Full wwPDB EM Validation Report

Mar 28, 2026 – 11:02 PM UTC

PDB ID	:	7UMH / pdb_00007umh
EMDB ID	:	EMD-26601
Title	:	Energetic robustness to large scale structural dynamics in a photosynthetic supercomplex
Authors	:	Harris, D.; Toporik, H.; Schlau-Cohen, G.S.; Mazor, Y.
Deposited on	:	2022-04-07
Resolution	:	2.60 Å(reported)
Based on initial model	:	6NWA

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

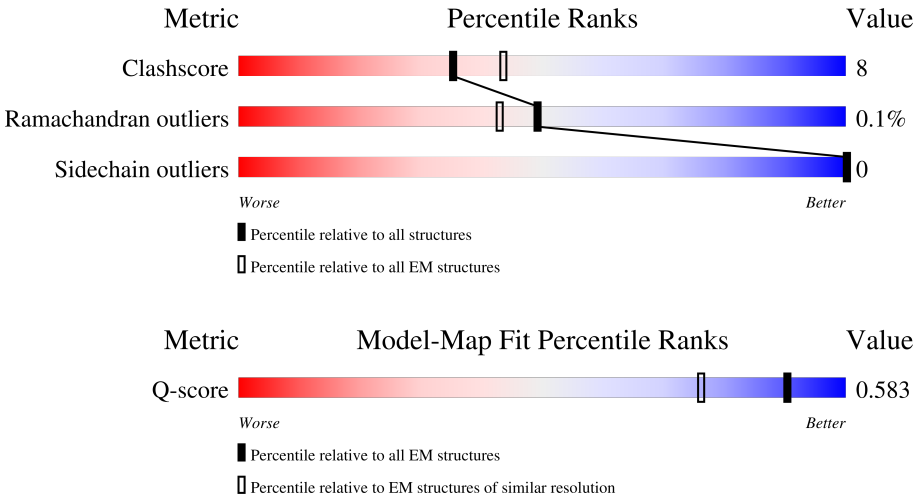
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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

Mol	Chain	Length	Quality of chain
1	A	751	83% 15%
1	H	751	82% 17%
1	a	751	83% 15%
2	B	731	85% 15%

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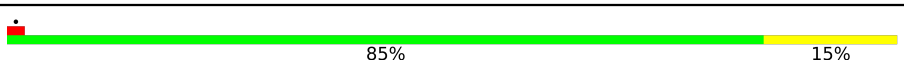
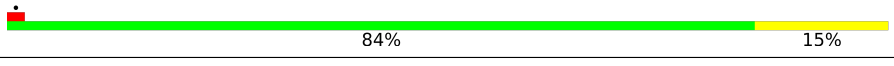
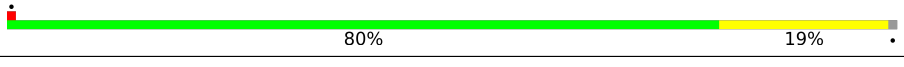
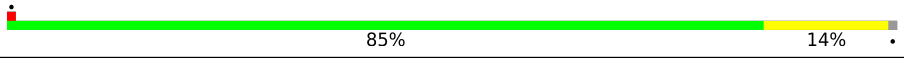
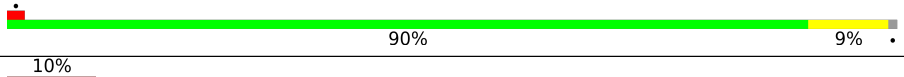
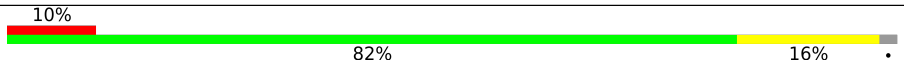
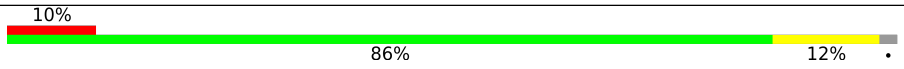
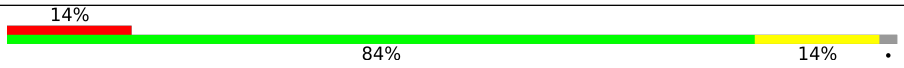
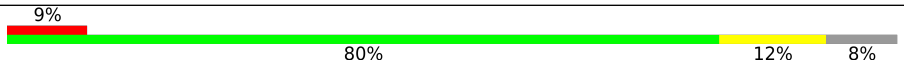
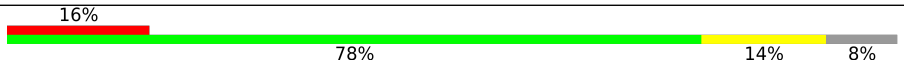
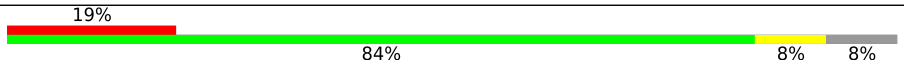
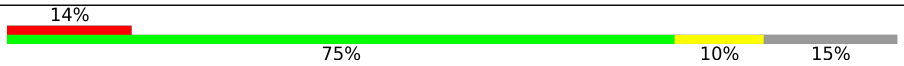
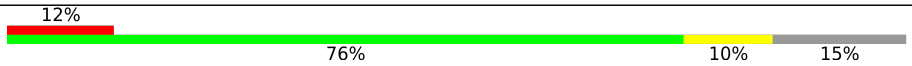
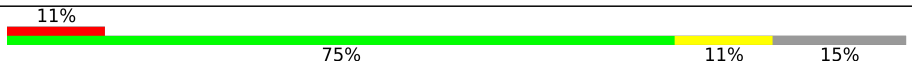
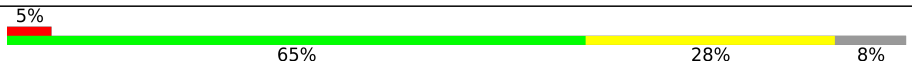
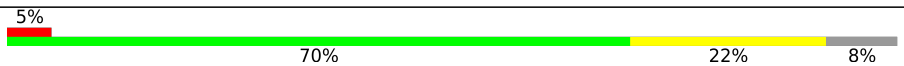
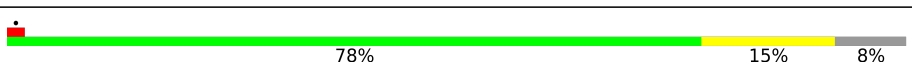
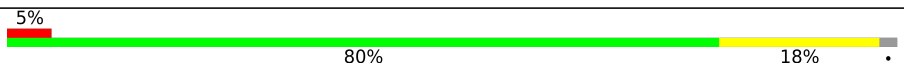
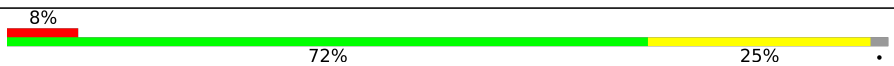
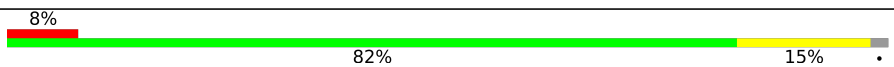
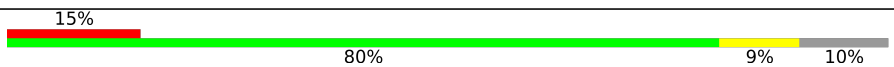
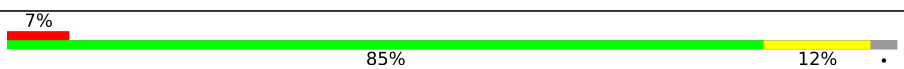
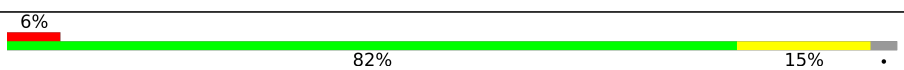
Mol	Chain	Length	Quality of chain
2	G	731	
2	b	731	
3	C	81	
3	N	81	
3	c	81	
4	D	141	
4	P	141	
4	d	141	
5	E	74	
5	O	74	
5	e	74	
6	F	165	
6	Q	165	
6	f	165	
7	I	40	
7	R	40	
7	i	40	
8	J	40	
8	S	40	
8	j	40	
9	K	86	
9	T	86	
9	k	86	
10	L	157	
10	U	157	

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Mol	Chain	Length	Quality of chain
10	l	157	8% 85% 12%
11	M	31	6% 94% 6%
11	V	31	6% 97%
11	m	31	6% 97%
12	W	342	15% 82% 16%
12	X	342	6% 82% 17%
12	Y	342	6% 82% 17%
12	Z	342	84% 15%
12	g	342	8% 82% 15%
12	h	342	29% 85% 11%
12	n	342	12% 82% 17%
12	o	342	7% 89% 11%
12	p	342	7% 86% 14%
12	q	342	5% 82% 16%
12	r	342	9% 82% 15%
12	s	342	6% 83% 15%
12	t	342	15% 85% 14%
12	u	342	7% 85% 14%
12	v	342	26% 84% 13%
12	w	342	85% 13%
12	x	342	9% 85% 12%
12	y	342	29% 82% 15%

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
15	CL0	A	1011	X	-	-	-
15	CL0	H	1011	X	-	-	-
15	CL0	a	1011	X	-	-	-
16	CLA	A	1013	X	-	-	-
16	CLA	A	1022	X	-	-	-
16	CLA	A	1101	X	-	-	-
16	CLA	A	1102	X	-	-	-
16	CLA	A	1103	X	-	-	-
16	CLA	A	1104	X	-	-	-
16	CLA	A	1105	X	-	-	-
16	CLA	A	1106	X	-	-	-
16	CLA	A	1109	X	-	-	-
16	CLA	A	1110	X	-	-	-
16	CLA	A	1111	X	-	-	-
16	CLA	A	1113	X	-	-	-
16	CLA	A	1114	X	-	-	-
16	CLA	A	1115	X	-	-	-
16	CLA	A	1116	X	-	-	-
16	CLA	A	1117	X	-	-	-
16	CLA	A	1119	X	-	-	-
16	CLA	A	1121	X	-	-	-
16	CLA	A	1122	X	-	-	-
16	CLA	A	1124	X	-	-	-
16	CLA	A	1126	X	-	-	-
16	CLA	A	1127	X	-	-	-
16	CLA	A	1128	X	-	-	-
16	CLA	A	1130	X	-	-	-
16	CLA	A	1132	X	-	-	-
16	CLA	A	1133	X	-	-	-
16	CLA	A	1135	X	-	-	-
16	CLA	A	1136	X	-	-	-
16	CLA	A	1137	X	-	-	-
16	CLA	A	1138	X	-	-	-
16	CLA	A	1139	X	-	-	-
16	CLA	A	1140	X	-	-	-
16	CLA	A	1237	X	-	-	-
16	CLA	A	1801	X	-	-	-
16	CLA	B	1012	X	-	-	-
16	CLA	B	1021	X	-	-	-
16	CLA	B	1201	X	-	-	-
16	CLA	B	1202	X	-	-	-
16	CLA	B	1203	X	-	-	-
16	CLA	B	1204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	1205	X	-	-	-
16	CLA	B	1206	X	-	-	-
16	CLA	B	1208	X	-	-	-
16	CLA	B	1209	X	-	-	-
16	CLA	B	1211	X	-	-	-
16	CLA	B	1212	X	-	-	-
16	CLA	B	1213	X	-	-	-
16	CLA	B	1214	X	-	-	-
16	CLA	B	1215	X	-	-	-
16	CLA	B	1220	X	-	-	-
16	CLA	B	1223	X	-	-	-
16	CLA	B	1224	X	-	-	-
16	CLA	B	1227	X	-	-	-
16	CLA	B	1229	X	-	-	-
16	CLA	B	1230	X	-	-	-
16	CLA	B	1231	X	-	-	-
16	CLA	B	1232	X	-	-	-
16	CLA	B	1234	X	-	-	-
16	CLA	B	1235	X	-	-	-
16	CLA	B	1236	X	-	-	-
16	CLA	B	1238	X	-	-	-
16	CLA	B	1240	X	-	-	-
16	CLA	F	1301	X	-	-	-
16	CLA	F	1302	X	-	-	-
16	CLA	G	1012	X	-	-	-
16	CLA	G	1021	X	-	-	-
16	CLA	G	1201	X	-	-	-
16	CLA	G	1202	X	-	-	-
16	CLA	G	1203	X	-	-	-
16	CLA	G	1204	X	-	-	-
16	CLA	G	1205	X	-	-	-
16	CLA	G	1206	X	-	-	-
16	CLA	G	1208	X	-	-	-
16	CLA	G	1209	X	-	-	-
16	CLA	G	1212	X	-	-	-
16	CLA	G	1213	X	-	-	-
16	CLA	G	1214	X	-	-	-
16	CLA	G	1215	X	-	-	-
16	CLA	G	1216	X	-	-	-
16	CLA	G	1220	X	-	-	-
16	CLA	G	1221	X	-	-	-
16	CLA	G	1223	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	G	1224	X	-	-	-
16	CLA	G	1225	X	-	-	-
16	CLA	G	1228	X	-	-	-
16	CLA	G	1229	X	-	-	-
16	CLA	G	1230	X	-	-	-
16	CLA	G	1231	X	-	-	-
16	CLA	G	1232	X	-	-	-
16	CLA	G	1234	X	-	-	-
16	CLA	G	1235	X	-	-	-
16	CLA	G	1238	X	-	-	-
16	CLA	G	1239	X	-	-	-
16	CLA	G	1240	X	-	-	-
16	CLA	H	1013	X	-	-	-
16	CLA	H	1022	X	-	-	-
16	CLA	H	1101	X	-	-	-
16	CLA	H	1102	X	-	-	-
16	CLA	H	1103	X	-	-	-
16	CLA	H	1104	X	-	-	-
16	CLA	H	1105	X	-	-	-
16	CLA	H	1106	X	-	-	-
16	CLA	H	1109	X	-	-	-
16	CLA	H	1110	X	-	-	-
16	CLA	H	1111	X	-	-	-
16	CLA	H	1113	X	-	-	-
16	CLA	H	1114	X	-	-	-
16	CLA	H	1116	X	-	-	-
16	CLA	H	1117	X	-	-	-
16	CLA	H	1119	X	-	-	-
16	CLA	H	1121	X	-	-	-
16	CLA	H	1124	X	-	-	-
16	CLA	H	1126	X	-	-	-
16	CLA	H	1127	X	-	-	-
16	CLA	H	1128	X	-	-	-
16	CLA	H	1131	X	-	-	-
16	CLA	H	1132	X	-	-	-
16	CLA	H	1136	X	-	-	-
16	CLA	H	1137	X	-	-	-
16	CLA	H	1138	X	-	-	-
16	CLA	H	1139	X	-	-	-
16	CLA	H	1140	X	-	-	-
16	CLA	H	1237	X	-	-	-
16	CLA	H	1801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	J	1302	X	-	-	-
16	CLA	K	4002	X	-	-	-
16	CLA	K	4003	X	-	-	-
16	CLA	K	4004	X	-	-	-
16	CLA	L	1503	X	-	-	-
16	CLA	Q	1301	X	-	-	-
16	CLA	Q	1302	X	-	-	-
16	CLA	S	1302	X	-	-	-
16	CLA	T	4002	X	-	-	-
16	CLA	T	4003	X	-	-	-
16	CLA	U	1503	X	-	-	-
16	CLA	W	501	X	-	-	-
16	CLA	W	502	X	-	-	-
16	CLA	W	503	X	-	-	-
16	CLA	W	504	X	-	-	-
16	CLA	W	505	X	-	-	-
16	CLA	W	508	X	-	-	-
16	CLA	W	509	X	-	-	-
16	CLA	W	511	X	-	-	-
16	CLA	W	512	X	-	-	-
16	CLA	W	514	X	-	-	-
16	CLA	W	515	X	-	-	-
16	CLA	W	517	X	-	-	-
16	CLA	X	502	X	-	-	-
16	CLA	X	505	X	-	-	-
16	CLA	X	506	X	-	-	-
16	CLA	X	508	X	-	-	-
16	CLA	X	509	X	-	-	-
16	CLA	X	511	X	-	-	-
16	CLA	X	514	X	-	-	-
16	CLA	X	515	X	-	-	-
16	CLA	Y	501	X	-	-	-
16	CLA	Y	502	X	-	-	-
16	CLA	Y	503	X	-	-	-
16	CLA	Y	504	X	-	-	-
16	CLA	Y	505	X	-	-	-
16	CLA	Y	508	X	-	-	-
16	CLA	Y	509	X	-	-	-
16	CLA	Y	511	X	-	-	-
16	CLA	Y	512	X	-	-	-
16	CLA	Y	514	X	-	-	-
16	CLA	Y	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	Z	501	X	-	-	-
16	CLA	Z	502	X	-	-	-
16	CLA	Z	503	X	-	-	-
16	CLA	Z	504	X	-	-	-
16	CLA	Z	505	X	-	-	-
16	CLA	Z	507	X	-	-	-
16	CLA	Z	508	X	-	-	-
16	CLA	Z	509	X	-	-	-
16	CLA	Z	511	X	-	-	-
16	CLA	Z	512	X	-	-	-
16	CLA	Z	514	X	-	-	-
16	CLA	Z	515	X	-	-	-
16	CLA	Z	516	X	-	-	-
16	CLA	Z	517	X	-	-	-
16	CLA	a	1013	X	-	-	-
16	CLA	a	1022	X	-	-	-
16	CLA	a	1101	X	-	-	-
16	CLA	a	1102	X	-	-	-
16	CLA	a	1103	X	-	-	-
16	CLA	a	1104	X	-	-	-
16	CLA	a	1105	X	-	-	-
16	CLA	a	1106	X	-	-	-
16	CLA	a	1109	X	-	-	-
16	CLA	a	1110	X	-	-	-
16	CLA	a	1111	X	-	-	-
16	CLA	a	1113	X	-	-	-
16	CLA	a	1114	X	-	-	-
16	CLA	a	1115	X	-	-	-
16	CLA	a	1116	X	-	-	-
16	CLA	a	1117	X	-	-	-
16	CLA	a	1119	X	-	-	-
16	CLA	a	1121	X	-	-	-
16	CLA	a	1124	X	-	-	-
16	CLA	a	1126	X	-	-	-
16	CLA	a	1127	X	-	-	-
16	CLA	a	1128	X	-	-	-
16	CLA	a	1132	X	-	-	-
16	CLA	a	1135	X	-	-	-
16	CLA	a	1136	X	-	-	-
16	CLA	a	1137	X	-	-	-
16	CLA	a	1138	X	-	-	-
16	CLA	a	1139	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	a	1237	X	-	-	-
16	CLA	a	1801	X	-	-	-
16	CLA	b	1012	X	-	-	-
16	CLA	b	1021	X	-	-	-
16	CLA	b	1201	X	-	-	-
16	CLA	b	1202	X	-	-	-
16	CLA	b	1203	X	-	-	-
16	CLA	b	1204	X	-	-	-
16	CLA	b	1205	X	-	-	-
16	CLA	b	1206	X	-	-	-
16	CLA	b	1208	X	-	-	-
16	CLA	b	1209	X	-	-	-
16	CLA	b	1210	X	-	-	-
16	CLA	b	1211	X	-	-	-
16	CLA	b	1212	X	-	-	-
16	CLA	b	1213	X	-	-	-
16	CLA	b	1214	X	-	-	-
16	CLA	b	1216	X	-	-	-
16	CLA	b	1221	X	-	-	-
16	CLA	b	1223	X	-	-	-
16	CLA	b	1224	X	-	-	-
16	CLA	b	1226	X	-	-	-
16	CLA	b	1227	X	-	-	-
16	CLA	b	1228	X	-	-	-
16	CLA	b	1229	X	-	-	-
16	CLA	b	1231	X	-	-	-
16	CLA	b	1232	X	-	-	-
16	CLA	b	1234	X	-	-	-
16	CLA	b	1235	X	-	-	-
16	CLA	b	1238	X	-	-	-
16	CLA	b	1240	X	-	-	-
16	CLA	f	1301	X	-	-	-
16	CLA	f	1302	X	-	-	-
16	CLA	g	502	X	-	-	-
16	CLA	g	504	X	-	-	-
16	CLA	g	505	X	-	-	-
16	CLA	g	507	X	-	-	-
16	CLA	g	508	X	-	-	-
16	CLA	g	509	X	-	-	-
16	CLA	g	511	X	-	-	-
16	CLA	g	512	X	-	-	-
16	CLA	g	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	g	515	X	-	-	-
16	CLA	g	516	X	-	-	-
16	CLA	h	502	X	-	-	-
16	CLA	h	503	X	-	-	-
16	CLA	h	506	X	-	-	-
16	CLA	h	507	X	-	-	-
16	CLA	h	508	X	-	-	-
16	CLA	h	509	X	-	-	-
16	CLA	h	511	X	-	-	-
16	CLA	h	513	X	-	-	-
16	CLA	h	515	X	-	-	-
16	CLA	h	516	X	-	-	-
16	CLA	h	517	X	-	-	-
16	CLA	k	4002	X	-	-	-
16	CLA	k	4003	X	-	-	-
16	CLA	k	4004	X	-	-	-
16	CLA	l	1503	X	-	-	-
16	CLA	n	501	X	-	-	-
16	CLA	n	502	X	-	-	-
16	CLA	n	503	X	-	-	-
16	CLA	n	505	X	-	-	-
16	CLA	n	507	X	-	-	-
16	CLA	n	508	X	-	-	-
16	CLA	n	509	X	-	-	-
16	CLA	n	512	X	-	-	-
16	CLA	n	514	X	-	-	-
16	CLA	n	515	X	-	-	-
16	CLA	n	517	X	-	-	-
16	CLA	o	502	X	-	-	-
16	CLA	o	505	X	-	-	-
16	CLA	o	506	X	-	-	-
16	CLA	o	508	X	-	-	-
16	CLA	o	509	X	-	-	-
16	CLA	o	511	X	-	-	-
16	CLA	o	512	X	-	-	-
16	CLA	o	514	X	-	-	-
16	CLA	o	515	X	-	-	-
16	CLA	p	501	X	-	-	-
16	CLA	p	502	X	-	-	-
16	CLA	p	503	X	-	-	-
16	CLA	p	508	X	-	-	-
16	CLA	p	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	p	511	X	-	-	-
16	CLA	p	512	X	-	-	-
16	CLA	p	514	X	-	-	-
16	CLA	p	515	X	-	-	-
16	CLA	p	516	X	-	-	-
16	CLA	q	501	X	-	-	-
16	CLA	q	502	X	-	-	-
16	CLA	q	503	X	-	-	-
16	CLA	q	504	X	-	-	-
16	CLA	q	505	X	-	-	-
16	CLA	q	506	X	-	-	-
16	CLA	q	507	X	-	-	-
16	CLA	q	508	X	-	-	-
16	CLA	q	509	X	-	-	-
16	CLA	q	512	X	-	-	-
16	CLA	q	514	X	-	-	-
16	CLA	q	515	X	-	-	-
16	CLA	q	516	X	-	-	-
16	CLA	r	501	X	-	-	-
16	CLA	r	502	X	-	-	-
16	CLA	r	504	X	-	-	-
16	CLA	r	507	X	-	-	-
16	CLA	r	508	X	-	-	-
16	CLA	r	511	X	-	-	-
16	CLA	r	512	X	-	-	-
16	CLA	r	514	X	-	-	-
16	CLA	r	515	X	-	-	-
16	CLA	r	516	X	-	-	-
16	CLA	s	501	X	-	-	-
16	CLA	s	502	X	-	-	-
16	CLA	s	503	X	-	-	-
16	CLA	s	504	X	-	-	-
16	CLA	s	505	X	-	-	-
16	CLA	s	508	X	-	-	-
16	CLA	s	509	X	-	-	-
16	CLA	s	511	X	-	-	-
16	CLA	s	512	X	-	-	-
16	CLA	s	514	X	-	-	-
16	CLA	s	515	X	-	-	-
16	CLA	t	501	X	-	-	-
16	CLA	t	502	X	-	-	-
16	CLA	t	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	t	504	X	-	-	-
16	CLA	t	506	X	-	-	-
16	CLA	t	507	X	-	-	-
16	CLA	t	508	X	-	-	-
16	CLA	t	509	X	-	-	-
16	CLA	t	511	X	-	-	-
16	CLA	t	512	X	-	-	-
16	CLA	t	514	X	-	-	-
16	CLA	t	515	X	-	-	-
16	CLA	t	516	X	-	-	-
16	CLA	t	517	X	-	-	-
16	CLA	u	502	X	-	-	-
16	CLA	u	505	X	-	-	-
16	CLA	u	506	X	-	-	-
16	CLA	u	507	X	-	-	-
16	CLA	u	508	X	-	-	-
16	CLA	u	509	X	-	-	-
16	CLA	u	511	X	-	-	-
16	CLA	u	514	X	-	-	-
16	CLA	u	516	X	-	-	-
16	CLA	v	502	X	-	-	-
16	CLA	v	503	X	-	-	-
16	CLA	v	504	X	-	-	-
16	CLA	v	506	X	-	-	-
16	CLA	v	508	X	-	-	-
16	CLA	v	511	X	-	-	-
16	CLA	v	513	X	-	-	-
16	CLA	v	514	X	-	-	-
16	CLA	v	515	X	-	-	-
16	CLA	v	516	X	-	-	-
16	CLA	v	517	X	-	-	-
16	CLA	w	501	X	-	-	-
16	CLA	w	502	X	-	-	-
16	CLA	w	503	X	-	-	-
16	CLA	w	504	X	-	-	-
16	CLA	w	507	X	-	-	-
16	CLA	w	508	X	-	-	-
16	CLA	w	509	X	-	-	-
16	CLA	w	511	X	-	-	-
16	CLA	w	512	X	-	-	-
16	CLA	w	514	X	-	-	-
16	CLA	w	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	w	516	X	-	-	-
16	CLA	w	517	X	-	-	-
16	CLA	x	502	X	-	-	-
16	CLA	x	504	X	-	-	-
16	CLA	x	505	X	-	-	-
16	CLA	x	507	X	-	-	-
16	CLA	x	508	X	-	-	-
16	CLA	x	509	X	-	-	-
16	CLA	x	514	X	-	-	-
16	CLA	x	515	X	-	-	-
16	CLA	x	516	X	-	-	-
16	CLA	y	501	X	-	-	-
16	CLA	y	502	X	-	-	-
16	CLA	y	503	X	-	-	-
16	CLA	y	505	X	-	-	-
16	CLA	y	506	X	-	-	-
16	CLA	y	508	X	-	-	-
16	CLA	y	509	X	-	-	-
16	CLA	y	511	X	-	-	-
16	CLA	y	513	X	-	-	-
16	CLA	y	515	X	-	-	-
16	CLA	y	516	X	-	-	-
16	CLA	y	517	X	-	-	-

