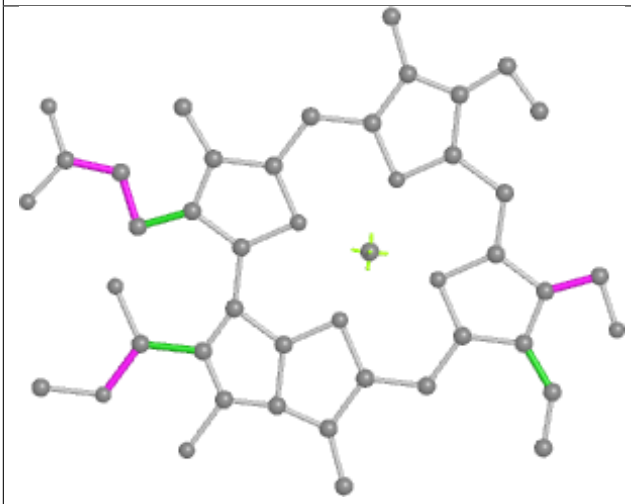


Bond angles



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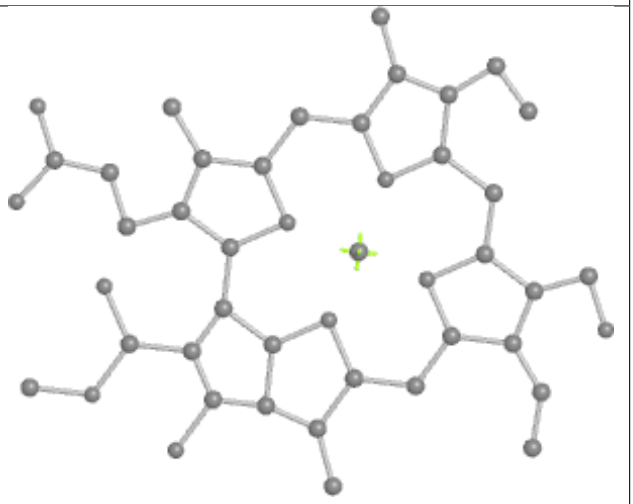
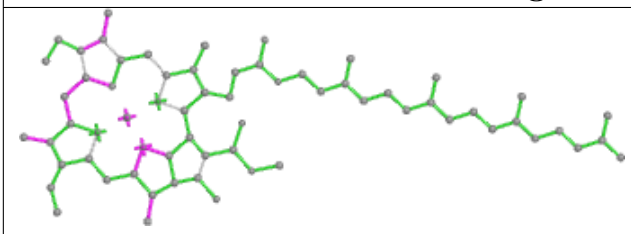


Rings

Ligand CLA y 613



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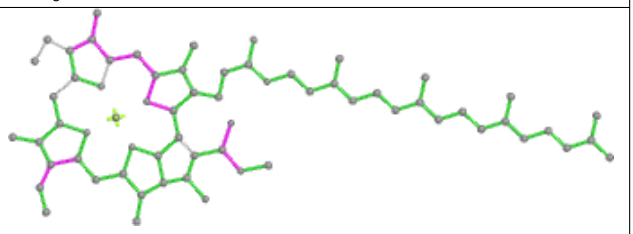
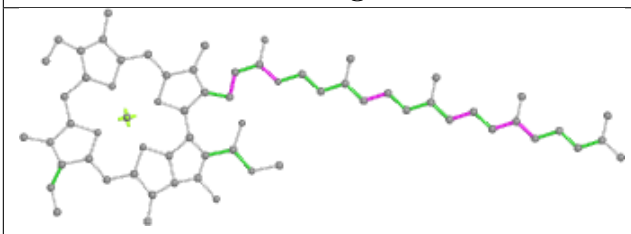


Bond angles



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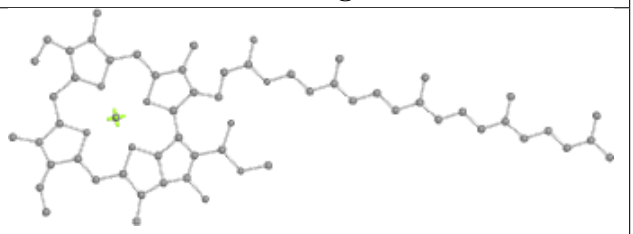
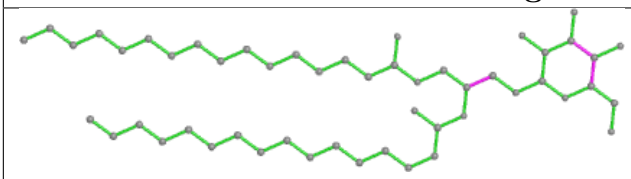


Rings

Ligand LMG z 101



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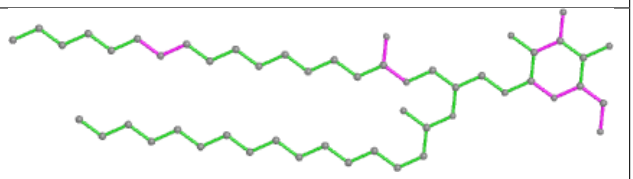
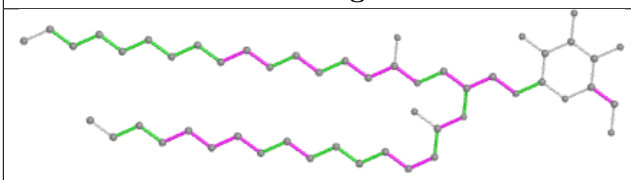
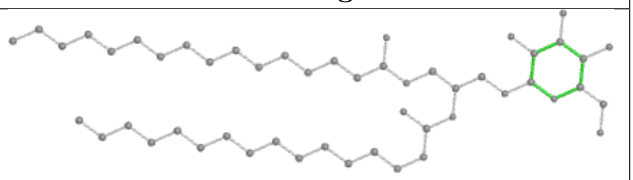


Bond angles

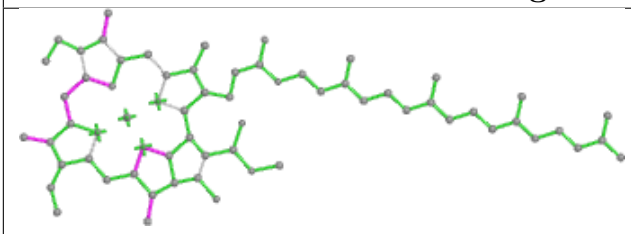


Torsions

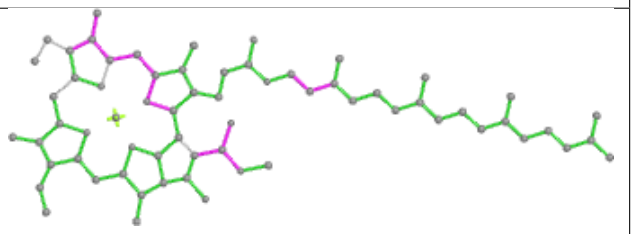


Rings

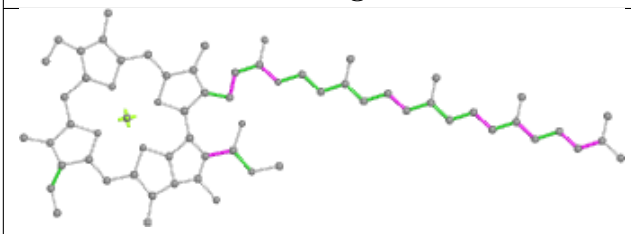
Ligand CLA c 505



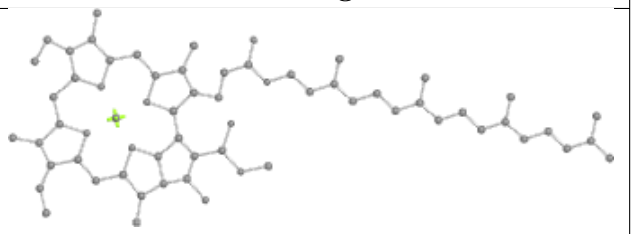
Bond lengths



Bond angles

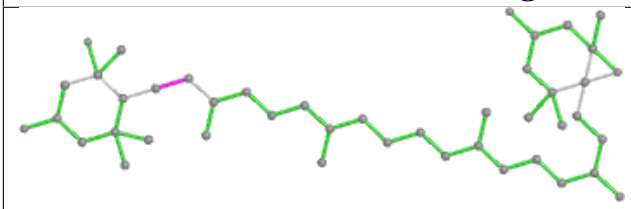


Torsions



Rings

Ligand NEX s 1623



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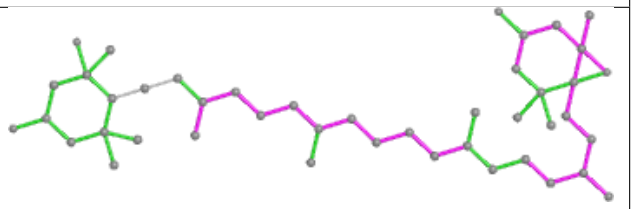
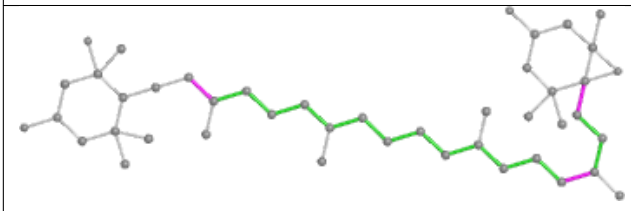


Bond angles



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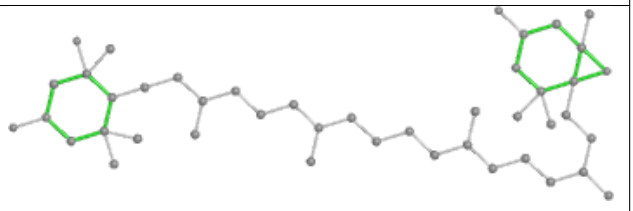
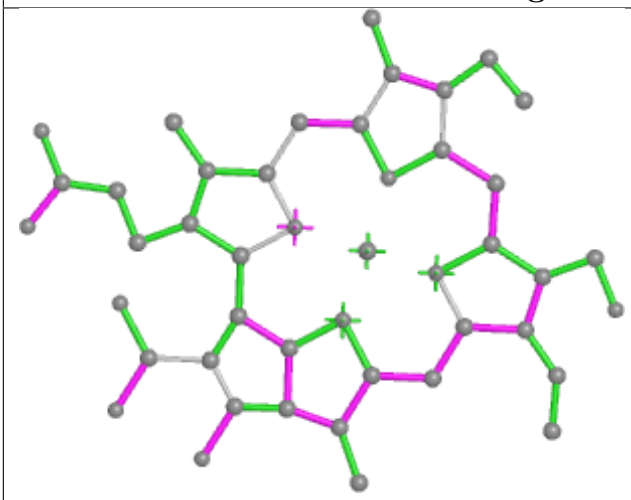


Rings

Ligand CHL 4 601



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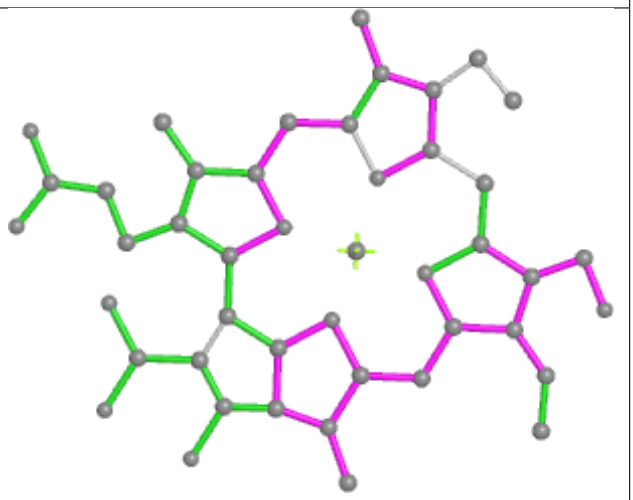
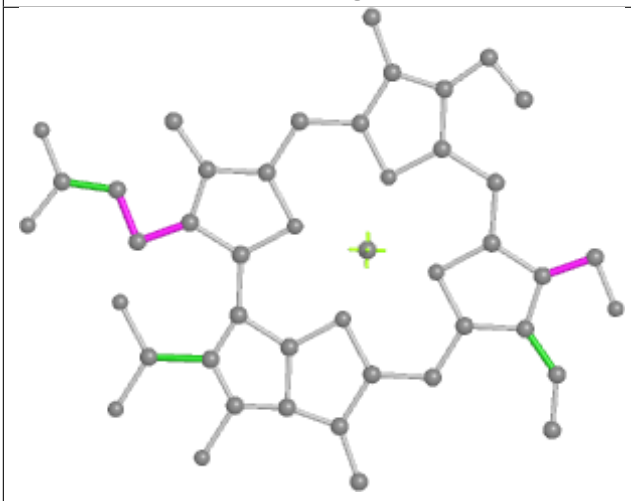


Bond angles



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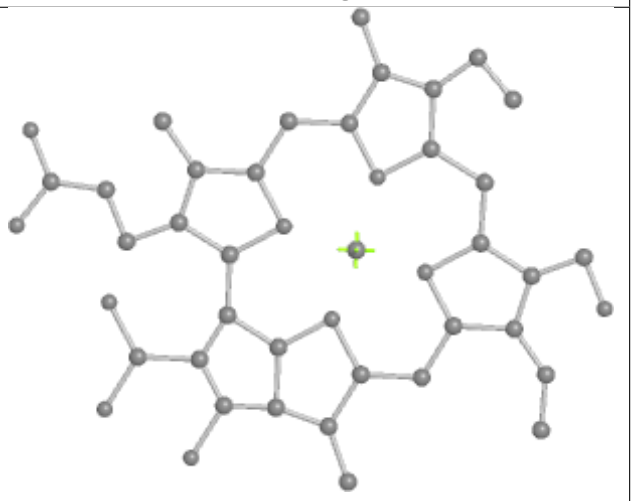
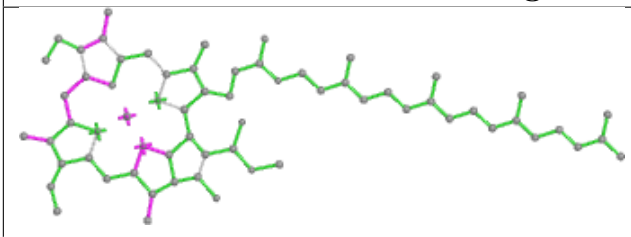


Rings

Ligand CLA Y 613



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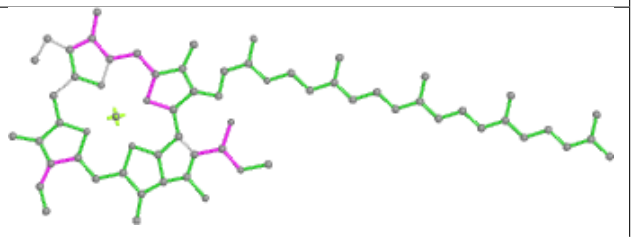
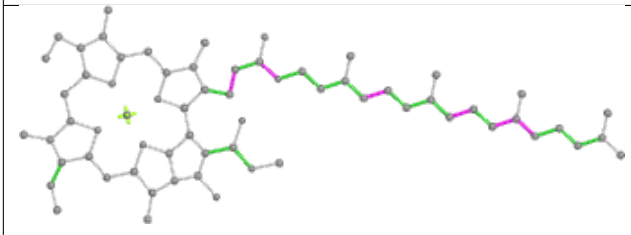


Bond angles



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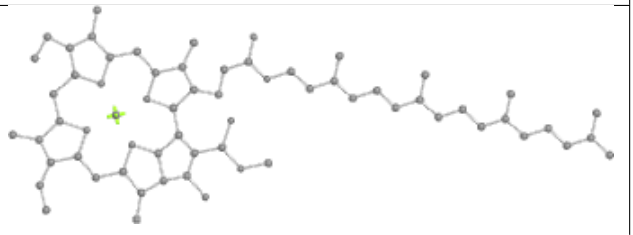
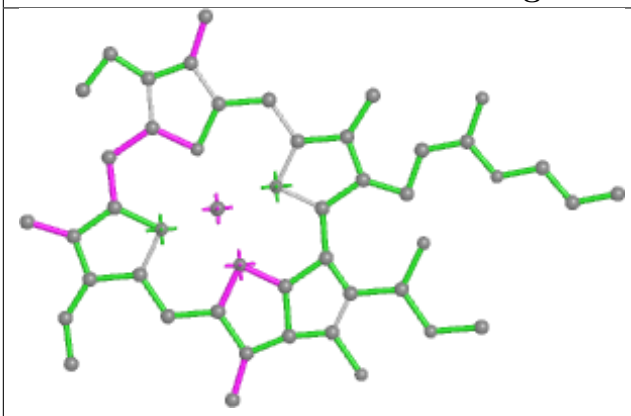


Rings

Ligand CLA N 614



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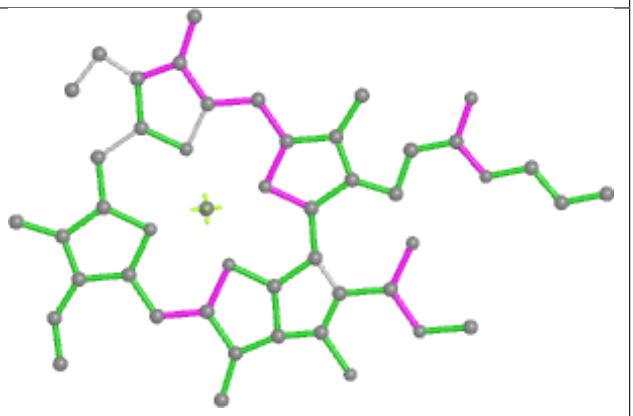
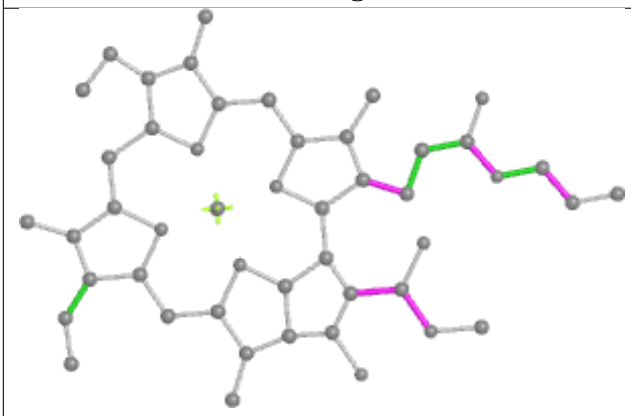


Bond angles



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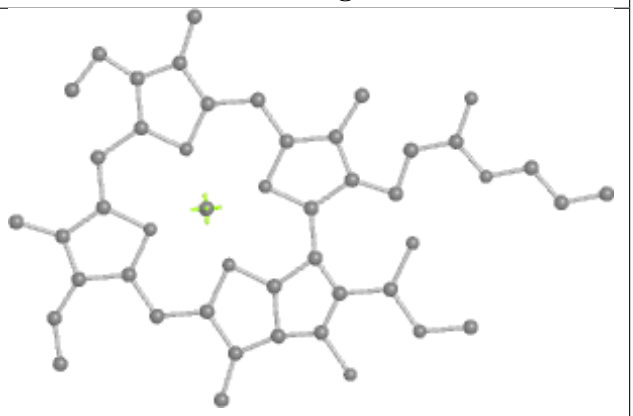
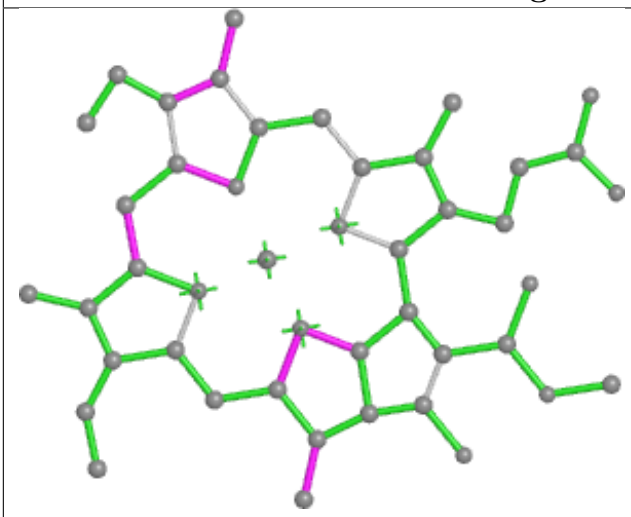


Rings

Ligand CLA s 603



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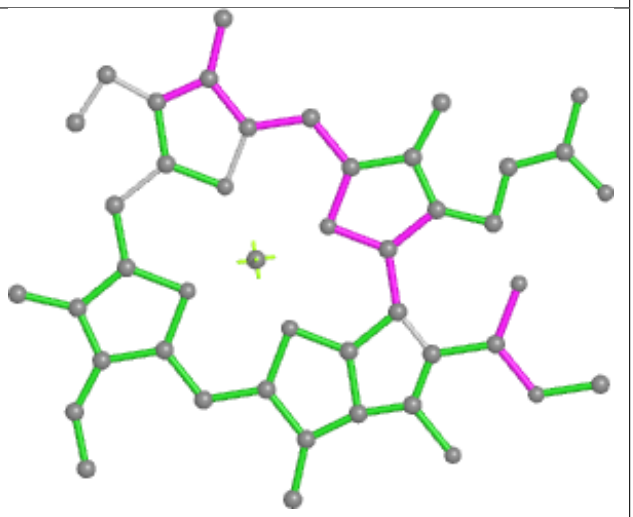
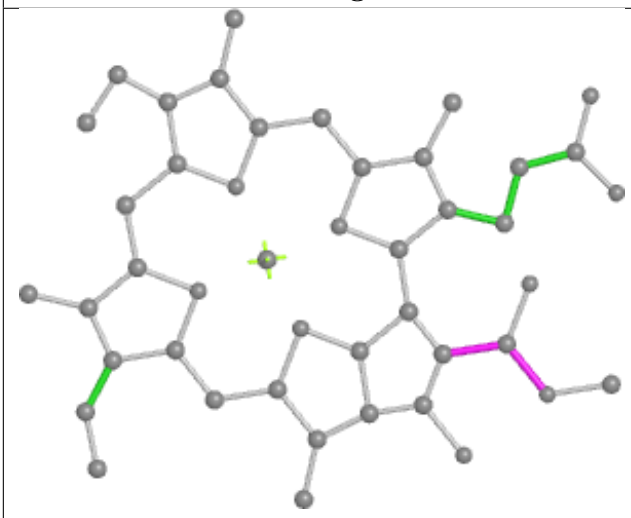


Bond angles



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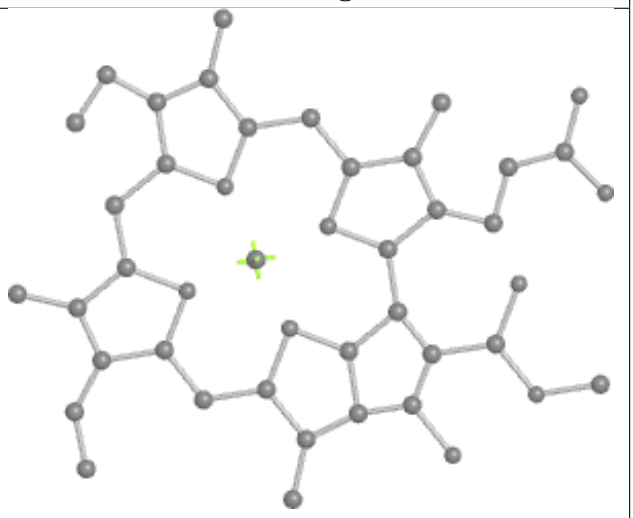
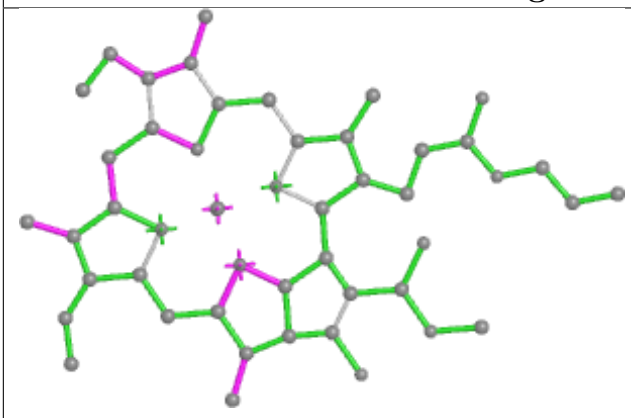


Rings

Ligand CLA g 614



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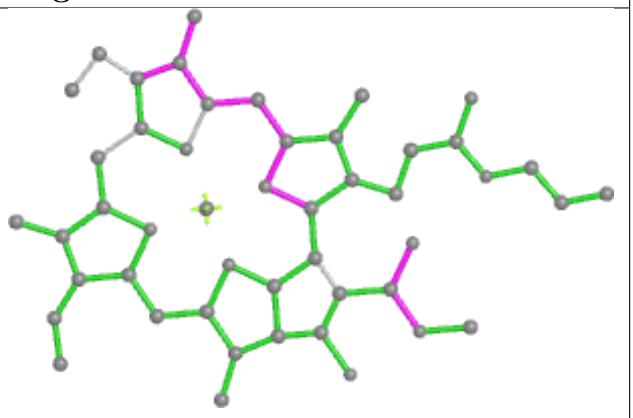
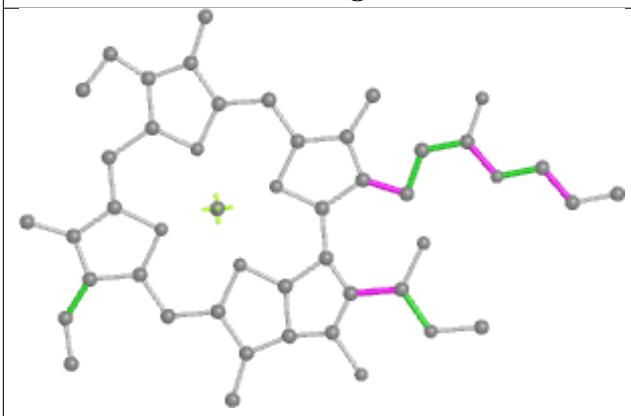


Bond angles



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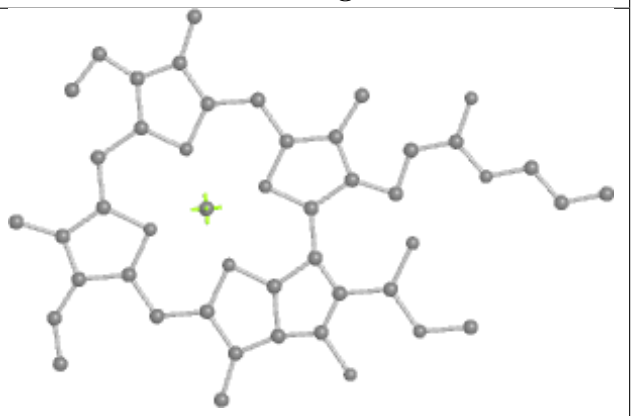
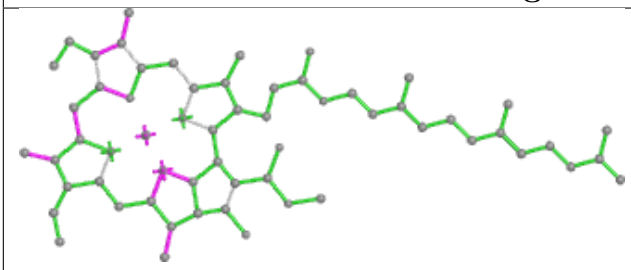


Rings

Ligand CLA Y 611



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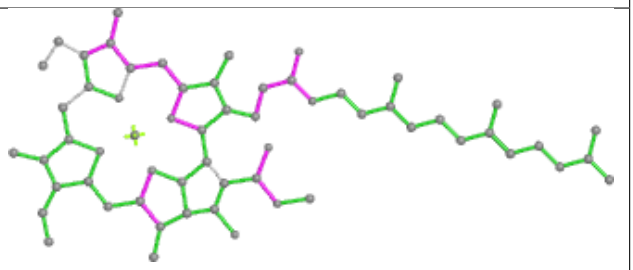
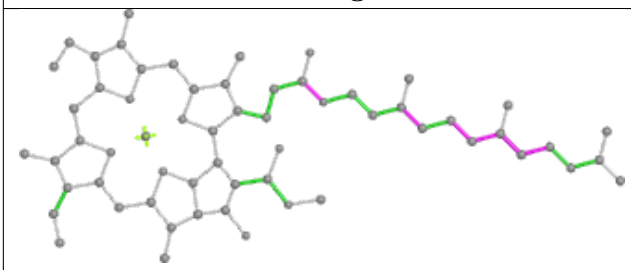
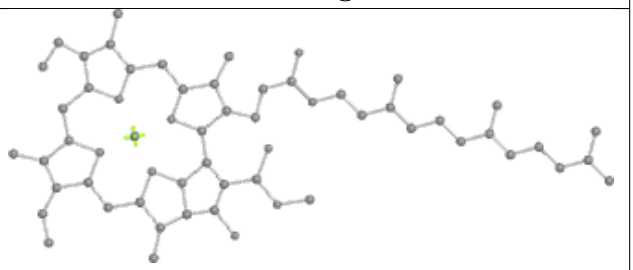


Bond angles

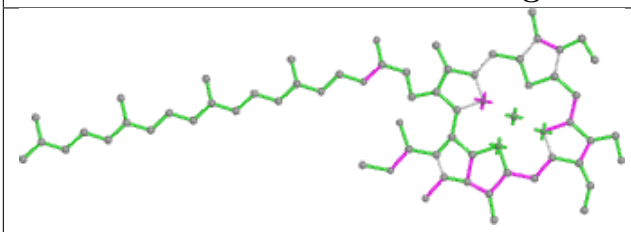


Torsions



Rings

Ligand CHL N 607



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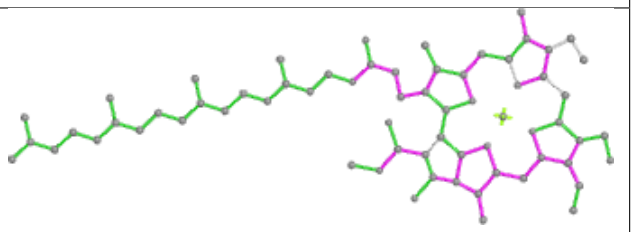
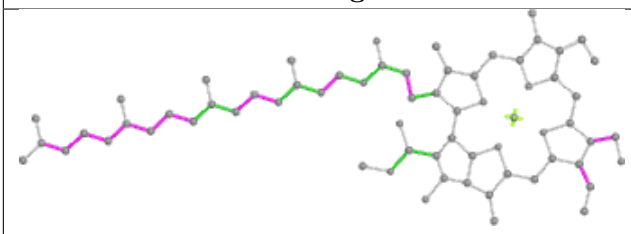
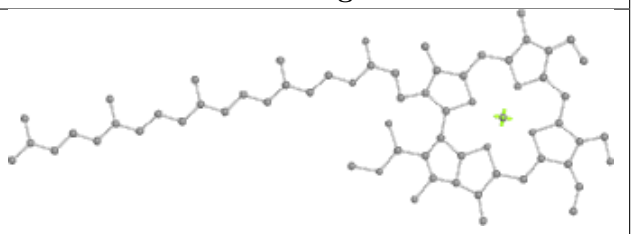


Bond angles

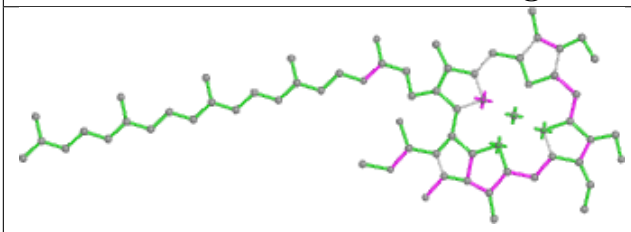


Torsions



Rings

Ligand CHL G 608



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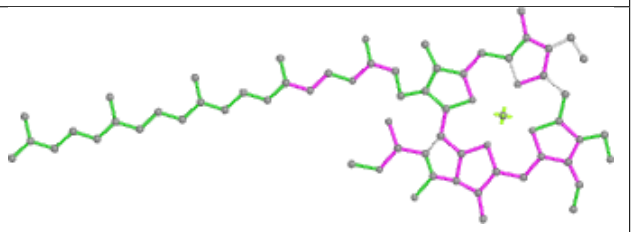
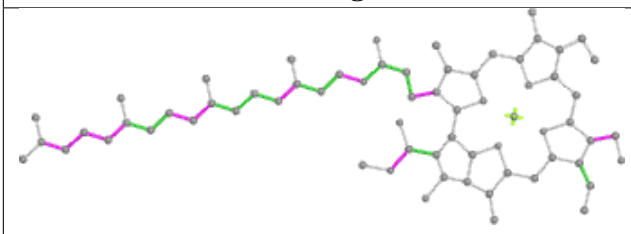


Bond angles



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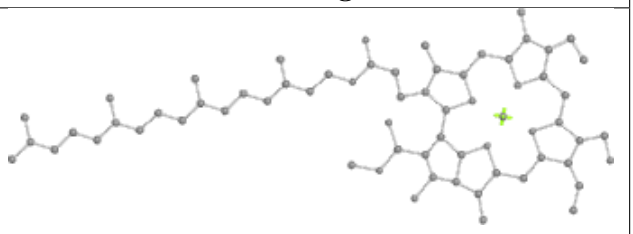
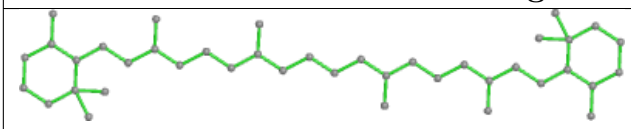


Rings

Ligand BCR c 517



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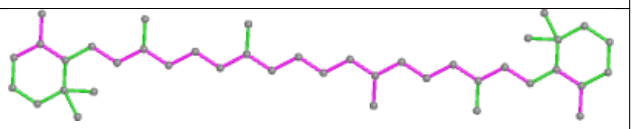
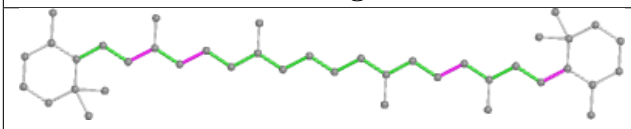


Bond angles



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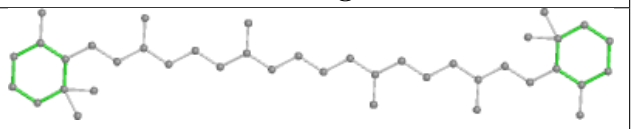
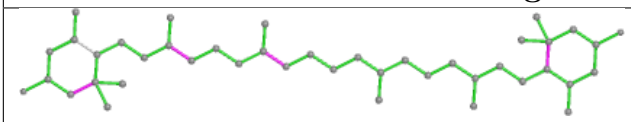


Rings

Ligand LUT R 620



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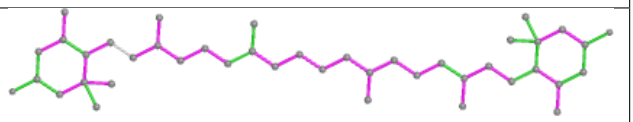
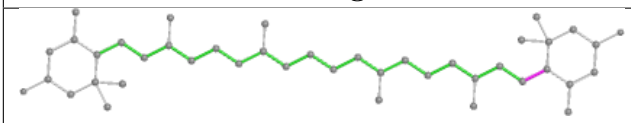


Bond angles



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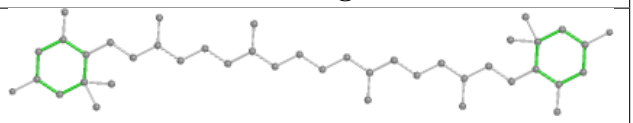
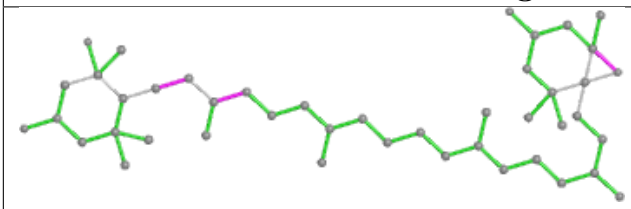


Rings

Ligand NEX n 1623



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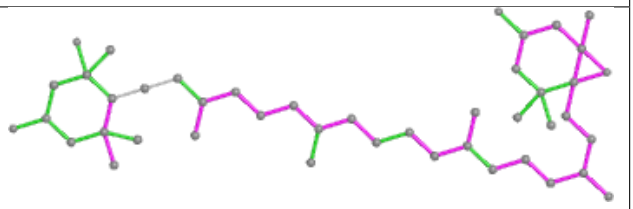
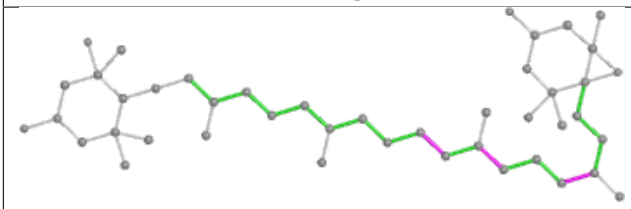


Bond angles



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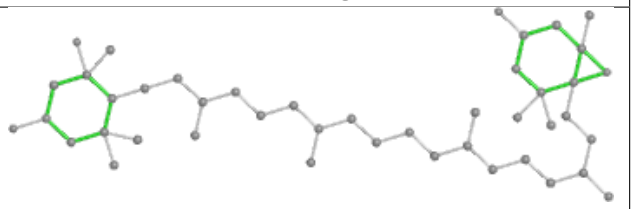
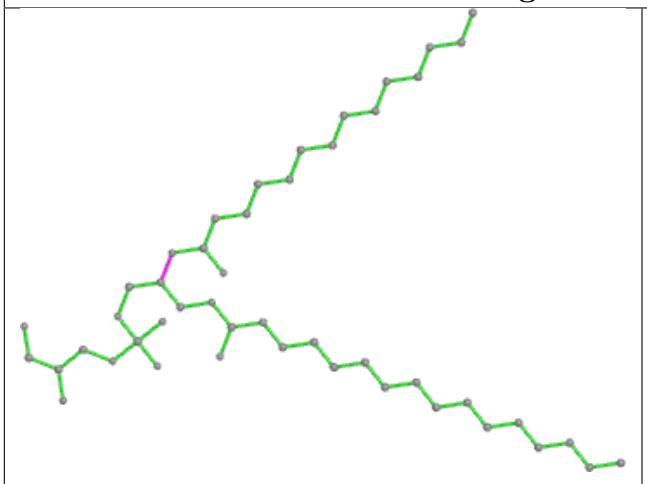
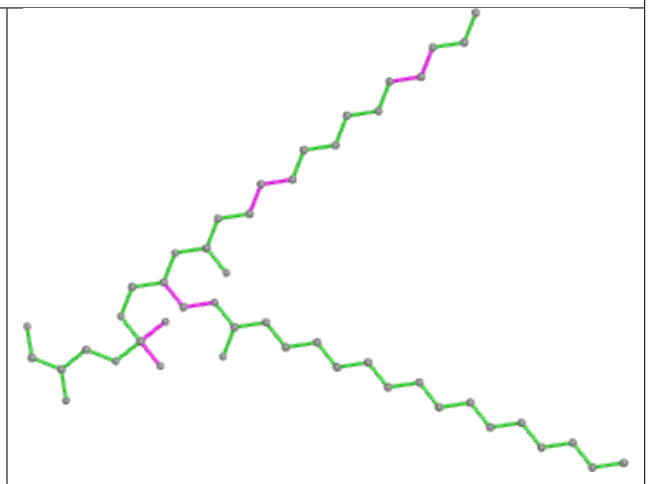


Rings

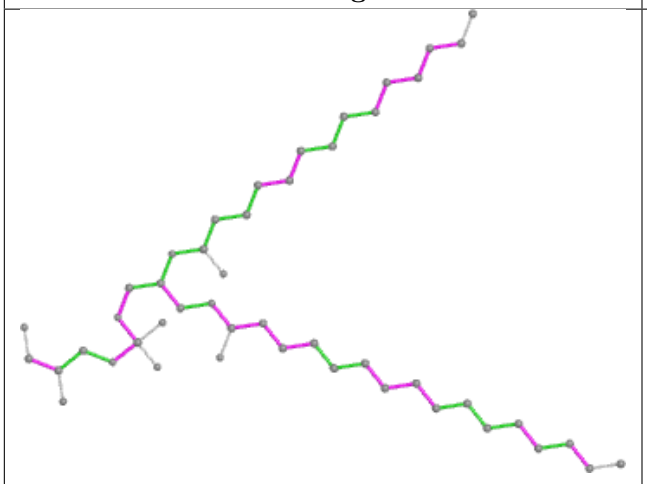
Ligand LHG 3 2630



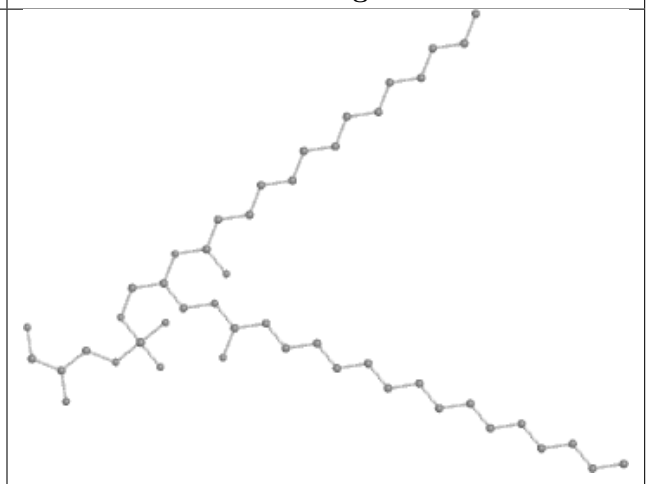
Bond lengths



Bond angles

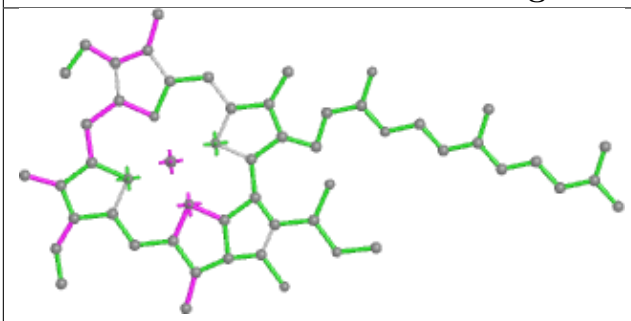


Torsions



Rings

Ligand CLA 3 603



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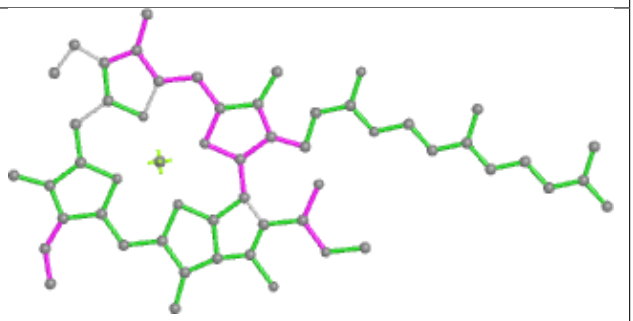

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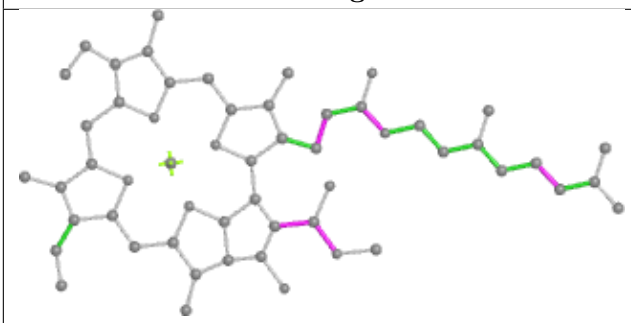

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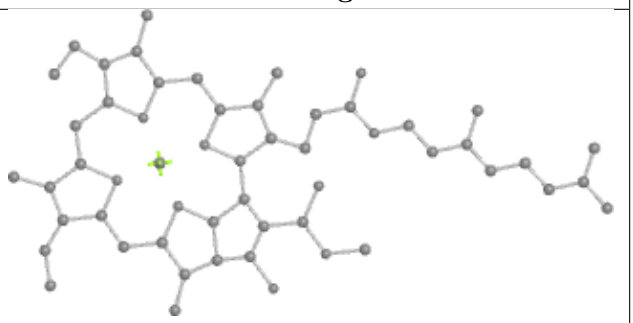
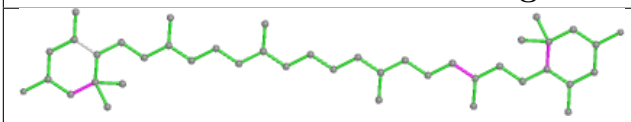


Rings

Ligand LUT 1 1621



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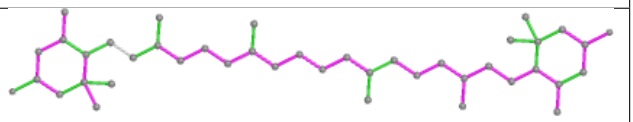

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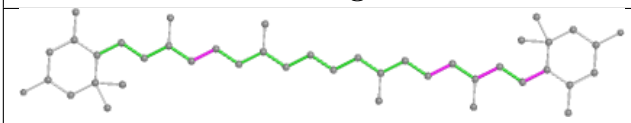
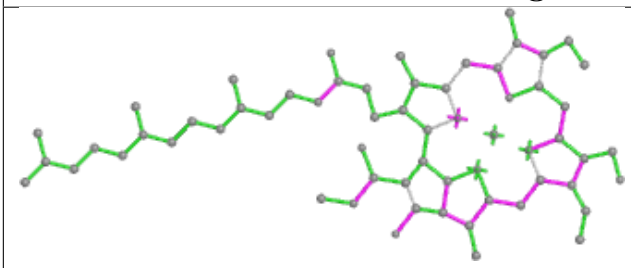


Torsions

Rings

Ligand CHL 3 609



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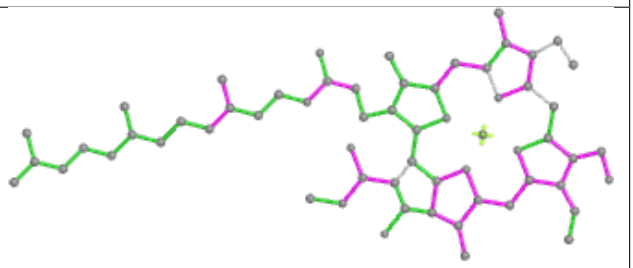

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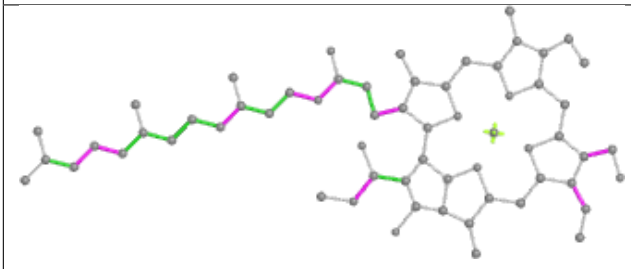

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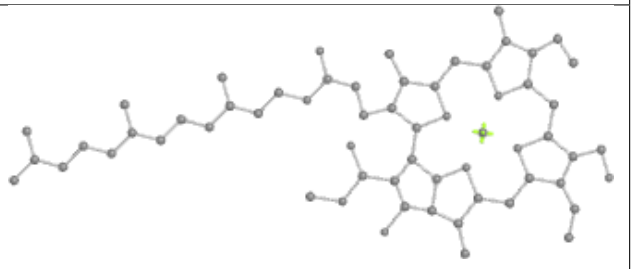
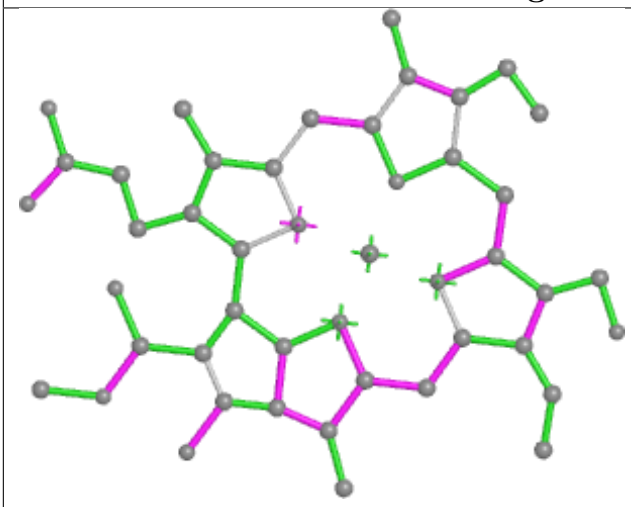


Rings

Ligand CHL 5 605



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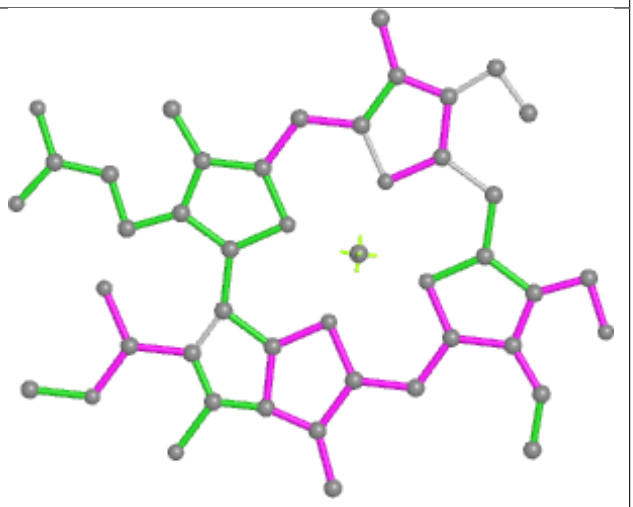
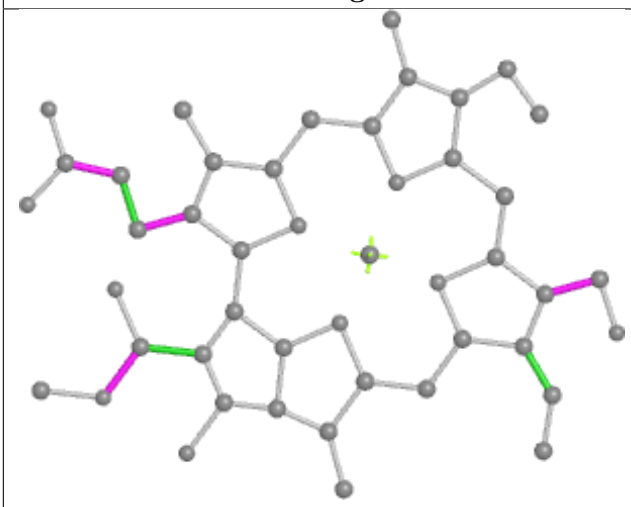


Bond angles



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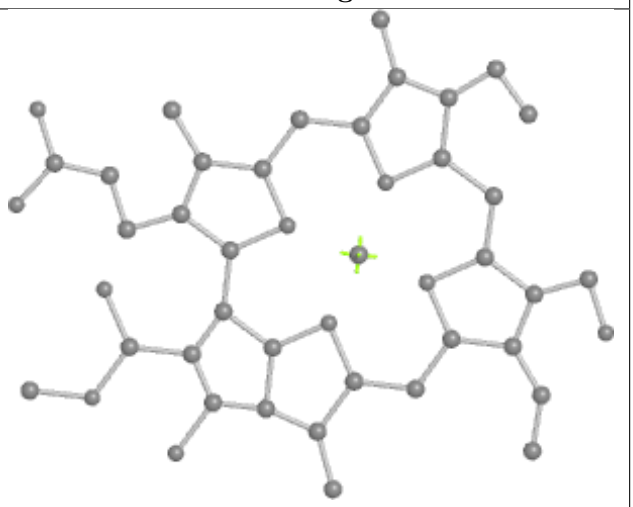
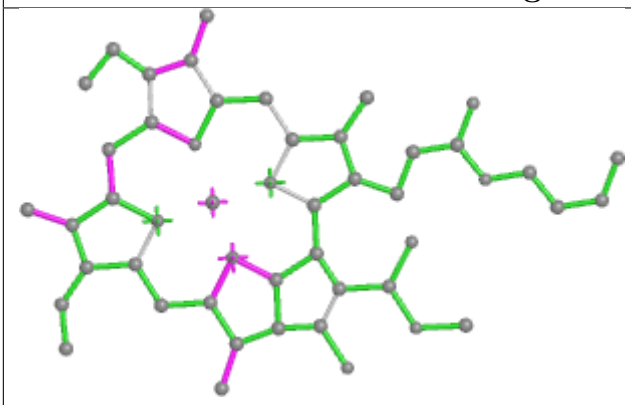
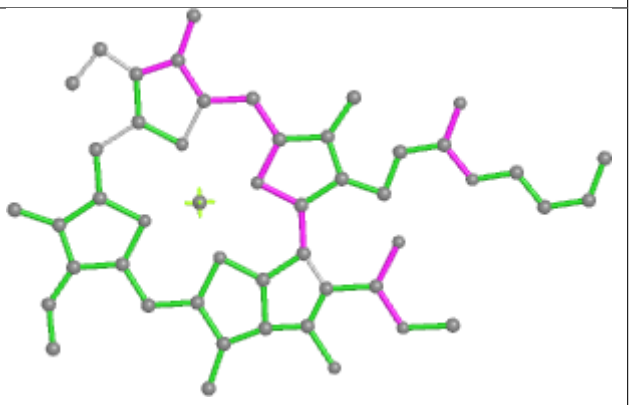
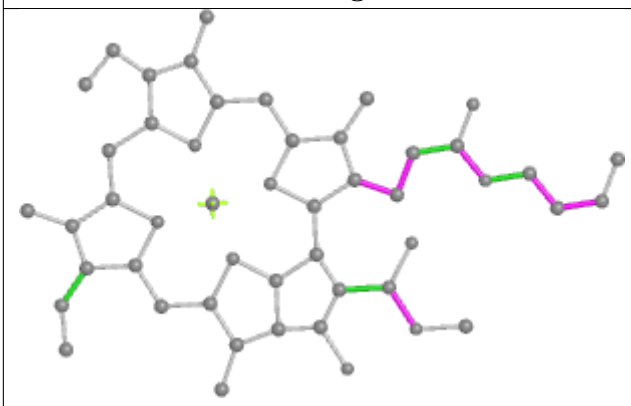
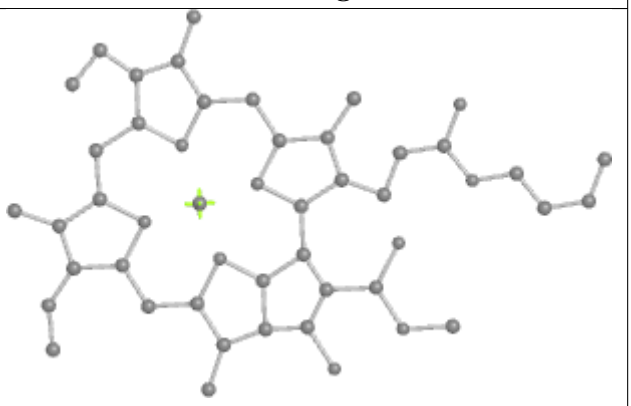
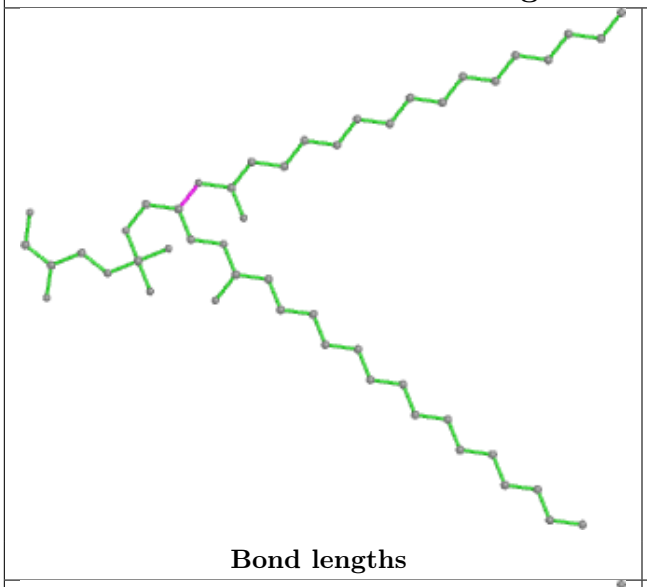


Rings

Ligand CLA R 611	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand LHG s 2630



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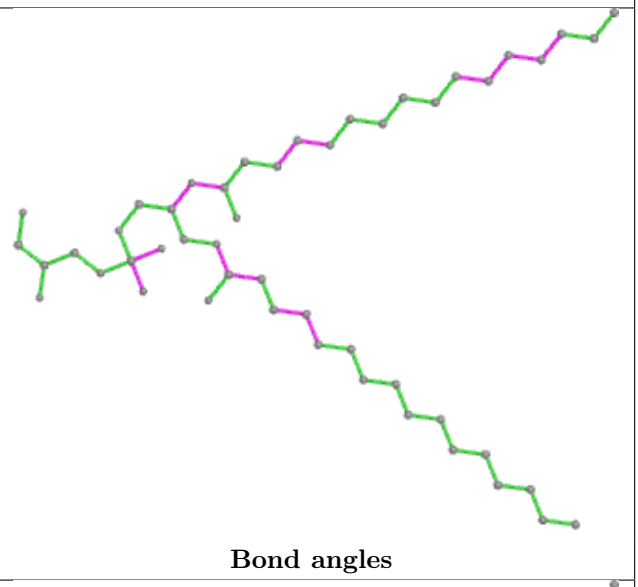
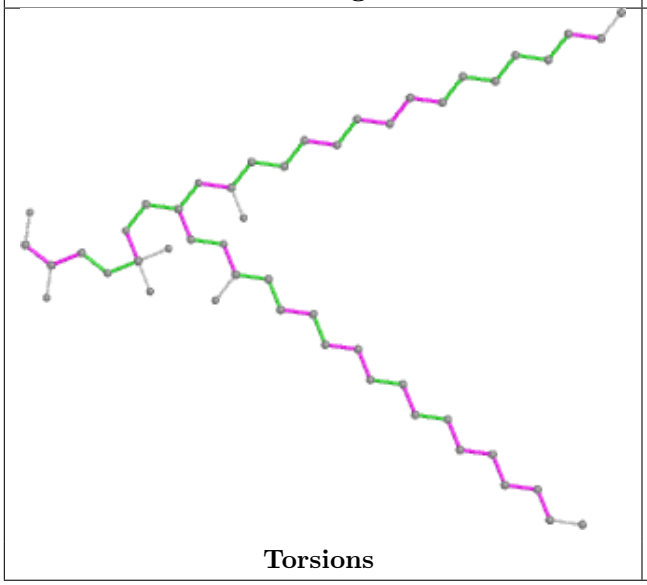
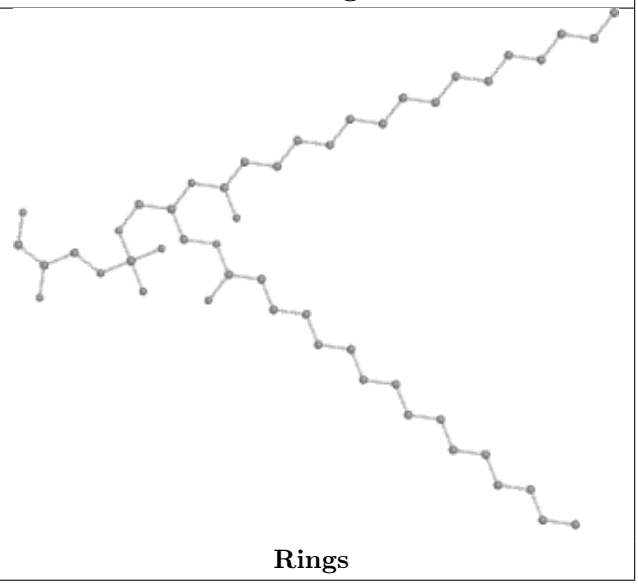


Bond angles

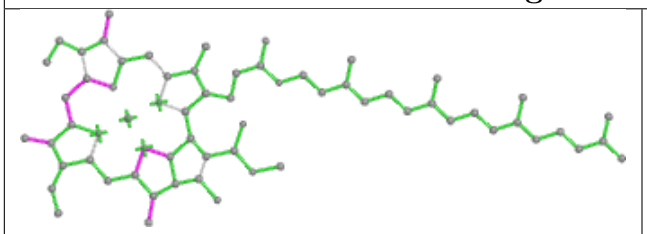


Torsions



Rings

Ligand CLA C 504



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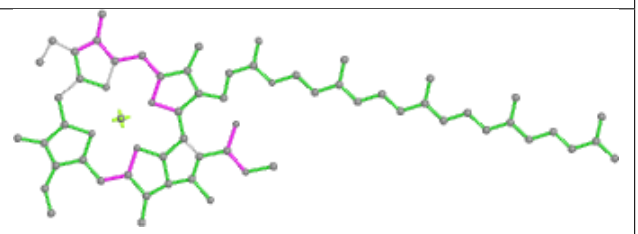
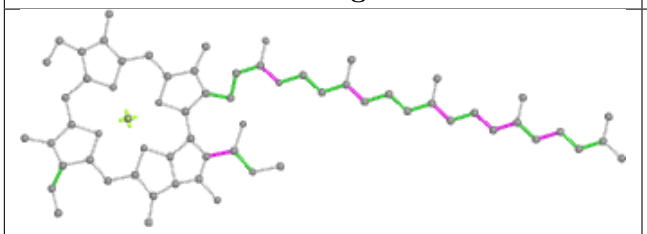


Bond angles



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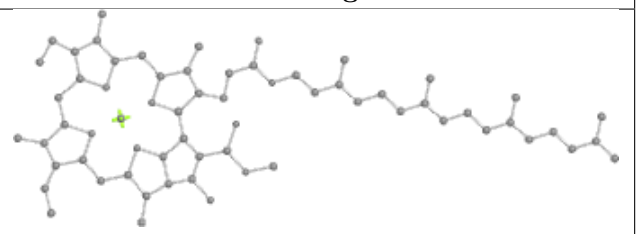
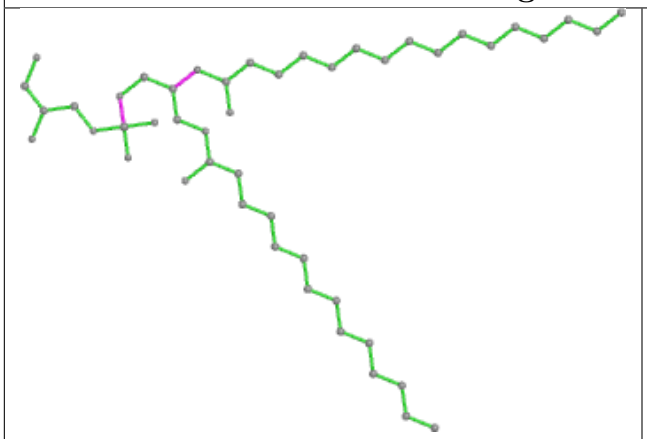


Rings

Ligand LHG b 2630



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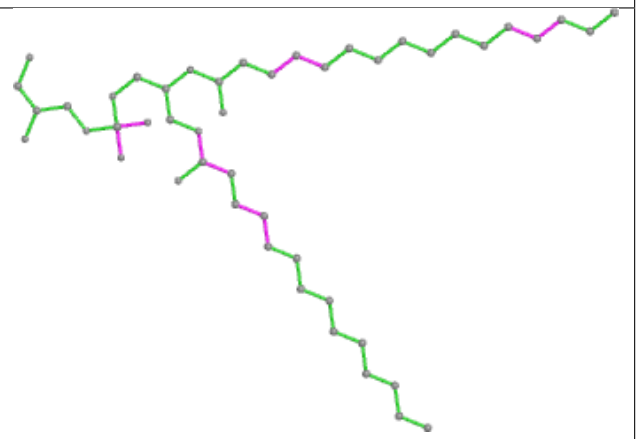

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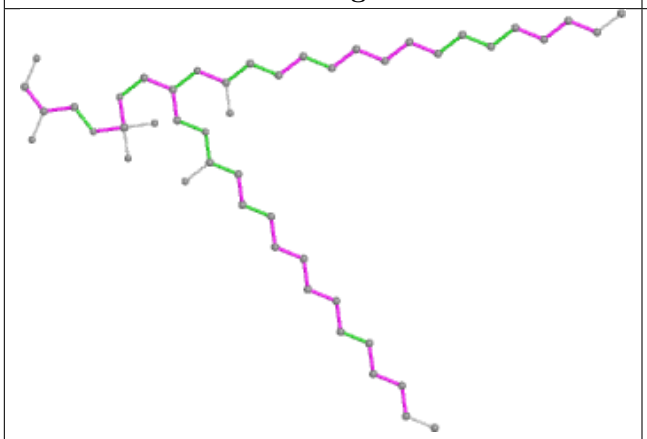

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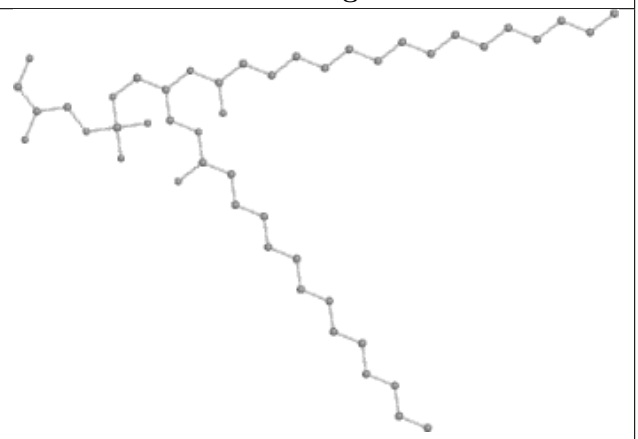
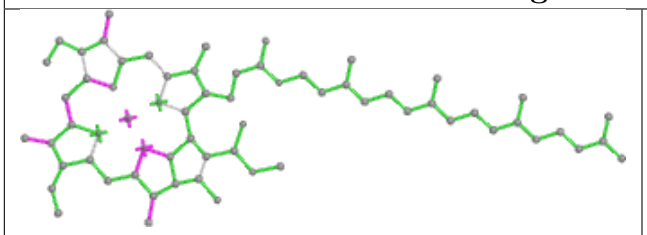


Rings

Ligand CLA c 509



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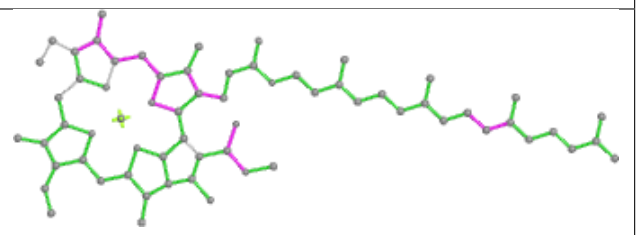
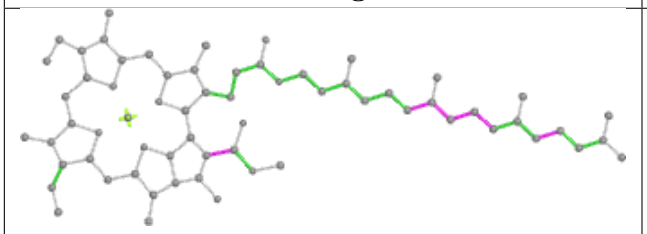


Bond angles



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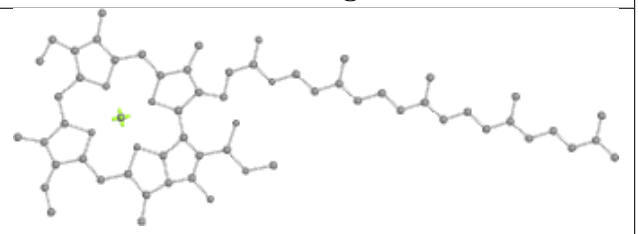
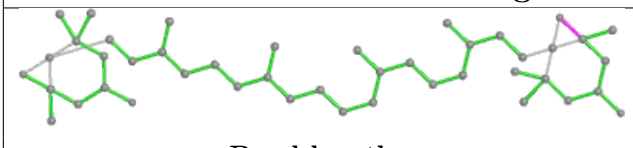


Rings

Ligand XAT G 1622



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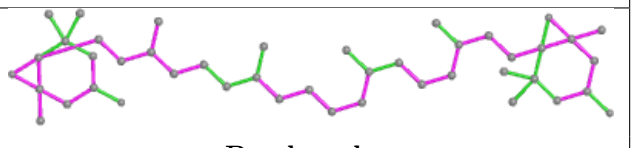
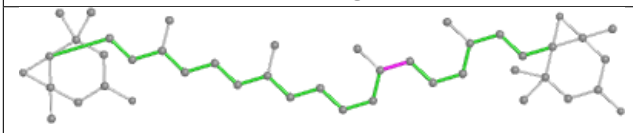


Bond angles



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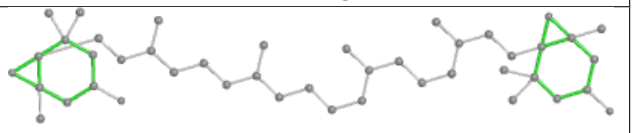
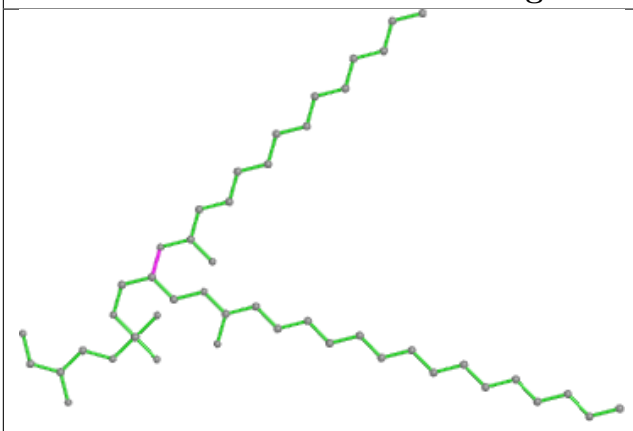


Rings

Ligand LHG d 408



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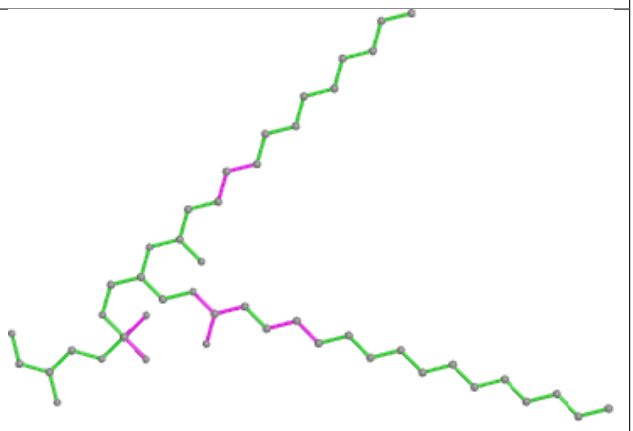
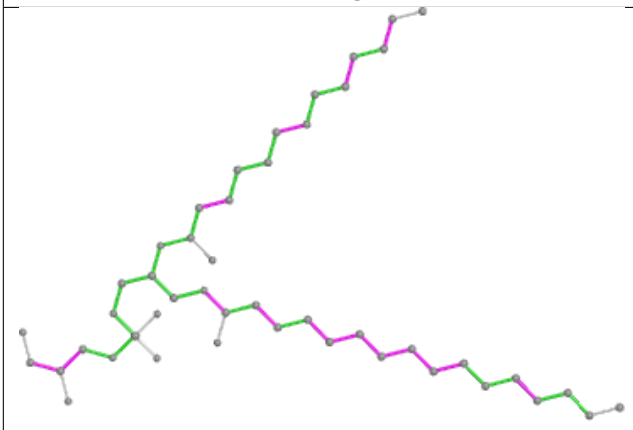


Bond angles



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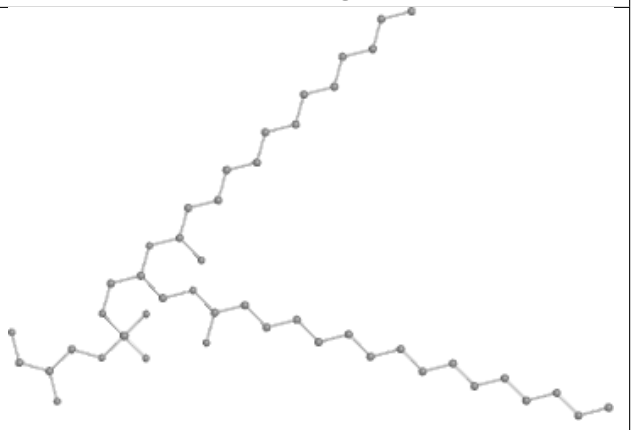
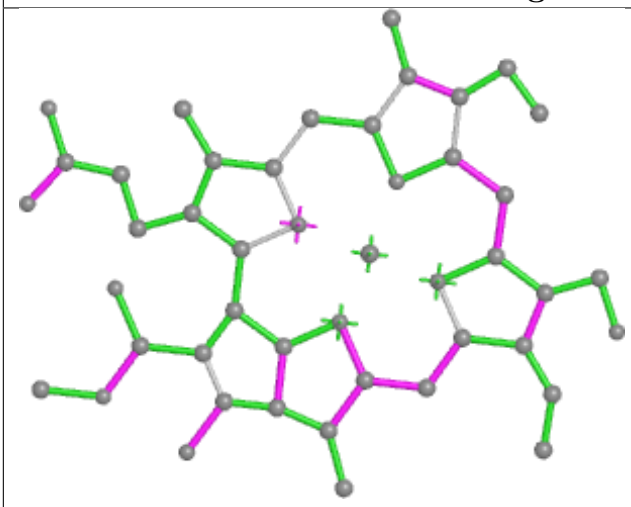


Rings

Ligand CHL 1 608



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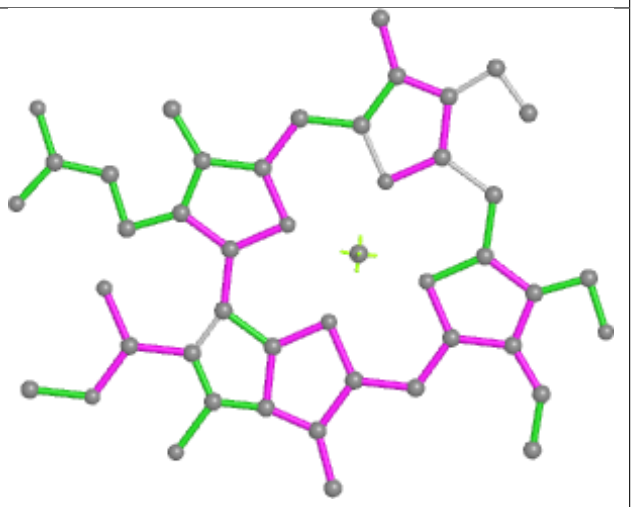
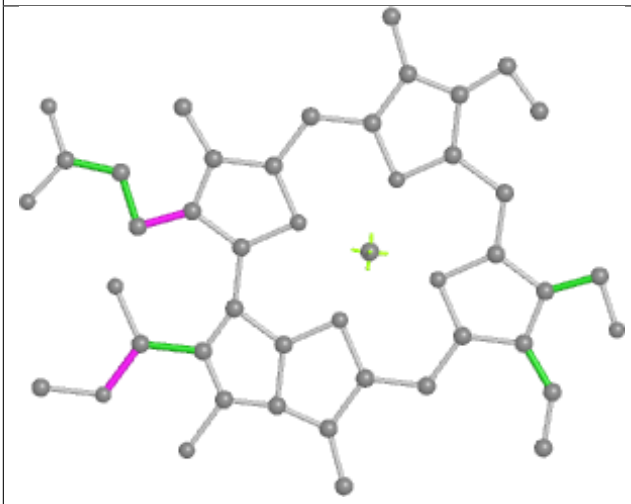


Bond angles



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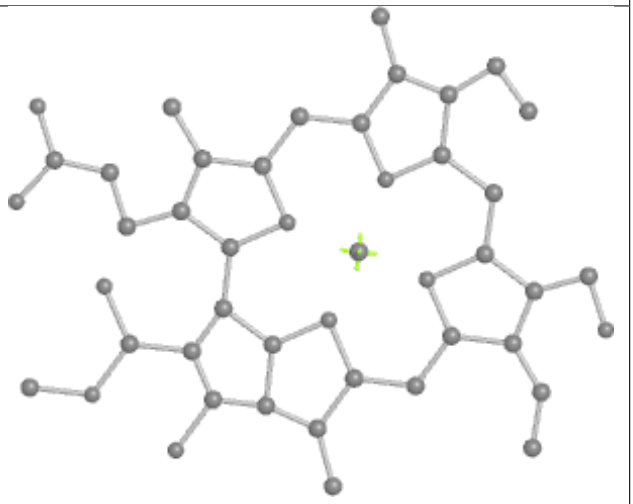
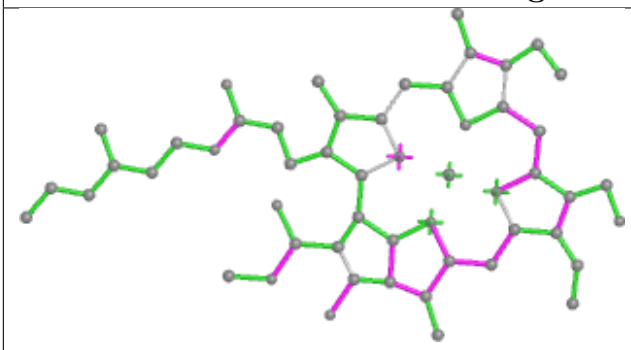


Rings

Ligand CHL 3 607



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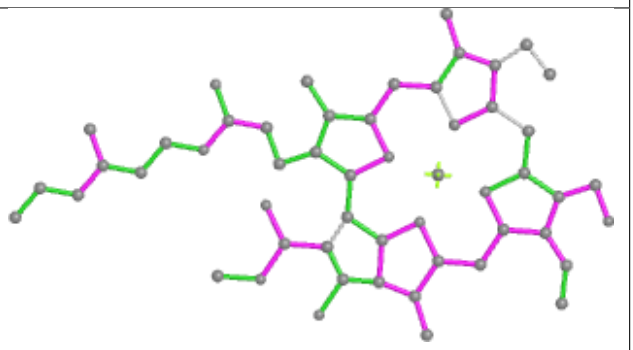
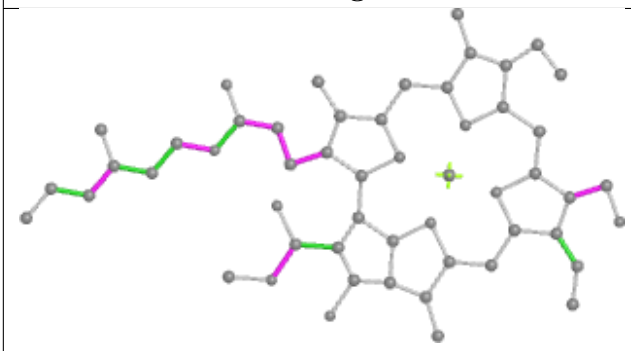


Bond angles



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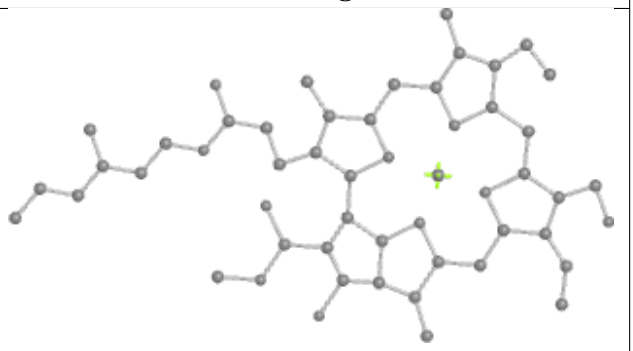
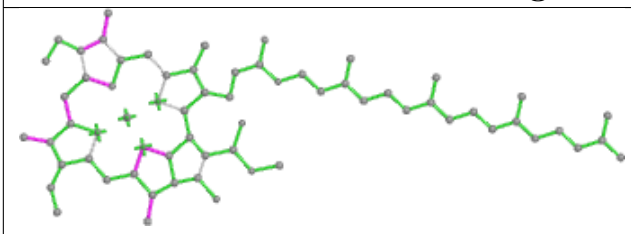
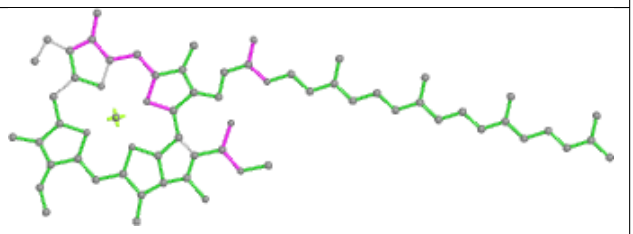


Rings

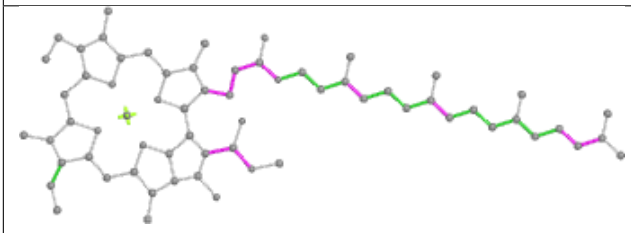
Ligand CLA c 501



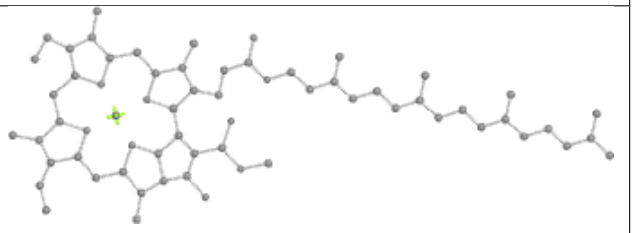
Bond lengths



Bond angles

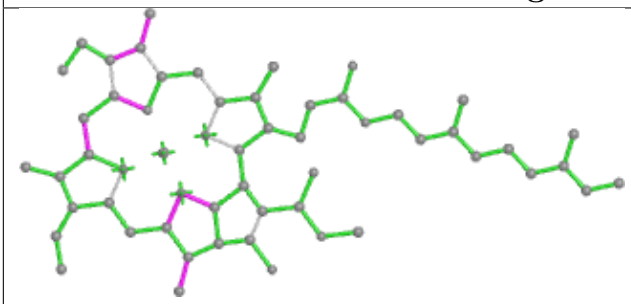


Torsions



Rings

Ligand CLA S 611



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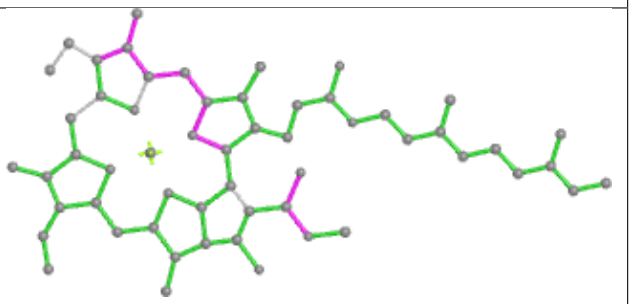

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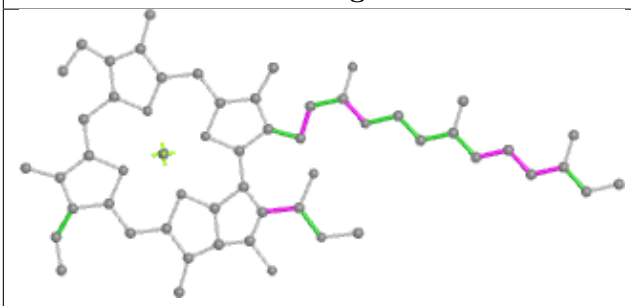

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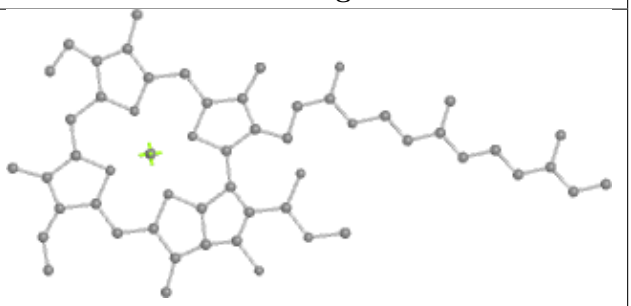
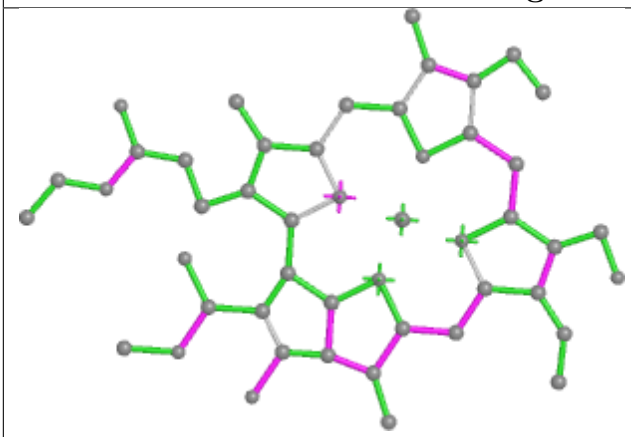


Rings

Ligand CHL n 605



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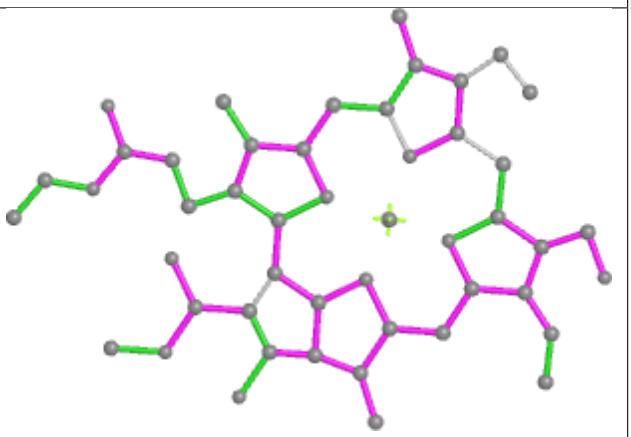
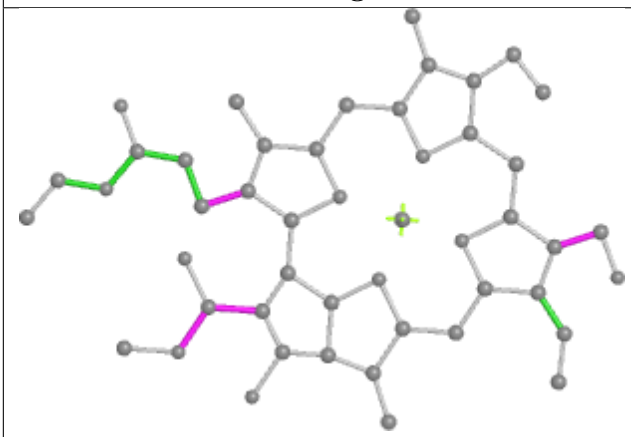


Bond angles



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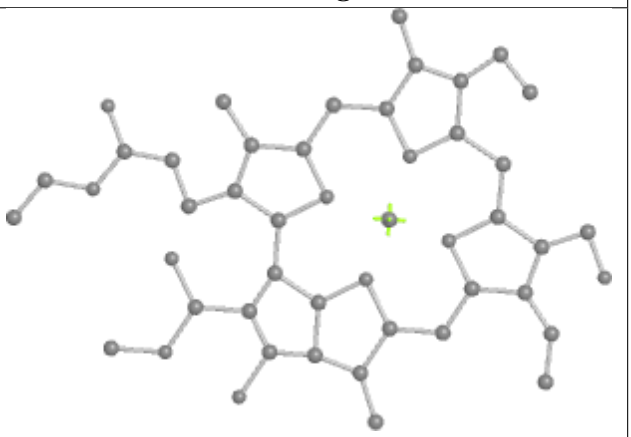
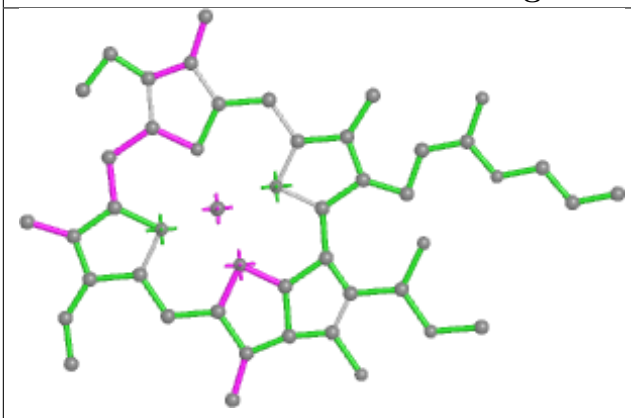


Rings

Ligand CLA R 604



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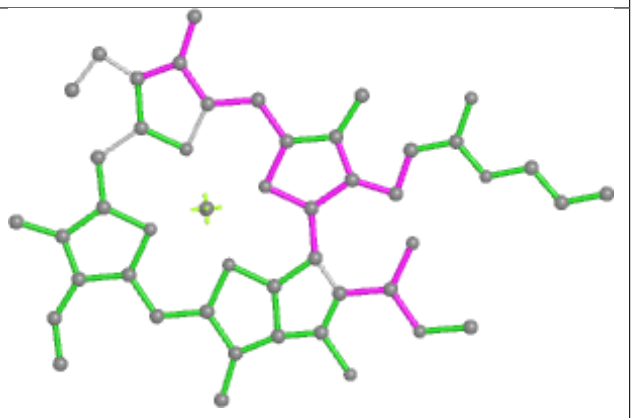
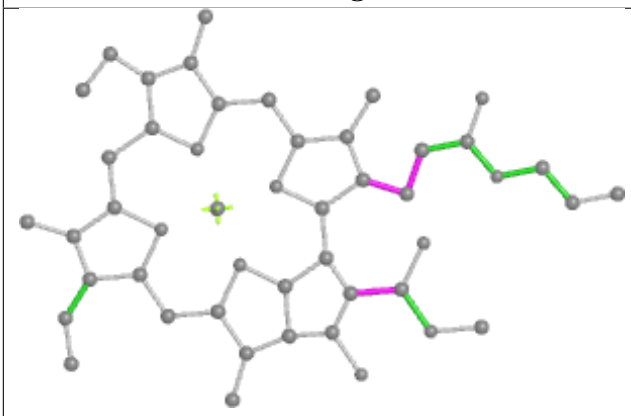


Bond angles



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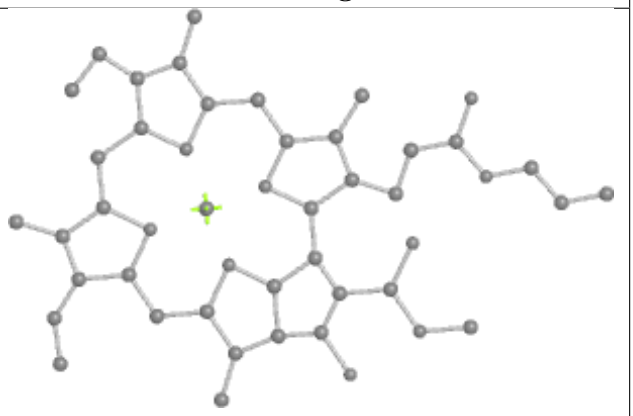
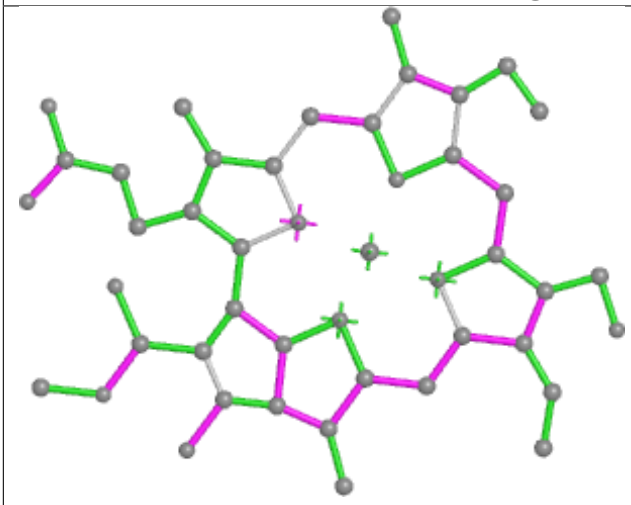


Rings

Ligand CHL S 606



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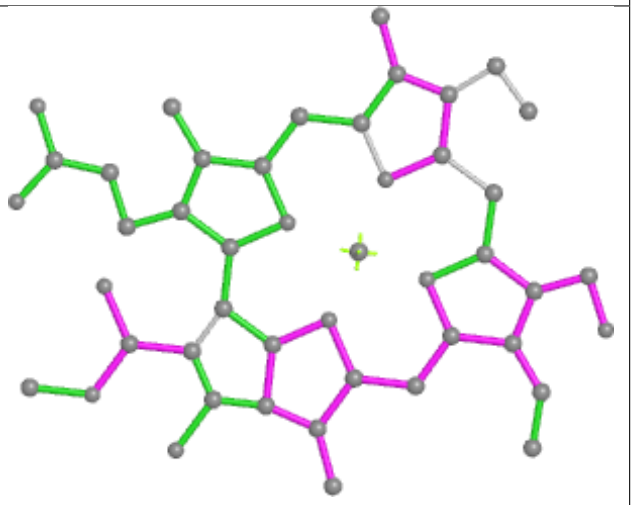

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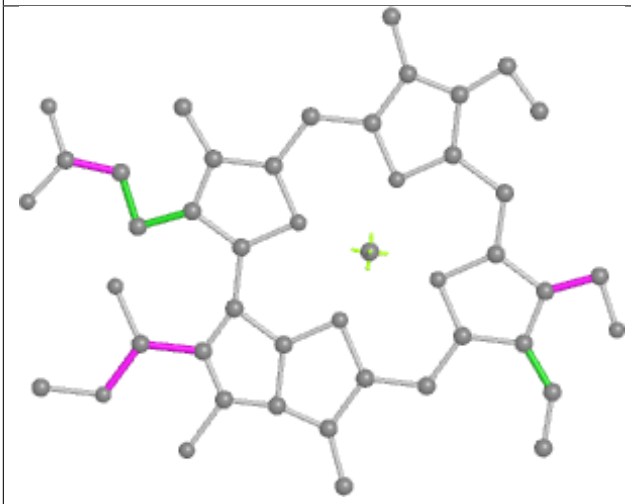

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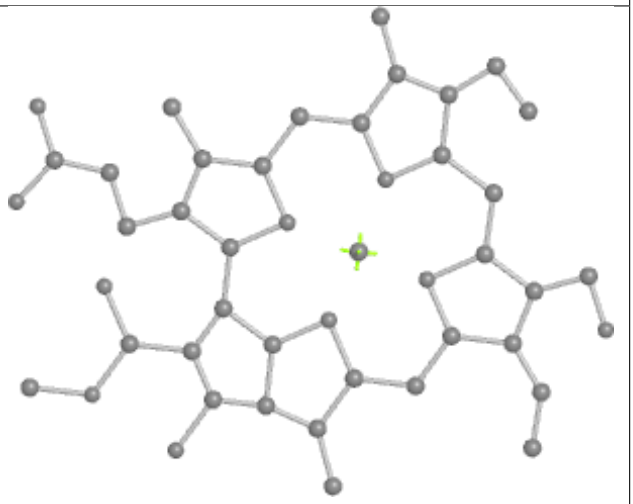

Rings

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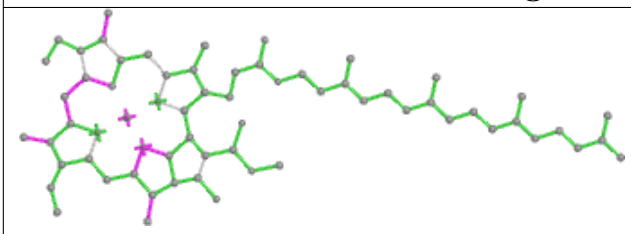

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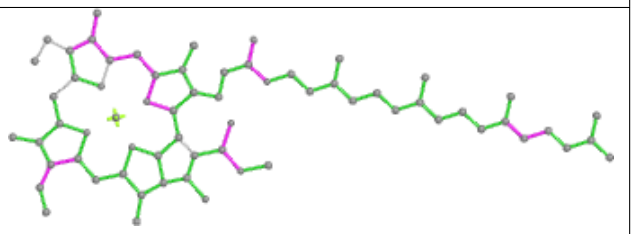

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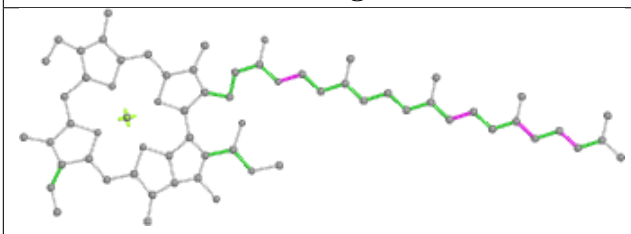

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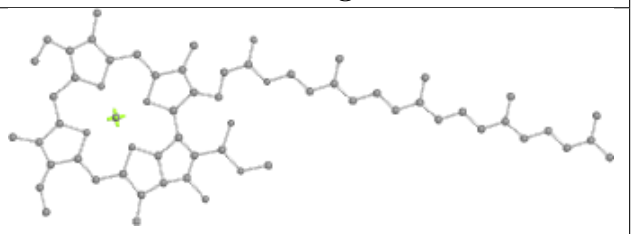
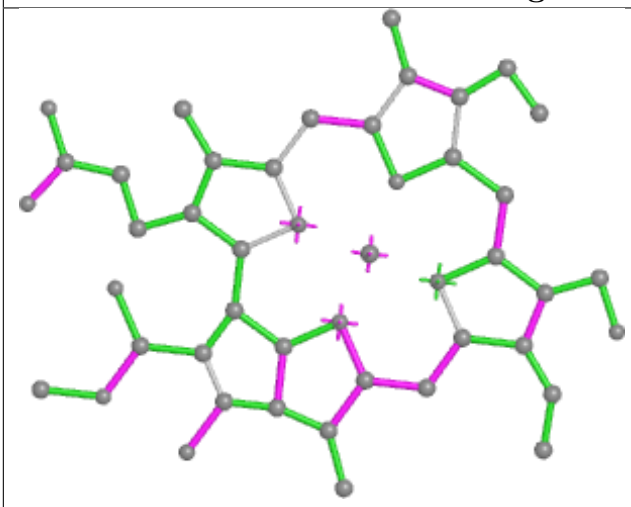


Rings

Ligand CHL 1 601



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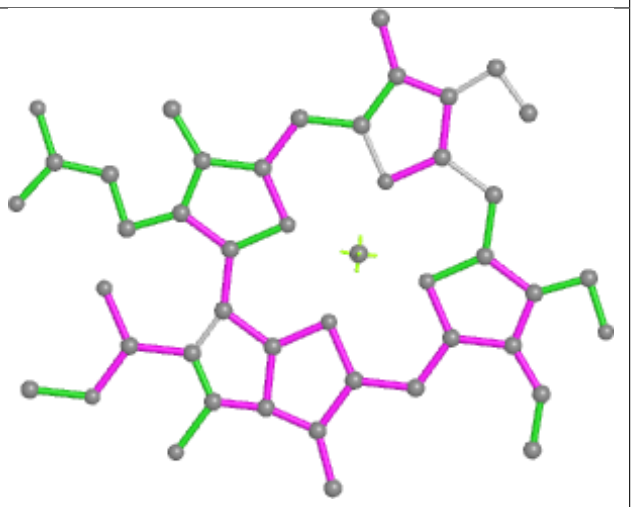

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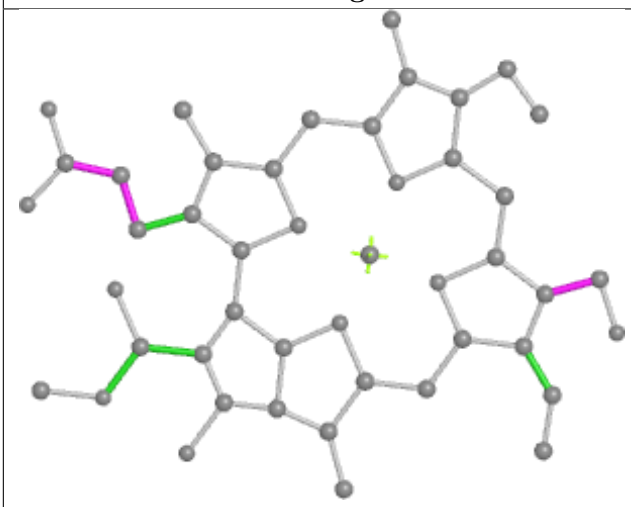

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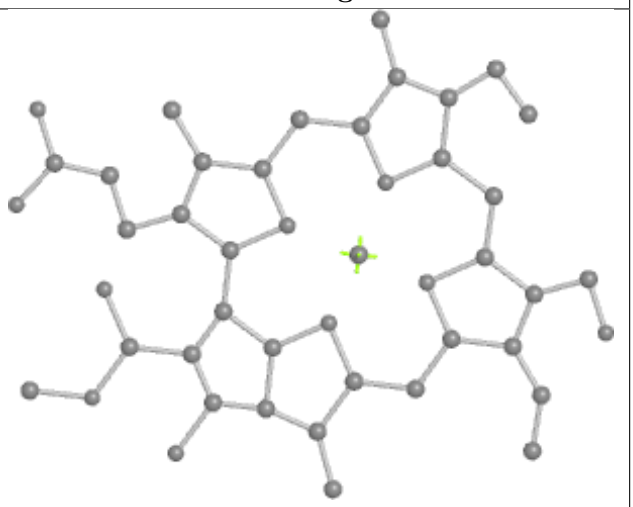
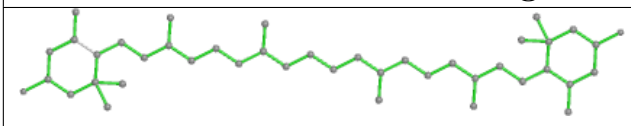


Rings

Ligand LUT 6 1620



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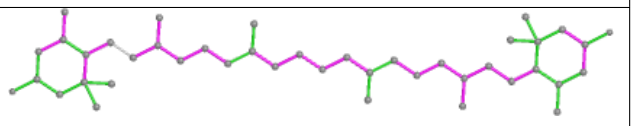

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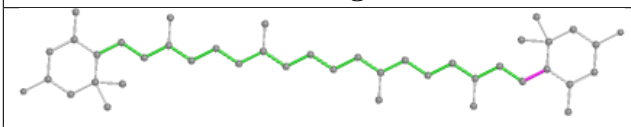

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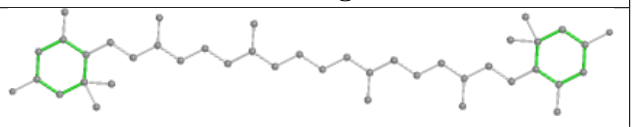
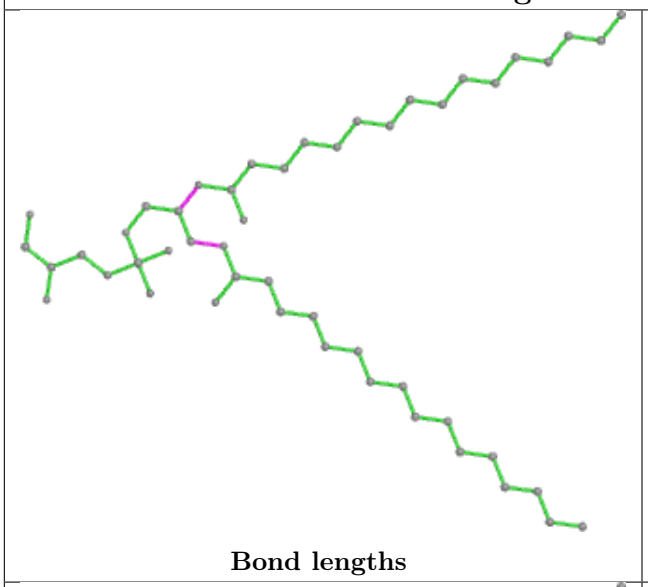


Rings

Ligand LHG Y 2630



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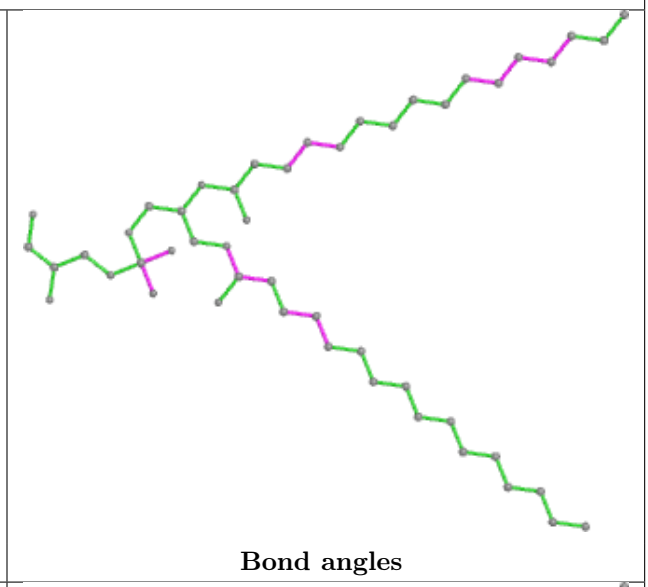
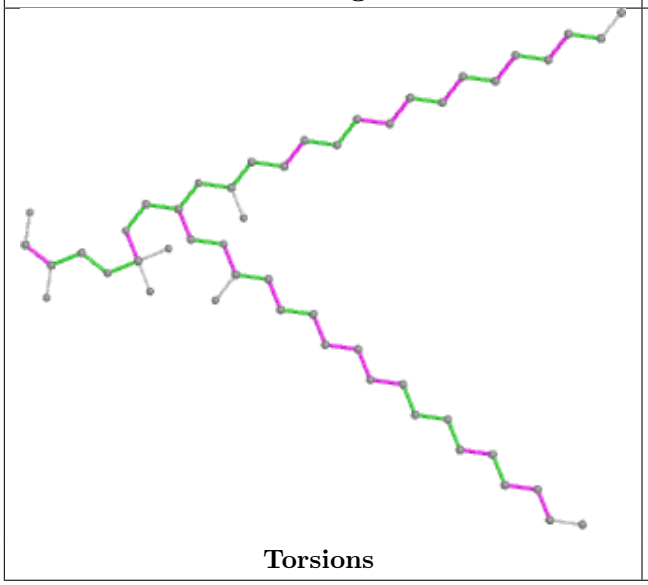


Bond angles



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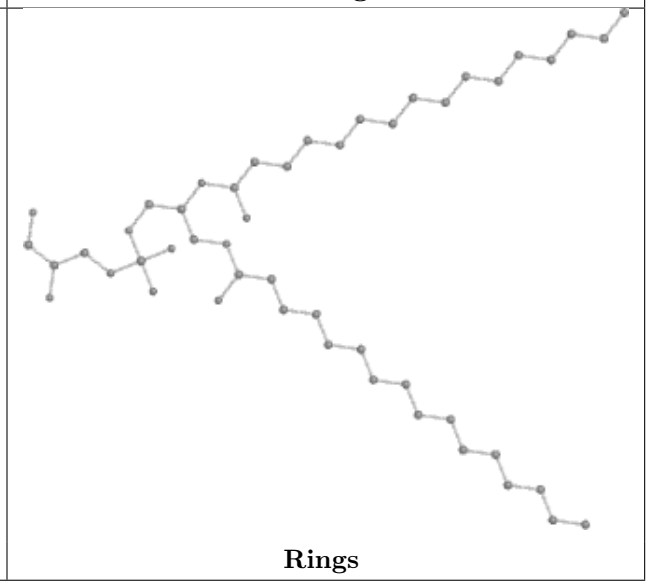
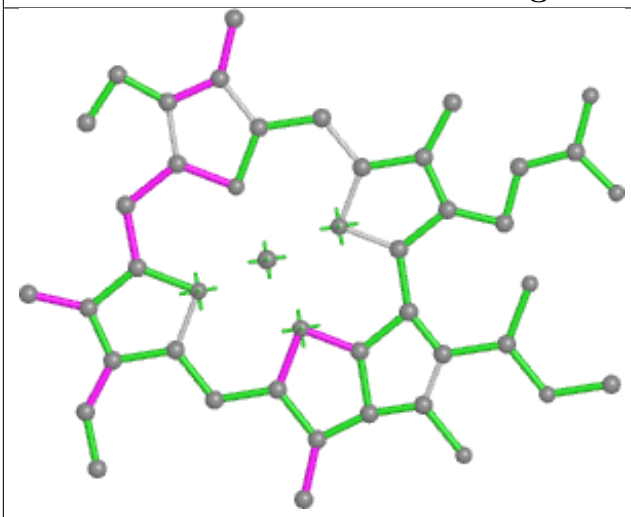


Rings

Ligand CLA r 616



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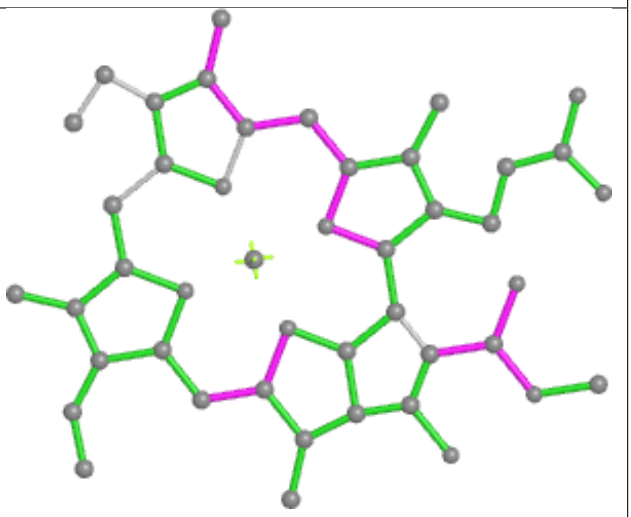

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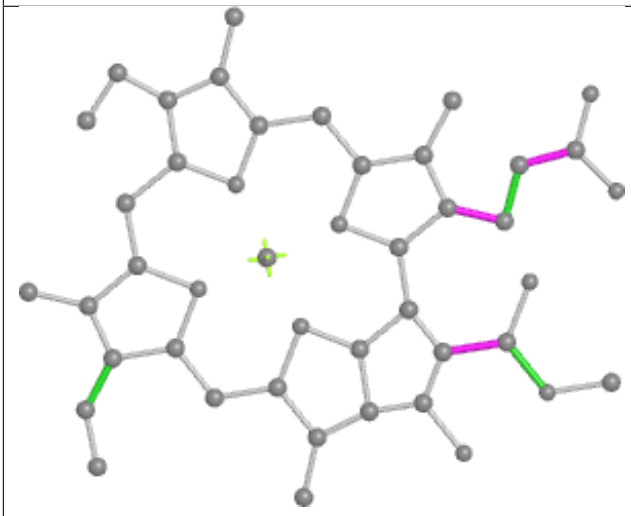

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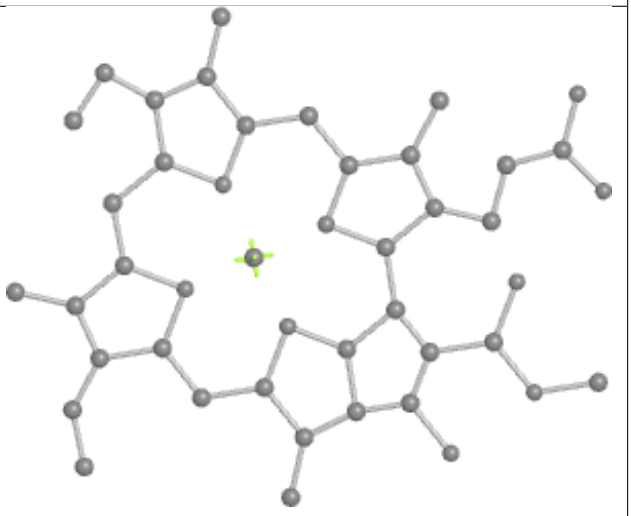
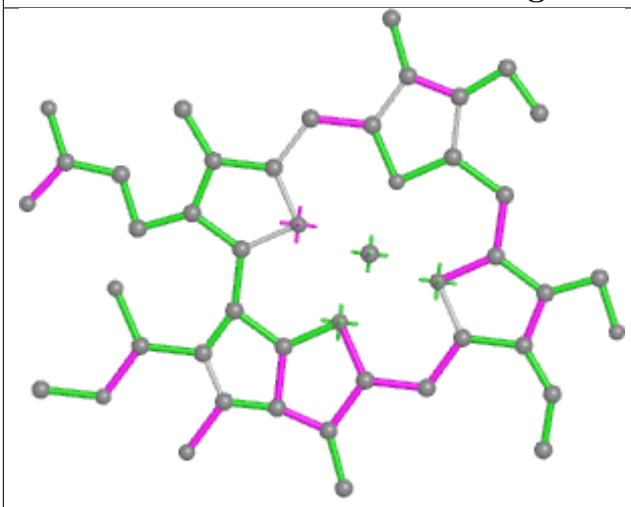


Rings

Ligand CHL 1 605



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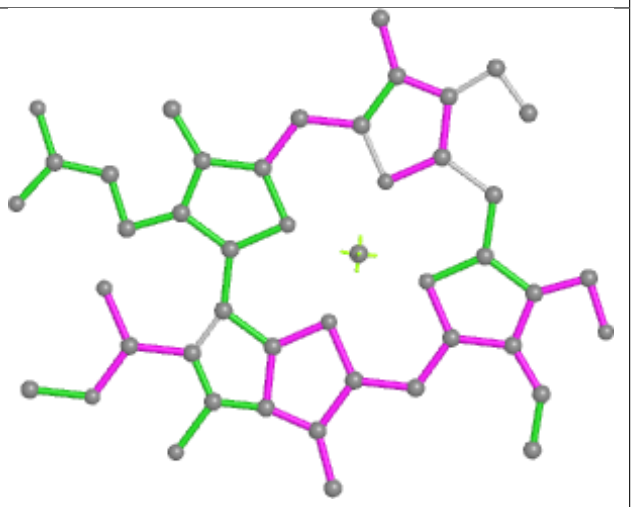

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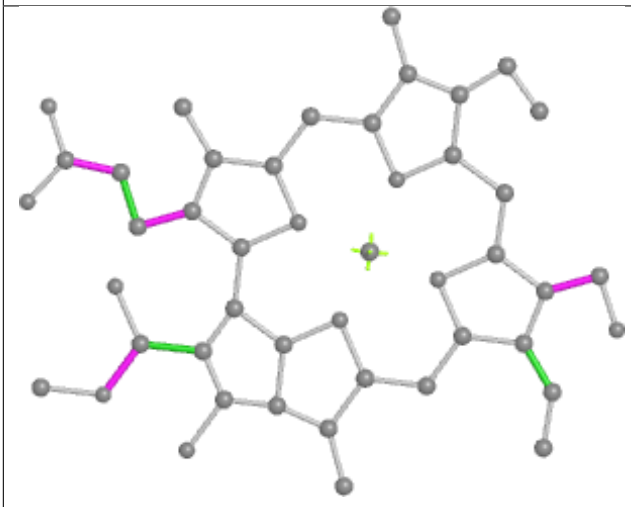

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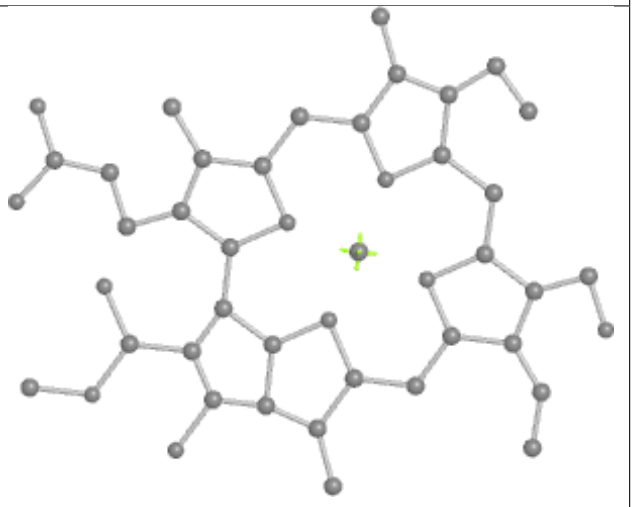

Rings

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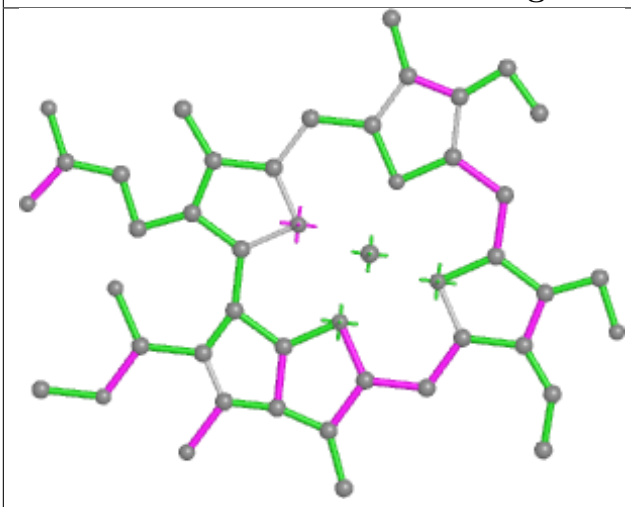

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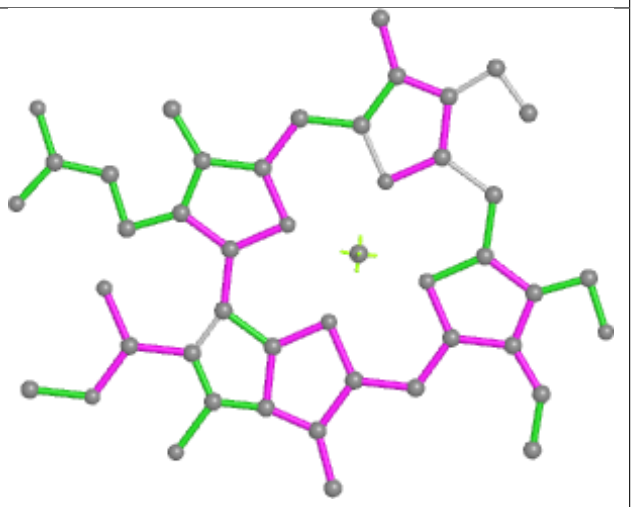
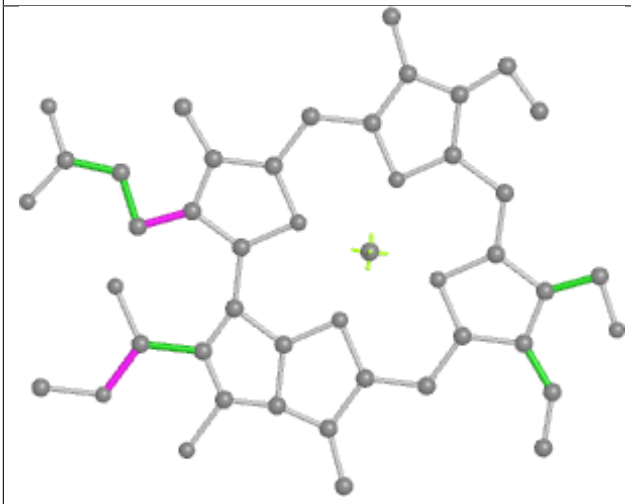
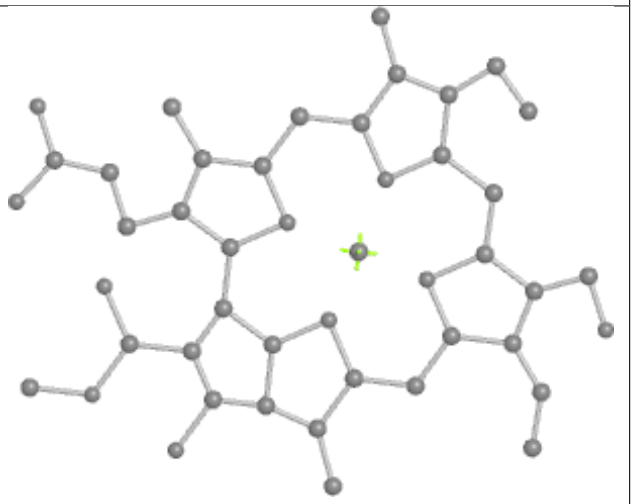


Bond angles

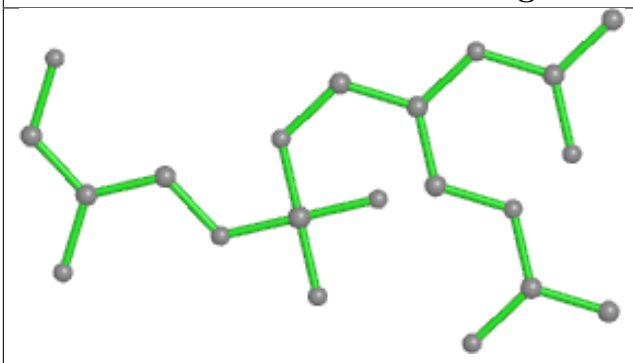


Torsions



Rings

Ligand LHG 4 2630



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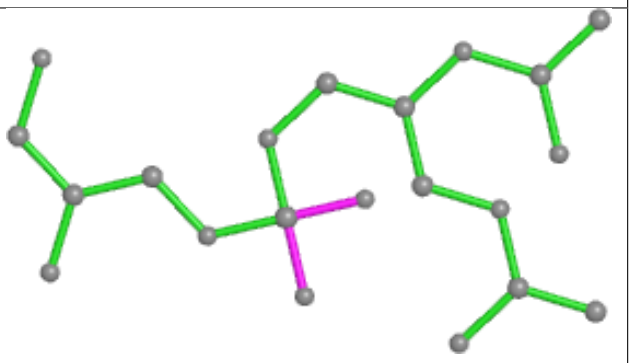
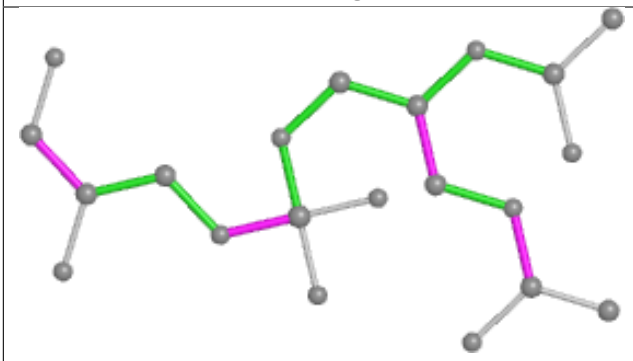


Bond angles



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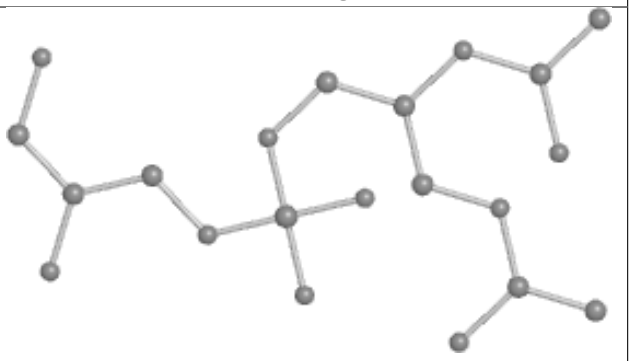
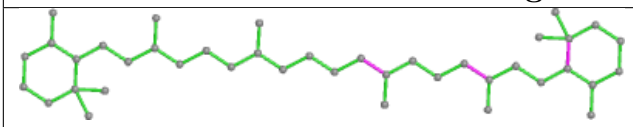


Rings

Ligand BCR b 618



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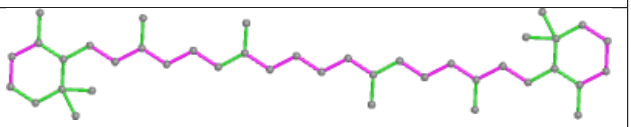
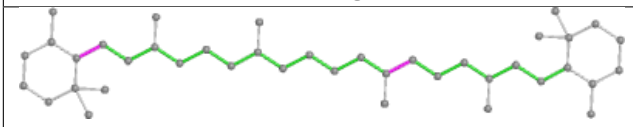
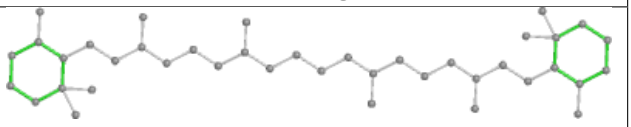


Bond angles

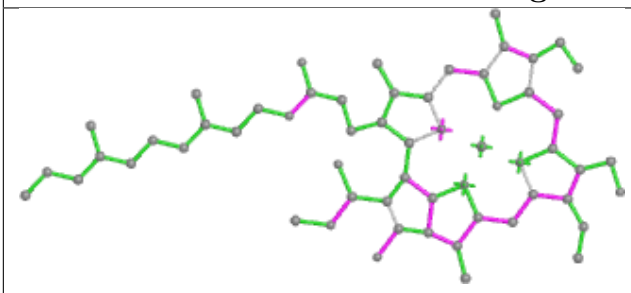


Torsions

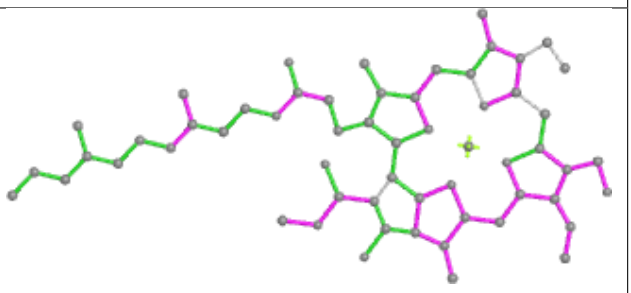


Rings

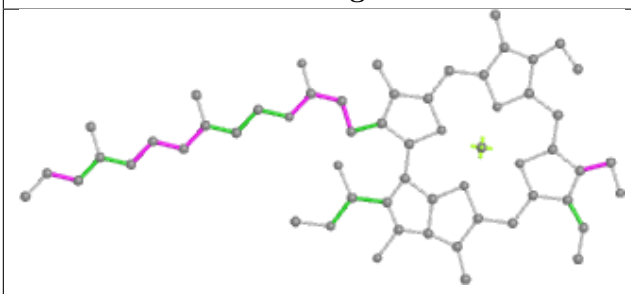
Ligand CHL s 607



Bond lengths



Bond angles



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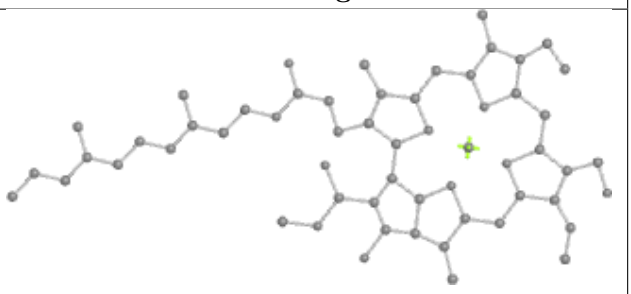
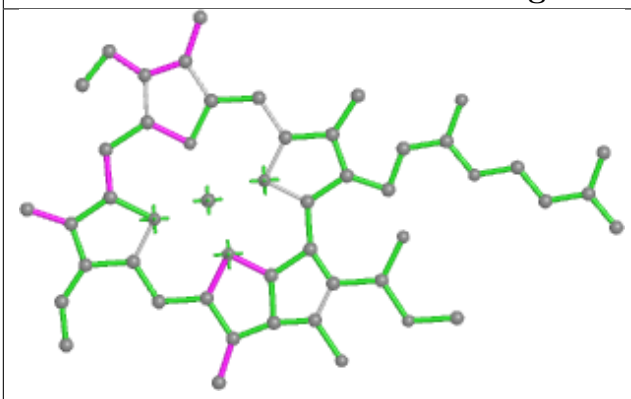


Rings

Ligand CLA 2 610



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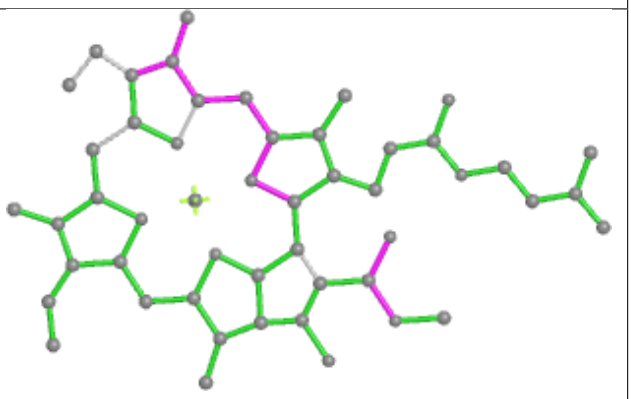
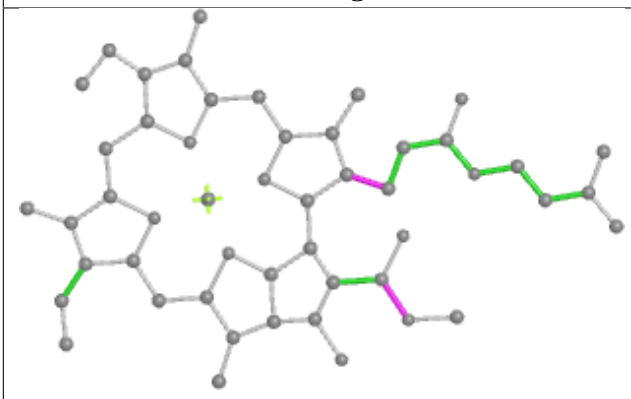


Bond angles



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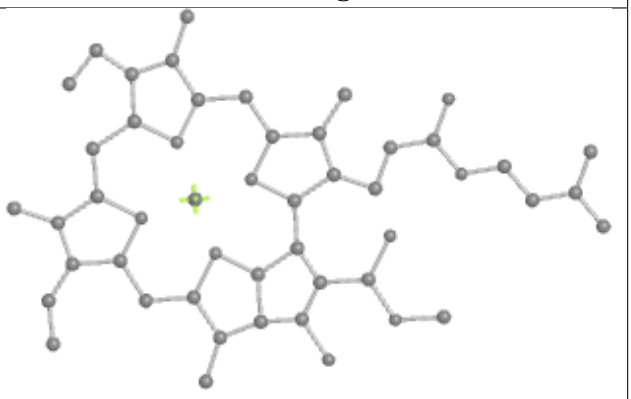
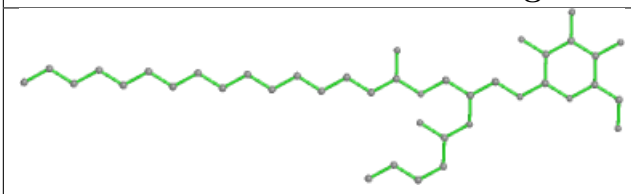


Rings

Ligand LMG a 415



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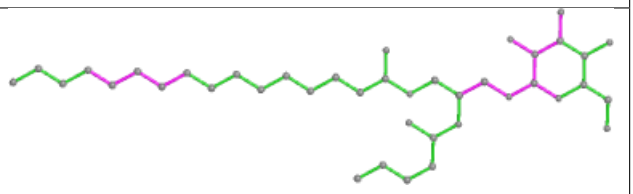
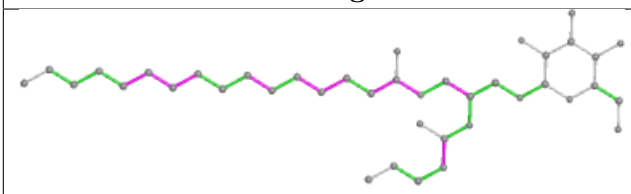


Bond angles



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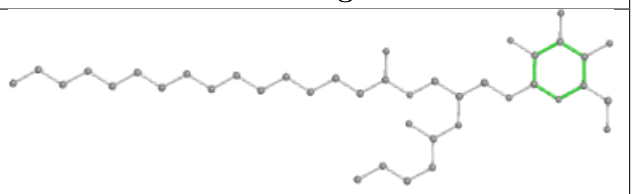
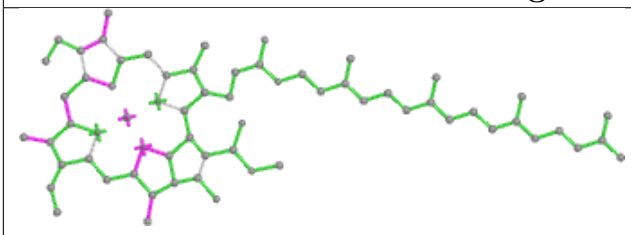


Rings

Ligand CLA g 602



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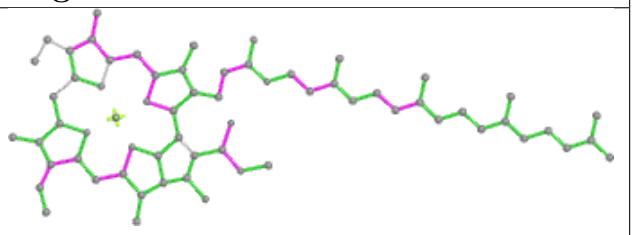
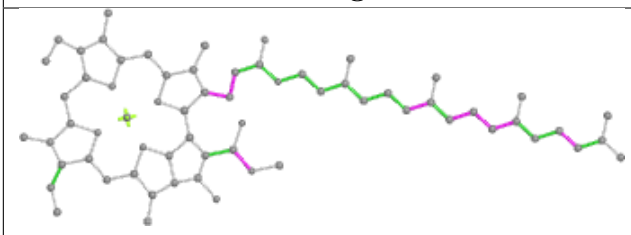


Bond angles



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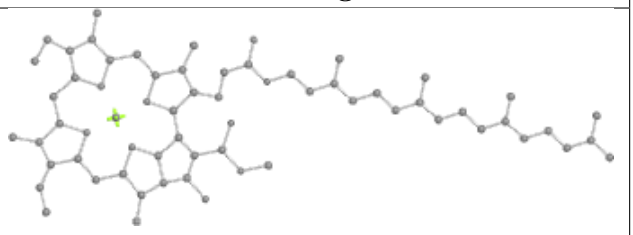
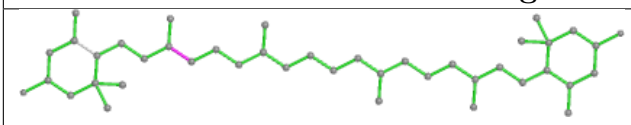


Rings

Ligand LUT g 1620



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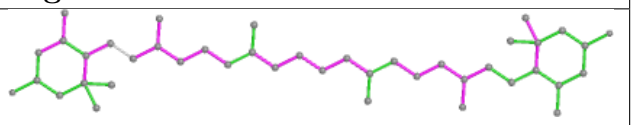
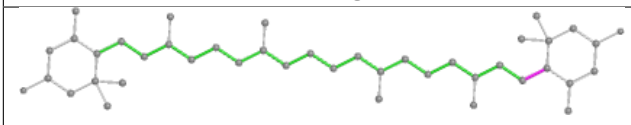


Bond angles



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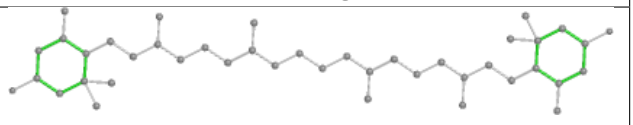
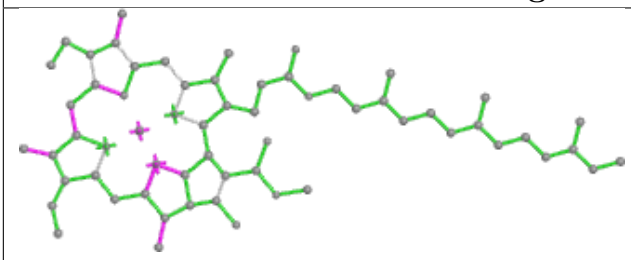


Rings

Ligand CLA 6 602



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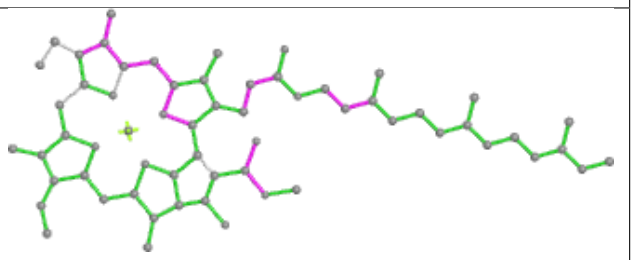

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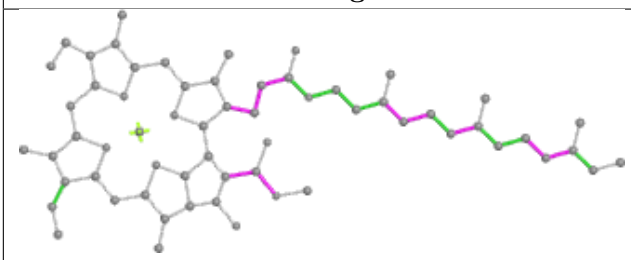

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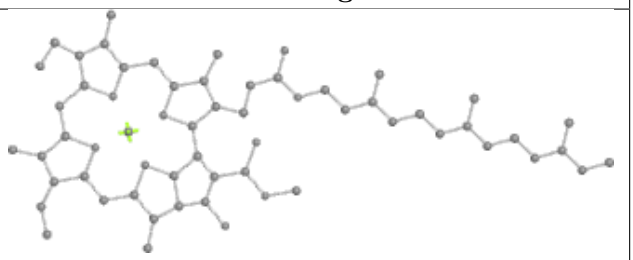
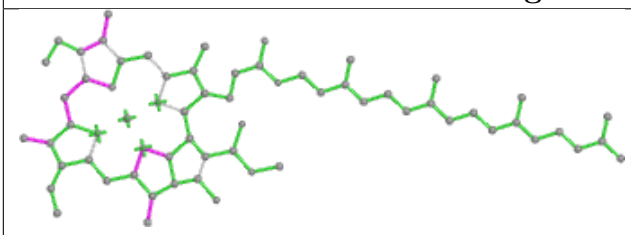


Rings

Ligand CLA B 617



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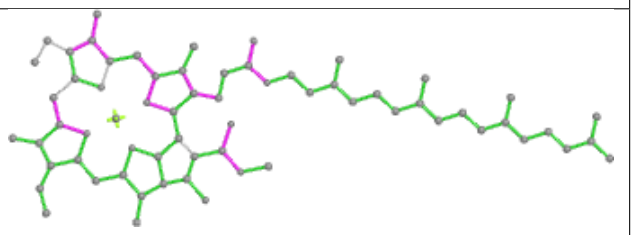

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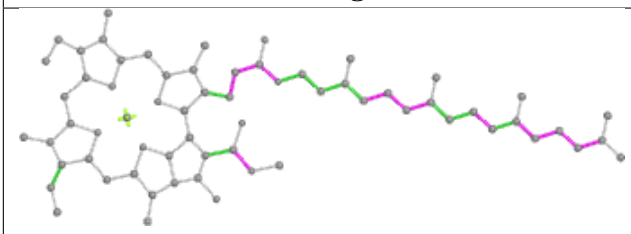

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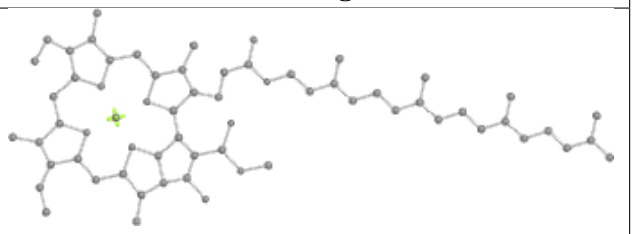
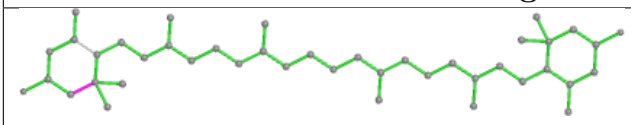


Rings

Ligand LUT 2 1621



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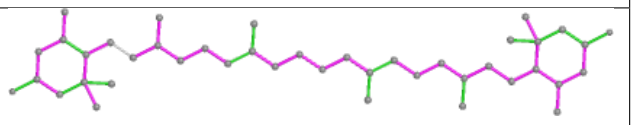
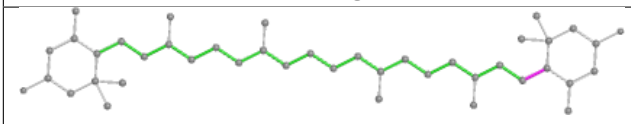


Bond angles



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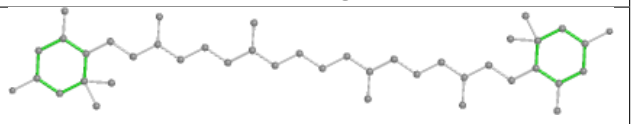
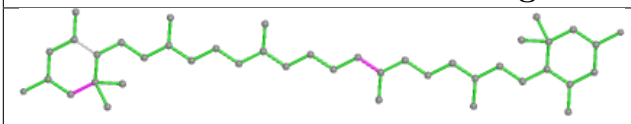


Rings

Ligand LUT n 1620



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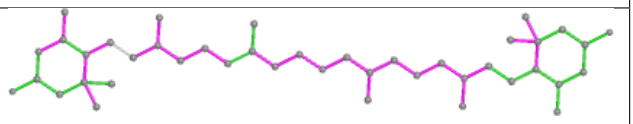

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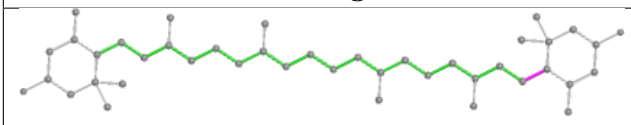

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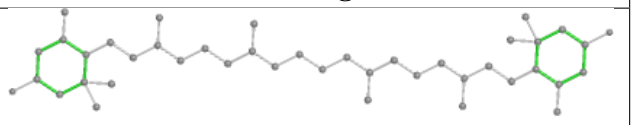
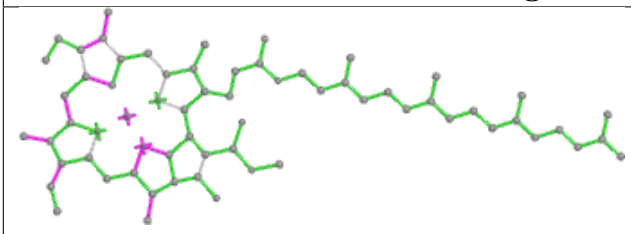


Rings

Ligand CLA N 603



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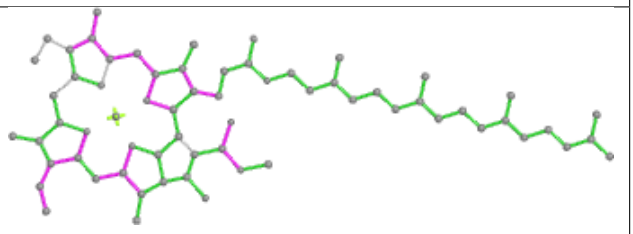
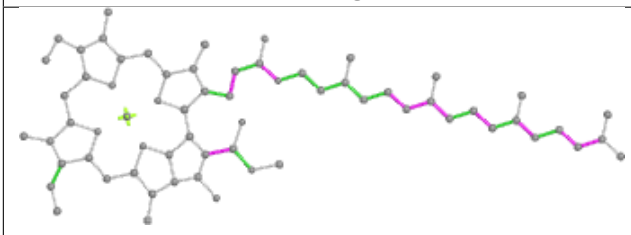


Bond angles



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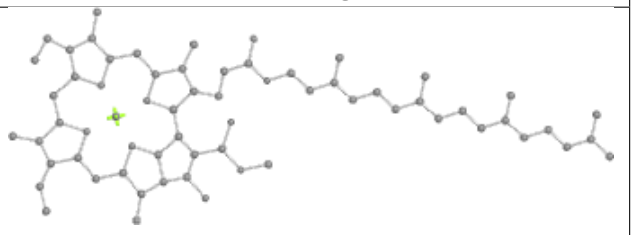
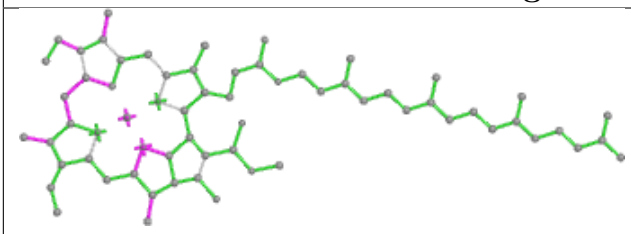


Rings

Ligand CLA D 403



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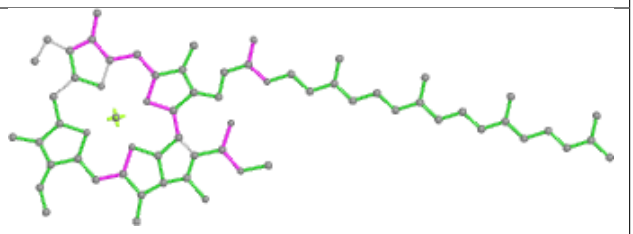
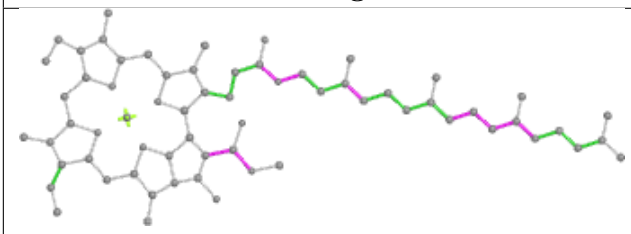


Bond angles



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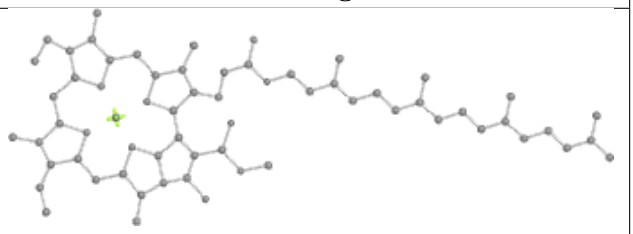
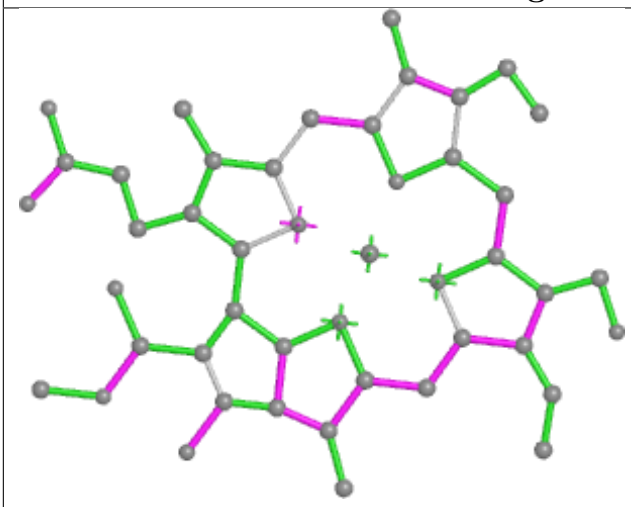


Rings

Ligand CHL 4 607



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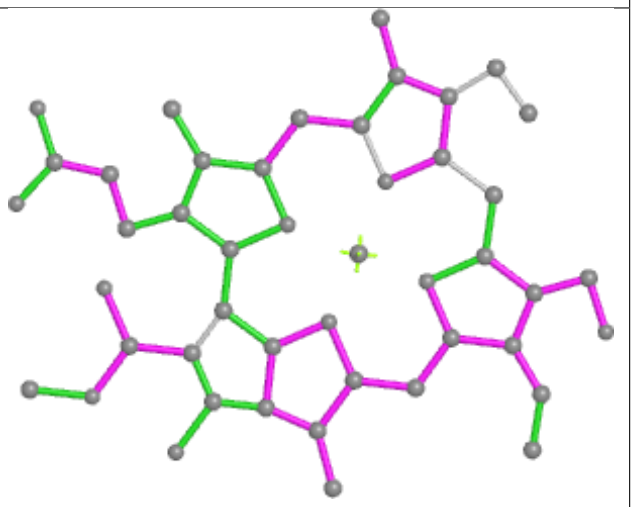
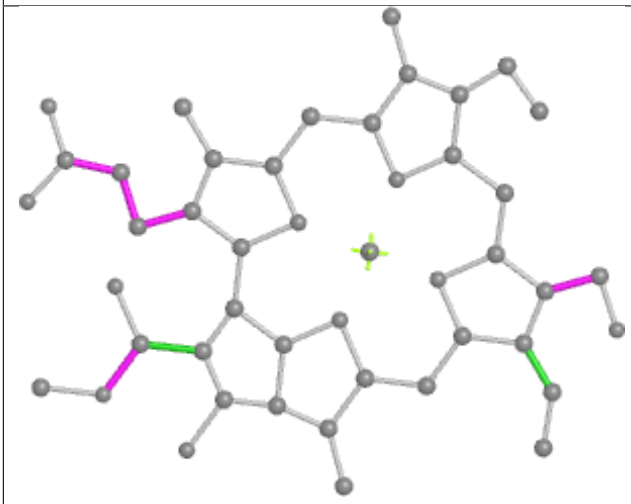


Bond angles



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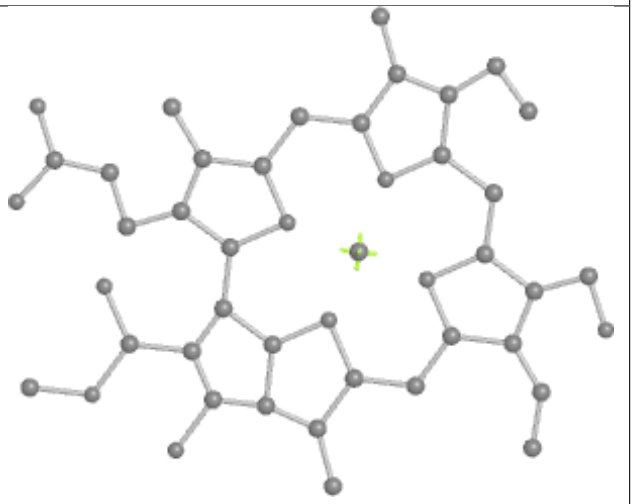
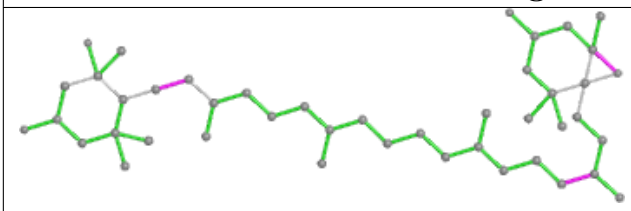


Rings

Ligand NEX r 623



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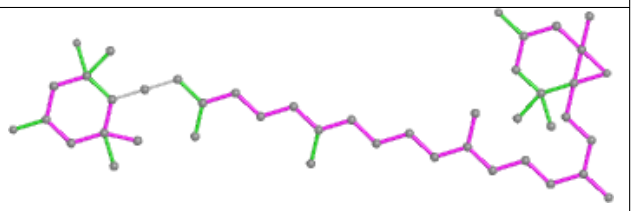
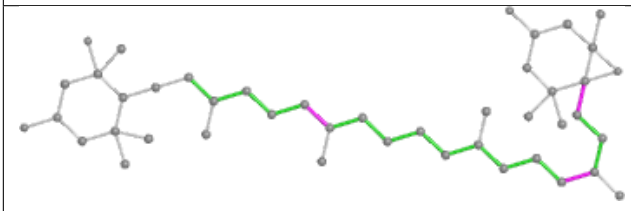


Bond angles



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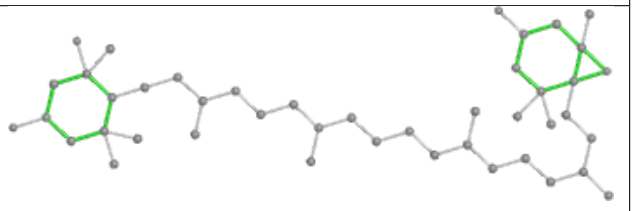
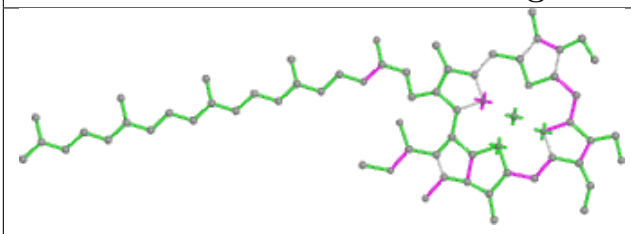
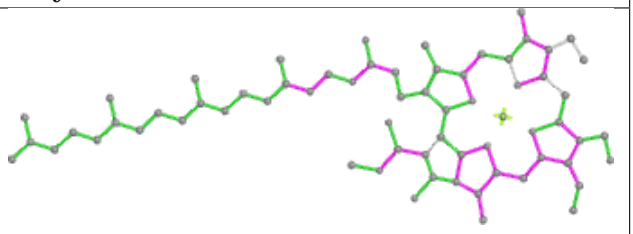


Rings

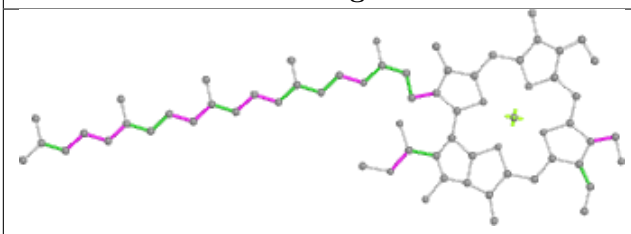
Ligand CHL y 608



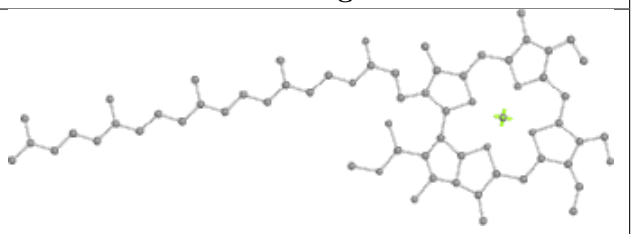
Bond lengths



Bond angles

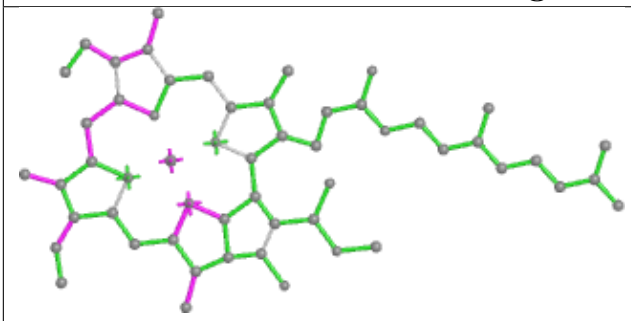


Torsions



Rings

Ligand CLA 1 603



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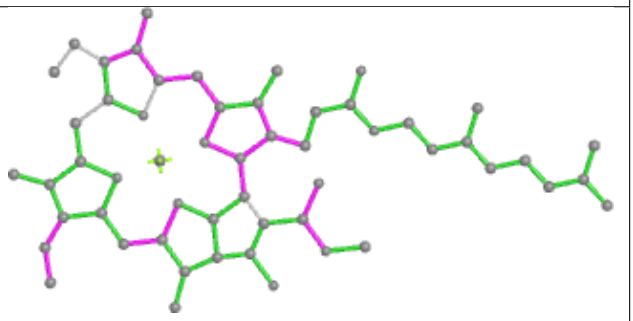

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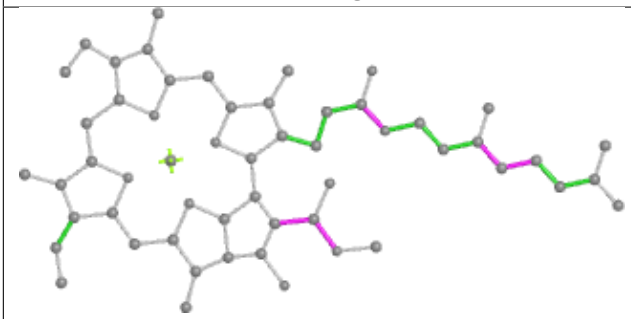

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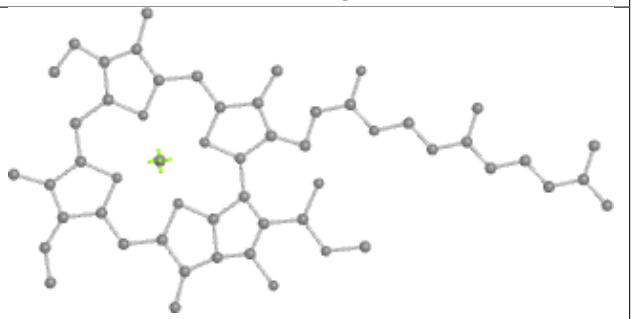
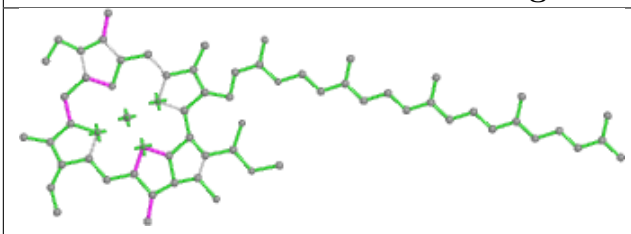


Rings

Ligand CLA c 511



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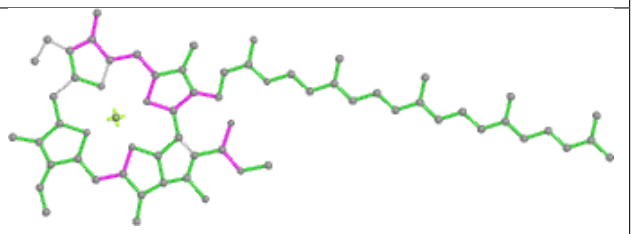
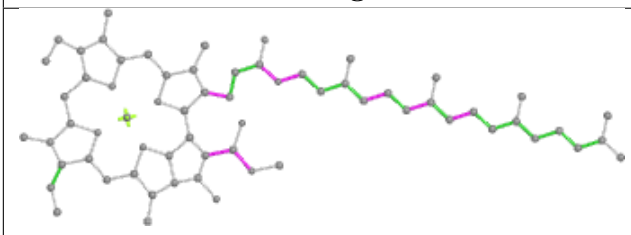


Bond angles



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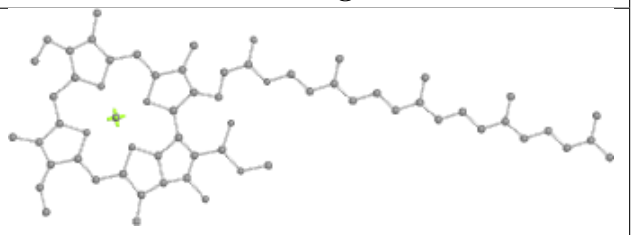
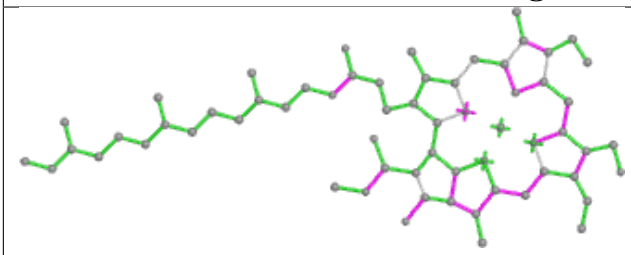


Rings

Ligand CHL 5 609



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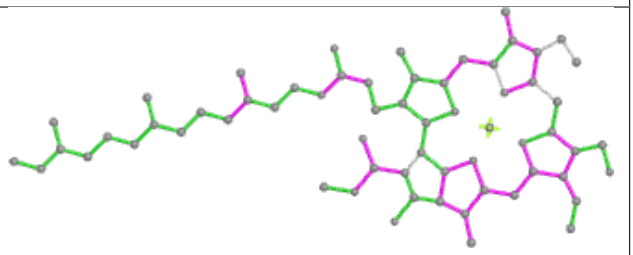
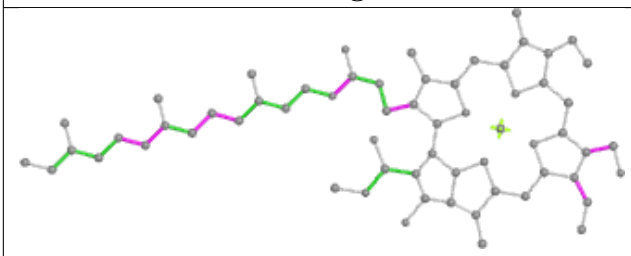


Bond angles



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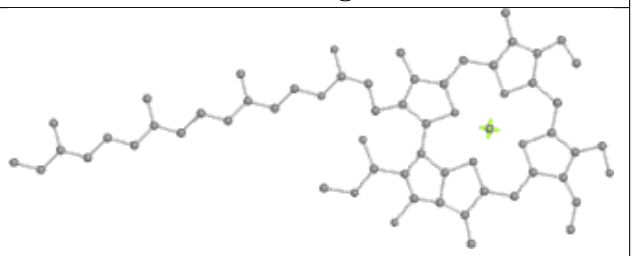
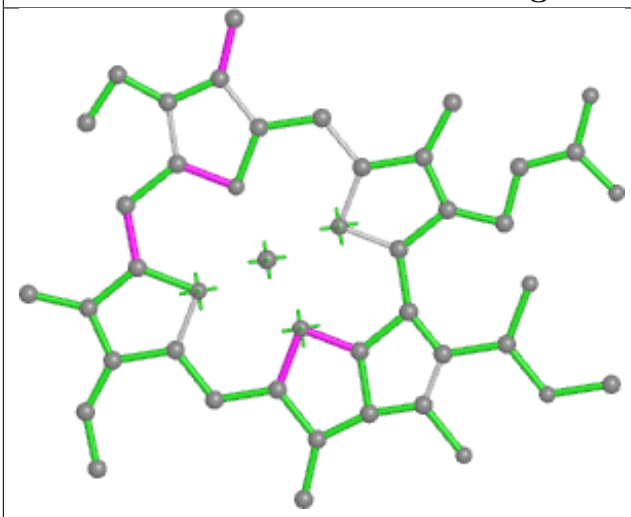


Rings

Ligand CLA s 609



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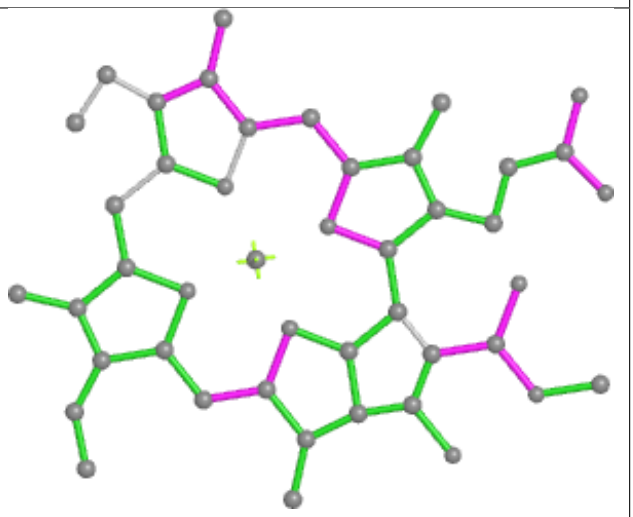

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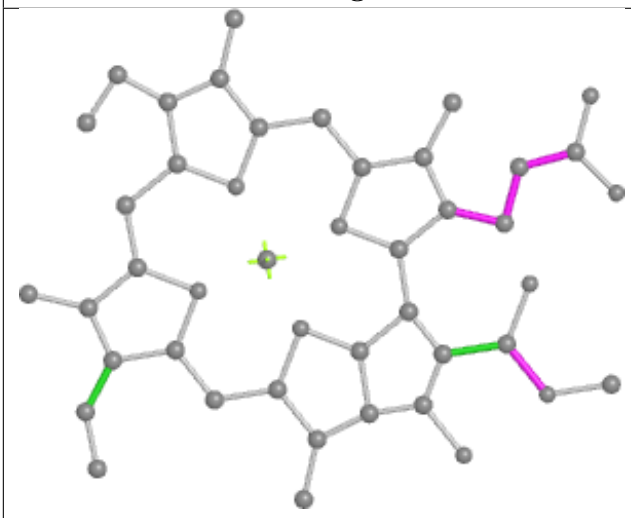

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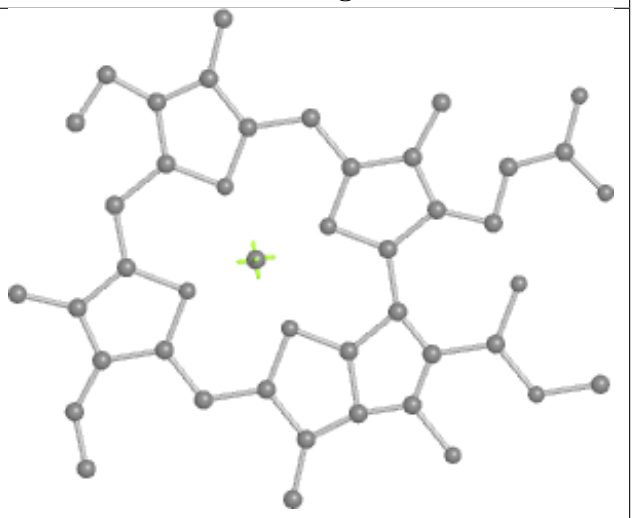
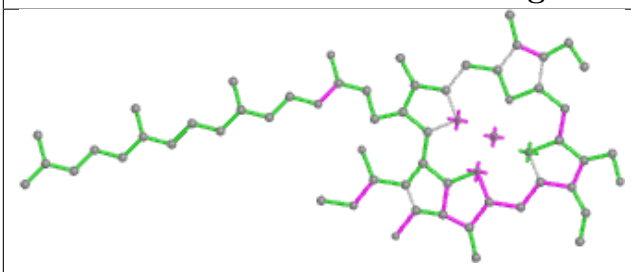


Rings

Ligand CHL 2 607



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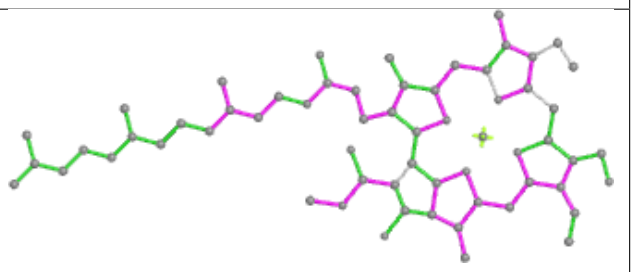
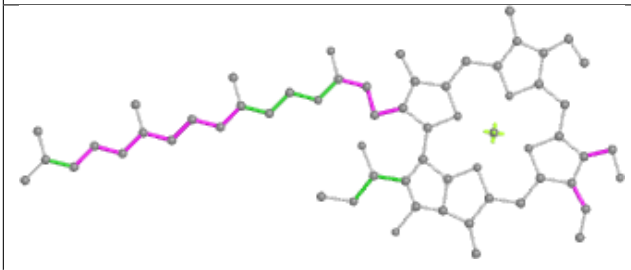


Bond angles



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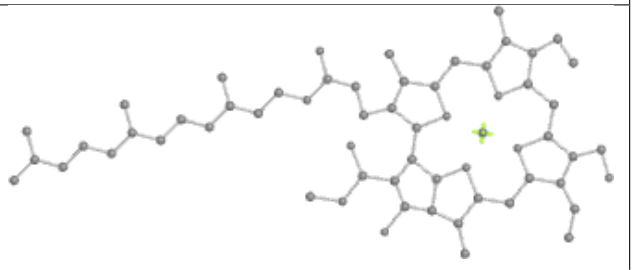
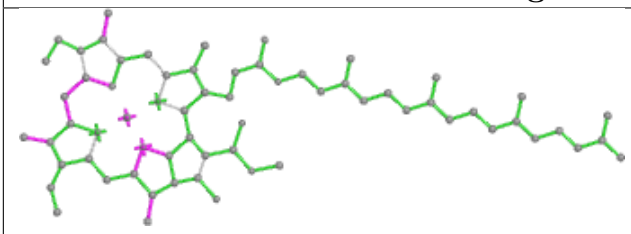


Rings

Ligand CLA b 609



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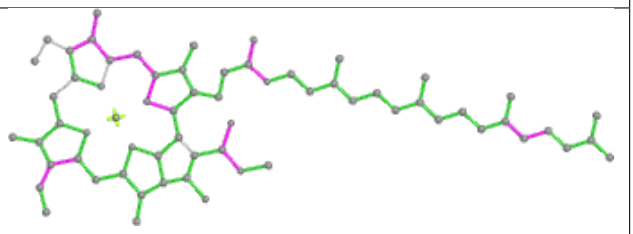

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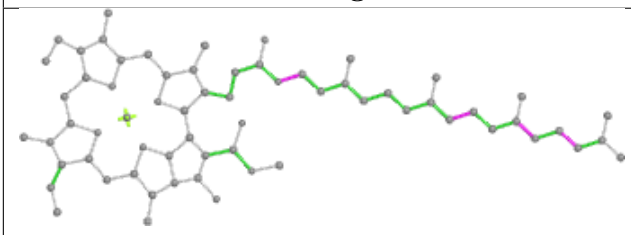

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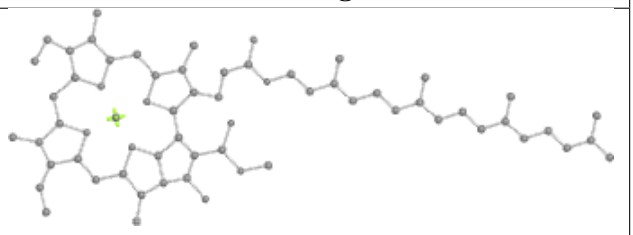

Rings

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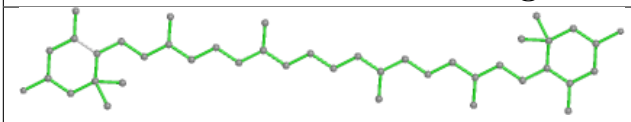

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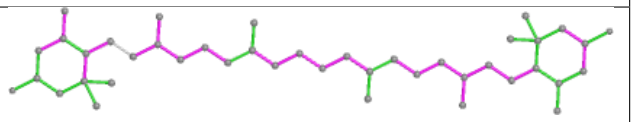

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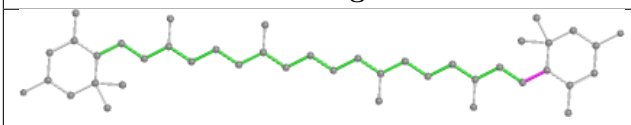

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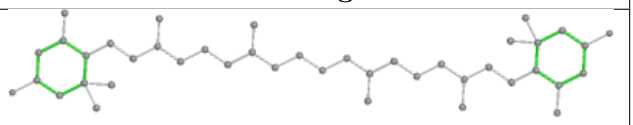
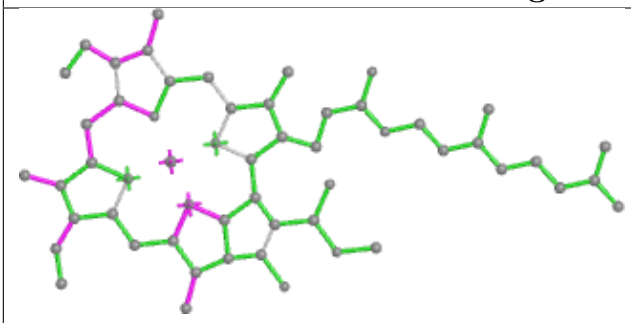


Rings

Ligand CLA 5 603



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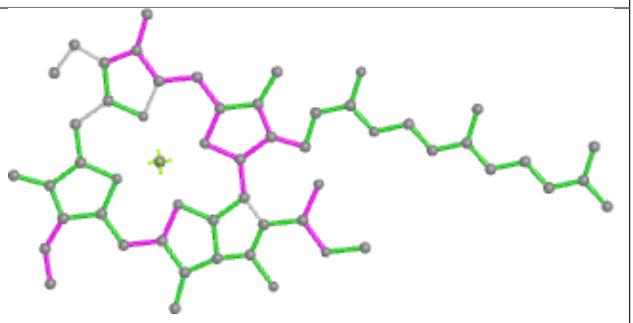
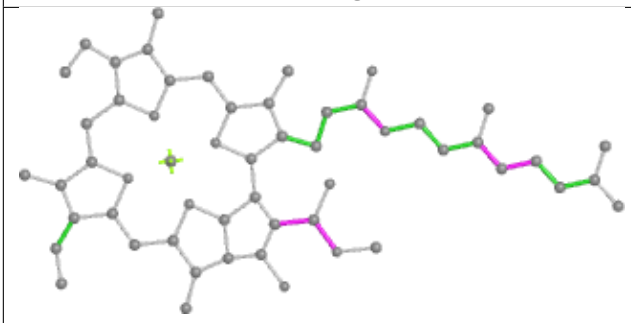