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 140516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	H	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	a	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	G	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		
2	b	730	Total	C	N	O	S	0	0
			5775	3801	968	991	15		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		
4	d	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			537	337	95	105		
5	O	68	Total	C	N	O	0	0
			537	337	95	105		
5	e	68	Total	C	N	O	0	0
			537	337	95	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	Q	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	f	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	R	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	i	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	52	3		
8	S	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	T	77	Total	C	N	O	S	0	0
			538	353	89	92	4		
9	k	77	Total	C	N	O	S	0	0
			538	353	89	92	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	U	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		
10	l	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		

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

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

- Molecule 12 is a protein called Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	X	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	Y	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		

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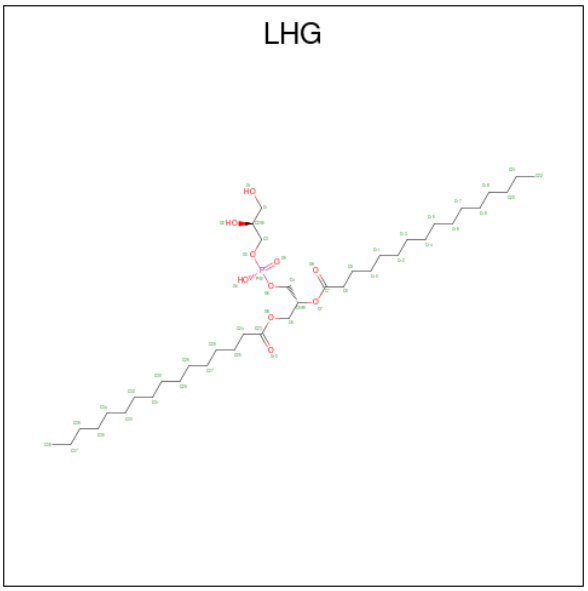
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	g	333	Total	C	N	O	S	0	0
			2573	1714	420	434	5		
12	h	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	n	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	o	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	p	340	Total	C	N	O	S	0	0
			2622	1744	428	445	5		
12	q	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	r	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	s	339	Total	C	N	O	S	0	0
			2617	1741	427	444	5		
12	t	338	Total	C	N	O	S	0	0
			2601	1732	422	442	5		
12	u	339	Total	C	N	O	S	0	0
			2622	1744	428	446	4		
12	v	330	Total	C	N	O	S	0	0
			2538	1692	412	429	5		
12	w	337	Total	C	N	O	S	0	0
			2603	1734	425	439	5		
12	x	332	Total	C	N	O	S	0	0
			2566	1709	419	433	5		
12	y	330	Total	C	N	O	S	0	0
			2532	1689	409	429	5		

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			43	32	10	1	
13	A	1	Total	C	O	P	0
			26	15	10	1	
13	B	1	Total	C	O	P	0
			38	27	10	1	
13	G	1	Total	C	O	P	0
			38	27	10	1	
13	H	1	Total	C	O	P	0
			43	32	10	1	
13	H	1	Total	C	O	P	0
			26	15	10	1	
13	I	1	Total	C	O	P	0
			40	29	10	1	
13	R	1	Total	C	O	P	0
			40	29	10	1	
13	X	1	Total	C	O	P	0
			27	16	10	1	
13	Y	1	Total	C	O	P	0
			32	21	10	1	
13	a	1	Total	C	O	P	0
			43	32	10	1	
13	a	1	Total	C	O	P	0
			26	15	10	1	
13	b	1	Total	C	O	P	0
			38	27	10	1	
13	g	1	Total	C	O	P	0
			31	20	10	1	

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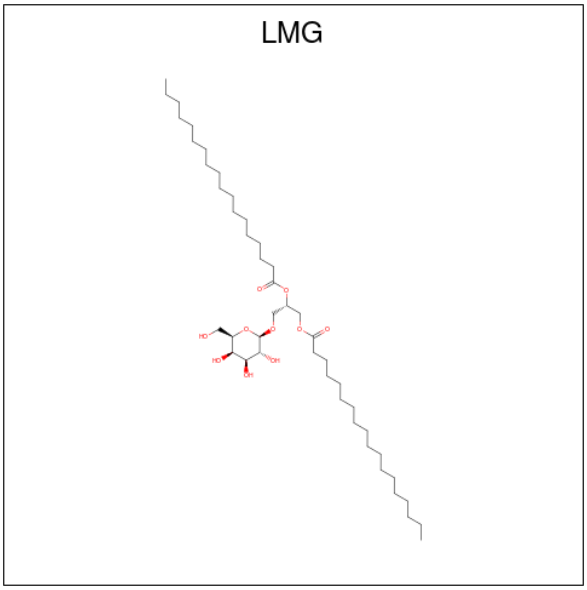
Mol	Chain	Residues	Atoms				AltConf
13	i	1	Total	C	O	P	0
			40	29	10	1	
13	o	1	Total	C	O	P	0
			27	16	10	1	
13	p	1	Total	C	O	P	0
			32	21	10	1	
13	r	1	Total	C	O	P	0
			31	20	10	1	
13	s	1	Total	C	O	P	0
			32	21	10	1	
13	u	1	Total	C	O	P	0
			27	16	10	1	
13	x	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 14 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			38	28	10	
14	A	1	Total	C	O	0
			46	36	10	
14	A	1	Total	C	O	0
			32	22	10	
14	B	1	Total	C	O	0
			43	33	10	

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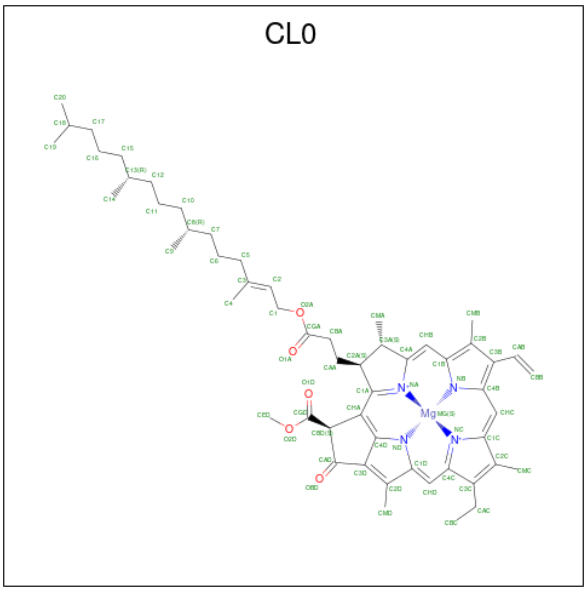
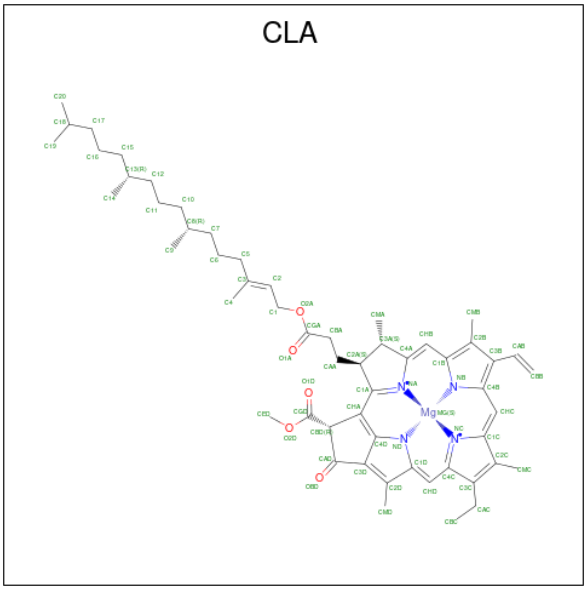
Mol	Chain	Residues	Atoms			AltConf
14	F	1	Total	C	O	0
			27	17	10	
14	G	1	Total	C	O	0
			43	33	10	
14	H	1	Total	C	O	0
			38	28	10	
14	H	1	Total	C	O	0
			46	36	10	
14	H	1	Total	C	O	0
			32	22	10	
14	Q	1	Total	C	O	0
			27	17	10	
14	a	1	Total	C	O	0
			38	28	10	
14	a	1	Total	C	O	0
			46	36	10	
14	a	1	Total	C	O	0
			32	22	10	
14	b	1	Total	C	O	0
			43	33	10	
14	f	1	Total	C	O	0
			27	17	10	

- Molecule 15 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
16	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	S	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
16	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	T	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	Y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	h	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	j	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
16	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
16	k	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	n	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	o	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	t	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	t	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	u	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	v	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
16	w	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	w	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	x	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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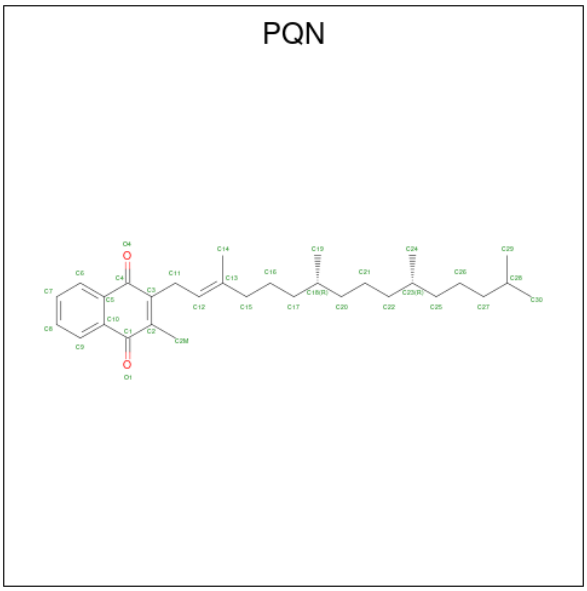
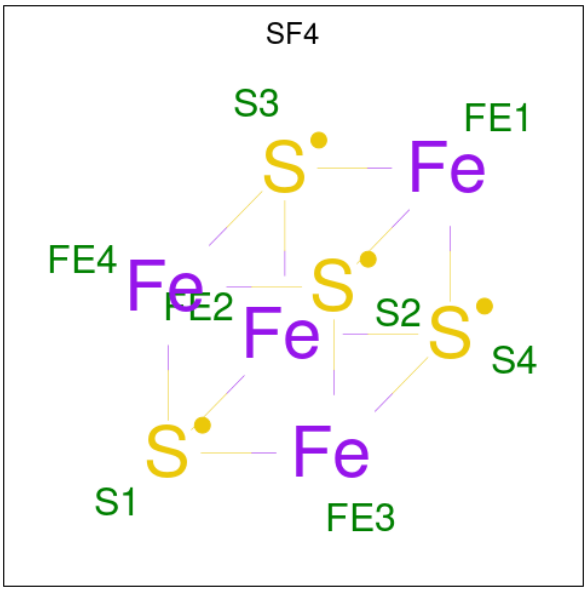
Mol	Chain	Residues	Atoms					AltConf
16	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
16	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	y	1	Total	C	Mg	N	O	0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

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



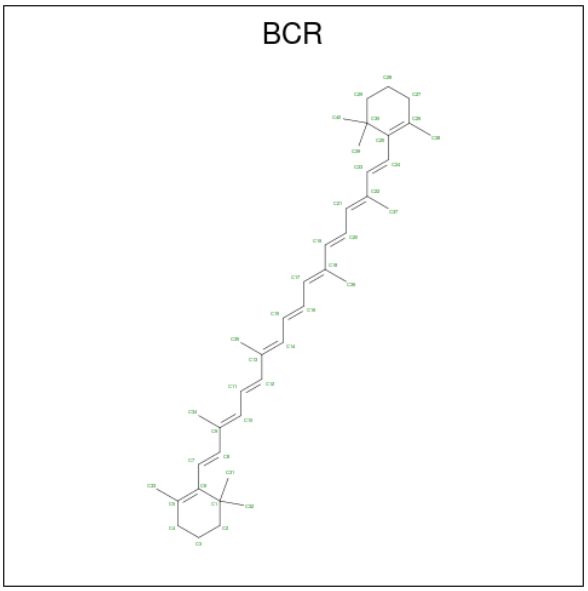
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C O 33 31 2	0
17	B	1	Total C O 33 31 2	0
17	G	1	Total C O 33 31 2	0
17	H	1	Total C O 33 31 2	0
17	a	1	Total C O 33 31 2	0
17	b	1	Total C O 33 31 2	0

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total Fe S 8 4 4	0
18	C	1	Total Fe S 8 4 4	0
18	C	1	Total Fe S 8 4 4	0
18	H	1	Total Fe S 8 4 4	0
18	N	1	Total Fe S 8 4 4	0
18	N	1	Total Fe S 8 4 4	0
18	a	1	Total Fe S 8 4 4	0
18	c	1	Total Fe S 8 4 4	0
18	c	1	Total Fe S 8 4 4	0

- Molecule 19 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	A	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 30 30	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	B	1	Total C 40 40	0
19	F	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C 30 30	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	G	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	H	1	Total C 40 40	0
19	I	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	J	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	K	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	L	1	Total C 40 40	0
19	Q	1	Total C 40 40	0
19	R	1	Total C 40 40	0
19	S	1	Total C 40 40	0
19	S	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	S	1	Total C 40 40	0
19	T	1	Total C 40 40	0
19	T	1	Total C 40 40	0
19	U	1	Total C 40 40	0
19	U	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	W	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	X	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Y	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	Z	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	a	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 30 30	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	b	1	Total C 40 40	0
19	f	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	g	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	h	1	Total C 40 40	0
19	i	1	Total C 40 40	0
19	j	1	Total C 40 40	0
19	j	1	Total C 40 40	0
19	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	k	1	Total C 40 40	0
19	k	1	Total C 40 40	0
19	l	1	Total C 40 40	0
19	l	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	n	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	o	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	p	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	q	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0
19	r	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
19	r	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	s	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	t	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	u	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	v	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	w	1	Total C 40 40	0
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0
19	x	1	Total C 40 40	0

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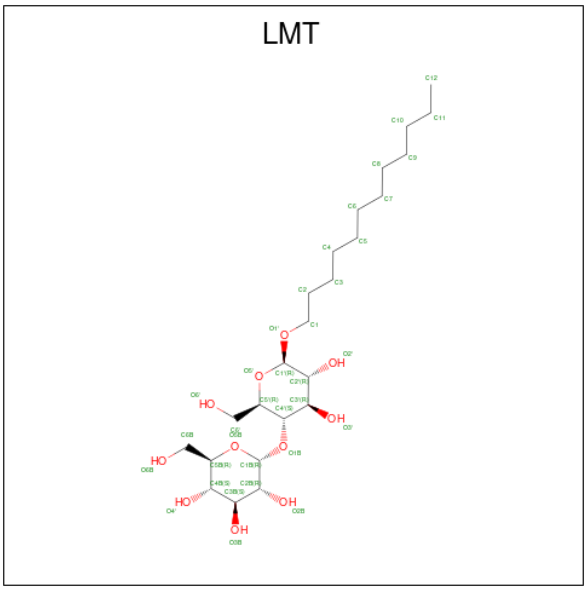
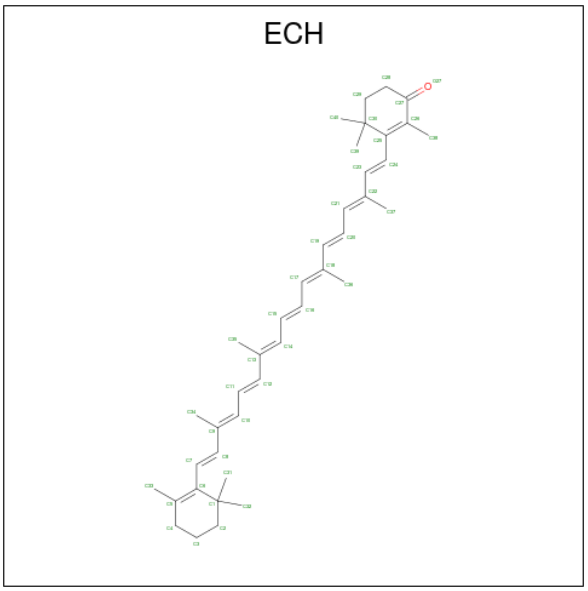
Mol	Chain	Residues	Atoms	AltConf
19	x	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0
19	y	1	Total C 40 40	0

- Molecule 20 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total C O 35 24 11	0
20	H	1	Total C O 35 24 11	0
20	L	1	Total C O 35 24 11	0
20	U	1	Total C O 35 24 11	0
20	a	1	Total C O 35 24 11	0
20	l	1	Total C O 35 24 11	0

- Molecule 21 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).