Bond angles



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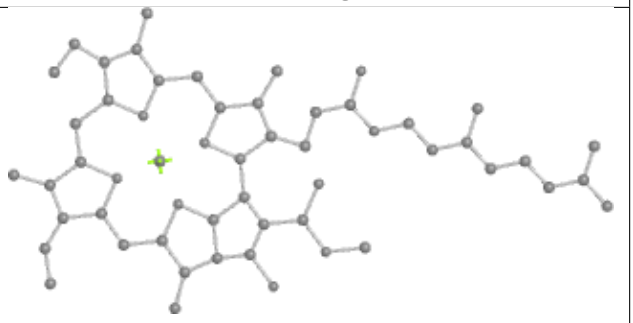
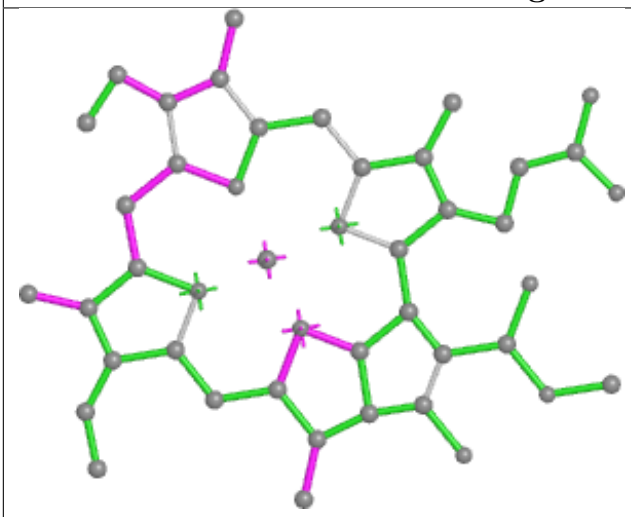


Rings

Ligand CLA 7 612



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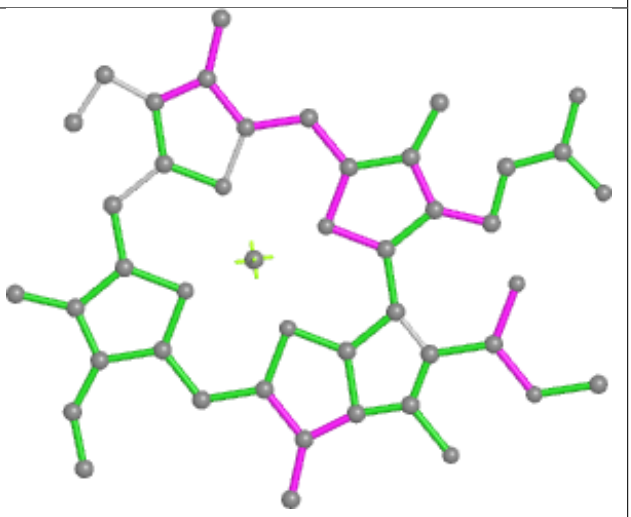
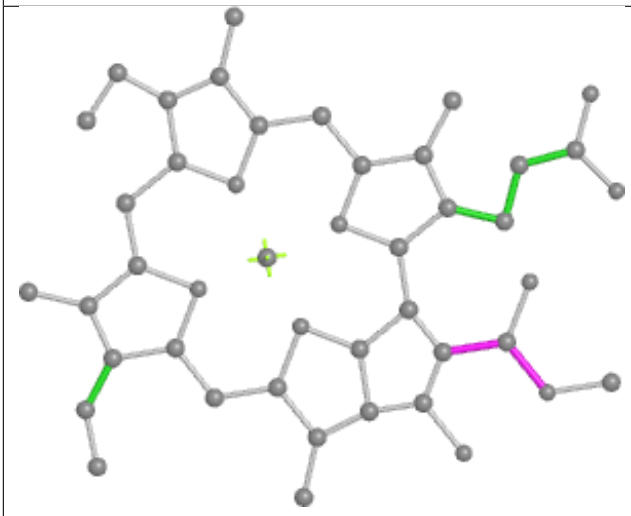


Bond angles



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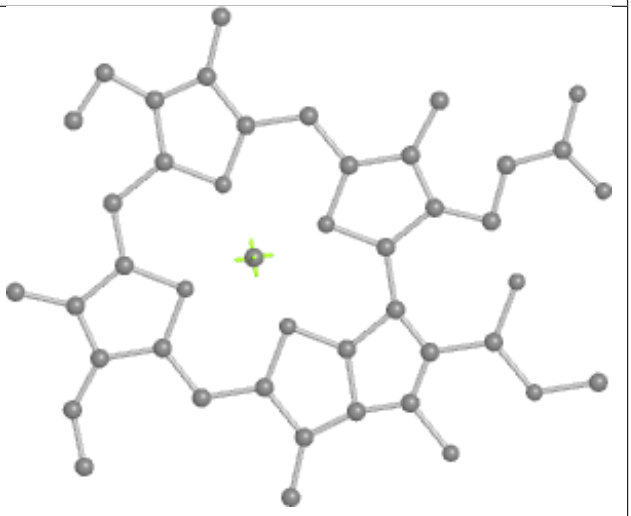
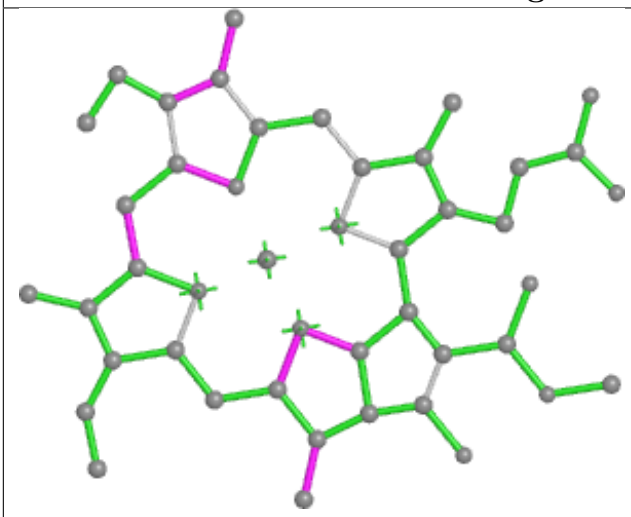


Rings

Ligand CLA S 603



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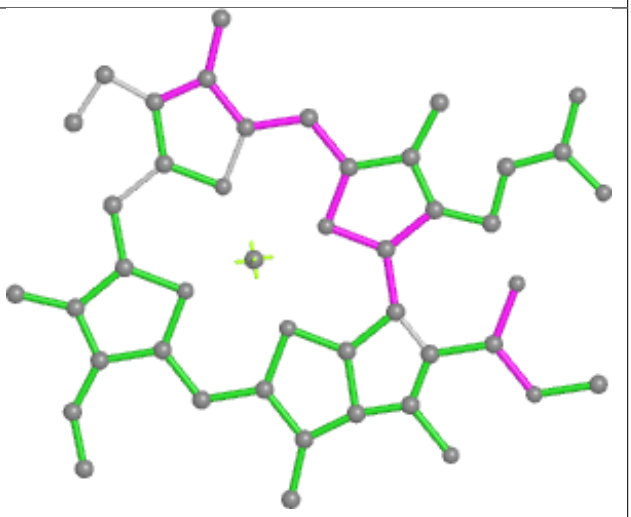
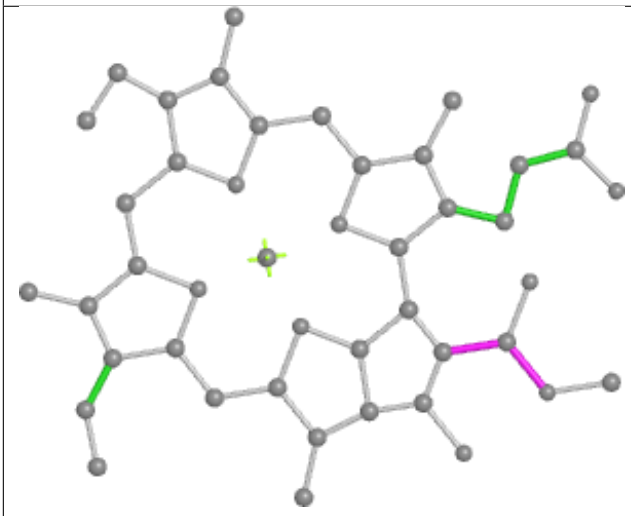


Bond angles



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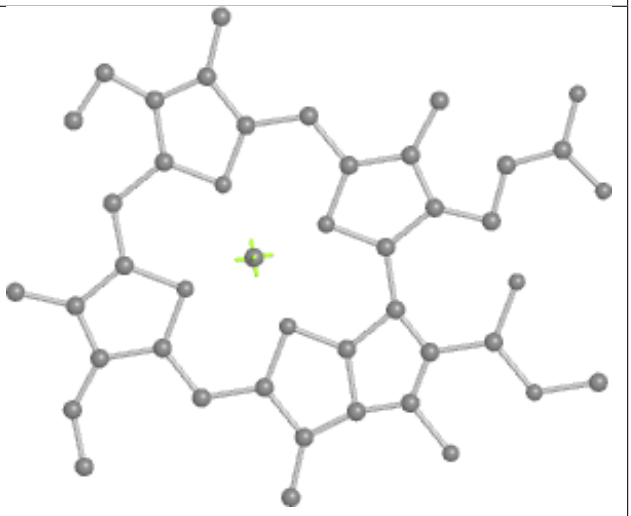
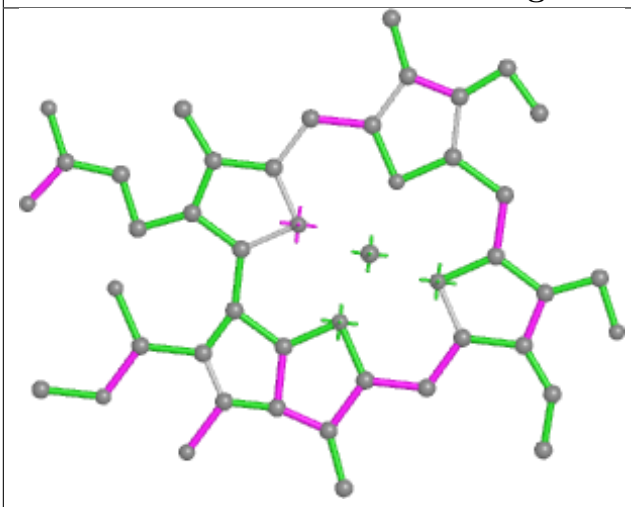


Rings

Ligand CHL 8 608



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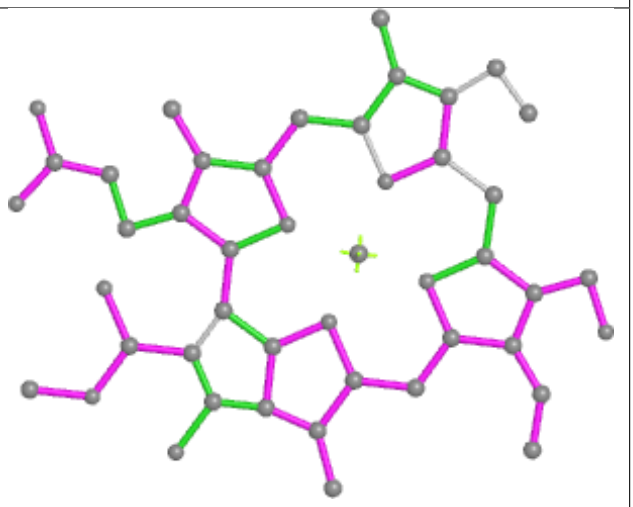
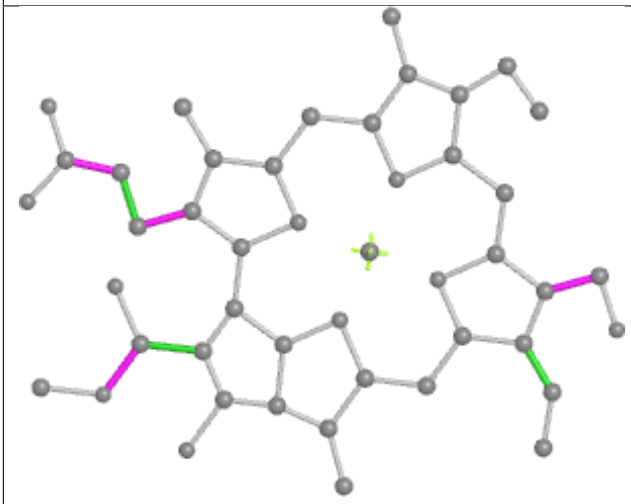


Bond angles



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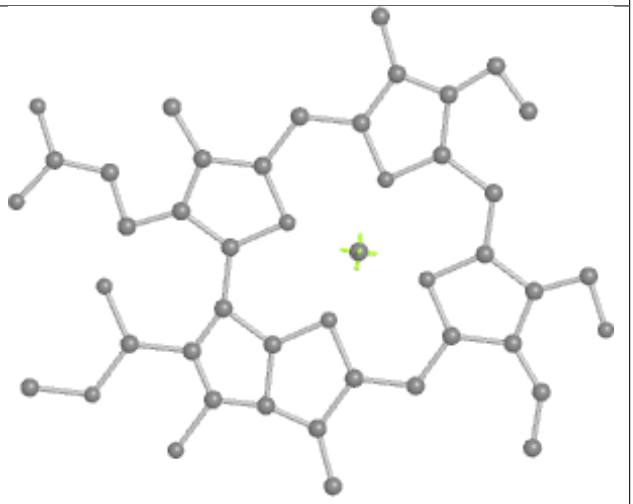
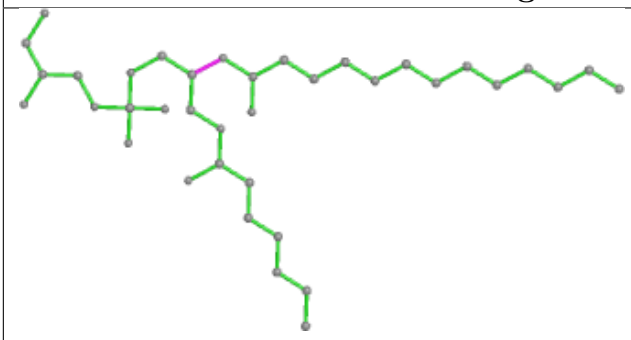


Rings

Ligand LHG 6 2630



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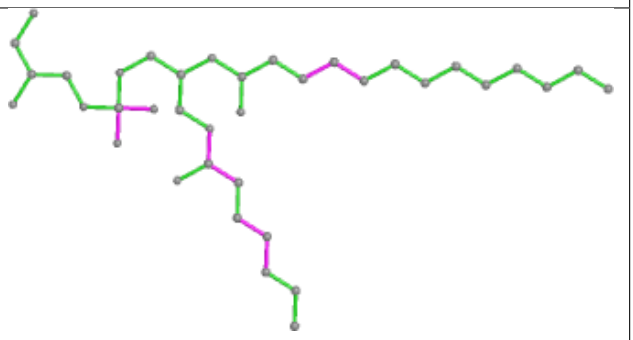
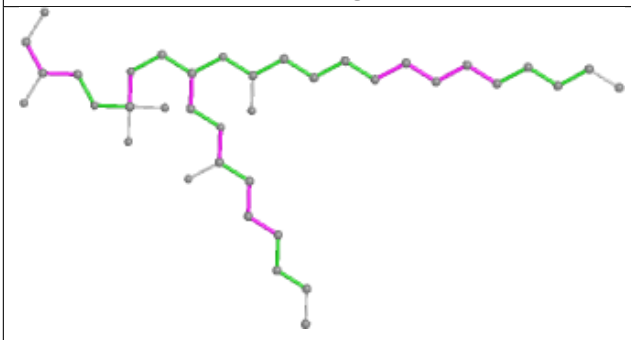


Bond angles



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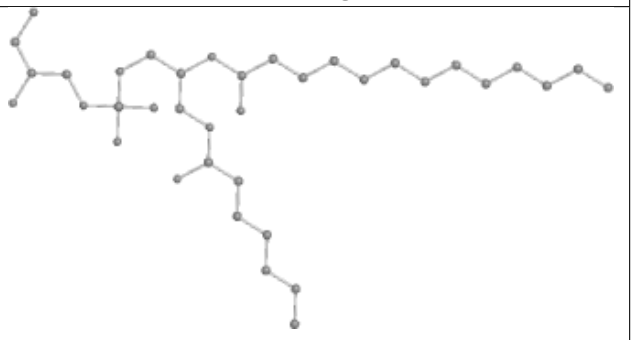
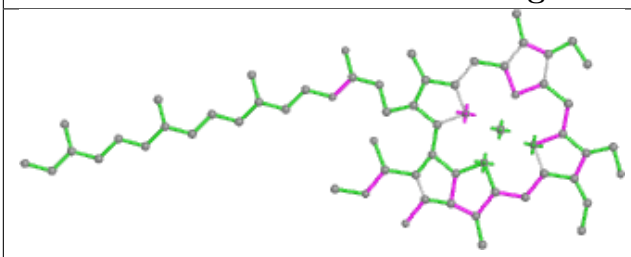


Rings

Ligand CHL 1 609



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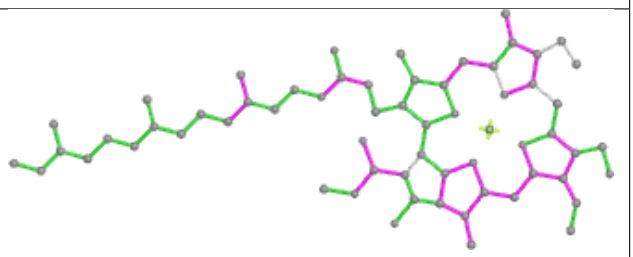

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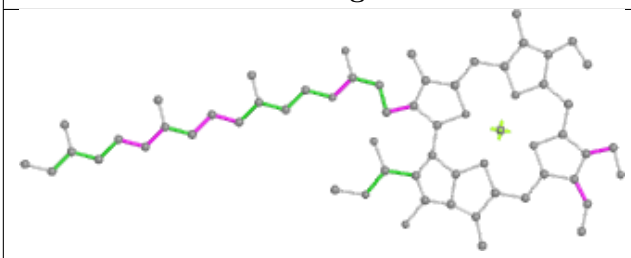
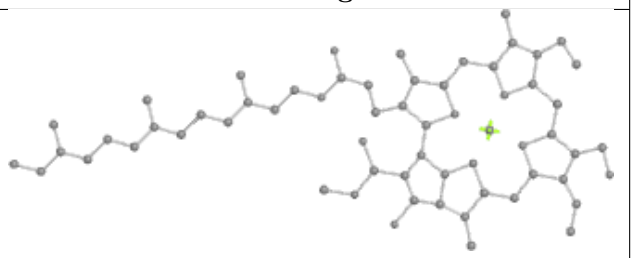
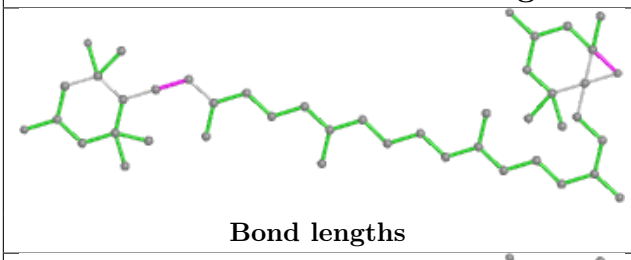


Torsions

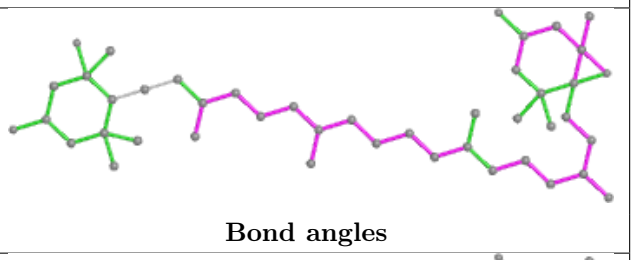


Rings

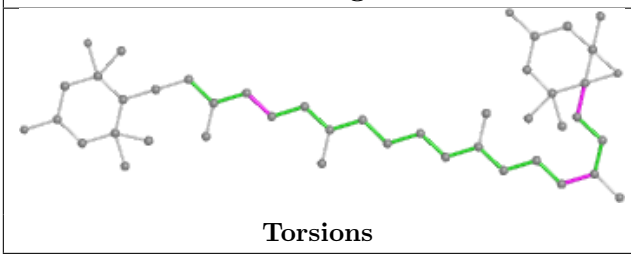
Ligand NEX 7 1623



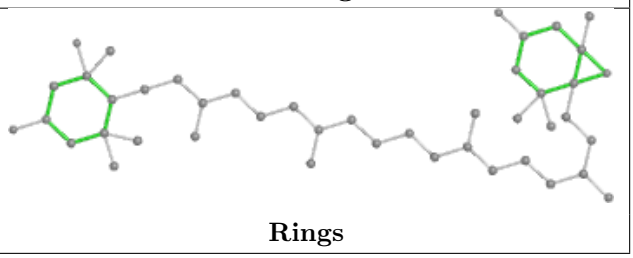
Bond lengths



Bond angles

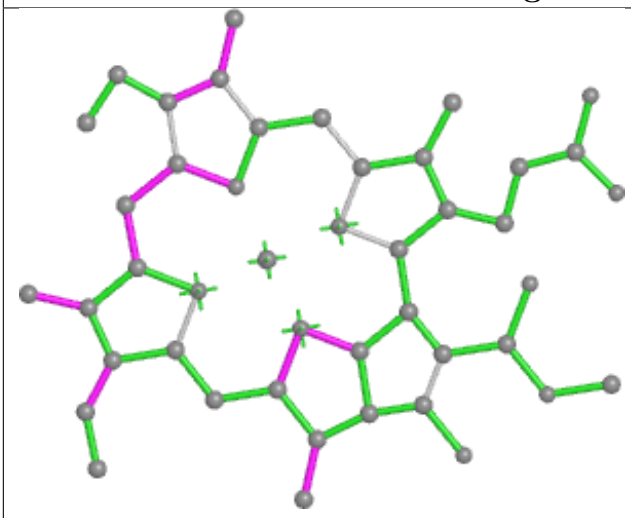


Torsions



Rings

Ligand CLA R 616



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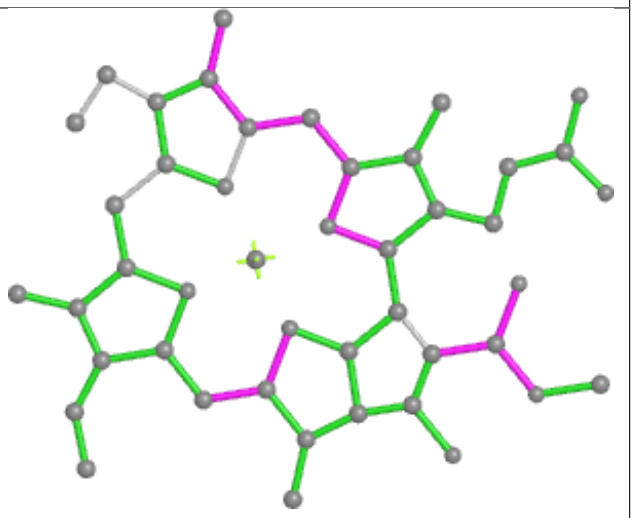
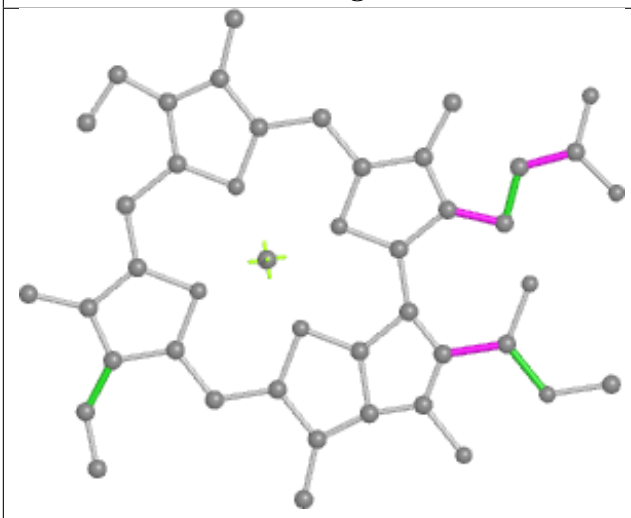


Bond angles



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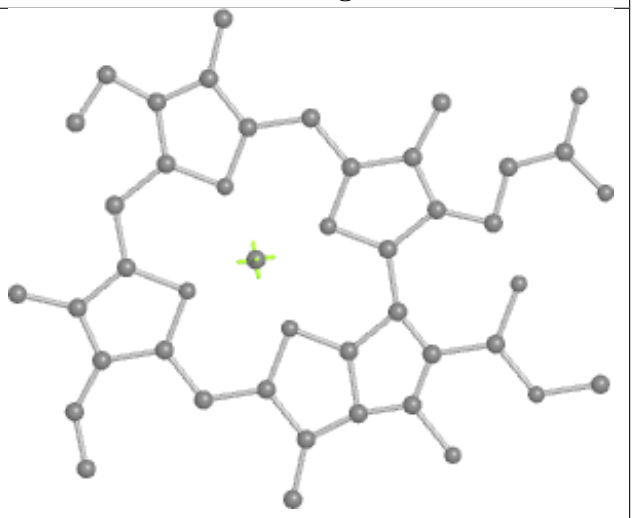
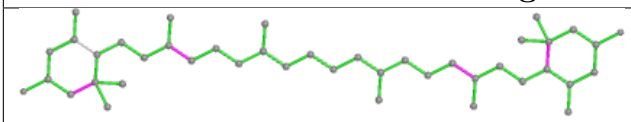


Rings

Ligand LUT y 1621



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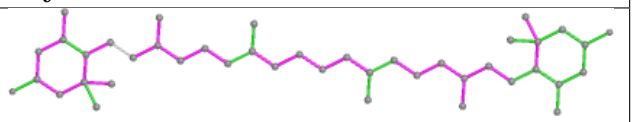
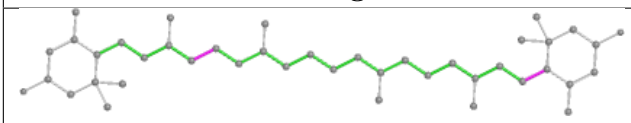


Bond angles



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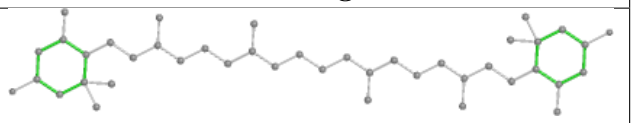
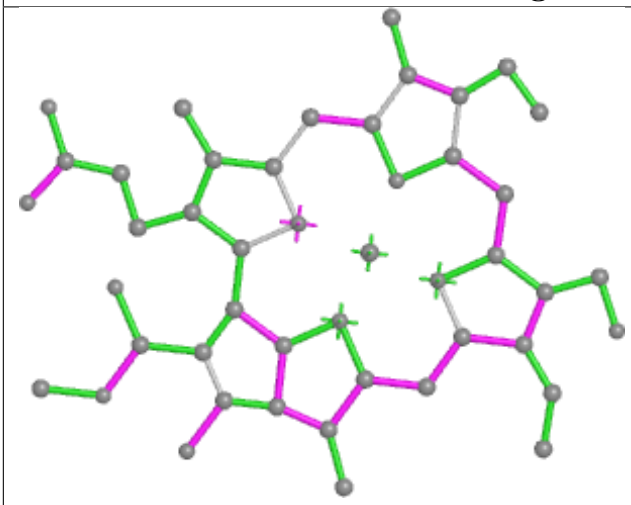


Rings

Ligand CHL s 606



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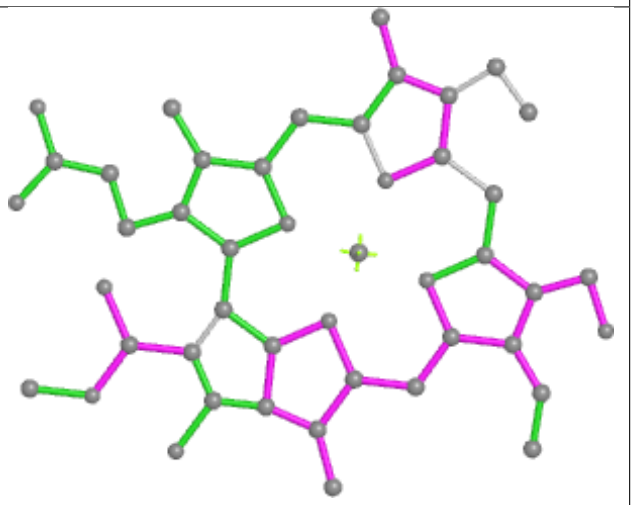
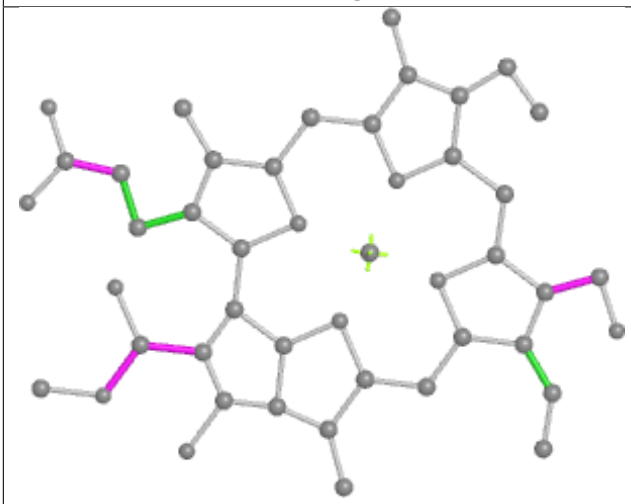
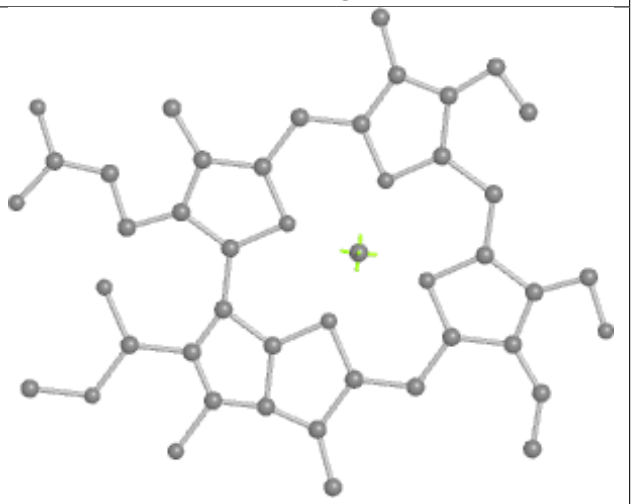


Bond angles

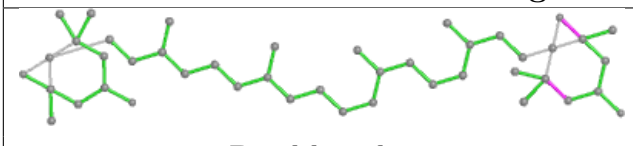


Torsions



Rings

Ligand XAT r 622



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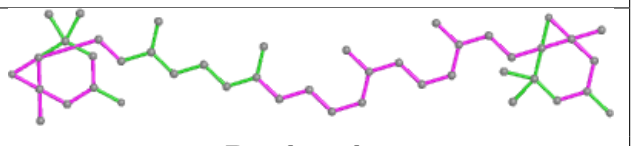

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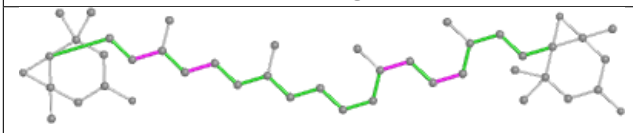

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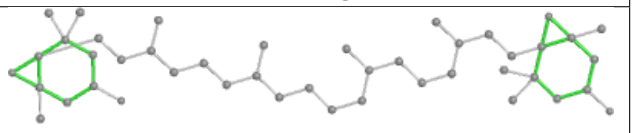
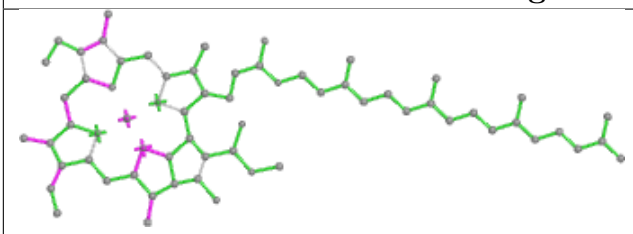


Rings

Ligand CLA g 603



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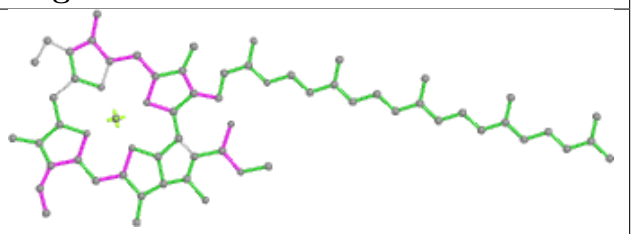
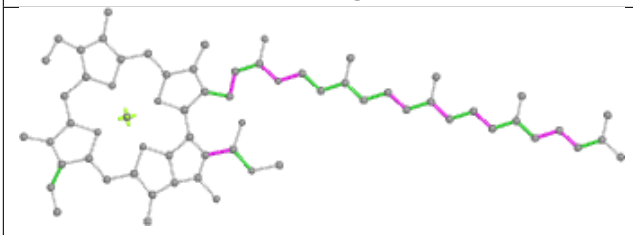


Bond angles



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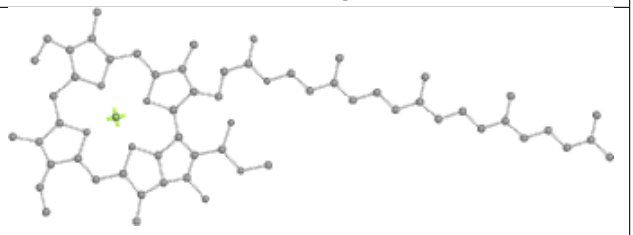
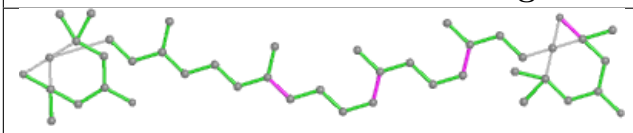


Rings

Ligand XAT y 1622



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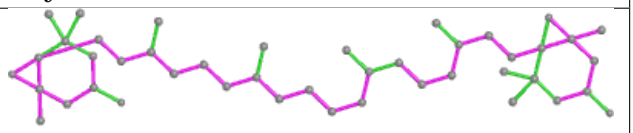
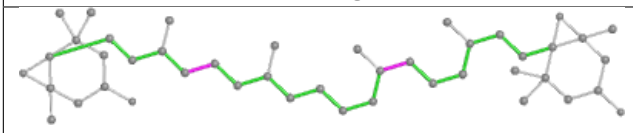


Bond angles



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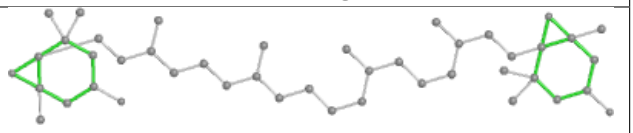
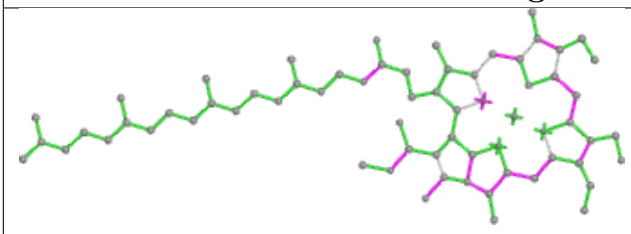


Rings

Ligand CHL g 608



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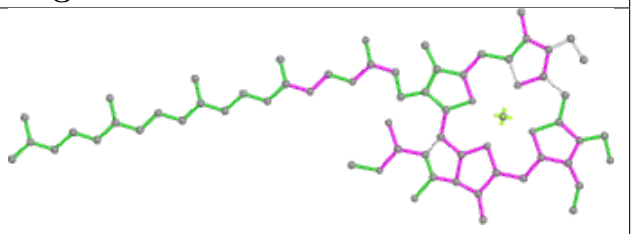
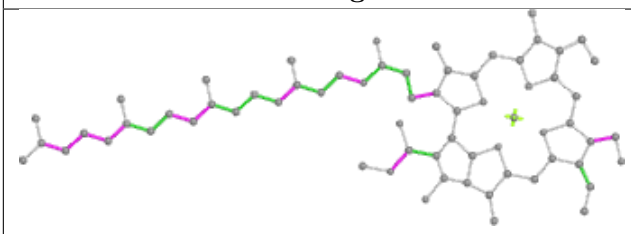


Bond angles



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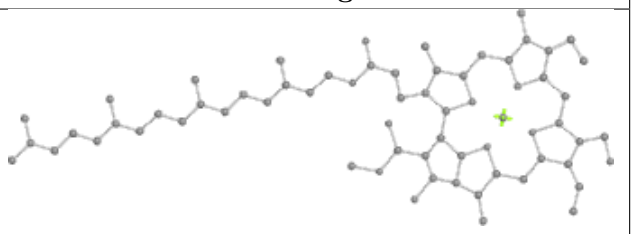
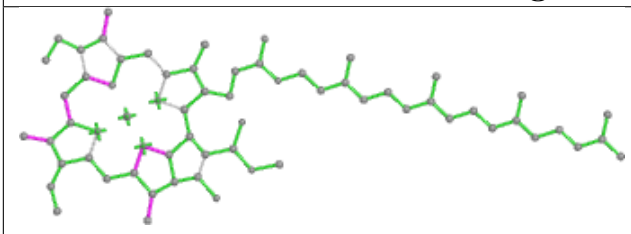


Rings

Ligand CLA c 504



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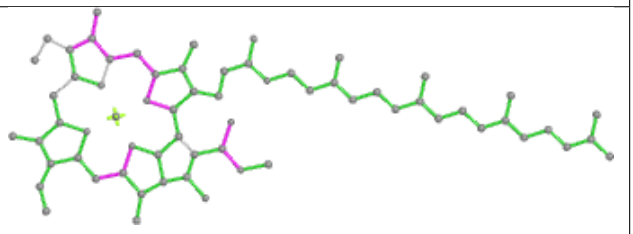
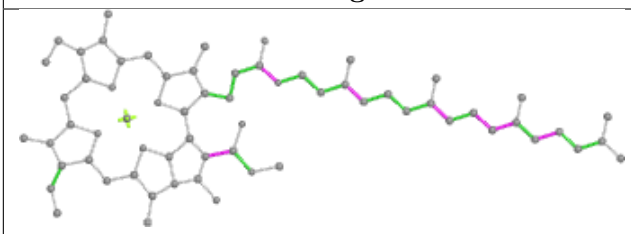


Bond angles



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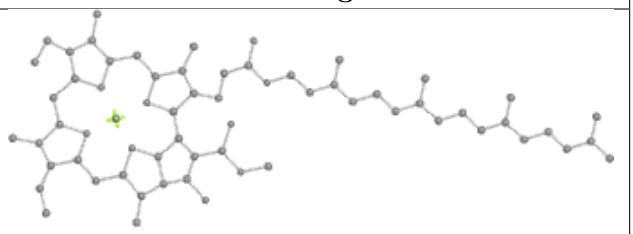
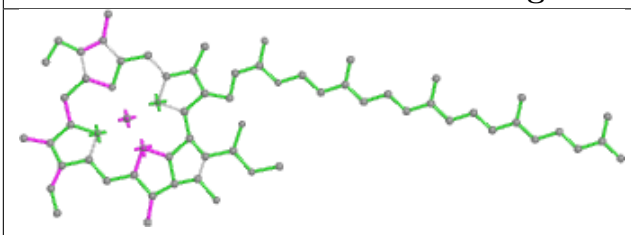


Rings

Ligand CLA n 603



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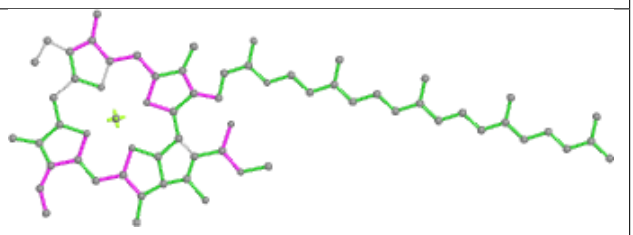

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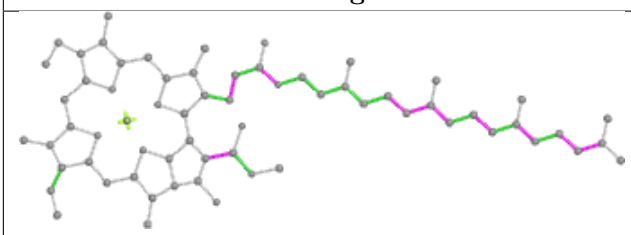

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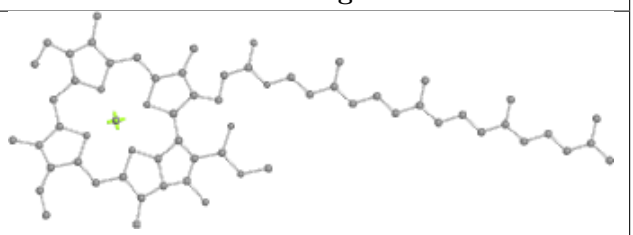
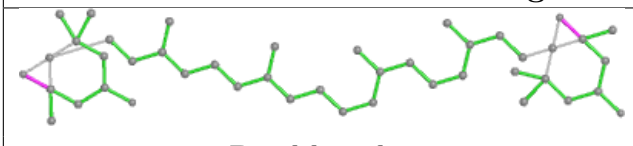


Rings

Ligand XAT 4 622



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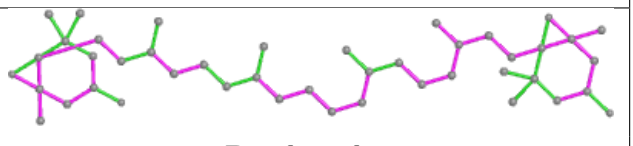
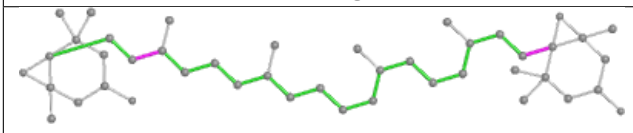


Bond angles



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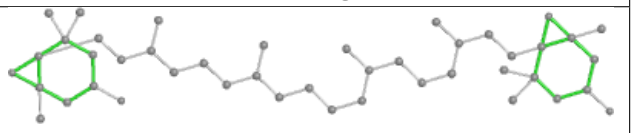
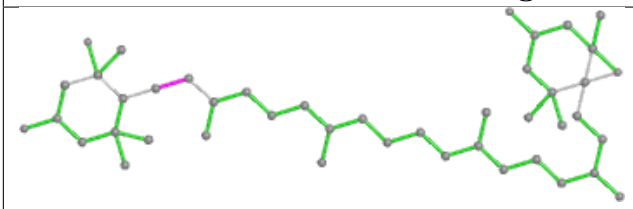


Rings

Ligand NEX 2 1623



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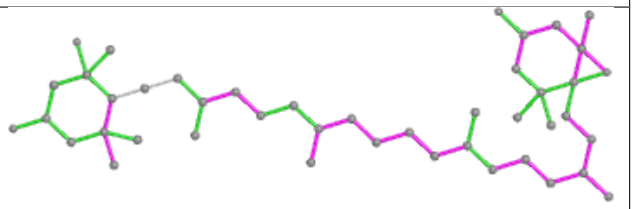
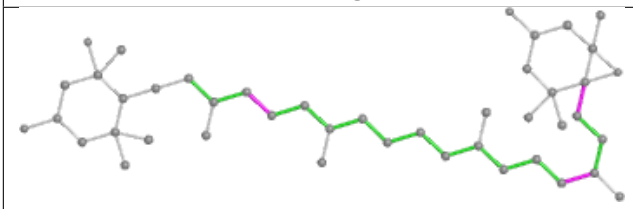


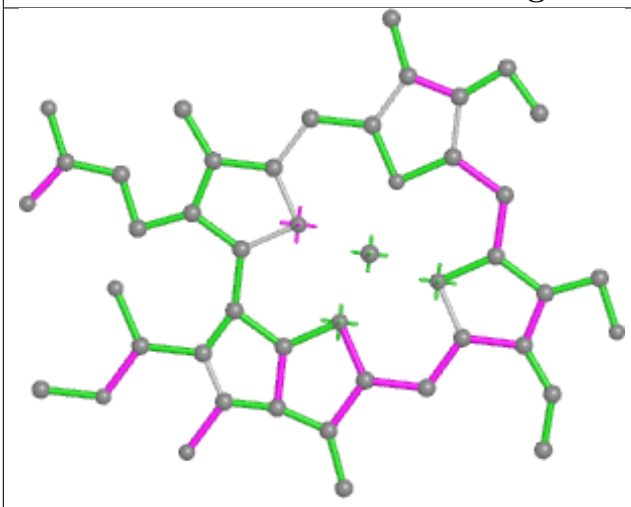
Bond angles



Torsions

Rings

Ligand CHL 3 606



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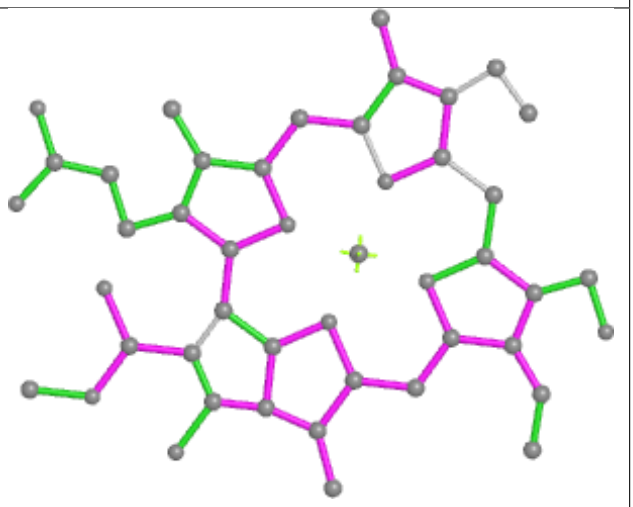
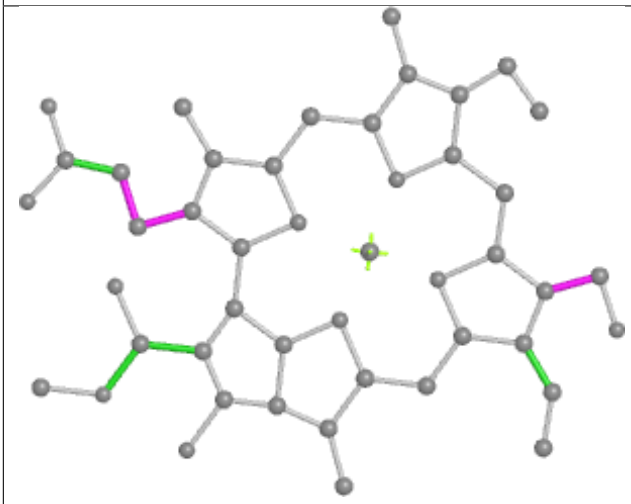
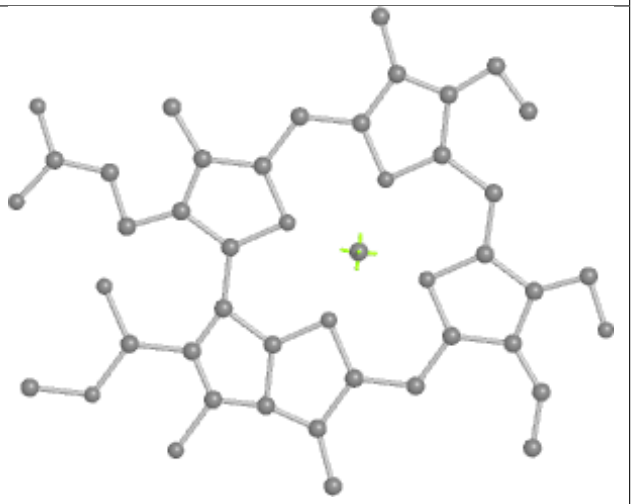


Bond angles

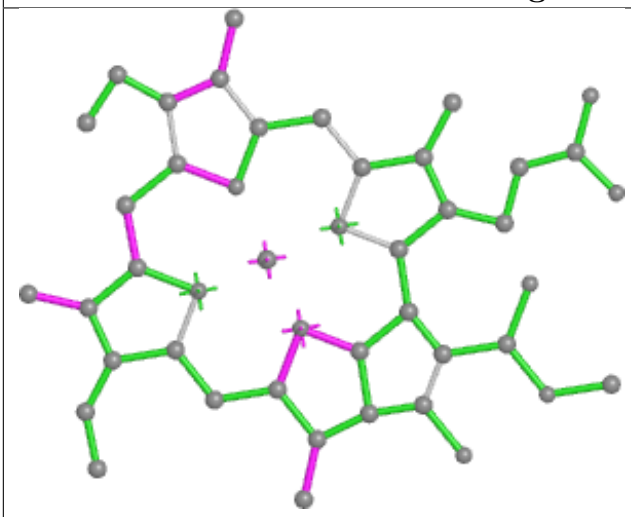


Torsions



Rings

Ligand CLA 8 603



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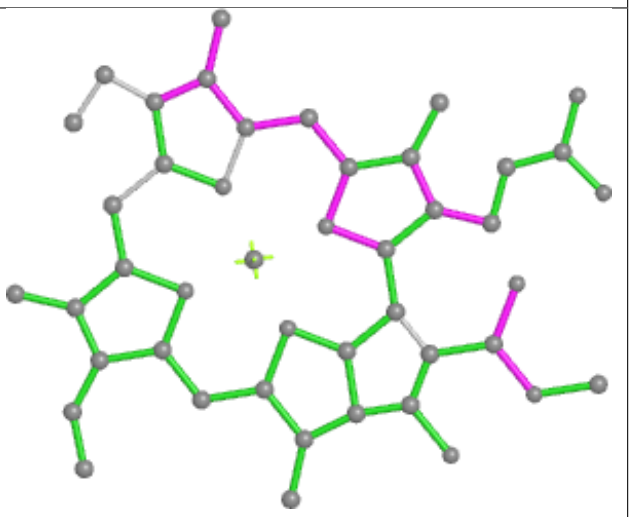
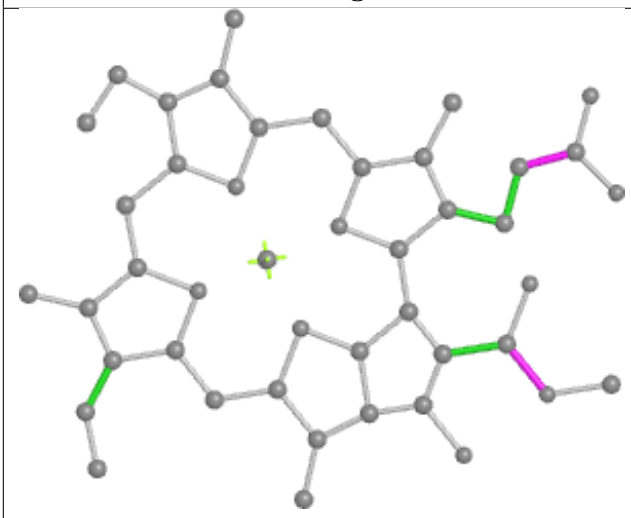
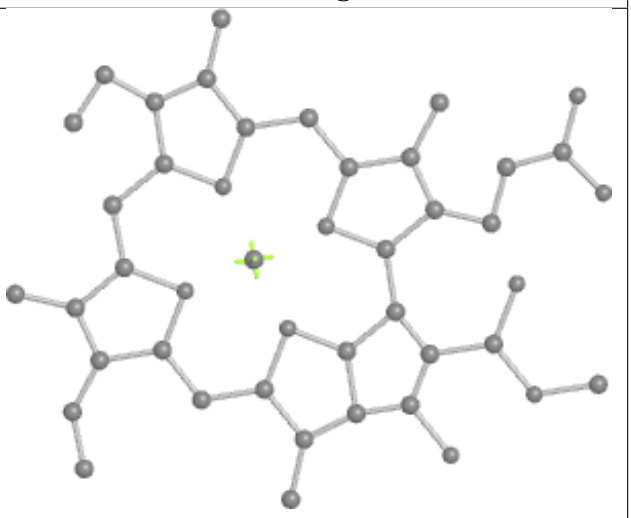


Bond angles

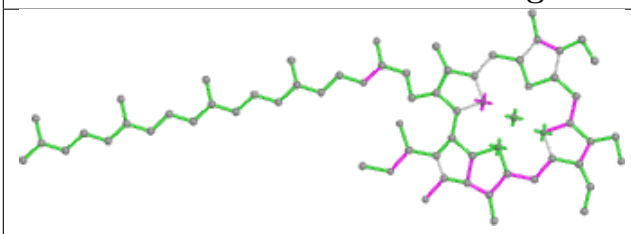


Torsions

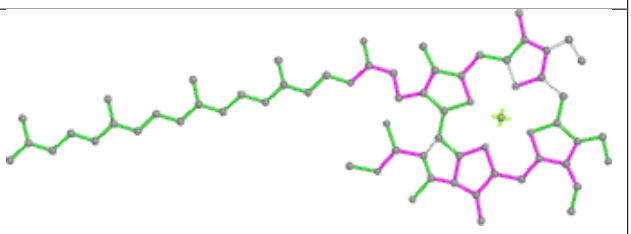


Rings

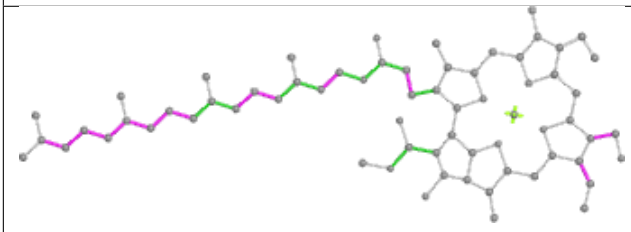
Ligand CHL n 607



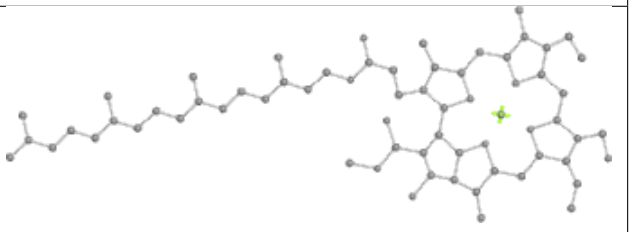
Bond lengths



Bond angles

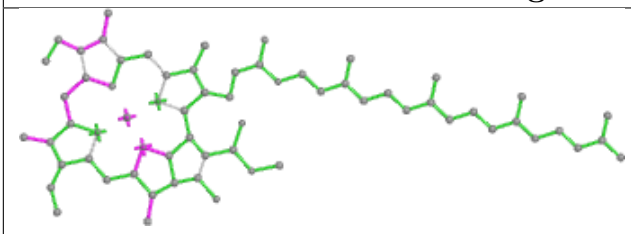


Torsions



Rings

Ligand CLA y 602



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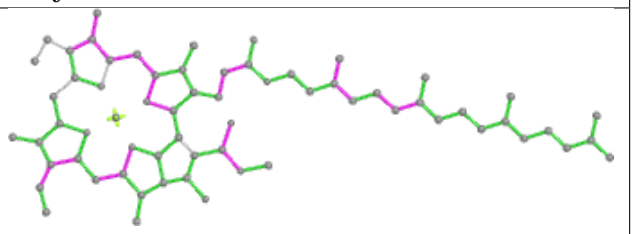
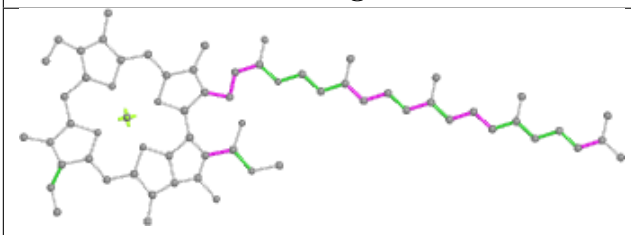
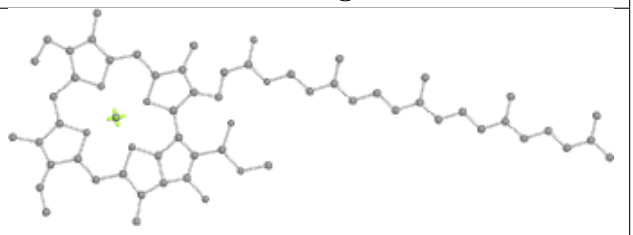


Bond angles

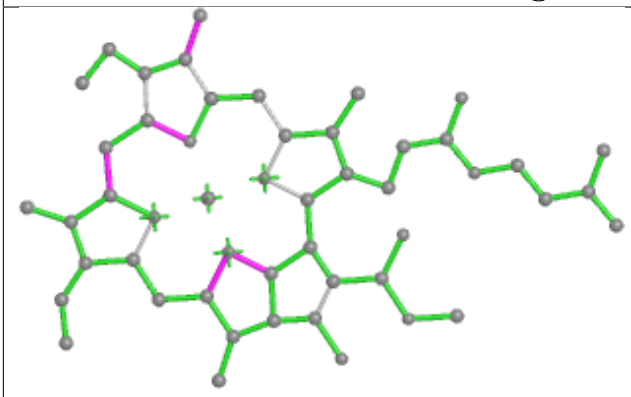


Torsions



Rings

Ligand CLA s 604



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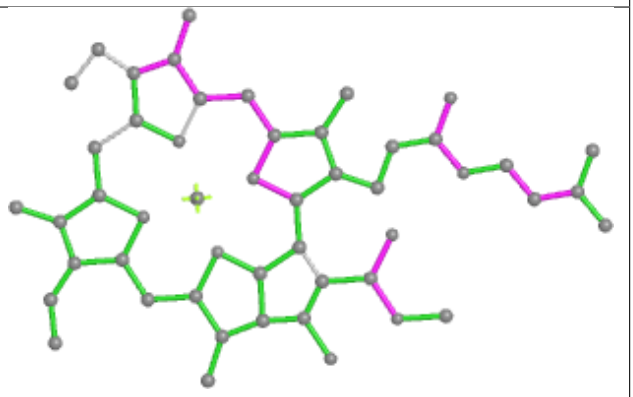
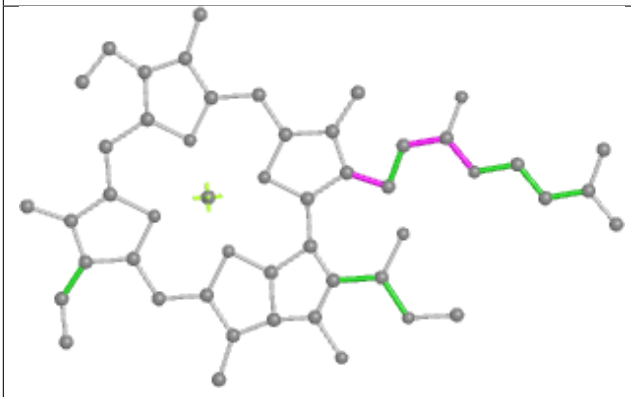


Bond angles



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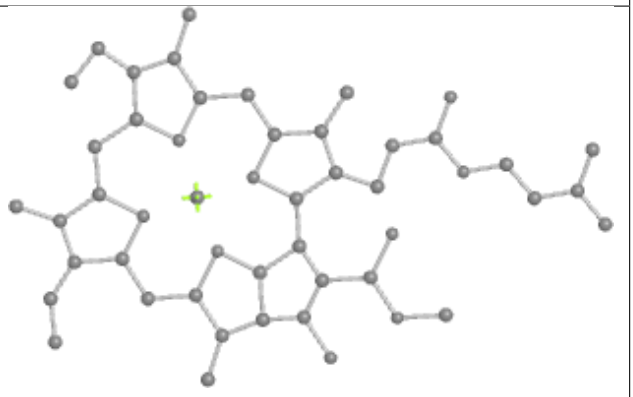
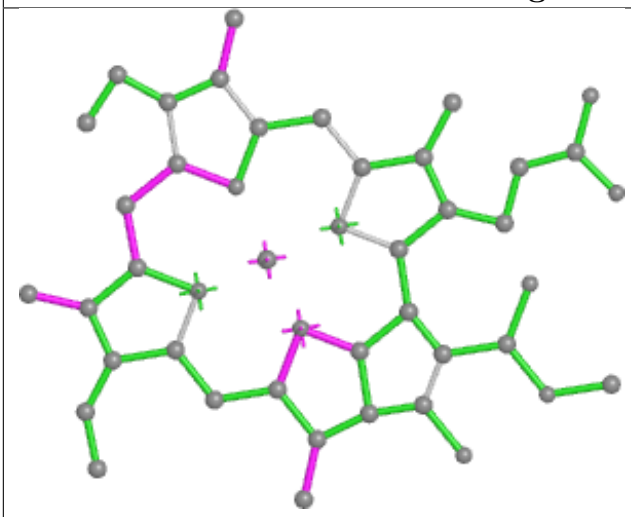


Rings

Ligand CLA 6 611



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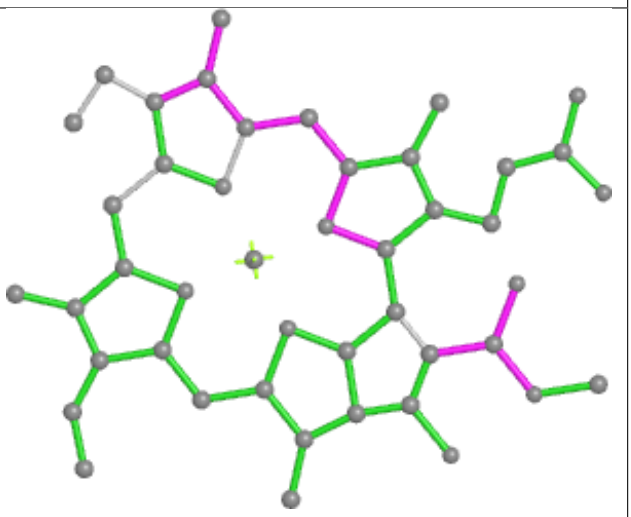
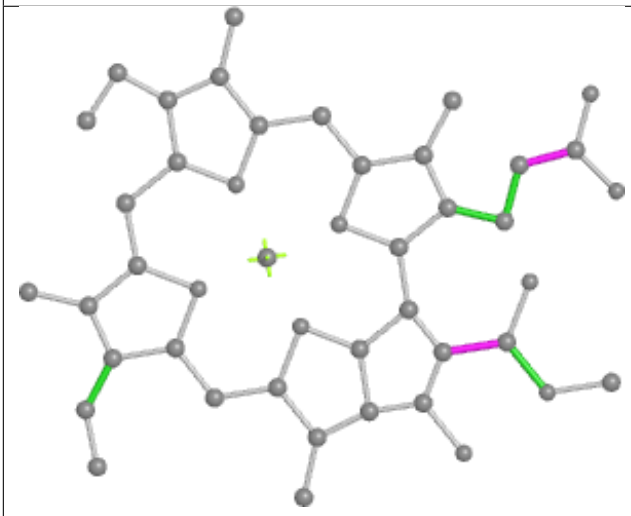


Bond angles



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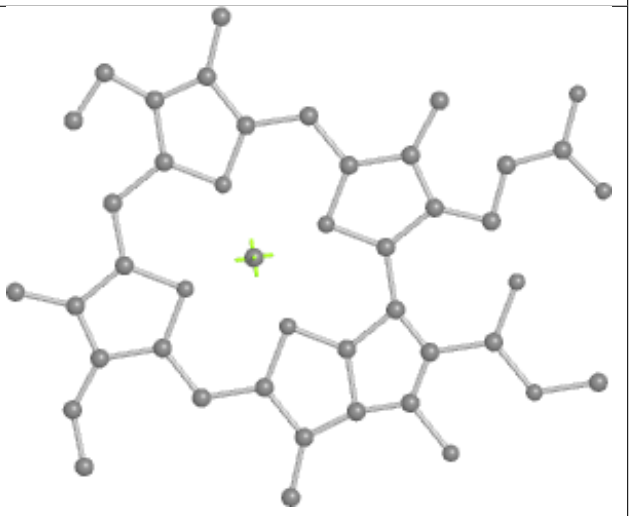
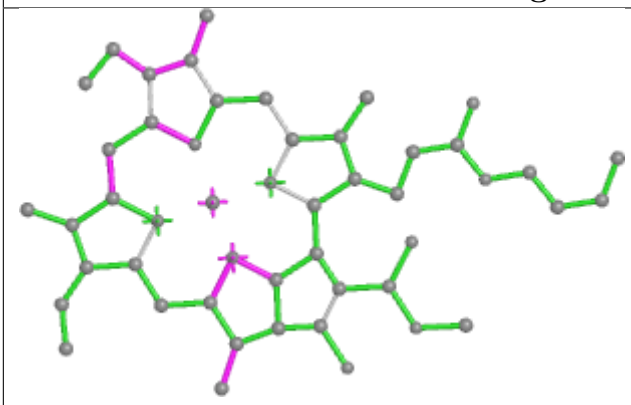


Rings

Ligand CLA r 601



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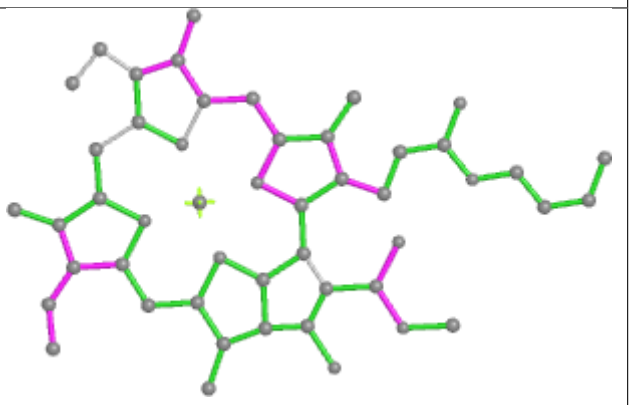
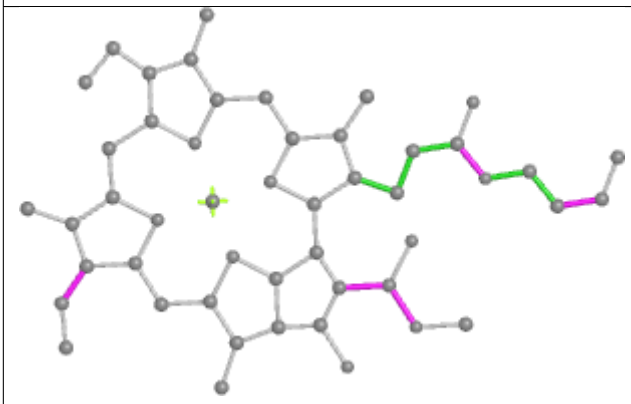


Bond angles



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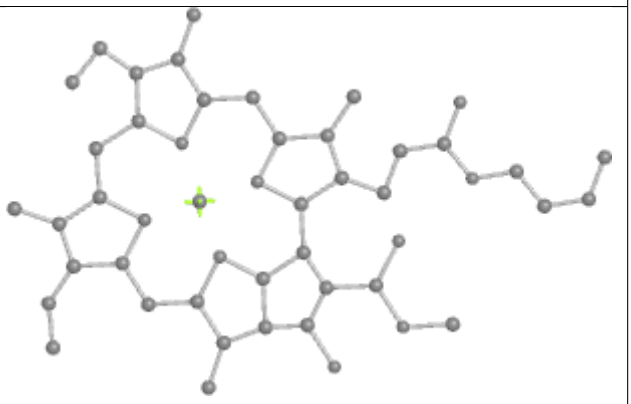
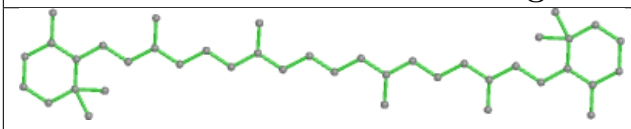
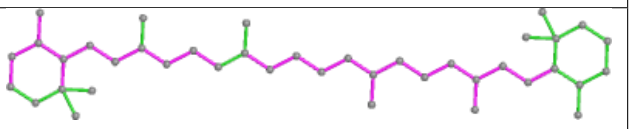


Rings

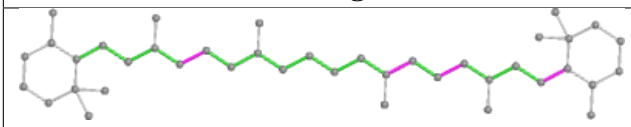
Ligand BCR c 515



Bond lengths



Bond angles



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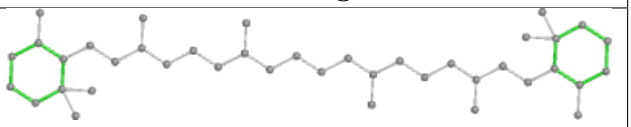
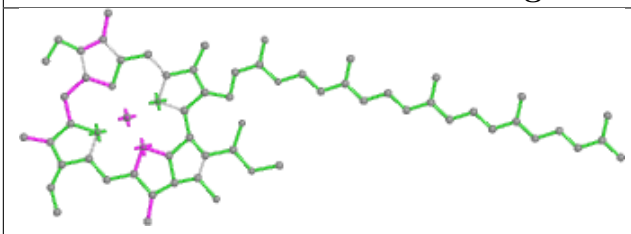
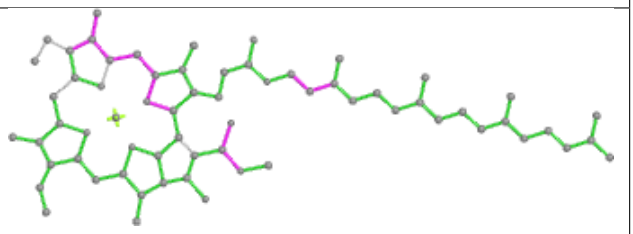
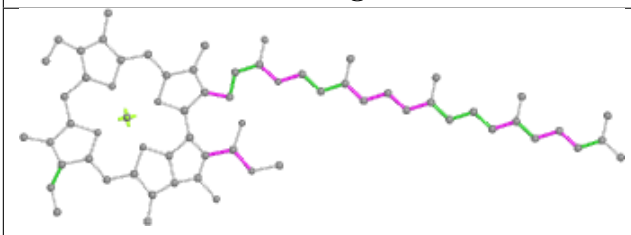
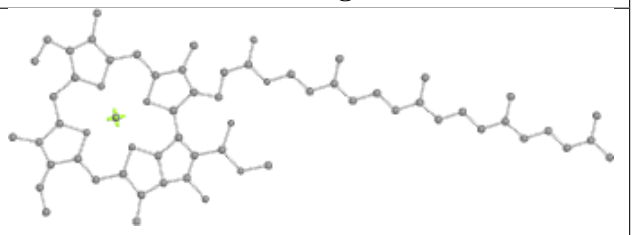
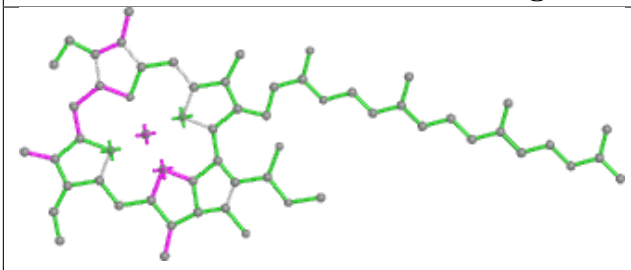
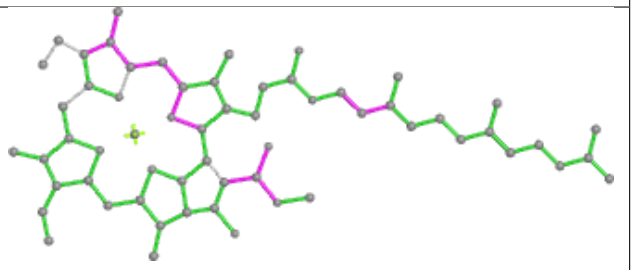
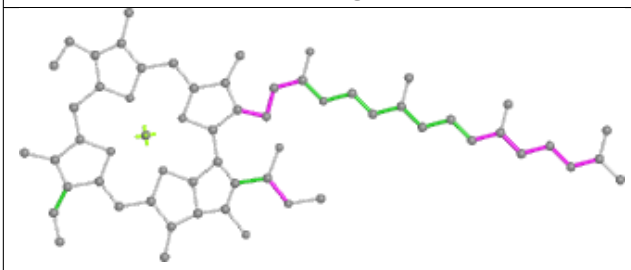
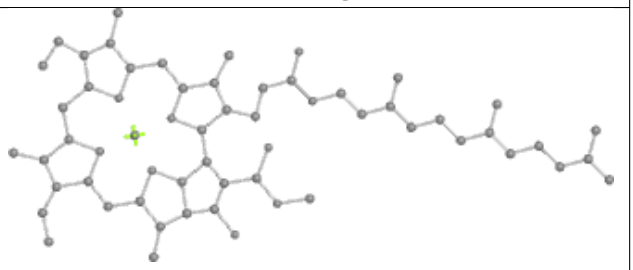
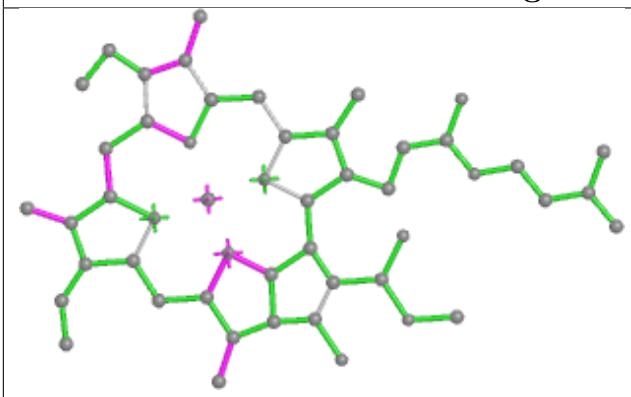


Rings

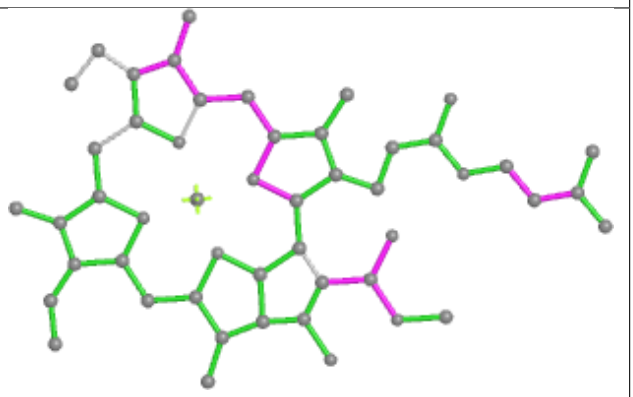
Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

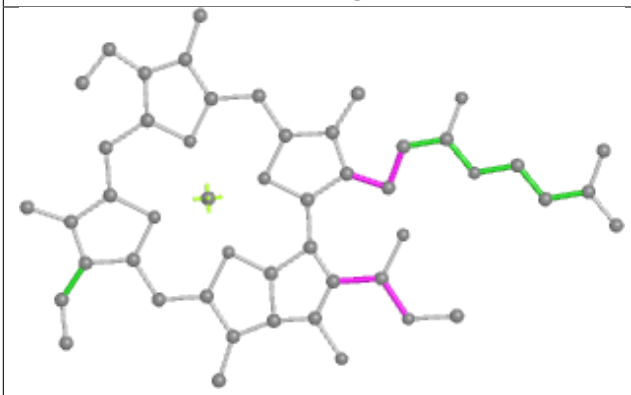
Ligand CLA Y 604



Bond lengths



Bond angles



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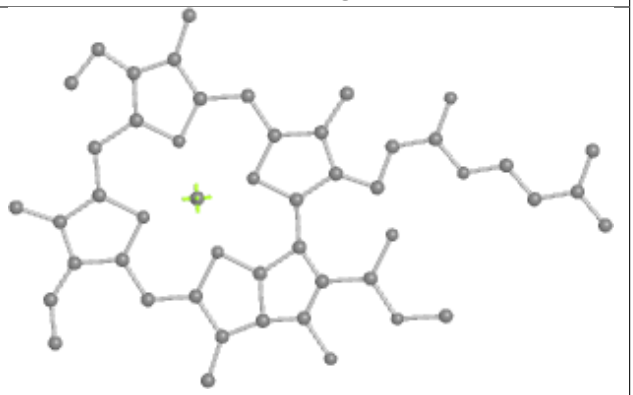
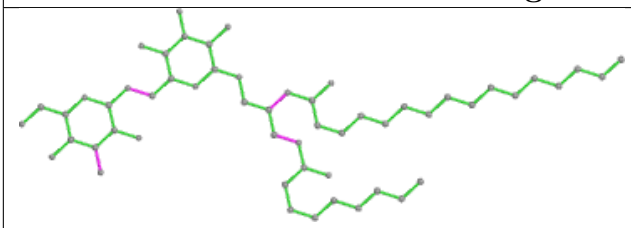


Rings

Ligand DGD c 518



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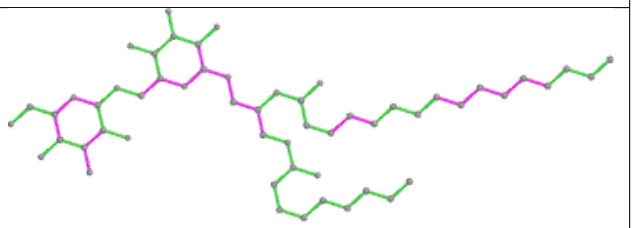
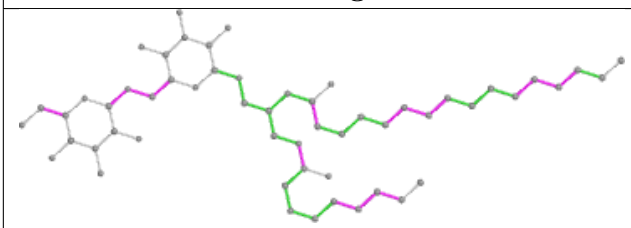


Bond angles



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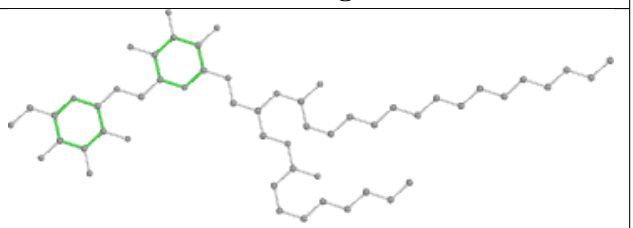
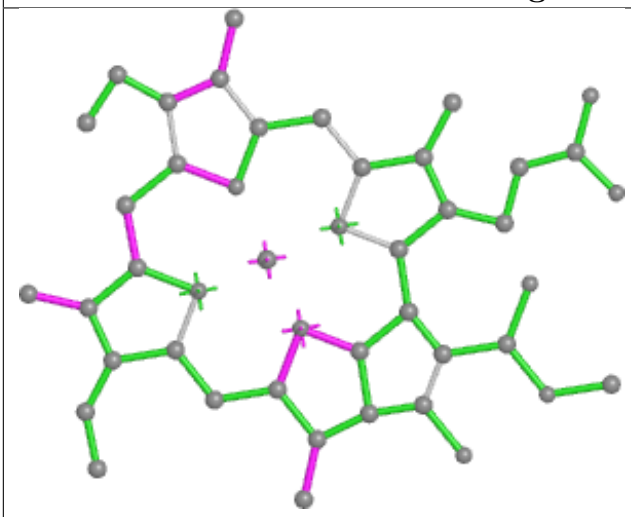


Rings

Ligand CLA 6 614



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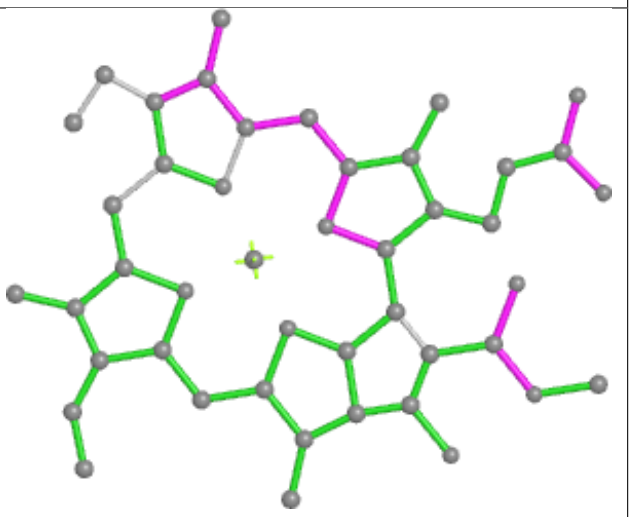
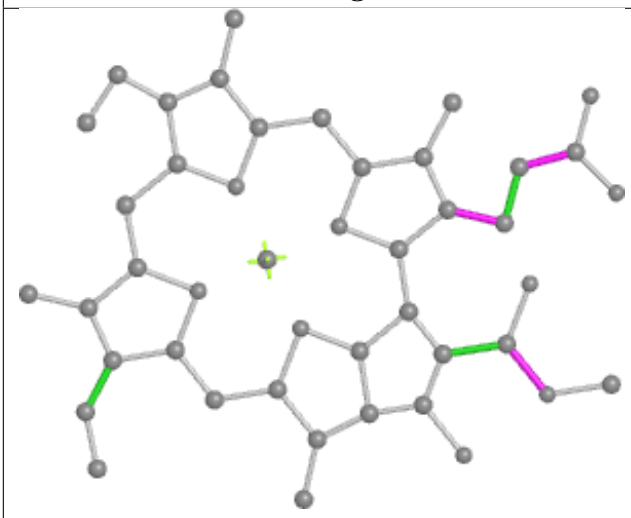


Bond angles



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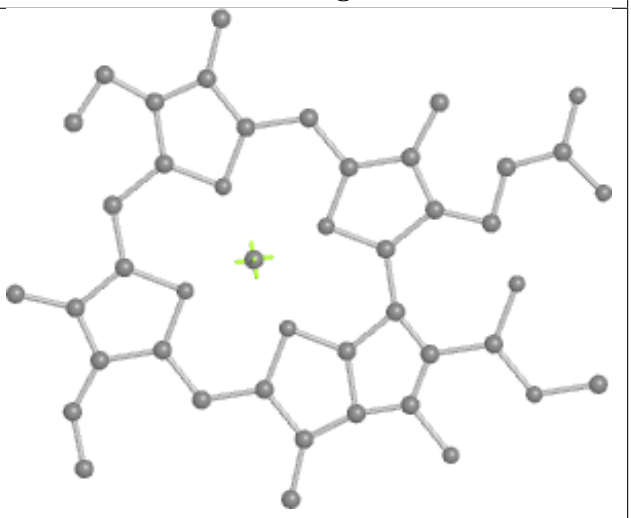
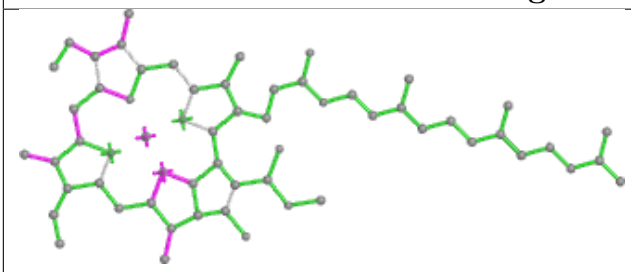


Rings

Ligand CLA 7 610



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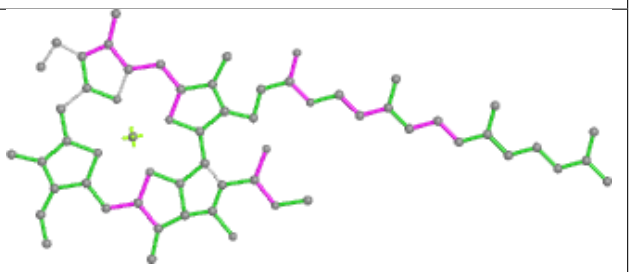
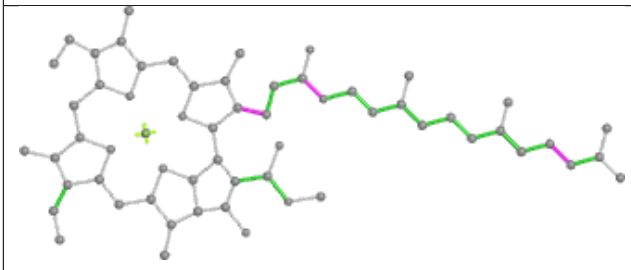


Bond angles



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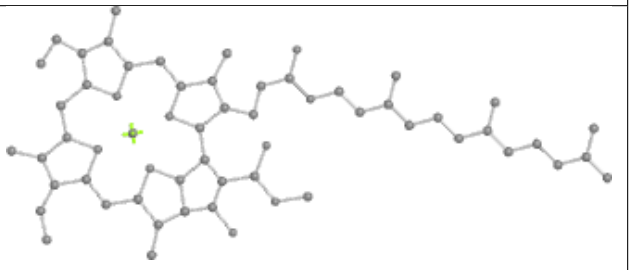
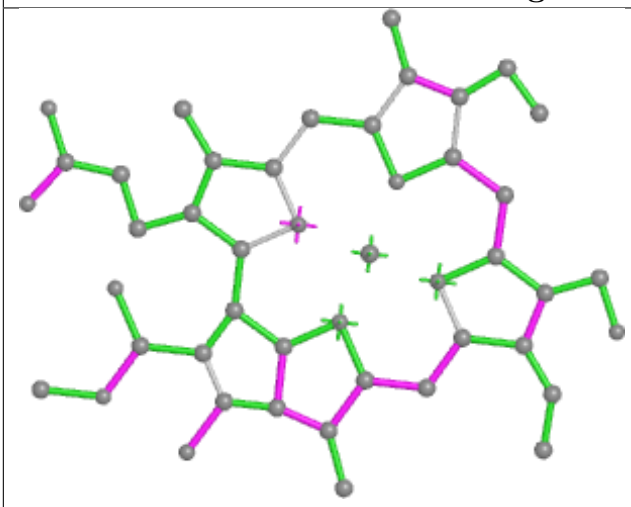
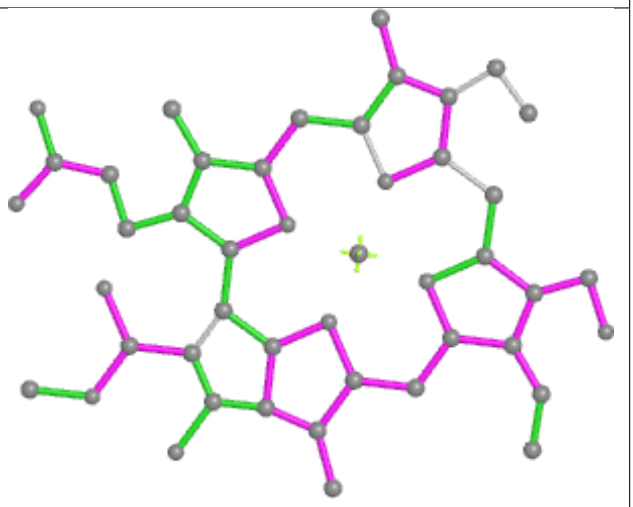


Rings

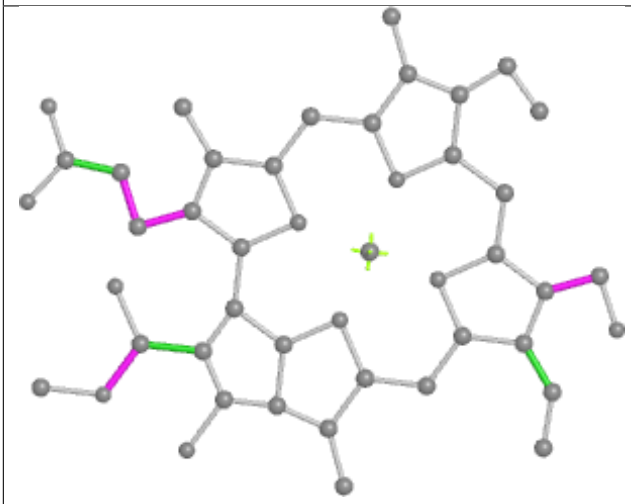
Ligand CHL 4 606



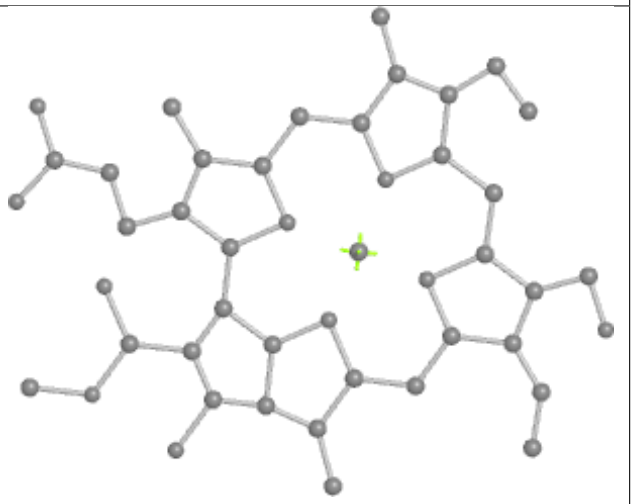
Bond lengths



Bond angles

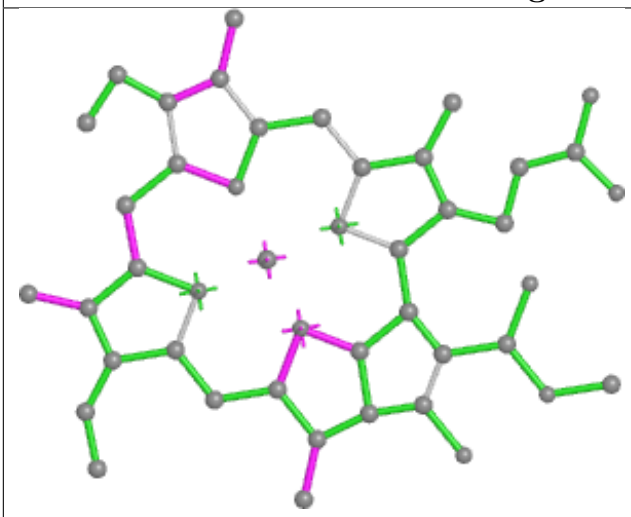


Torsions

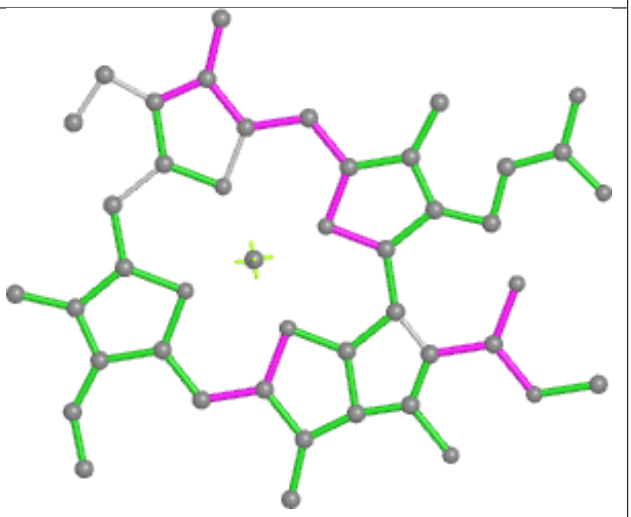


Rings

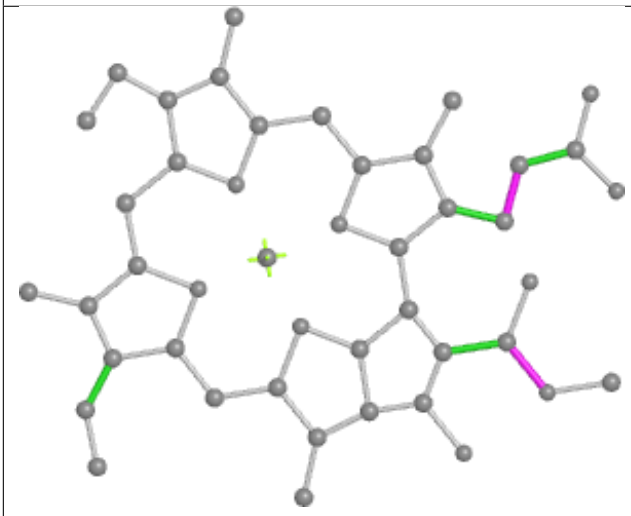
Ligand CLA 8 602



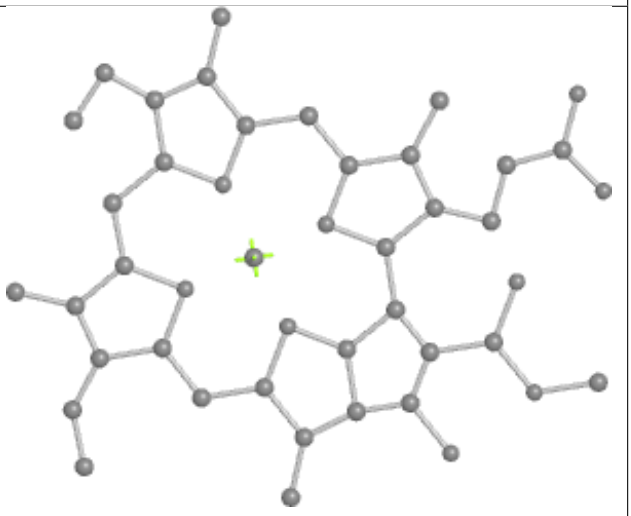
Bond lengths



Bond angles

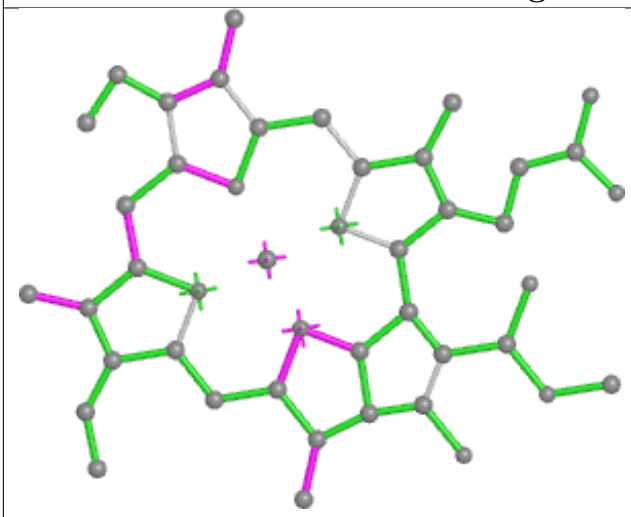


Torsions



Rings

Ligand CLA 4 603



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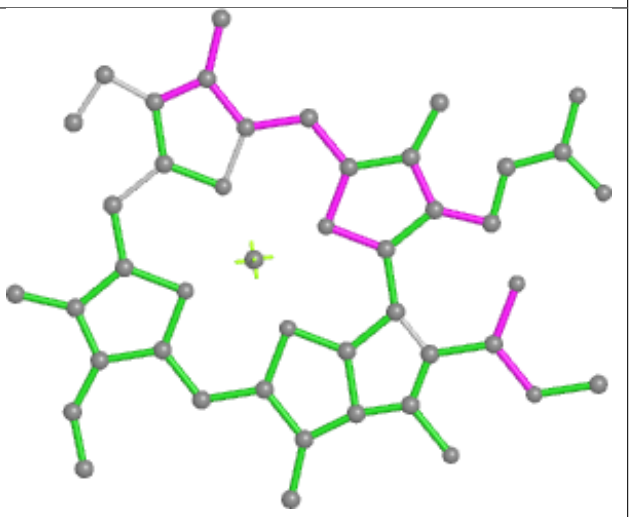
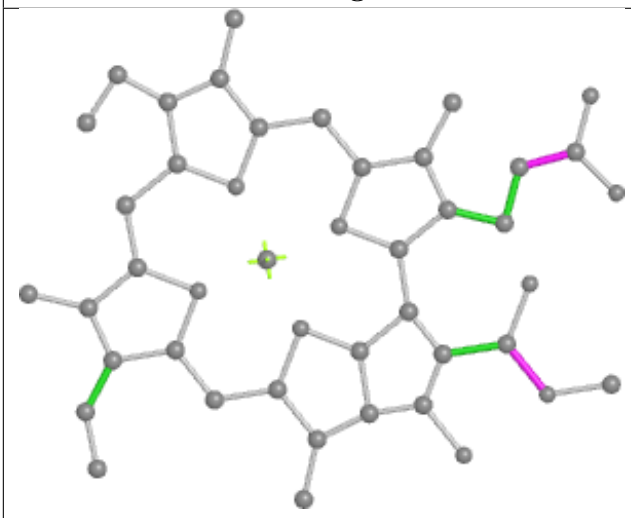


Bond angles



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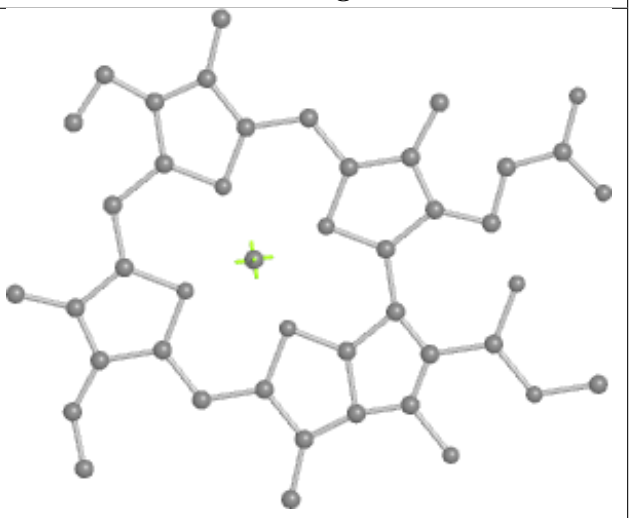
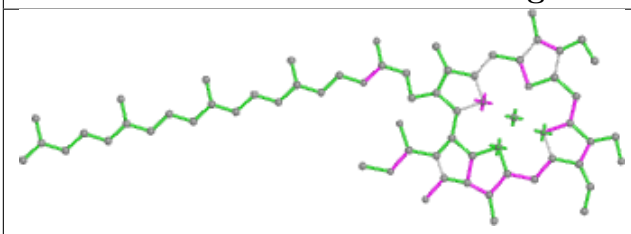


Rings

Ligand CHL y 609



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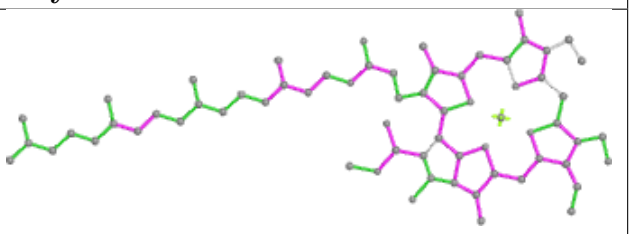
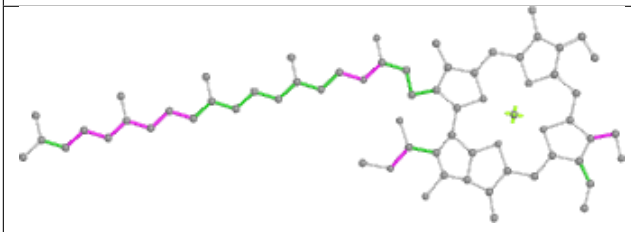


Bond angles



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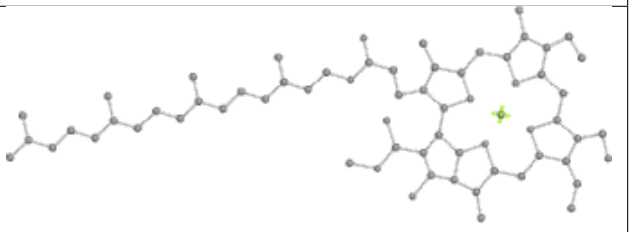
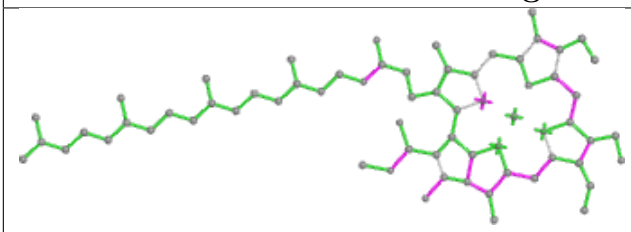


Rings

Ligand CHL N 608



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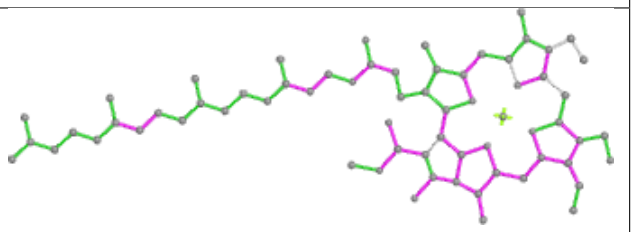

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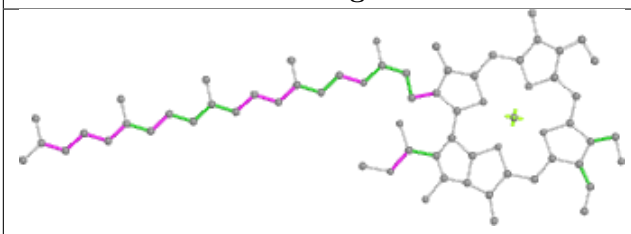

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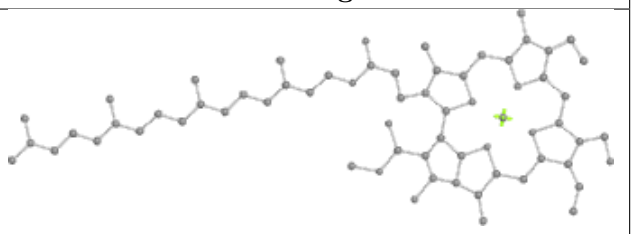
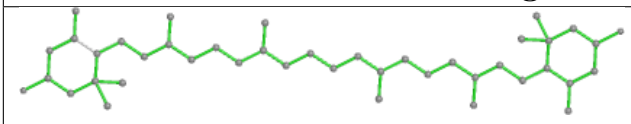


Rings

Ligand LUT s 1621



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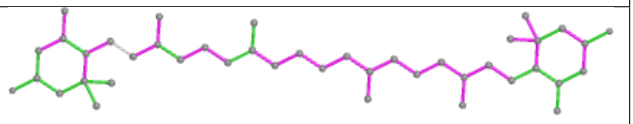

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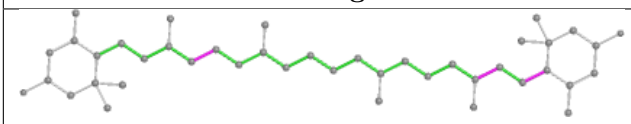

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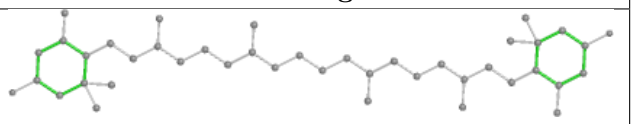
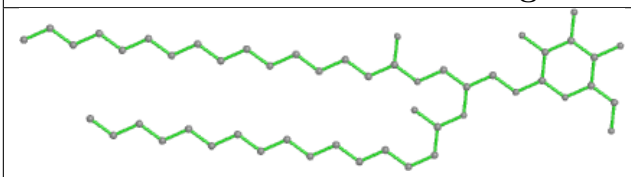


Rings

Ligand LMG C 521



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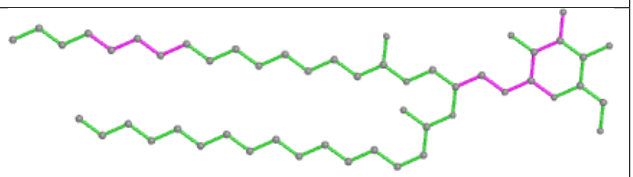
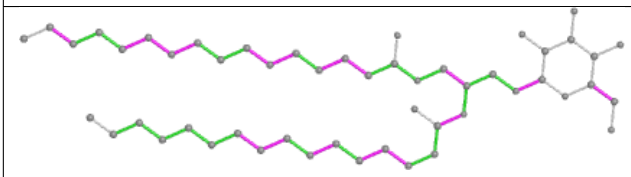


Bond angles



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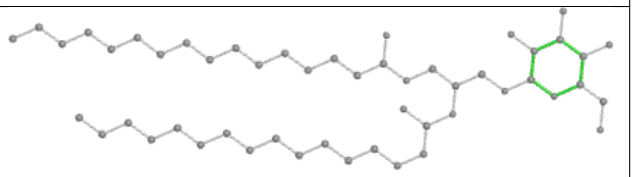
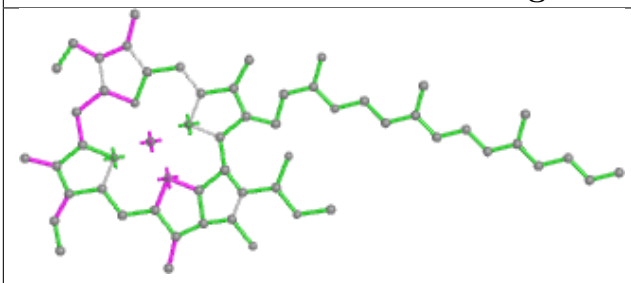
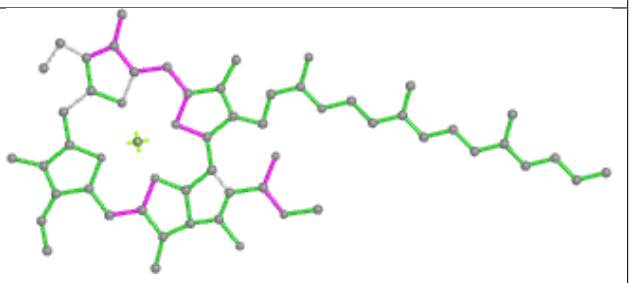
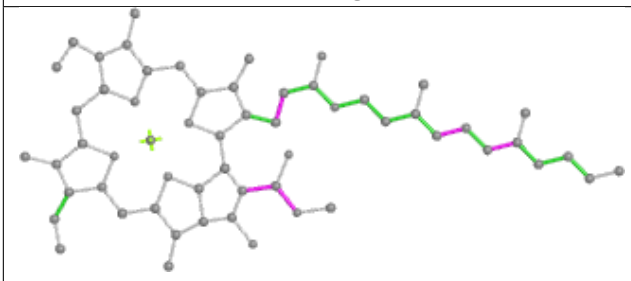
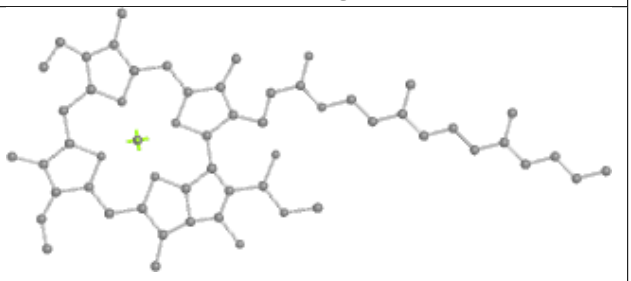


Rings

Ligand CLA 3 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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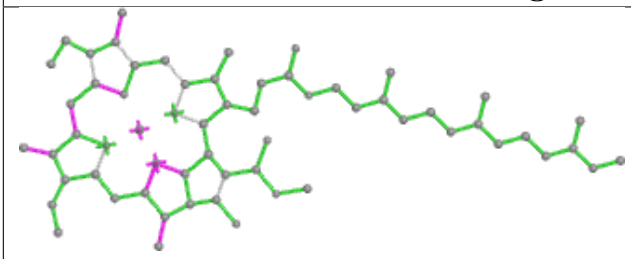
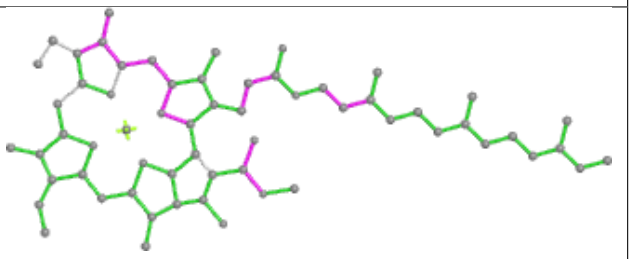
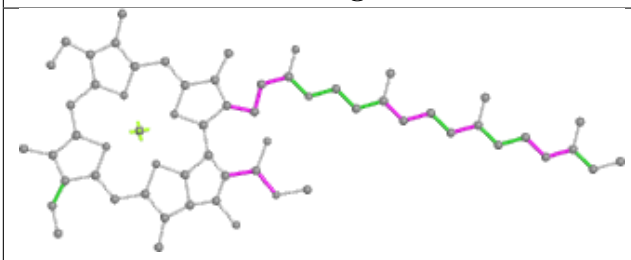
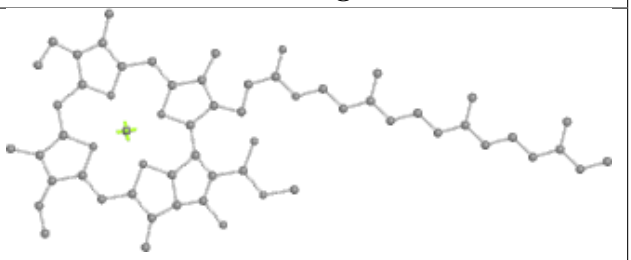
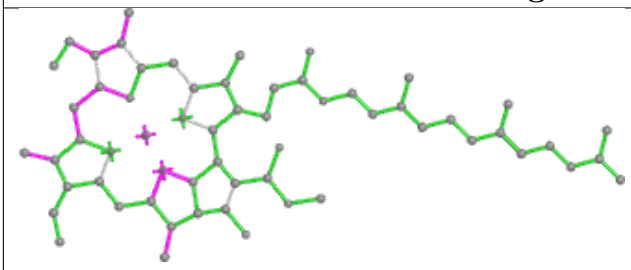
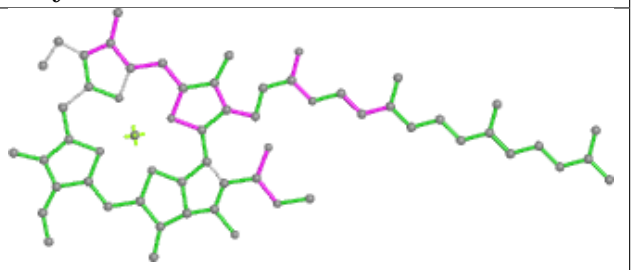
 Bond lengths	 Bond angles
 Torsions	 Rings

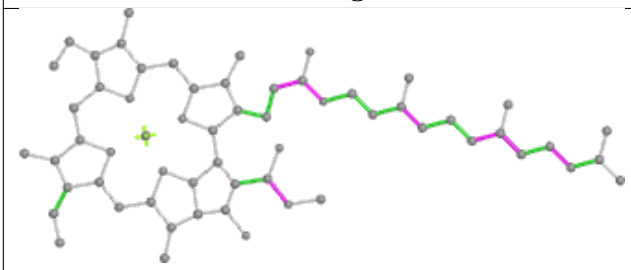
Ligand CLA y 612



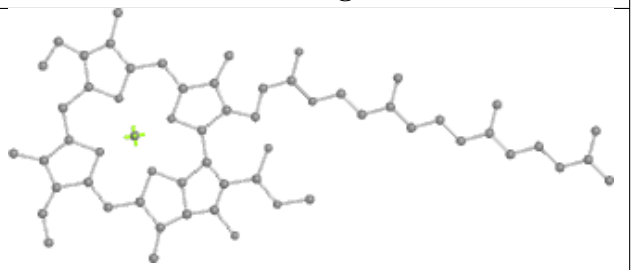
Bond lengths



Bond angles

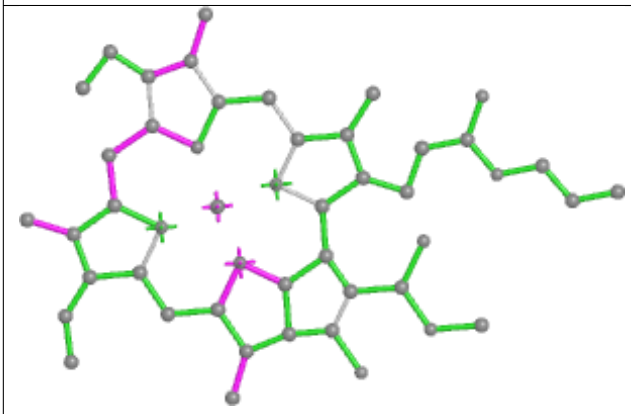


Torsions



Rings

Ligand CLA r 604



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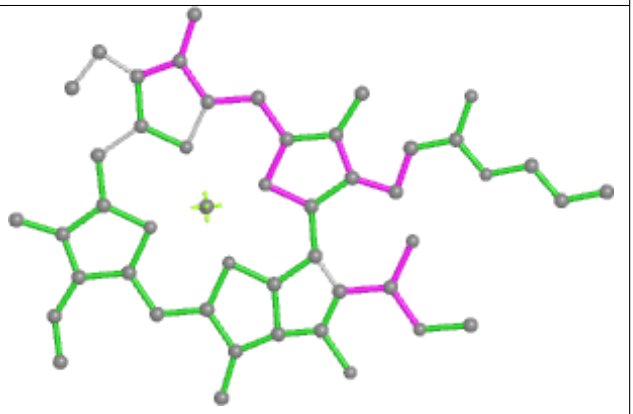
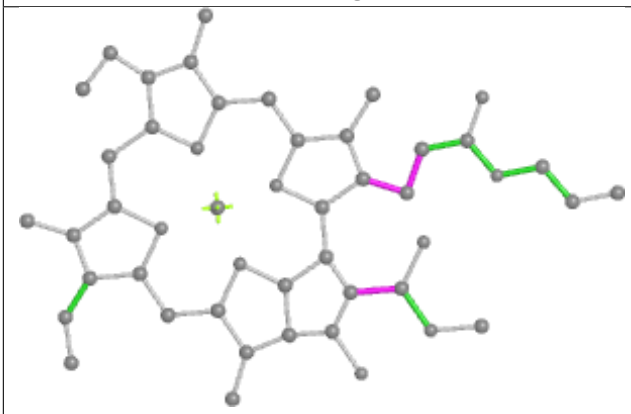


Bond angles



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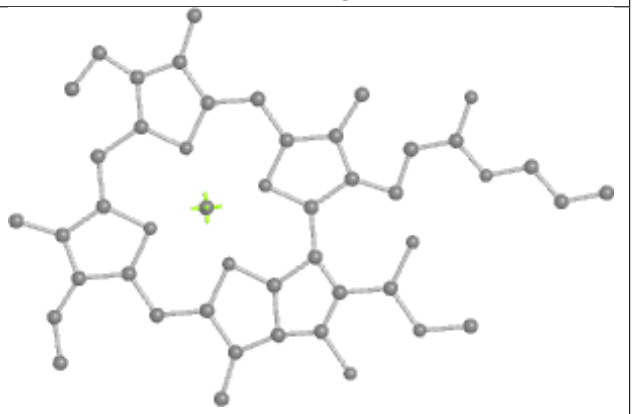
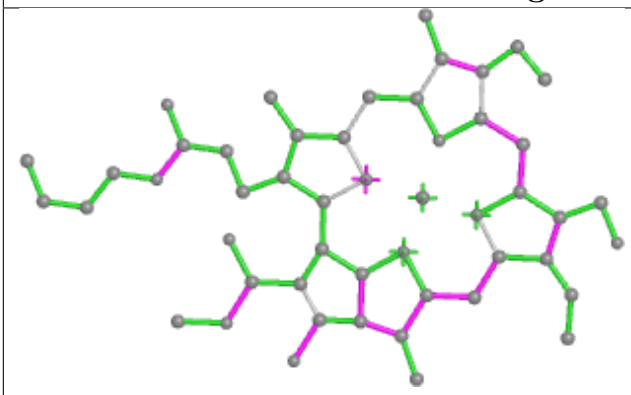


Rings

Ligand CHL g 606



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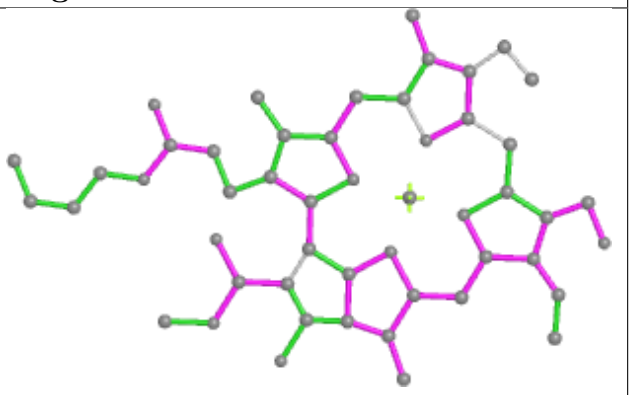
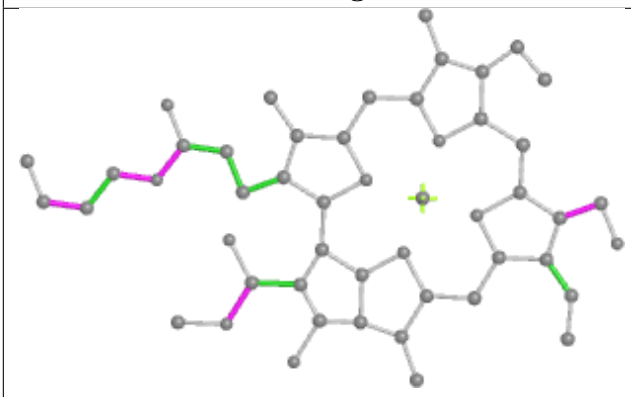


Bond angles



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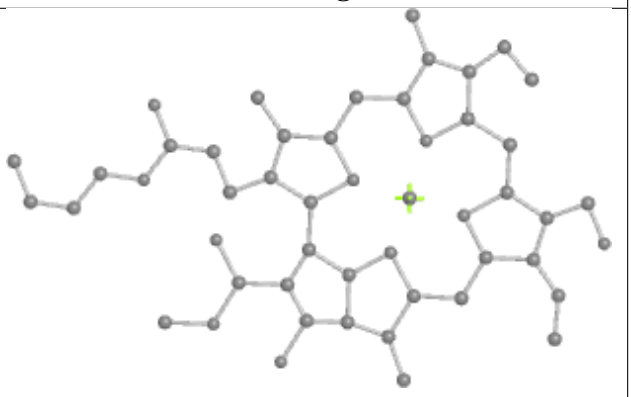
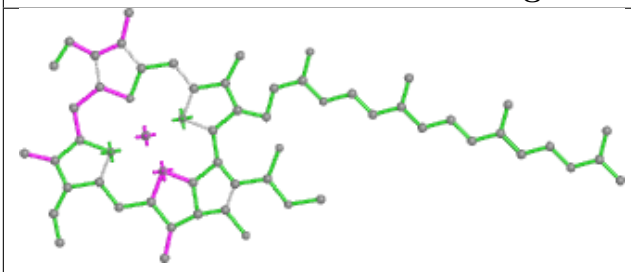


Rings

Ligand CLA Y 612



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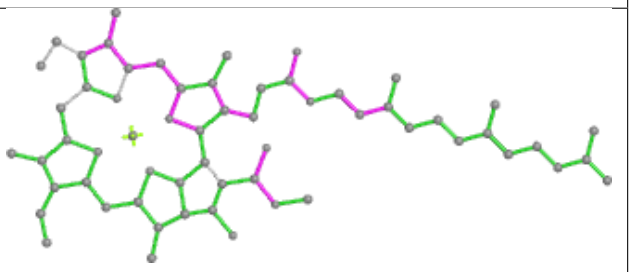
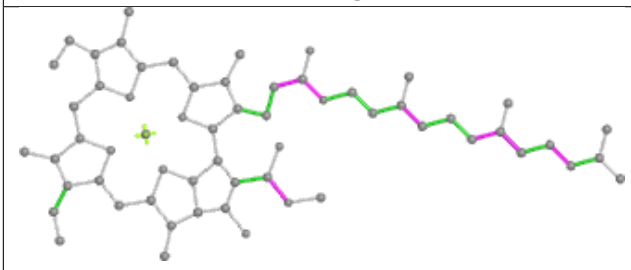


Bond angles



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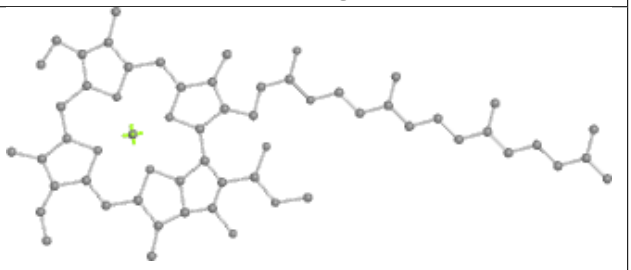
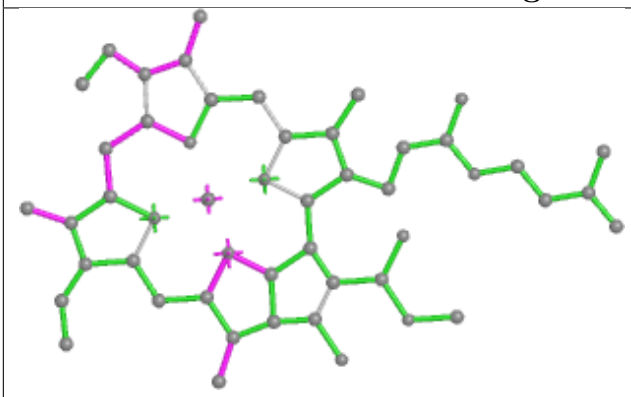


Rings

Ligand CLA G 604



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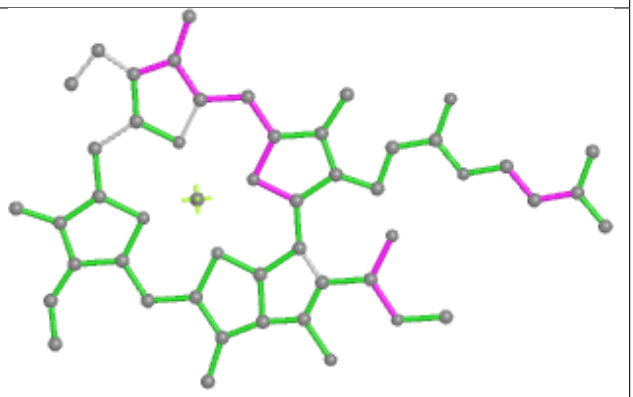
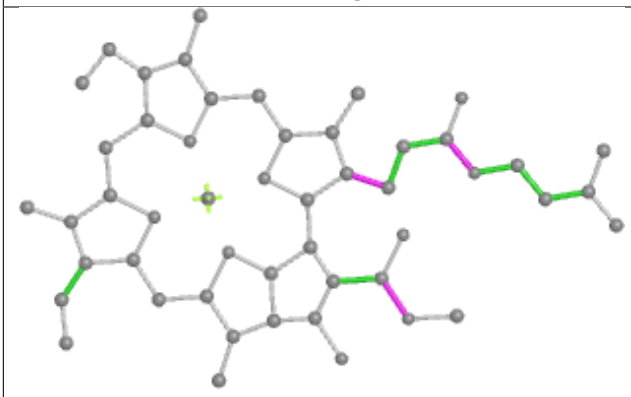


Bond angles



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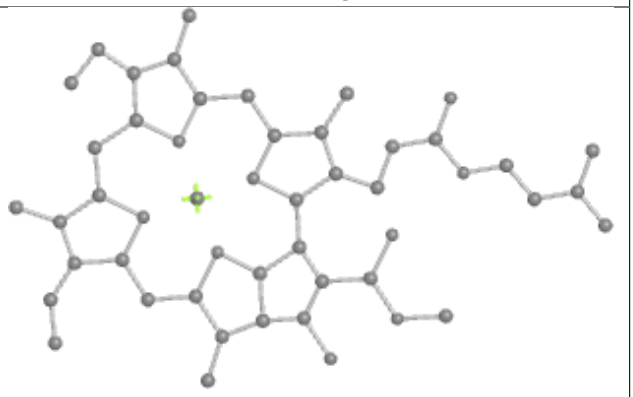
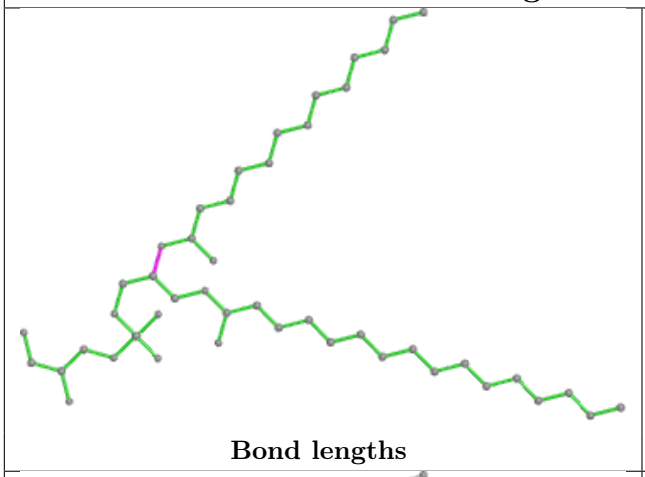


Rings

Ligand LHG D 408



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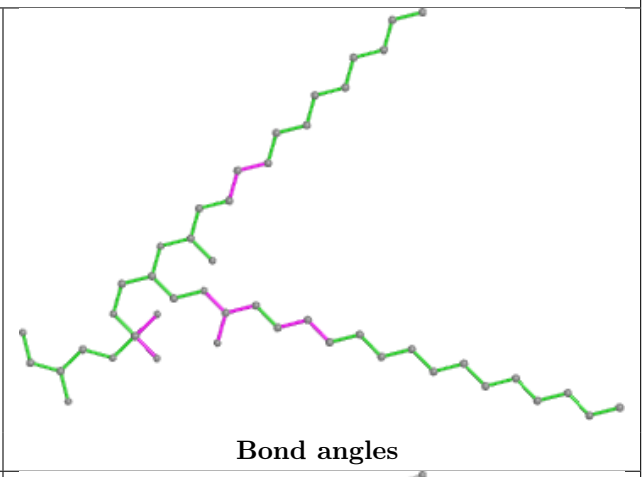
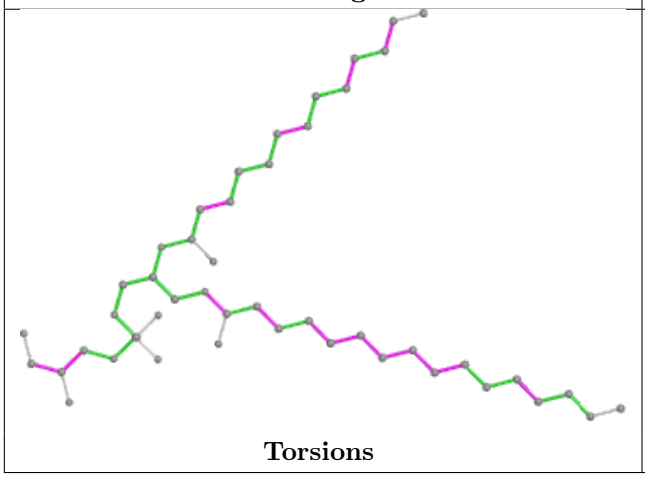
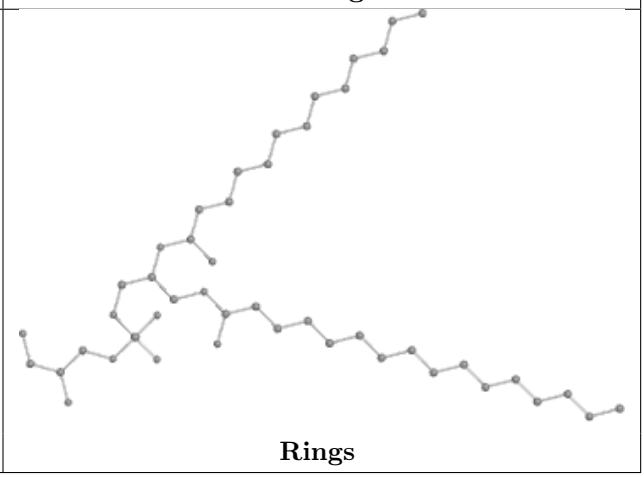


Bond angles

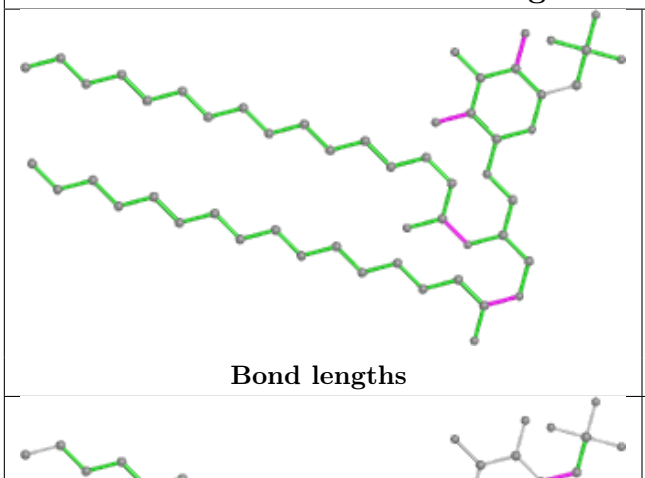


Torsions



Rings

Ligand SQD b 621



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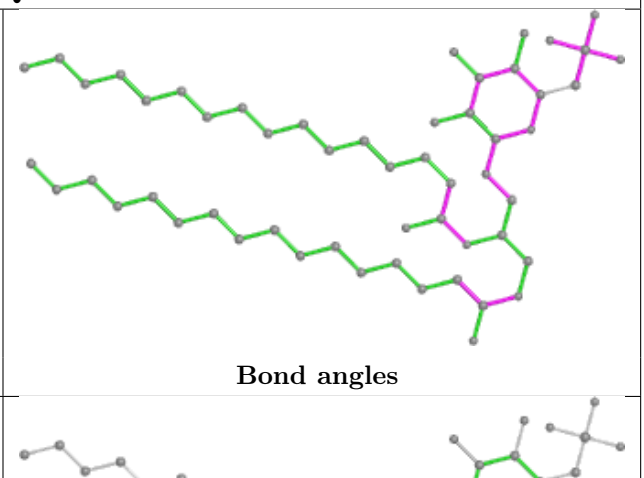
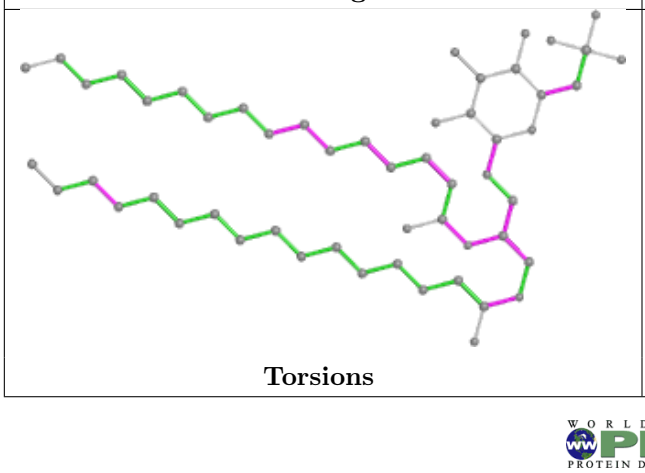


Bond angles



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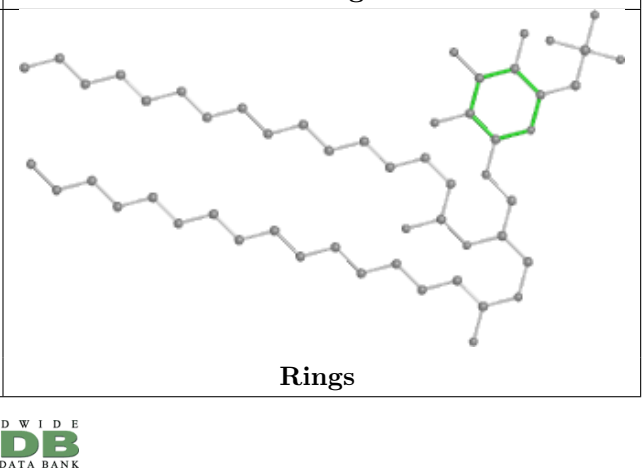
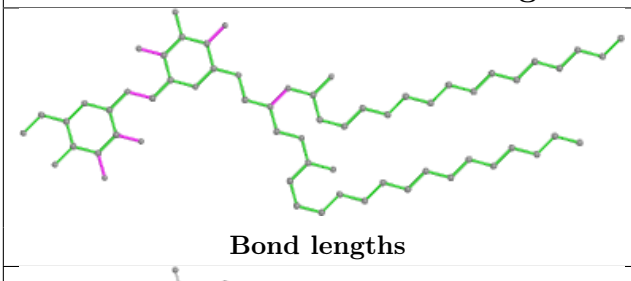


Rings

Ligand DGD H 102



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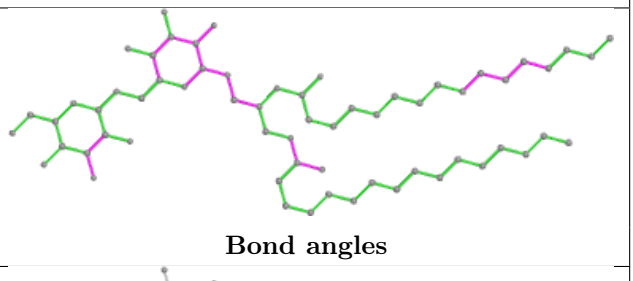
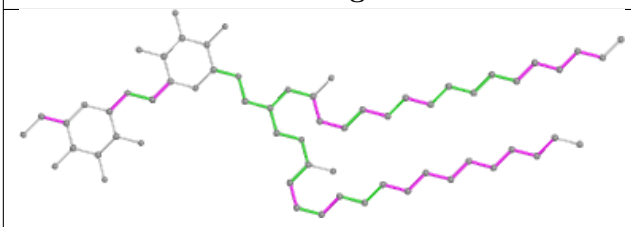
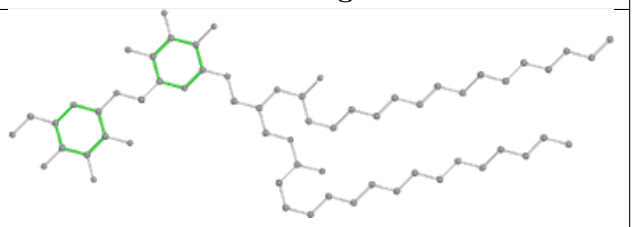


Bond angles

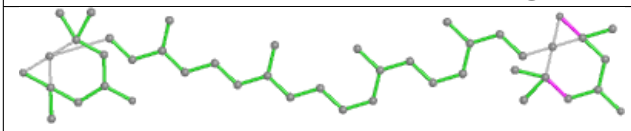


Torsions



Rings

Ligand XAT R 622



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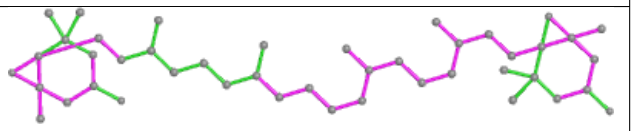
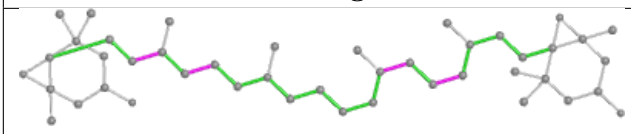


Bond angles



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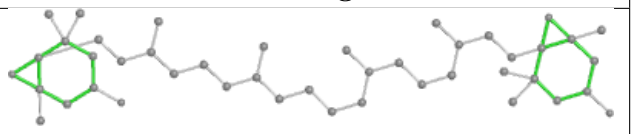
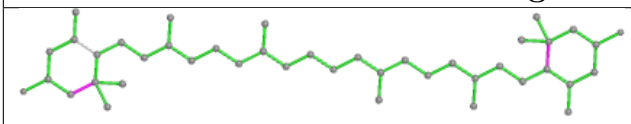


Rings

Ligand LUT 8 620



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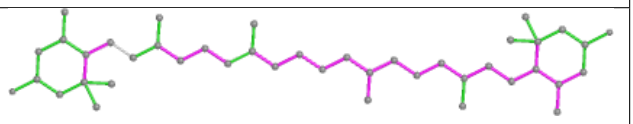
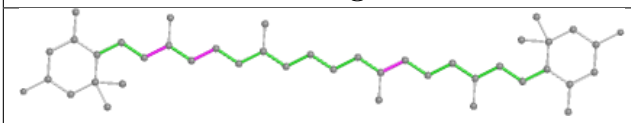


Bond angles



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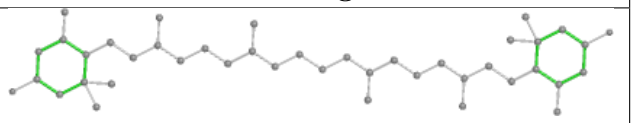
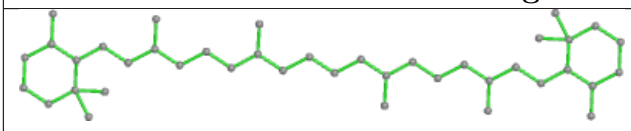


Rings

Ligand BCR C 516



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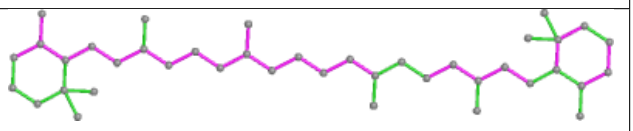
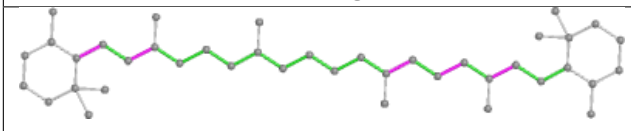


Bond angles



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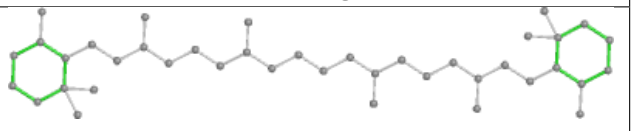
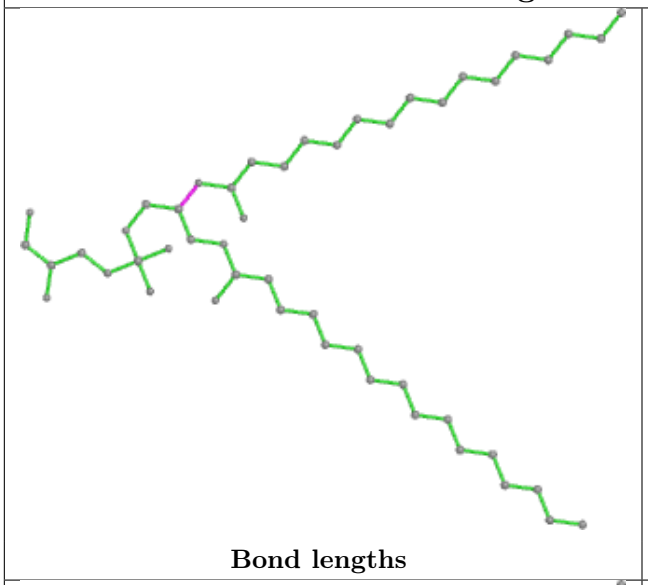


Rings

Ligand LHG b 2631



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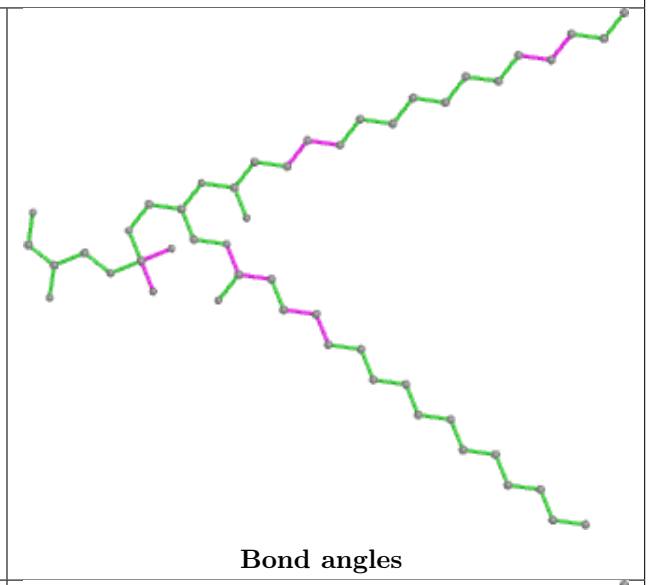

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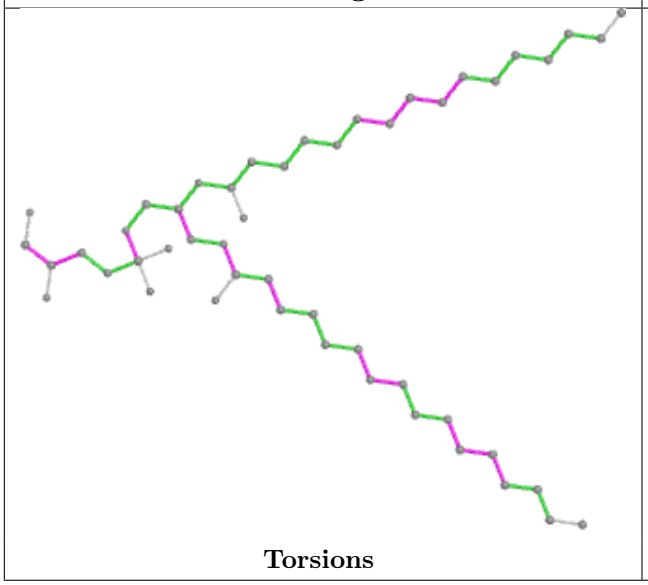

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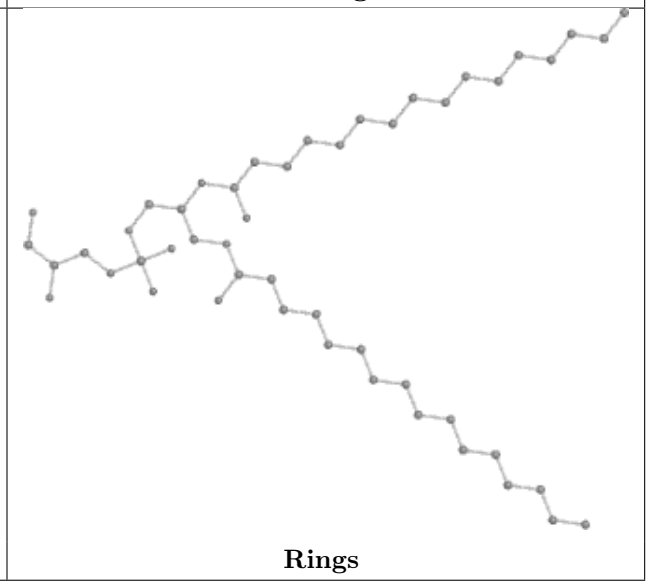
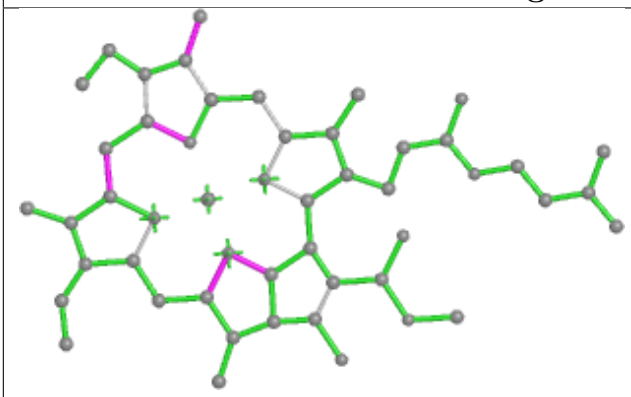


Rings

Ligand CLA S 604



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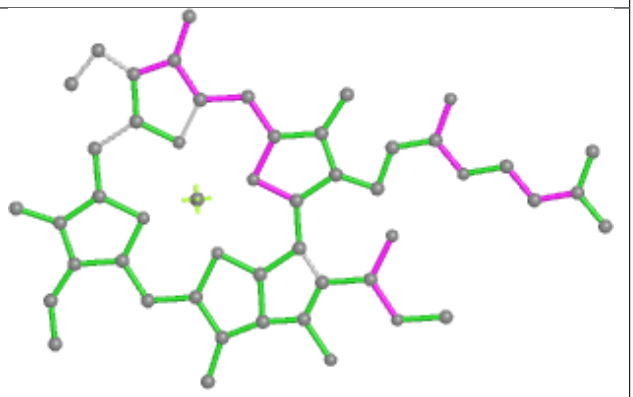

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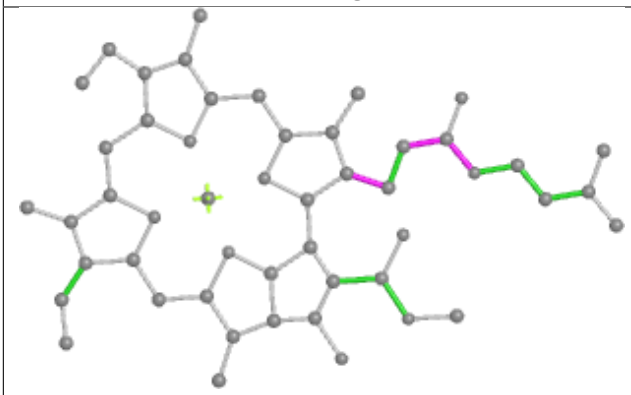

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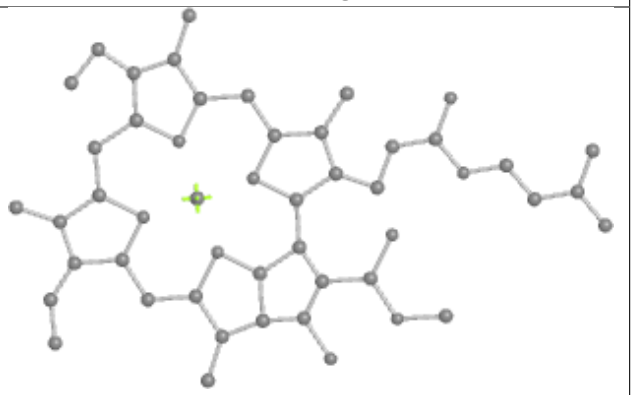
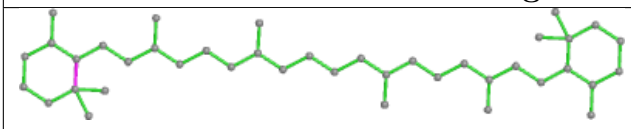


Rings

Ligand BCR B 620



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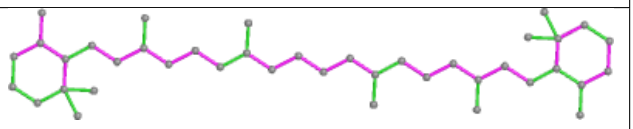
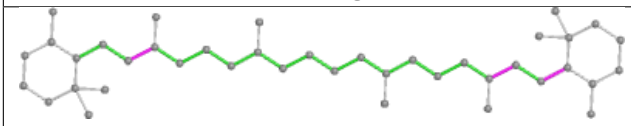


Bond angles



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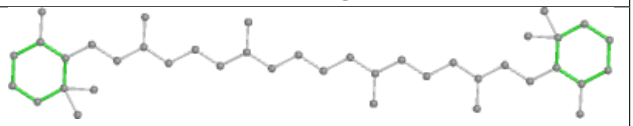
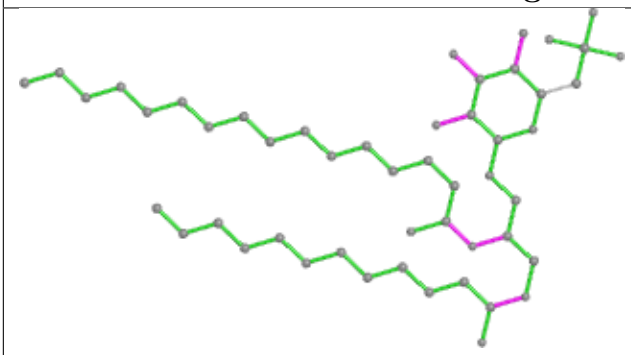


Rings

Ligand SQD A 412



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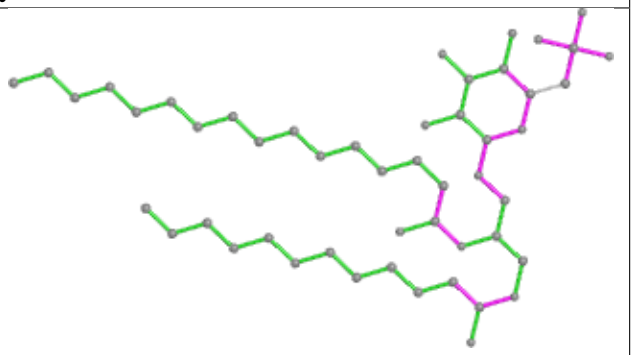
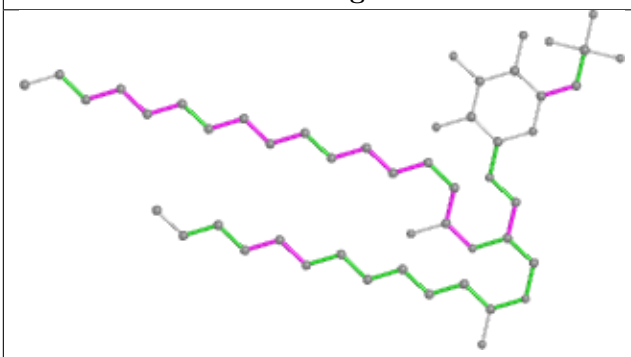


Bond angles



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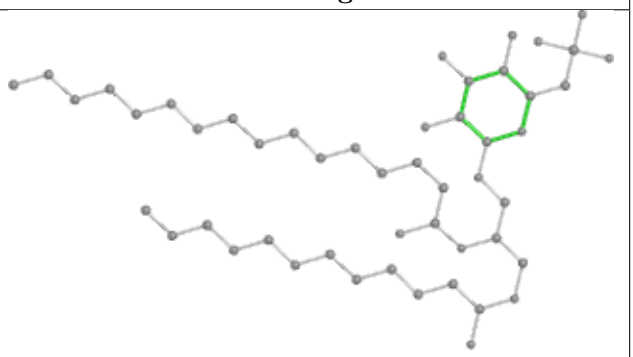
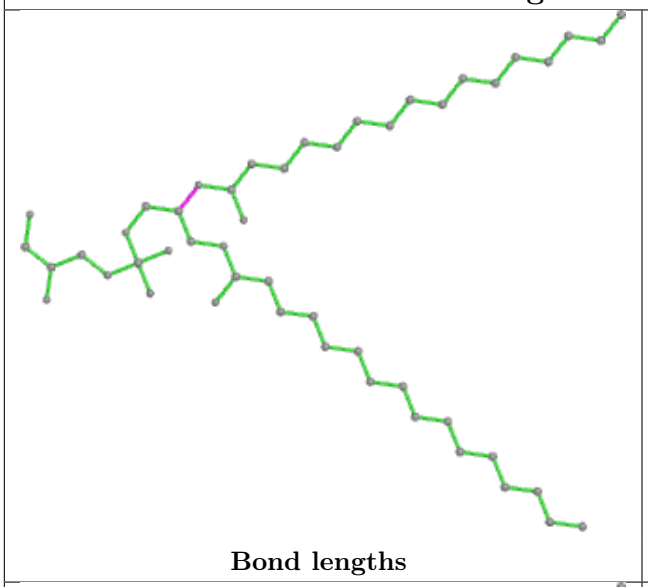


Rings

Ligand LHG d 409



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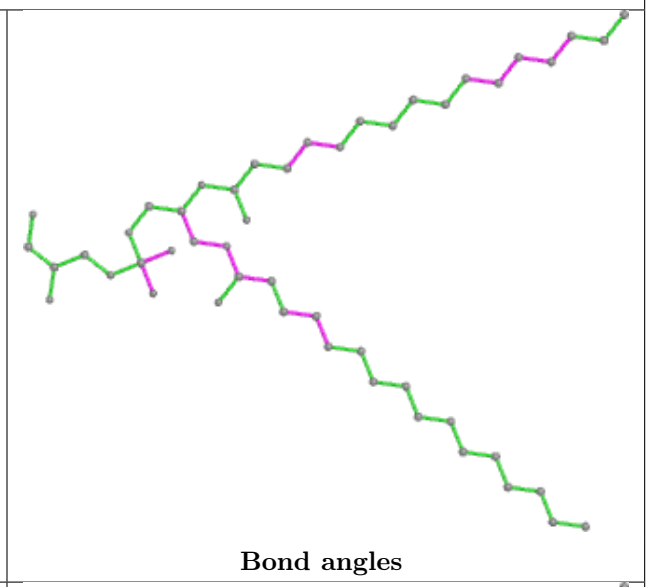
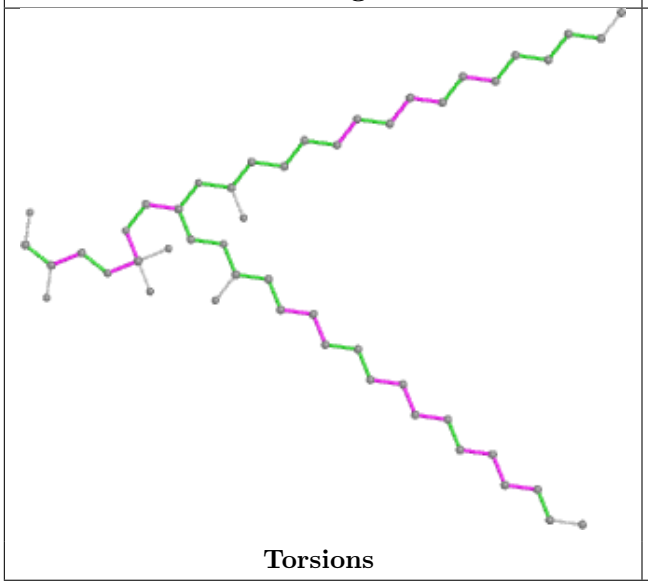


Bond angles



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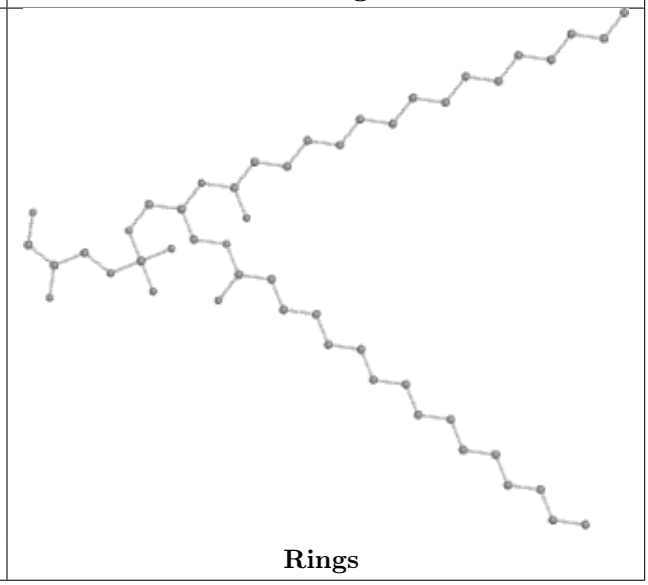
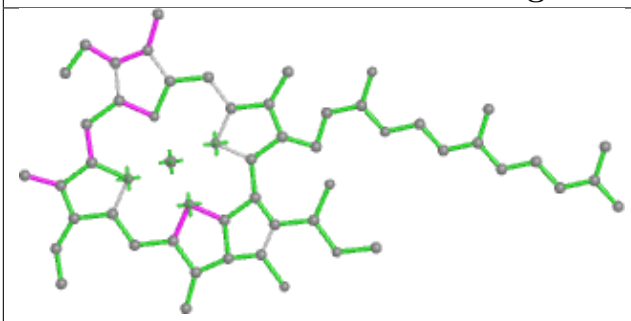


Rings

Ligand CLA S 610



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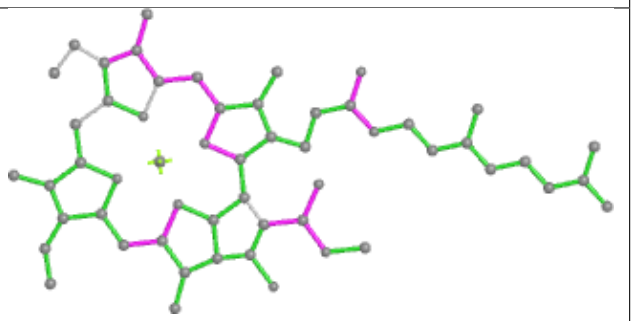

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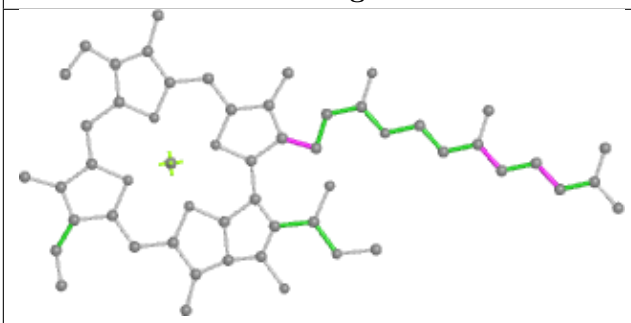

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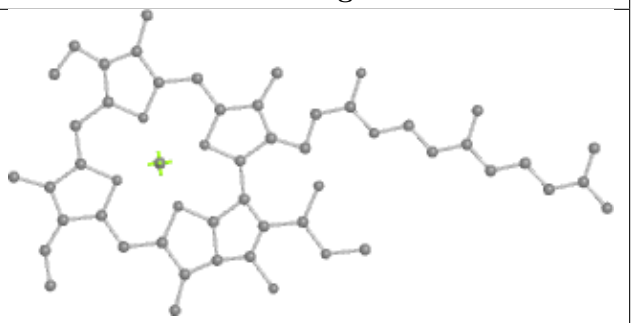
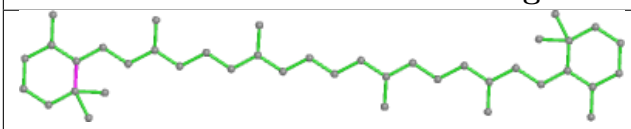


Rings

Ligand BCR T 101



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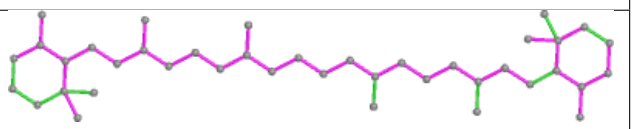
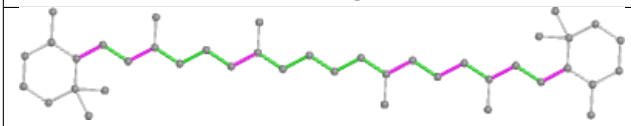


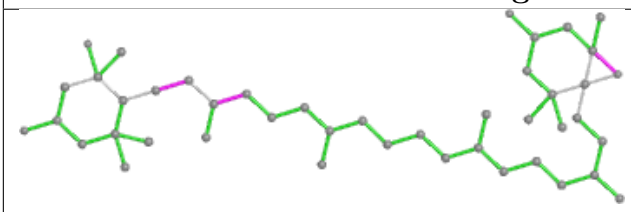
Bond angles



Torsions

Rings

Ligand NEX N 1623



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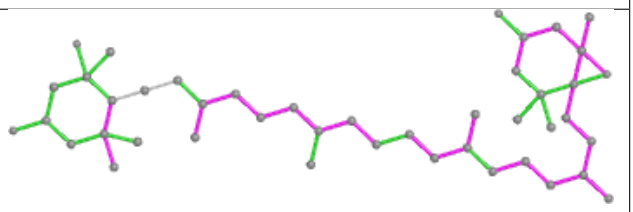
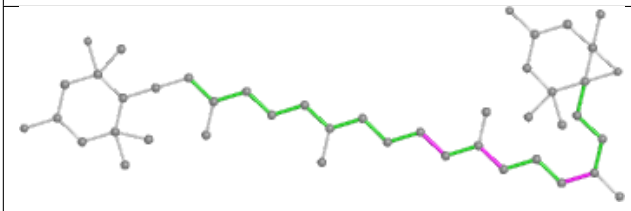


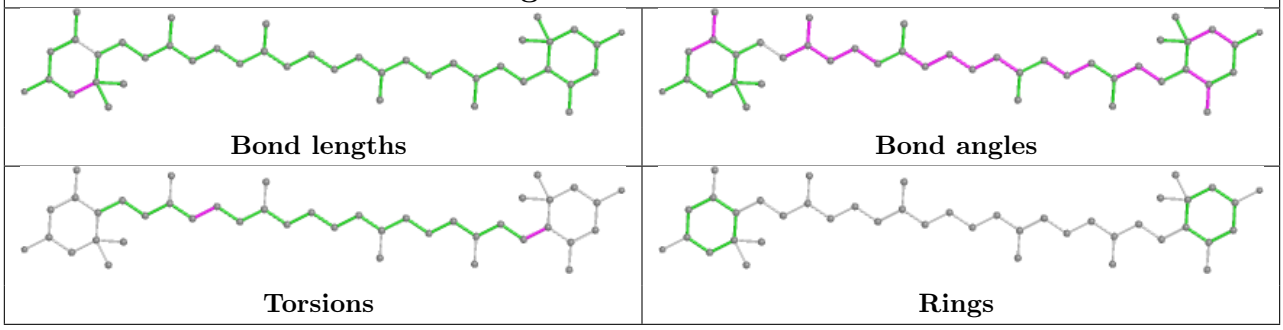
Bond angles



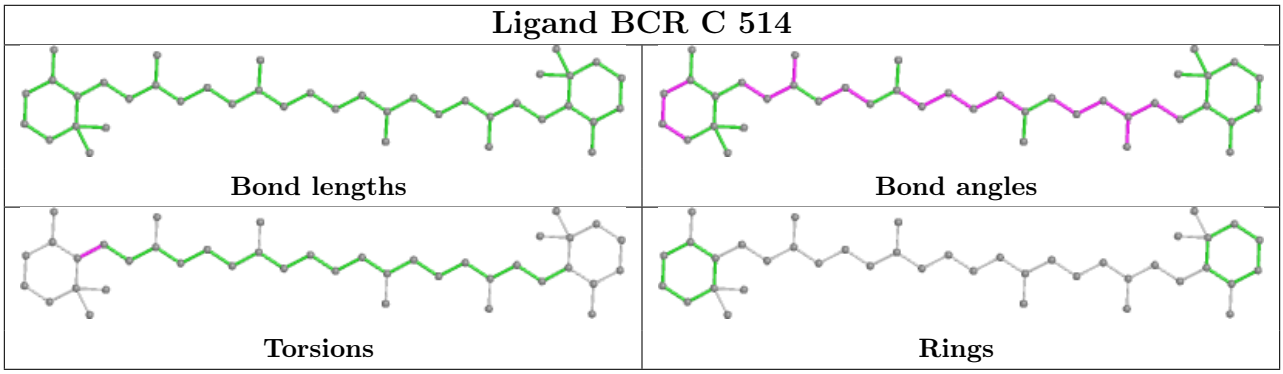
Torsions

Rings

Ligand LUT 7 1621



Ligand BCR C 514



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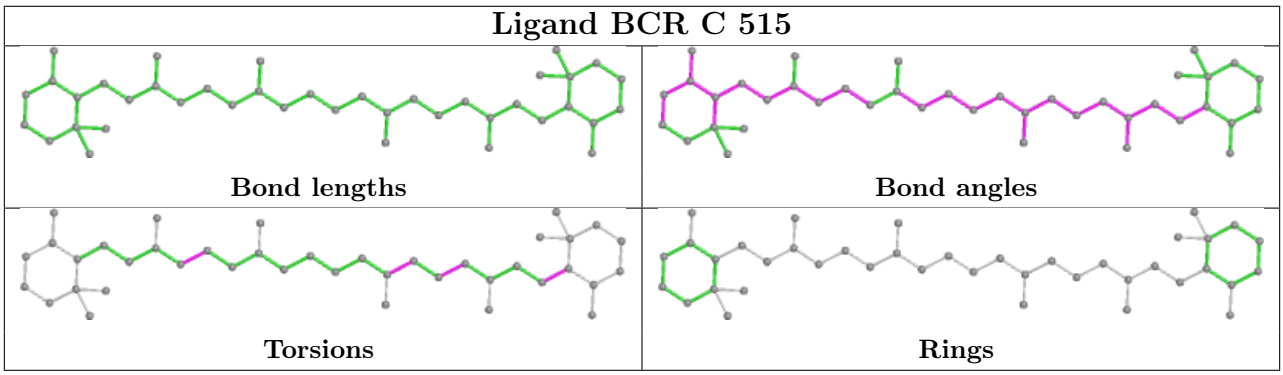
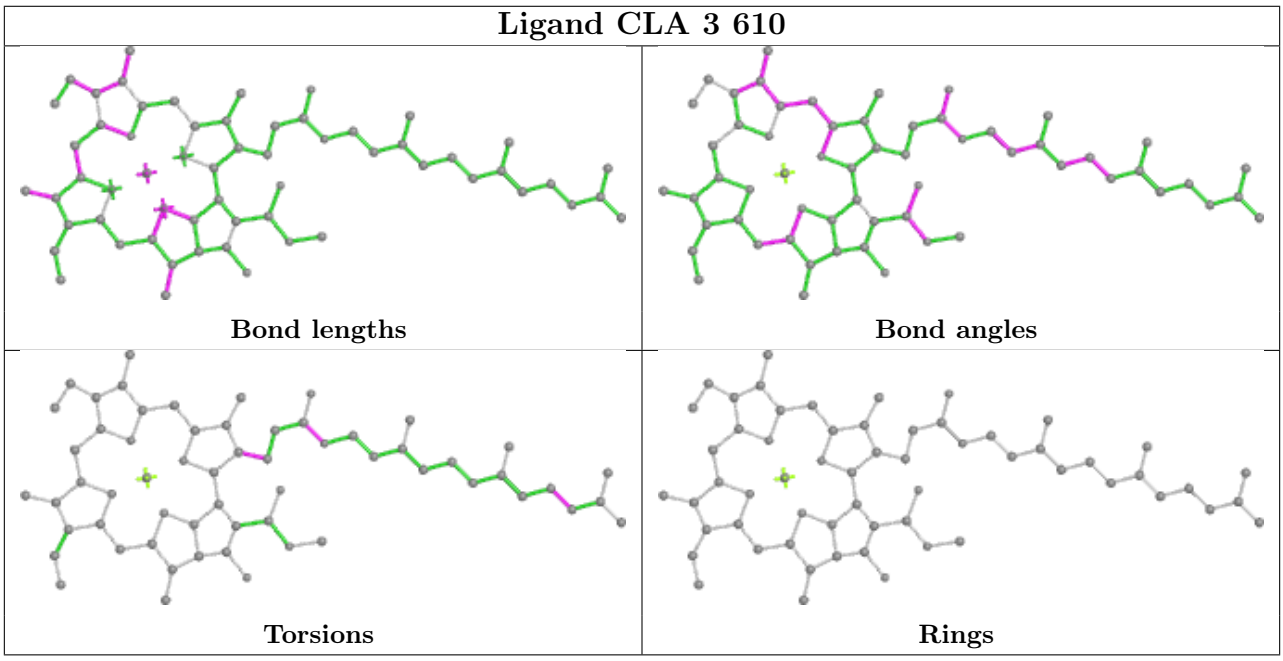
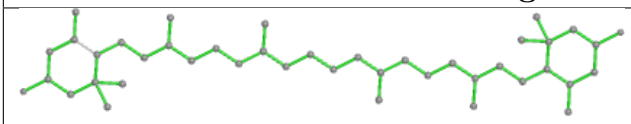
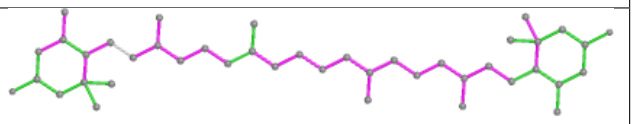


Ligand CLA 3 610



Ligand LUT S 1620


Bond lengths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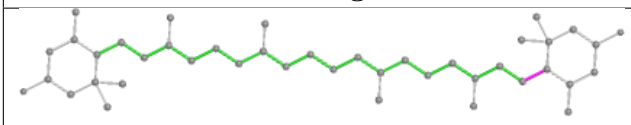
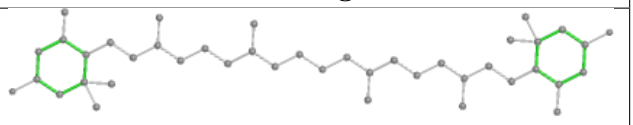
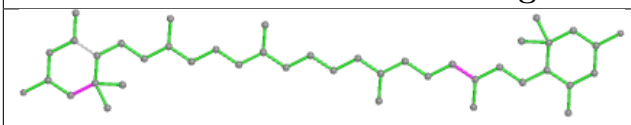

Torsions


Rings

Ligand LUT n 1621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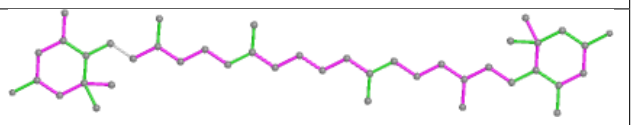
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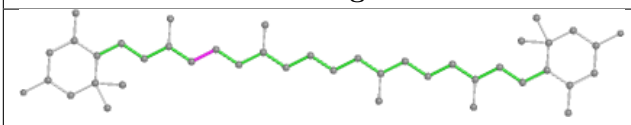
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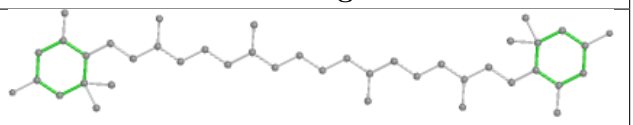
Rings

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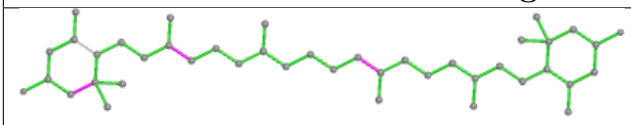
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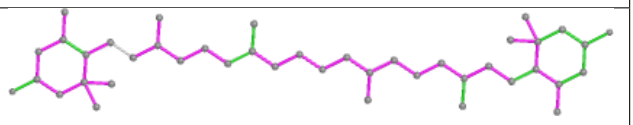
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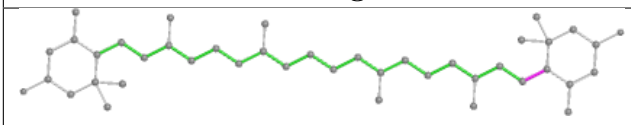
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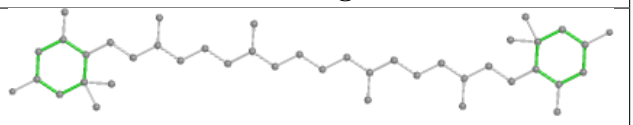
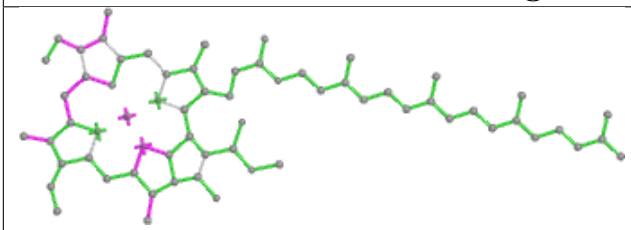