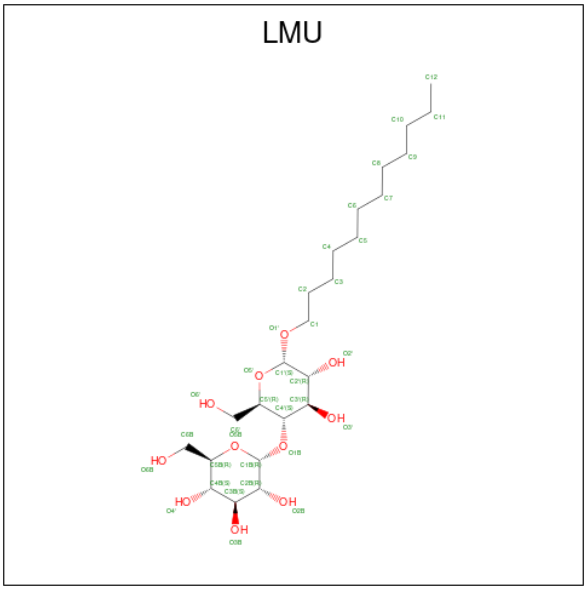


Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C O 41 40 1	0
21	G	1	Total C O 41 40 1	0
21	I	1	Total C O 41 40 1	0
21	M	1	Total C O 41 40 1	0
21	R	1	Total C O 41 40 1	0
21	V	1	Total C O 41 40 1	0
21	b	1	Total C O 41 40 1	0
21	i	1	Total C O 41 40 1	0
21	m	1	Total C O 41 40 1	0

- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

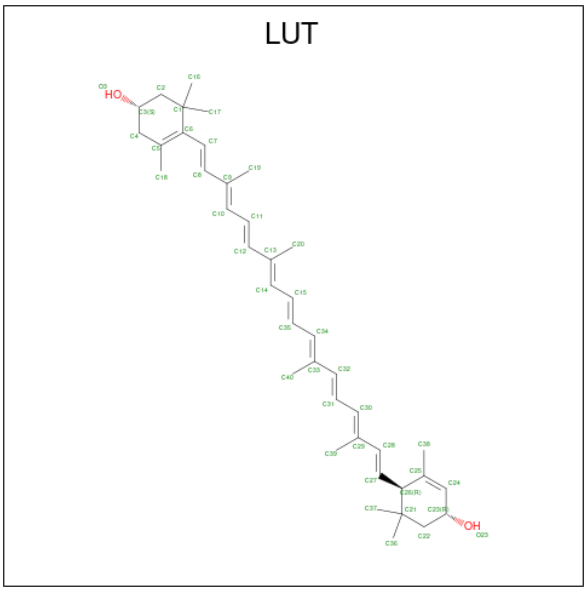
Mol	Chain	Residues	Atoms	AltConf
22	L	1	Total Ca 1 1	0
22	U	1	Total Ca 1 1	0
22	l	1	Total Ca 1 1	0

- Molecule 23 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
23	Y	1	Total	C	O	0
			35	24	11	
23	Z	1	Total	C	O	0
			35	24	11	
23	g	1	Total	C	O	0
			35	24	11	
23	p	1	Total	C	O	0
			35	24	11	
23	q	1	Total	C	O	0
			35	24	11	
23	r	1	Total	C	O	0
			35	24	11	
23	s	1	Total	C	O	0
			35	24	11	
23	w	1	Total	C	O	0
			35	24	11	
23	x	1	Total	C	O	0
			35	24	11	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
24	Z	1	Total C O 42 40 2	0
24	q	1	Total C O 42 40 2	0
24	w	1	Total C O 42 40 2	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	AltConf
25	A	56	Total O 56 56	0
25	B	52	Total O 52 52	0
25	C	7	Total O 7 7	0
25	D	3	Total O 3 3	0
25	E	4	Total O 4 4	0
25	F	3	Total O 3 3	0
25	G	55	Total O 55 55	0
25	H	52	Total O 52 52	0
25	I	1	Total O 1 1	0

Continued on next page...

Continued from previous page...

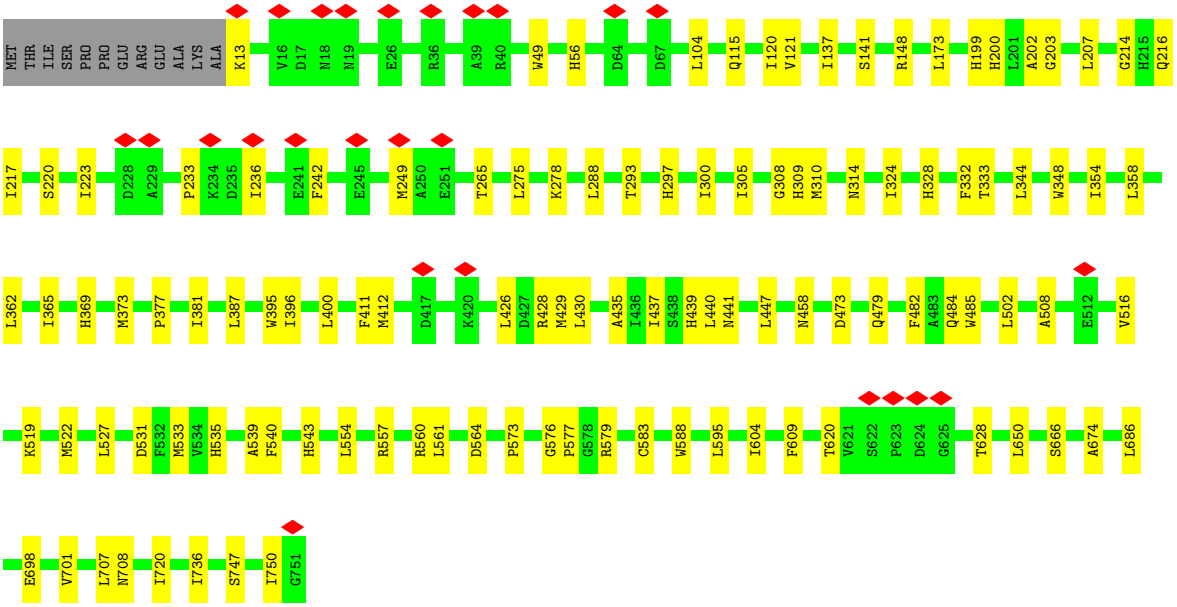
Mol	Chain	Residues	Atoms	AltConf
25	J	1	Total O 1 1	0
25	L	5	Total O 5 5	0
25	N	13	Total O 13 13	0
25	O	11	Total O 11 11	0
25	P	6	Total O 6 6	0
25	Q	4	Total O 4 4	0
25	R	1	Total O 1 1	0
25	S	3	Total O 3 3	0
25	U	3	Total O 3 3	0
25	a	57	Total O 57 57	0
25	b	74	Total O 74 74	0
25	c	17	Total O 17 17	0
25	d	7	Total O 7 7	0
25	e	10	Total O 10 10	0
25	f	7	Total O 7 7	0
25	i	1	Total O 1 1	0
25	j	1	Total O 1 1	0
25	k	1	Total O 1 1	0
25	l	6	Total O 6 6	0

3 Residue-property plots (i)

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

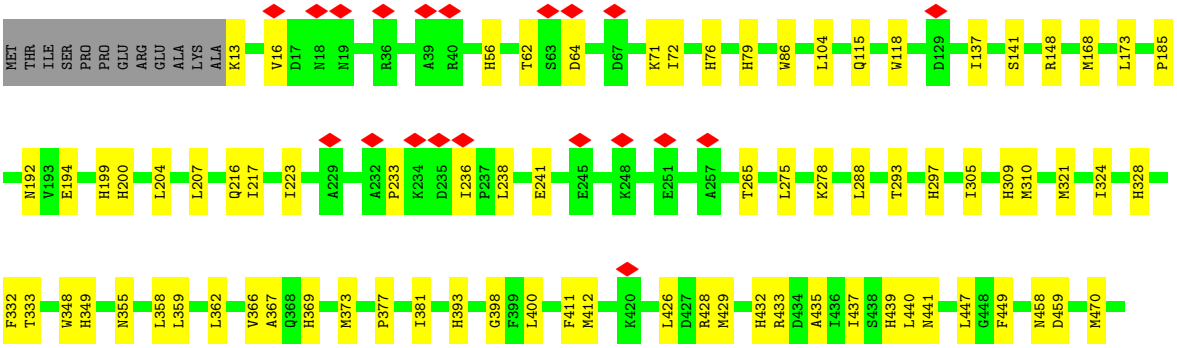
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

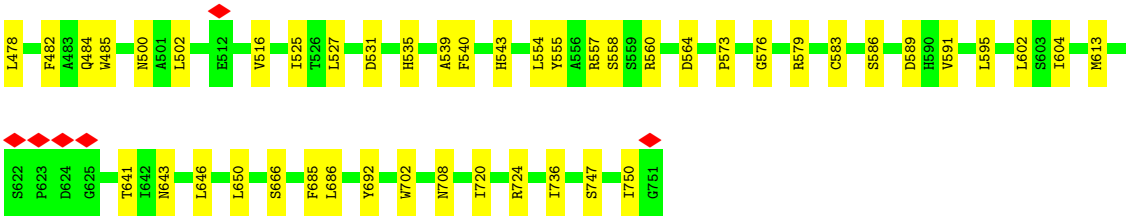
Chain A:



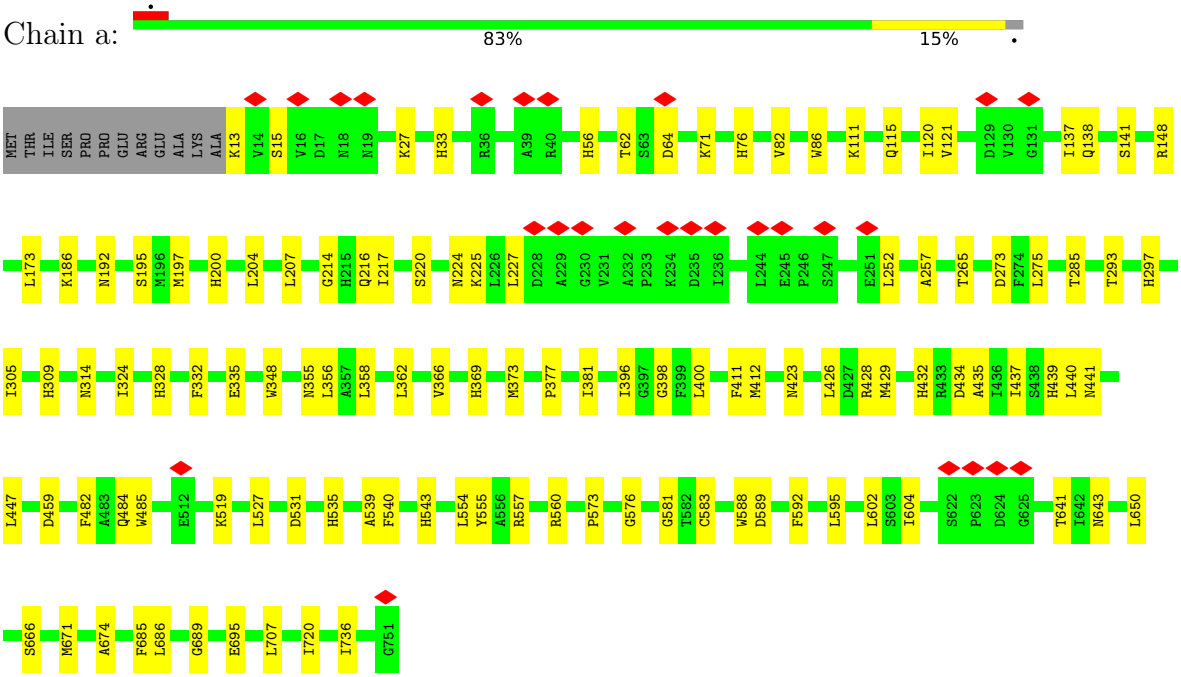
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain H:

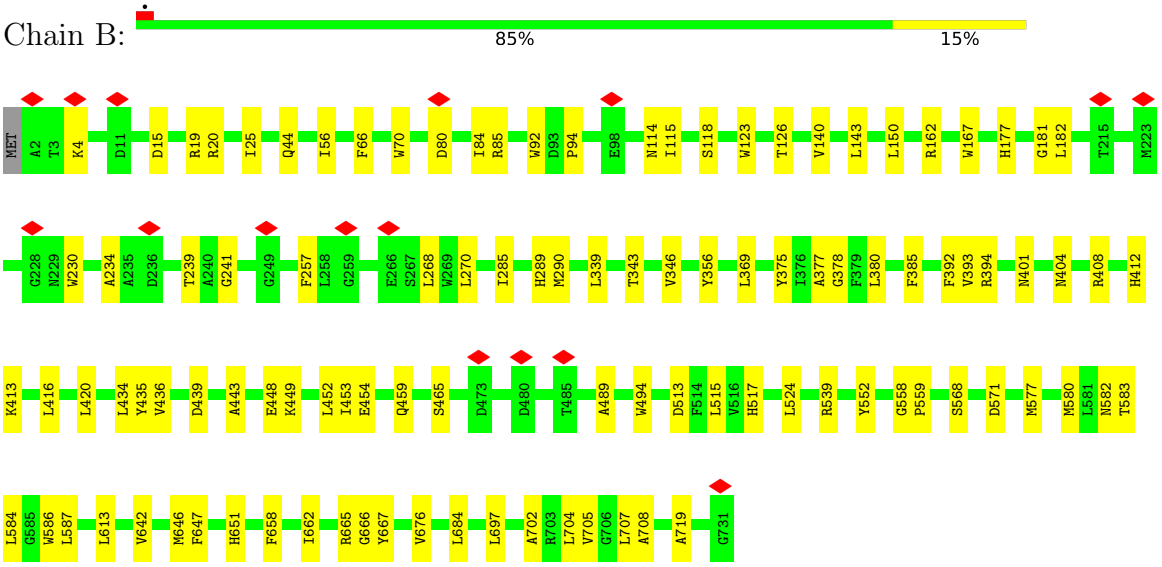




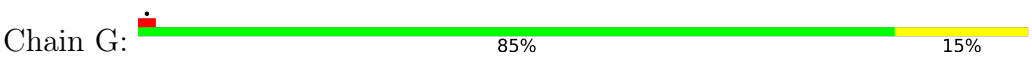
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

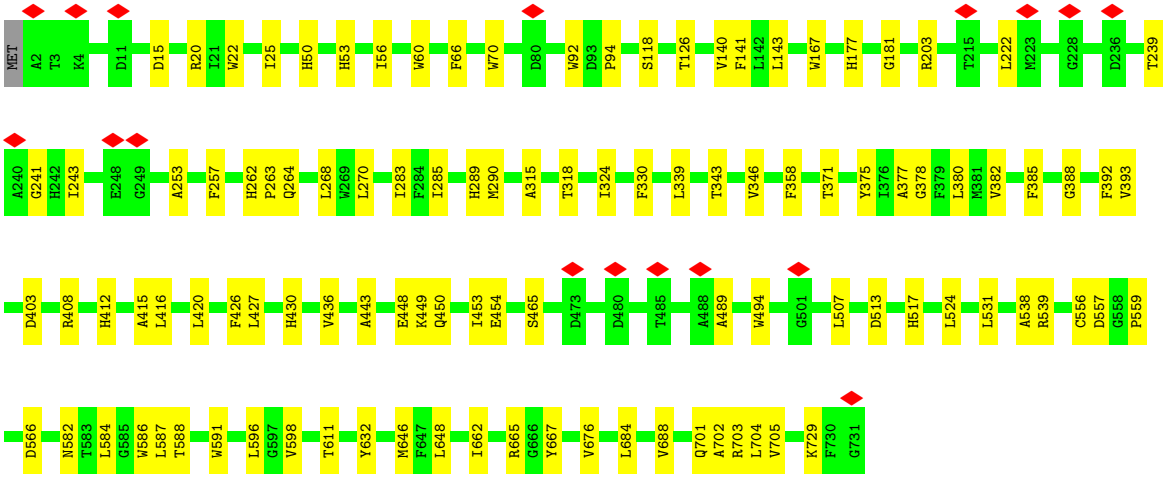


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



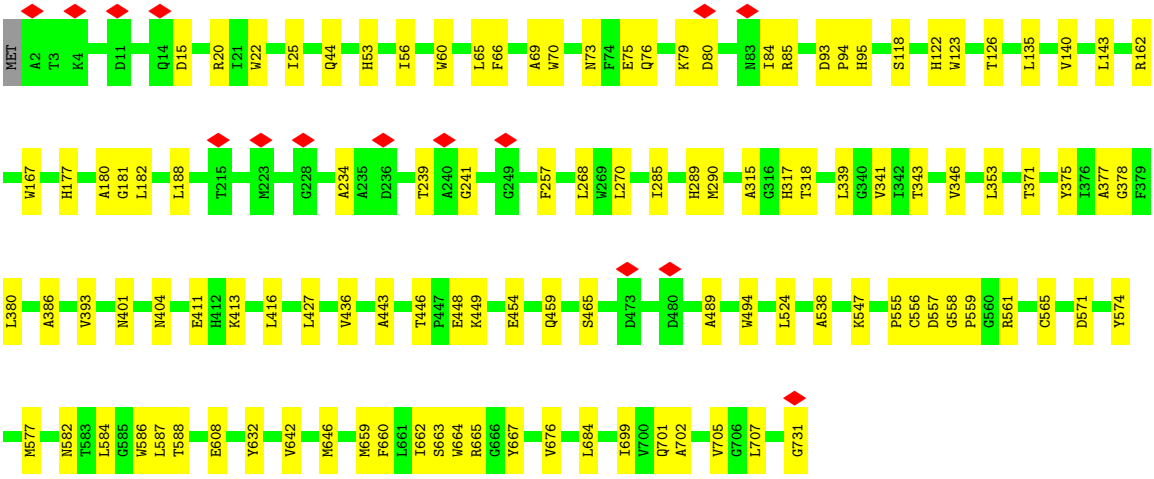
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





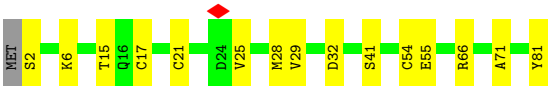
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



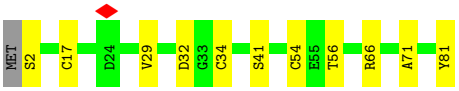
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



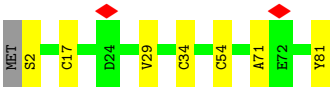
• Molecule 3: Photosystem I iron-sulfur center

Chain N:



• Molecule 3: Photosystem I iron-sulfur center

Chain c:

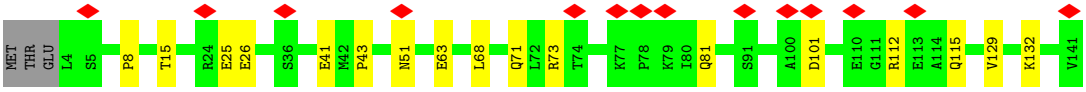


• Molecule 4: Photosystem I reaction center subunit II

Chain D:

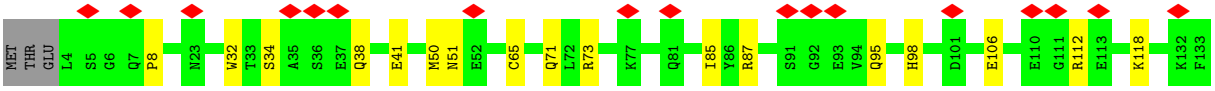
• Molecule 4: Photosystem I reaction center subunit II

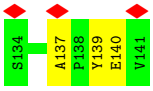
Chain P:



• Molecule 4: Photosystem I reaction center subunit II

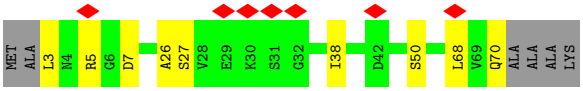
Chain d:





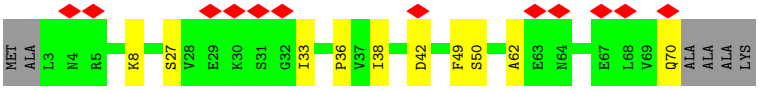
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



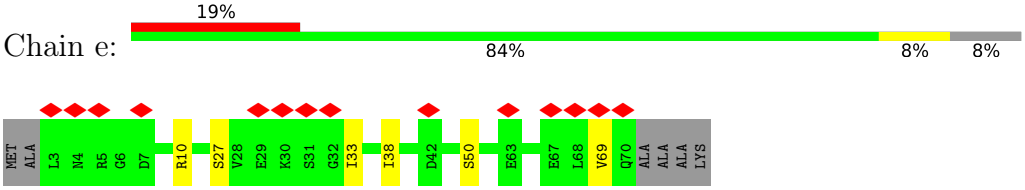
• Molecule 5: Photosystem I reaction center subunit IV

Chain O:



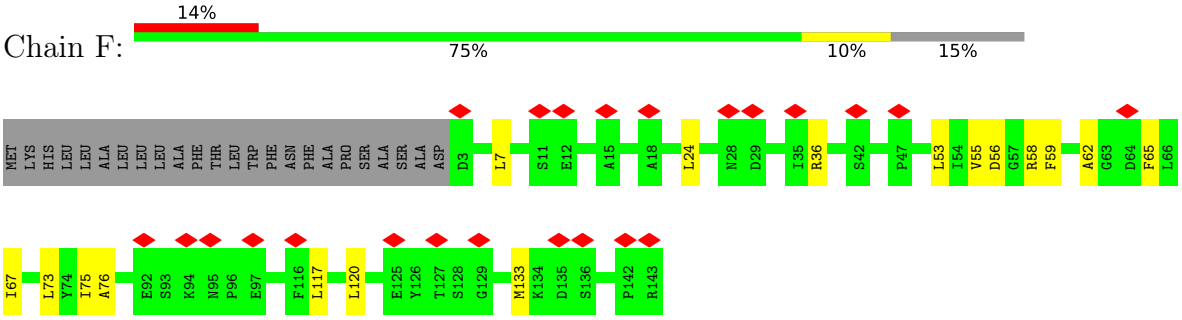
• Molecule 5: Photosystem I reaction center subunit IV

Chain e:



• Molecule 6: Photosystem I reaction center subunit III

Chain F:



• Molecule 6: Photosystem I reaction center subunit III

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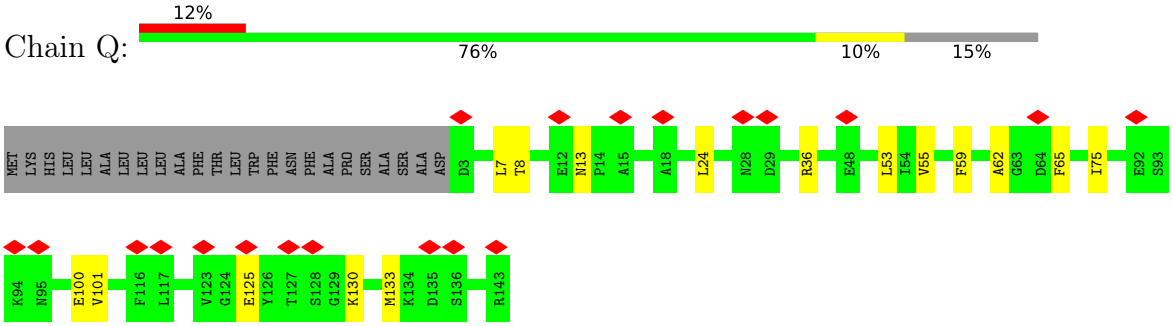
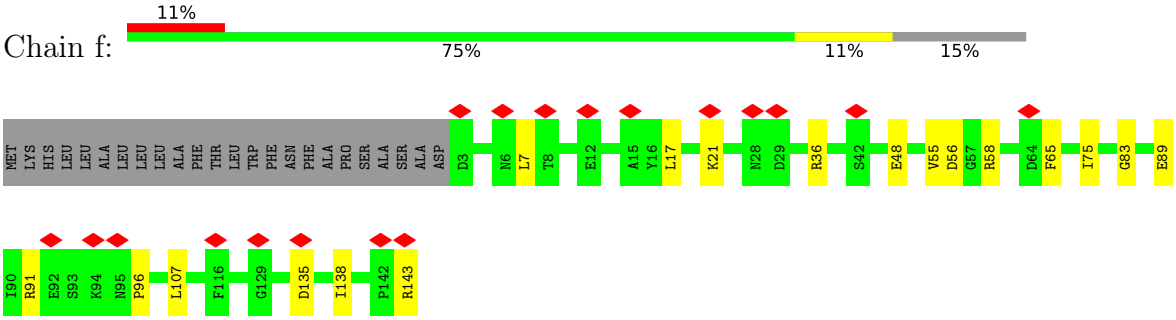


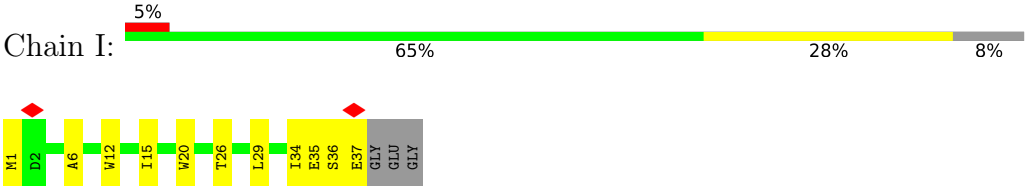
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



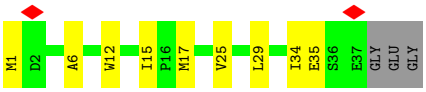
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



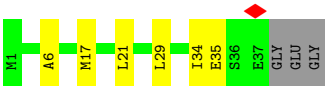
• Molecule 7: Photosystem I reaction center subunit VIII

Chain R:



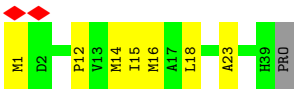
• Molecule 7: Photosystem I reaction center subunit VIII

Chain i:



• Molecule 8: Photosystem I reaction center subunit IX

Chain J:

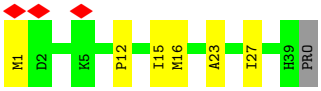


• Molecule 8: Photosystem I reaction center subunit IX

Chain S:

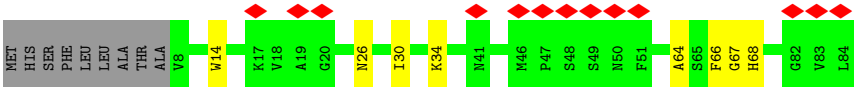
• Molecule 8: Photosystem I reaction center subunit IX

Chain j:



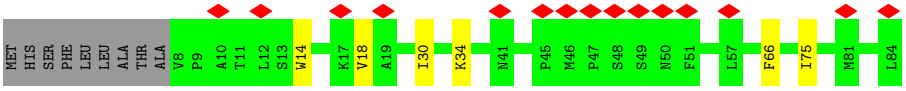
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:

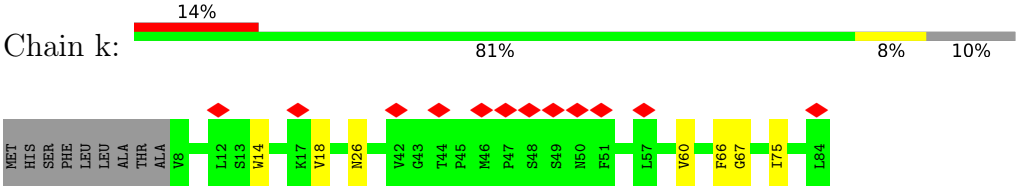


• Molecule 9: Photosystem I reaction center subunit PsaK 1

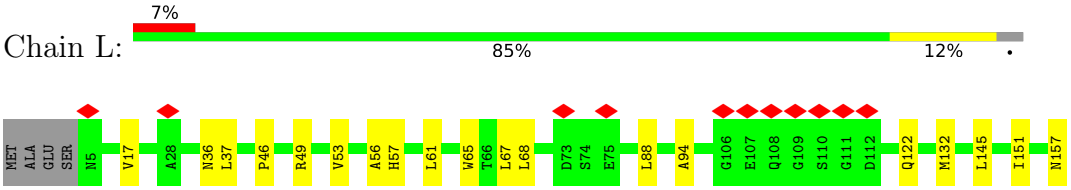
Chain T:



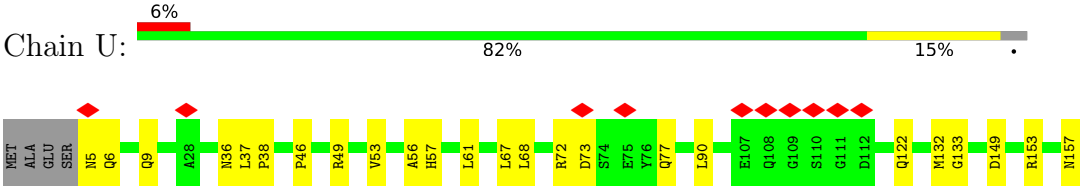
• Molecule 9: Photosystem I reaction center subunit PsaK 1



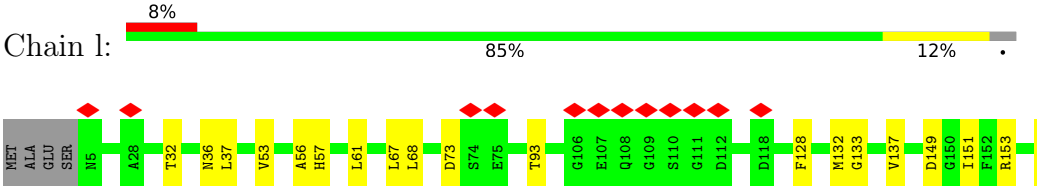
• Molecule 10: Photosystem I reaction center subunit XI



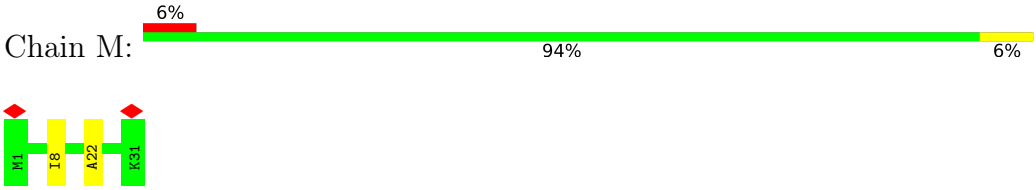
• Molecule 10: Photosystem I reaction center subunit XI



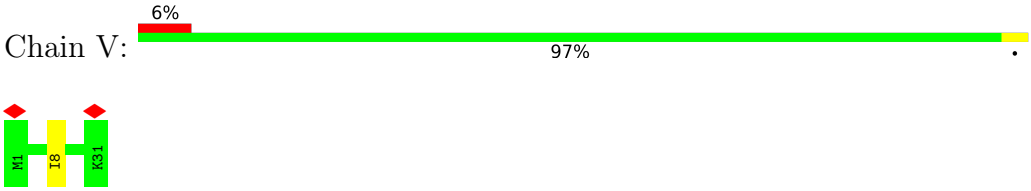
• Molecule 10: Photosystem I reaction center subunit XI



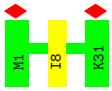
• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 11: Photosystem I reaction center subunit XII

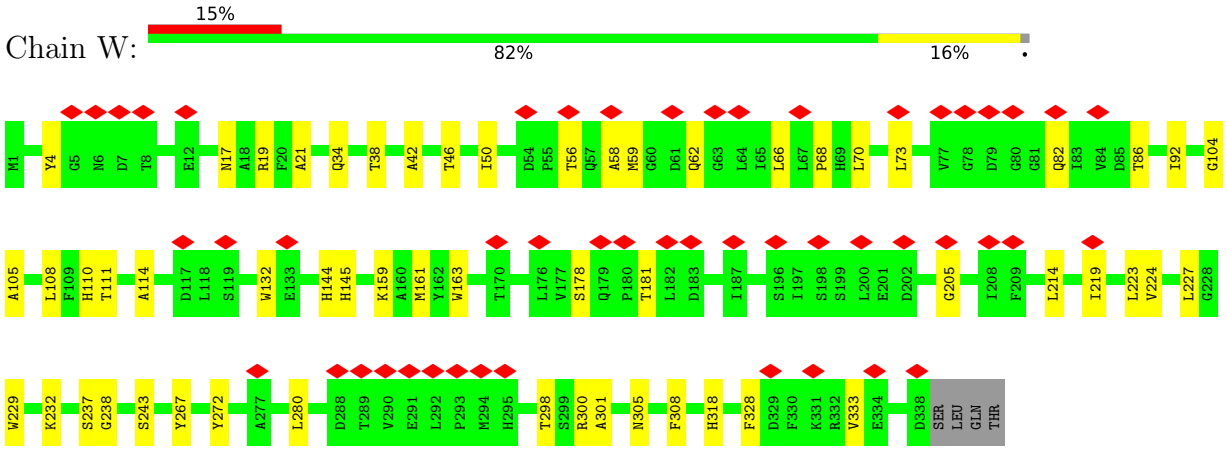


• Molecule 11: Photosystem I reaction center subunit XII



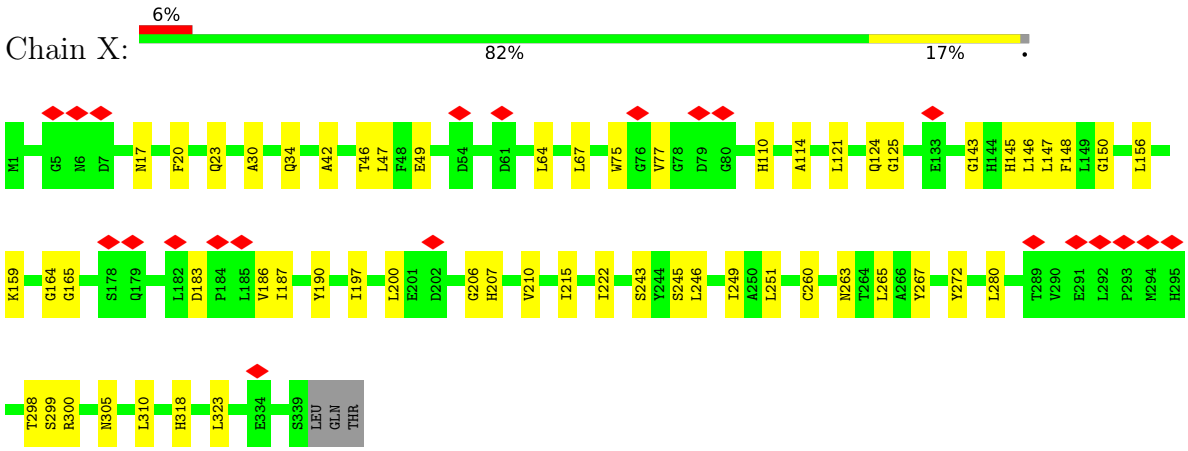
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain W:



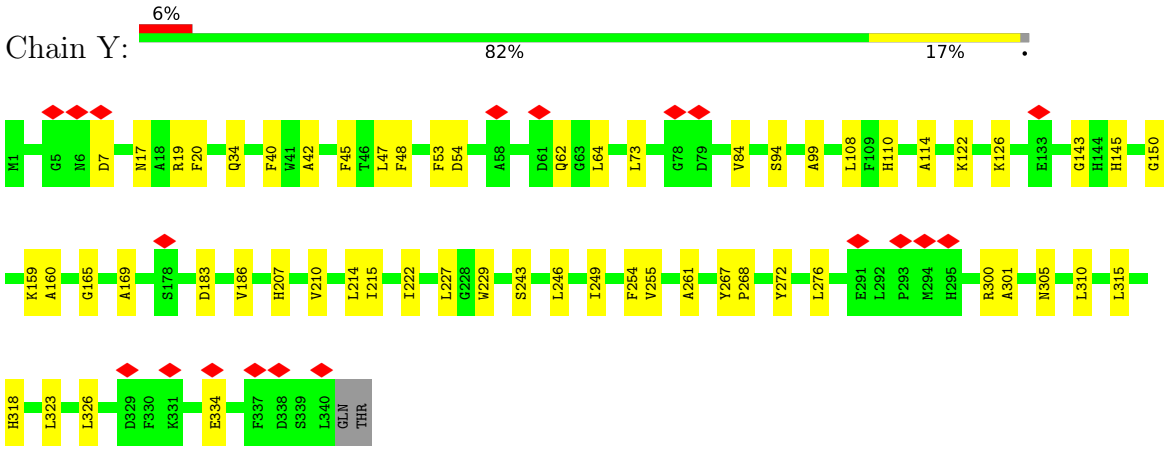
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain X:



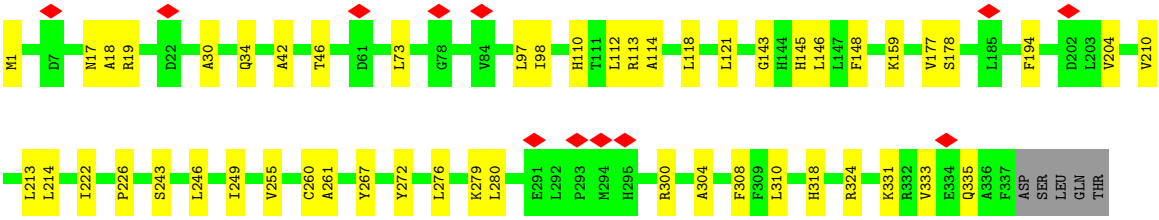
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Y:



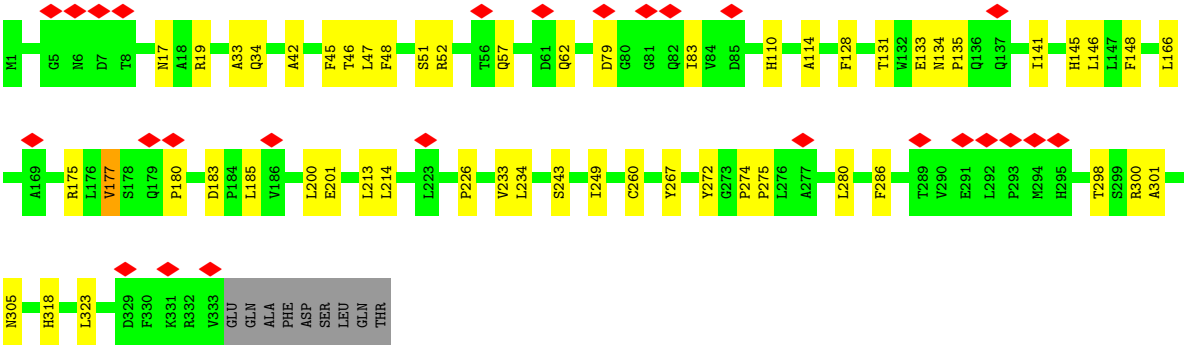
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain Z:



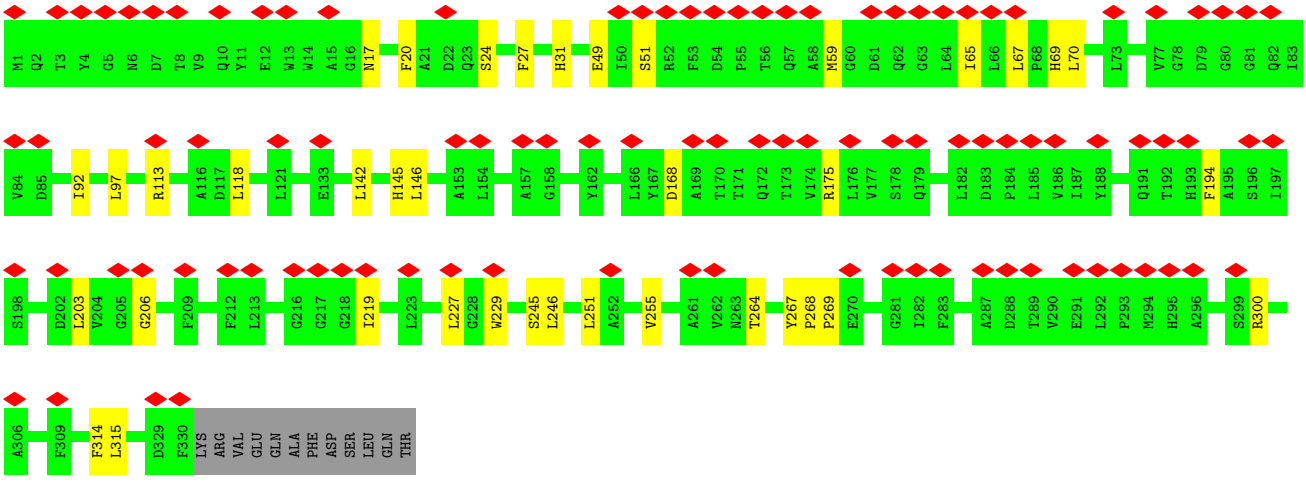
• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain g:



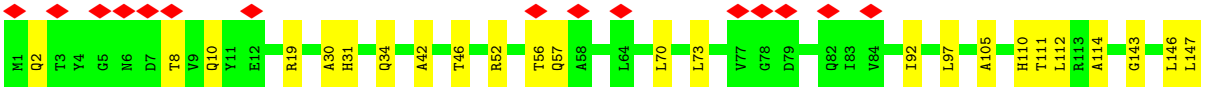
• Molecule 12: Iron stress-induced chlorophyll-binding protein

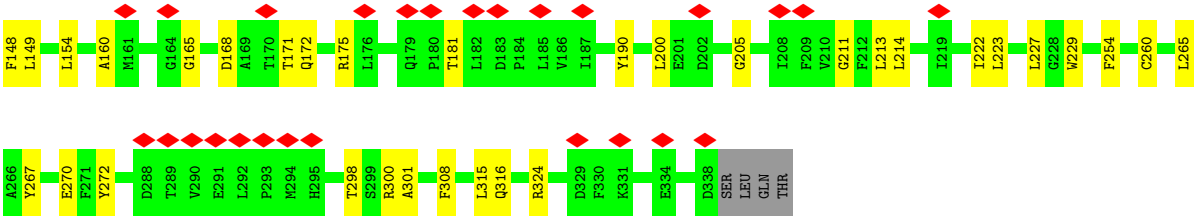
Chain h:



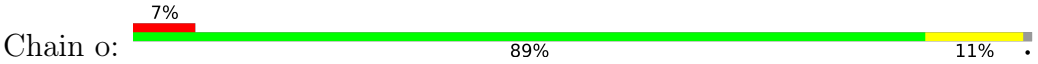
• Molecule 12: Iron stress-induced chlorophyll-binding protein

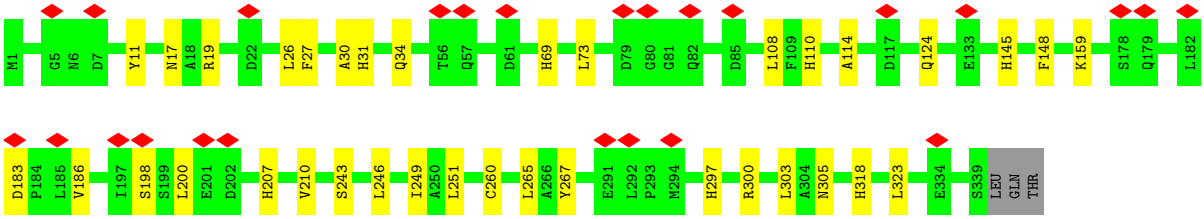
Chain n:



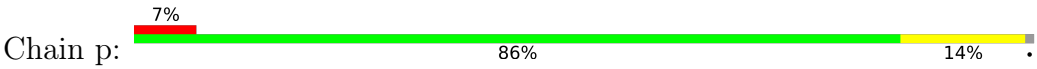


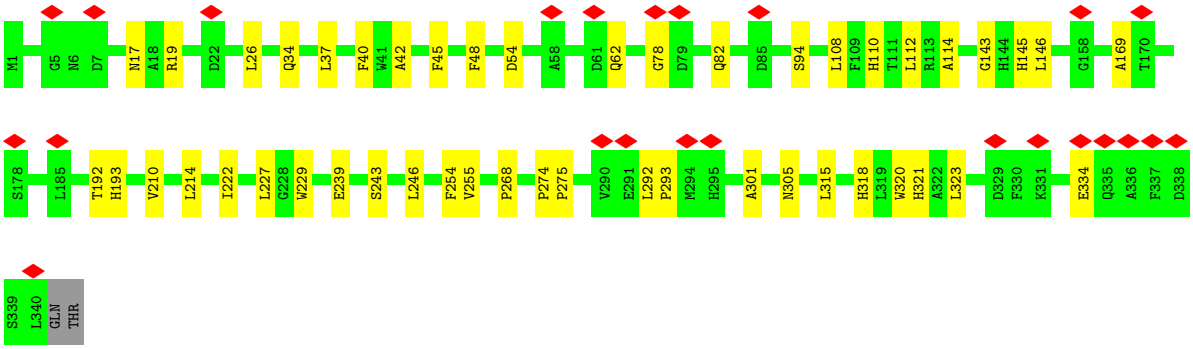
• Molecule 12: Iron stress-induced chlorophyll-binding protein