Rings

Ligand CLA B 615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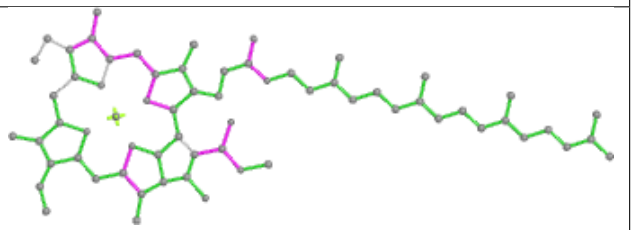
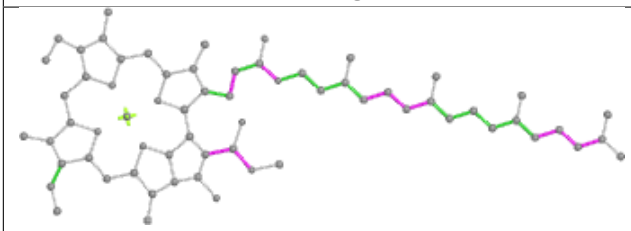

Bond angles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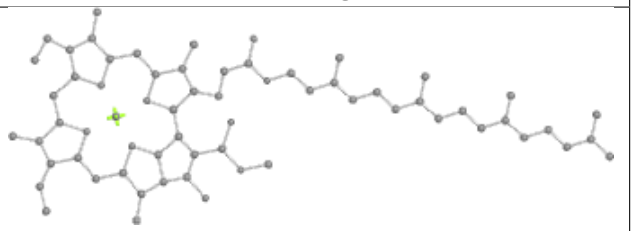
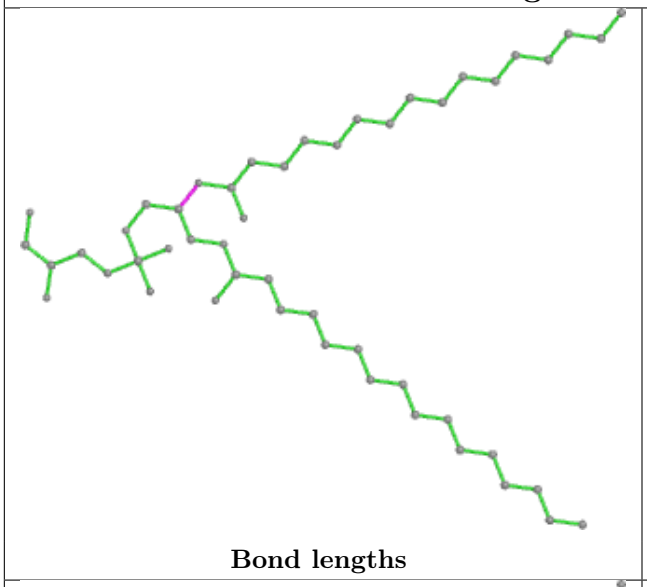

Rings

Ligand LHG C 523



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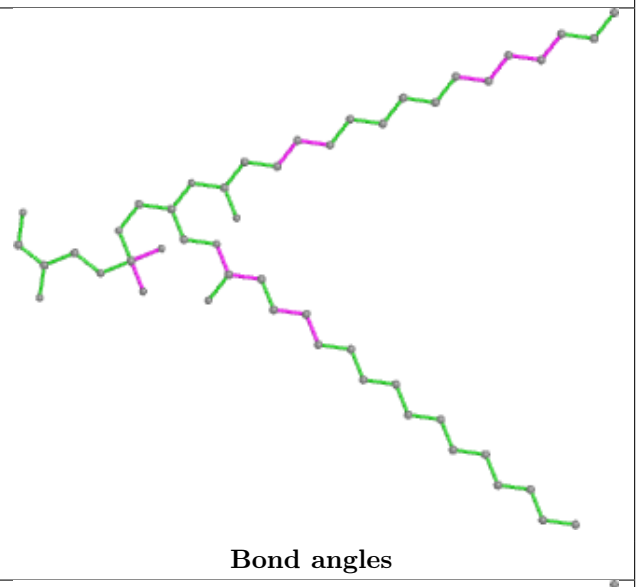

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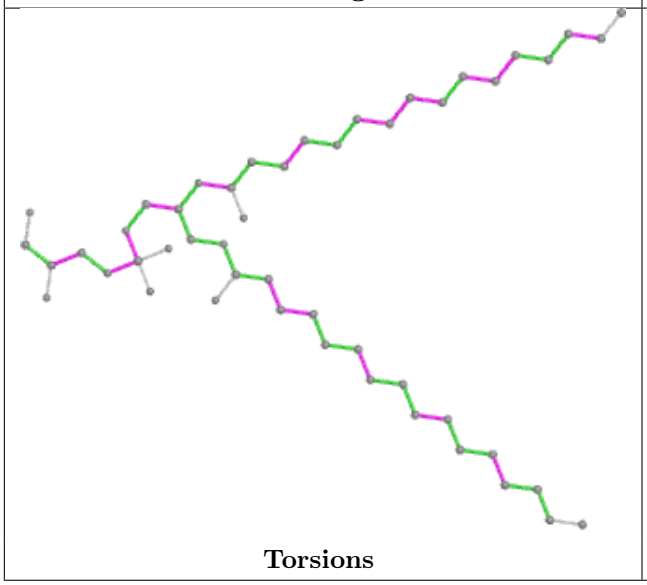

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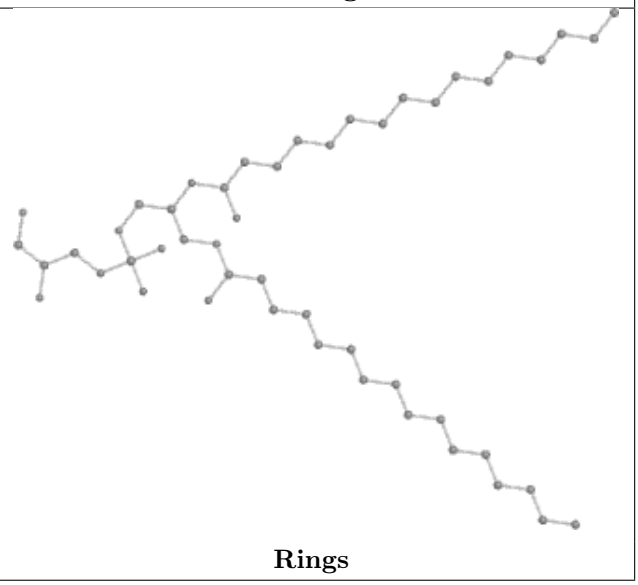
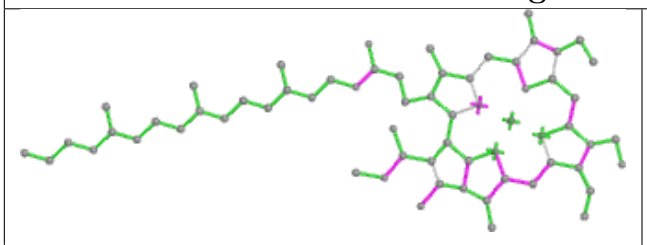


Rings

Ligand CHL 7 601



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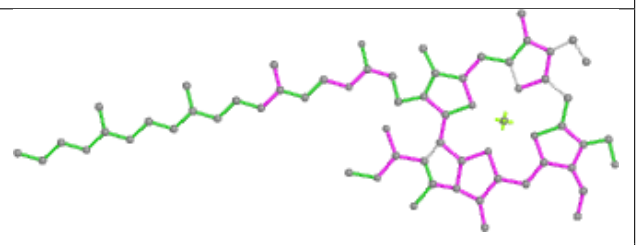

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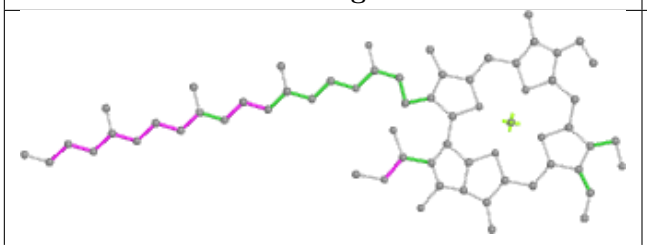

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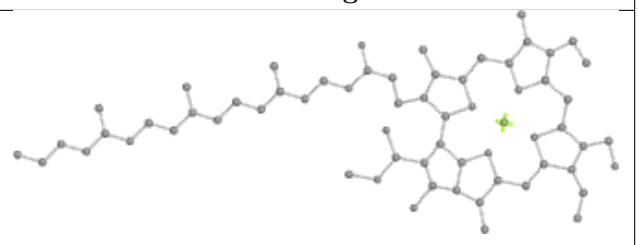
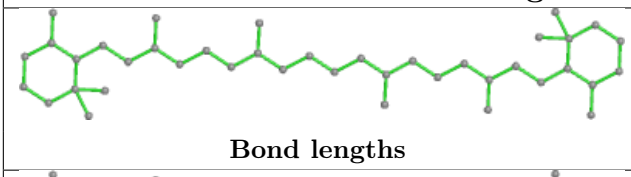


Rings

Ligand BCR 8 623



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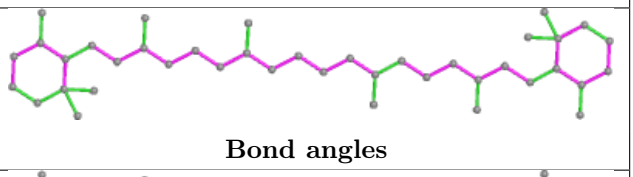
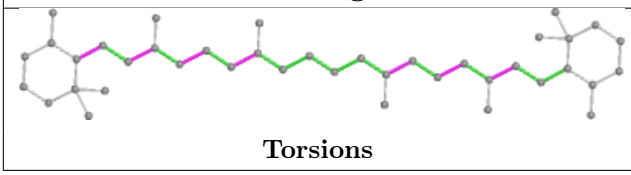


Bond angles



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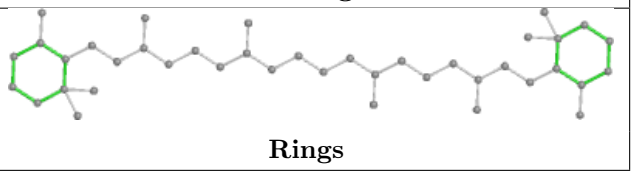
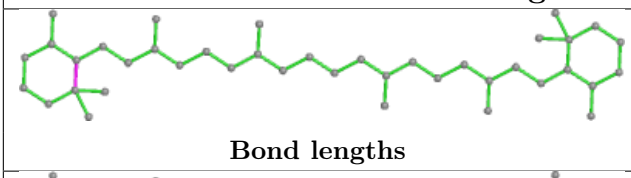


Rings

Ligand BCR t 101



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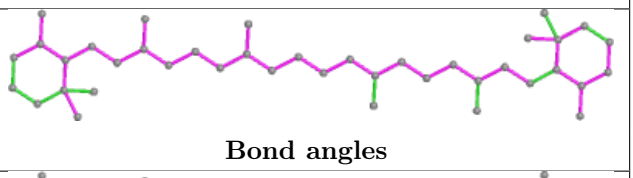

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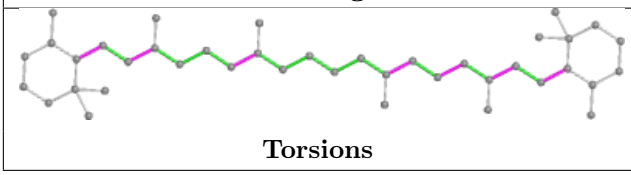

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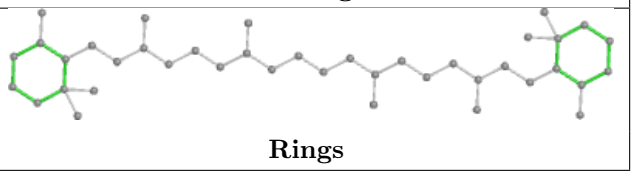
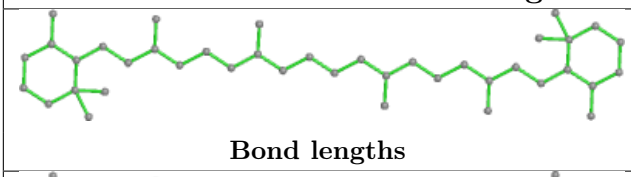


Rings

Ligand BCR h 101



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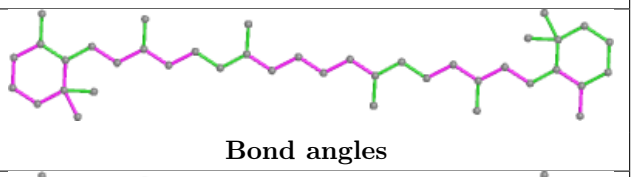
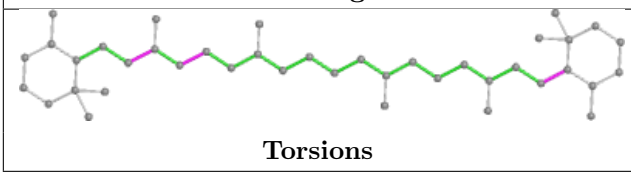


Bond angles



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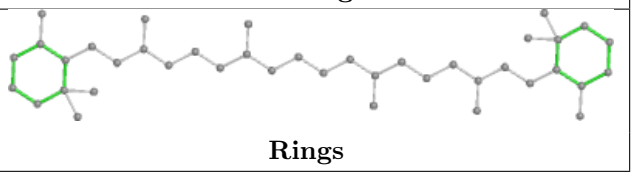
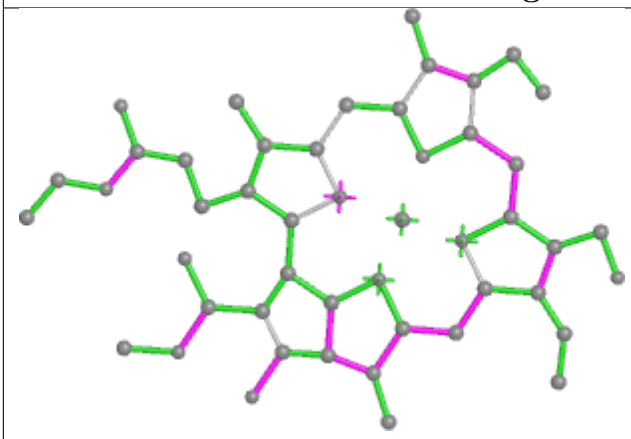


Rings

Ligand CHL N 605



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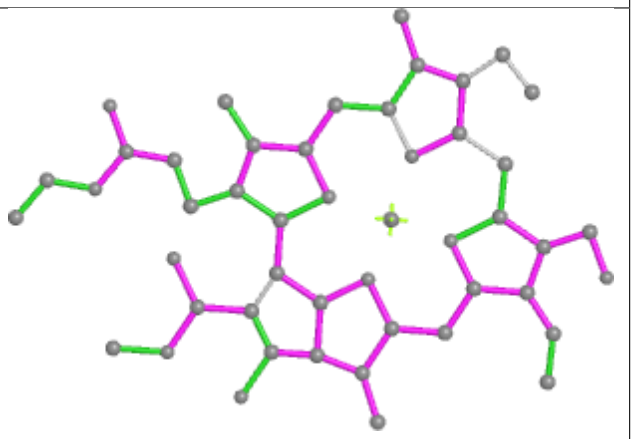

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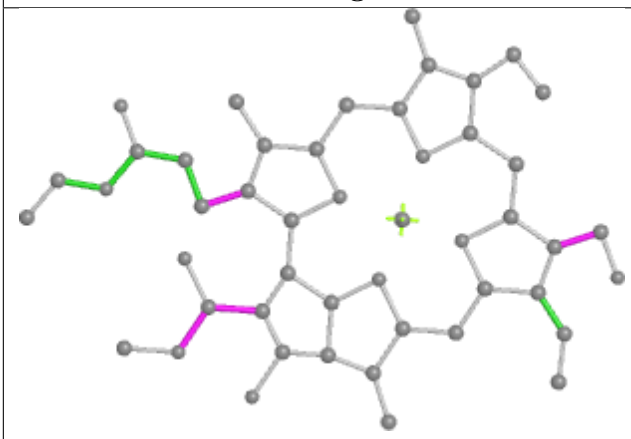

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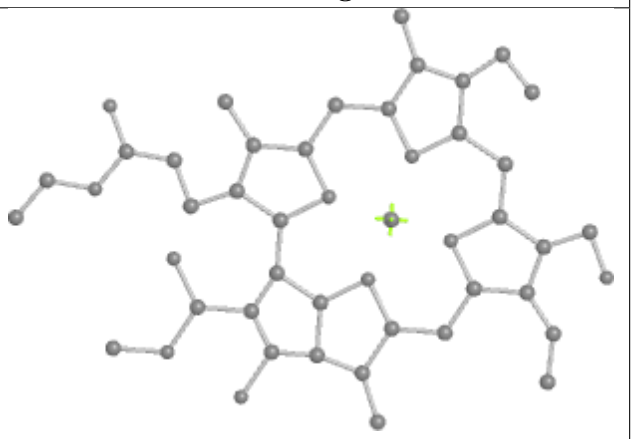

Rings

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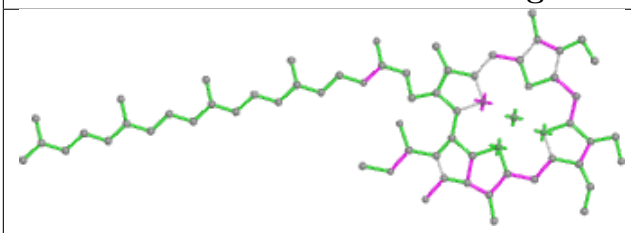

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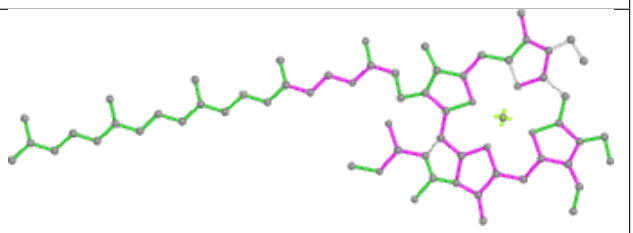
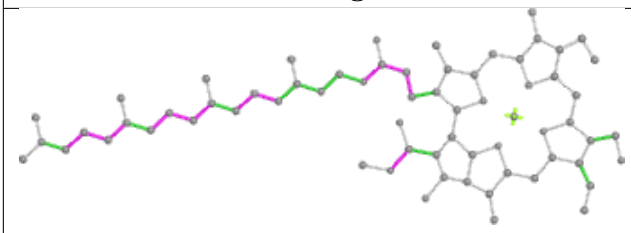


Bond angles



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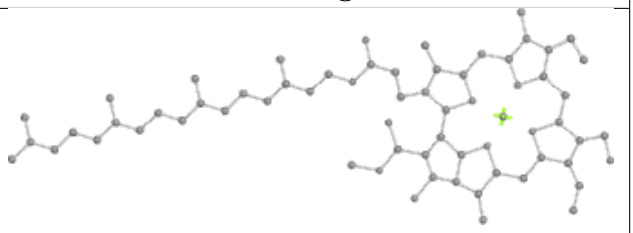

Rings

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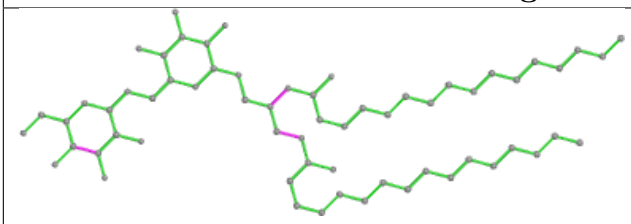

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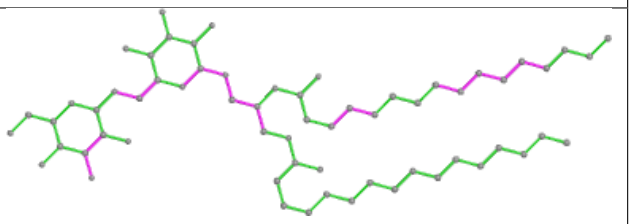
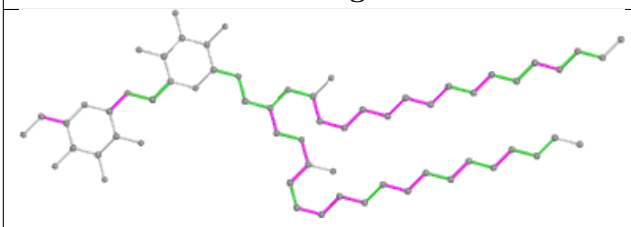


Bond angles



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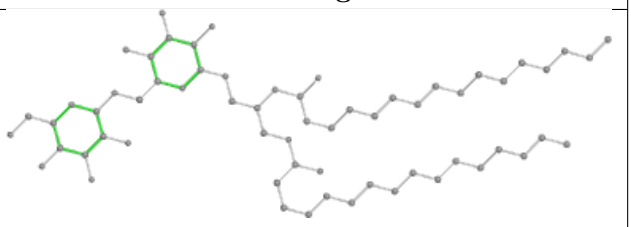
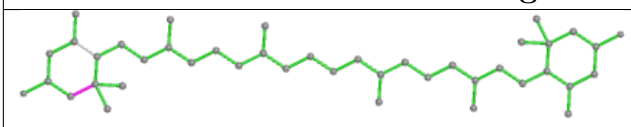


Rings

Ligand LUT 3 1621



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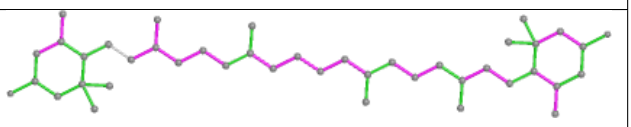
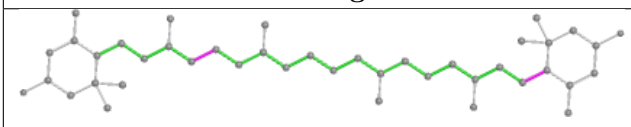


Bond angles



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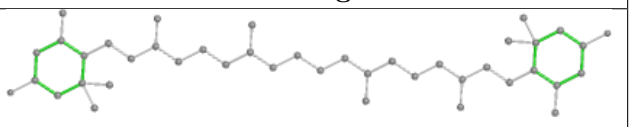
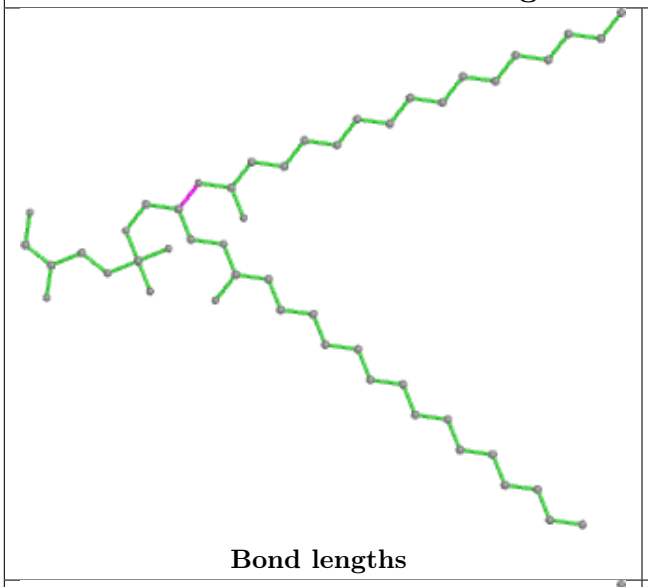
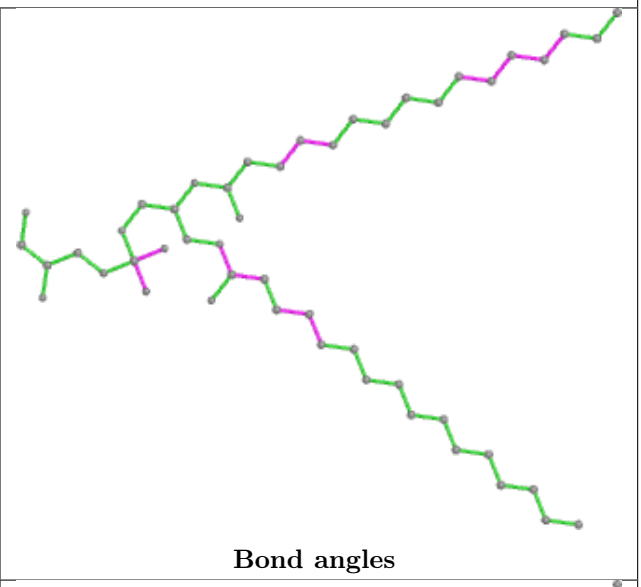


Rings

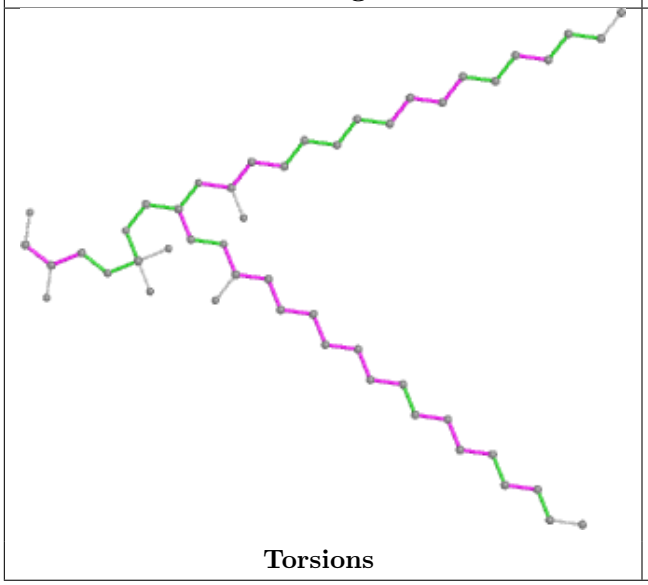
Ligand LHG c 2630



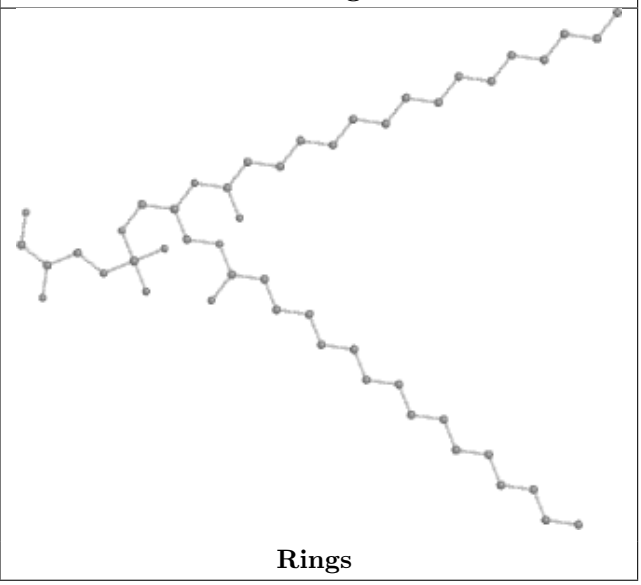
Bond lengths



Bond angles

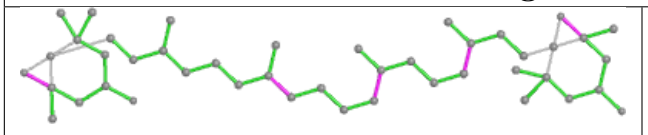


Torsions



Rings

Ligand XAT 3 1622



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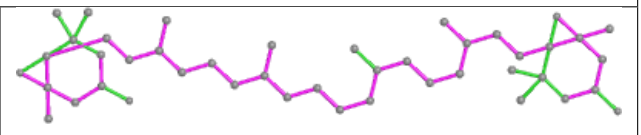

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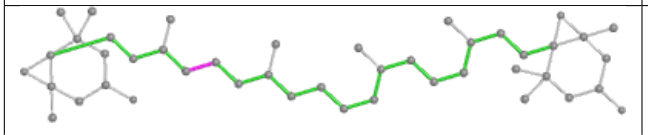

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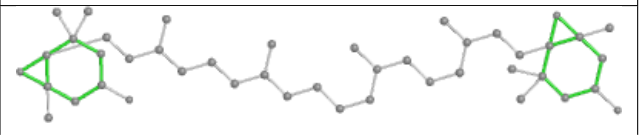
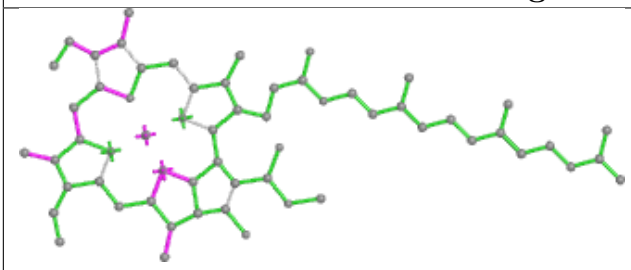


Rings

Ligand CLA a 410



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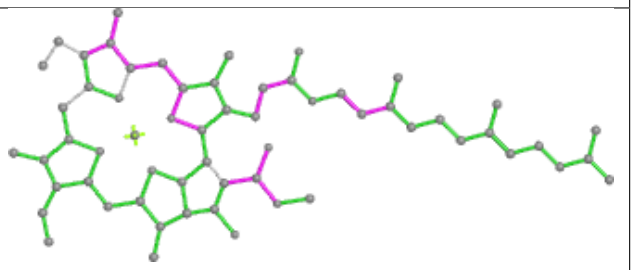
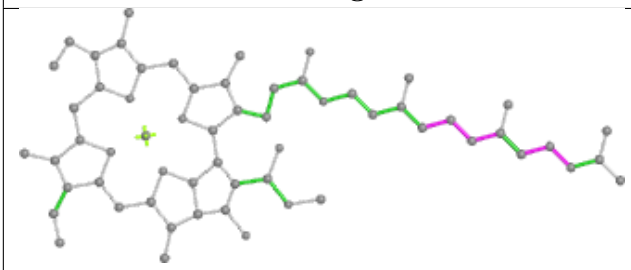


Bond angles



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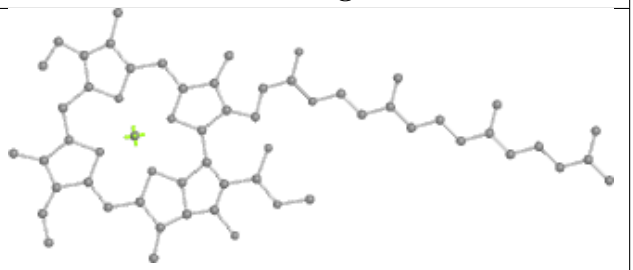
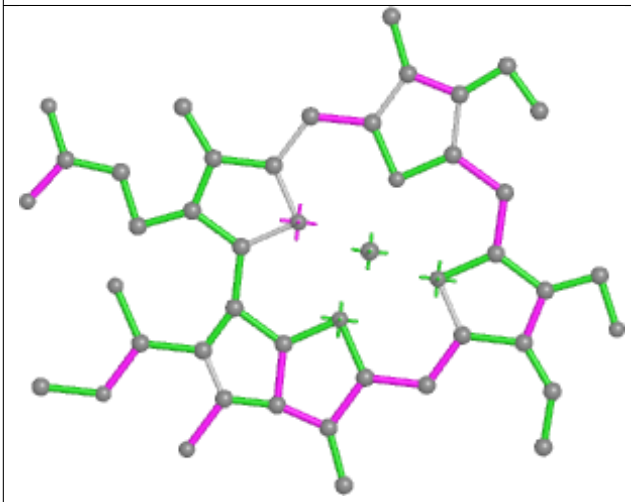


Rings

Ligand CHL g 605



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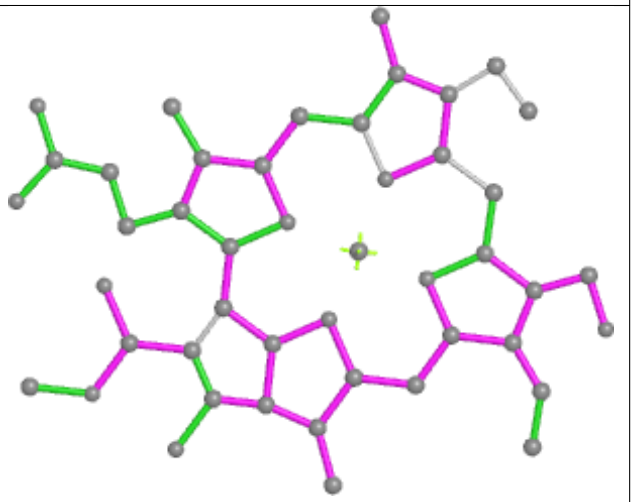
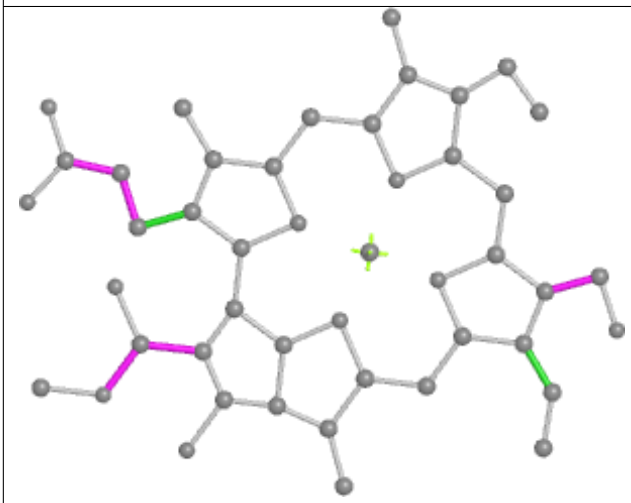


Bond angles



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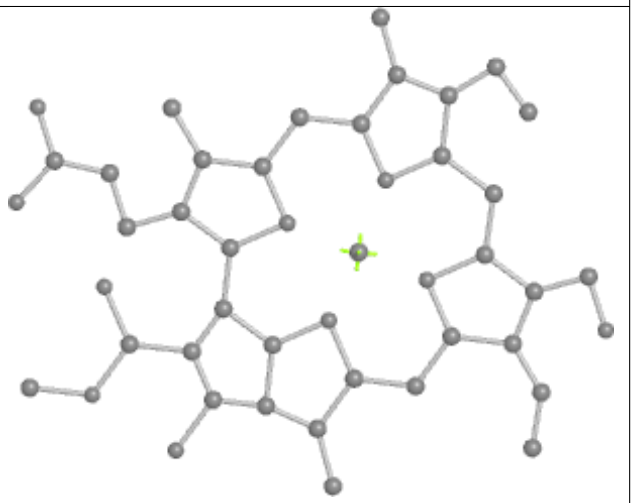
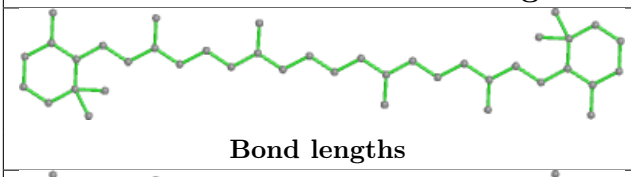


Rings

Ligand BCR H 101



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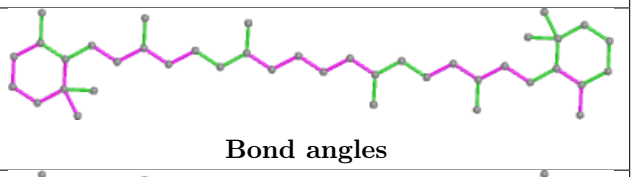

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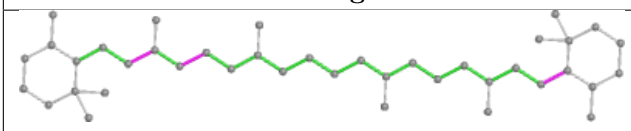

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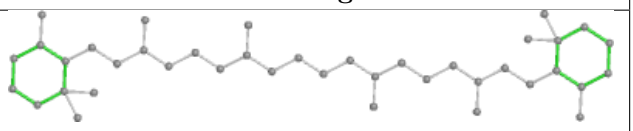

Rings

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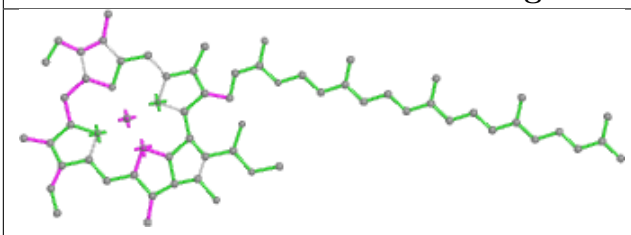

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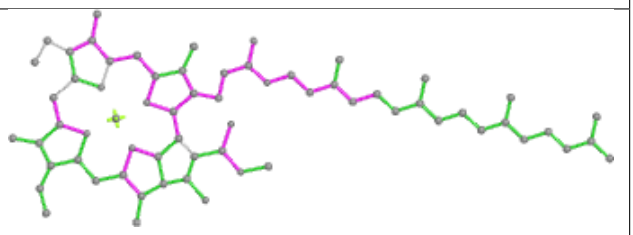

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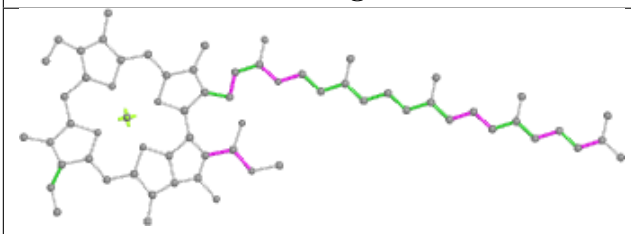

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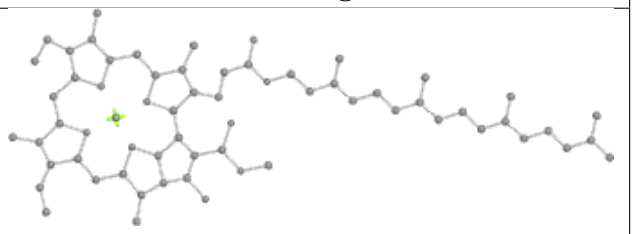
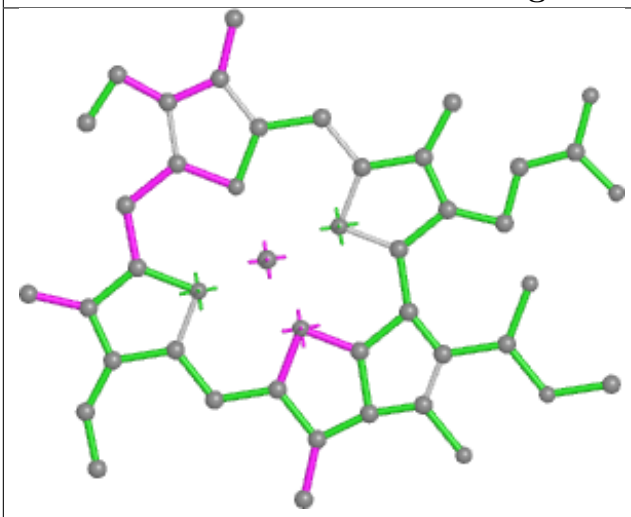


Rings

Ligand CLA 7 604



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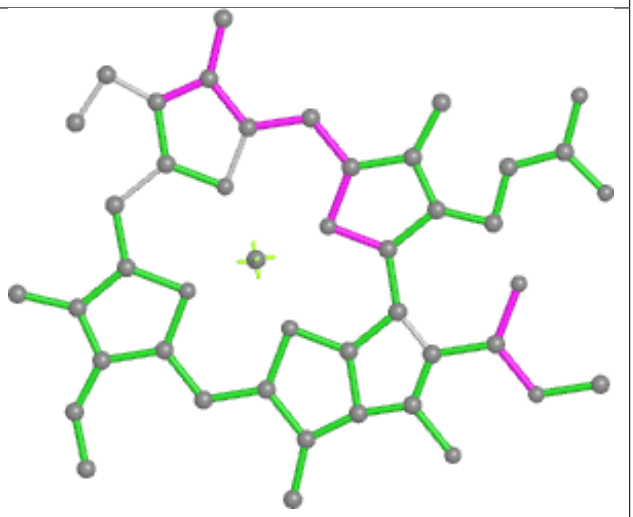

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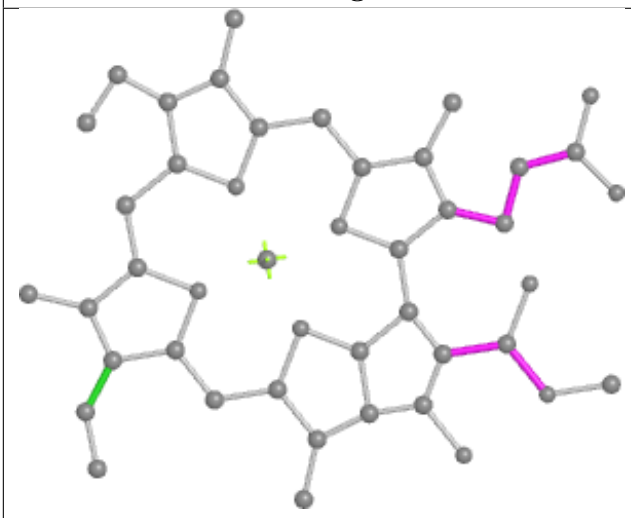

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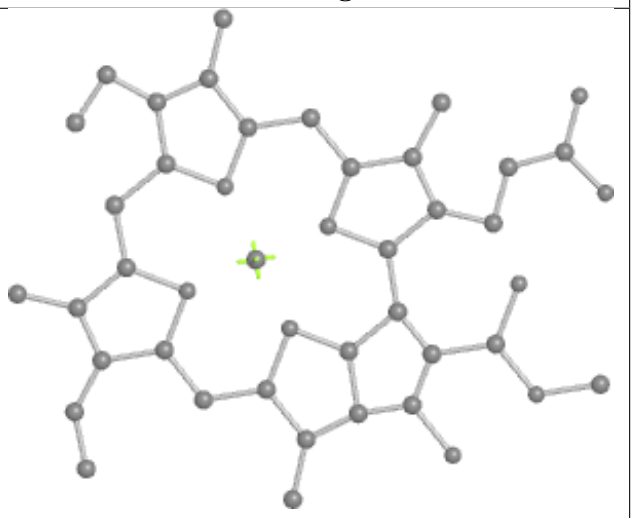
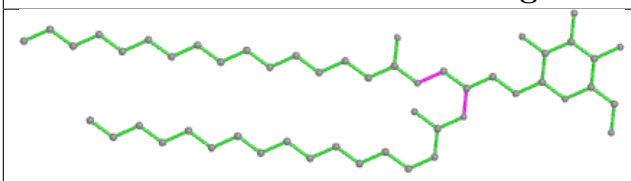


Rings

Ligand LMG B 622



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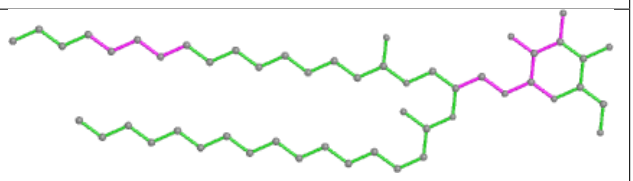
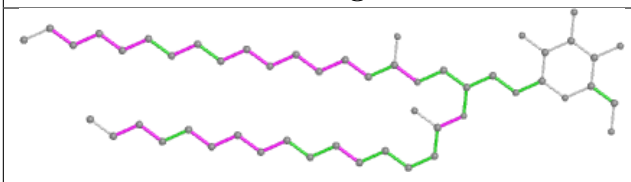


Bond angles



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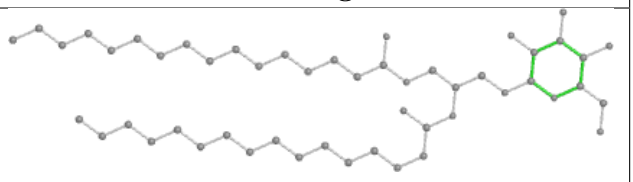
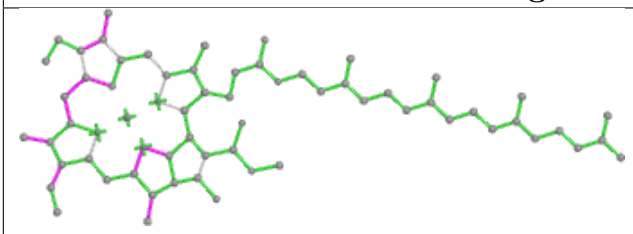


Rings

Ligand CLA a 406



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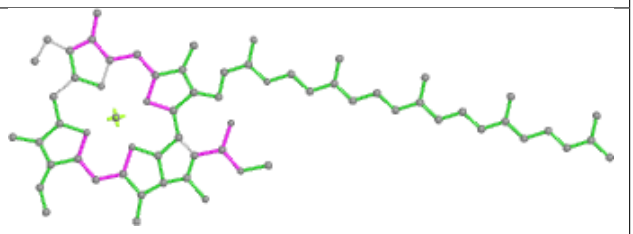
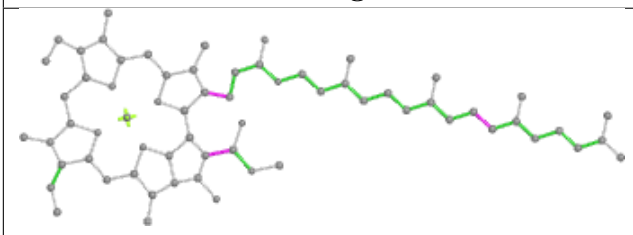


Bond angles



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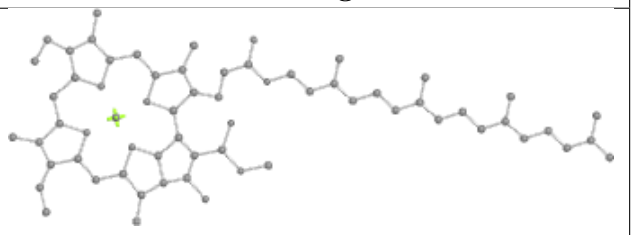
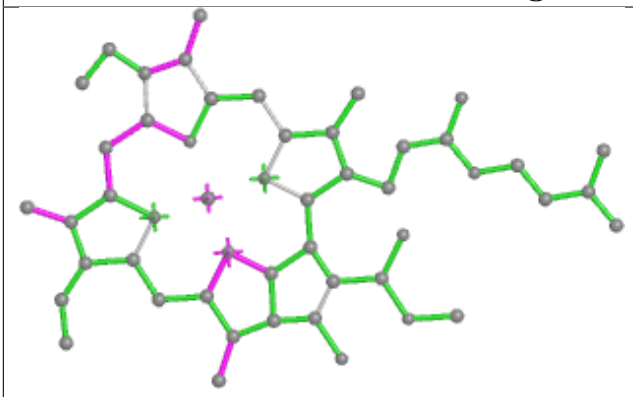


Rings

Ligand CLA n 604



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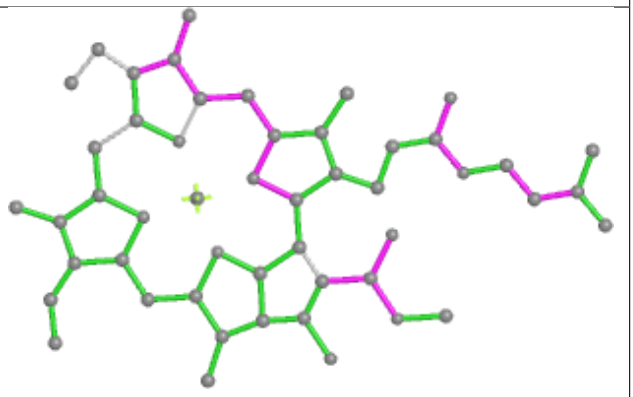

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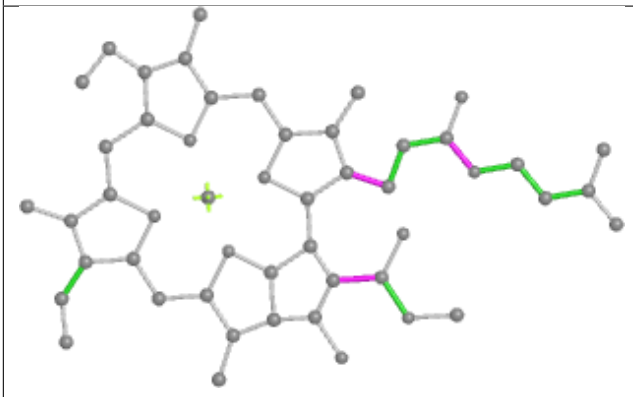

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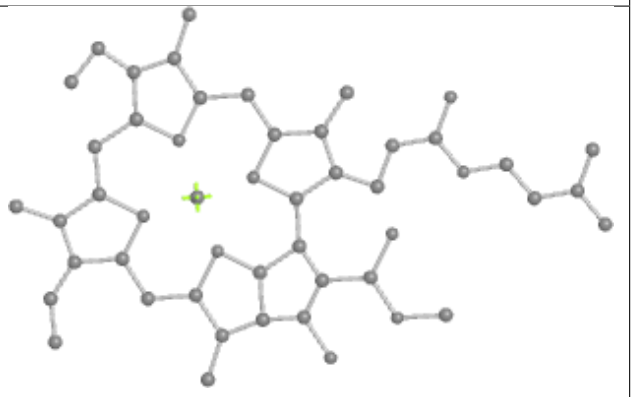
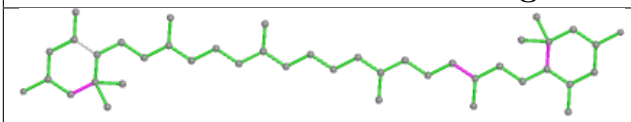


Rings

Ligand LUT 5 1621



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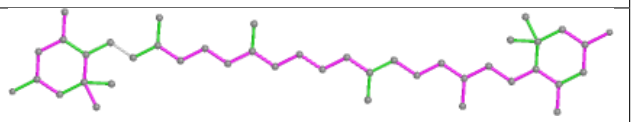

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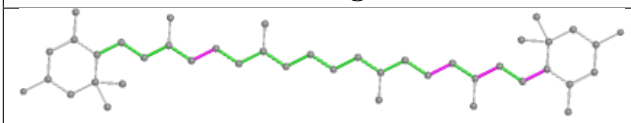

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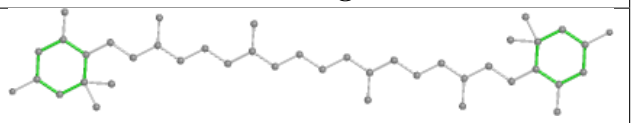

Rings

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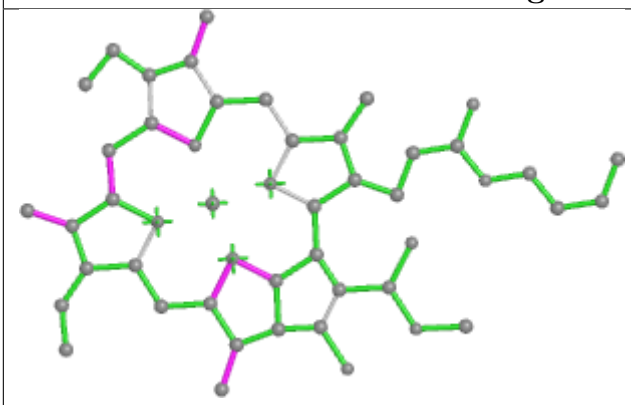

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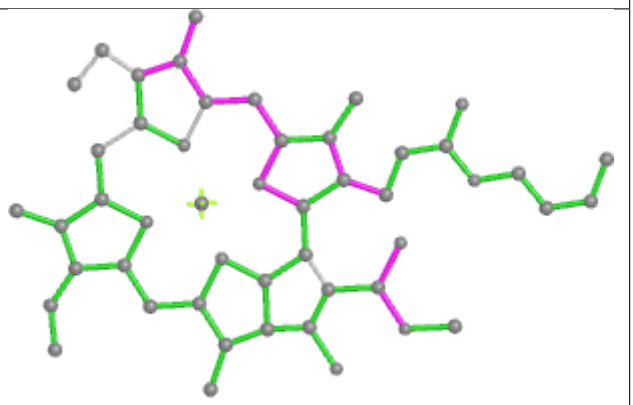
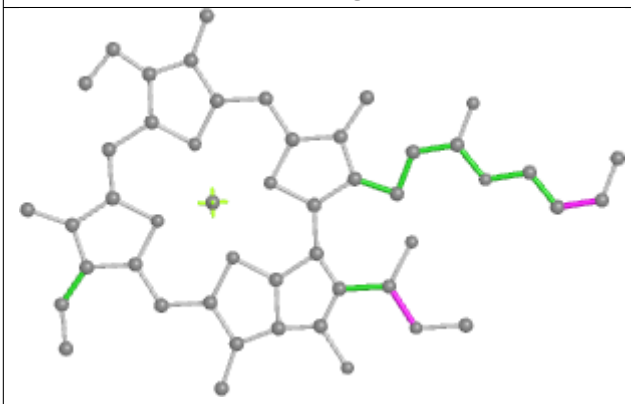


Bond angles



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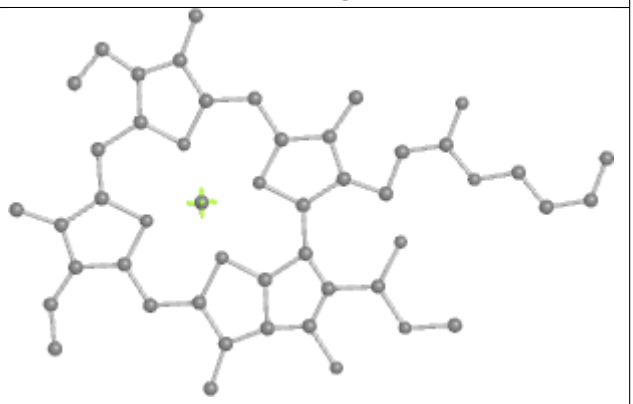
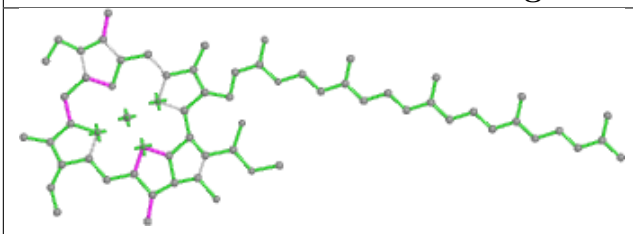


Rings

Ligand CLA C 512



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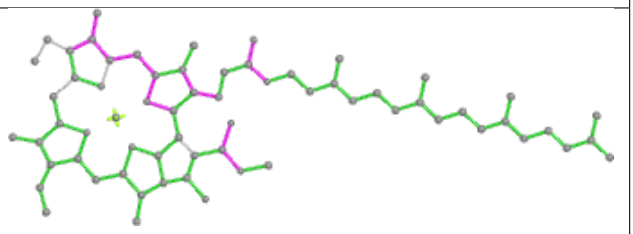
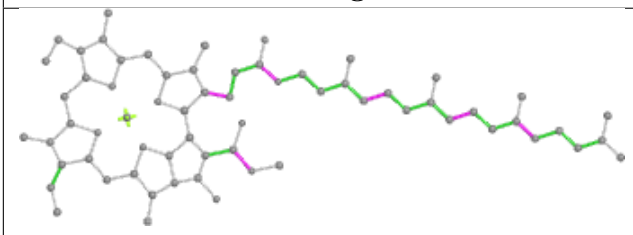


Bond angles



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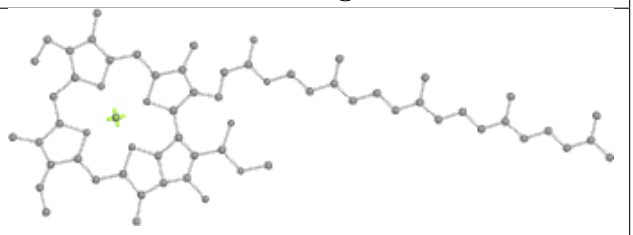
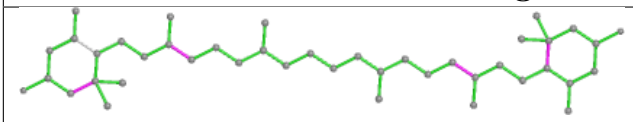


Rings

Ligand LUT G 1621



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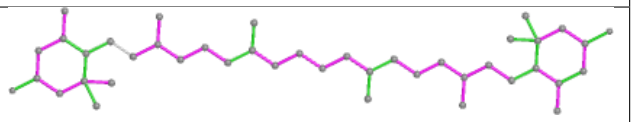
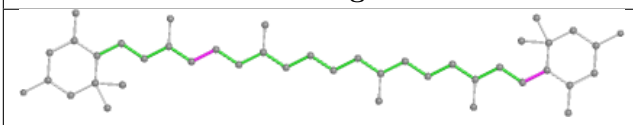
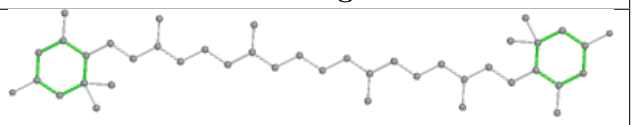


Bond angles

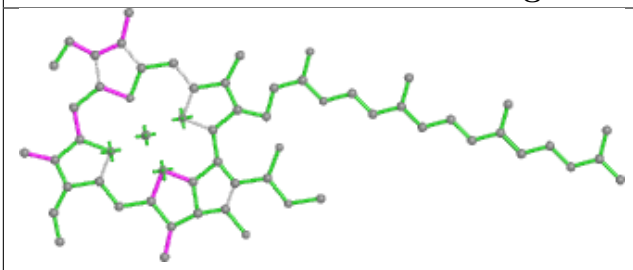


Torsions

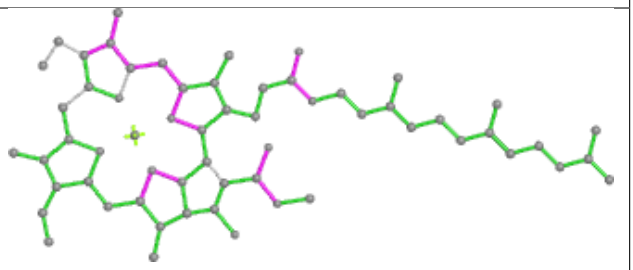


Rings

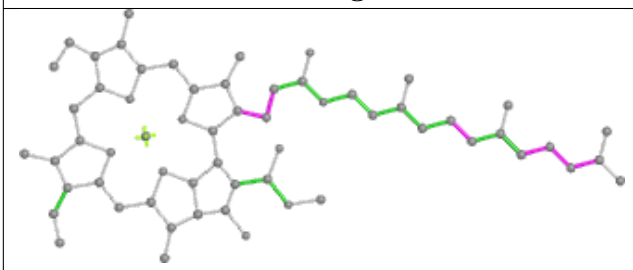
Ligand CLA Y 610



Bond lengths



Bond angles



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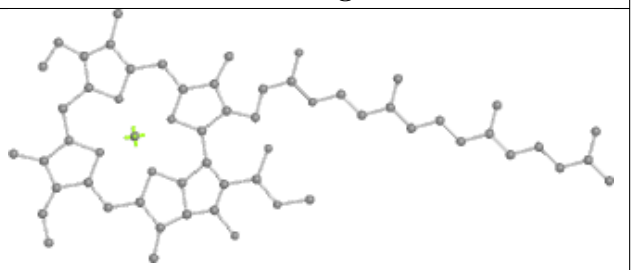
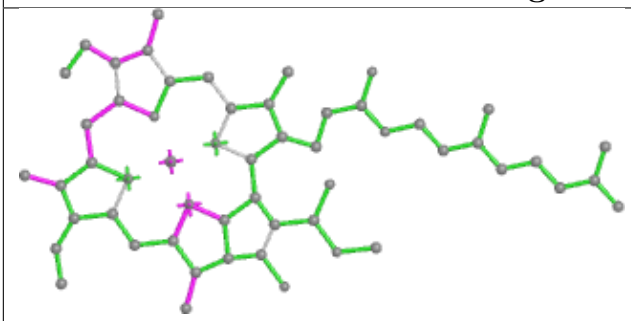


Rings

Ligand CLA 5 613



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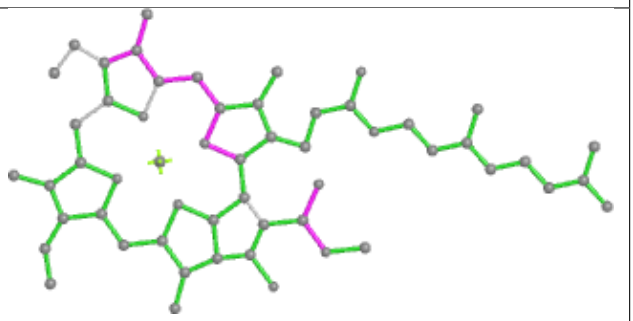

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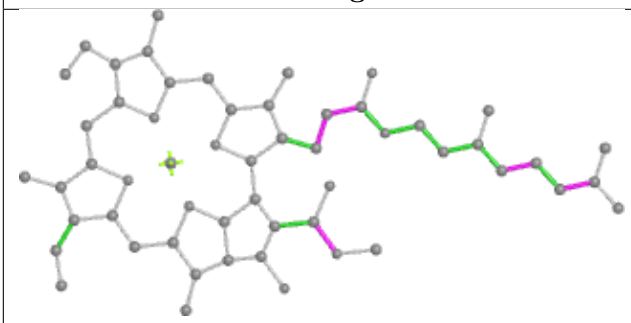

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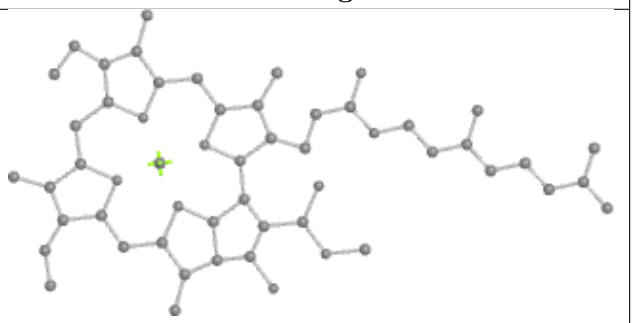
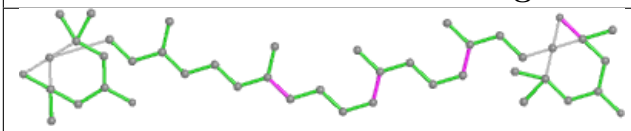


Rings

Ligand XAT Y 1622



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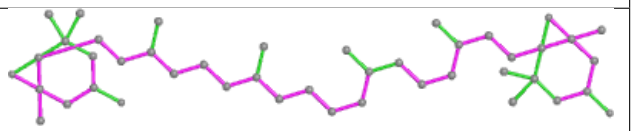
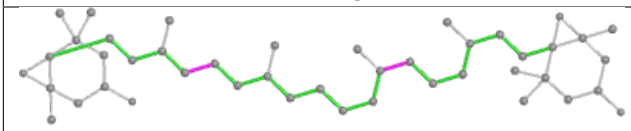


Bond angles



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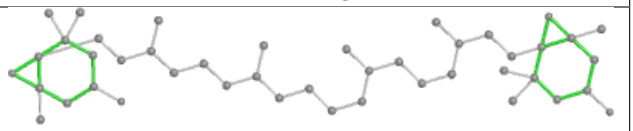
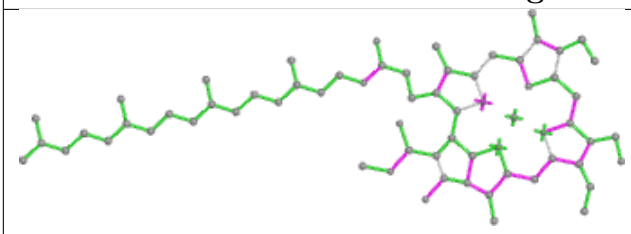


Rings

Ligand CHL n 609



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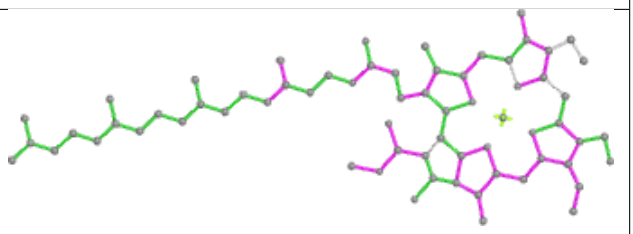
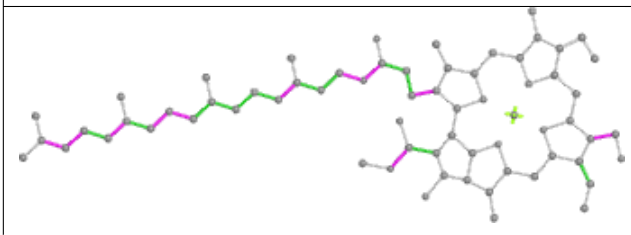


Bond angles



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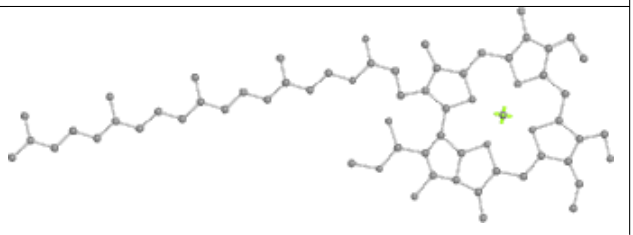
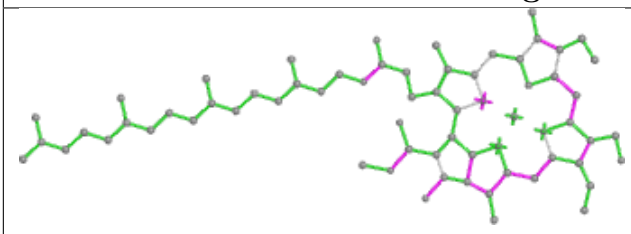


Rings

Ligand CHL G 601



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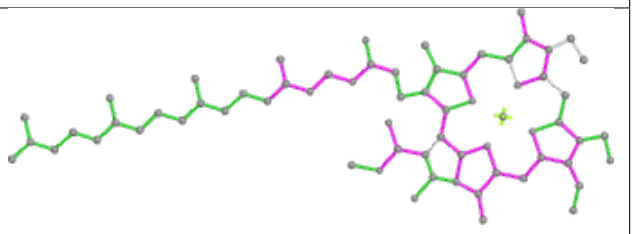

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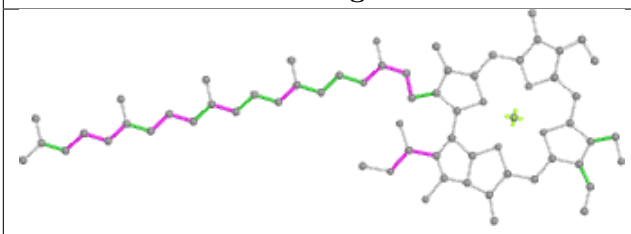

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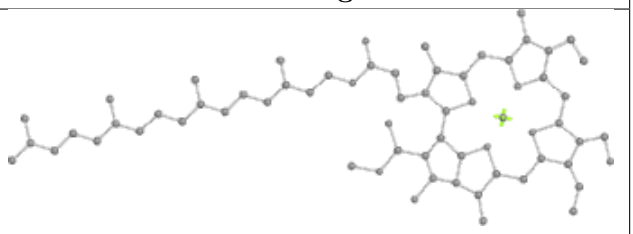
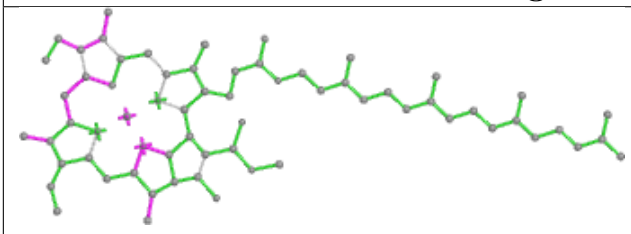


Rings

Ligand CLA b 615



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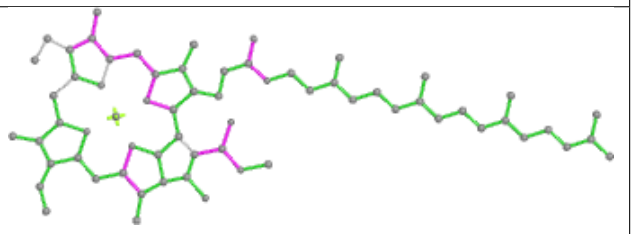

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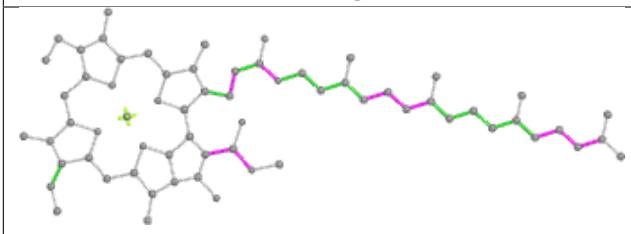

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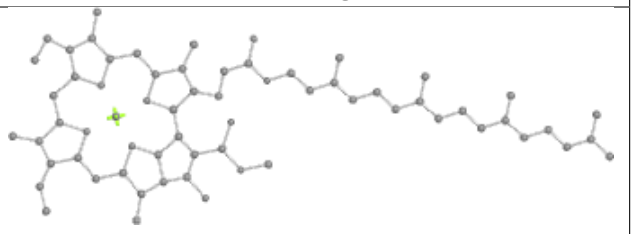
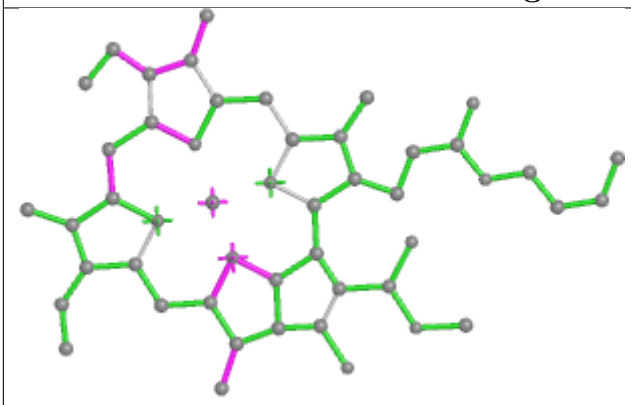


Rings

Ligand CLA R 601



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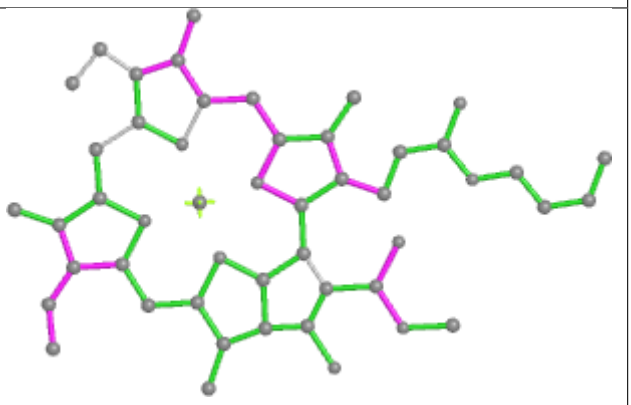

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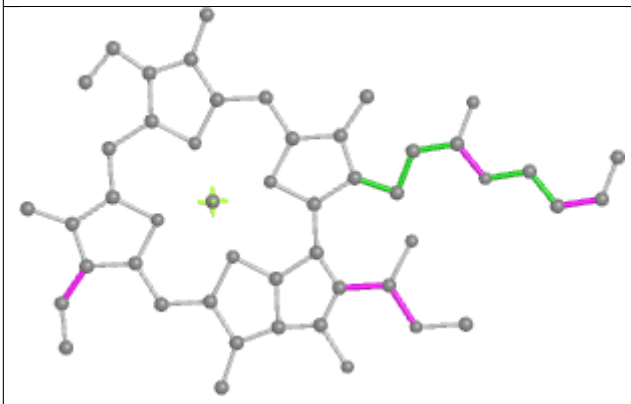

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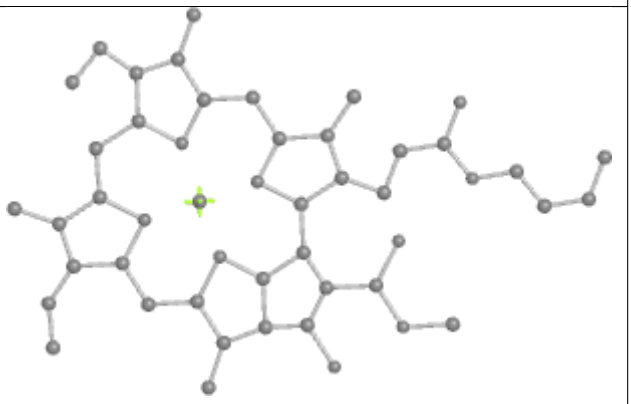
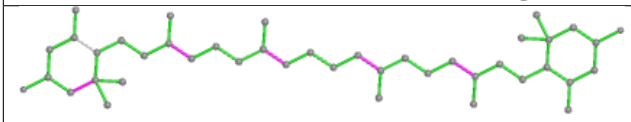


Rings

Ligand LUT Y 1620



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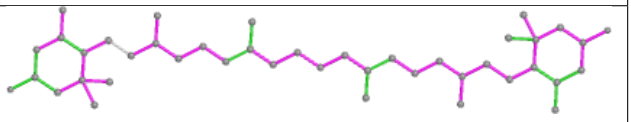

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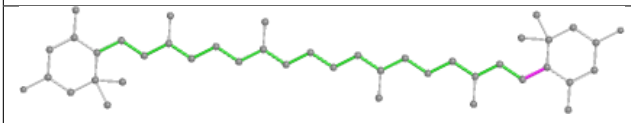

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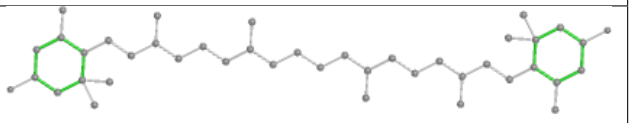
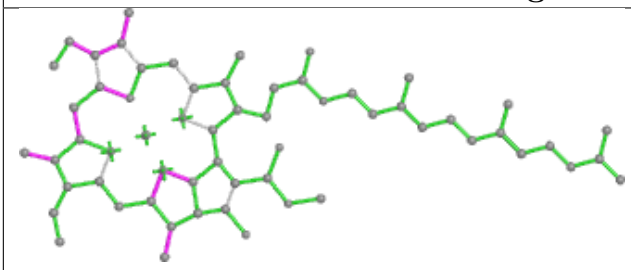


Rings

Ligand CLA n 611



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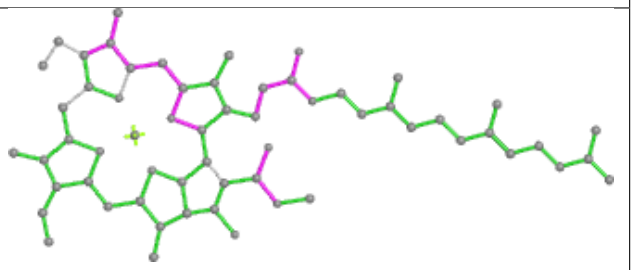
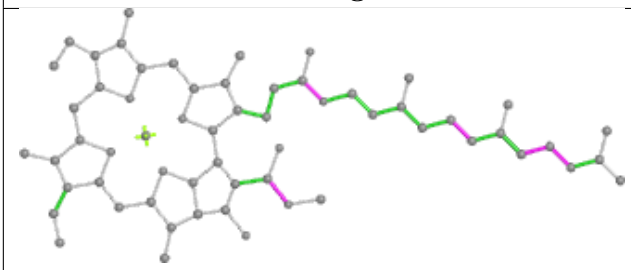


Bond angles



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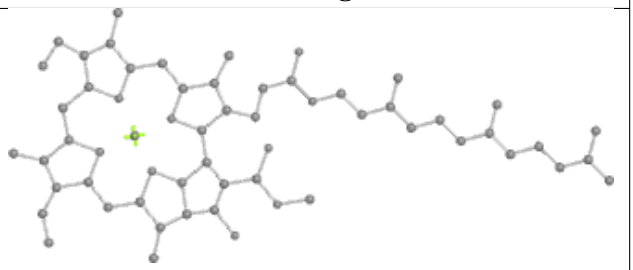
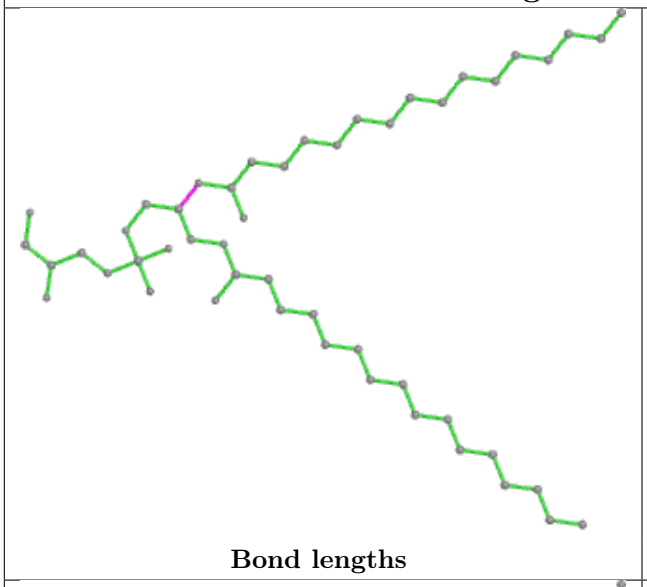


Rings

Ligand LHG D 409



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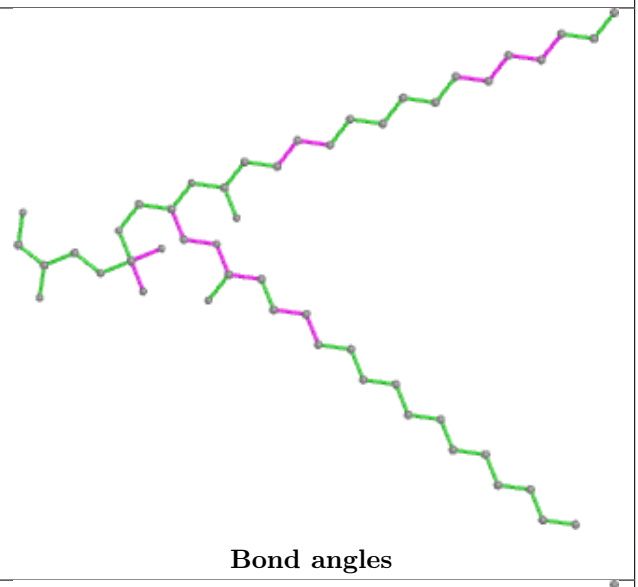

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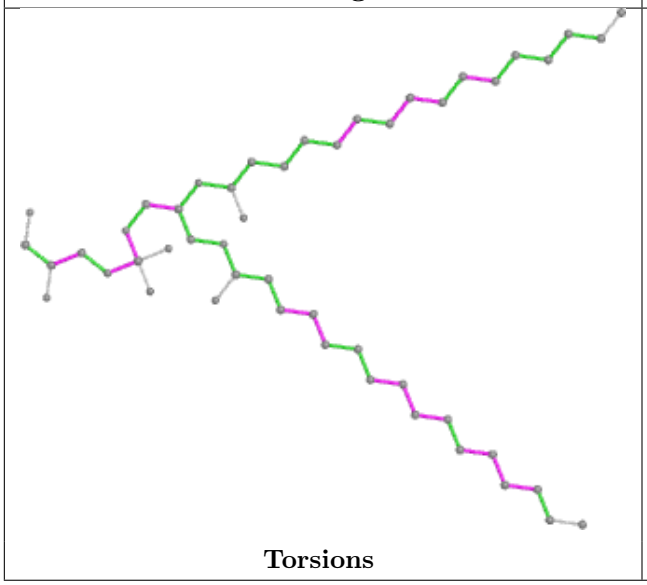

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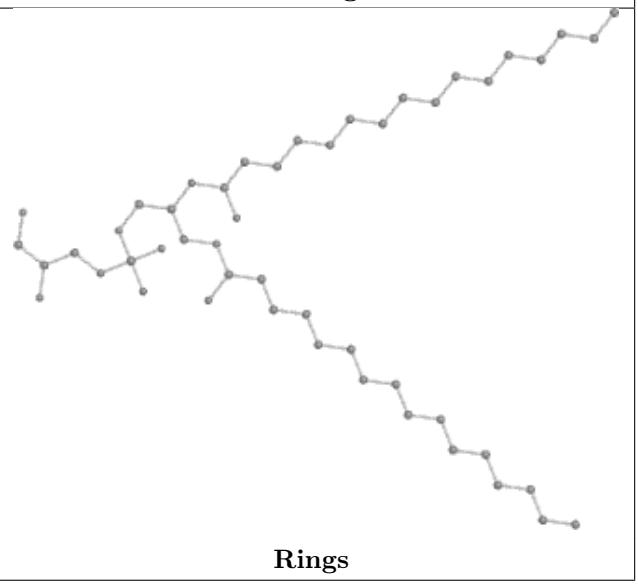
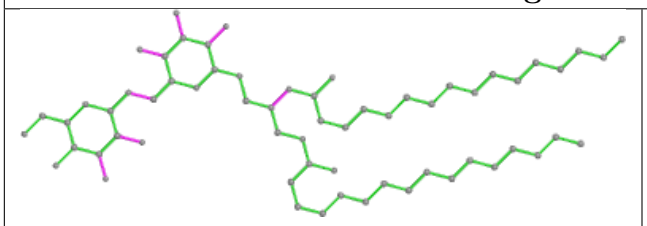


Rings

Ligand DGD h 102



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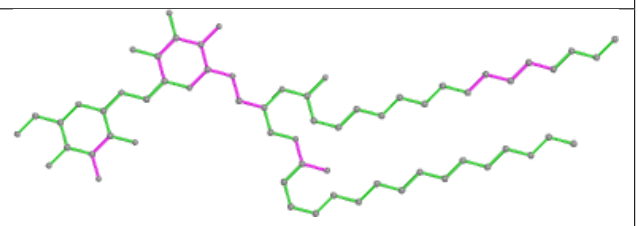

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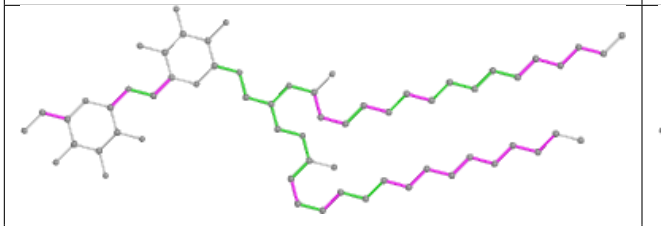

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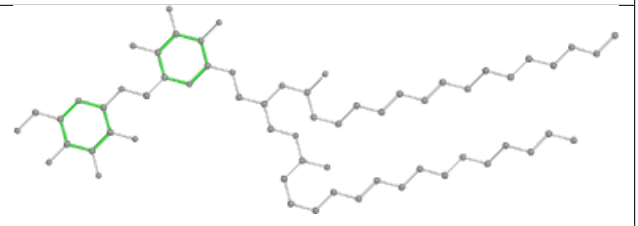
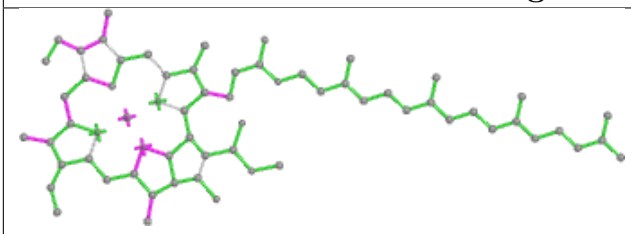


Rings

Ligand CLA b 614



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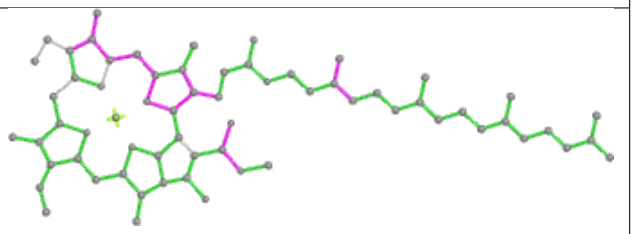
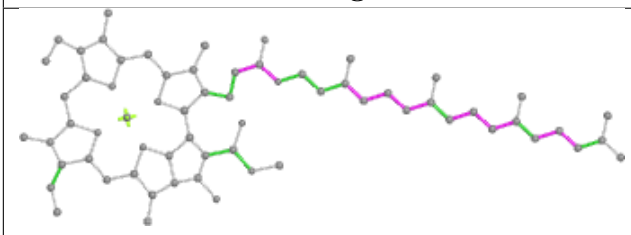


Bond angles



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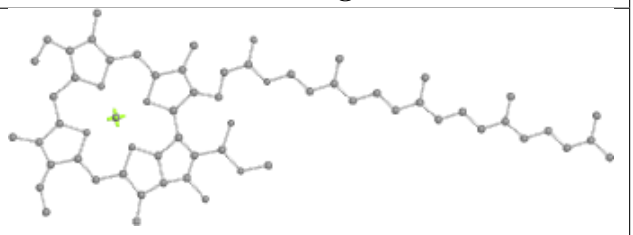
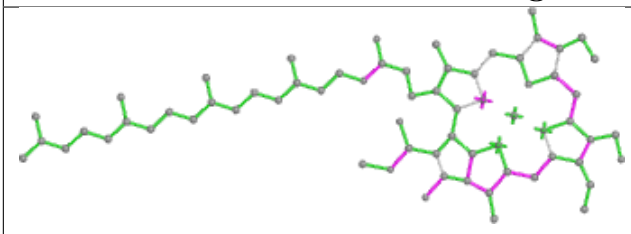


Rings

Ligand CHL g 601



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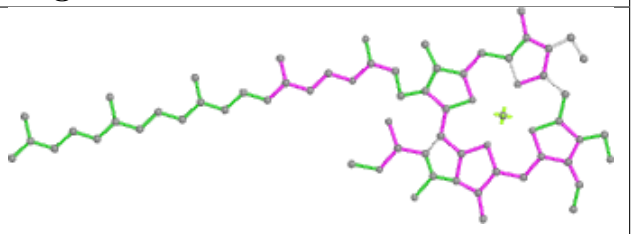
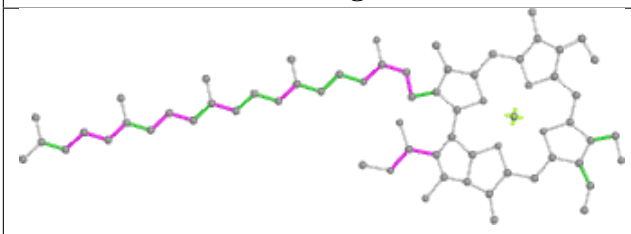