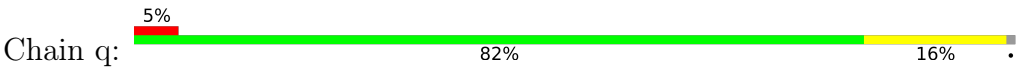


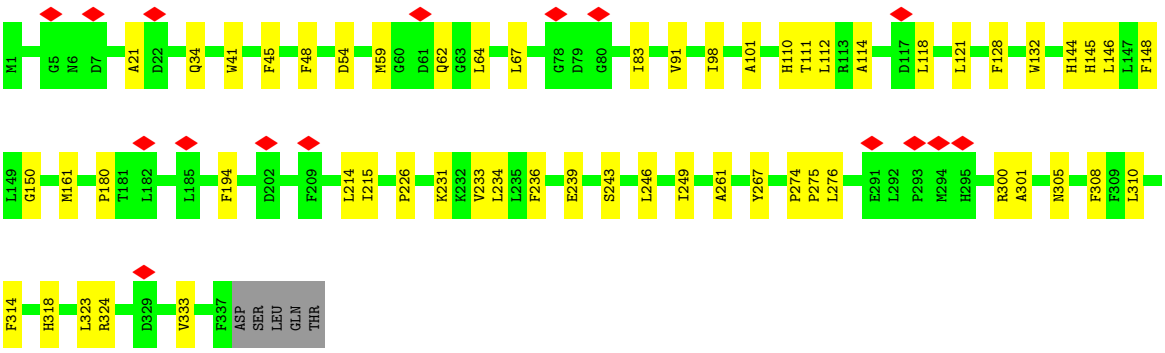
• Molecule 12: Iron stress-induced chlorophyll-binding protein



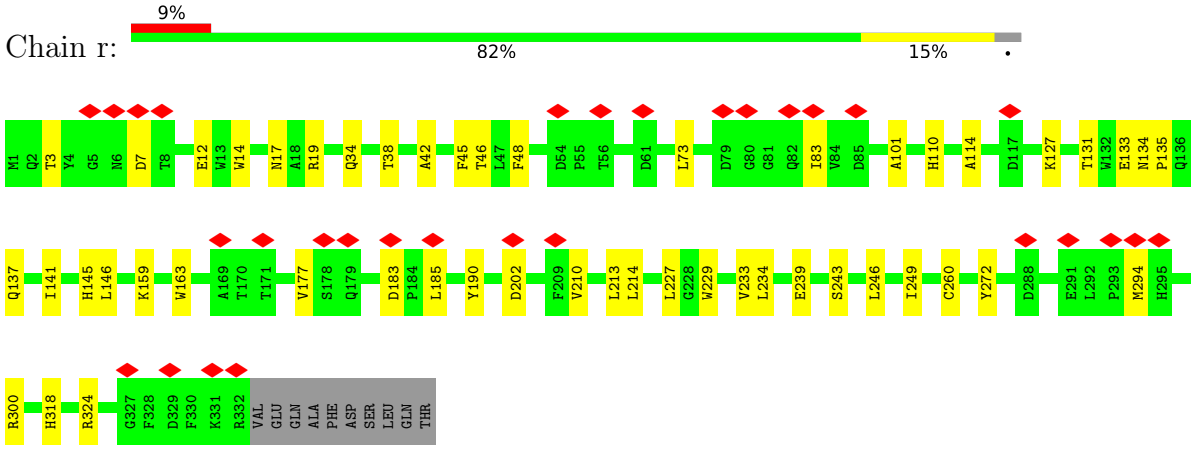


• Molecule 12: Iron stress-induced chlorophyll-binding protein

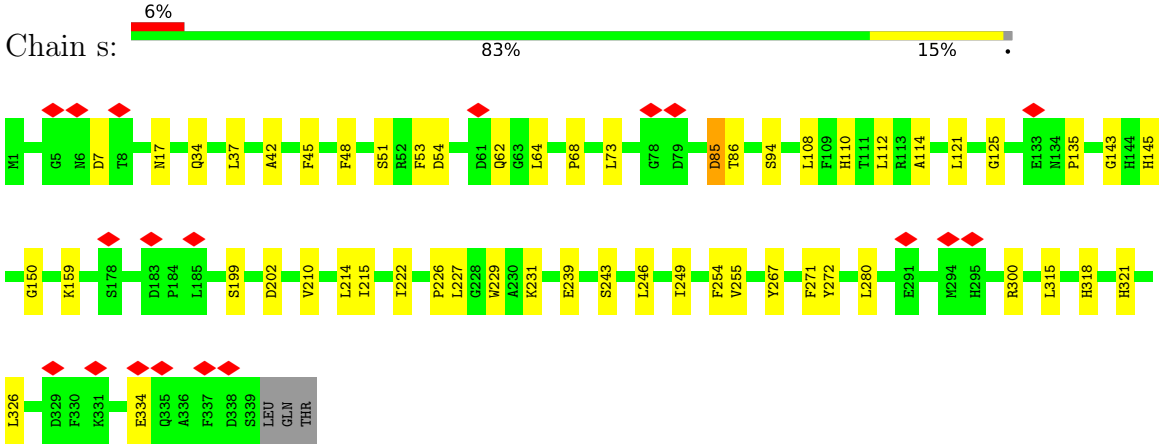




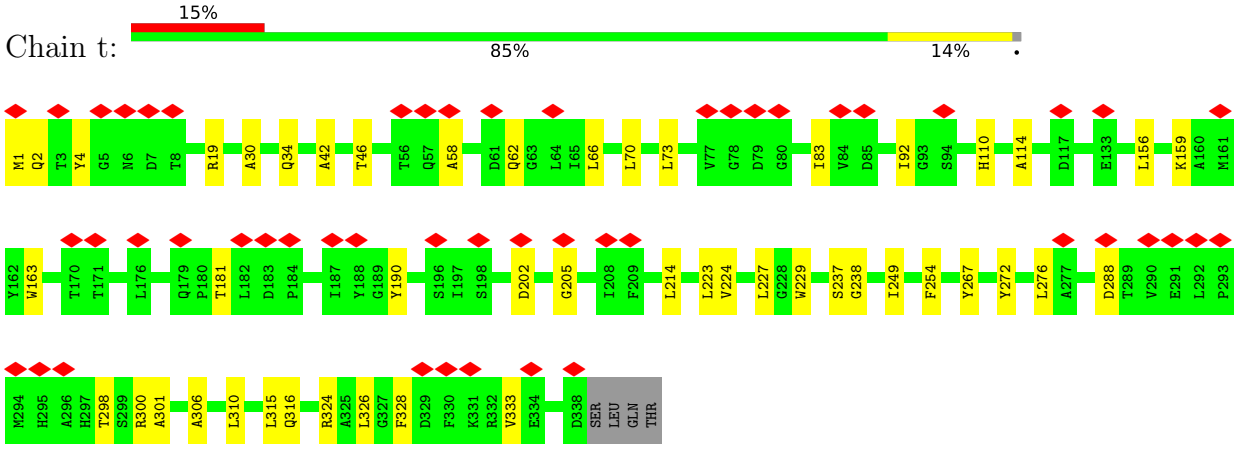
• Molecule 12: Iron stress-induced chlorophyll-binding protein



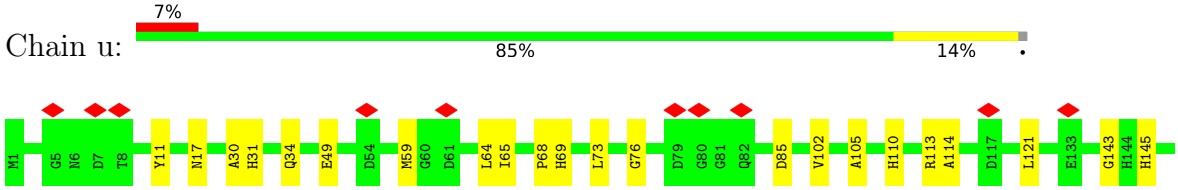
• Molecule 12: Iron stress-induced chlorophyll-binding protein

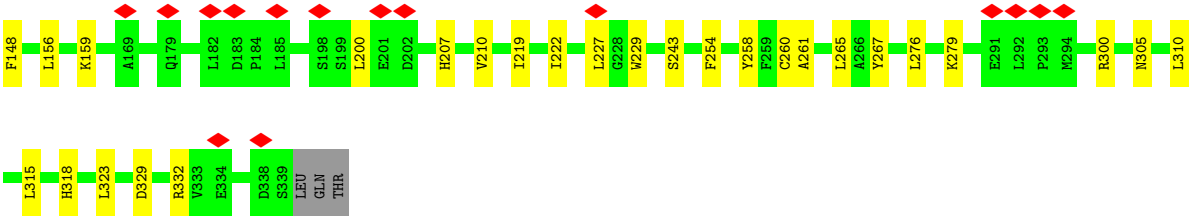


• Molecule 12: Iron stress-induced chlorophyll-binding protein

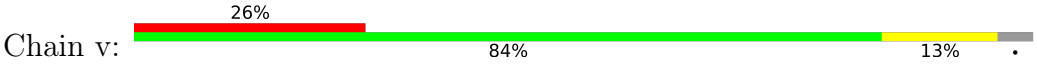


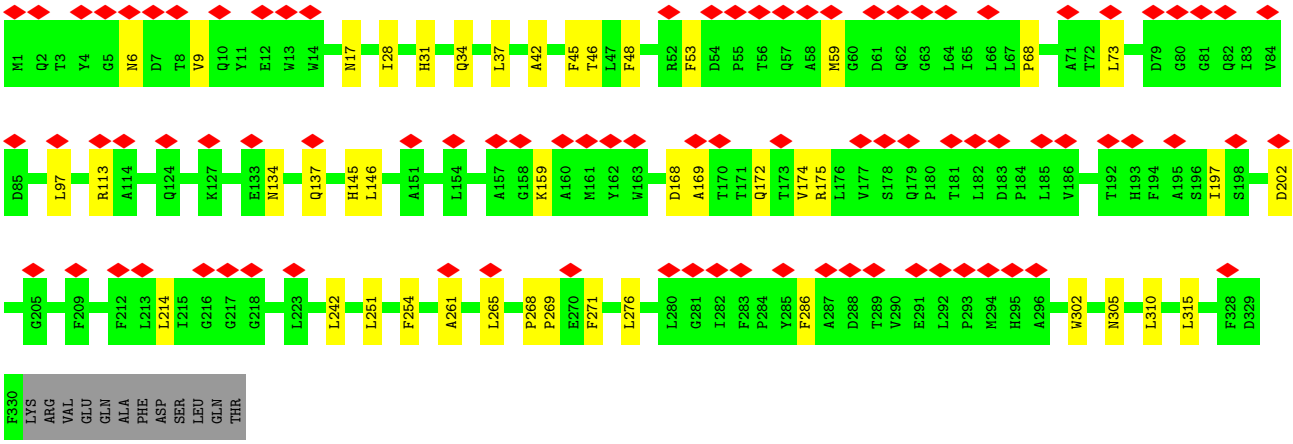
• Molecule 12: Iron stress-induced chlorophyll-binding protein



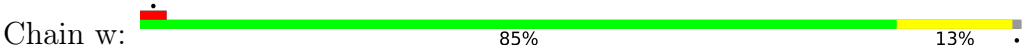


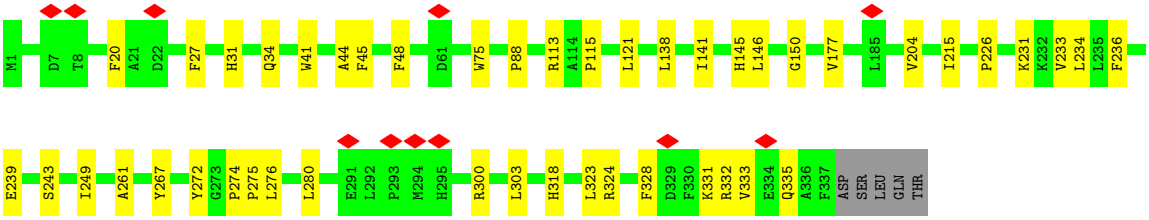
• Molecule 12: Iron stress-induced chlorophyll-binding protein



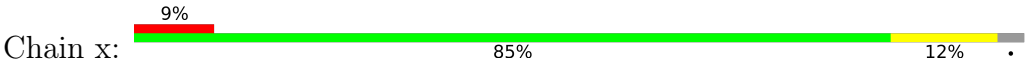


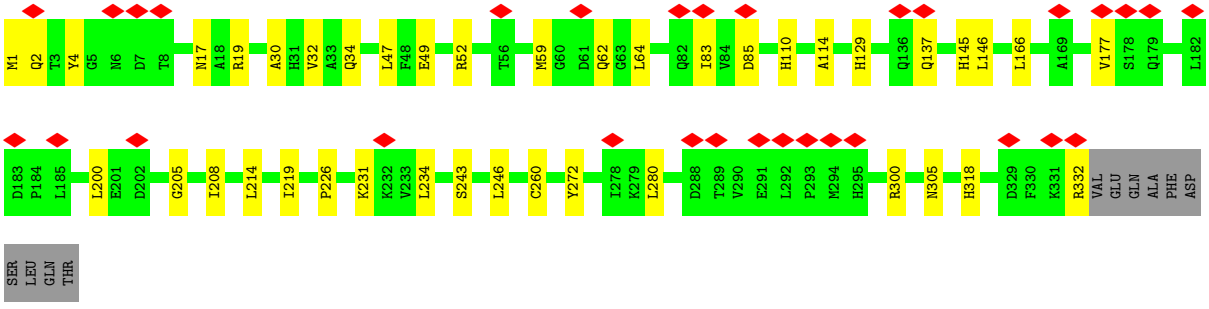
• Molecule 12: Iron stress-induced chlorophyll-binding protein





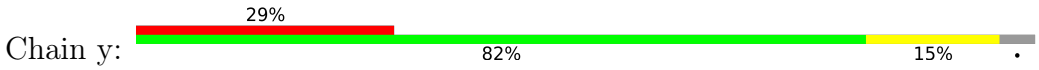
• Molecule 12: Iron stress-induced chlorophyll-binding protein

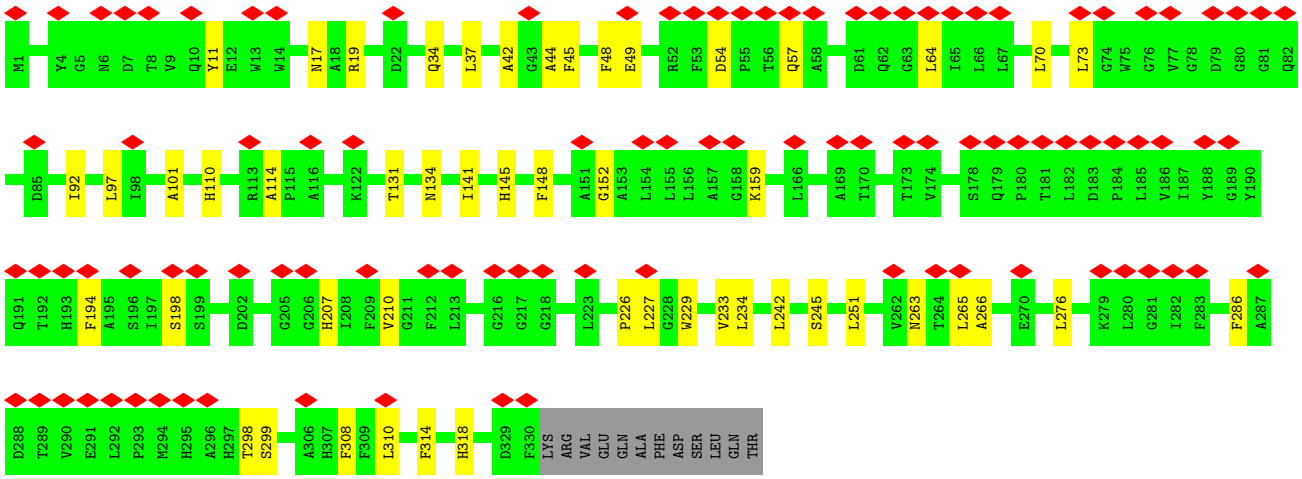




• Molecule 12: Iron stress-induced chlorophyll-binding protein

Chain y:


29%
82%
15%


M1 Y4 G5 N6 D7 T8 V9 Q10 Y11 E12 W13 W14 N17 A18 R19 D22 Q34 L37 A42 G43 A44 F45 F48 E49 R52 F53 D54 P55 T56 Q57 A58 D61 Q62 G63 L64 I65 L66 L67 L70 L73 G74 W75 G76 V77 G78 D79 G80 G81 Q82
D85 I92 L97 I98 A101 H110 R113 A114 P115 A116 K122 T131 N134 I141 H145 F148 A151 G152 A153 L154 L155 L156 A157 G158 K159 L166 A169 T170 T173 V174 S178 Q179 P180 T181 L182 D183 P184 L185 V186 I187 Y188 G189 Y190
Q191 T192 H193 F194 A195 S196 I197 S198 S199 D202 G205 G206 H207 I208 F209 V210 G211 F212 L213 G216 G217 G218 L223 P226 L227 G228 W229 V233 L234 L242 S245 L251 V262 N263 T264 L265 A266 E270 L276 K279 L280 G281 I282 F283 F286 A287
D288 T289 V290 E291 L292 P293 M294 H295 A296 H297 T298 S299 A306 H307 F308 F309 L310 F314 H318 D329 F330 LYS ARG VAL GLU GLN ALA PHE ASP SER LEU GLN THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	70.466	Depositor
Minimum map value	-42.667	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	2.305	Depositor
Recommended contour level	9.2	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, SF4, CA, LUT, CL0, LHG, LMU, CLA, ECH, PQN, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.23	0/5985	0.43	0/8158
1	H	0.23	0/5985	0.44	0/8158
1	a	0.23	0/5985	0.45	0/8158
2	B	0.22	0/5986	0.44	0/8185
2	G	0.23	0/5986	0.45	0/8185
2	b	0.23	0/5986	0.45	0/8185
3	C	0.20	0/610	0.48	0/826
3	N	0.21	0/610	0.48	0/826
3	c	0.22	0/610	0.51	0/826
4	D	0.19	0/1102	0.44	0/1485
4	P	0.18	0/1102	0.38	0/1485
4	d	0.18	0/1102	0.40	0/1485
5	E	0.13	0/546	0.31	0/738
5	O	0.13	0/546	0.32	0/738
5	e	0.14	0/546	0.33	0/738
6	F	0.20	0/1130	0.43	0/1535
6	Q	0.22	0/1130	0.46	0/1535
6	f	0.21	0/1130	0.44	0/1535
7	I	0.27	0/304	0.55	0/416
7	R	0.30	0/304	0.57	0/416
7	i	0.31	0/304	0.61	0/416
8	J	0.20	0/319	0.45	0/431
8	S	0.22	0/319	0.47	0/431
8	j	0.30	0/319	0.48	0/431
9	K	0.15	0/549	0.36	0/745
9	T	0.16	0/549	0.43	0/745
9	k	0.16	0/549	0.44	0/745
10	L	0.20	0/1180	0.47	0/1603
10	U	0.21	0/1180	0.49	0/1603
10	l	0.21	0/1180	0.46	0/1603
11	M	0.19	0/241	0.38	0/326
11	V	0.22	0/241	0.45	0/326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	m	0.24	0/241	0.50	0/326
12	W	0.18	0/2691	0.44	1/3678 (0.0%)
12	X	0.20	0/2712	0.47	0/3703
12	Y	0.21	0/2712	0.45	0/3704
12	Z	0.20	0/2693	0.44	1/3678 (0.0%)
12	g	0.19	0/2662	0.45	0/3636
12	h	0.17	0/2627	0.42	0/3592
12	n	0.16	0/2691	0.37	0/3678
12	o	0.20	0/2712	0.47	0/3703
12	p	0.20	0/2712	0.43	0/3704
12	q	0.18	0/2693	0.39	0/3678
12	r	0.20	0/2655	0.49	0/3626
12	s	0.20	0/2707	0.42	0/3697
12	t	0.17	0/2691	0.41	0/3678
12	u	0.20	0/2712	0.45	0/3703
12	v	0.16	0/2627	0.40	0/3592
12	w	0.19	0/2693	0.43	0/3678
12	x	0.18	0/2655	0.45	2/3626 (0.1%)
12	y	0.16	0/2621	0.40	0/3585
All	All	0.21	0/102122	0.44	4/139283 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
12	Y	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	x	85	ASP	CA-C-N	5.76	131.60	122.61
12	x	85	ASP	C-N-CA	5.76	131.60	122.61
12	W	308	PHE	N-CA-C	-5.49	106.25	113.12
12	Z	333	VAL	N-CA-C	-5.27	108.36	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	Y	84	VAL	Peptide
2	b	664	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5787	0	5648	95	0
1	H	5787	0	5648	100	0
1	a	5787	0	5648	90	0
2	B	5775	0	5554	86	0
2	G	5775	0	5554	86	0
2	b	5775	0	5554	85	0
3	C	600	0	589	12	0
3	N	600	0	589	9	0
3	c	600	0	589	5	0
4	D	1078	0	1076	17	0
4	P	1078	0	1076	11	0
4	d	1078	0	1076	12	0
5	E	537	0	520	5	0
5	O	537	0	520	7	0
5	e	537	0	520	4	0
6	F	1100	0	1096	14	0
6	Q	1100	0	1096	12	0
6	f	1100	0	1096	13	0
7	I	293	0	292	10	0
7	R	293	0	292	8	0
7	i	293	0	292	4	0
8	J	311	0	321	7	0
8	S	311	0	321	10	0
8	j	311	0	321	6	0
9	K	538	0	565	6	0
9	T	538	0	565	5	0
9	k	538	0	565	5	0
10	L	1150	0	1122	19	0
10	U	1150	0	1122	23	0
10	l	1150	0	1122	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	238	0	260	2	0
11	V	238	0	260	1	0
11	m	238	0	260	1	0
12	W	2601	0	2532	39	0
12	X	2622	0	2567	47	0
12	Y	2622	0	2561	43	0
12	Z	2603	0	2550	38	0
12	g	2573	0	2526	39	0
12	h	2538	0	2476	32	0
12	n	2601	0	2532	47	0
12	o	2622	0	2567	32	0
12	p	2622	0	2561	34	0
12	q	2603	0	2550	44	0
12	r	2566	0	2517	36	0
12	s	2617	0	2559	38	0
12	t	2601	0	2532	34	0
12	u	2622	0	2567	38	0
12	v	2538	0	2476	33	0
12	w	2603	0	2550	37	0
12	x	2566	0	2517	29	0
12	y	2532	0	2465	35	0
13	A	69	0	78	2	0
13	B	38	0	49	1	0
13	G	38	0	49	1	0
13	H	69	0	78	2	0
13	I	40	0	50	2	0
13	R	40	0	50	2	0
13	X	27	0	24	1	0
13	Y	32	0	34	0	0
13	a	69	0	78	0	0
13	b	38	0	49	3	0
13	g	31	0	32	0	0
13	i	40	0	50	2	0
13	o	27	0	24	1	0
13	p	32	0	34	1	0
13	r	31	0	32	2	0
13	s	32	0	34	1	0
13	u	27	0	24	1	0
13	x	31	0	32	0	0
14	A	116	0	142	6	0
14	B	43	0	56	2	0
14	F	27	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	G	43	0	56	2	0
14	H	116	0	142	8	0
14	Q	27	0	24	1	0
14	a	116	0	142	3	0
14	b	43	0	56	0	0
14	f	27	0	24	1	0
15	A	65	0	72	3	0
15	H	65	0	72	4	0
15	a	65	0	72	4	0
16	A	2545	0	2497	100	0
16	B	2309	0	2201	99	0
16	F	91	0	66	1	0
16	G	2310	0	2204	89	0
16	H	2545	0	2497	105	0
16	J	82	0	58	1	0
16	K	145	0	115	3	0
16	L	185	0	190	11	0
16	Q	91	0	66	3	0
16	S	82	0	58	0	0
16	T	145	0	115	3	0
16	U	185	0	190	11	0
16	W	963	0	910	26	0
16	X	959	0	904	40	0
16	Y	973	0	936	33	0
16	Z	977	0	942	37	0
16	a	2540	0	2487	97	0
16	b	2310	0	2204	84	0
16	f	91	0	66	2	0
16	g	978	0	949	31	0
16	h	969	0	930	32	0
16	j	82	0	58	0	0
16	k	145	0	115	2	0
16	l	185	0	190	15	0
16	n	968	0	923	41	0
16	o	959	0	904	34	0
16	p	973	0	936	36	0
16	q	977	0	942	43	0
16	r	978	0	949	38	0
16	s	973	0	936	34	0
16	t	968	0	923	24	0
16	u	959	0	904	32	0
16	v	969	0	930	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	w	977	0	942	35	0
16	x	978	0	949	35	0
16	y	969	0	930	38	0
17	A	33	0	46	4	0
17	B	33	0	46	5	0
17	G	33	0	46	5	0
17	H	33	0	46	4	0
17	a	33	0	46	4	0
17	b	33	0	46	2	0
18	A	8	0	0	0	0
18	C	16	0	0	0	0
18	H	8	0	0	0	0
18	N	16	0	0	0	0
18	a	8	0	0	0	0
18	c	16	0	0	0	0
19	A	200	0	280	12	0
19	B	230	0	319	15	0
19	F	40	0	56	4	0
19	G	230	0	319	16	0
19	H	200	0	280	13	0
19	I	40	0	56	3	0
19	J	120	0	168	8	0
19	K	80	0	112	5	0
19	L	80	0	112	9	0
19	Q	40	0	56	2	0
19	R	40	0	56	0	0
19	S	120	0	168	9	0
19	T	80	0	112	3	0
19	U	80	0	112	13	0
19	W	120	0	168	6	0
19	X	160	0	224	11	0
19	Y	160	0	224	6	0
19	Z	120	0	168	4	0
19	a	200	0	280	15	0
19	b	230	0	319	15	0
19	f	40	0	56	4	0
19	g	160	0	224	12	0
19	h	120	0	168	9	0
19	i	40	0	56	5	0
19	j	120	0	168	7	0
19	k	80	0	112	4	0
19	l	80	0	112	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	n	120	0	168	9	0
19	o	160	0	224	5	0
19	p	160	0	224	10	0
19	q	120	0	168	13	0
19	r	160	0	224	7	0
19	s	160	0	224	11	0
19	t	120	0	168	5	0
19	u	160	0	224	8	0
19	v	120	0	168	7	0
19	w	120	0	168	8	0
19	x	160	0	224	9	0
19	y	120	0	168	11	0
20	A	35	0	46	1	0
20	H	35	0	46	1	0
20	L	35	0	46	3	0
20	U	35	0	46	2	0
20	a	35	0	45	1	0
20	l	35	0	46	3	0
21	B	41	0	54	3	0
21	G	41	0	54	2	0
21	I	41	0	54	2	0
21	M	41	0	54	2	0
21	R	41	0	54	2	0
21	V	41	0	54	4	0
21	b	41	0	54	2	0
21	i	41	0	54	1	0
21	m	41	0	54	2	0
22	L	1	0	0	0	0
22	U	1	0	0	0	0
22	l	1	0	0	0	0
23	Y	35	0	46	1	0
23	Z	35	0	46	0	0
23	g	35	0	46	1	0
23	p	35	0	46	1	0
23	q	35	0	46	2	0
23	r	35	0	46	3	0
23	s	35	0	46	0	0
23	w	35	0	46	0	0
23	x	35	0	46	2	0
24	Z	42	0	55	0	0
24	q	42	0	55	1	0
24	w	42	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	56	0	0	1	0
25	B	52	0	0	1	0
25	C	7	0	0	0	0
25	D	3	0	0	0	0
25	E	4	0	0	0	0
25	F	3	0	0	0	0
25	G	55	0	0	1	0
25	H	52	0	0	0	0
25	I	1	0	0	0	0
25	J	1	0	0	0	0
25	L	5	0	0	0	0
25	N	13	0	0	0	0
25	O	11	0	0	0	0
25	P	6	0	0	0	0
25	Q	4	0	0	0	0
25	R	1	0	0	0	0
25	S	3	0	0	0	0
25	U	3	0	0	0	0
25	a	57	0	0	0	0
25	b	74	0	0	1	0
25	c	17	0	0	0	0
25	d	7	0	0	0	0
25	e	10	0	0	0	0
25	f	7	0	0	0	0
25	i	1	0	0	0	0
25	j	1	0	0	0	0
25	k	1	0	0	0	0
25	l	6	0	0	0	0
All	All	140516	0	138986	2192	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HB2	16:A:1137:CLA:HBB1	1.61	0.81
16:b:1206:CLA:H3A	16:b:1207:CLA:HBB1	1.64	0.78
16:H:1107:CLA:HBB1	19:S:4012:BCR:HC7	1.67	0.77
16:B:1206:CLA:H3A	16:B:1207:CLA:HBB1	1.66	0.77
1:a:440:LEU:HB2	16:a:1137:CLA:HBB1	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:41:GLU:H	4:d:71:GLN:HE22	1.34	0.75
16:G:1238:CLA:H2	16:G:1239:CLA:H122	1.66	0.75
9:T:66:PHE:HB2	19:T:4001:BCR:H23C	1.69	0.74
16:G:1206:CLA:H3A	16:G:1207:CLA:HBB1	1.68	0.74
1:H:440:LEU:HB2	16:H:1137:CLA:HBB1	1.70	0.74
16:Z:505:CLA:HBB2	16:Z:510:CLA:H92	1.70	0.73
16:g:508:CLA:H3A	16:g:508:CLA:H43	1.71	0.73
16:Y:505:CLA:HBB2	16:Y:510:CLA:H92	1.72	0.72
9:k:66:PHE:HB2	19:k:4001:BCR:H23C	1.73	0.71
16:s:505:CLA:HBB2	16:s:510:CLA:H92	1.73	0.71
16:a:1108:CLA:HBB2	16:a:1111:CLA:HMA3	1.73	0.71
16:A:1138:CLA:H41	19:B:4014:BCR:H19C	1.73	0.71
16:G:1215:CLA:HBB2	16:G:1221:CLA:H201	1.73	0.71
12:r:146:LEU:HD21	16:r:516:CLA:HAB	1.71	0.70
16:g:505:CLA:HBB2	16:g:510:CLA:H92	1.72	0.70
16:B:1238:CLA:H2	16:B:1239:CLA:H122	1.72	0.70
16:A:1101:CLA:H93	19:B:4014:BCR:H20C	1.73	0.70
16:B:1223:CLA:H152	19:B:4010:BCR:H14C	1.73	0.70
1:a:736:ILE:HG23	16:a:1126:CLA:HAB	1.74	0.69
16:r:506:CLA:HBB2	16:r:507:CLA:H151	1.74	0.69
16:b:1208:CLA:HBB2	16:b:1210:CLA:HMA3	1.75	0.69
16:B:1227:CLA:HBB2	16:B:1236:CLA:HMC2	1.73	0.69
1:a:356:LEU:HD21	16:a:1128:CLA:HAB	1.75	0.69
16:b:1215:CLA:HBB2	16:b:1221:CLA:H201	1.75	0.69
12:W:219:ILE:HG12	16:W:501:CLA:HBB2	1.75	0.69
16:H:1108:CLA:HBB2	16:H:1111:CLA:HMA3	1.73	0.68
16:p:505:CLA:HBB2	16:p:510:CLA:H92	1.73	0.68
16:G:1222:CLA:HBB1	16:G:1236:CLA:HHB	1.75	0.68
16:q:505:CLA:HBB2	16:q:510:CLA:H92	1.75	0.68
16:B:1208:CLA:HBB2	16:B:1210:CLA:HMA3	1.74	0.68
16:H:1128:CLA:H171	16:H:1140:CLA:H3A	1.75	0.68
16:y:517:CLA:H12	16:y:517:CLA:H3A	1.77	0.67
16:A:1104:CLA:HMA2	16:A:1104:CLA:H2	1.76	0.67
16:o:505:CLA:HBB2	16:o:510:CLA:H92	1.76	0.67
16:A:1107:CLA:HBB1	19:J:4012:BCR:HC7	1.76	0.67
16:A:1120:CLA:HMD2	19:K:4001:BCR:H24C	1.76	0.66
16:q:506:CLA:HBB2	16:q:507:CLA:H151	1.77	0.66
16:B:1219:CLA:HMA1	16:B:1240:CLA:HBB2	1.78	0.66
1:H:458:ASN:HD22	1:H:470:MET:HE2	1.61	0.66
16:w:505:CLA:HBB2	16:w:510:CLA:H92	1.77	0.66
1:H:398:GLY:HA3	1:H:602:LEU:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:w:506:CLA:HBB2	16:w:507:CLA:H151	1.78	0.65
12:Z:146:LEU:HD21	16:Z:516:CLA:HAB	1.78	0.65
16:a:1128:CLA:H171	16:a:1140:CLA:H3A	1.78	0.65
10:U:46:PRO:HA	10:U:49:ARG:HG2	1.78	0.65
10:L:46:PRO:HA	10:L:49:ARG:HG2	1.78	0.65
16:v:504:CLA:H141	16:v:507:CLA:HBB2	1.78	0.65
16:A:1108:CLA:HBB2	16:A:1111:CLA:HMA3	1.78	0.65
12:W:227:LEU:HD12	12:W:229:TRP:H	1.62	0.65
16:B:1222:CLA:HBB1	16:B:1236:CLA:HHB	1.78	0.64
16:p:504:CLA:H172	16:p:507:CLA:HBB2	1.79	0.64
12:q:146:LEU:HD21	16:q:516:CLA:HAB	1.79	0.64
12:x:146:LEU:HD21	16:x:516:CLA:HAB	1.79	0.64
12:t:227:LEU:HD12	12:t:229:TRP:H	1.63	0.64
16:Z:505:CLA:HBB1	16:Z:505:CLA:H62	1.78	0.64
10:l:132:MET:HG3	19:l:4022:BCR:H23C	1.80	0.64
16:b:1223:CLA:H152	19:b:4010:BCR:H14C	1.78	0.64
16:b:1238:CLA:H2	16:b:1239:CLA:H122	1.78	0.64
16:H:1129:CLA:HBB2	16:H:1137:CLA:HMC2	1.79	0.64
12:x:332:ARG:HH21	16:y:512:CLA:H12	1.63	0.64
16:B:1204:CLA:HMB3	16:B:1205:CLA:H3A	1.80	0.64
16:v:505:CLA:HBB1	19:v:603:BCR:H21C	1.81	0.63
12:w:34:GLN:HE21	16:w:509:CLA:HHB	1.64	0.63
16:Y:504:CLA:H172	16:Y:507:CLA:HBB2	1.81	0.63
12:g:17:ASN:HB2	16:g:511:CLA:HBA1	1.80	0.63
16:G:1203:CLA:HMC2	19:G:4005:BCR:H401	1.79	0.63
16:G:1204:CLA:H2A	16:G:1206:CLA:HED1	1.81	0.63
16:g:507:CLA:H93	19:g:601:BCR:H14C	1.80	0.63
16:A:1101:CLA:H92	17:A:2001:PQN:H201	1.81	0.63
12:v:146:LEU:HD21	16:v:516:CLA:HAB	1.80	0.63
16:X:505:CLA:HBB2	16:X:510:CLA:H92	1.80	0.63
16:B:1215:CLA:HBB2	16:B:1221:CLA:H201	1.80	0.63
16:b:1210:CLA:H43	19:b:4005:BCR:H19C	1.80	0.63
12:y:263:ASN:HD21	12:y:266:ALA:HB3	1.63	0.62
1:A:736:ILE:HG21	16:A:1126:CLA:HMC2	1.80	0.62
1:H:173:LEU:HD21	16:H:1109:CLA:H151	1.82	0.62
12:Y:20:PHE:HZ	16:Y:509:CLA:HAB	1.63	0.62
16:B:1228:CLA:H71	19:F:4016:BCR:H14C	1.81	0.62
1:A:141:SER:HA	16:A:1126:CLA:HMA2	1.82	0.62
16:H:1119:CLA:H12	16:H:1122:CLA:HBA2	1.80	0.62
1:A:583:CYS:HB2	2:B:665:ARG:H	1.64	0.62
3:c:17:CYS:HB2	3:c:54:CYS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:1228:CLA:H71	19:Q:4016:BCR:H14C	1.81	0.62
3:N:17:CYS:HB2	3:N:54:CYS:HB2	1.81	0.62
10:U:132:MET:HG3	19:U:4022:BCR:H23C	1.82	0.62
16:G:1204:CLA:HMB3	16:G:1205:CLA:H3A	1.81	0.61
4:P:41:GLU:H	4:P:71:GLN:HE22	1.47	0.61
16:q:515:CLA:H12	19:q:603:BCR:HC7	1.82	0.61
3:C:17:CYS:HB2	3:C:54:CYS:HB2	1.82	0.61
2:G:454:GLU:HG3	6:Q:7:LEU:HD11	1.80	0.61
16:h:507:CLA:H3A	16:h:511:CLA:HBB1	1.83	0.61
2:G:15:ASP:HB3	2:G:20:ARG:HB2	1.81	0.61
1:A:278:LYS:HG3	1:A:502:LEU:HD12	1.82	0.61
16:B:1204:CLA:H2A	16:B:1206:CLA:HED1	1.83	0.61
16:G:1210:CLA:H43	19:G:4005:BCR:H19C	1.83	0.61
1:a:429:MET:HE2	16:a:1119:CLA:H171	1.83	0.61
8:S:1:MET:HB3	12:s:334:GLU:HG3	1.83	0.61
12:v:242:LEU:HD11	16:v:511:CLA:HBB1	1.83	0.61
16:A:1119:CLA:H12	16:A:1122:CLA:HBA2	1.82	0.61
12:u:49:GLU:HB2	12:u:64:LEU:HD22	1.81	0.60
16:x:505:CLA:H201	16:x:510:CLA:HBB1	1.82	0.60
2:b:339:LEU:HD11	16:b:1202:CLA:H52	1.83	0.60
12:t:34:GLN:HB2	16:t:509:CLA:HMB2	1.83	0.60
16:s:504:CLA:H172	16:s:507:CLA:HBB2	1.84	0.60
1:a:82:VAL:HG21	16:a:1102:CLA:HBB1	1.83	0.60
12:w:272:TYR:HB3	12:w:300:ARG:HB3	1.82	0.60
1:a:173:LEU:HD21	16:a:1109:CLA:H151	1.83	0.60
12:r:272:TYR:HB3	12:r:300:ARG:HB2	1.84	0.60
12:Y:210:VAL:HG21	16:Y:505:CLA:HAB	1.84	0.60
19:s:604:BCR:H362	16:u:508:CLA:H2	1.83	0.60
16:A:1140:CLA:H171	8:J:23:ALA:HB2	1.85	0.59
16:G:1227:CLA:HBB2	16:G:1236:CLA:HMC2	1.84	0.59