Bond angles



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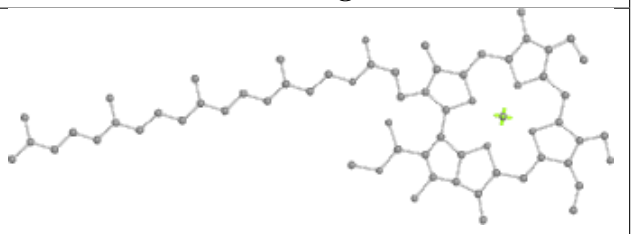
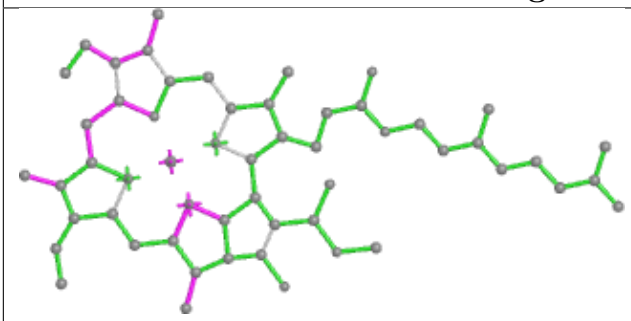
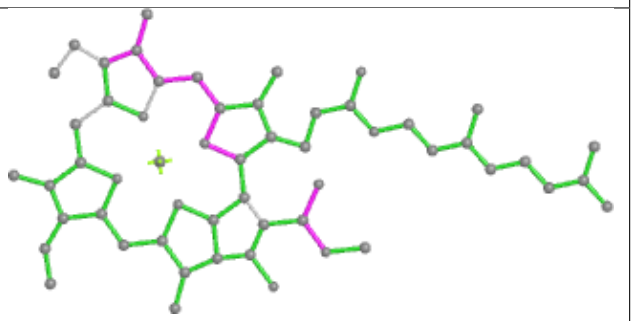


Rings

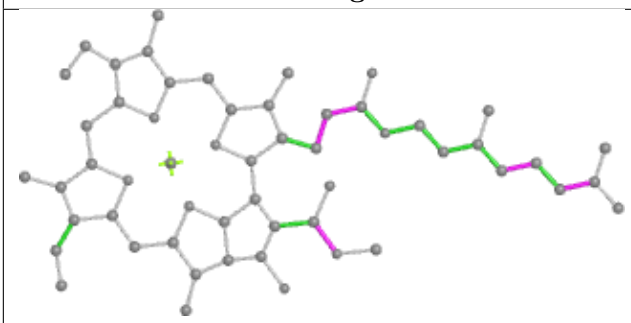
Ligand CLA 1 613



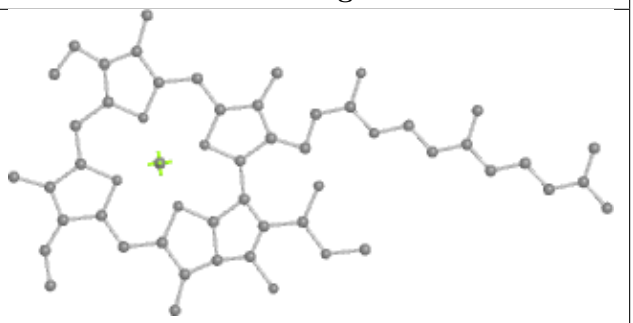
Bond lengths



Bond angles

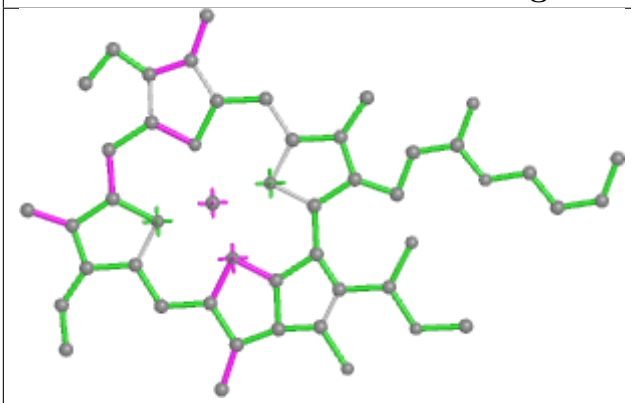


Torsions



Rings

Ligand CLA r 612



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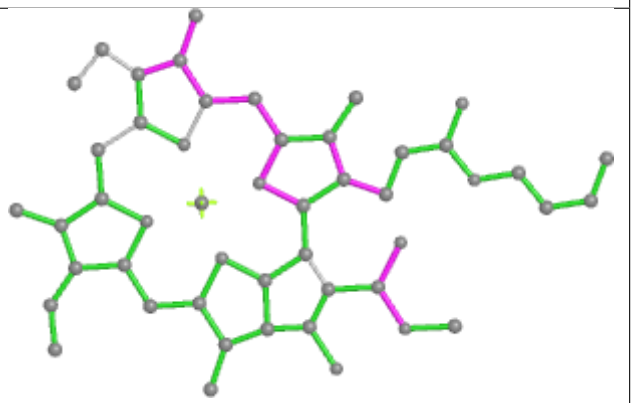
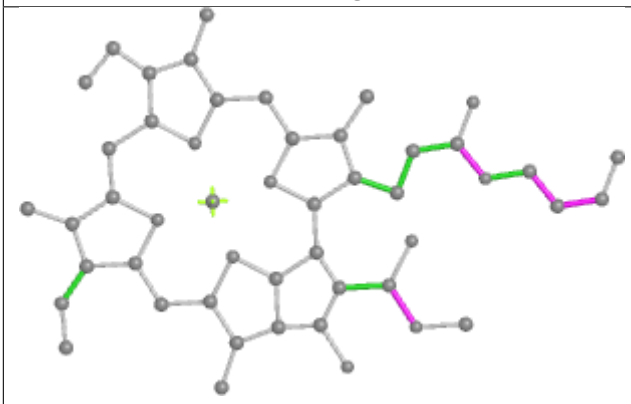


Bond angles



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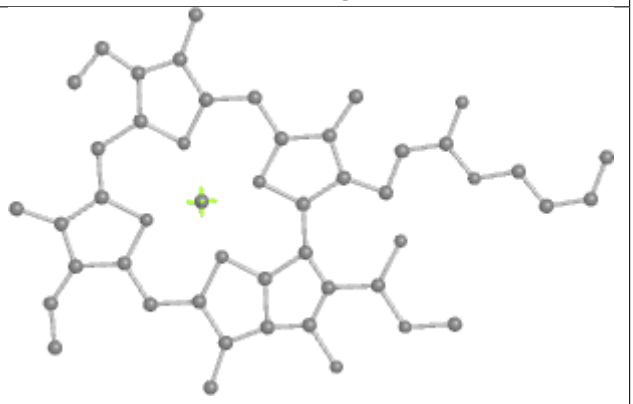
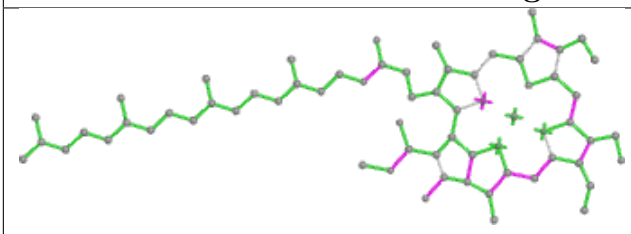


Rings

Ligand CHL Y 601



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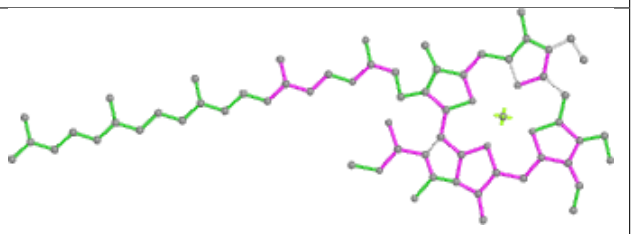
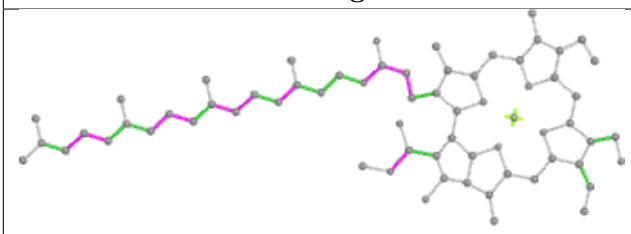
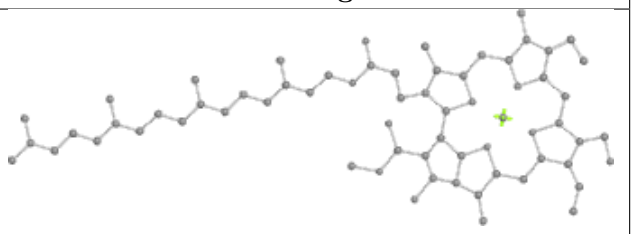


Bond angles

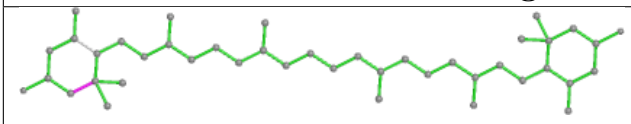


Torsions



Rings

Ligand LUT 6 1621



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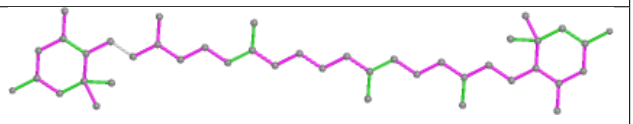
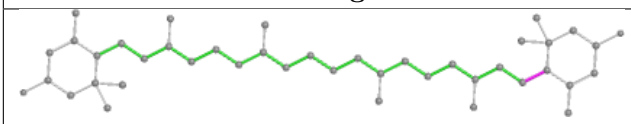


Bond angles



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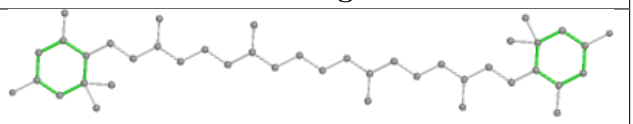
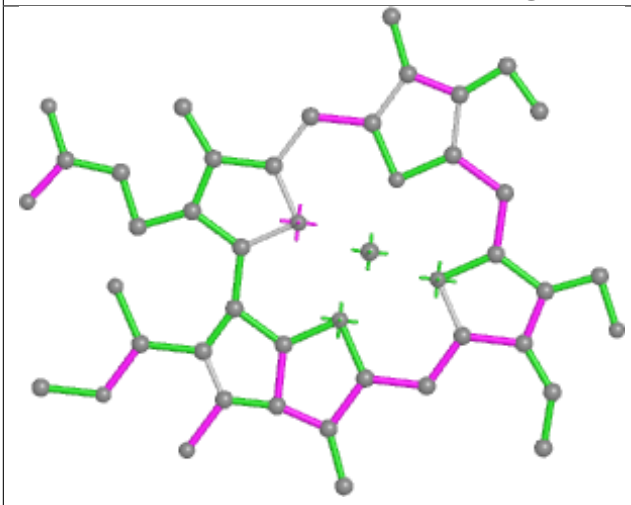


Rings

Ligand CHL G 605



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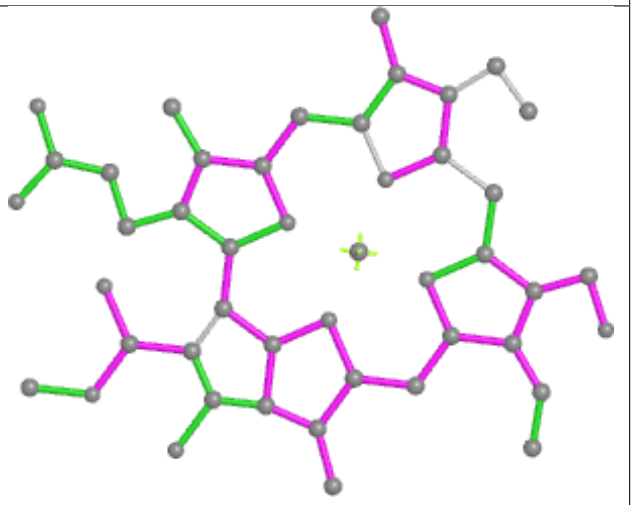
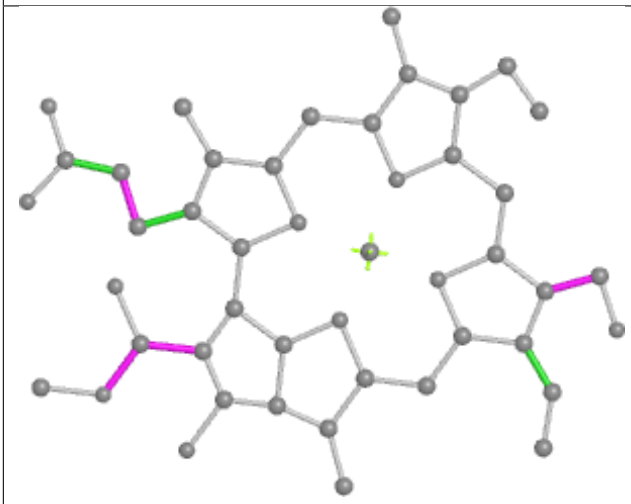


Bond angles



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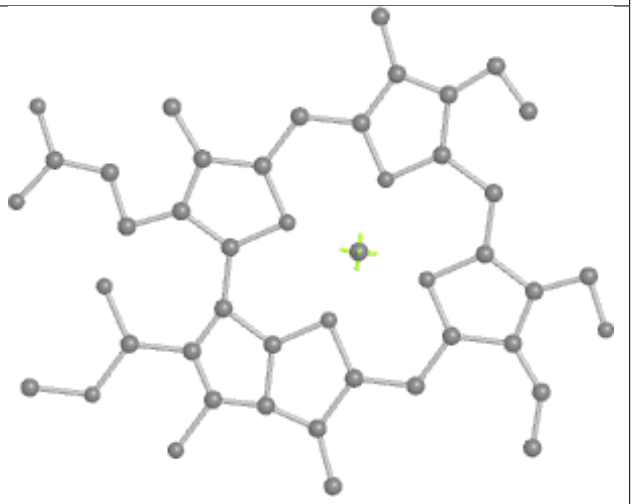
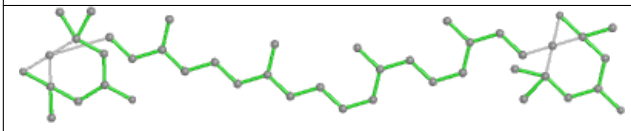


Rings

Ligand XAT 6 1622



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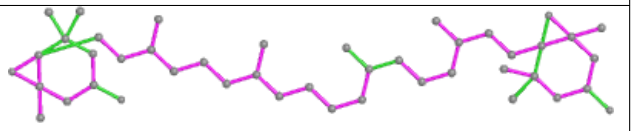
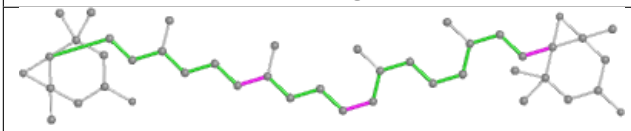


Bond angles



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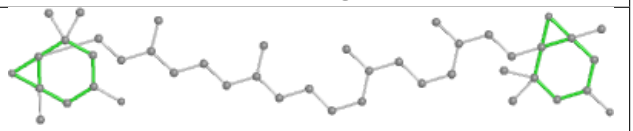
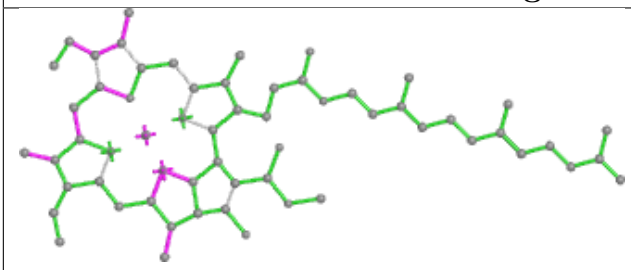


Rings

Ligand CLA A 410



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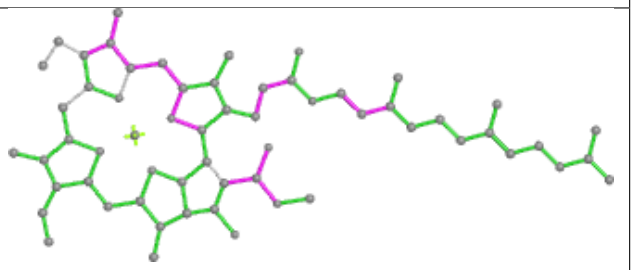
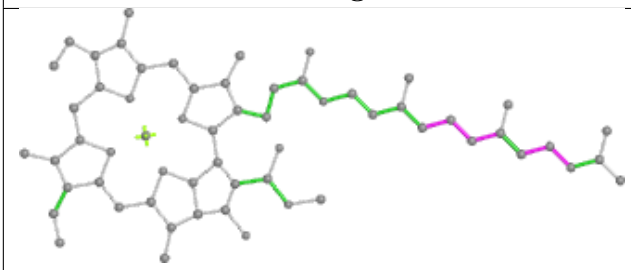


Bond angles



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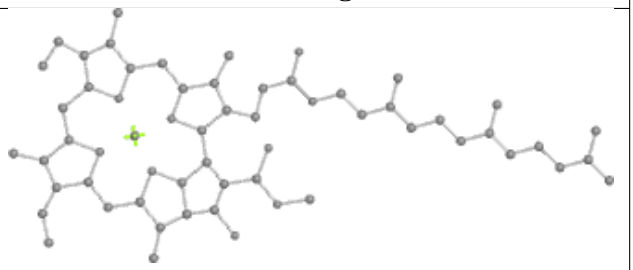
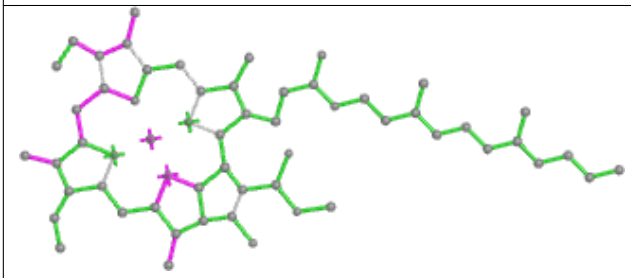


Rings

Ligand CLA R 609



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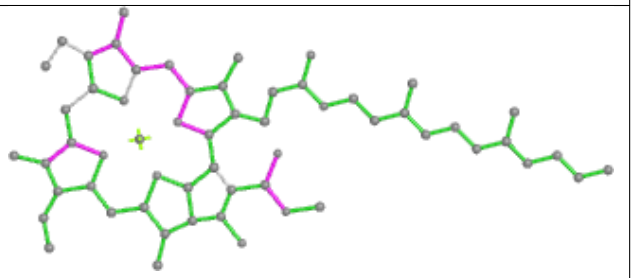
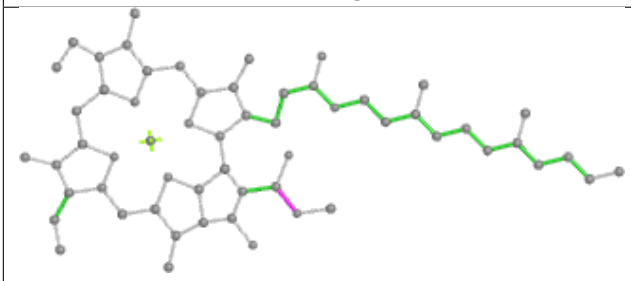


Bond angles



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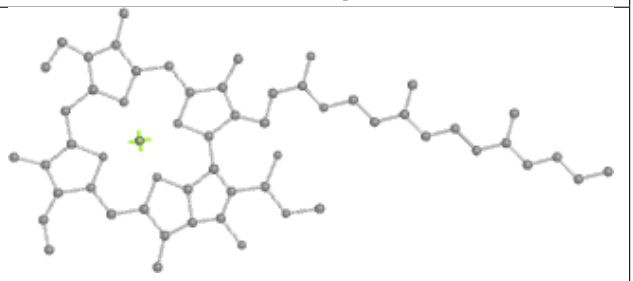
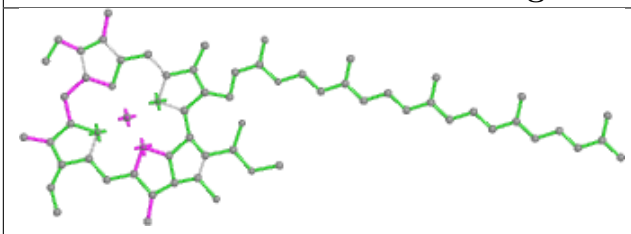


Rings

Ligand CLA d 403



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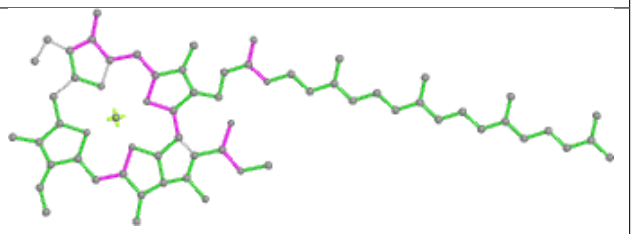
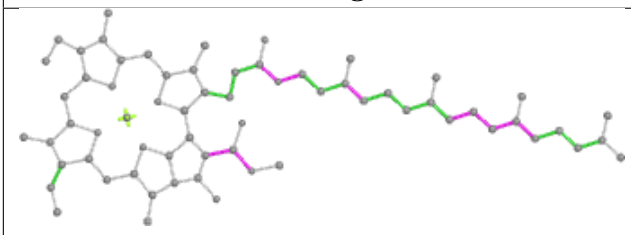
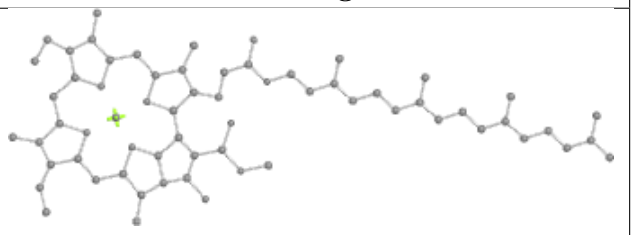


Bond angles

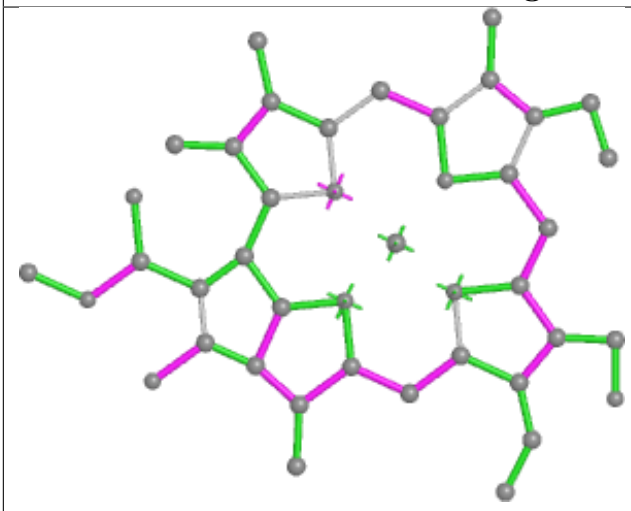


Torsions



Rings

Ligand CHL R 614



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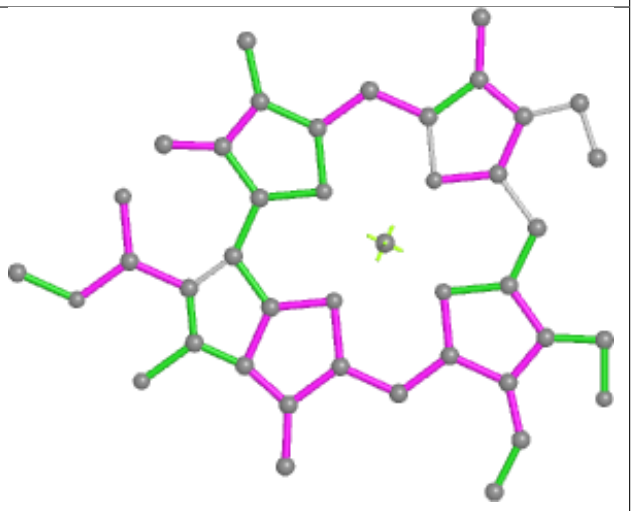
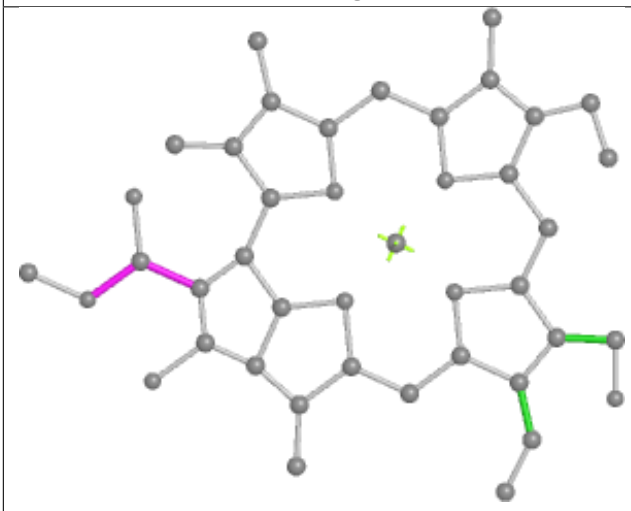


Bond angles



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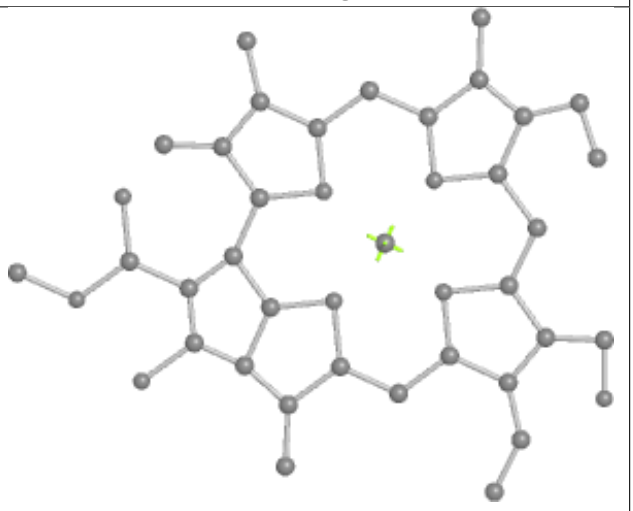
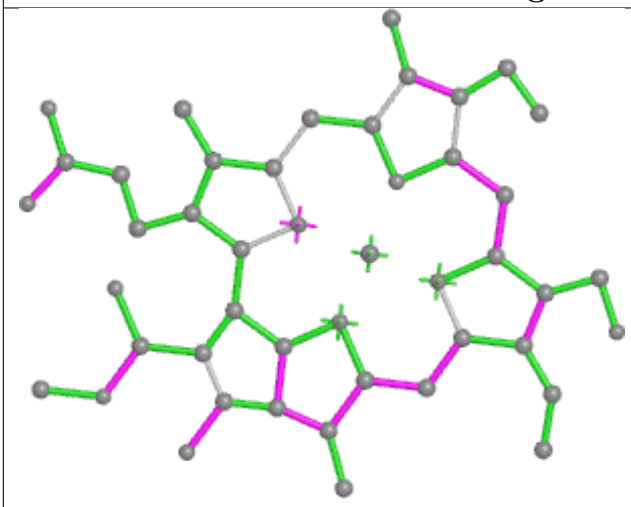


Rings

Ligand CHL 3 605



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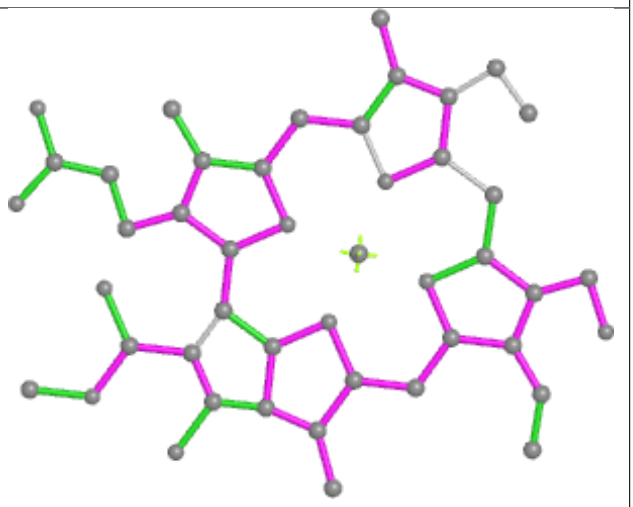
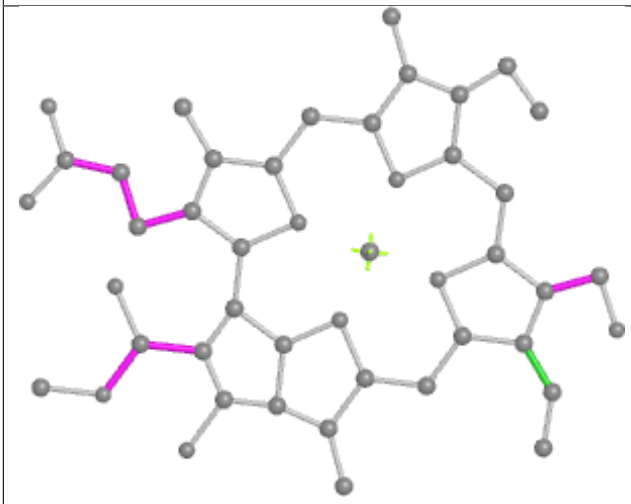


Bond angles



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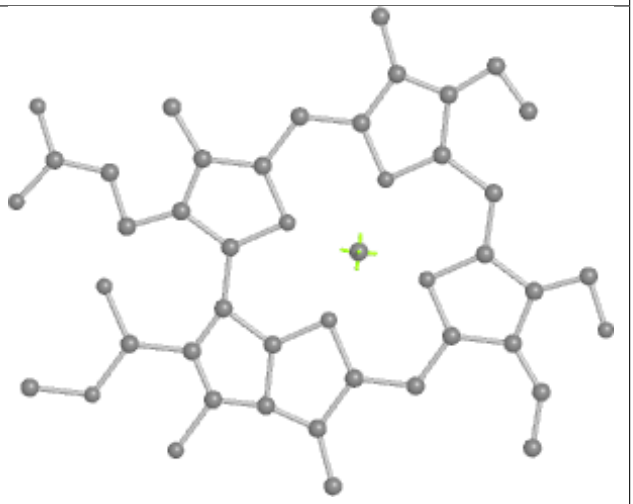
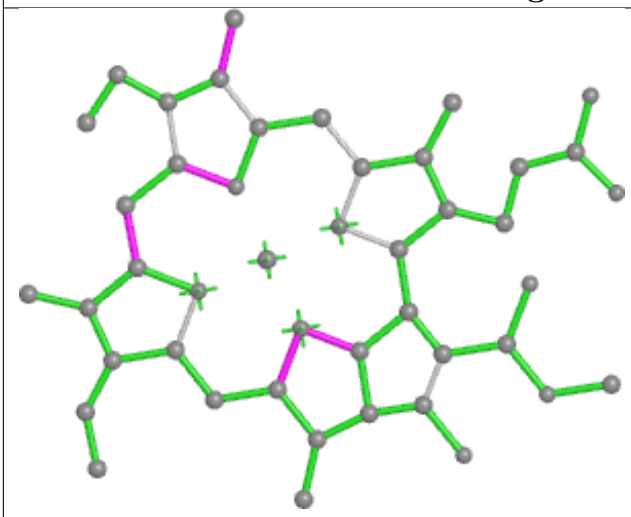


Rings

Ligand CLA S 609



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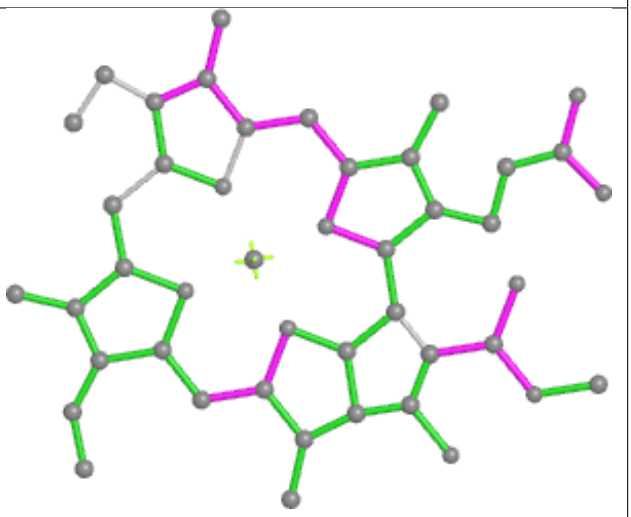
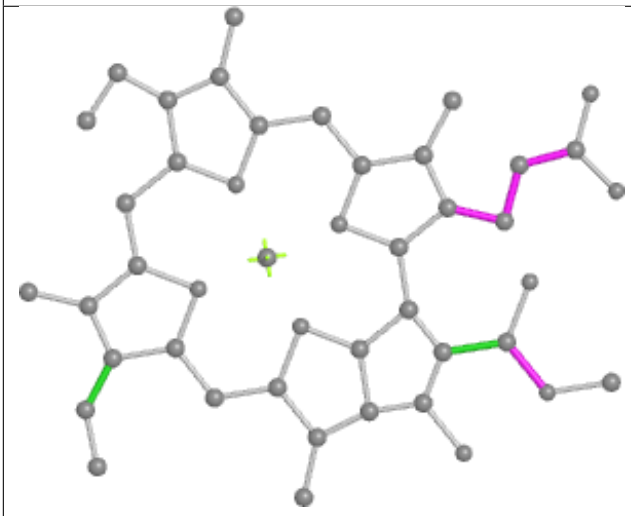


Bond angles



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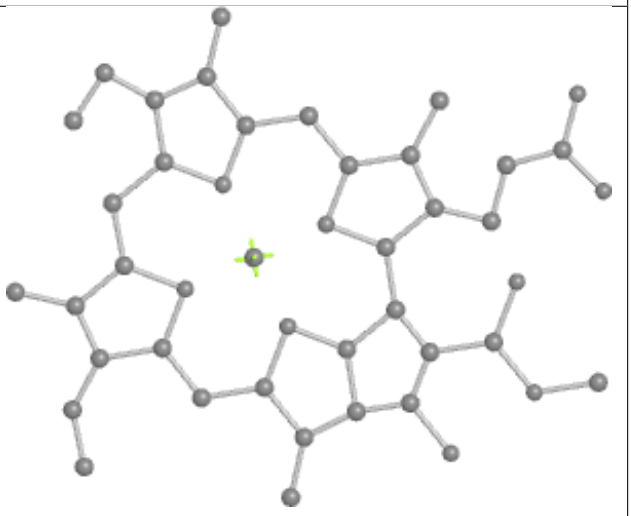
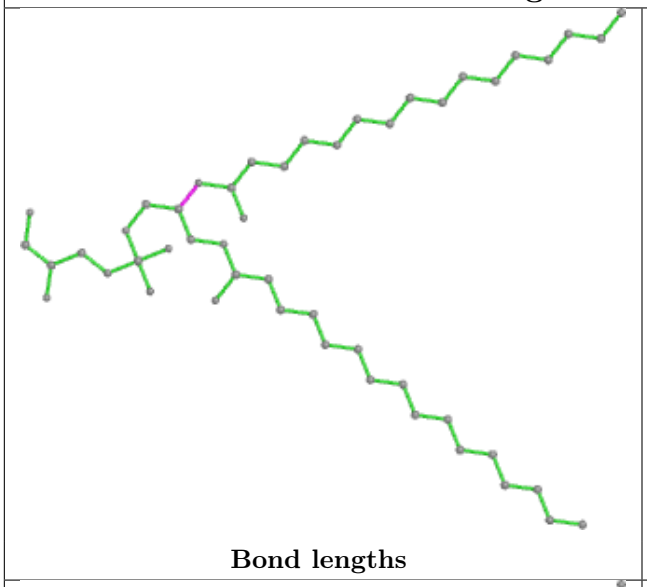


Rings

Ligand LHG L 101



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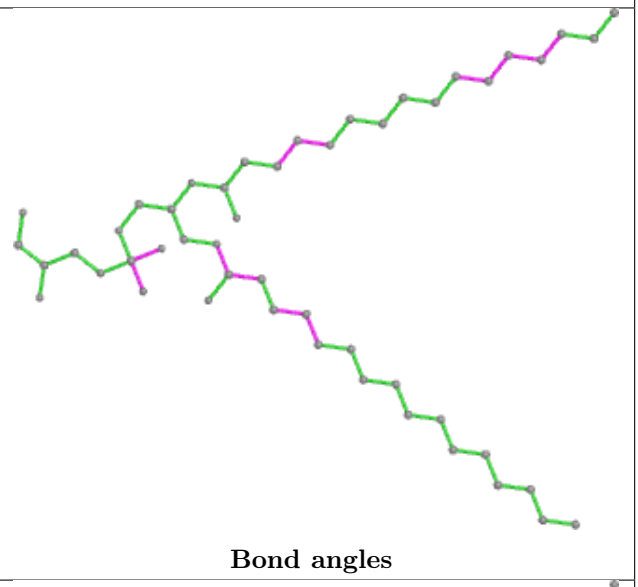
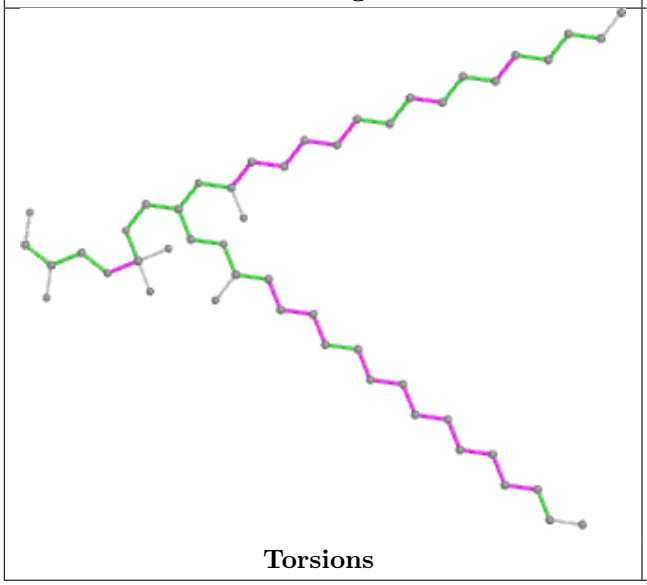


Bond angles



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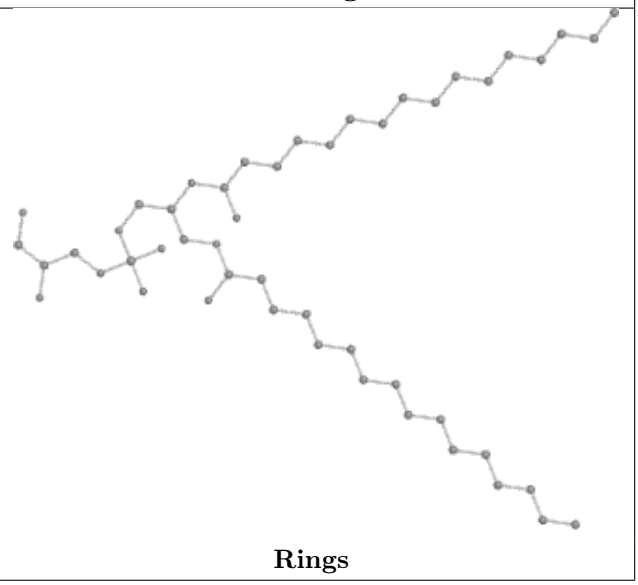
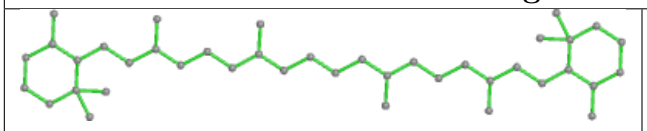
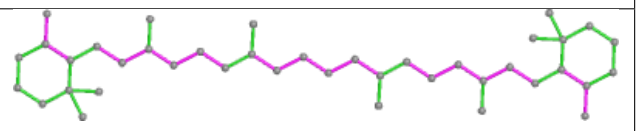


Rings

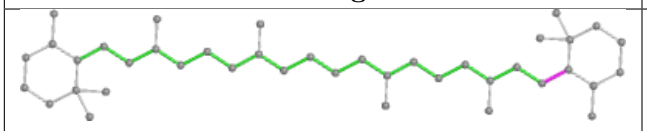
Ligand BCR A 411



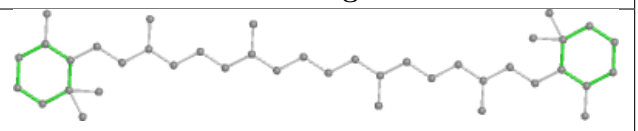
Bond lengths



Bond angles

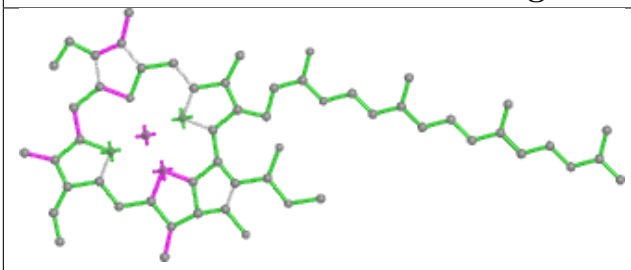


Torsions

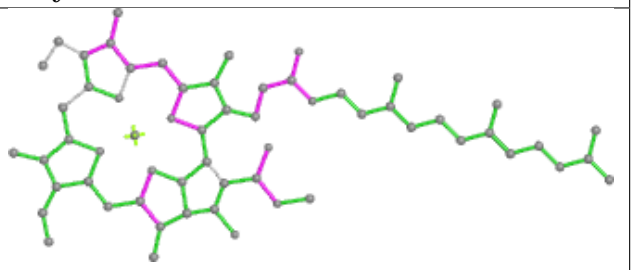


Rings

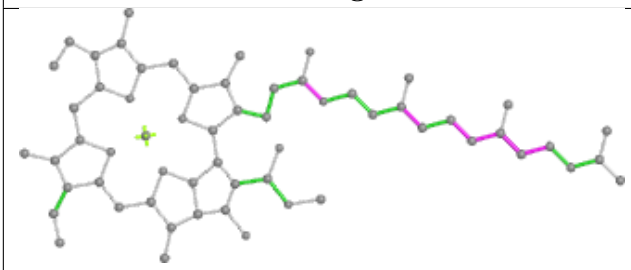
Ligand CLA y 611



Bond lengths



Bond angles



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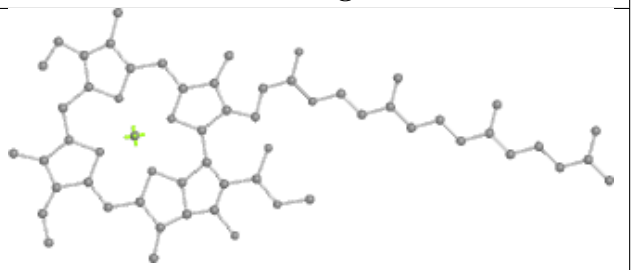
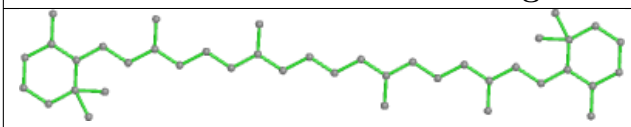


Rings

Ligand BCR C 517



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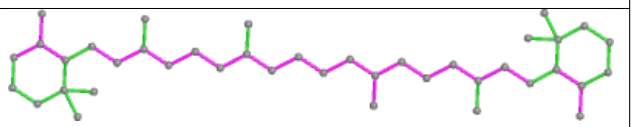
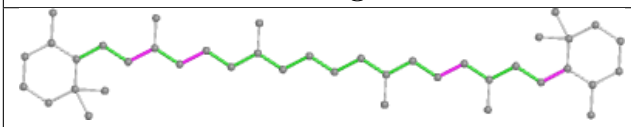


Bond angles



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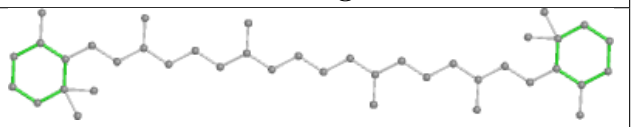
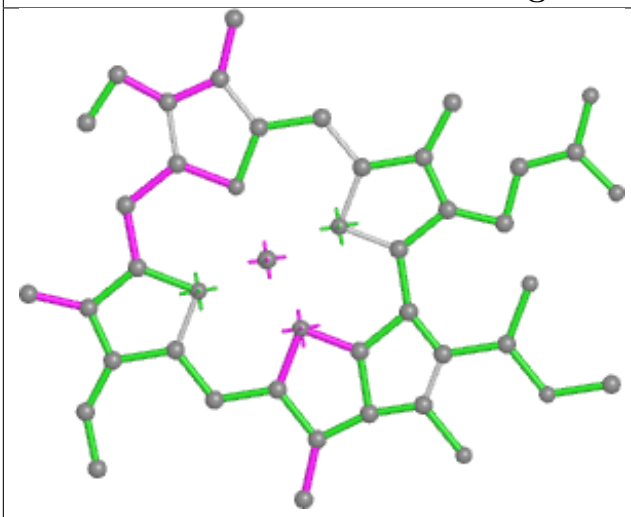


Rings

Ligand CLA 3 604



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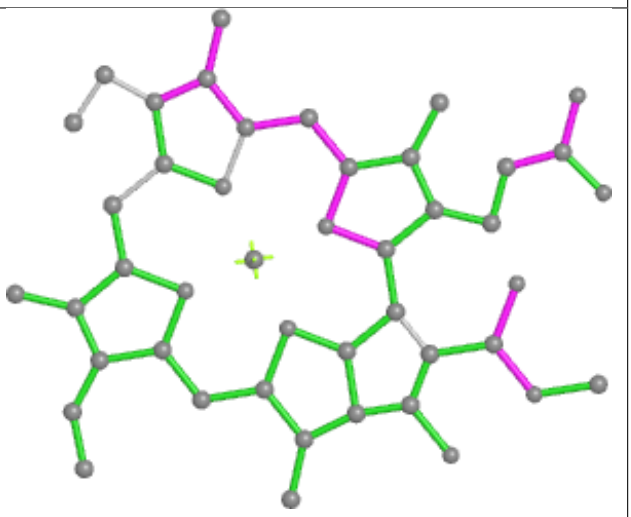
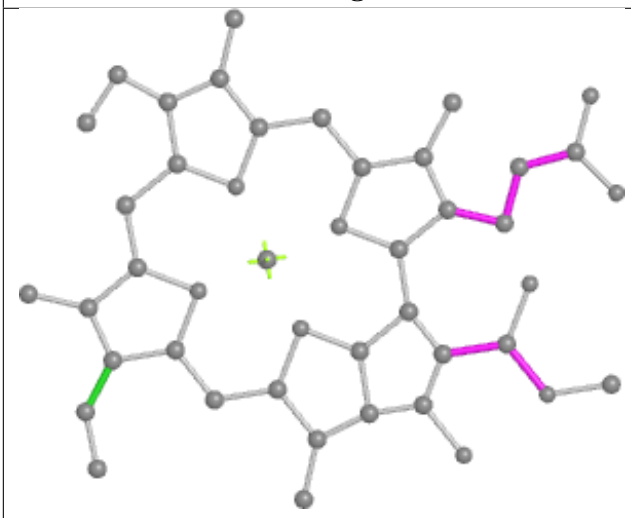


Bond angles



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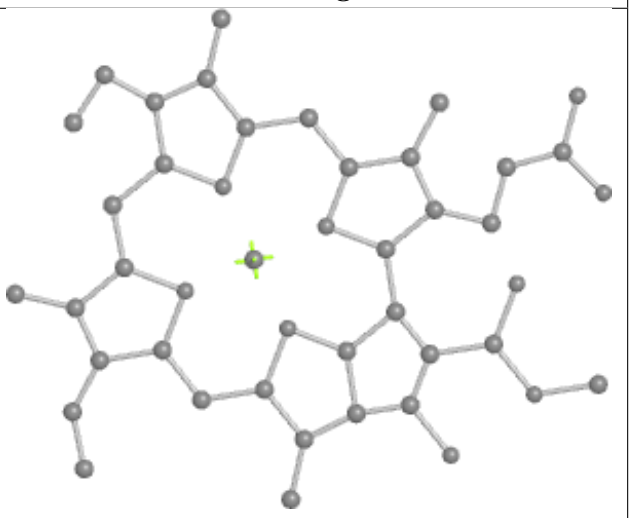
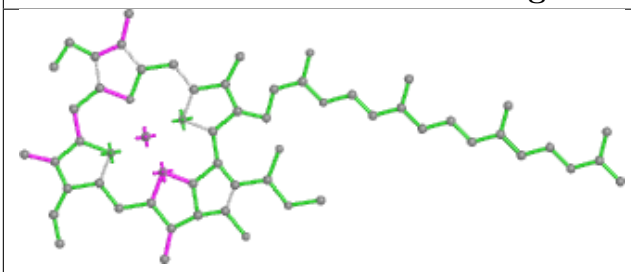


Rings

Ligand CLA g 612



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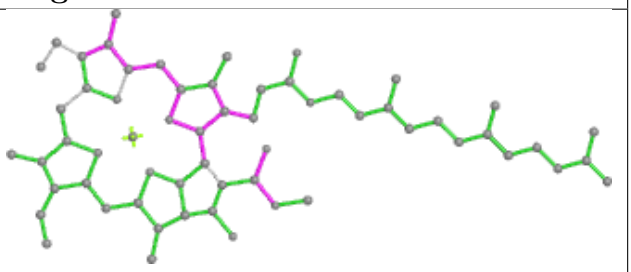
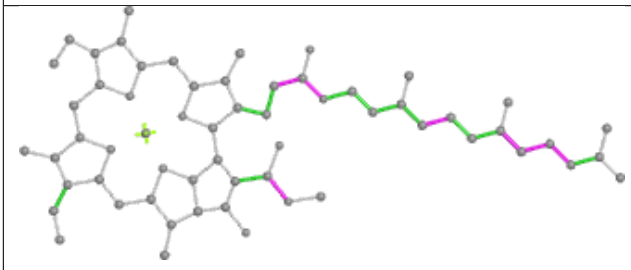


Bond angles



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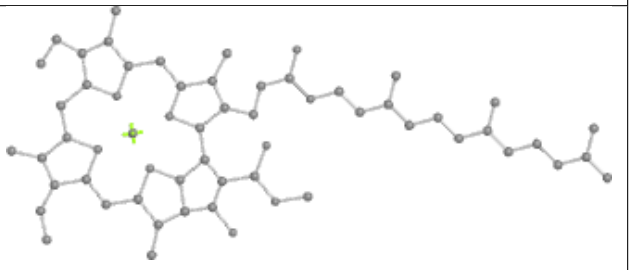
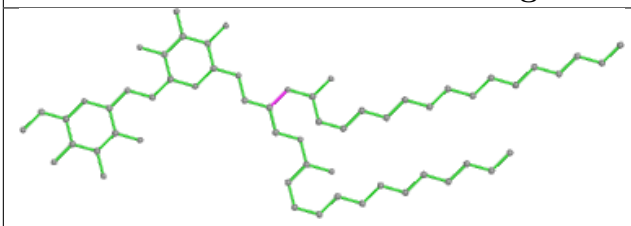


Rings

Ligand DGD B 626



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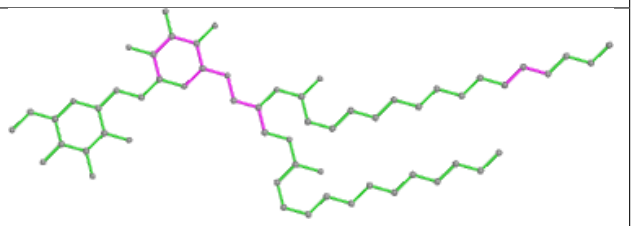
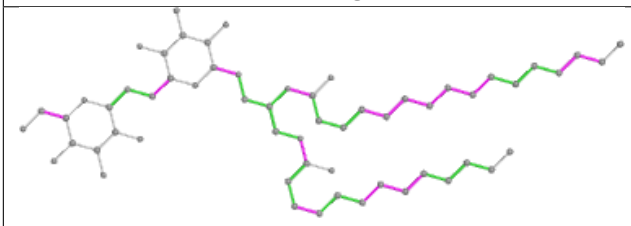


Bond angles



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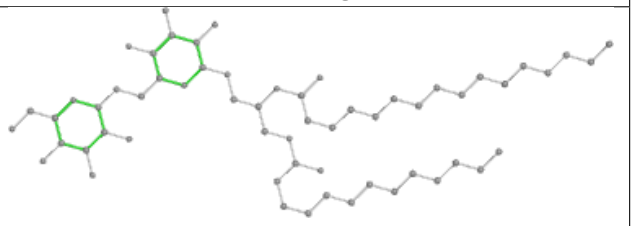
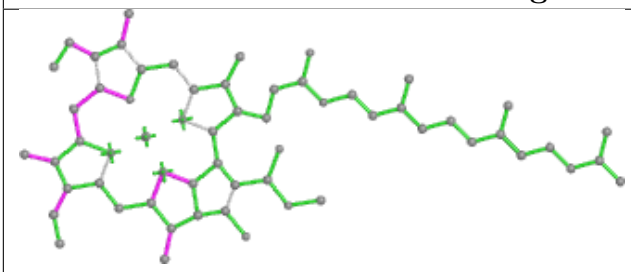


Rings

Ligand CLA r 602



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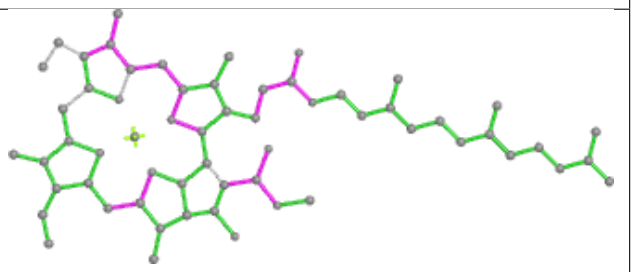
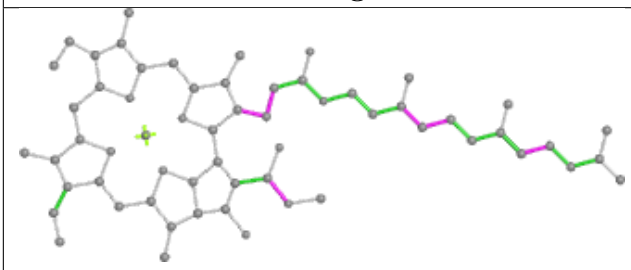


Bond angles



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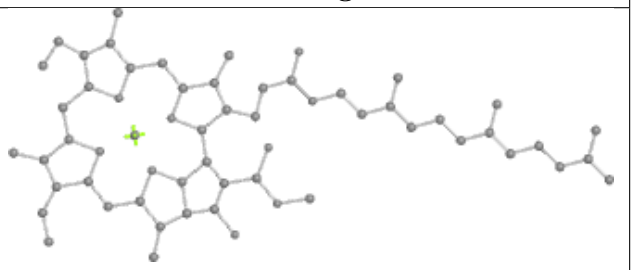
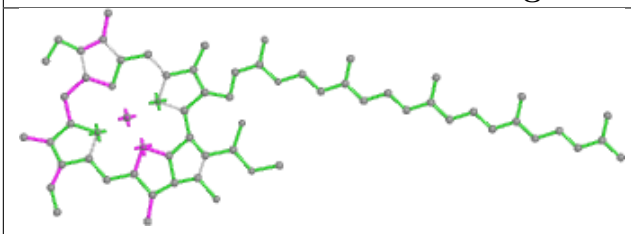


Rings

Ligand CLA Y 603



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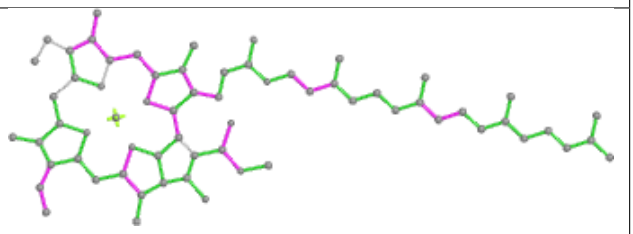

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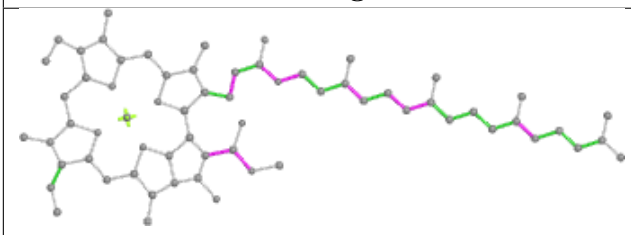

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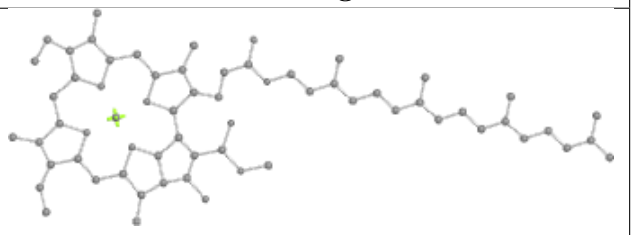
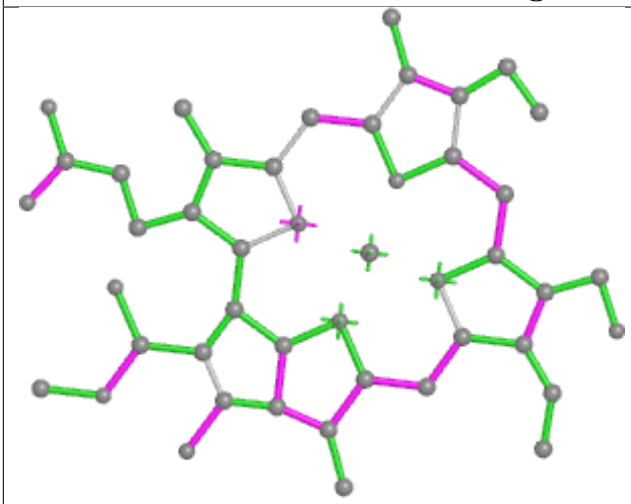


Rings

Ligand CHL 2 605



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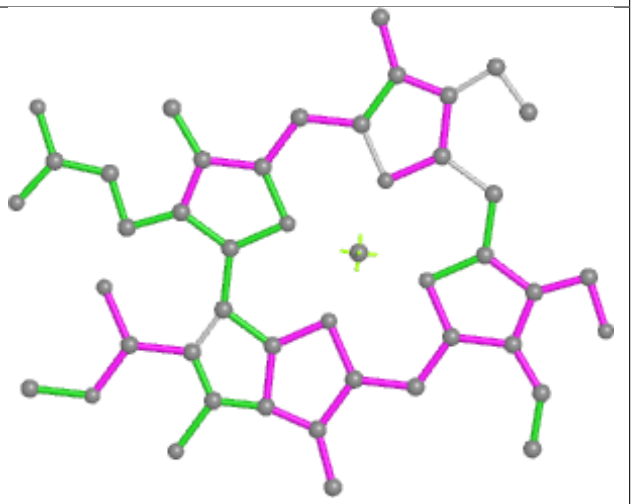
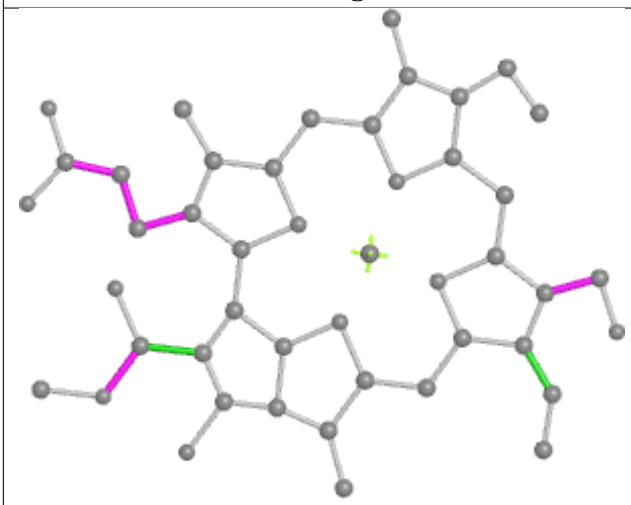


Bond angles



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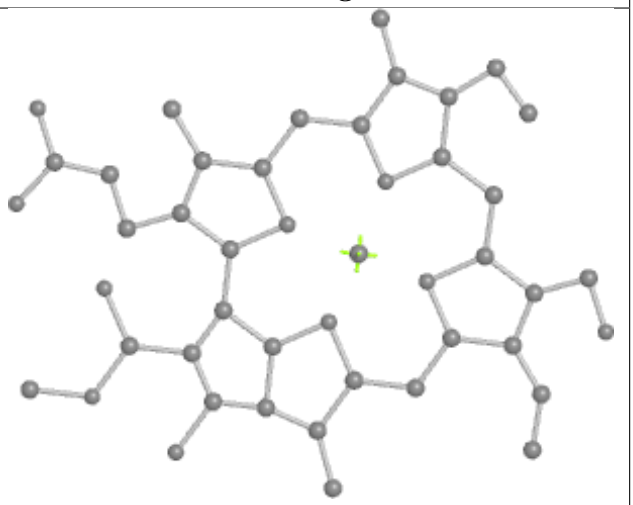
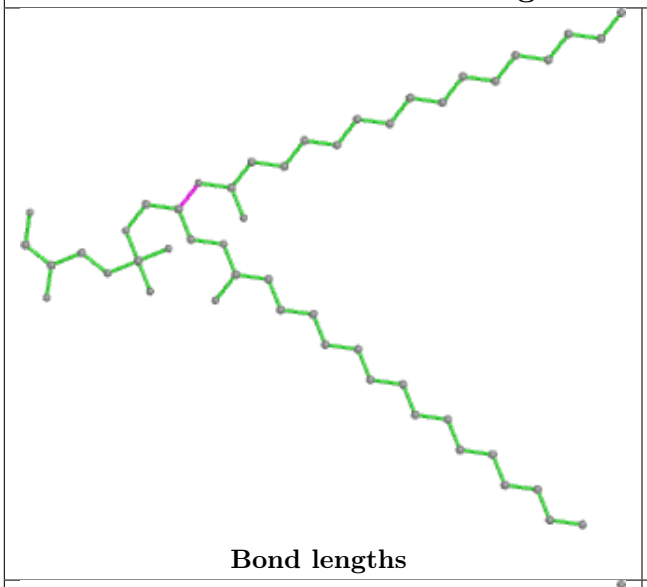


Rings

Ligand LHG S 2630



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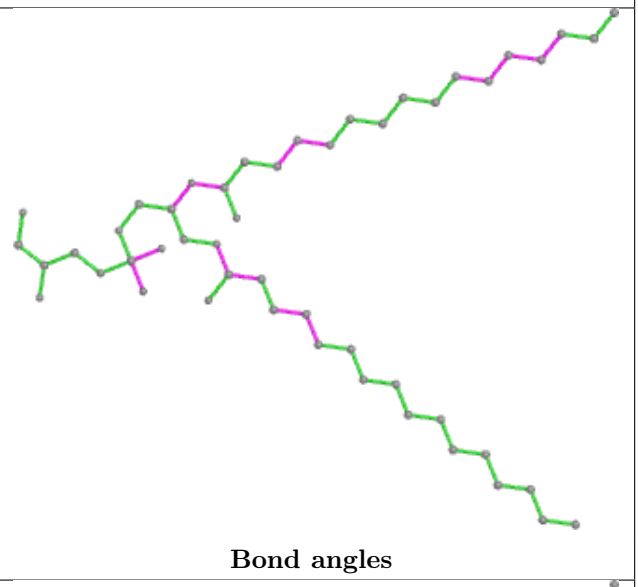
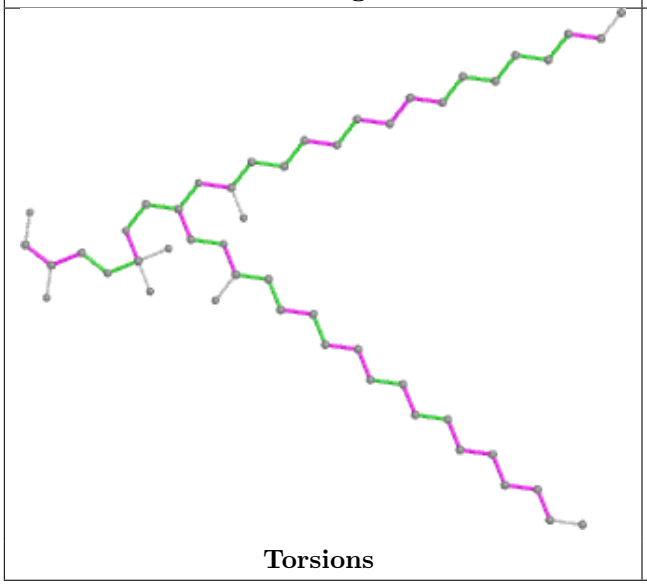


Bond angles



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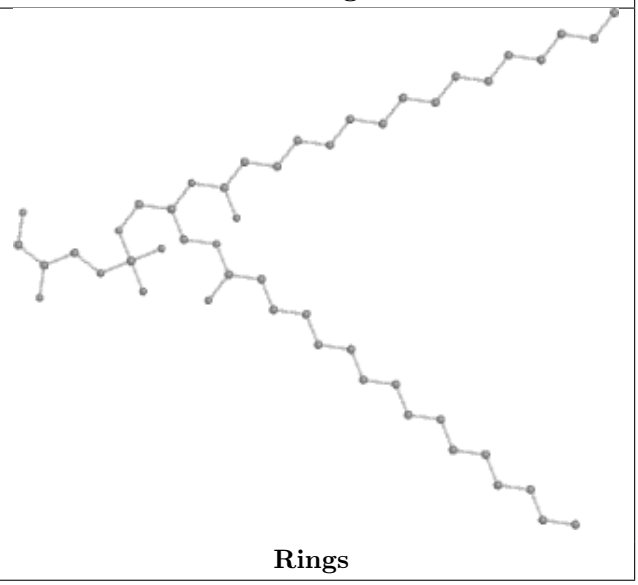
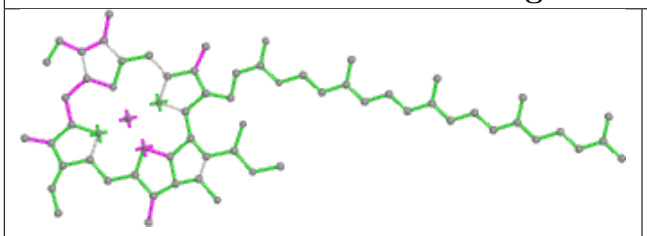


Rings

Ligand CLA B 613



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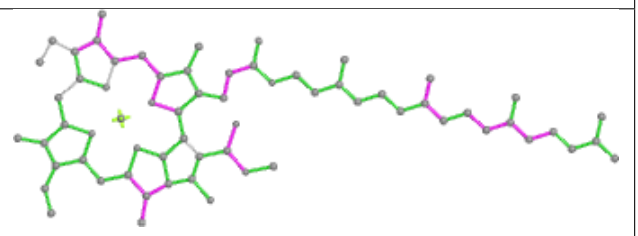
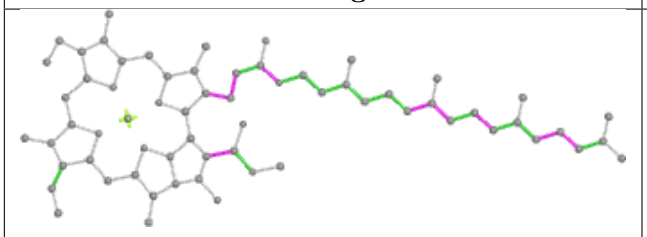


Bond angles



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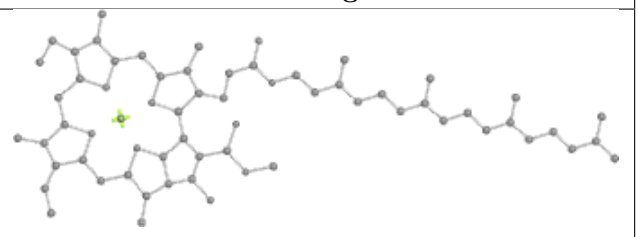
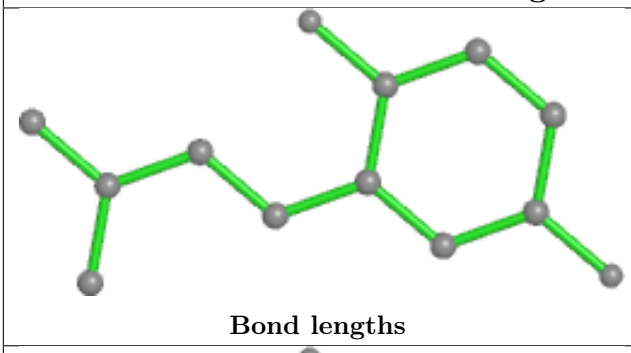


Rings

Ligand PL9 A 414



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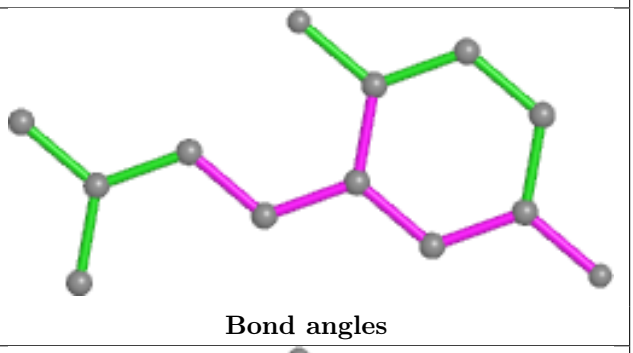
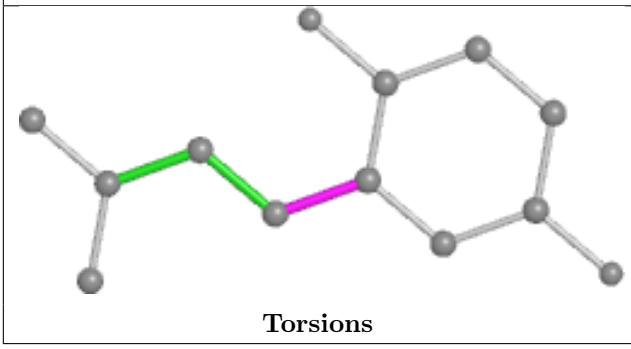


Bond angles



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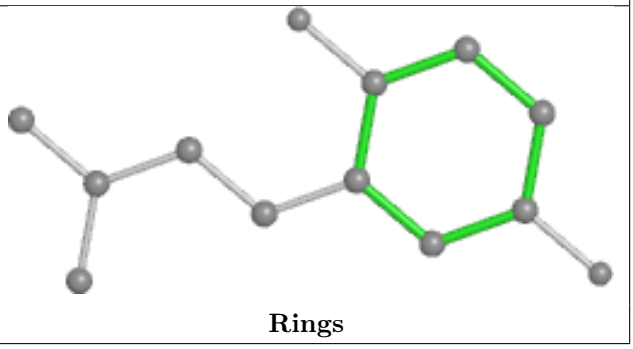
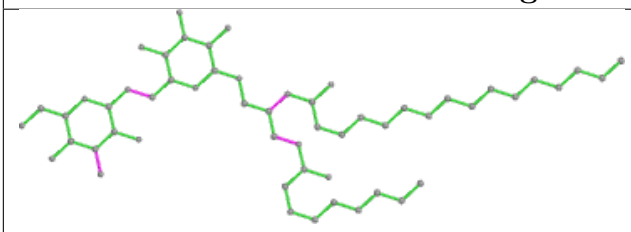


Rings

Ligand DGD C 518



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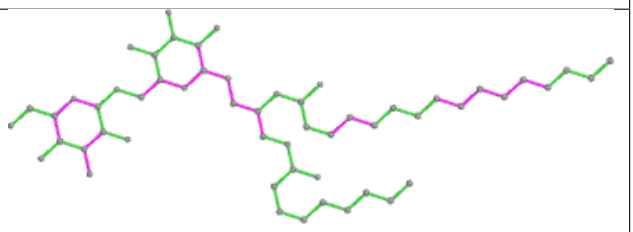
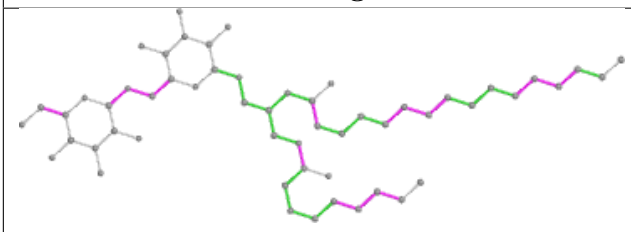


Bond angles



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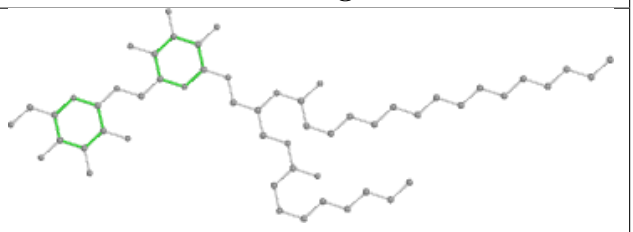
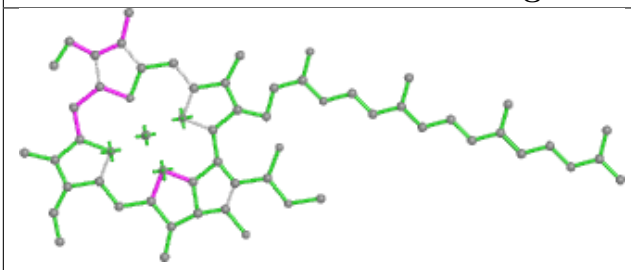


Rings

Ligand CLA R 613



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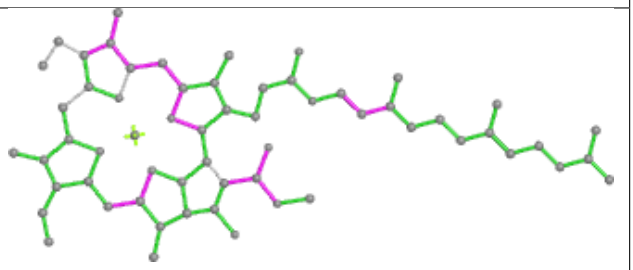
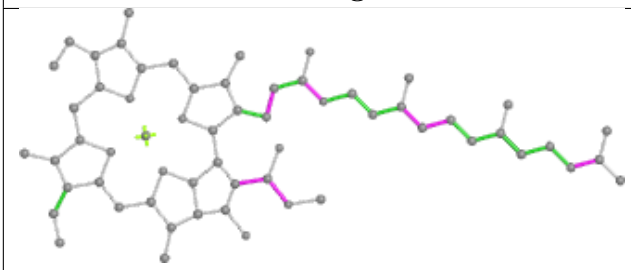


Bond angles



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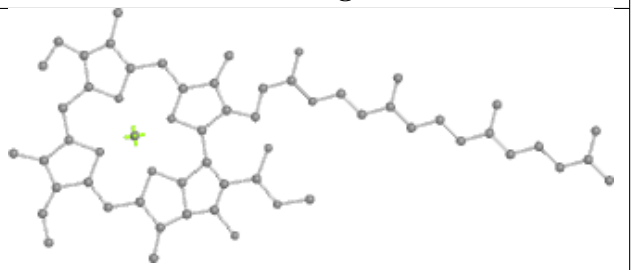
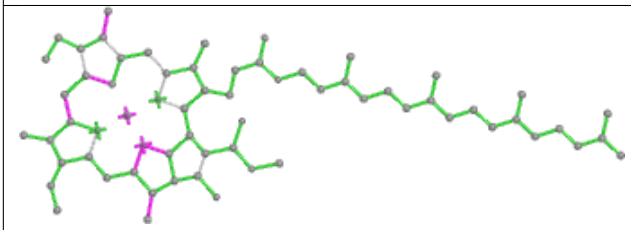
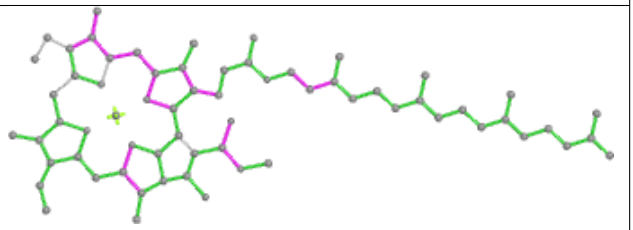


Rings

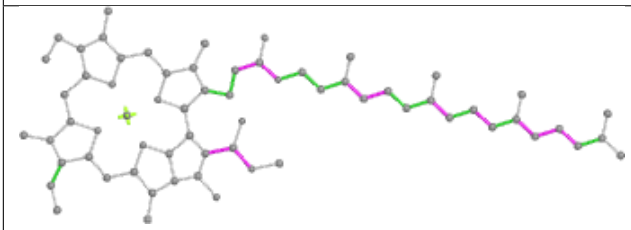
Ligand CLA C 510



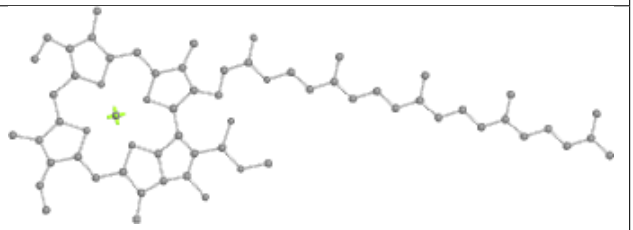
Bond lengths



Bond angles

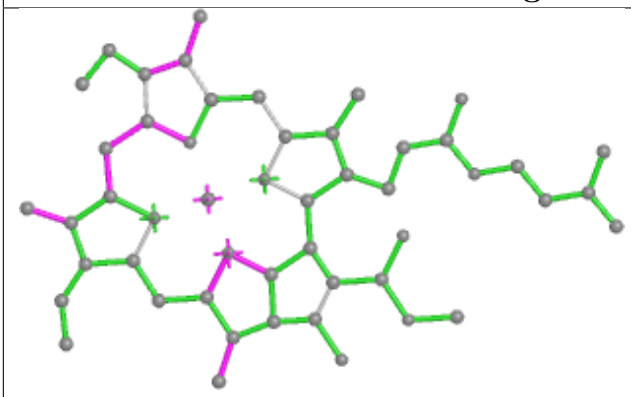


Torsions



Rings

Ligand CLA N 604



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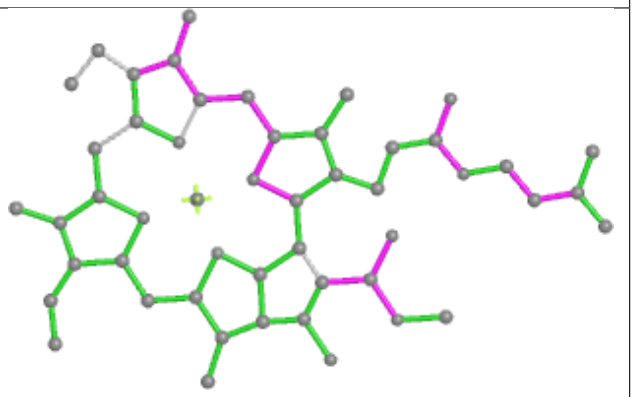
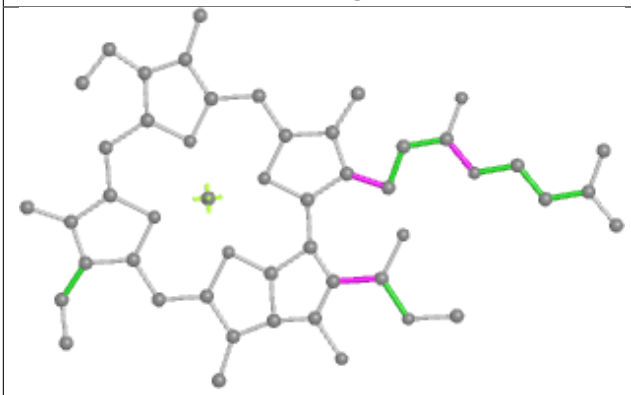


Bond angles



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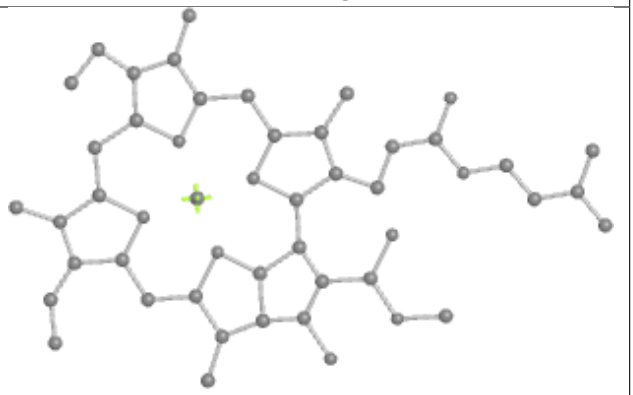
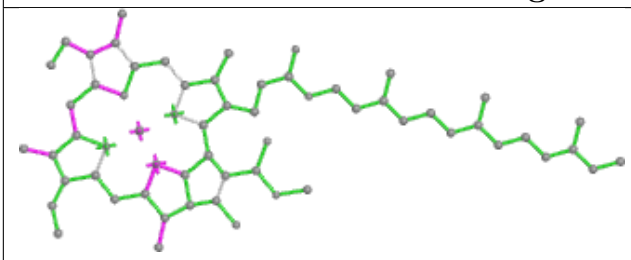


Rings

Ligand CLA 1 602



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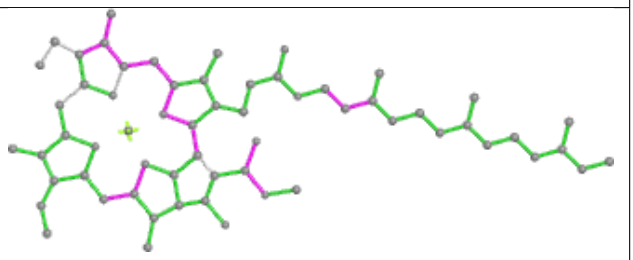
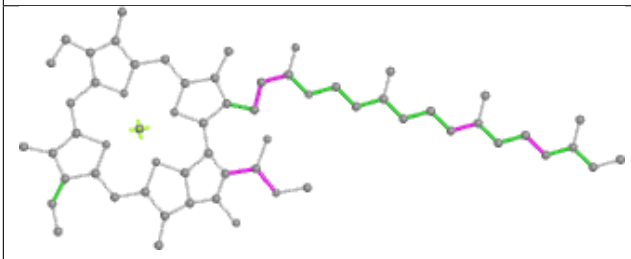


Bond angles



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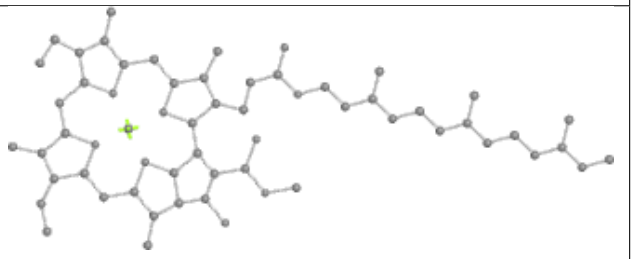
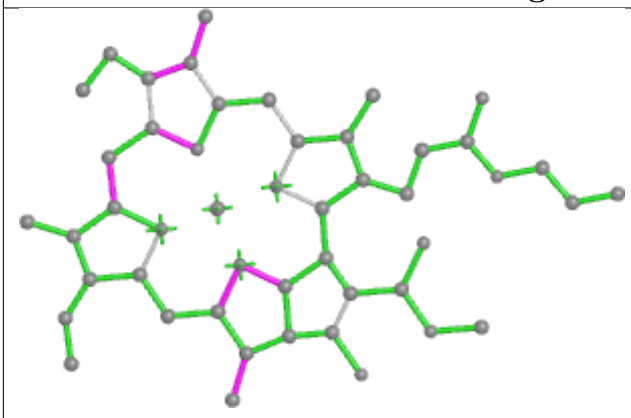


Rings

Ligand CLA 7 614



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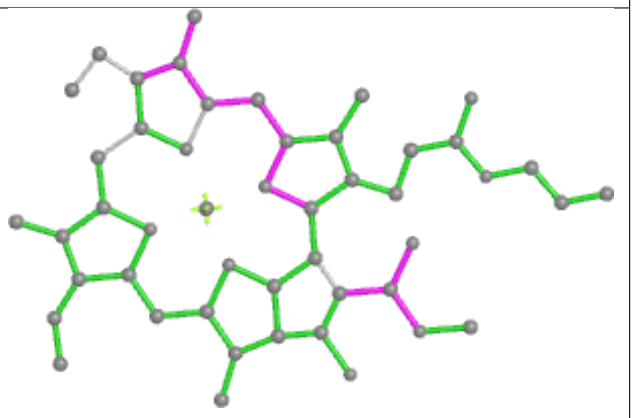
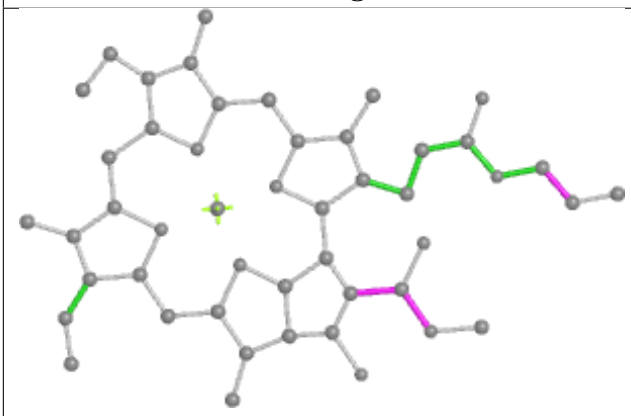


Bond angles



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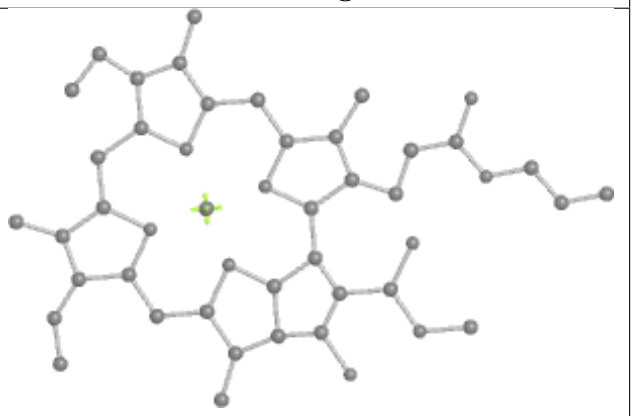
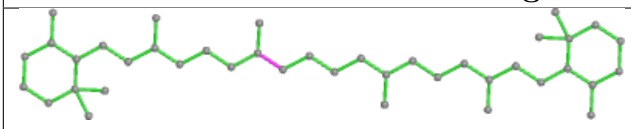


Rings

Ligand BCR B 619



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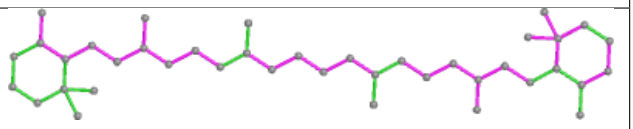
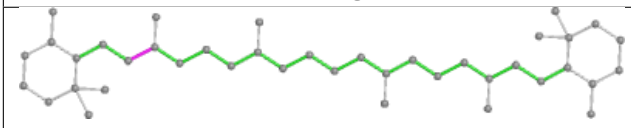


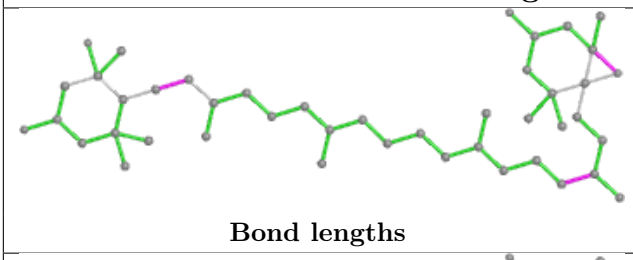
Bond angles



Torsions

Rings

Ligand NEX R 623



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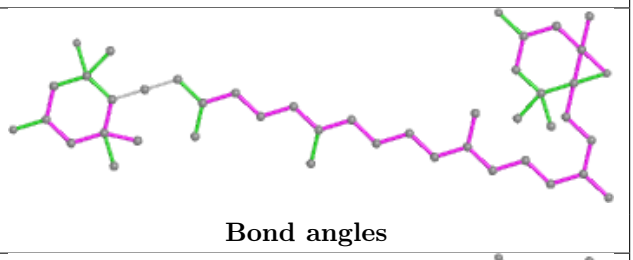
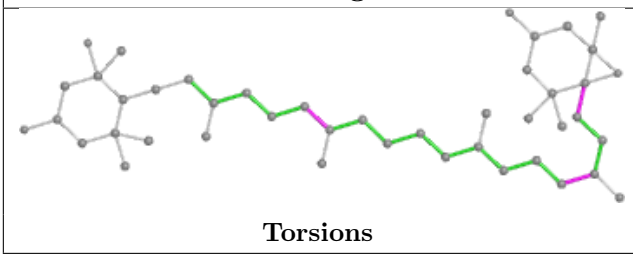


Bond angles



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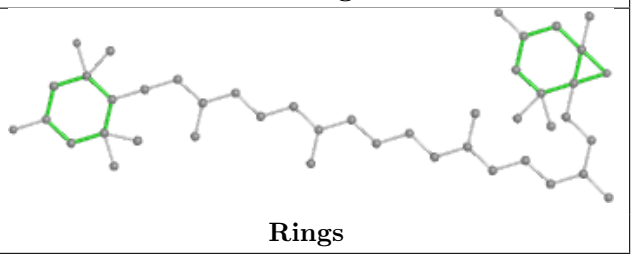
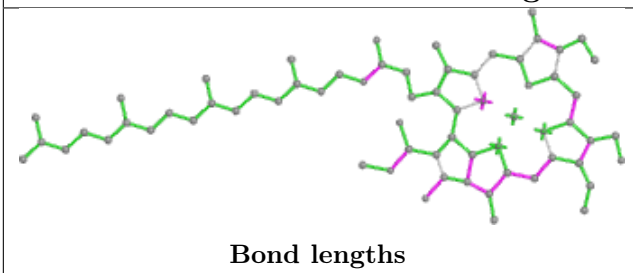


Rings

Ligand CHL G 607



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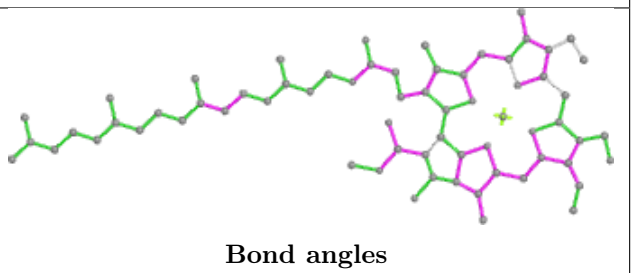
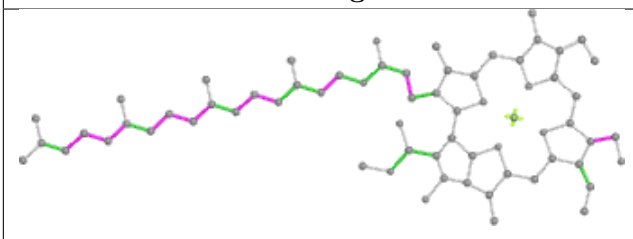


Bond angles



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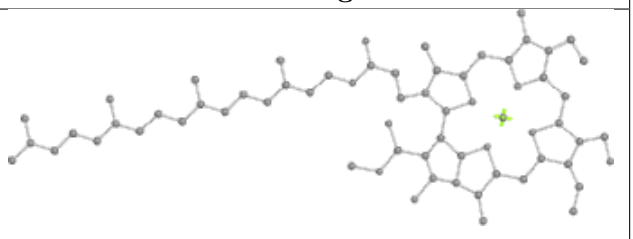
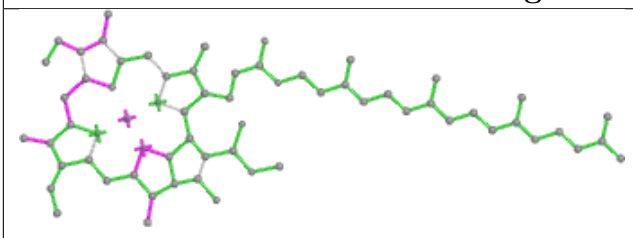


Rings

Ligand CLA B 607



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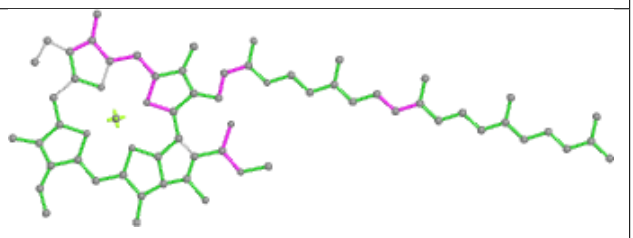
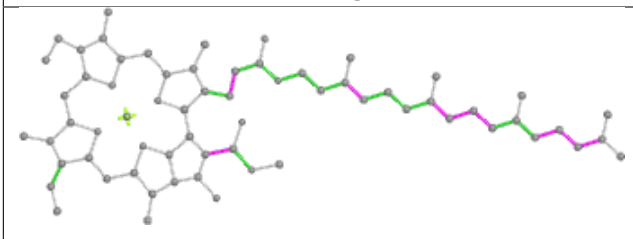


Bond angles



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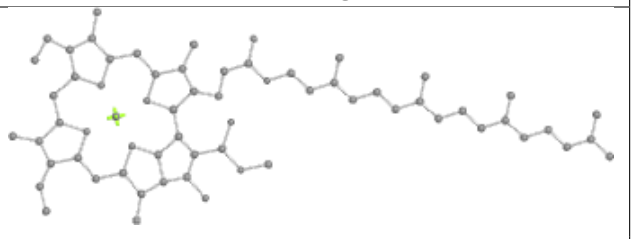
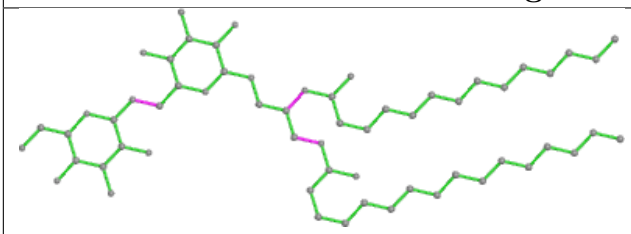


Rings

Ligand DGD c 520



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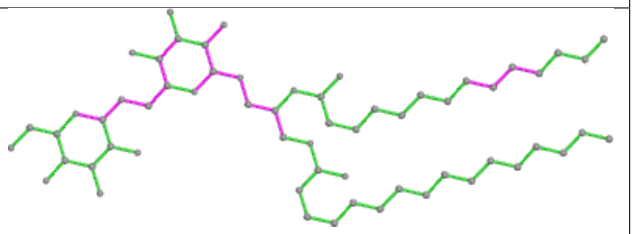
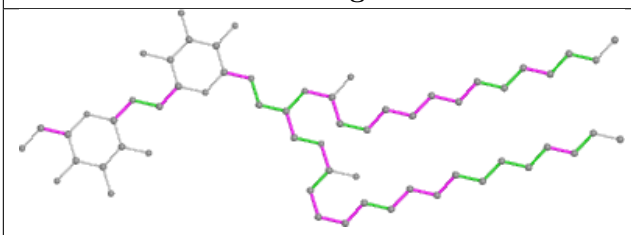
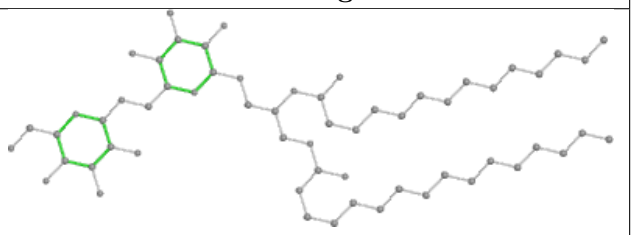


Bond angles

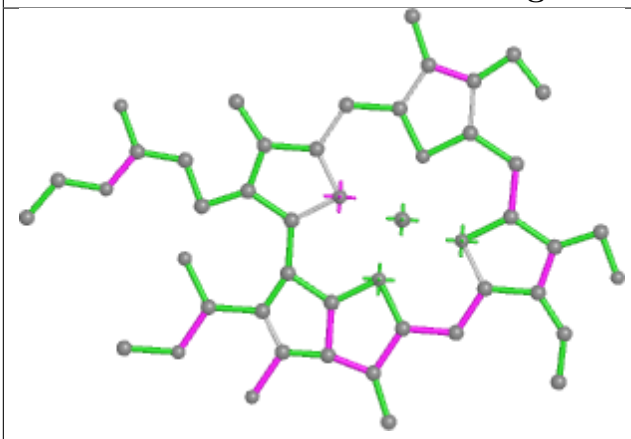


Torsions



Rings

Ligand CHL y 605



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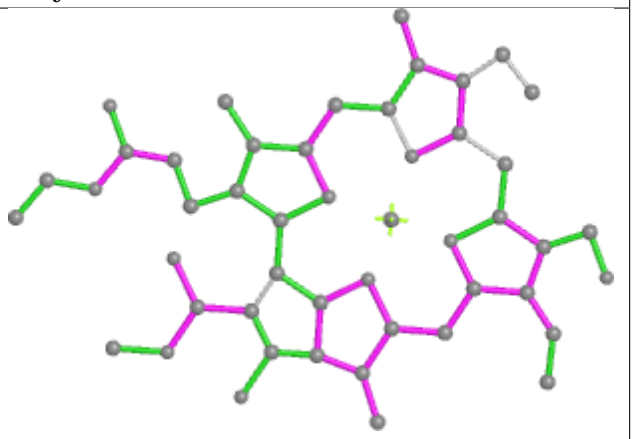
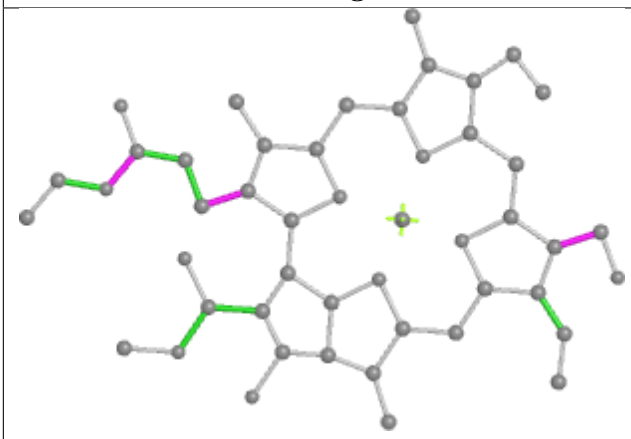


Bond angles



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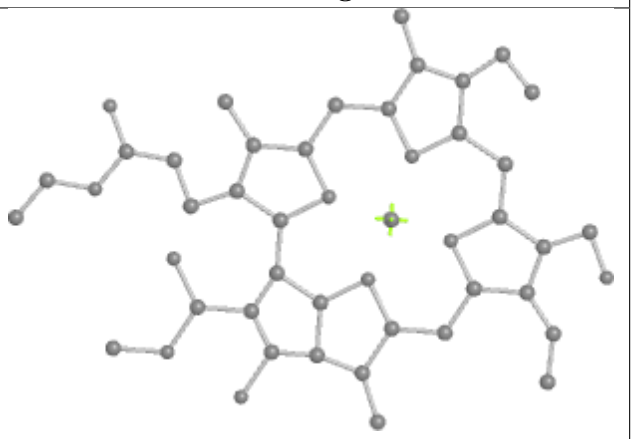
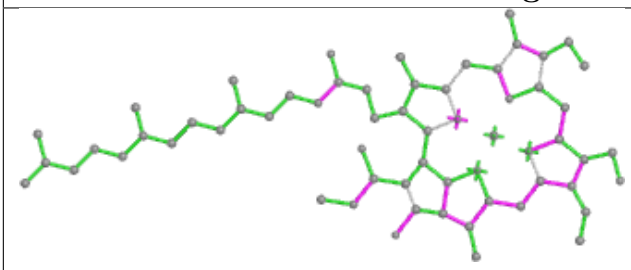


Rings

Ligand CHL G 609



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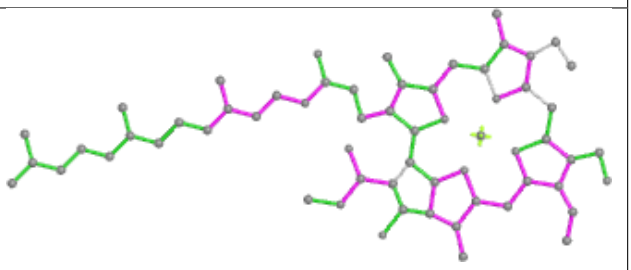
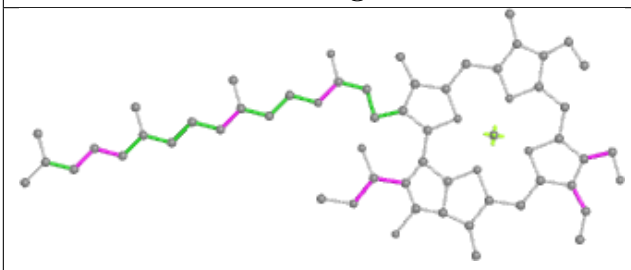
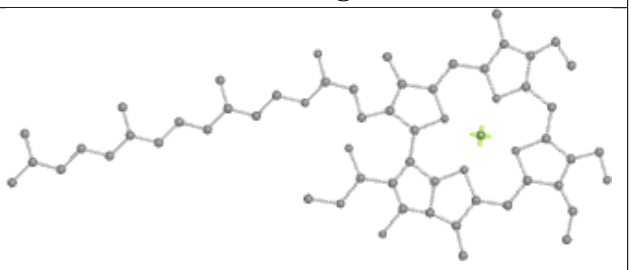


Bond angles

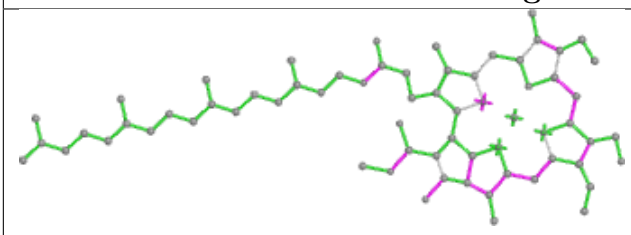


Torsions



Rings

Ligand CHL R 606



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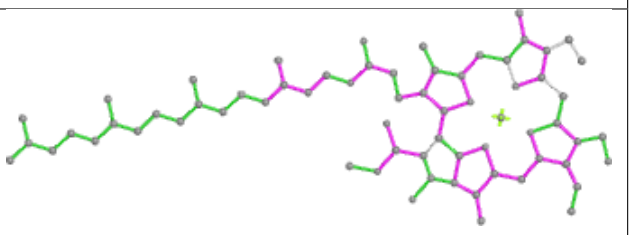
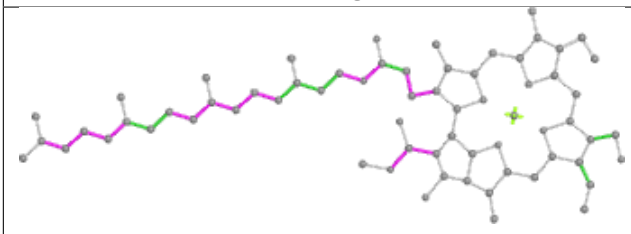


Bond angles



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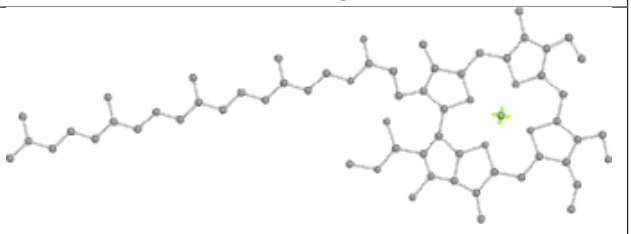
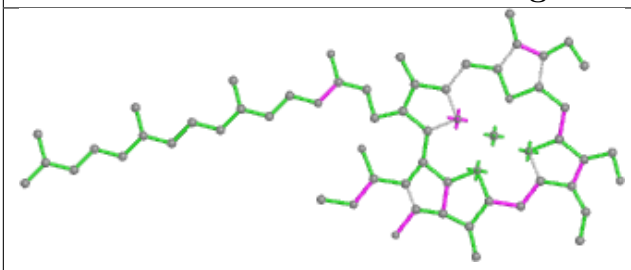
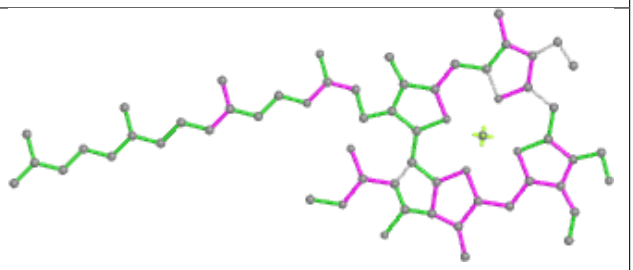


Rings

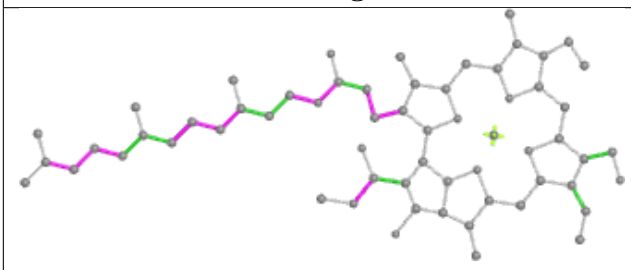
Ligand CHL r 608



Bond lengths



Bond angles



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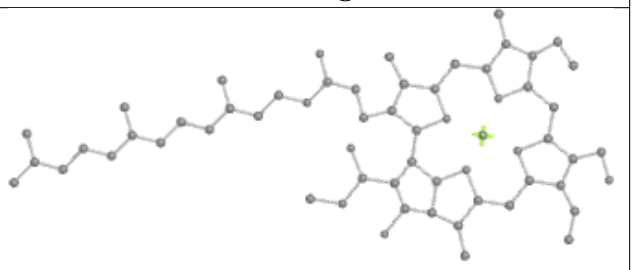
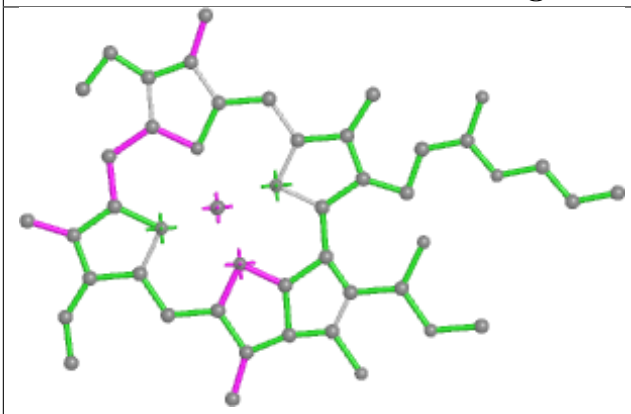


Rings

Ligand CLA n 614



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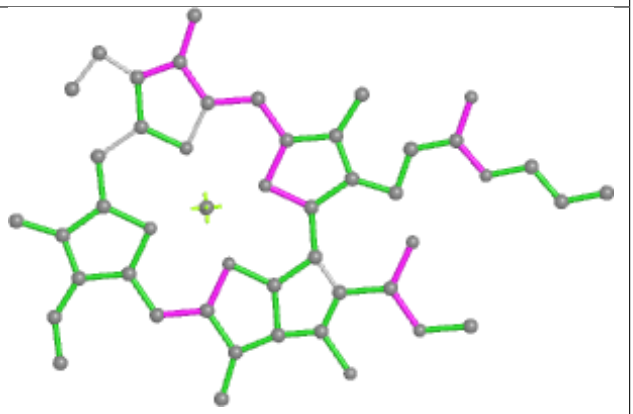
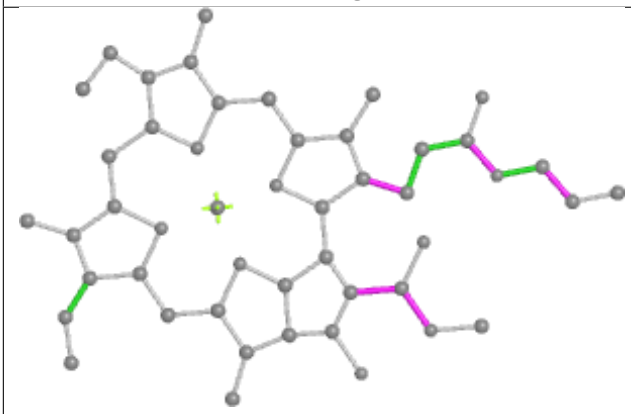
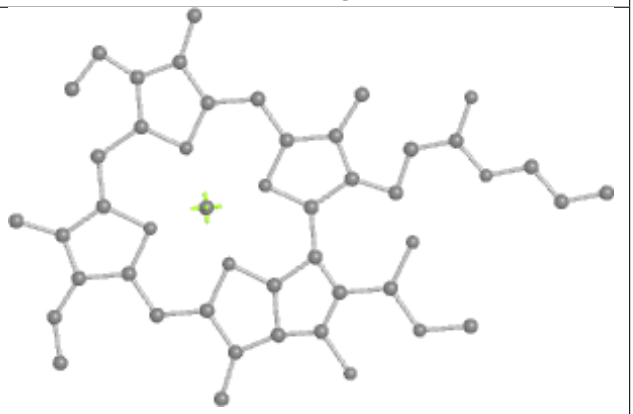


Bond angles

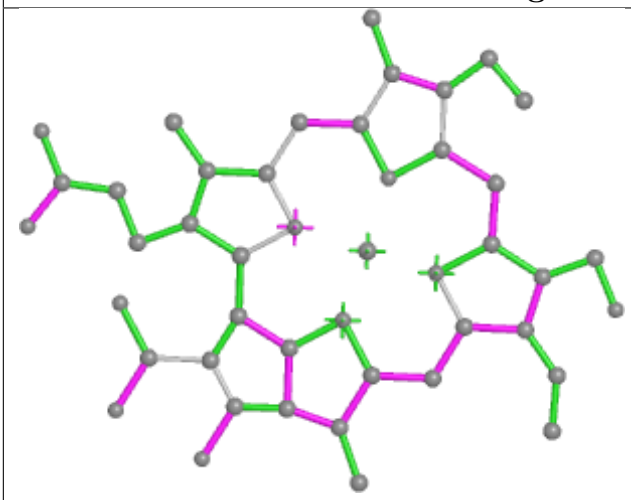


Torsions

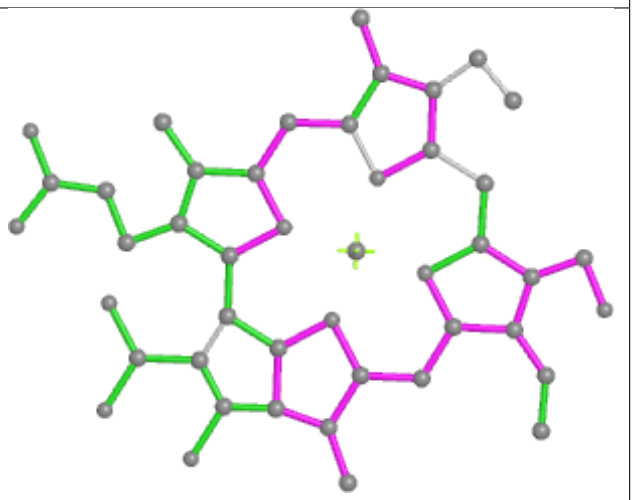


Rings

Ligand CHL 8 601



Bond lengths



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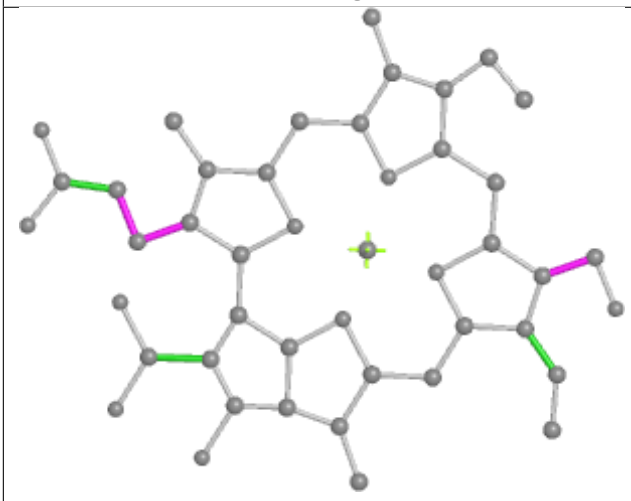
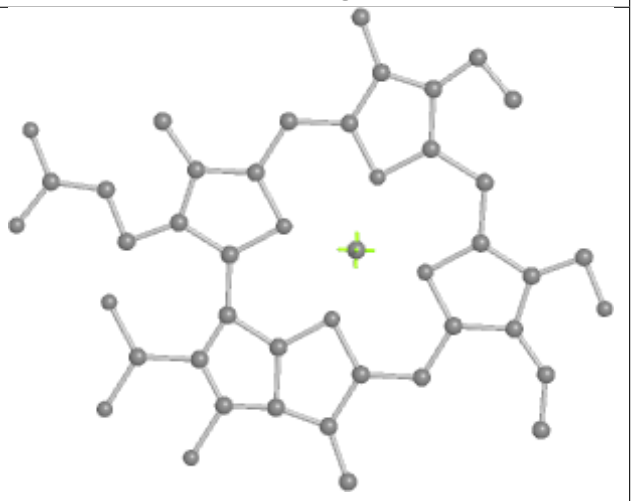
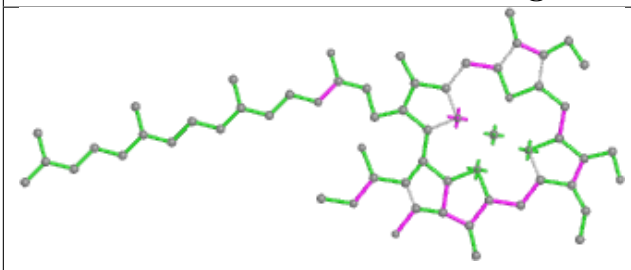


Torsions



Rings

Ligand CHL 6 609



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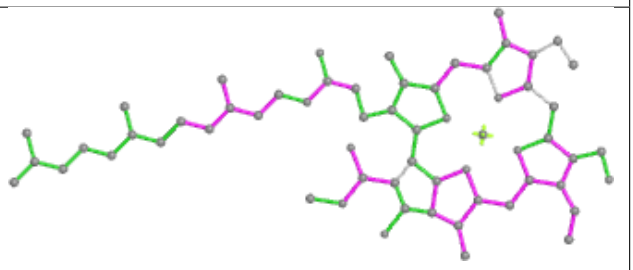

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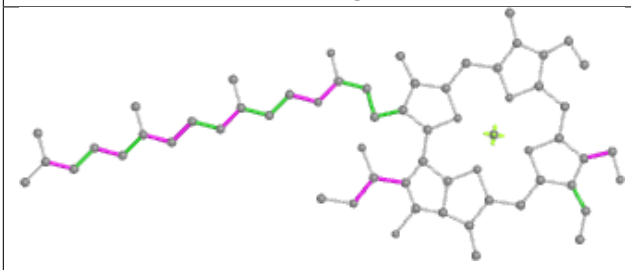

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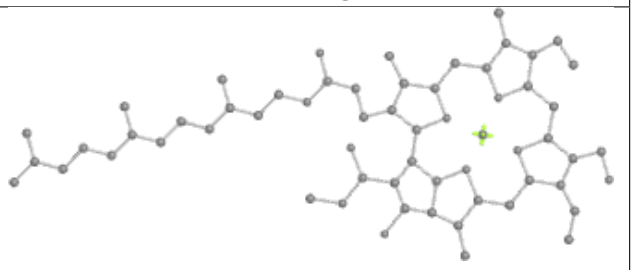
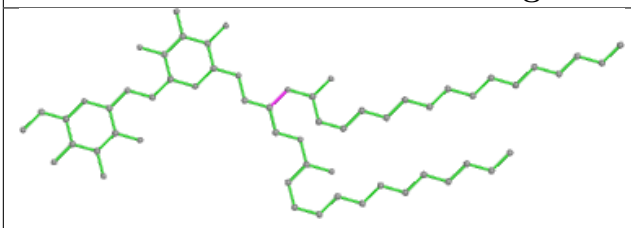


Rings

Ligand DGD b 626



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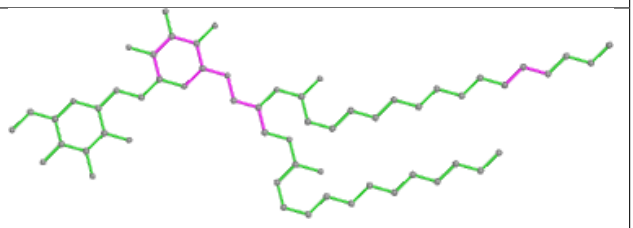

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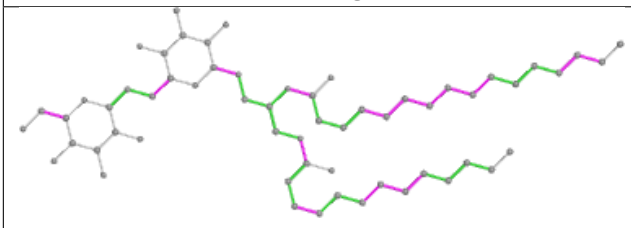

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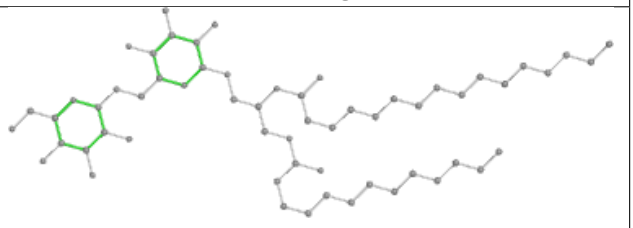
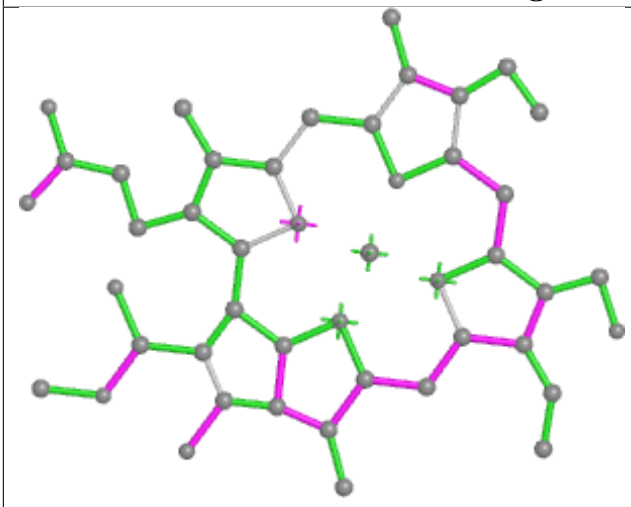


Rings

Ligand CHL 2 608



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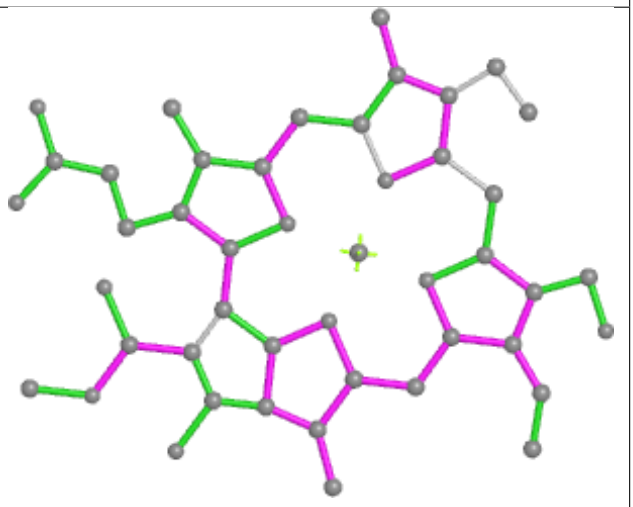

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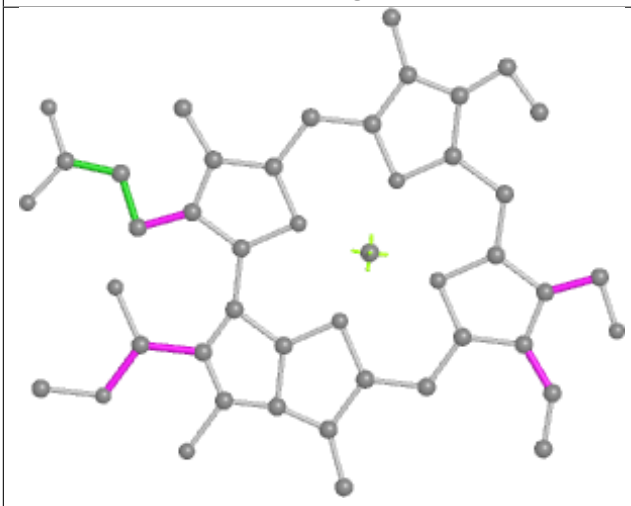

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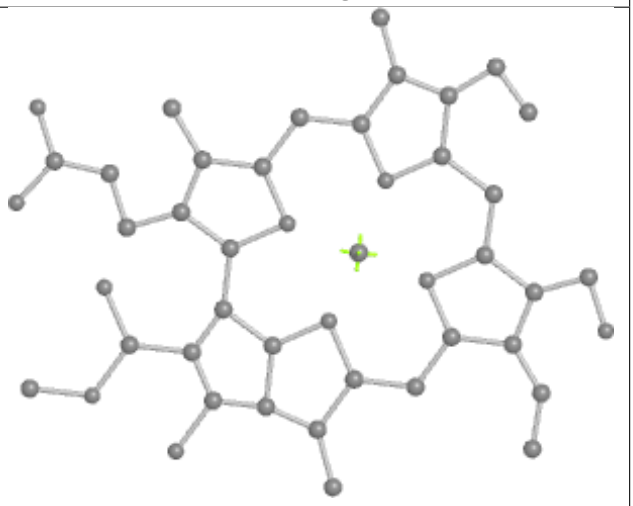

Rings

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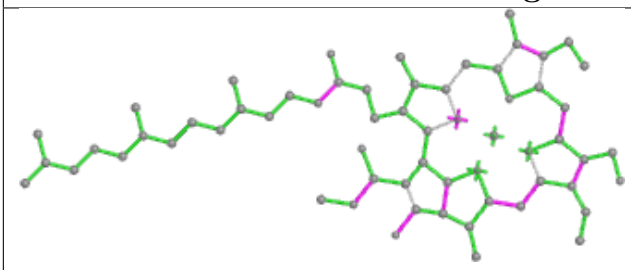

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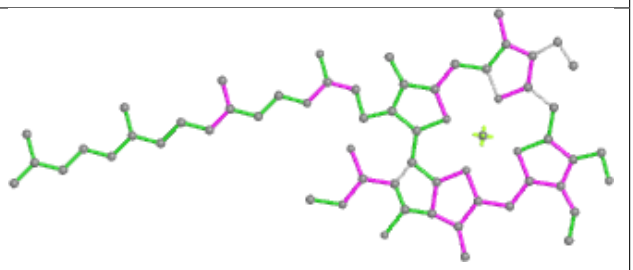

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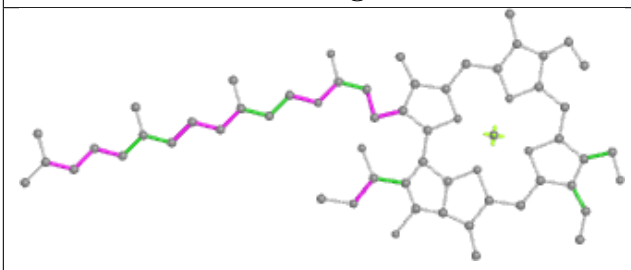

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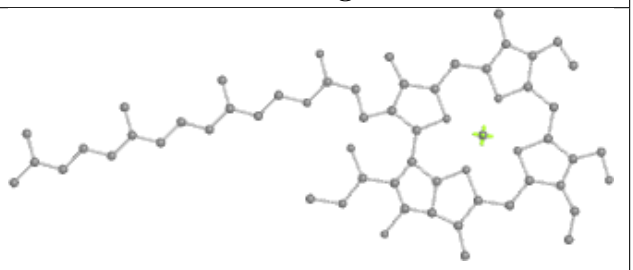
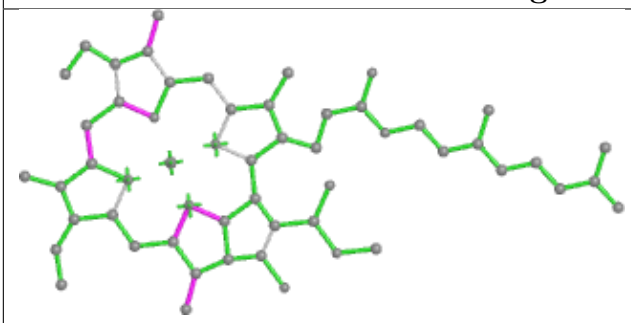


Rings

Ligand CLA s 613



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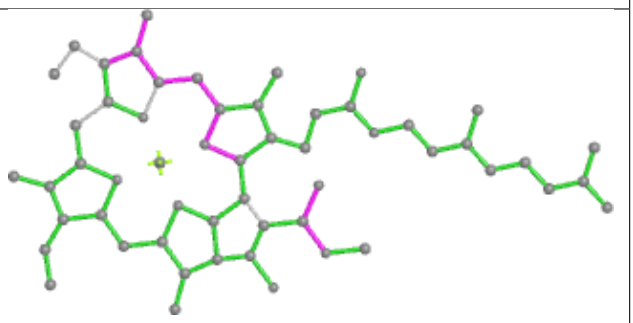

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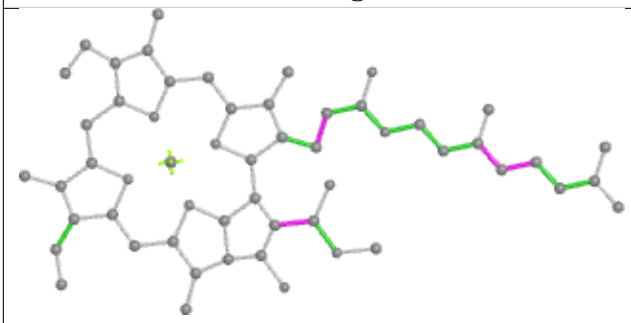

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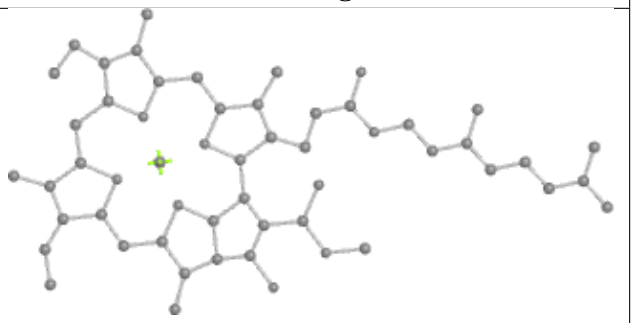

Rings

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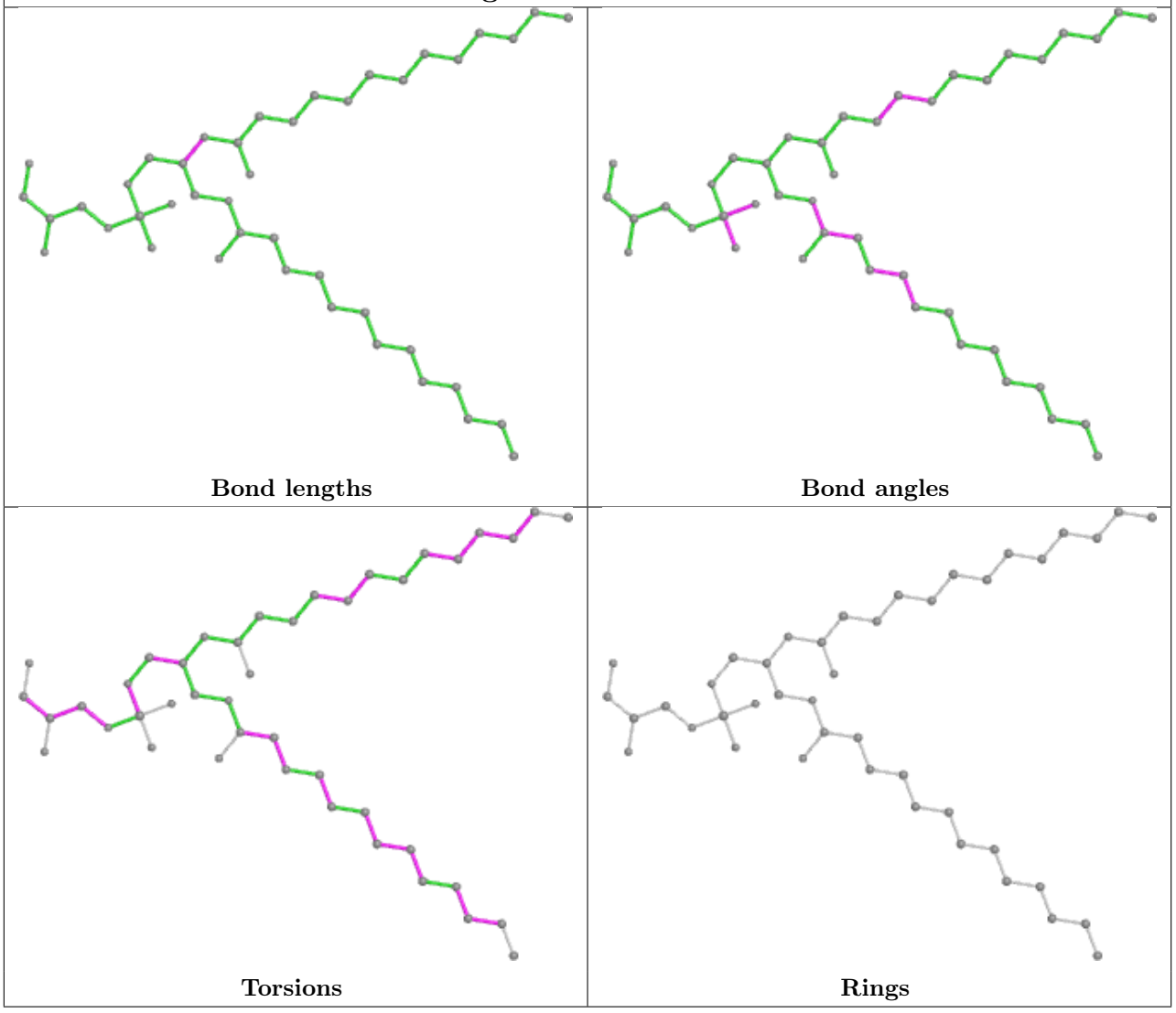

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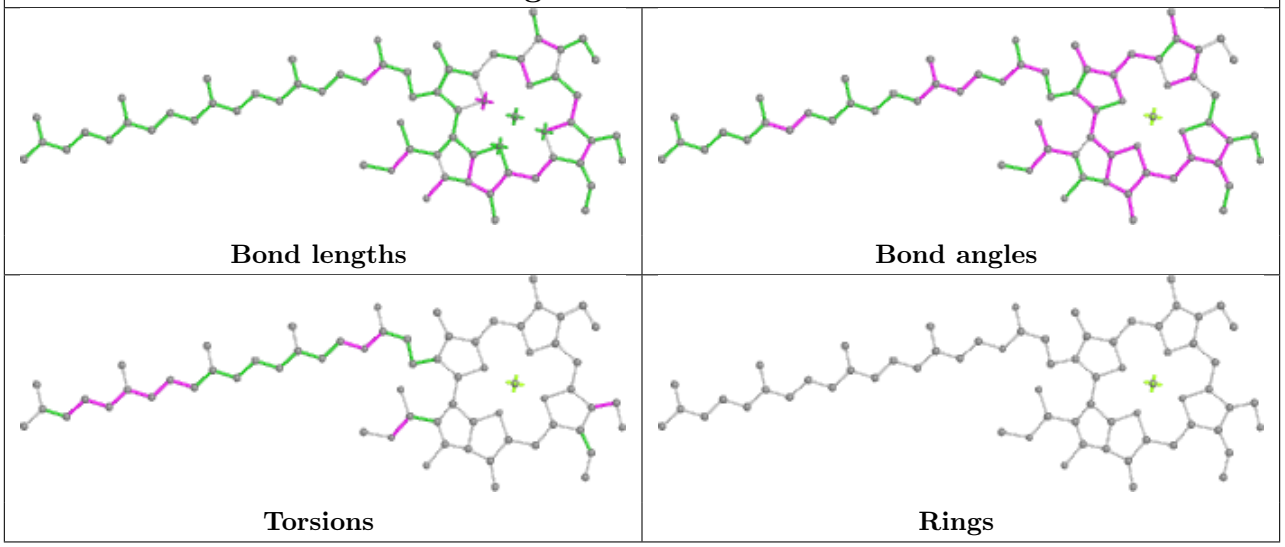

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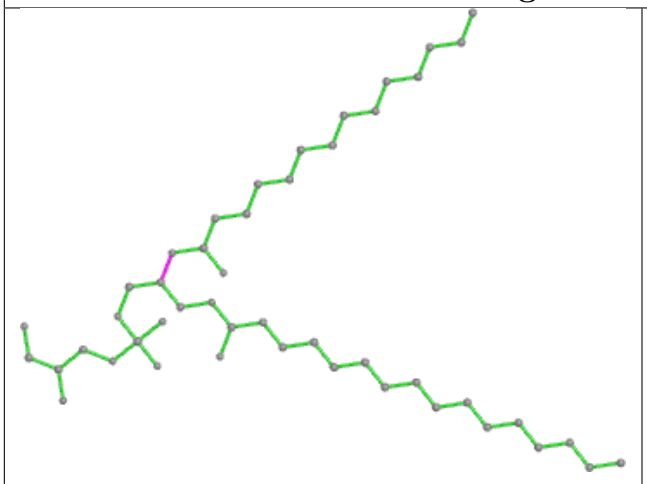

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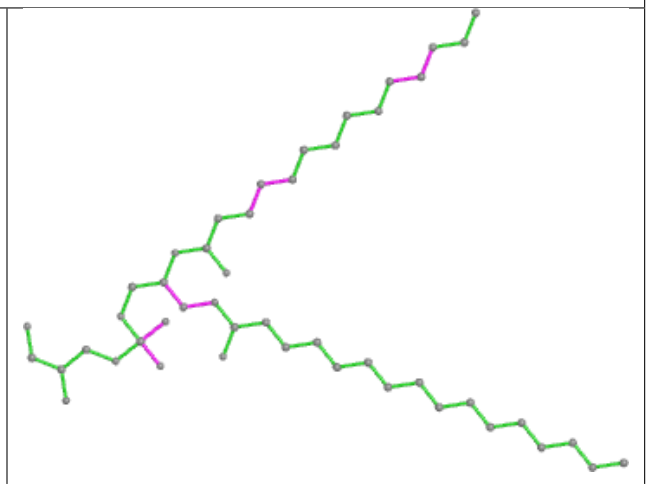
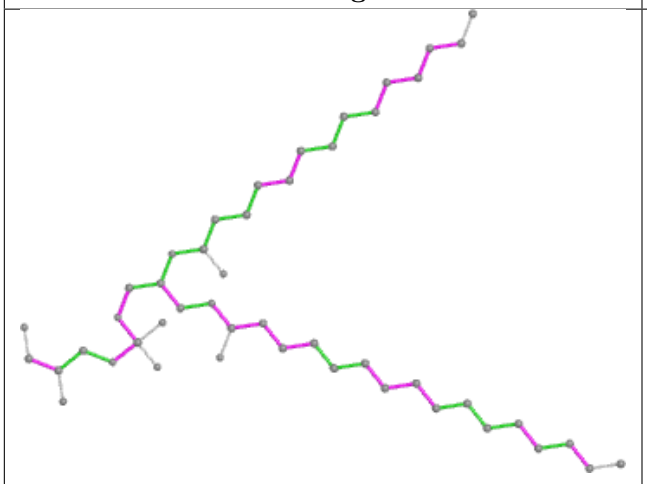


Bond angles



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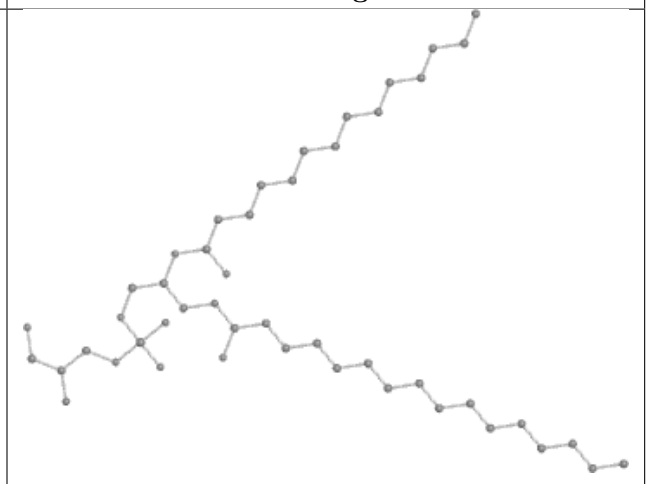

Rings

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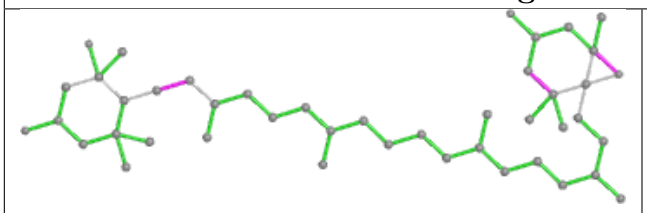

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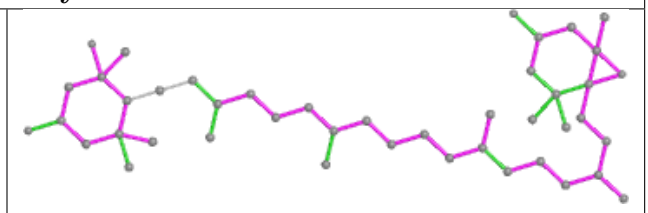

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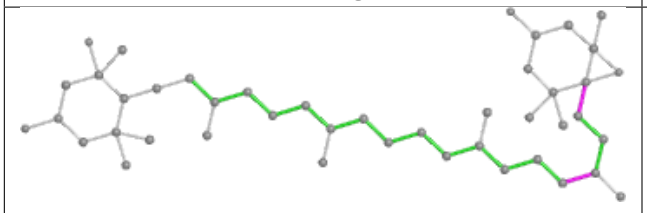

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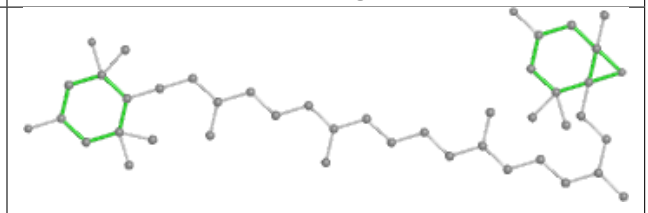
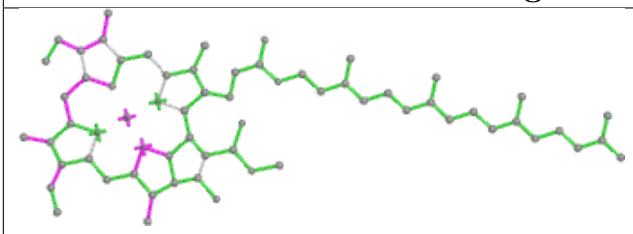


Rings

Ligand CLA B 606



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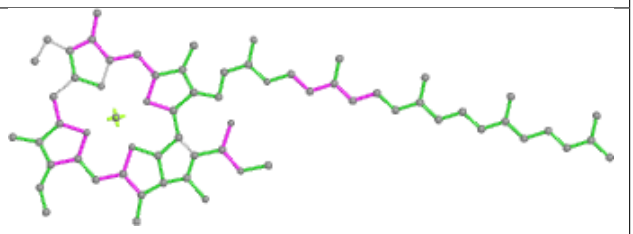

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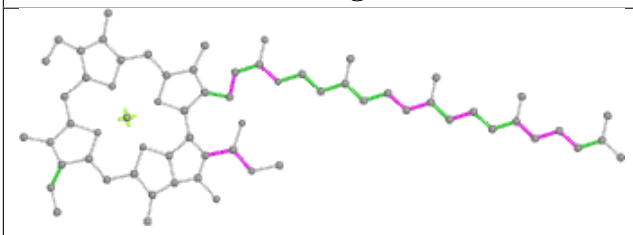

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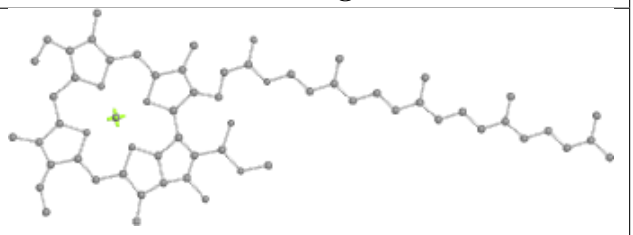

Rings

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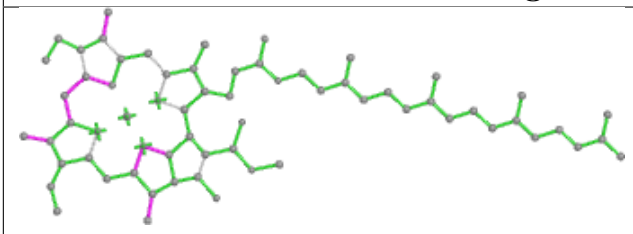

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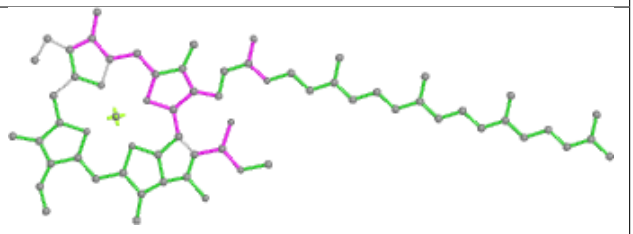

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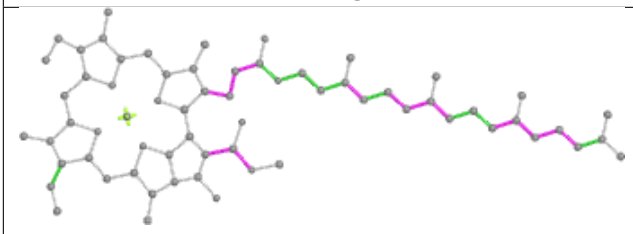

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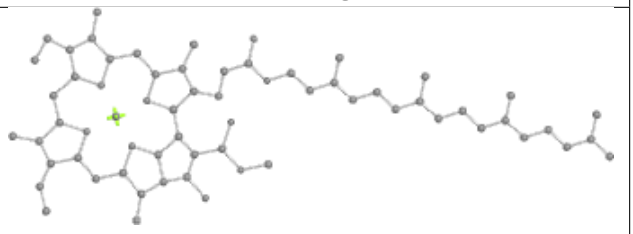
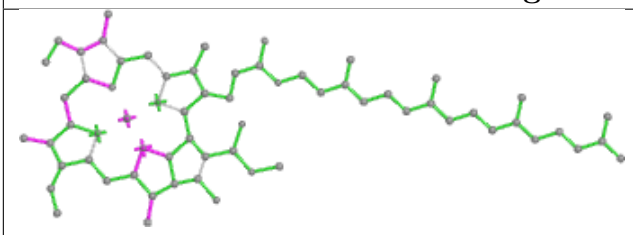


Rings

Ligand CLA N 602



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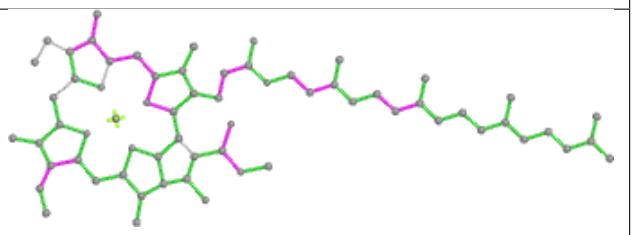
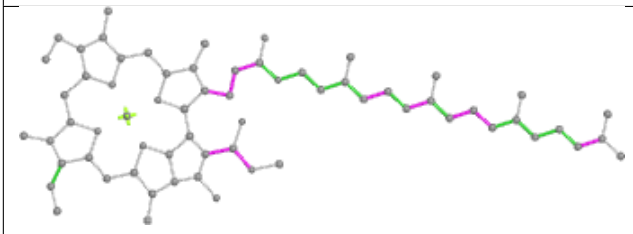


Bond angles



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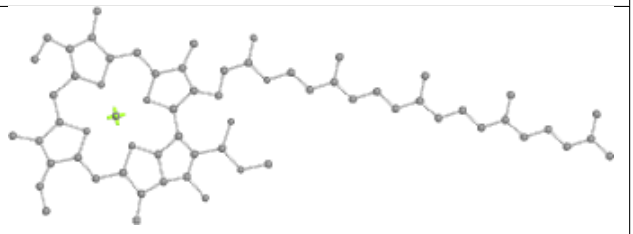
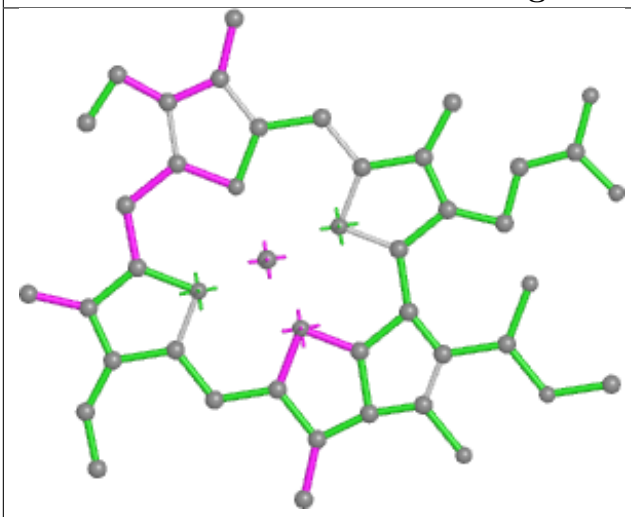


Rings

Ligand CLA 3 612



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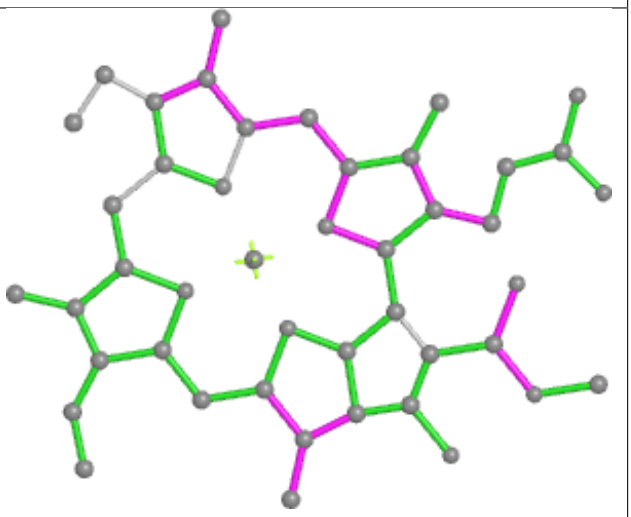
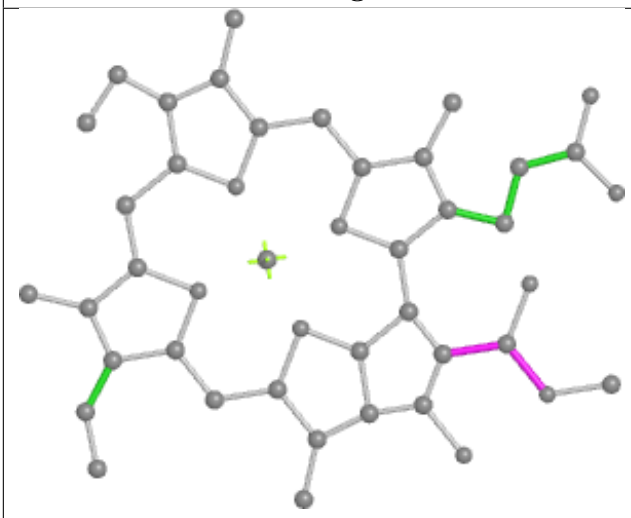


Bond angles



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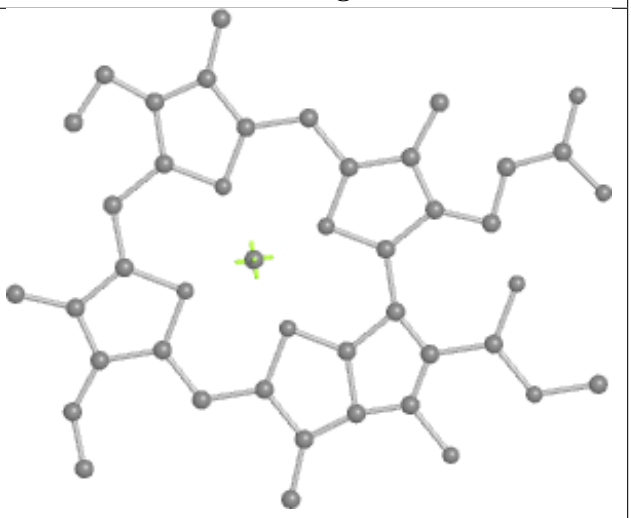
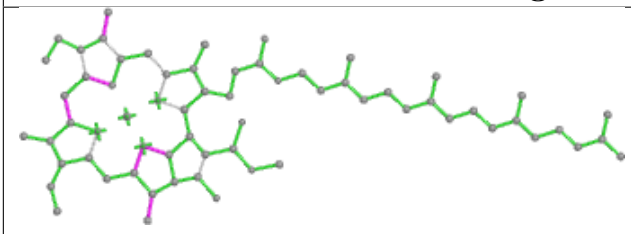


Rings

Ligand CLA c 512



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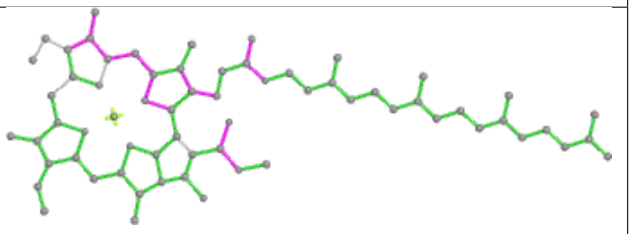

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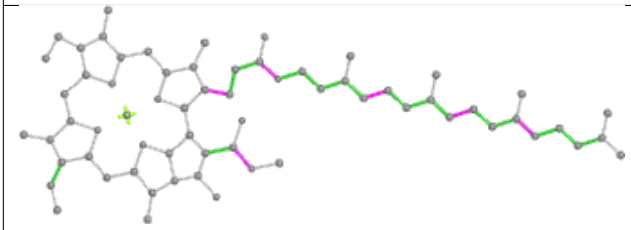

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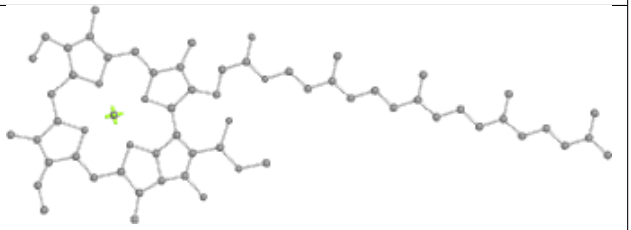
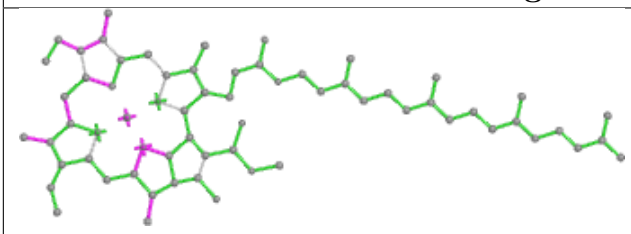
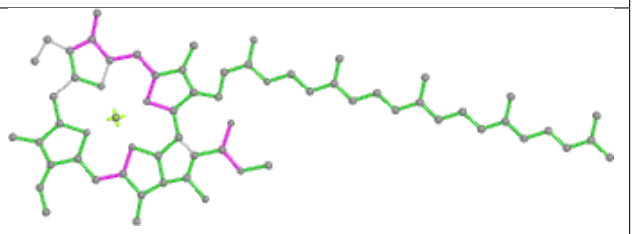


Rings

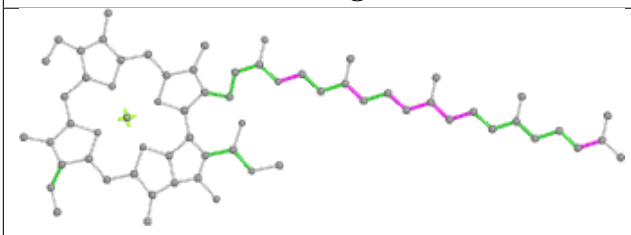
Ligand CLA B 603



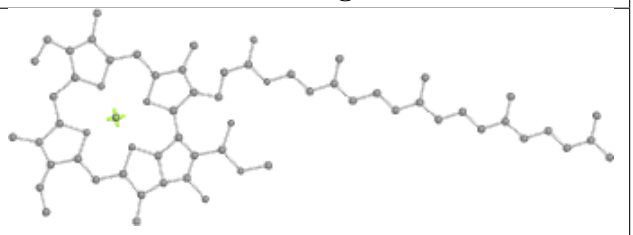
Bond lengths



Bond angles

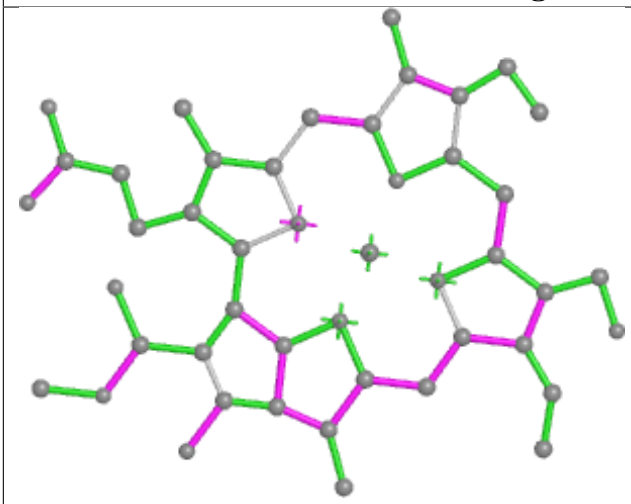


Torsions



Rings

Ligand CHL s 608



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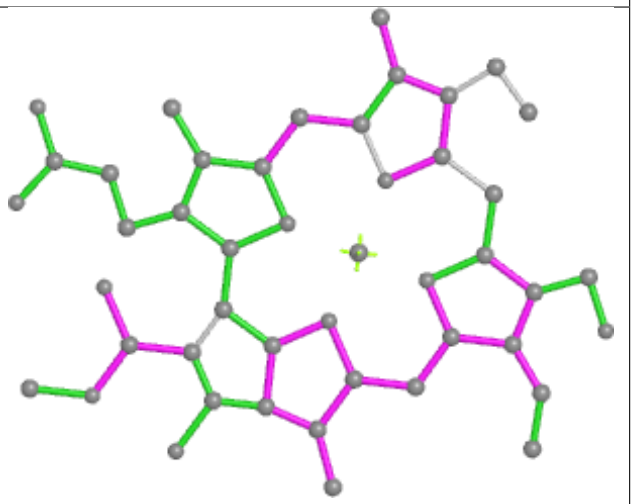

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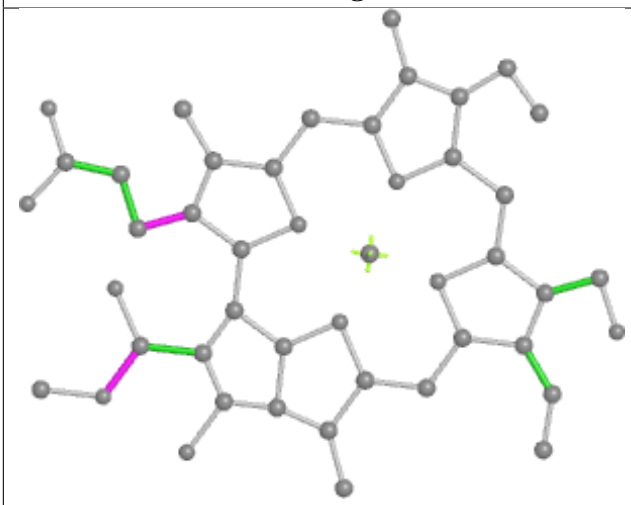

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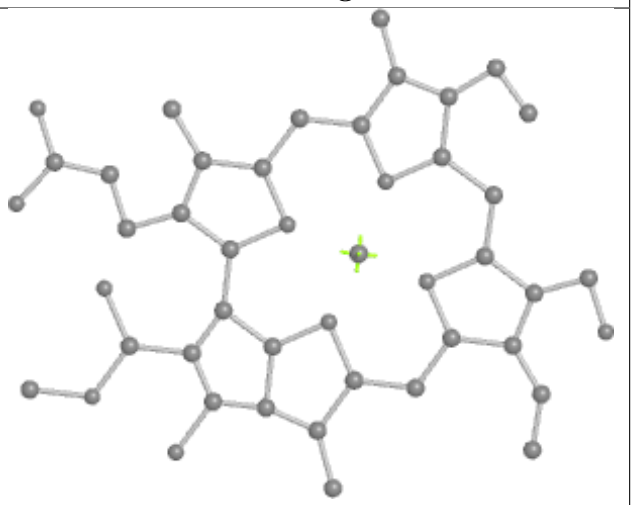
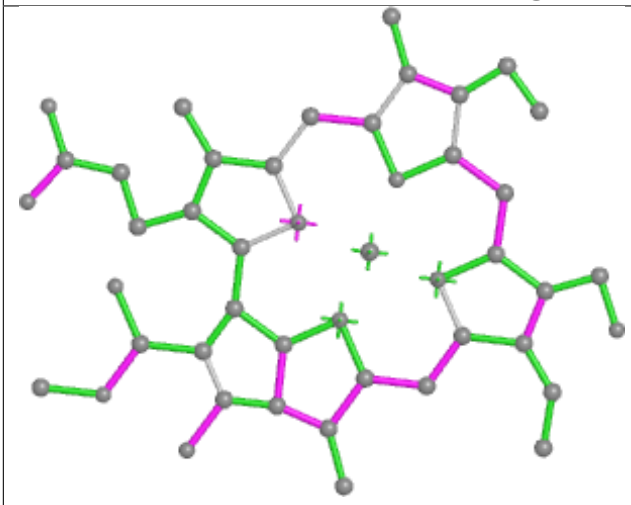


Rings

Ligand CHL 6 605



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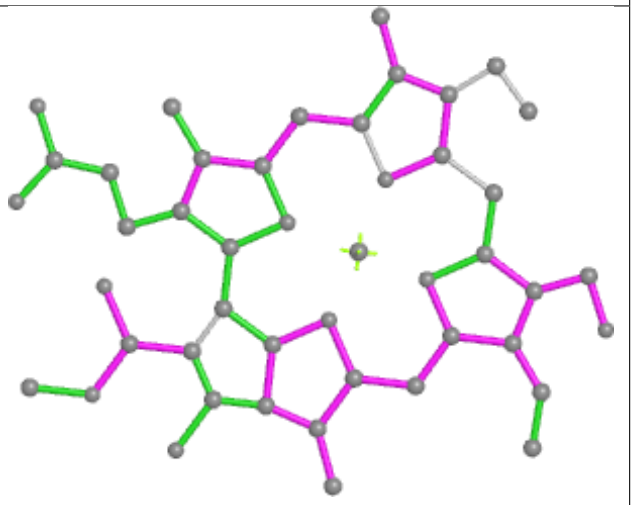
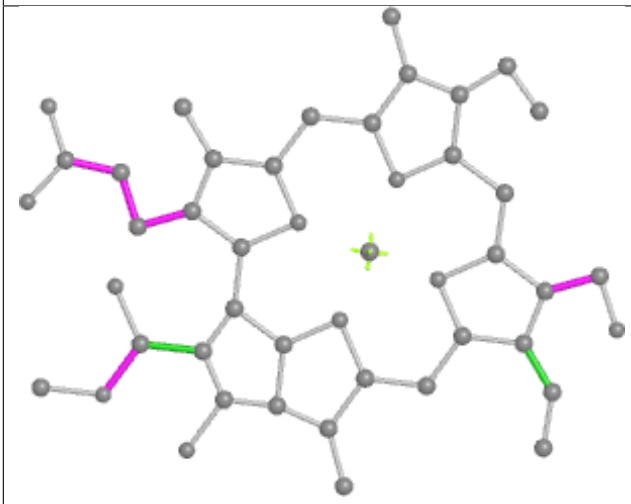


Bond angles



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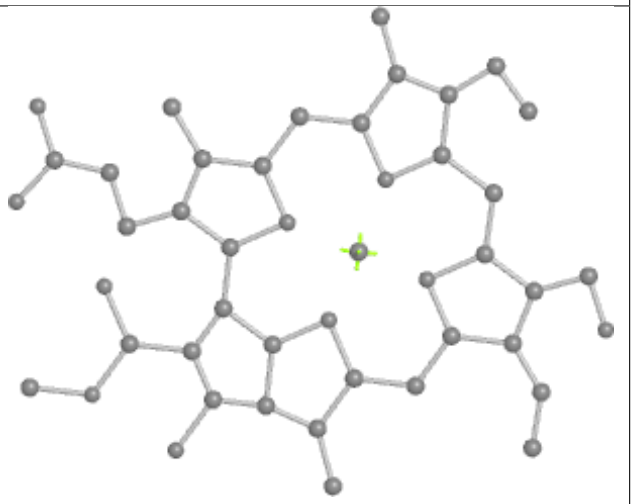
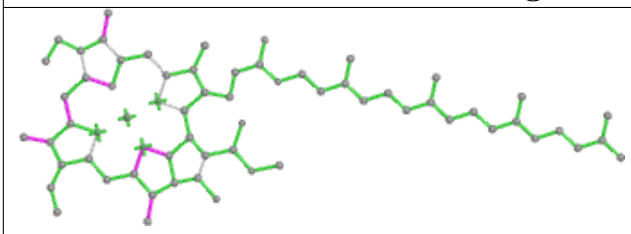


Rings

Ligand CLA C 513



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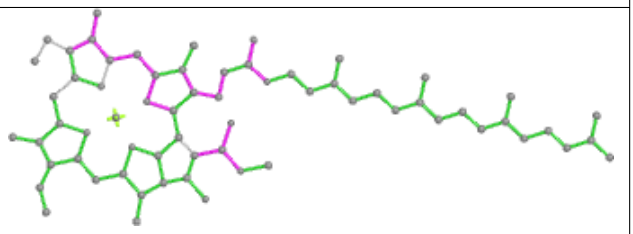
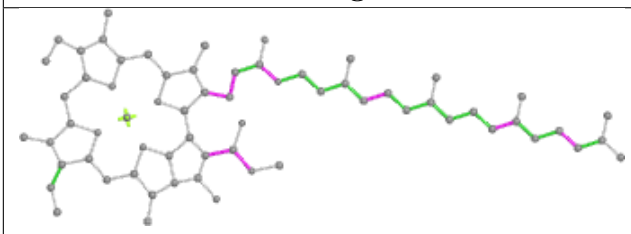


Bond angles



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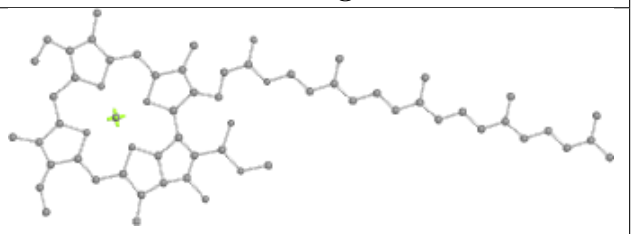
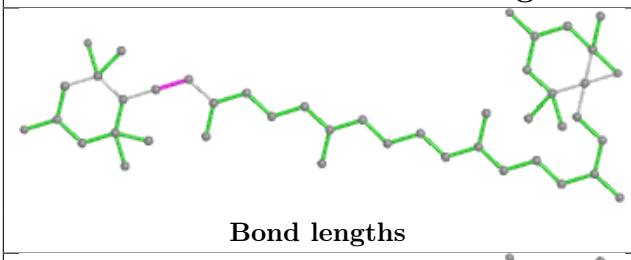


Rings

Ligand NEX S 1623



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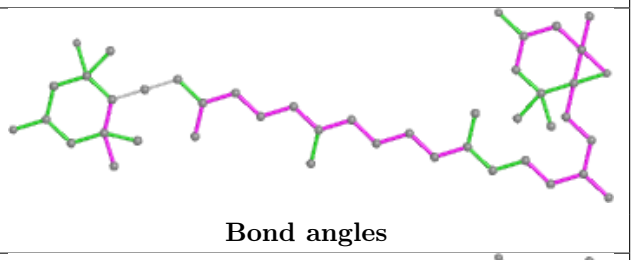
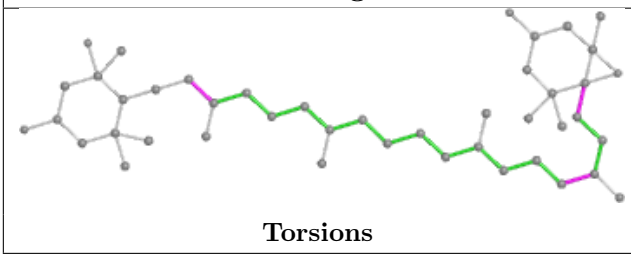


Bond angles



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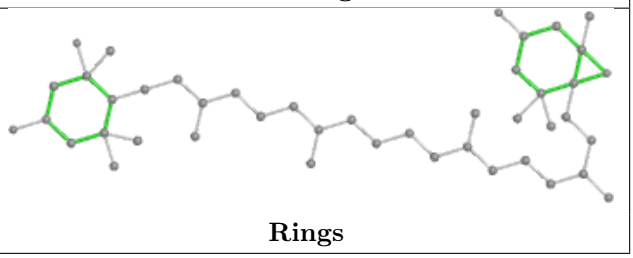
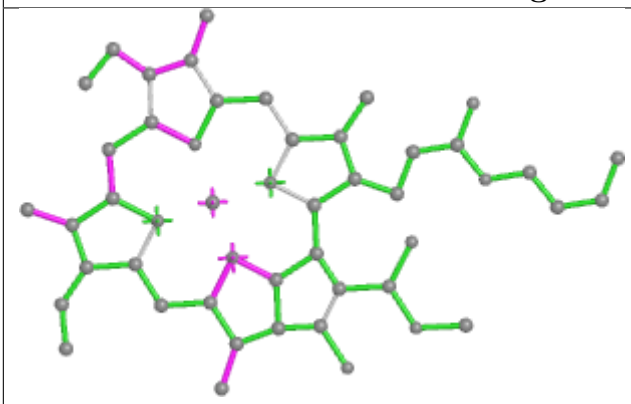


Rings

Ligand CLA r 611



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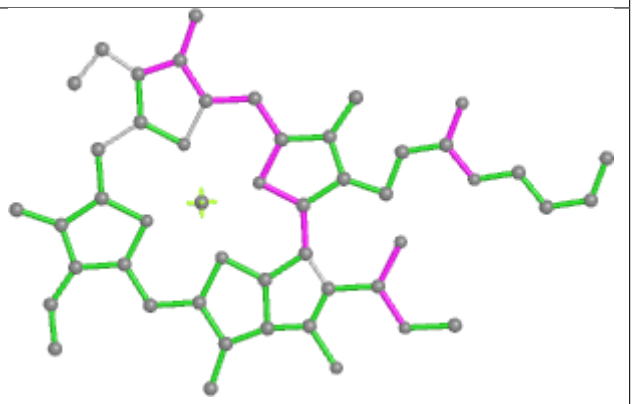
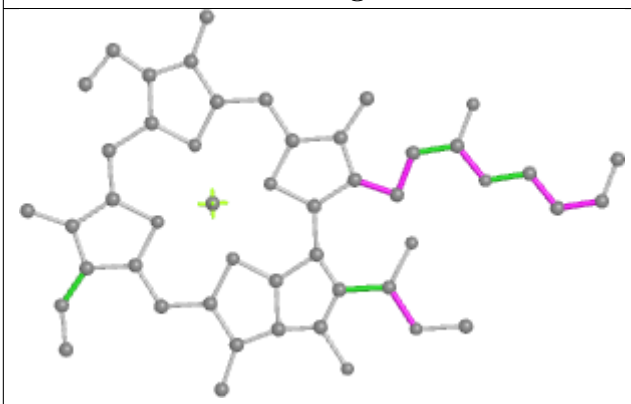


Bond angles



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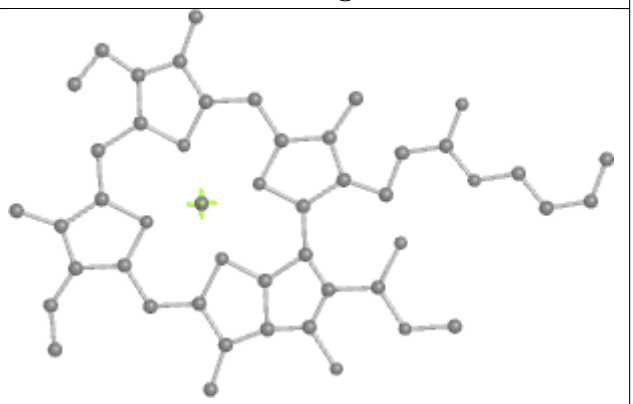
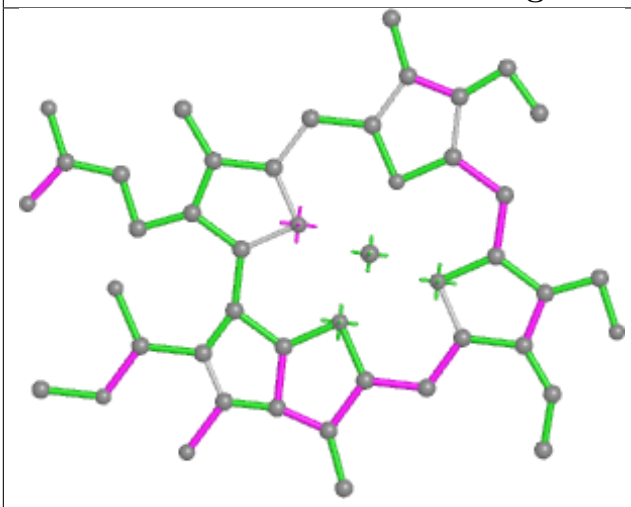


Rings

Ligand CHL S 601



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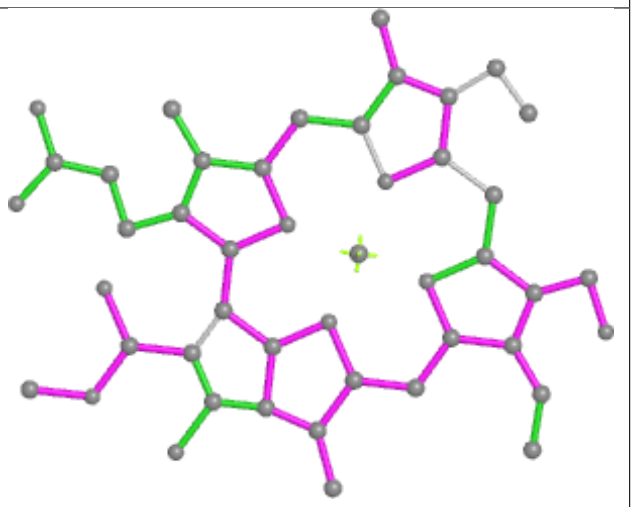

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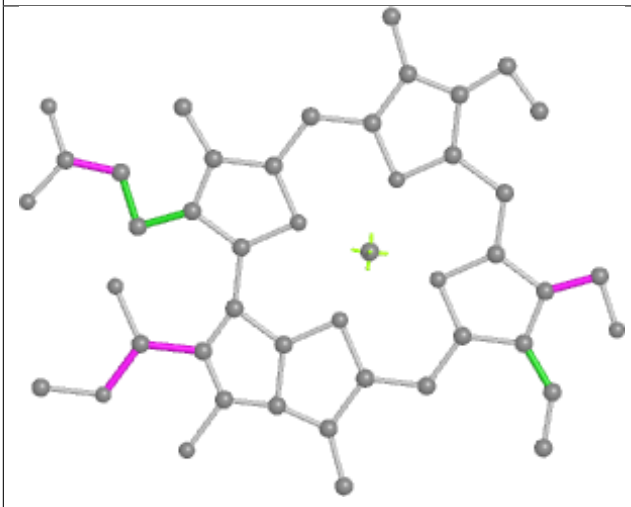