16:W:512:CLA:H2	16:W:512:CLA:H111	1.83	0.59
16:H:1120:CLA:HMD2	19:T:4001:BCR:H24C	1.83	0.59
12:s:94:SER:HB3	19:s:602:BCR:H323	1.84	0.59
12:w:146:LEU:HD21	16:w:516:CLA:HAB	1.84	0.59
19:G:4017:BCR:H12C	16:H:1022:CLA:H121	1.82	0.59
1:a:216:GLN:NE2	16:a:1117:CLA:O1D	2.36	0.59
12:Y:110:HIS:HA	12:Y:114:ALA:HB3	1.85	0.59
16:b:1203:CLA:HMC2	19:b:4005:BCR:H401	1.83	0.59
16:b:1228:CLA:H71	19:f:4016:BCR:H14C	1.83	0.59
16:a:1120:CLA:HMD2	19:k:4001:BCR:H24C	1.85	0.59
12:s:108:LEU:HD22	12:u:323:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:SER:HB2	4:D:115:GLN:H	1.67	0.59
16:H:1138:CLA:HAB	16:H:1138:CLA:H112	1.84	0.59
12:x:17:ASN:HB2	16:x:511:CLA:HBA1	1.84	0.59
16:r:505:CLA:HBB2	16:r:510:CLA:H92	1.85	0.58
12:t:223:LEU:HD12	12:t:224:VAL:HG23	1.85	0.58
2:B:587:LEU:HD22	16:B:1234:CLA:HBB2	1.85	0.58
12:X:323:LEU:HD11	12:Y:108:LEU:HD22	1.84	0.58
2:b:15:ASP:HB3	2:b:20:ARG:HB2	1.84	0.58
16:h:510:CLA:H111	19:h:603:BCR:H16C	1.85	0.58
1:H:429:MET:HE3	1:H:554:LEU:HD21	1.85	0.58
12:p:94:SER:HB3	19:p:602:BCR:H323	1.85	0.58
16:q:505:CLA:HBB1	16:q:505:CLA:H52	1.84	0.58
16:w:504:CLA:H172	16:w:507:CLA:HBB2	1.84	0.58
6:Q:24:LEU:O	6:Q:36:ARG:NH2	2.35	0.58
16:b:1216:CLA:HBB1	16:b:1221:CLA:H112	1.84	0.58
16:h:511:CLA:HMD2	19:h:601:BCR:HC8	1.85	0.58
2:B:454:GLU:HG3	6:F:7:LEU:HD11	1.85	0.58
1:H:358:LEU:HD11	16:H:1119:CLA:H51	1.84	0.58
16:A:1101:CLA:H41	16:A:1138:CLA:HMC1	1.84	0.58
14:a:852:LMG:H292	7:i:29:LEU:HB3	1.85	0.58
1:A:120:ILE:HG12	1:A:121:VAL:HG13	1.86	0.58
12:w:20:PHE:HZ	16:w:509:CLA:HAB	1.68	0.58
12:y:34:GLN:HG2	16:y:509:CLA:H3A	1.84	0.58
16:L:1503:CLA:HBD	16:L:1503:CLA:H2	1.86	0.58
12:Y:272:TYR:HB3	12:Y:300:ARG:HB2	1.86	0.58
16:o:503:CLA:HBB1	19:o:602:BCR:H23C	1.86	0.58
12:x:219:ILE:HG12	16:x:501:CLA:HBB2	1.84	0.58
12:W:73:LEU:O	12:W:159:LYS:NZ	2.37	0.58
12:n:214:LEU:HD11	16:n:510:CLA:H71	1.84	0.58
16:t:512:CLA:H102	16:t:512:CLA:H2	1.86	0.58
16:X:502:CLA:H2	19:X:602:BCR:H373	1.85	0.58
16:B:1239:CLA:HAC1	17:B:2002:PQN:H172	1.86	0.57
16:Z:503:CLA:HED3	16:Z:503:CLA:HBA1	1.85	0.57
16:a:1119:CLA:H71	19:a:4008:BCR:H12C	1.86	0.57
2:b:454:GLU:HG3	6:f:7:LEU:HD11	1.85	0.57
2:b:702:ALA:HA	2:b:705:VAL:HB	1.85	0.57
12:h:97:LEU:HD13	19:h:604:BCR:H10C	1.86	0.57
12:w:145:HIS:ND1	16:w:510:CLA:OBD	2.34	0.57
2:G:448:GLU:OE2	6:Q:36:ARG:NH1	2.37	0.57
2:b:25:ILE:HA	16:b:1201:CLA:HMD3	1.86	0.57
16:s:510:CLA:H121	16:s:516:CLA:HMC2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:GLN:HB3	1:H:137:ILE:HB	1.87	0.57
16:t:505:CLA:HBB2	16:t:510:CLA:H71	1.86	0.57
8:J:1:MET:HB3	12:Y:334:GLU:HG3	1.87	0.57
12:W:223:LEU:HD12	12:W:224:VAL:HG23	1.85	0.57
3:c:29:VAL:HG12	4:d:112:ARG:HB3	1.86	0.57
12:x:145:HIS:ND1	16:x:510:CLA:OBD	2.32	0.57
4:P:73:ARG:HD2	4:P:81:GLN:HG2	1.86	0.57
2:G:385:PHE:HZ	16:G:1222:CLA:HAB	1.70	0.57
16:a:1119:CLA:H12	16:a:1122:CLA:HBA2	1.85	0.57
12:h:264:THR:HG22	12:h:300:ARG:HH12	1.69	0.57
12:w:34:GLN:HB2	16:w:509:CLA:HMB2	1.85	0.57
16:v:512:CLA:H2	16:v:512:CLA:H101	1.87	0.57
16:H:1104:CLA:HMB2	16:H:1128:CLA:HBB2	1.86	0.57
16:b:1214:CLA:H41	16:b:1231:CLA:HAA1	1.86	0.57
12:h:219:ILE:HG22	16:h:501:CLA:HBB2	1.87	0.57
16:H:1140:CLA:H171	8:S:23:ALA:HB2	1.86	0.57
12:X:49:GLU:HB2	12:X:64:LEU:HD22	1.85	0.57
12:X:305:ASN:HD22	19:X:601:BCR:H393	1.68	0.57
12:v:97:LEU:HD13	19:v:604:BCR:H10C	1.86	0.57
6:Q:75:ILE:HG23	16:Q:1301:CLA:HAA1	1.86	0.57
12:u:34:GLN:HB2	16:u:509:CLA:HMB2	1.87	0.57
2:B:339:LEU:HD11	16:B:1202:CLA:H52	1.87	0.56
16:b:1204:CLA:H61	19:i:4018:BCR:HC31	1.87	0.56
16:x:506:CLA:HBB2	16:x:507:CLA:H151	1.88	0.56
16:X:515:CLA:HBC2	19:X:603:BCR:H341	1.87	0.56
16:a:1138:CLA:HBB2	6:f:83:GLY:HA3	1.87	0.56
12:g:260:CYS:O	12:g:300:ARG:NH1	2.38	0.56
12:y:141:ILE:HG21	16:y:509:CLA:H202	1.87	0.56
14:A:852:LMG:H292	7:I:29:LEU:HB3	1.86	0.56
4:D:71:GLN:HG3	4:D:75:LYS:HG3	1.87	0.56
16:G:1239:CLA:HAC1	17:G:2002:PQN:H172	1.86	0.56
1:H:79:HIS:HB2	16:H:1103:CLA:HMB2	1.86	0.56
16:W:504:CLA:H122	16:W:507:CLA:HBB2	1.88	0.56
12:Z:73:LEU:O	12:Z:159:LYS:NZ	2.38	0.56
1:a:595:LEU:HD21	16:a:1128:CLA:HBC1	1.85	0.56
16:b:1023:CLA:HBA2	16:b:1023:CLA:HED3	1.88	0.56
16:b:1220:CLA:HBB1	13:b:4018:LHG:H261	1.86	0.56
12:o:34:GLN:HB2	16:o:509:CLA:HMB2	1.88	0.56
16:p:515:CLA:HBC2	19:p:603:BCR:H341	1.86	0.56
12:s:272:TYR:HB3	12:s:300:ARG:HB2	1.86	0.56
16:w:504:CLA:H102	16:w:510:CLA:H42	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:NE2	16:A:1107:CLA:OBD	2.37	0.56
10:L:37:LEU:HD22	16:L:1502:CLA:HBD	1.86	0.56
1:a:141:SER:HA	16:a:1126:CLA:HMA2	1.87	0.56
16:g:505:CLA:H201	16:g:510:CLA:HBB1	1.88	0.56
16:B:1240:CLA:HED3	16:B:1240:CLA:H2A	1.87	0.56
1:H:141:SER:HA	16:H:1126:CLA:HMA2	1.88	0.56
12:Z:97:LEU:HB3	19:Z:604:BCR:H10C	1.86	0.56
12:o:73:LEU:O	12:o:159:LYS:NZ	2.38	0.56
16:B:1204:CLA:H61	19:I:4018:BCR:HC31	1.88	0.56
1:H:531:ASP:O	1:H:535:HIS:ND1	2.35	0.56
12:Y:94:SER:HB3	19:Y:602:BCR:H323	1.86	0.56
16:A:1123:CLA:HBA1	16:A:1127:CLA:H203	1.87	0.56
12:p:145:HIS:ND1	16:p:510:CLA:OBD	2.36	0.56
2:B:646:MET:HE1	16:B:1205:CLA:H41	1.88	0.56
2:G:140:VAL:HA	2:G:143:LEU:HD12	1.88	0.56
12:n:148:PHE:HD2	16:n:502:CLA:H3A	1.70	0.56
16:n:505:CLA:H172	16:n:516:CLA:HAB	1.87	0.56
12:s:135:PRO:HG2	12:s:231:LYS:HE3	1.87	0.56
12:v:145:HIS:ND1	16:v:510:CLA:OBD	2.39	0.56
12:W:66:LEU:HB3	16:W:504:CLA:HED1	1.88	0.56
12:W:181:THR:HB	12:W:205:GLY:HA3	1.87	0.56
16:Z:507:CLA:HMA2	16:Z:507:CLA:H11	1.88	0.56
12:r:131:THR:HG23	12:r:133:GLU:H	1.70	0.56
12:y:226:PRO:HA	16:y:516:CLA:HED3	1.88	0.56
17:B:2002:PQN:H301	19:L:4019:BCR:HC7	1.89	0.55
2:b:587:LEU:HD22	16:b:1234:CLA:HBB2	1.88	0.55
12:g:141:ILE:HG21	16:g:509:CLA:H192	1.87	0.55
12:t:73:LEU:O	12:t:159:LYS:NZ	2.39	0.55
1:A:173:LEU:HD21	16:A:1109:CLA:H151	1.88	0.55
2:B:56:ILE:HD11	21:M:4021:ECH:H23	1.89	0.55
16:G:1204:CLA:H3A	16:G:1205:CLA:HMB3	1.88	0.55
12:n:272:TYR:HB3	12:n:300:ARG:HB2	1.89	0.55
12:t:159:LYS:HA	12:t:163:TRP:HB2	1.88	0.55
16:x:510:CLA:HED1	16:x:510:CLA:H2	1.88	0.55
1:A:400:LEU:HD21	16:A:1104:CLA:H142	1.89	0.55
2:B:420:LEU:HG	16:B:1236:CLA:HBB1	1.88	0.55
5:E:27:SER:HB3	5:E:38:ILE:HD12	1.88	0.55
2:G:25:ILE:HA	16:G:1201:CLA:HMD3	1.88	0.55
12:p:42:ALA:HB1	16:p:504:CLA:HED3	1.88	0.55
12:s:34:GLN:HG2	16:s:509:CLA:HHB	1.88	0.55
12:s:214:LEU:HD21	16:s:510:CLA:H72	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:v:214:LEU:HD21	16:v:510:CLA:H71	1.88	0.55
16:A:1013:CLA:H101	19:A:4011:BCR:H23C	1.88	0.55
2:B:140:VAL:HA	2:B:143:LEU:HD12	1.88	0.55
14:H:4101:LMG:H112	10:U:67:LEU:HB3	1.87	0.55
5:O:8:LYS:H	5:O:70:GLN:HG2	1.71	0.55
1:a:435:ALA:O	1:a:439:HIS:ND1	2.40	0.55
16:b:1229:CLA:H72	19:f:4016:BCR:HC32	1.88	0.55
16:r:510:CLA:HED1	16:r:510:CLA:H2	1.89	0.55
12:t:110:HIS:HA	12:t:114:ALA:HB3	1.88	0.55
12:W:110:HIS:HA	12:W:114:ALA:HB3	1.89	0.55
12:t:272:TYR:HB3	12:t:300:ARG:HB2	1.89	0.55
12:u:59:MET:HG3	12:u:68:PRO:HG3	1.89	0.55
16:B:1204:CLA:H162	16:B:1205:CLA:H201	1.87	0.55
16:B:1207:CLA:H193	16:U:1501:CLA:H12	1.87	0.55
2:b:448:GLU:OE2	6:f:36:ARG:NH1	2.39	0.55
16:u:503:CLA:HBB1	19:u:602:BCR:H23C	1.88	0.55
16:L:1501:CLA:H12	16:b:1207:CLA:H193	1.88	0.55
1:a:369:HIS:ND1	16:a:1116:CLA:OBD	2.40	0.55
12:r:141:ILE:HG21	16:r:509:CLA:H192	1.88	0.55
12:t:333:VAL:HA	16:u:512:CLA:H8	1.89	0.55
16:n:502:CLA:HED3	16:n:503:CLA:HBB2	1.89	0.55
16:B:1235:CLA:HBC2	19:J:4015:BCR:HC7	1.89	0.55
12:n:2:GLN:NE2	12:n:324:ARG:O	2.40	0.55
12:y:45:PHE:HA	12:y:48:PHE:HB3	1.89	0.55
16:B:1222:CLA:HMA1	19:B:4010:BCR:H17C	1.88	0.55
2:G:346:VAL:HG21	16:G:1225:CLA:HHD	1.88	0.55
16:H:1124:CLA:HMB2	16:H:1137:CLA:HAA1	1.89	0.55
12:r:17:ASN:HB2	16:r:511:CLA:HBA1	1.89	0.55
12:t:19:ARG:NH1	16:t:512:CLA:OBD	2.40	0.55
2:G:257:PHE:HD2	2:G:489:ALA:HB3	1.71	0.54
10:l:67:LEU:HD12	16:l:1503:CLA:HHB	1.88	0.54
12:p:210:VAL:HG21	16:p:505:CLA:HAB	1.88	0.54
16:r:507:CLA:H93	19:r:601:BCR:H14C	1.88	0.54
16:r:515:CLA:HBC2	19:r:603:BCR:H341	1.89	0.54
16:s:504:CLA:H13	16:s:506:CLA:HMD2	1.89	0.54
1:A:214:GLY:HA3	16:A:1113:CLA:HAB	1.88	0.54
17:A:2001:PQN:H142	19:B:4014:BCR:H271	1.89	0.54
19:G:4014:BCR:H19C	16:H:1138:CLA:H41	1.88	0.54
1:H:573:PRO:HG3	5:O:50:SER:HB3	1.88	0.54
16:o:505:CLA:H122	16:o:510:CLA:H61	1.90	0.54
12:r:3:THR:HB	12:r:7:ASP:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:LEU:HD21	16:A:1128:CLA:HBC1	1.87	0.54
1:H:595:LEU:HD21	16:H:1128:CLA:HBC1	1.89	0.54
16:W:502:CLA:H12	16:W:504:CLA:HMC2	1.90	0.54
12:X:34:GLN:HB2	16:X:509:CLA:HMB2	1.89	0.54
4:d:65:CYS:HB3	4:d:85:ILE:HD13	1.89	0.54
16:q:503:CLA:HED3	16:q:503:CLA:HBA1	1.89	0.54
12:t:181:THR:HB	12:t:205:GLY:HA3	1.90	0.54
1:A:560:ARG:NH2	4:D:15:THR:O	2.41	0.54
2:B:393:VAL:HG23	2:B:394:ARG:HG3	1.89	0.54
2:G:702:ALA:HA	2:G:705:VAL:HB	1.90	0.54
1:H:435:ALA:O	1:H:439:HIS:ND1	2.41	0.54
4:P:8:PRO:O	4:P:51:ASN:ND2	2.40	0.54
4:d:8:PRO:O	4:d:51:ASN:ND2	2.41	0.54
12:r:260:CYS:O	12:r:300:ARG:NH1	2.39	0.54
12:s:255:VAL:HG21	16:s:505:CLA:H92	1.89	0.54
1:A:573:PRO:HG3	5:E:50:SER:HB3	1.89	0.54
16:L:1503:CLA:H161	16:b:1207:CLA:H111	1.90	0.54
12:X:272:TYR:HB3	12:X:300:ARG:HB2	1.89	0.54
2:b:181:GLY:HA3	16:b:1210:CLA:HBB1	1.90	0.54
16:g:504:CLA:H172	16:g:507:CLA:HBB2	1.90	0.54
16:y:505:CLA:H171	16:y:510:CLA:H122	1.88	0.54
2:b:454:GLU:OE1	2:b:459:GLN:NE2	2.39	0.54
12:w:239:GLU:OE2	12:w:324:ARG:NH1	2.41	0.54
3:C:29:VAL:HG12	4:D:112:ARG:HB3	1.88	0.54
2:G:587:LEU:HD22	16:G:1234:CLA:HBB2	1.89	0.54
6:f:75:ILE:HG23	16:f:1301:CLA:HAA1	1.88	0.54
14:f:4017:LMG:H121	14:f:4017:LMG:H301	1.89	0.54
12:p:255:VAL:HG21	16:p:505:CLA:H92	1.90	0.54
12:q:267:TYR:O	12:q:300:ARG:NH2	2.40	0.54
2:B:25:ILE:HA	16:B:1201:CLA:HMD3	1.89	0.54
6:F:75:ILE:HG23	16:F:1301:CLA:HAA1	1.90	0.54
3:N:41:SER:HB2	4:P:115:GLN:H	1.73	0.54
12:o:124:GLN:NE2	16:o:501:CLA:OBD	2.41	0.54
12:t:214:LEU:HD11	16:t:510:CLA:H72	1.90	0.54
16:v:504:CLA:H102	16:v:504:CLA:H41	1.89	0.54
2:B:257:PHE:HD2	2:B:489:ALA:HB3	1.73	0.54
2:B:448:GLU:OE2	6:F:36:ARG:NH1	2.41	0.54
2:B:702:ALA:HA	2:B:705:VAL:HB	1.90	0.54
16:H:1013:CLA:H101	19:H:4011:BCR:H23C	1.89	0.54
10:L:151:ILE:HG23	16:b:1207:CLA:HBA1	1.90	0.54
16:X:503:CLA:HBB1	19:X:602:BCR:H23C	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:401:ASN:OD1	2:b:404:ASN:ND2	2.40	0.54
12:n:181:THR:HB	12:n:205:GLY:HA3	1.89	0.54
2:G:268:LEU:HD13	16:G:1214:CLA:HMA2	1.90	0.54
1:H:369:HIS:ND1	16:H:1116:CLA:OBD	2.40	0.54
10:L:46:PRO:HB2	10:L:122:GLN:HB2	1.89	0.54
12:W:267:TYR:O	12:W:300:ARG:NH2	2.41	0.54
1:a:583:CYS:HB2	2:b:665:ARG:H	1.73	0.54
16:b:1221:CLA:HMA2	16:b:1221:CLA:H11	1.90	0.54
12:s:45:PHE:HA	12:s:48:PHE:HB3	1.90	0.54
12:Z:213:LEU:HD21	16:Z:510:CLA:H142	1.89	0.53
16:q:504:CLA:H111	16:q:510:CLA:H12	1.90	0.53
12:x:260:CYS:O	12:x:300:ARG:NH1	2.41	0.53
1:A:686:LEU:HB3	2:B:662:ILE:HG12	1.90	0.53
19:U:4022:BCR:H363	16:l:1501:CLA:HAA2	1.91	0.53
9:k:60:VAL:HG13	16:k:4003:CLA:HAC2	1.90	0.53
12:r:145:HIS:ND1	16:r:510:CLA:OBD	2.37	0.53
13:A:851:LHG:HC62	16:A:1801:CLA:HMB3	1.89	0.53
1:H:216:GLN:NE2	16:H:1117:CLA:O1D	2.42	0.53
2:b:140:VAL:HA	2:b:143:LEU:HD12	1.88	0.53
12:n:31:HIS:HD2	16:n:509:CLA:H91	1.74	0.53
12:o:26:LEU:HD13	16:o:512:CLA:HAA2	1.90	0.53
16:r:505:CLA:H201	16:r:510:CLA:HBB1	1.89	0.53
1:A:369:HIS:ND1	16:A:1116:CLA:OBD	2.41	0.53
19:G:4014:BCR:H271	17:H:2001:PQN:H142	1.90	0.53
1:H:115:GLN:NE2	16:H:1107:CLA:OBD	2.37	0.53
16:H:1112:CLA:HAB	19:H:4002:BCR:H14C	1.89	0.53
16:H:1122:CLA:H121	16:H:1137:CLA:HAA2	1.90	0.53
16:H:1237:CLA:H203	10:U:61:LEU:HD11	1.90	0.53
12:W:50:ILE:HD11	12:W:86:THR:HB	1.91	0.53
16:a:1107:CLA:HBB1	19:j:4012:BCR:HC7	1.91	0.53
2:b:646:MET:HE1	16:b:1205:CLA:H41	1.90	0.53
16:n:507:CLA:H93	19:n:601:BCR:H14C	1.91	0.53
16:p:504:CLA:H13	16:p:506:CLA:HMD2	1.91	0.53
12:u:200:LEU:HD12	12:u:265:LEU:HD11	1.91	0.53
12:y:42:ALA:HB1	16:y:504:CLA:HED3	1.91	0.53
16:A:1124:CLA:H42	16:A:1136:CLA:HBA1	1.89	0.53
16:B:1235:CLA:H152	19:F:4016:BCR:H402	1.89	0.53
17:B:2002:PQN:H142	19:B:4017:BCR:H271	1.89	0.53
17:G:2002:PQN:H142	19:G:4017:BCR:H271	1.90	0.53
12:X:49:GLU:HG3	12:X:67:LEU:HG	1.91	0.53
12:Y:255:VAL:HG21	16:Y:505:CLA:H92	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:194:PHE:HZ	19:r:602:BCR:H312	1.73	0.53
12:v:34:GLN:HG2	16:v:509:CLA:HHB	1.90	0.53
12:w:267:TYR:O	12:w:300:ARG:NH2	2.42	0.53
2:b:69:ALA:HB2	2:b:135:LEU:HB2	1.91	0.53
2:b:257:PHE:HD2	2:b:489:ALA:HB3	1.73	0.53
12:h:145:HIS:ND1	16:h:510:CLA:OBD	2.40	0.53
12:s:326:LEU:HD13	12:w:113:ARG:HB2	1.90	0.53
16:s:502:CLA:H11	16:s:504:CLA:HMC2	1.91	0.53
1:A:216:GLN:HA	1:A:220:SER:HB2	1.91	0.53
1:A:604:ILE:HD12	15:A:1011:CL0:H53	1.89	0.53
12:W:70:LEU:HD22	12:W:92:ILE:HD13	1.91	0.53
12:g:146:LEU:HD22	12:g:214:LEU:HD22	1.91	0.53
16:g:506:CLA:HBB2	16:g:507:CLA:H151	1.90	0.53
16:p:515:CLA:H162	12:q:98:ILE:HG12	1.91	0.53
16:s:506:CLA:HBB2	16:s:507:CLA:H151	1.90	0.53
2:B:339:LEU:HB3	2:B:380:LEU:HD13	1.91	0.53
10:U:6:GLN:O	10:U:9:GLN:NE2	2.42	0.53
2:b:577:MET:HG3	2:b:707:LEU:HD21	1.91	0.53
16:b:1240:CLA:HED3	16:b:1240:CLA:H2A	1.91	0.53
16:o:508:CLA:H2	19:p:604:BCR:H362	1.91	0.53
12:q:145:HIS:HB3	16:q:509:CLA:H91	1.90	0.53
16:v:507:CLA:H152	16:v:511:CLA:H202	1.91	0.53
12:X:200:LEU:HD12	12:X:265:LEU:HD11	1.91	0.53
12:Y:42:ALA:HB1	16:Y:504:CLA:HED3	1.90	0.53
12:Y:323:LEU:HD22	12:Z:112:LEU:HD12	1.91	0.53
12:Z:267:TYR:O	12:Z:300:ARG:NH2	2.42	0.53
16:a:1124:CLA:HAB	19:a:4008:BCR:H311	1.91	0.53
10:l:37:LEU:HD22	16:l:1502:CLA:HBD	1.91	0.53