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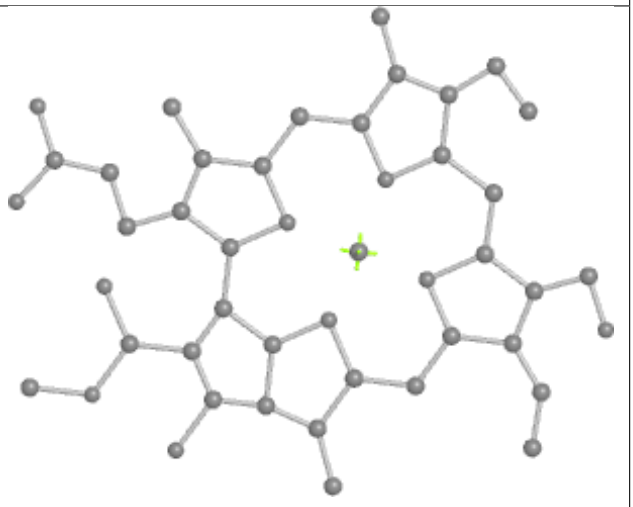
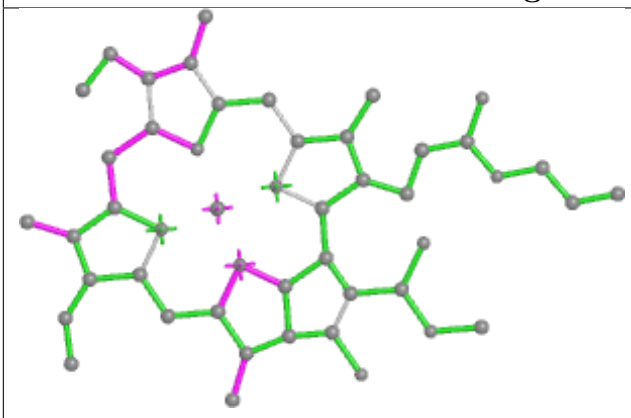


Rings

Ligand CLA Y 614



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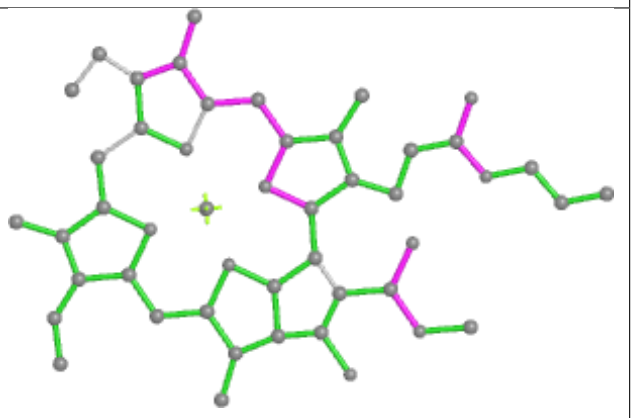
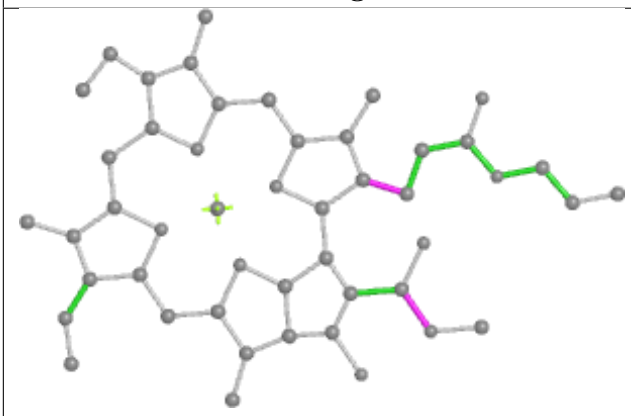


Bond angles



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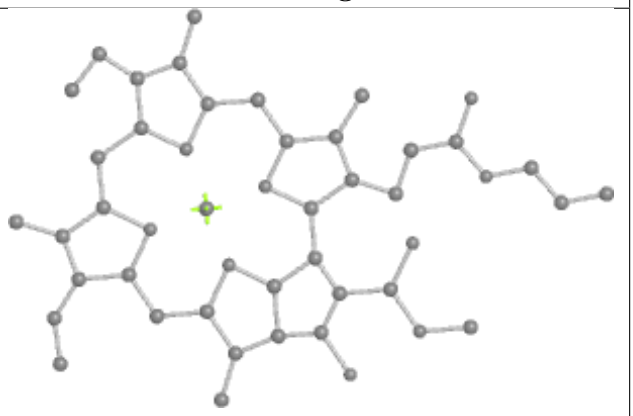
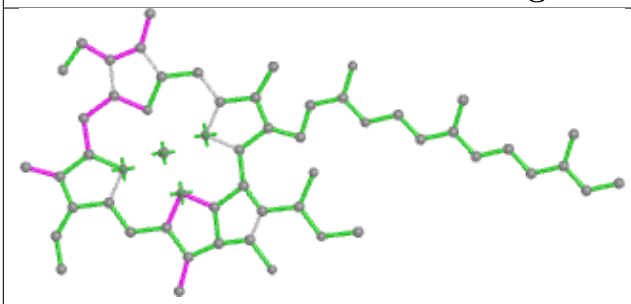


Rings

Ligand CLA 1 610



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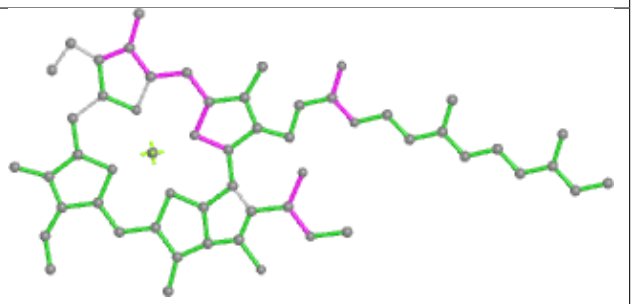
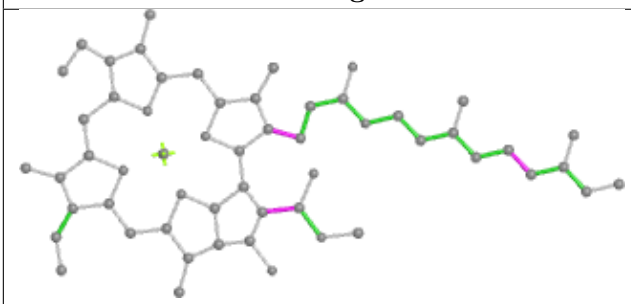


Bond angles



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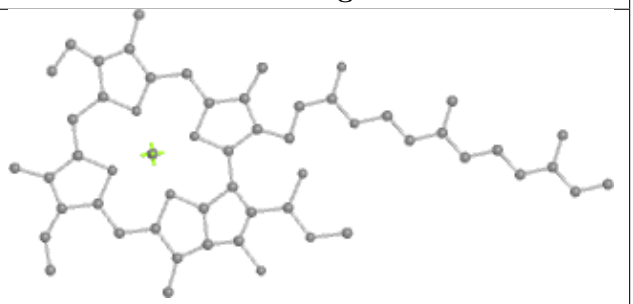
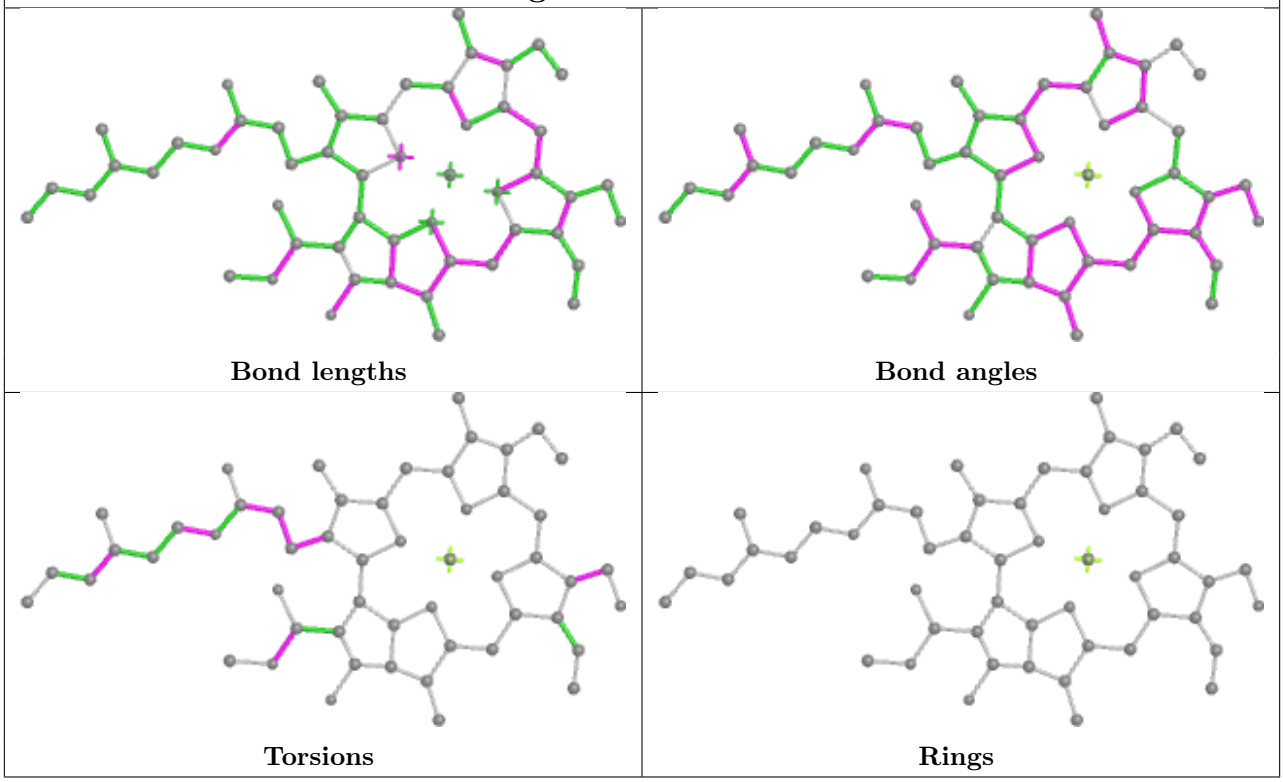
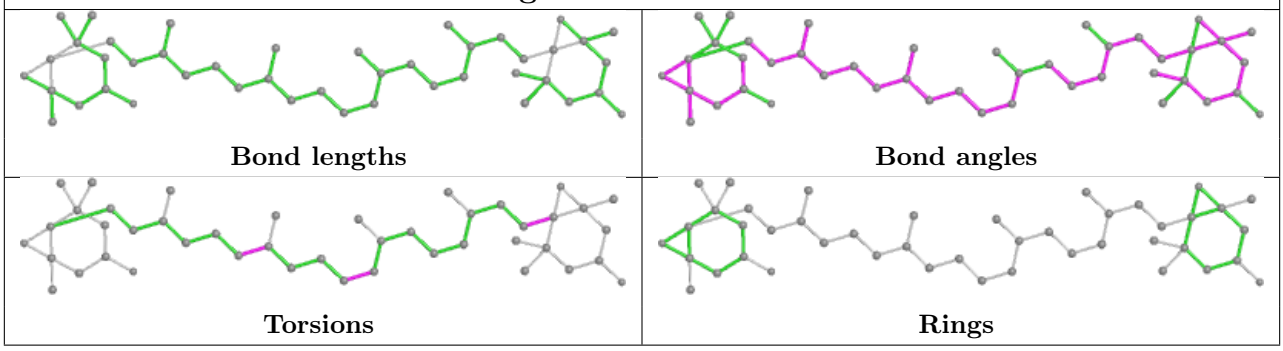


Rings

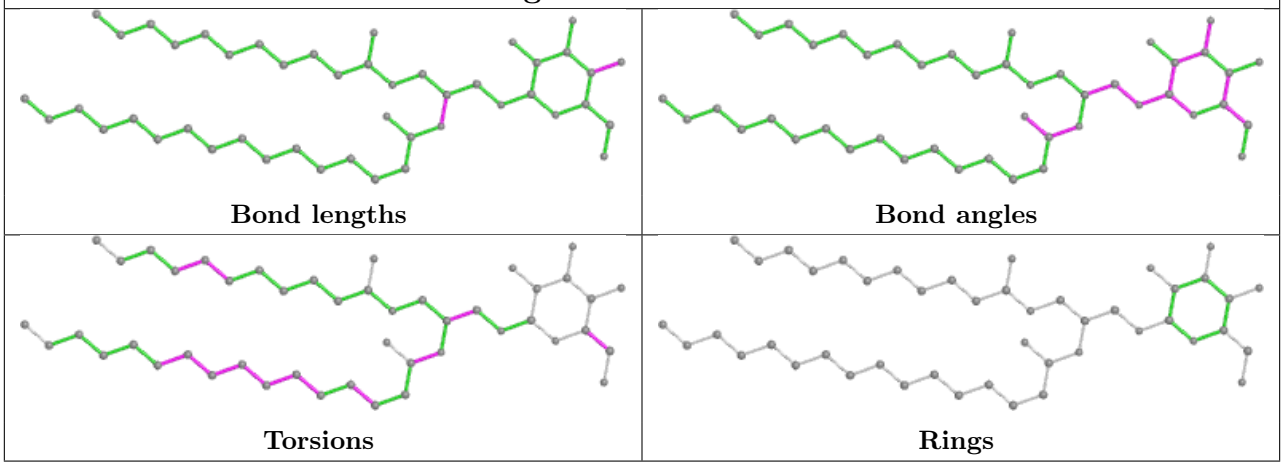
Ligand CHL 7 607



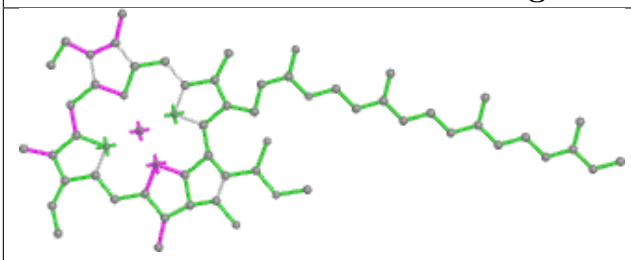
Ligand XAT 2 1622



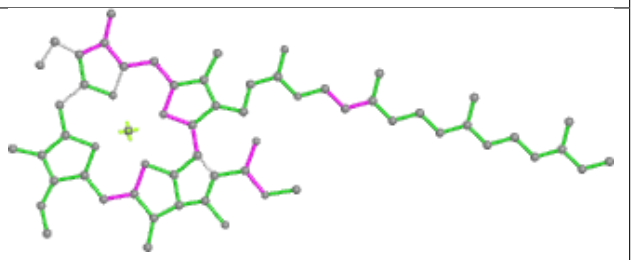
Ligand LMG d 411



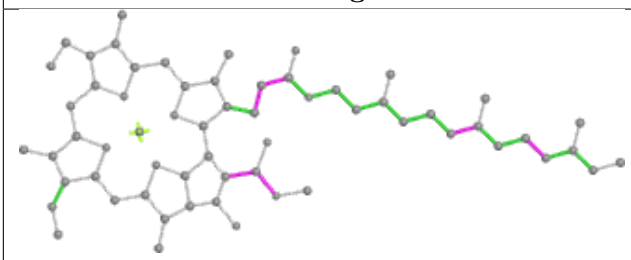
Ligand CLA 5 602



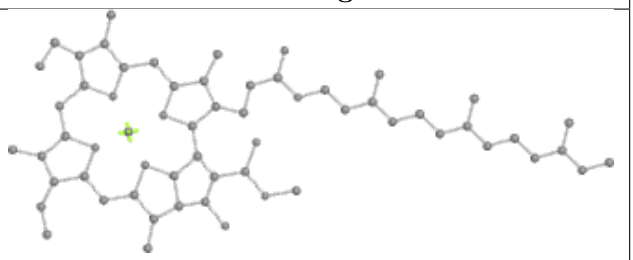
Bond lengths



Bond angles

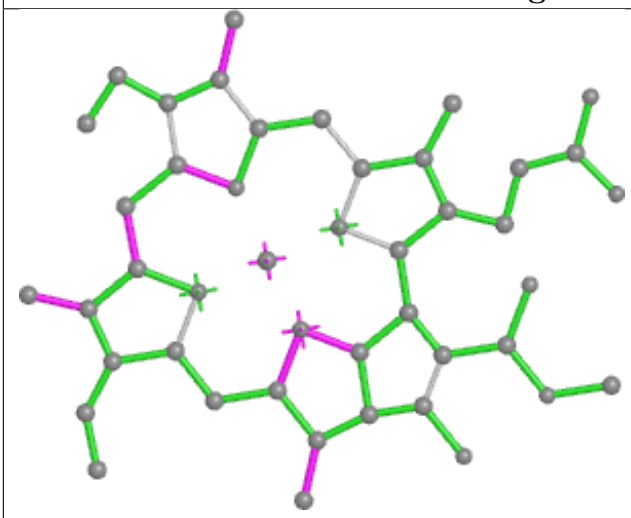


Torsions



Rings

Ligand CLA 8 612



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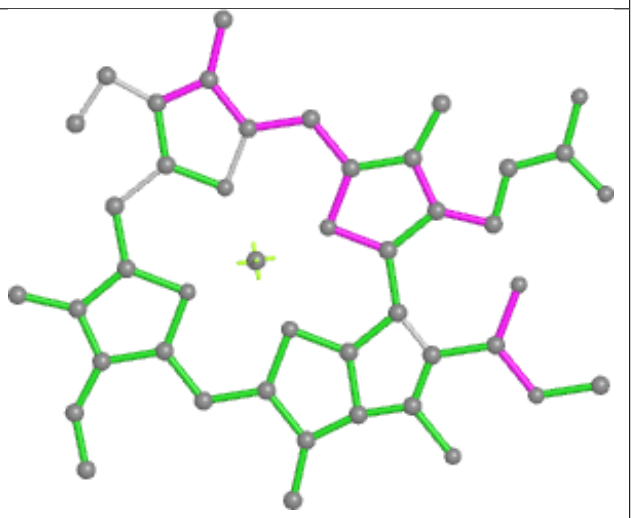
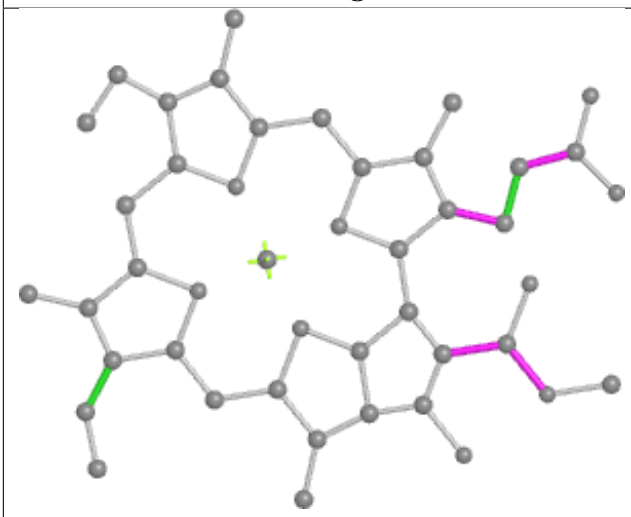


Bond angles



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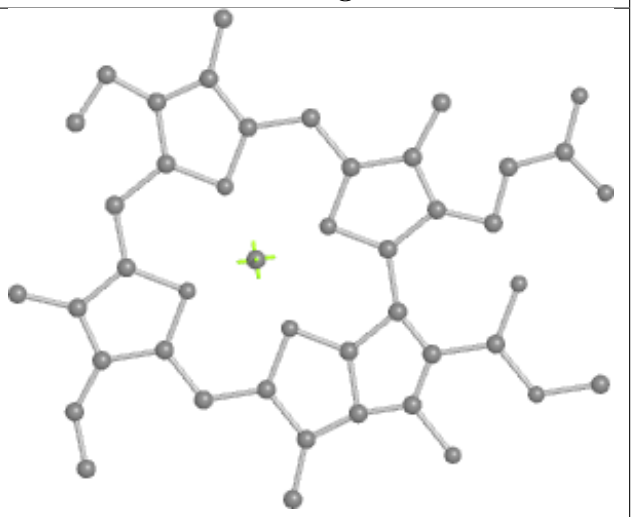
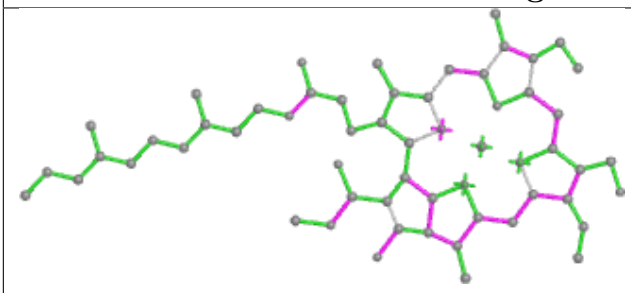


Rings

Ligand CHL S 607



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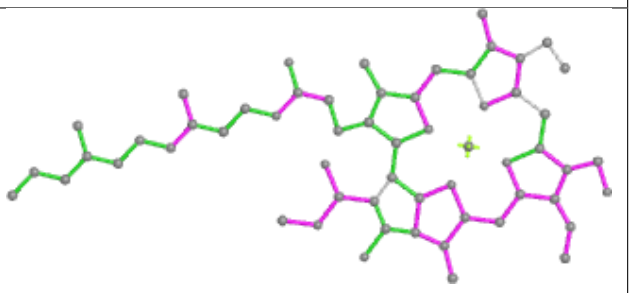
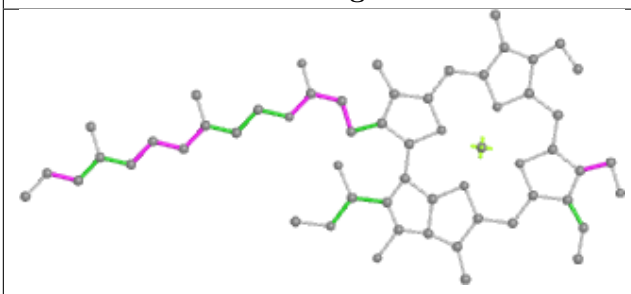
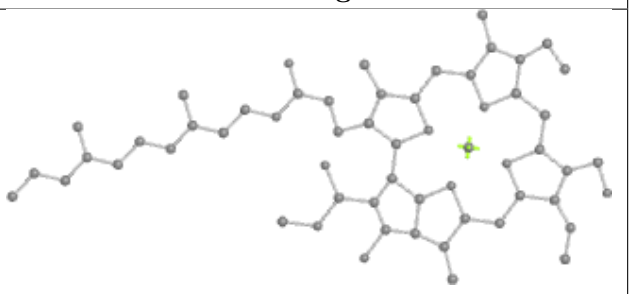


Bond angles

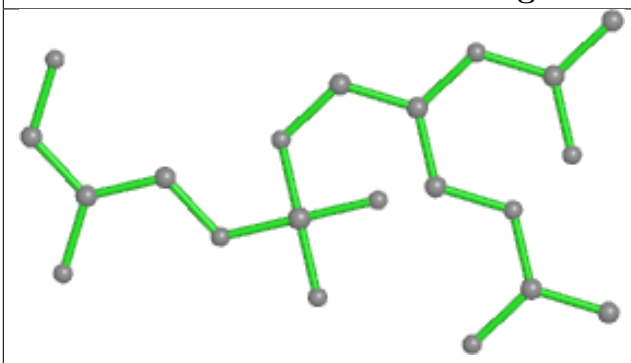


Torsions



Rings

Ligand LHG 8 2630



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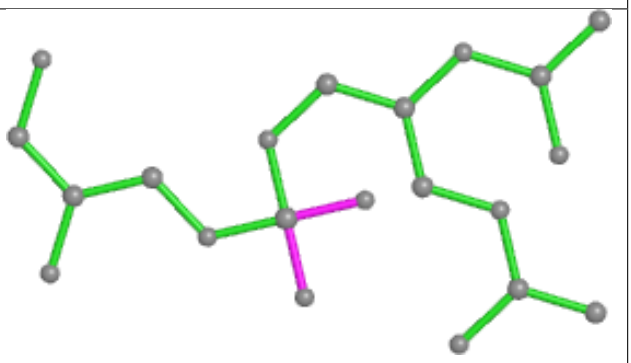
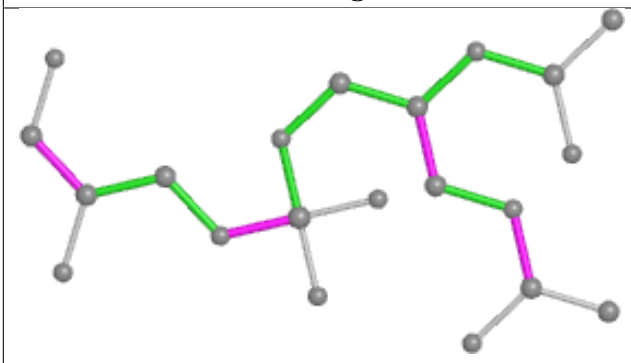
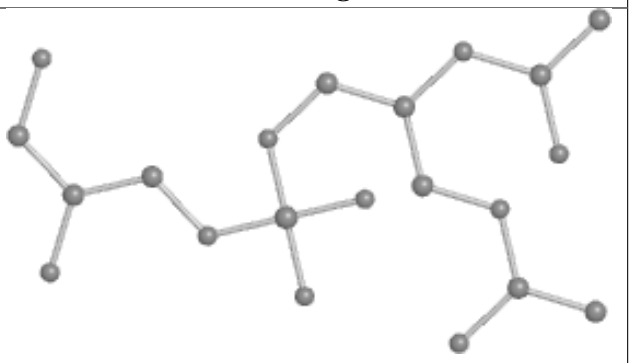


Bond angles

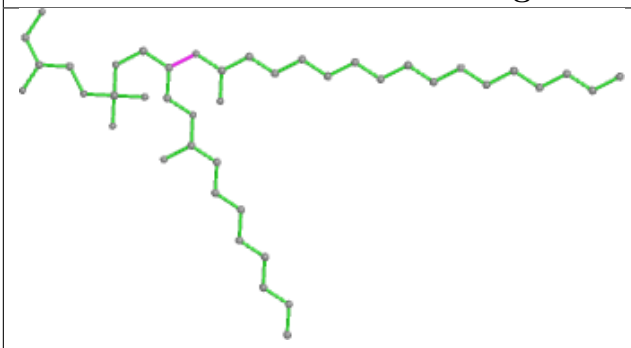


Torsions

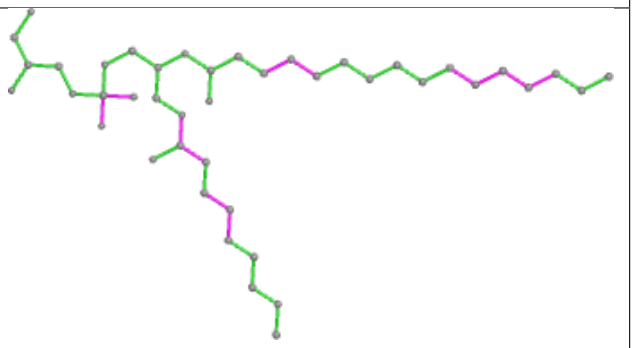


Rings

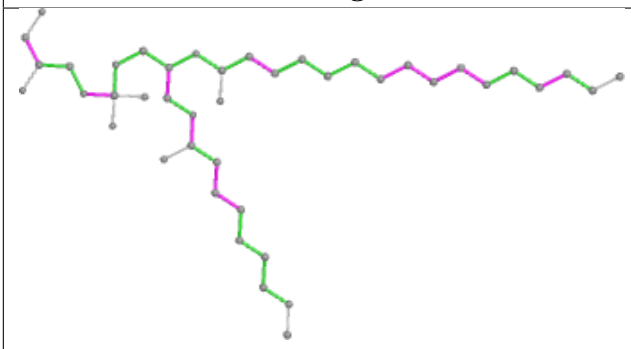
Ligand LHG R 2630



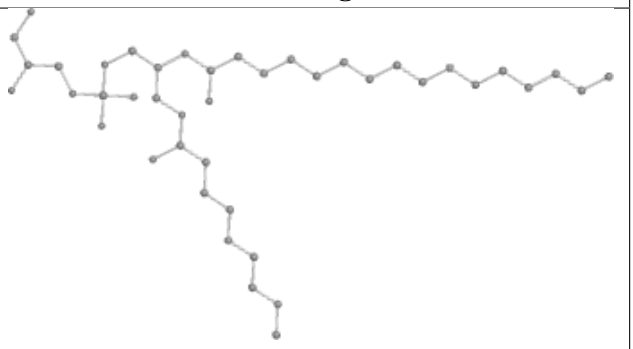
Bond lengths



Bond angles

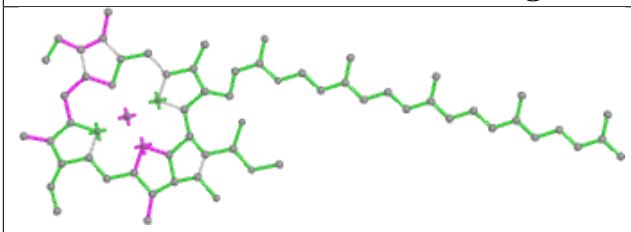


Torsions

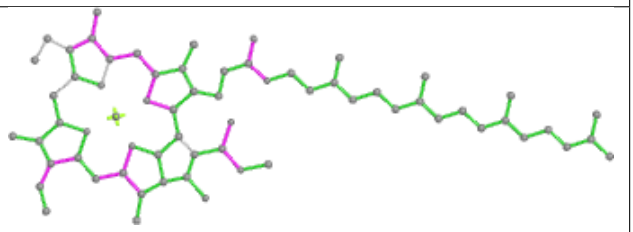


Rings

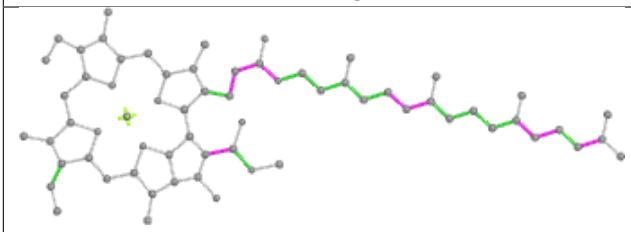
Ligand CLA B 602



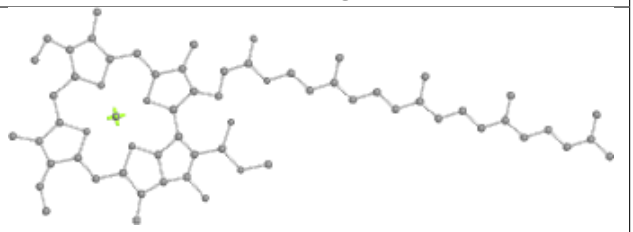
Bond lengths



Bond angles

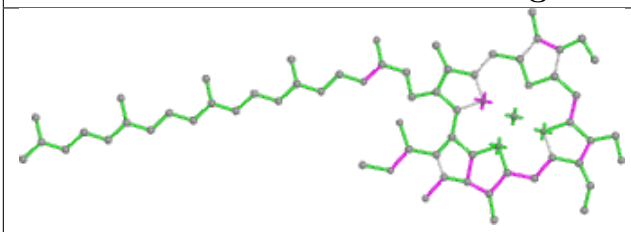


Torsions



Rings

Ligand CHL r 606



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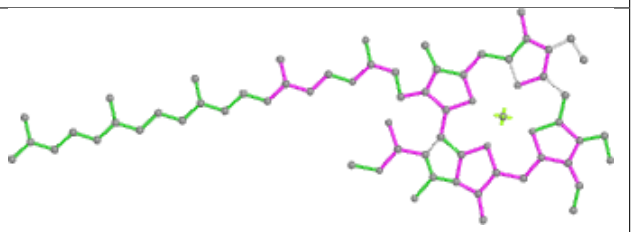
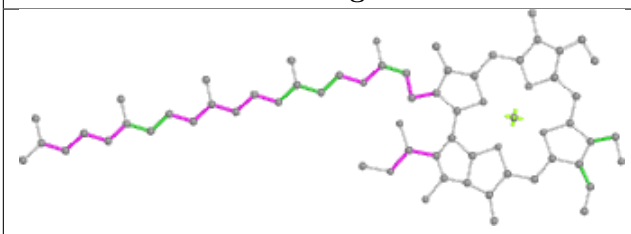


Bond angles



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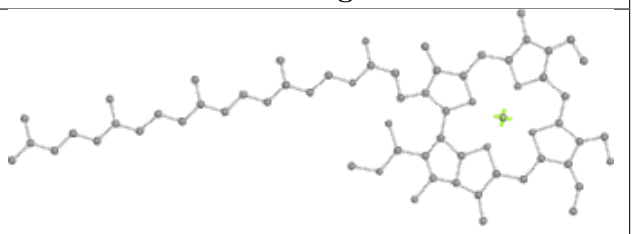
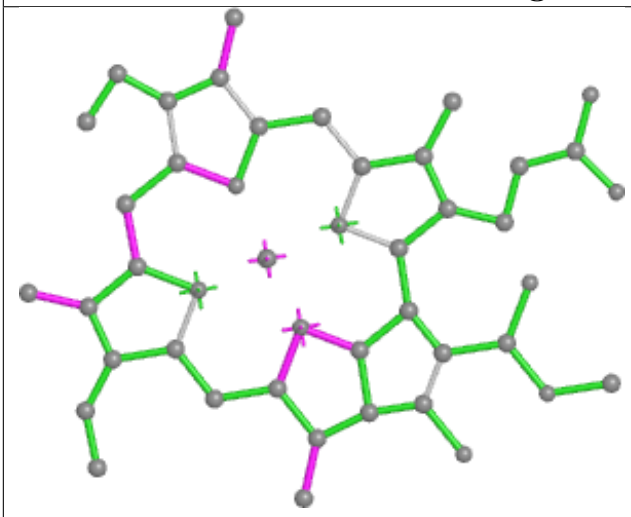
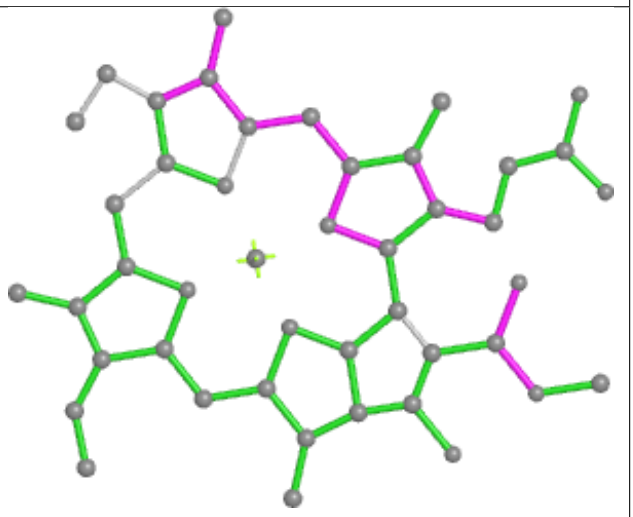


Rings

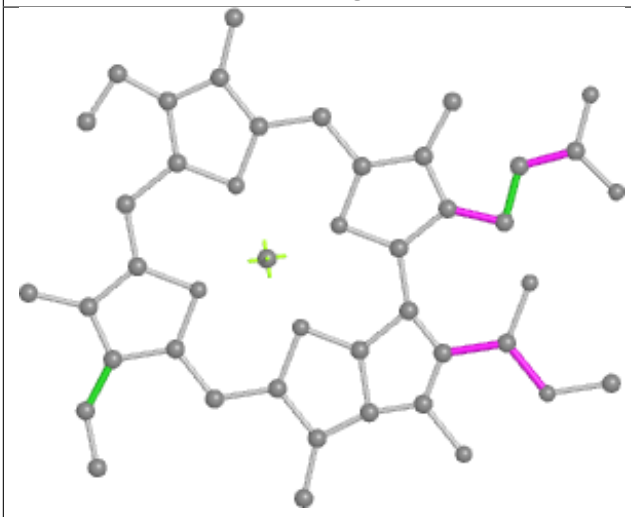
Ligand CLA 4 612



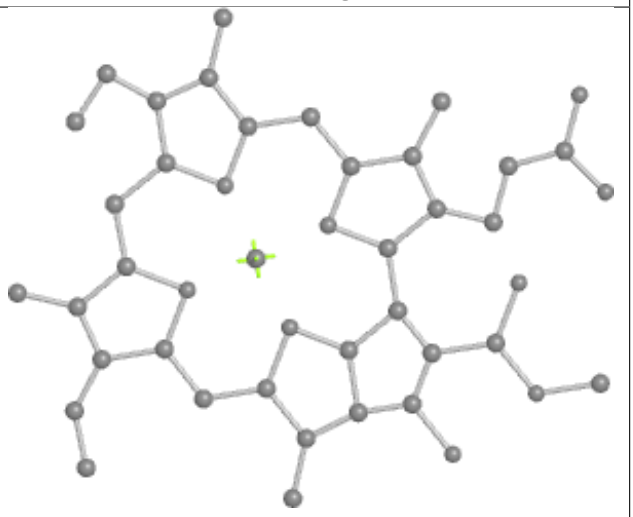
Bond lengths



Bond angles

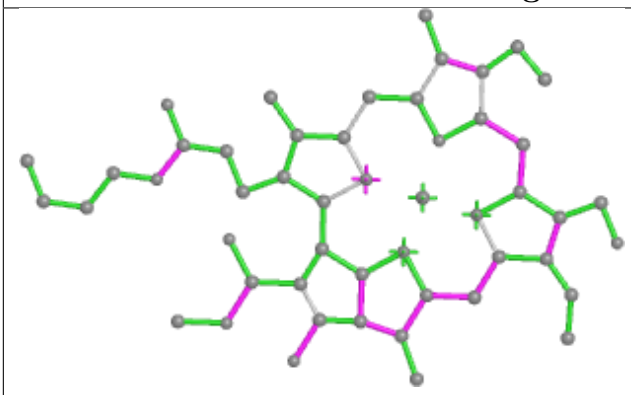


Torsions



Rings

Ligand CHL G 606



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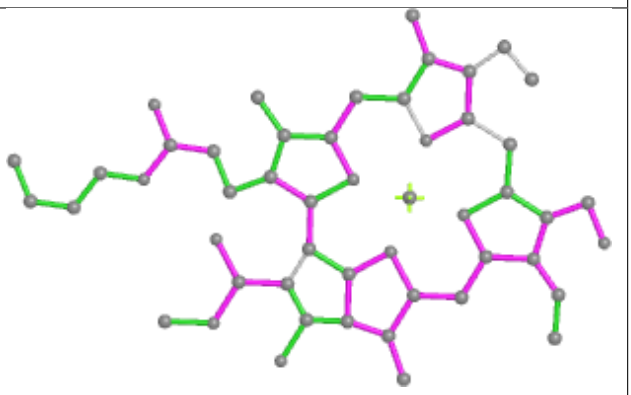
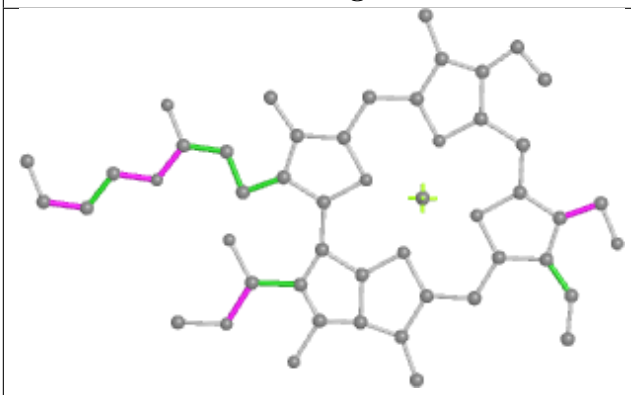
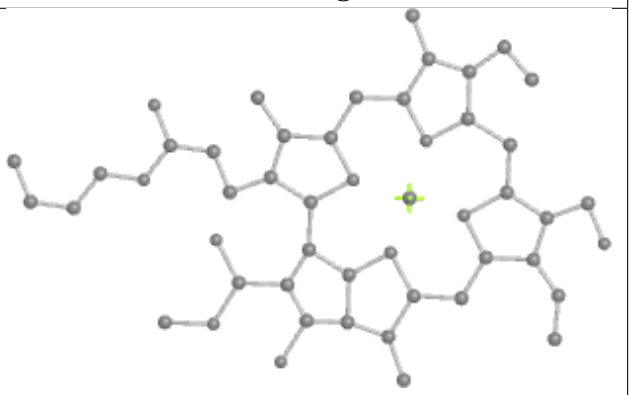


Bond angles

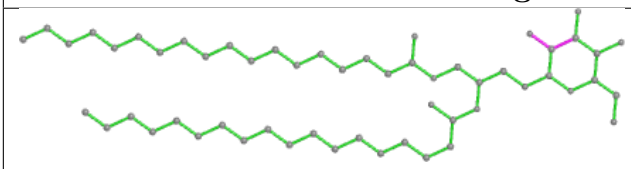


Torsions

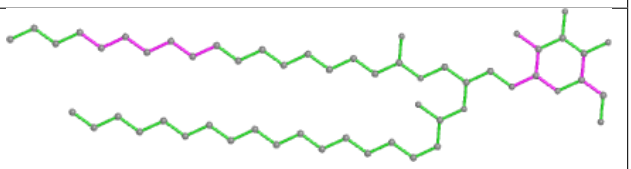


Rings

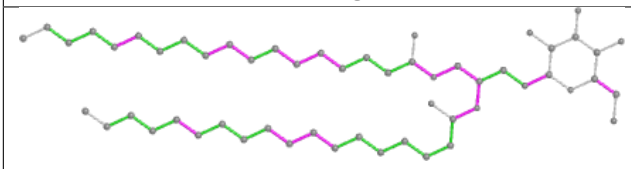
Ligand LMG b 2633



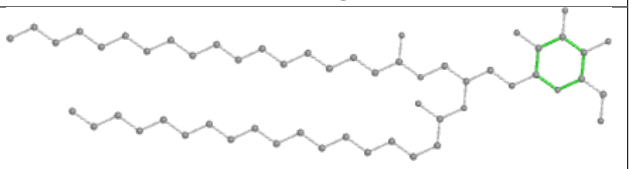
Bond lengths



Bond angles

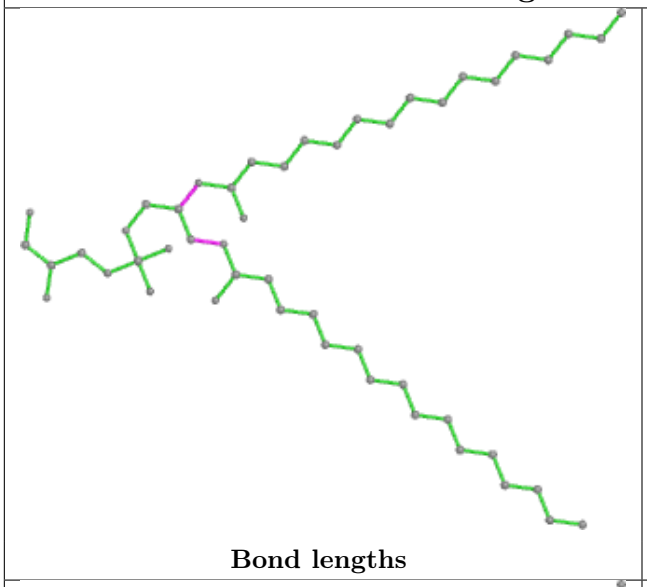


Torsions



Rings

Ligand LHG y 2630



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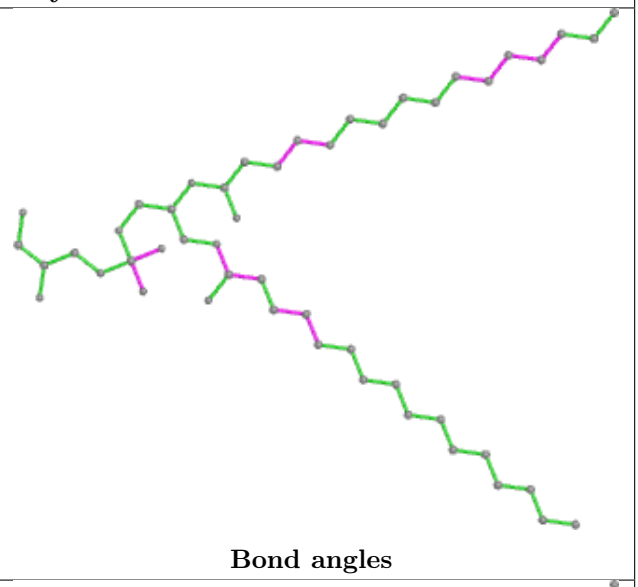
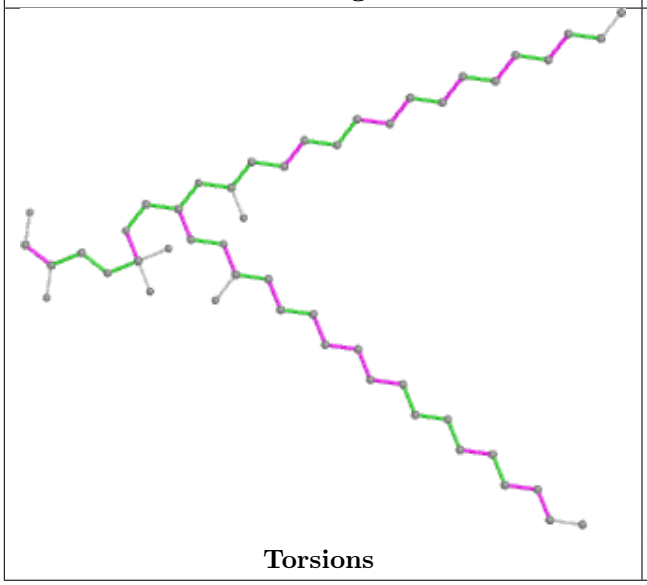
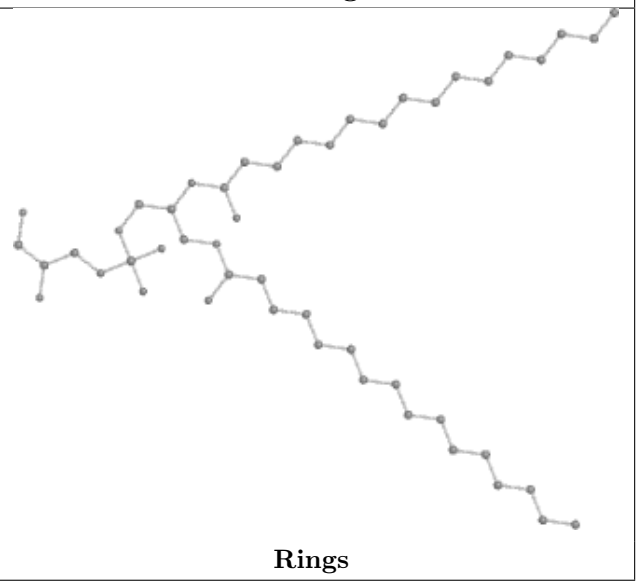


Bond angles

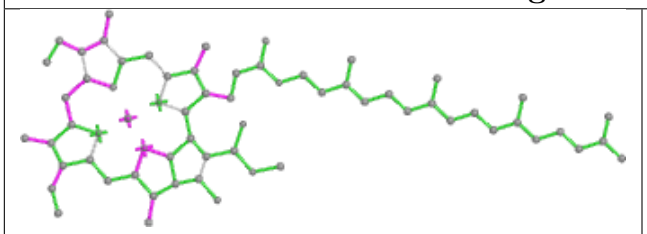


Torsions

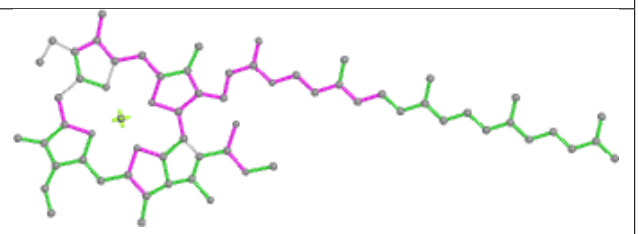


Rings

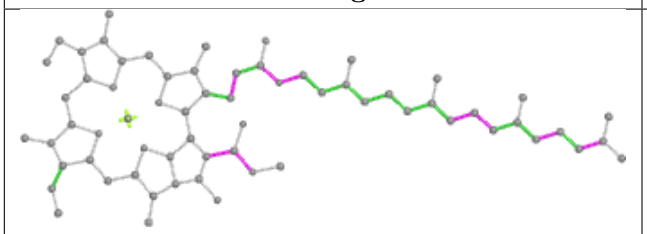
Ligand CLA b 605



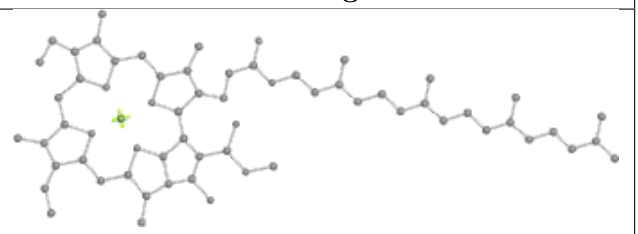
Bond lengths



Bond angles

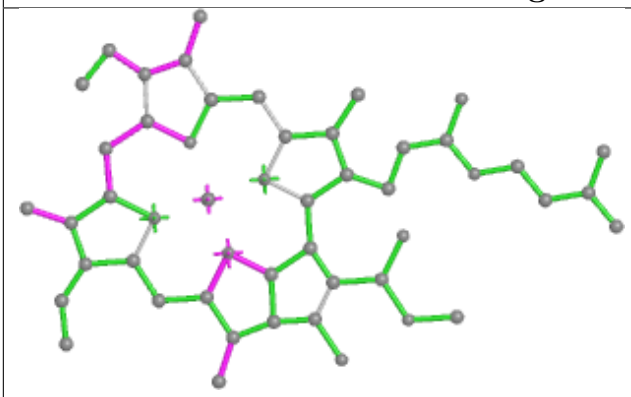


Torsions

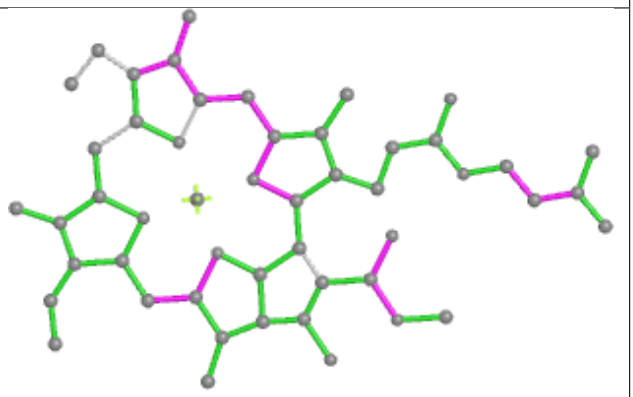


Rings

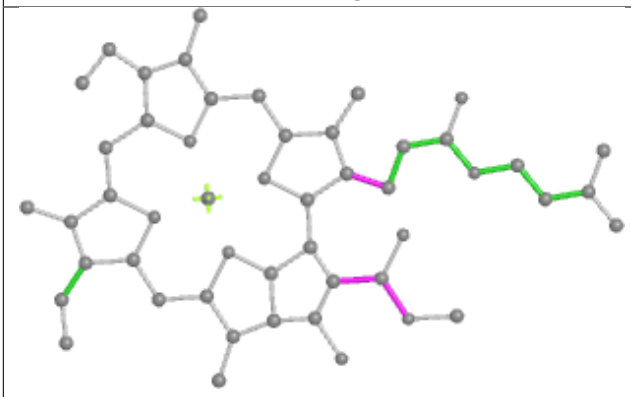
Ligand CLA a 407



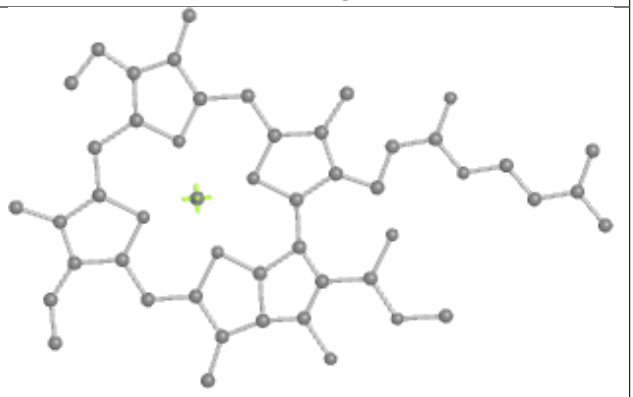
Bond lengths



Bond angles

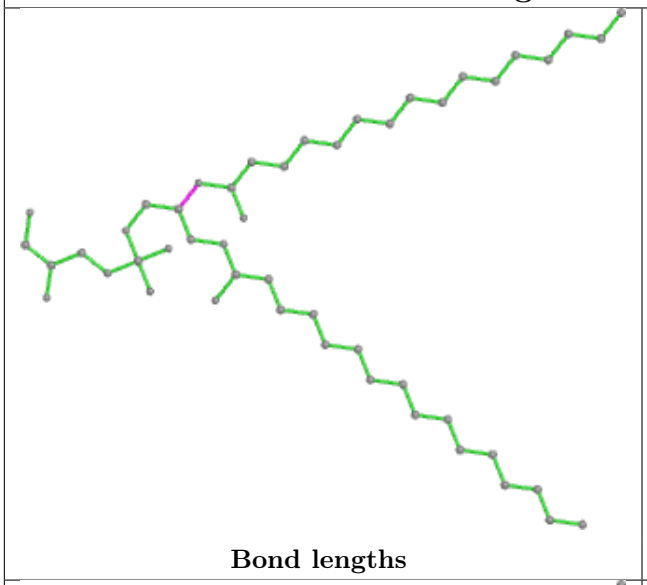


Torsions

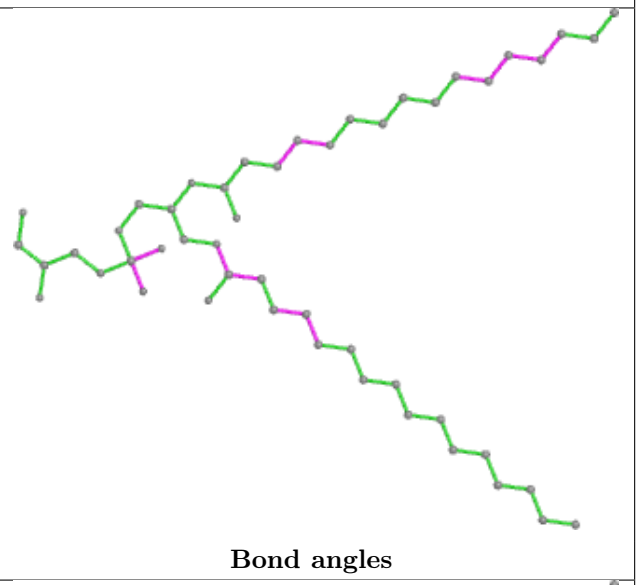


Rings

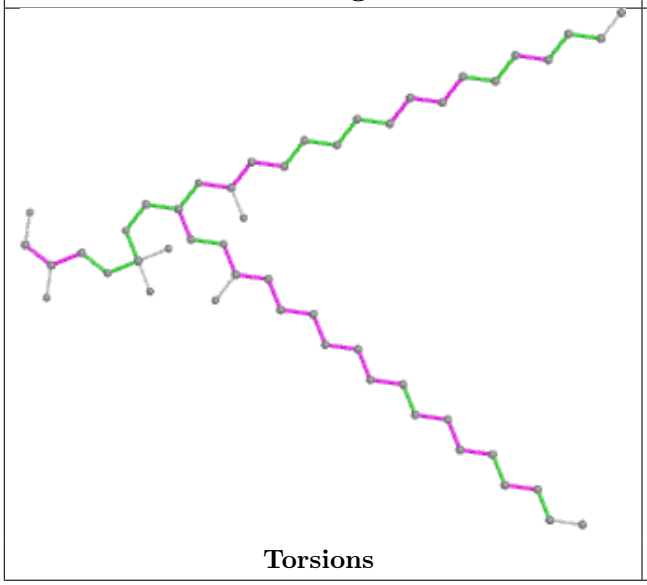
Ligand LHG C 2630



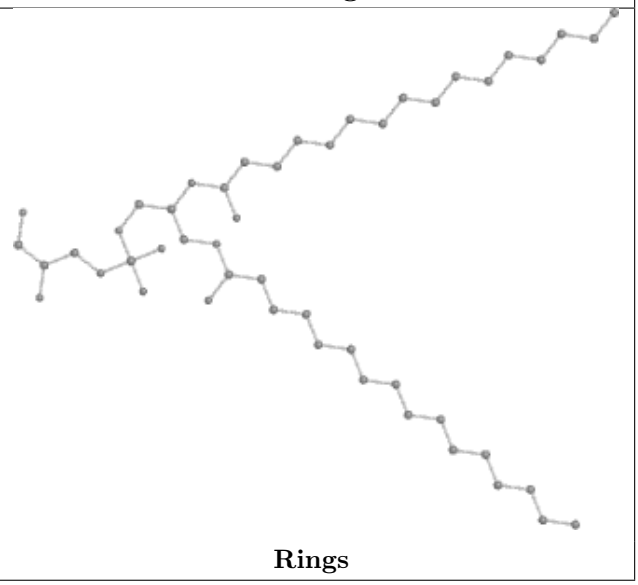
Bond lengths



Bond angles

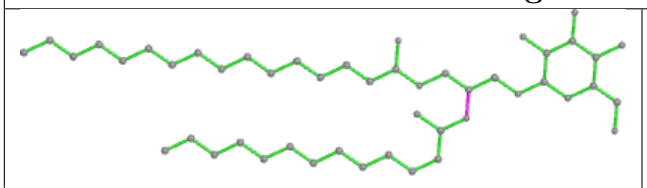


Torsions

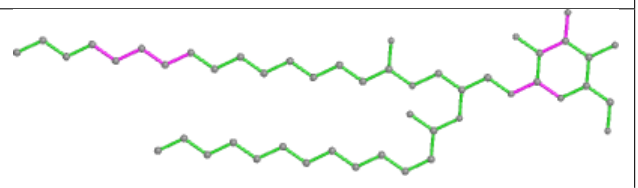


Rings

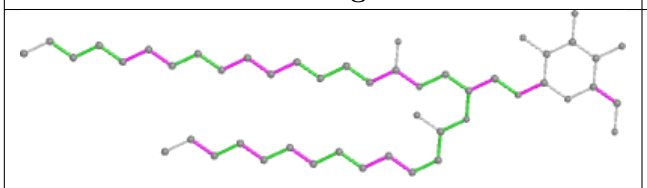
Ligand LMG a 413



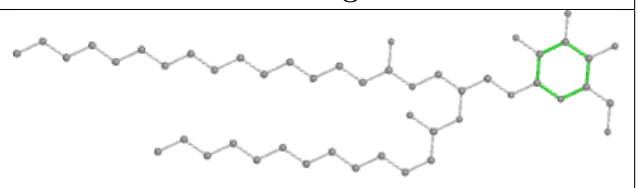
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

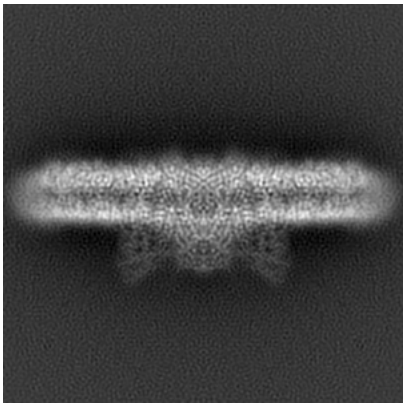
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6742. These allow visual inspection of the internal detail of the map and identification of artifacts.

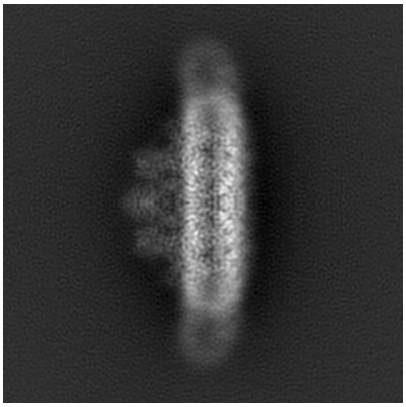
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

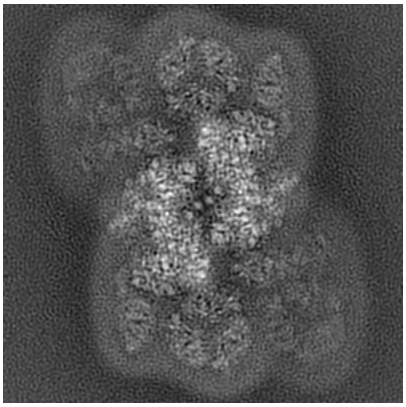
6.1.1 Primary map



X



Y

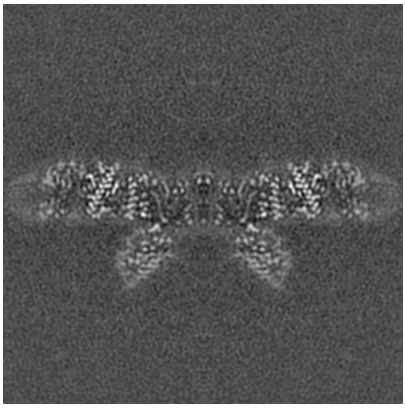


Z

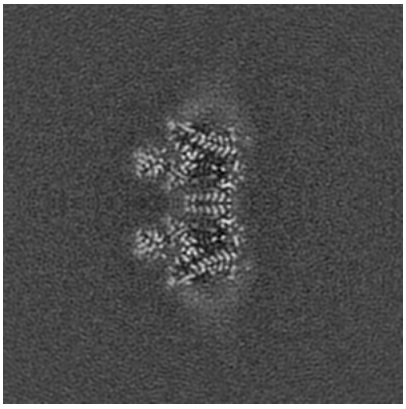
The images above show the map projected in three orthogonal directions.

6.2 Central slices

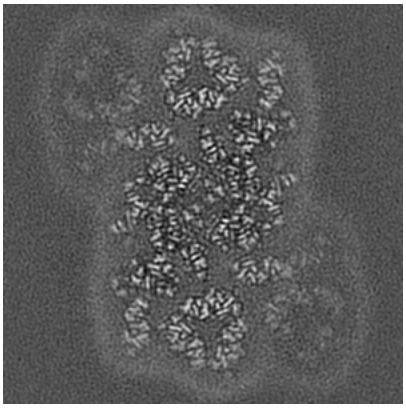
6.2.1 Primary map



X Index: 150



Y Index: 150

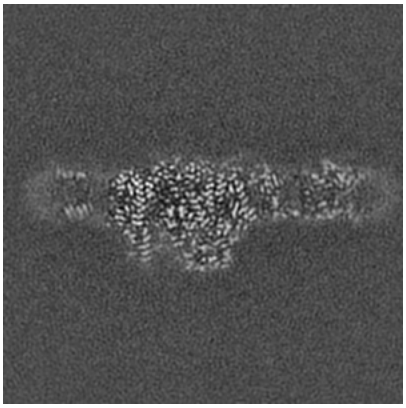


Z Index: 150

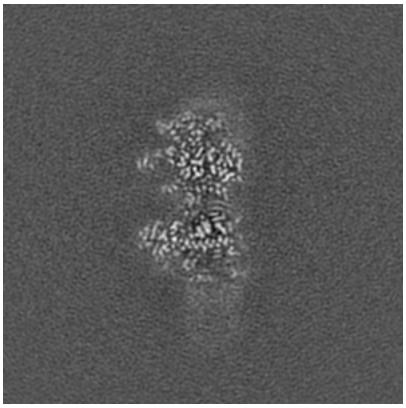
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

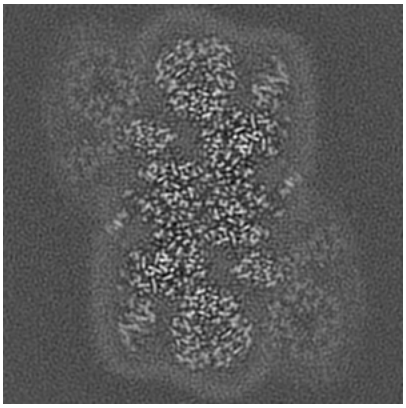
6.3.1 Primary map



X Index: 122



Y Index: 162

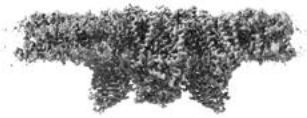


Z Index: 164

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

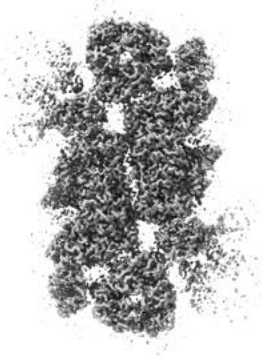
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

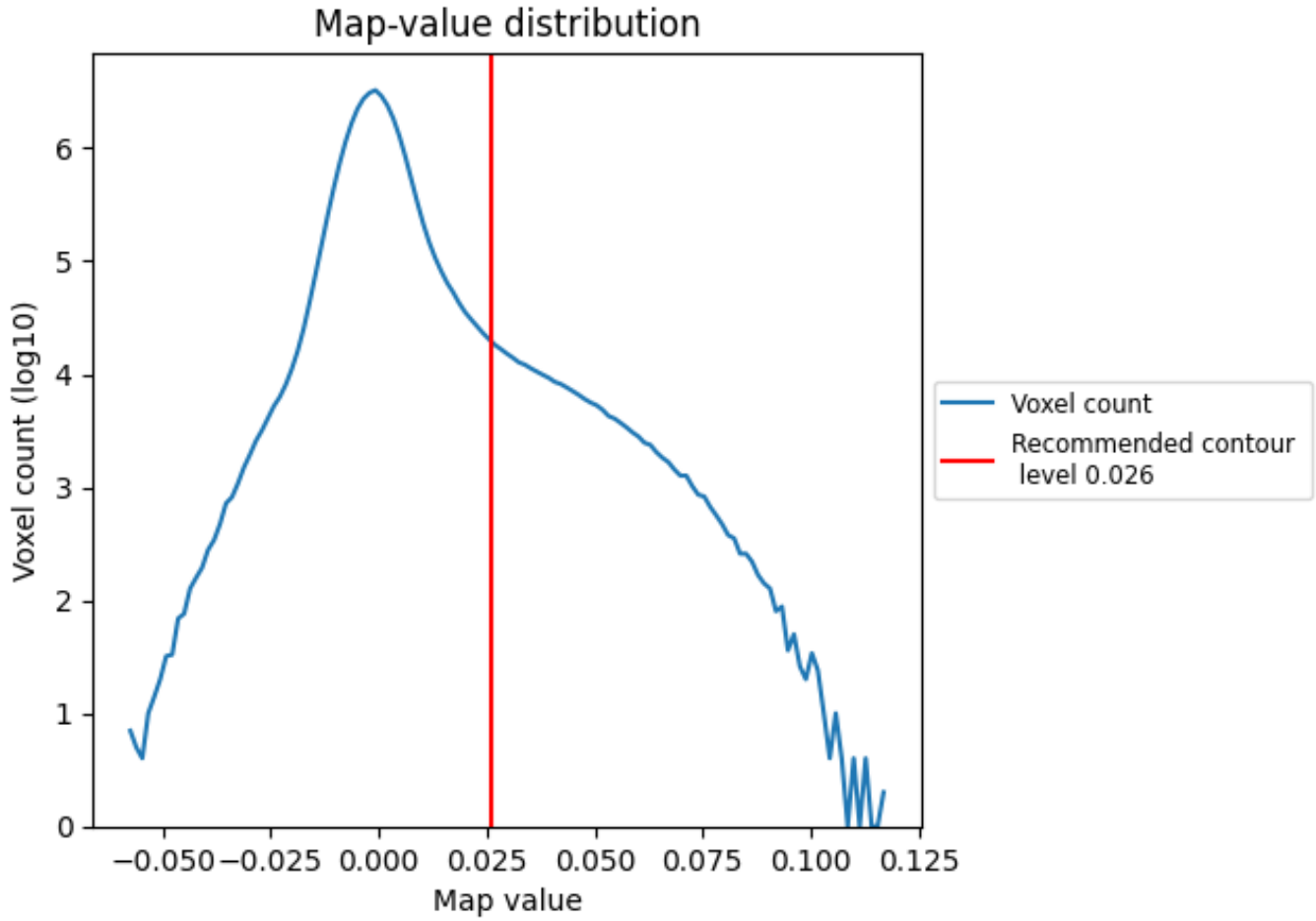
6.5 Mask visualisation (i)

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

7 Map analysis

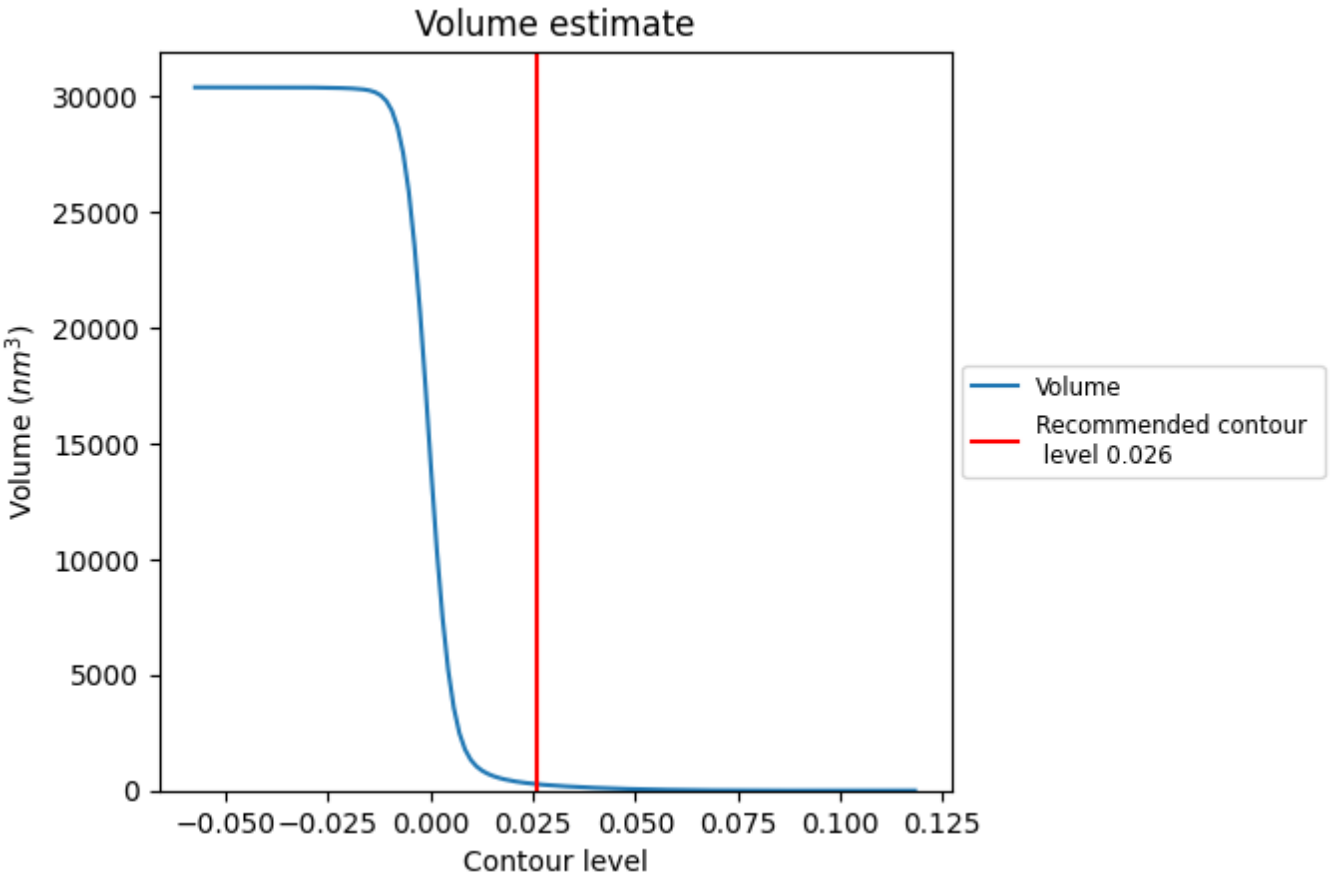
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

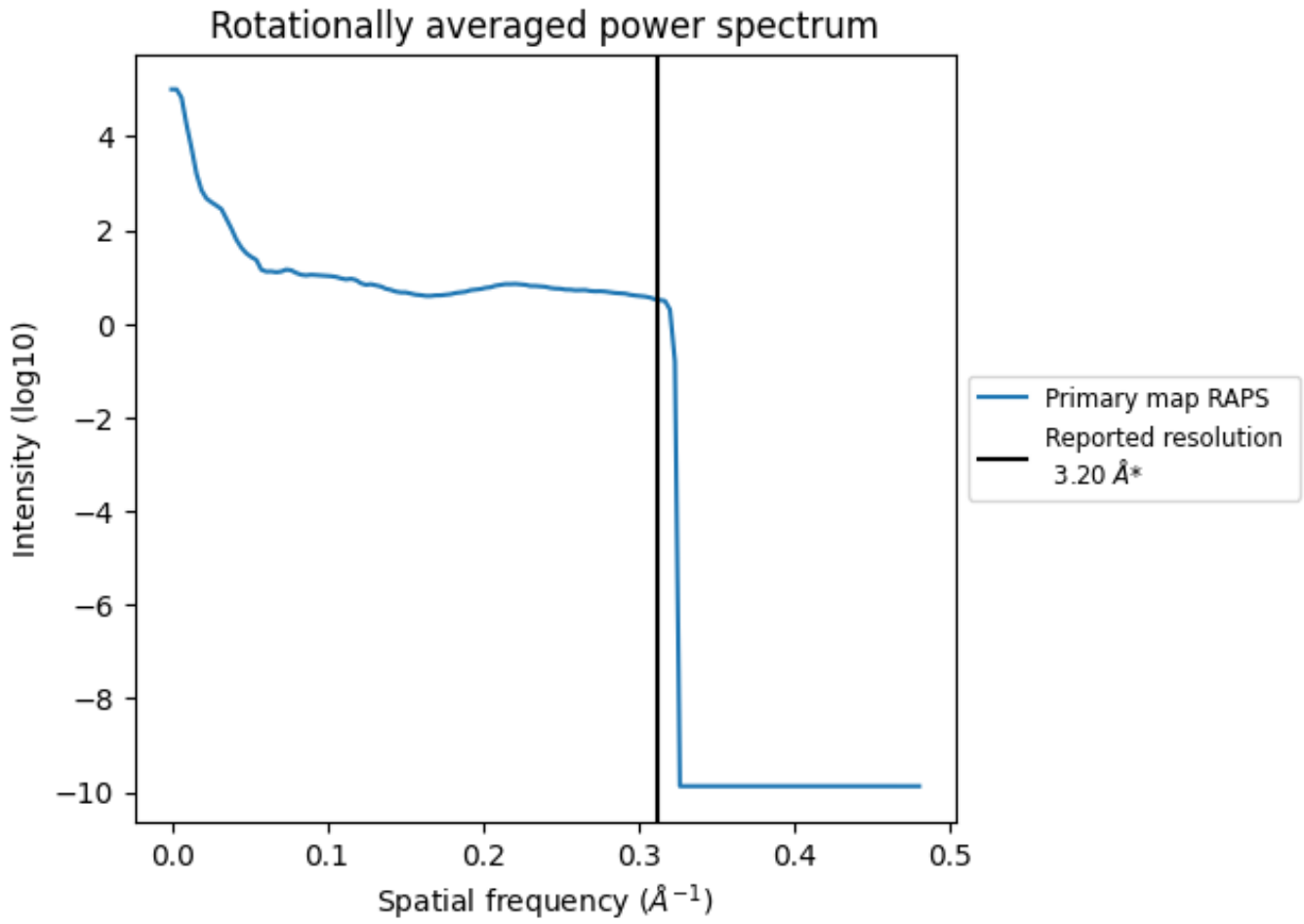
7.2 Volume estimate



The volume at the recommended contour level is 276 nm^3; this corresponds to an approximate mass of 249 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 0.312 Å^{-1}

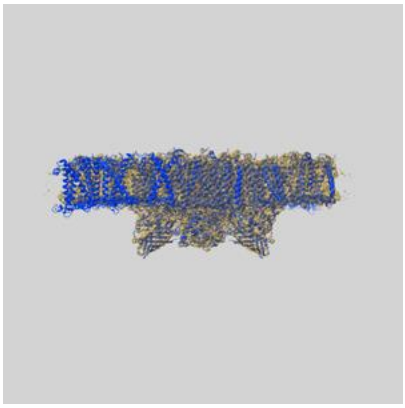
8 Fourier-Shell correlation

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

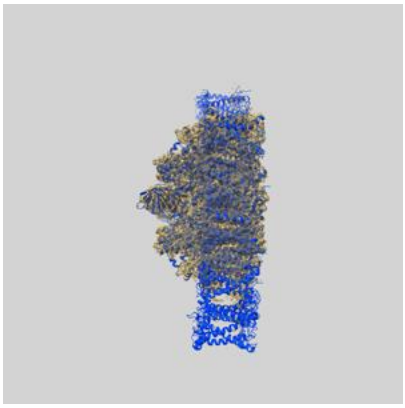
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6742 and PDB model 5XNM. Per-residue inclusion information can be found in section 3 on page 48.

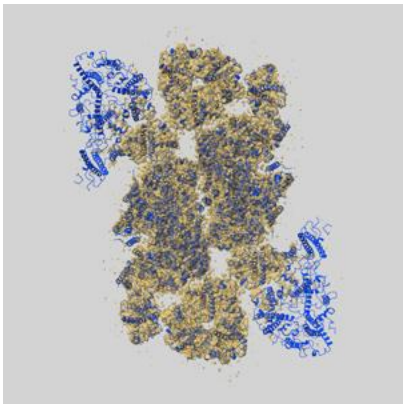
9.1 Map-model overlay



X



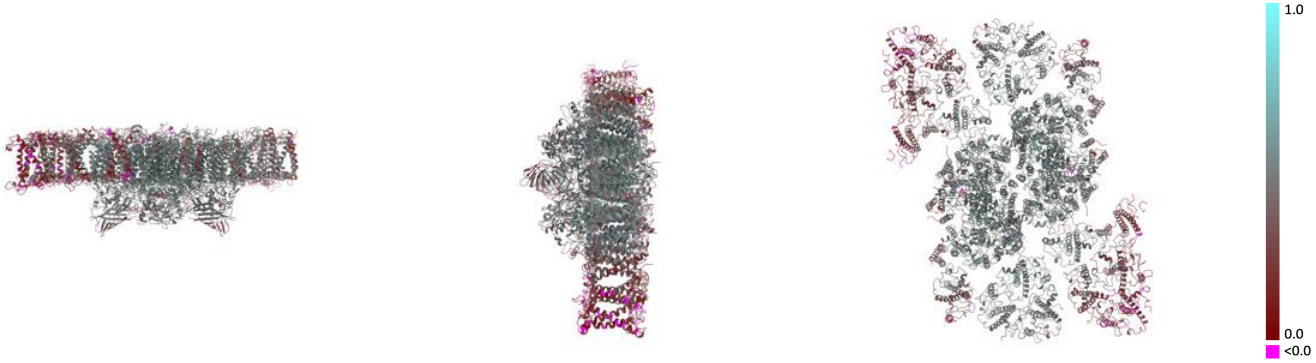
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

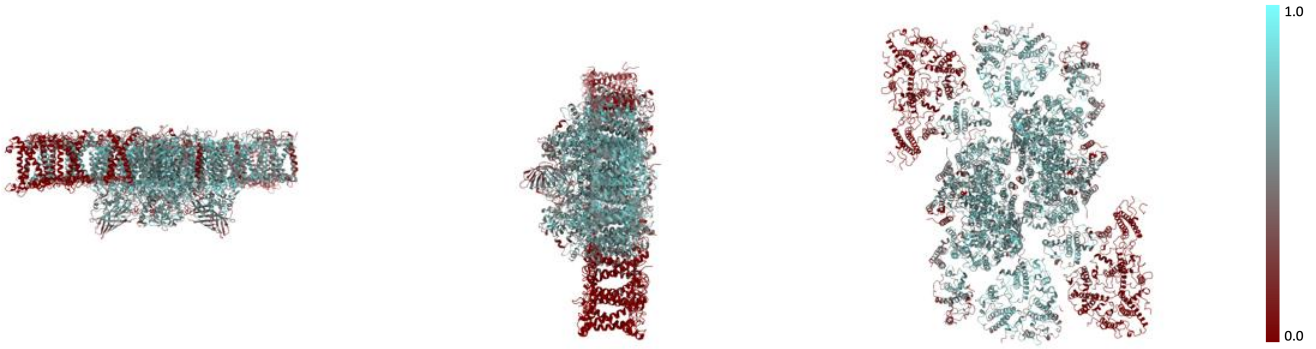
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

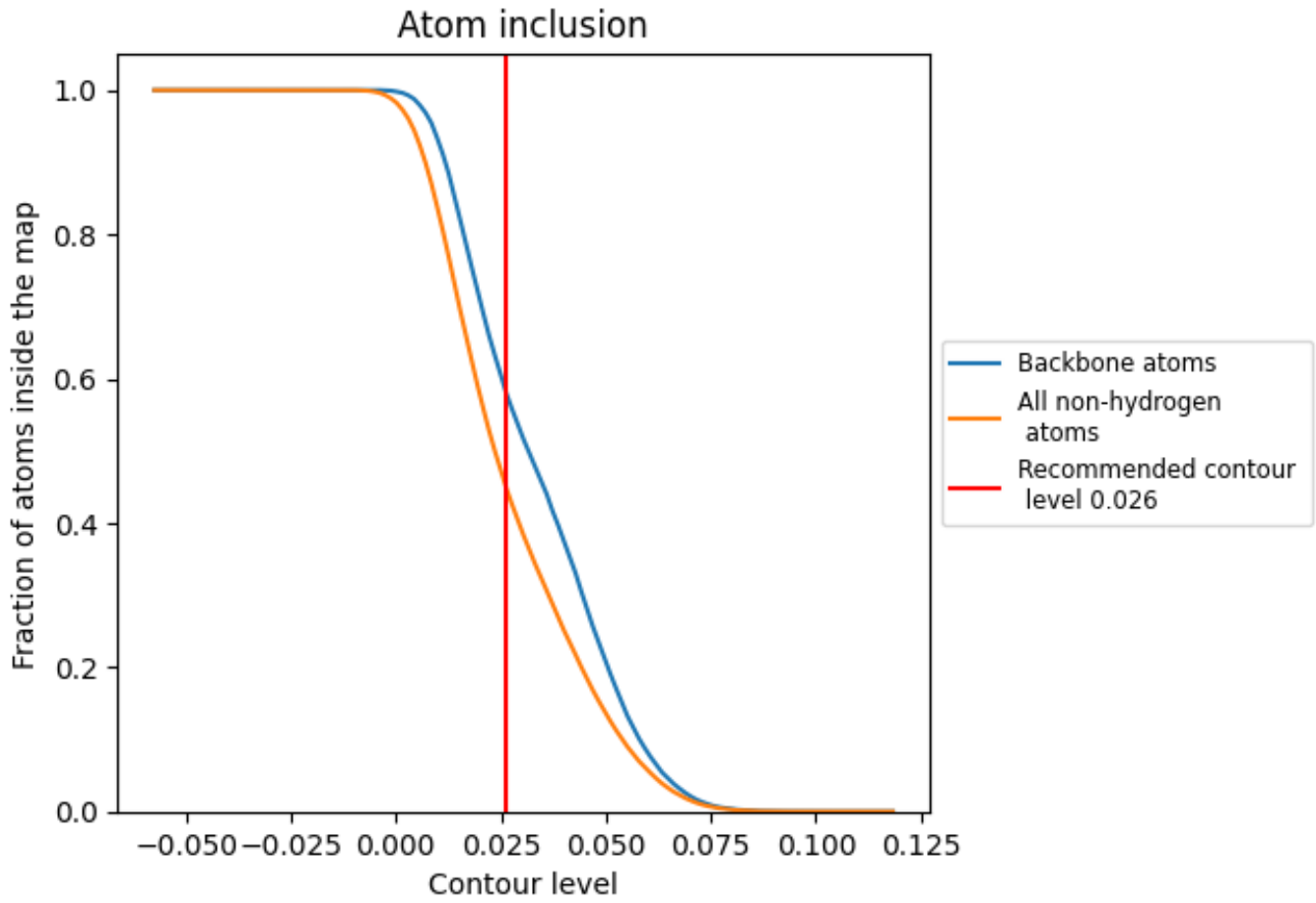
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4538	0.4380
1	0.0861	0.2990
2	0.0028	0.1580
3	0.0402	0.2970
4	0.0388	0.2450
5	0.0869	0.2990
6	0.0028	0.1560
7	0.0387	0.2950
8	0.0393	0.2440
A	0.6452	0.5320
B	0.6120	0.5170
C	0.5923	0.5110
D	0.6601	0.5410
E	0.4807	0.4190
F	0.5236	0.4390
G	0.5320	0.4690
H	0.5594	0.5160
I	0.6667	0.5430
J	0.0909	0.3730
K	0.5828	0.4850
L	0.5944	0.5140
M	0.4784	0.4670
N	0.5507	0.4770
O	0.4202	0.4010
R	0.5309	0.4820
S	0.4282	0.3750
T	0.5101	0.5200
U	0.3422	0.4140
W	0.5763	0.4860
X	0.4197	0.4390
Y	0.6593	0.5350
Z	0.3879	0.4010
a	0.6480	0.5320
b	0.6145	0.5180
c	0.5940	0.5110

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Chain	Atom inclusion	Q-score
d	0.6578	0.5400
e	0.4756	0.4190
f	0.5200	0.4380
g	0.5309	0.4630
h	0.5539	0.5110
i	0.6850	0.5440
j	0.0950	0.3710
k	0.5894	0.4840
l	0.5944	0.5190
m	0.4667	0.4620
n	0.5492	0.4720
o	0.4202	0.4030
r	0.5257	0.4830
s	0.4282	0.3740
t	0.5067	0.5170
u	0.3476	0.4170
w	0.5787	0.4920
x	0.4270	0.4410
y	0.6612	0.5320
z	0.3879	0.3920