12:p:54:ASP:OD1	12:p:62:GLN:NE2	2.42	0.53
12:v:134:ASN:ND2	12:v:137:GLN:OE1	2.42	0.53
2:B:434:LEU:HD12	2:B:515:LEU:HD21	1.91	0.53
4:D:89:TYR:HB2	4:D:93:GLU:HB3	1.91	0.53
2:G:339:LEU:HD11	16:G:1202:CLA:H52	1.91	0.53
12:W:34:GLN:HB2	16:W:509:CLA:HMB2	1.90	0.53
16:a:1013:CLA:H151	16:a:1101:CLA:H202	1.90	0.53
12:h:246:LEU:HD13	16:h:511:CLA:HAB	1.90	0.53
12:q:145:HIS:ND1	16:q:510:CLA:OBD	2.37	0.53
16:B:1220:CLA:HBB1	13:B:4018:LHG:H261	1.91	0.52
2:G:375:TYR:HA	2:G:584:LEU:HD13	1.91	0.52
1:a:224:ASN:HA	1:a:227:LEU:HB2	1.90	0.52
1:a:434:ASP:OD2	1:a:560:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:b:1229:CLA:HMB2	19:b:4014:BCR:H10C	1.91	0.52
12:h:17:ASN:ND2	16:h:507:CLA:O1A	2.42	0.52
12:p:110:HIS:HA	12:p:114:ALA:HB3	1.91	0.52
12:p:214:LEU:HD21	16:p:510:CLA:H72	1.90	0.52
16:p:515:CLA:H141	19:q:604:BCR:H11C	1.90	0.52
19:s:603:BCR:HC42	16:w:503:CLA:HMB3	1.91	0.52
12:t:70:LEU:HD22	12:t:92:ILE:HD13	1.90	0.52
16:t:502:CLA:H12	16:t:504:CLA:HMC2	1.91	0.52
16:G:1222:CLA:HMA1	19:G:4010:BCR:H17C	1.91	0.52
10:U:37:LEU:HD22	16:U:1502:CLA:HBD	1.90	0.52
1:A:217:ILE:HD11	1:A:275:LEU:HD21	1.91	0.52
1:A:579:ARG:NH1	25:A:902:HOH:O	2.41	0.52
17:a:2001:PQN:H292	8:j:16:MET:HE1	1.90	0.52
12:n:267:TYR:O	12:n:300:ARG:NH2	2.43	0.52
12:p:17:ASN:ND2	16:p:507:CLA:O1A	2.43	0.52
16:A:1124:CLA:H91	19:A:4008:BCR:H23C	1.90	0.52
2:G:582:ASN:HB2	16:G:1012:CLA:HBC2	1.92	0.52
16:H:1104:CLA:H2	16:H:1104:CLA:HMA2	1.92	0.52
8:S:26:LEU:O	8:S:30:ASN:ND2	2.43	0.52
16:a:1122:CLA:H2A	16:a:1122:CLA:HED3	1.90	0.52
16:b:1235:CLA:HBC2	19:j:4015:BCR:HC7	1.90	0.52
12:r:214:LEU:HD21	16:r:510:CLA:H72	1.92	0.52
2:B:392:PHE:HB3	2:B:539:ARG:HG3	1.92	0.52
16:G:1207:CLA:H151	19:U:4022:BCR:H362	1.91	0.52
16:Y:510:CLA:H121	16:Y:516:CLA:HMC2	1.92	0.52
1:a:573:PRO:HG3	5:e:50:SER:HB3	1.90	0.52
12:p:292:LEU:HD12	12:p:293:PRO:HD2	1.90	0.52
16:r:504:CLA:H172	16:r:507:CLA:HBB2	1.91	0.52
12:u:310:LEU:HD13	16:u:506:CLA:HMC3	1.90	0.52
2:G:56:ILE:HD11	21:V:4021:ECH:H23	1.92	0.52
16:X:504:CLA:H2	16:X:506:CLA:H11	1.92	0.52
2:b:85:ARG:NH1	2:b:731:GLY:O	2.43	0.52
12:s:226:PRO:O	12:s:231:LYS:NZ	2.43	0.52
12:v:17:ASN:ND2	16:v:507:CLA:O1A	2.42	0.52
16:B:1207:CLA:H151	19:L:4022:BCR:H362	1.90	0.52
2:G:403:ASP:OD1	2:G:408:ARG:NH1	2.40	0.52
1:H:72:ILE:O	1:H:76:HIS:ND1	2.42	0.52
17:H:2001:PQN:H292	8:S:16:MET:HE1	1.91	0.52
12:g:131:THR:HG23	12:g:133:GLU:H	1.75	0.52
12:q:54:ASP:O	12:q:62:GLN:NE2	2.43	0.52
16:w:503:CLA:HED3	16:w:503:CLA:HBA1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:2001:PQN:H292	8:J:16:MET:HE1	1.92	0.52
4:D:8:PRO:O	4:D:51:ASN:ND2	2.43	0.52
16:G:1223:CLA:H111	19:G:4009:BCR:H373	1.91	0.52
16:a:1124:CLA:H42	16:a:1136:CLA:HBA1	1.91	0.52
12:v:169:ALA:HB3	12:v:265:LEU:HD12	1.92	0.52
16:B:1214:CLA:H41	16:B:1231:CLA:HAA1	1.92	0.52
19:L:4022:BCR:H363	16:U:1501:CLA:HAA2	1.92	0.52
19:L:4022:BCR:H281	19:U:4022:BCR:H282	1.92	0.52
16:b:1201:CLA:HED2	16:b:1201:CLA:H2A	1.92	0.52
16:b:1215:CLA:H92	16:b:1221:CLA:H41	1.92	0.52
12:v:73:LEU:HB3	12:v:159:LYS:HE3	1.92	0.52
12:x:59:MET:HA	12:x:62:GLN:HE21	1.75	0.52
16:x:504:CLA:H172	16:x:507:CLA:HBB2	1.91	0.52
1:A:293:THR:O	1:A:297:HIS:ND1	2.42	0.51
10:L:157:ASN:ND2	2:b:94:PRO:O	2.43	0.51
12:X:110:HIS:HA	12:X:114:ALA:HB3	1.92	0.51
12:n:168:ASP:OD2	12:n:175:ARG:NH1	2.43	0.51
16:r:508:CLA:HBC2	13:r:605:LHG:H131	1.92	0.51
12:w:332:ARG:HG3	12:w:335:GLN:HE21	1.75	0.51
16:A:1122:CLA:H2A	16:A:1122:CLA:HED3	1.92	0.51
16:G:1214:CLA:H41	16:G:1231:CLA:HAA1	1.91	0.51
16:H:1013:CLA:H3A	16:H:1013:CLA:H43	1.91	0.51
1:a:348:TRP:HB3	16:a:1103:CLA:HAC1	1.93	0.51
12:s:54:ASP:OD1	12:s:62:GLN:NE2	2.43	0.51
1:A:473:ASP:OD1	1:A:479:GLN:NE2	2.43	0.51
1:A:539:ALA:HB1	16:A:1136:CLA:HMB3	1.92	0.51
16:A:1106:CLA:HBB2	16:A:1126:CLA:H142	1.93	0.51
16:G:1239:CLA:H12	17:G:2002:PQN:H293	1.93	0.51
16:H:1105:CLA:H2A	16:H:1107:CLA:HED1	1.93	0.51
16:H:1126:CLA:H193	19:S:4012:BCR:H10C	1.92	0.51
1:a:400:LEU:HD21	16:a:1104:CLA:H142	1.91	0.51
2:b:239:THR:HG23	2:b:241:GLY:H	1.74	0.51
12:g:286:PHE:H	12:g:305:ASN:HD21	1.58	0.51
1:A:362:LEU:HD21	16:A:1117:CLA:H93	1.93	0.51
10:L:145:LEU:HD11	16:L:1503:CLA:H42	1.92	0.51
12:W:161:MET:HB2	12:W:178:SER:HA	1.93	0.51
16:W:505:CLA:HBB1	16:W:510:CLA:H41	1.92	0.51
19:a:4011:BCR:H271	16:b:1229:CLA:HMB3	1.91	0.51
16:b:1204:CLA:H2A	16:b:1206:CLA:HED1	1.92	0.51
12:u:267:TYR:O	12:u:300:ARG:NH2	2.42	0.51
13:u:605:LHG:H241	13:u:605:LHG:HC91	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:v:169:ALA:O	12:v:172:GLN:NE2	2.44	0.51
1:A:435:ALA:O	1:A:439:HIS:ND1	2.44	0.51
16:B:1201:CLA:H11	13:I:103:LHG:H291	1.92	0.51
16:G:1225:CLA:H61	21:G:4006:ECH:H39A	1.93	0.51
12:Y:54:ASP:OD1	12:Y:62:GLN:NE2	2.43	0.51
12:Z:145:HIS:ND1	16:Z:510:CLA:OBD	2.39	0.51
16:a:1122:CLA:HHB	16:a:1801:CLA:HAB	1.91	0.51
16:p:502:CLA:H11	16:p:504:CLA:HMC2	1.92	0.51
12:y:314:PHE:O	12:y:318:HIS:N	2.42	0.51
2:B:70:TRP:NE1	7:I:6:ALA:O	2.34	0.51
1:H:650:LEU:HD11	15:H:1011:CL0:H43	1.91	0.51
12:X:251:LEU:HD21	16:X:513:CLA:HBB1	1.91	0.51
12:Z:34:GLN:HB2	16:Z:509:CLA:HMB2	1.92	0.51
1:a:62:THR:HG22	1:a:64:ASP:H	1.74	0.51
16:a:1132:CLA:H201	16:l:1502:CLA:HBA1	1.93	0.51
8:j:12:PRO:HB2	19:j:4013:BCR:H271	1.91	0.51
10:l:36:ASN:HB3	16:l:1501:CLA:HBC2	1.91	0.51
12:s:145:HIS:ND1	16:s:510:CLA:OBD	2.36	0.51
12:v:146:LEU:HD22	12:v:214:LEU:HD22	1.92	0.51
12:v:302:TRP:CD2	16:v:514:CLA:H3A	2.46	0.51
12:x:34:GLN:HB2	16:x:509:CLA:HMB2	1.92	0.51
16:x:515:CLA:H112	16:x:515:CLA:HMC2	1.92	0.51
1:H:412:MET:O	1:H:557:ARG:NH1	2.40	0.51
19:U:4022:BCR:H393	10:l:133:GLY:HA3	1.93	0.51
12:g:243:SER:O	12:g:318:HIS:ND1	2.43	0.51
12:g:323:LEU:HD22	16:g:508:CLA:HMD1	1.93	0.51
12:s:34:GLN:HB2	16:s:509:CLA:HMB2	1.92	0.51
12:y:145:HIS:ND1	16:y:510:CLA:OBD	2.37	0.51
16:A:1117:CLA:H92	16:A:1127:CLA:H91	1.93	0.51
5:E:5:ARG:NH1	5:E:26:ALA:O	2.44	0.51
1:H:293:THR:O	1:H:297:HIS:ND1	2.44	0.51
6:Q:55:VAL:HG12	6:Q:65:PHE:HB2	1.93	0.51
12:Z:308:PHE:HZ	16:Z:517:CLA:HAB	1.75	0.51
16:b:1222:CLA:HMA1	19:b:4010:BCR:H17C	1.92	0.51
12:o:145:HIS:ND1	16:o:510:CLA:OBD	2.43	0.51
16:A:1140:CLA:H152	19:J:4012:BCR:H353	1.92	0.51
16:G:1220:CLA:HBB1	13:G:4018:LHG:H261	1.93	0.51
1:H:204:LEU:HD11	16:H:1111:CLA:H42	1.93	0.51
1:H:539:ALA:O	1:H:543:HIS:ND1	2.44	0.51
16:H:1134:CLA:HMB1	19:H:4008:BCR:H281	1.92	0.51
16:Y:508:CLA:HMA2	16:Y:517:CLA:H93	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:510:CLA:H121	16:Z:516:CLA:HMC2	1.93	0.51
16:p:510:CLA:H121	16:p:516:CLA:HMC2	1.93	0.51
12:w:233:VAL:HG13	12:w:234:LEU:HG	1.92	0.51
16:A:1101:CLA:H141	19:A:4011:BCR:H292	1.92	0.51
2:G:285:ILE:O	2:G:289:HIS:ND1	2.42	0.51
1:H:604:ILE:HD12	15:H:1011:CL0:H53	1.93	0.51
10:L:36:ASN:HB3	16:L:1501:CLA:HBC2	1.92	0.51
12:Y:249:ILE:HG12	16:Y:506:CLA:HAC1	1.93	0.51
1:a:650:LEU:HD11	15:a:1011:CL0:H43	1.93	0.51
16:a:1101:CLA:H171	19:a:4011:BCR:H401	1.92	0.51
16:p:504:CLA:H203	16:p:506:CLA:H42	1.92	0.51
16:q:504:CLA:H172	16:q:507:CLA:HBB2	1.91	0.51
16:q:505:CLA:HMB2	19:q:603:BCR:H23C	1.93	0.51
12:r:34:GLN:HB2	16:r:509:CLA:HMB2	1.93	0.51
12:y:73:LEU:HB3	12:y:159:LYS:HE3	1.92	0.51
16:A:1126:CLA:H141	19:J:4012:BCR:H14C	1.91	0.50
2:B:704:LEU:HD11	14:B:848:LMG:H341	1.92	0.50
2:G:388:GLY:HA2	19:G:4010:BCR:HC22	1.93	0.50
1:a:115:GLN:HB3	1:a:137:ILE:HB	1.93	0.50
1:a:604:ILE:HD12	15:a:1011:CL0:H53	1.93	0.50
12:t:2:GLN:NE2	12:t:324:ARG:O	2.44	0.50
2:B:667:TYR:OH	16:B:1023:CLA:OBD	2.28	0.50
16:G:1207:CLA:HBA1	10:l:151:ILE:HG23	1.93	0.50
1:H:348:TRP:HB3	16:H:1103:CLA:HAC1	1.92	0.50
1:H:400:LEU:HD21	16:H:1104:CLA:H142	1.92	0.50
16:H:1106:CLA:HBB2	16:H:1126:CLA:H142	1.93	0.50
19:U:4022:BCR:H322	16:a:1130:CLA:H101	1.93	0.50
19:U:4022:BCR:H15C	10:l:56:ALA:HA	1.93	0.50
16:s:515:CLA:H92	16:s:515:CLA:H41	1.92	0.50
12:u:305:ASN:HB3	19:u:601:BCR:H382	1.93	0.50
16:x:505:CLA:HBB2	16:x:510:CLA:H92	1.92	0.50
2:b:290:MET:HA	16:b:1218:CLA:HHD	1.93	0.50
2:b:378:GLY:HA3	2:b:584:LEU:HD11	1.92	0.50
12:r:239:GLU:OE1	12:r:324:ARG:NH1	2.44	0.50
12:s:42:ALA:HB1	16:s:504:CLA:HED3	1.93	0.50
16:y:508:CLA:HAC2	16:y:511:CLA:HAC2	1.92	0.50
1:A:447:LEU:HB3	1:A:540:PHE:HB2	1.93	0.50
1:H:482:PHE:HB3	16:H:1135:CLA:H12	1.93	0.50
16:a:1022:CLA:H122	19:b:4017:BCR:H12C	1.92	0.50
12:h:59:MET:N	12:h:59:MET:SD	2.85	0.50
16:s:508:CLA:HMA2	16:s:517:CLA:H93	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:x:508:CLA:HBC1	16:x:511:CLA:HMD3	1.93	0.50
16:A:1139:CLA:H72	8:J:18:LEU:HD12	1.93	0.50
16:B:1203:CLA:HBB1	16:B:1225:CLA:HMC2	1.94	0.50
16:H:1119:CLA:HBA1	16:H:1125:CLA:H91	1.92	0.50
16:Y:504:CLA:H13	16:Y:506:CLA:HMD2	1.93	0.50
16:a:1103:CLA:H72	19:a:4003:BCR:H23C	1.93	0.50
16:a:1131:CLA:H101	16:b:1239:CLA:H72	1.92	0.50
2:b:660:PHE:HB3	2:b:702:ALA:HB1	1.93	0.50
16:b:1203:CLA:H62	16:b:1226:CLA:H8	1.93	0.50
12:n:111:THR:HG23	12:n:112:LEU:HG	1.91	0.50
1:A:115:GLN:HB3	1:A:137:ILE:HB	1.93	0.50
6:F:55:VAL:HG12	6:F:65:PHE:HB2	1.94	0.50
1:a:531:ASP:O	1:a:535:HIS:ND1	2.39	0.50
1:a:539:ALA:HB1	16:a:1136:CLA:HMB3	1.92	0.50
16:p:505:CLA:H72	16:p:505:CLA:HBB1	1.94	0.50
2:G:688:VAL:HG11	16:H:1237:CLA:HAB	1.94	0.50
16:G:1220:CLA:HMA1	16:G:1240:CLA:HMC1	1.94	0.50
7:R:25:VAL:HG22	16:l:1501:CLA:H111	1.93	0.50
16:X:512:CLA:H143	19:X:604:BCR:H292	1.94	0.50
12:s:73:LEU:HG	12:s:159:LYS:HE3	1.93	0.50
12:u:148:PHE:HD2	16:u:502:CLA:H3A	1.76	0.50
16:x:510:CLA:H8	19:x:603:BCR:H17C	1.92	0.50
2:B:375:TYR:HA	2:B:584:LEU:HD13	1.94	0.50
16:G:1206:CLA:HMB2	16:H:1022:CLA:H172	1.93	0.50
1:H:305:ILE:O	1:H:309:HIS:ND1	2.43	0.50
12:Y:169:ALA:HB2	12:Y:268:PRO:HB3	1.94	0.50
16:n:506:CLA:HBB2	16:n:507:CLA:H151	1.94	0.50
12:s:54:ASP:OD1	12:s:54:ASP:N	2.45	0.50
16:y:513:CLA:HMD3	19:y:603:BCR:H382	1.94	0.50
16:A:1131:CLA:H101	16:B:1239:CLA:H71	1.93	0.50
16:B:1206:CLA:H202	7:I:26:THR:HG21	1.94	0.50
1:H:217:ILE:HD11	1:H:275:LEU:HD21	1.93	0.50
16:H:1237:CLA:H201	16:U:1502:CLA:HAB	1.94	0.50
12:Z:177:VAL:HG21	12:Z:204:VAL:HG21	1.93	0.50
4:d:137:ALA:HB3	4:d:140:GLU:HG3	1.93	0.50
12:t:249:ILE:HG12	16:t:506:CLA:HAC1	1.94	0.50
12:w:249:ILE:HG12	16:w:506:CLA:HAC1	1.94	0.50
16:A:1132:CLA:HMA2	10:L:68:LEU:HB3	1.94	0.49
2:B:44:GLN:OE1	2:B:162:ARG:NH1	2.42	0.49
2:B:343:THR:HB	2:B:377:ALA:HB2	1.94	0.49
1:H:62:THR:HG22	1:H:64:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:560:ARG:NH2	4:P:15:THR:O	2.44	0.49
12:Y:34:GLN:HG2	16:Y:509:CLA:HHB	1.94	0.49
1:a:15:SER:HB2	1:a:186:LYS:HD3	1.94	0.49
12:g:19:ARG:NH1	16:g:512:CLA:OBD	2.40	0.49
12:q:249:ILE:HG12	16:q:506:CLA:HAC1	1.94	0.49
12:s:210:VAL:HG21	16:s:505:CLA:HAB	1.94	0.49
12:u:73:LEU:O	12:u:159:LYS:NZ	2.45	0.49
1:A:200:HIS:ND1	16:A:1123:CLA:OBD	2.45	0.49
16:B:1220:CLA:HMA1	16:B:1240:CLA:HMC1	1.94	0.49
12:W:272:TYR:HB3	12:W:300:ARG:HB2	1.94	0.49
12:n:52:ARG:HH12	16:n:514:CLA:HED3	1.78	0.49
12:q:236:PHE:HE1	16:q:510:CLA:HMC1	1.77	0.49
12:q:323:LEU:HD22	16:q:508:CLA:HMD1	1.95	0.49
1:A:531:ASP:O	1:A:535:HIS:ND1	2.39	0.49
16:A:1106:CLA:HAB	16:A:1126:CLA:H112	1.94	0.49
16:A:1121:CLA:HAB	16:A:1801:CLA:HAB	1.94	0.49
16:A:1130:CLA:H101	19:l:4022:BCR:H322	1.93	0.49
14:A:4101:LMG:H171	14:A:4201:LMG:H151	1.94	0.49
16:B:1211:CLA:H162	19:B:4005:BCR:H14C	1.94	0.49
3:C:6:LYS:HD2	4:D:118:LYS:HD3	1.94	0.49
2:G:94:PRO:O	10:l:157:ASN:ND2	2.46	0.49
2:G:378:GLY:HA3	2:G:584:LEU:HD11	1.94	0.49
4:P:43:PRO:HD3	4:P:68:LEU:HD12	1.95	0.49
12:W:17:ASN:HB2	16:W:511:CLA:HAA2	1.94	0.49
12:Y:54:ASP:OD1	12:Y:54:ASP:N	2.45	0.49
5:e:27:SER:HB3	5:e:38:ILE:HD12	1.93	0.49
12:u:17:ASN:HB2	16:u:511:CLA:HAA2	1.93	0.49
2:B:4:LYS:HZ2	7:I:36:SER:HB3	1.77	0.49
2:B:385:PHE:HZ	16:B:1222:CLA:HAB	1.77	0.49
1:H:692:TYR:OH	16:H:1013:CLA:OBD	2.25	0.49
12:Y:160:ALA:HA	12:Y:165:GLY:HA2	1.94	0.49
12:Z:42:ALA:O	12:Z:46:THR:OG1	2.28	0.49
12:Z:146:LEU:HD22	12:Z:214:LEU:HD22	1.94	0.49
19:a:4002:BCR:H19C	19:a:4003:BCR:H311	1.94	0.49
12:g:145:HIS:ND1	16:g:510:CLA:OBD	2.39	0.49
10:l:73:ASP:OD1	10:l:73:ASP:N	2.44	0.49
2:B:268:LEU:HD13	16:B:1214:CLA:HMA2	1.93	0.49
2:G:426:PHE:O	2:G:430:HIS:ND1	2.37	0.49
2:G:684:LEU:HD11	10:U:37:LEU:HD13	1.93	0.49
12:g:180:PRO:HA	12:g:201:GLU:HB3	1.93	0.49
12:p:246:LEU:HD23	16:p:509:CLA:HED1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:239:GLU:OE2	12:q:324:ARG:NE	2.42	0.49
12:s:53:PHE:HB2	12:s:64:LEU:HD21	1.94	0.49
16:y:508:CLA:H42	16:y:517:CLA:H92	1.95	0.49
16:H:1122:CLA:HMB2	16:H:1801:CLA:HBB1	1.93	0.49
1:a:214:GLY:HA3	16:a:1113:CLA:HAB	1.94	0.49
1:a:412:MET:O	1:a:557:ARG:NH1	2.43	0.49
2:b:60:TRP:NE1	16:b:1224:CLA:OBD	2.39	0.49
16:b:1239:CLA:H42	19:i:4018:BCR:H351	1.94	0.49
12:g:128:PHE:HD2	16:g:503:CLA:H3A	1.77	0.49
12:h:27:PHE:O	12:h:31:HIS:ND1	2.44	0.49
12:n:267:TYR:OH	16:n:506:CLA:O1D	2.31	0.49
12:p:143:GLY:HA3	12:p:222:ILE:HG13	1.94	0.49
1:A:348:TRP:HB3	16:A:1103:CLA:HAC1	1.94	0.49
1:A:708:ASN:HB2	6:F:133:MET:HE3	1.95	0.49
2:B:66:PHE:HZ	11:M:8:ILE:HG23	1.77	0.49
4:D:87:ARG:HB2	4:D:97:LEU:HD11	1.95	0.49
2:G:382:VAL:HG22	2:G:531:LEU:HD11	1.94	0.49
12:W:104:GLY:HA3	16:y:515:CLA:H93	1.95	0.49
2:B:181:GLY:HA3	16:B:1210:CLA:HBB1	1.95	0.49
19:B:4014:BCR:HC32	19:J:4015:BCR:H16C	1.94	0.49
2:G:662:ILE:HG12	1:H:686:LEU:HB3	1.94	0.49
1:H:484:GLN:NE2	1:H:527:LEU:O	2.43	0.49
12:W:58:ALA:H	12:W:62:GLN:HE21	1.61	0.49
16:g:510:CLA:H112	19:g:603:BCR:H362	1.95	0.49
12:h:70:LEU:HD11	12:h:92:ILE:HG21	1.93	0.49
12:o:19:ARG:NH1	16:o:512:CLA:OBD	2.40	0.49
12:o:200:LEU:HD12	12:o:265:LEU:HD11	1.94	0.49
12:t:306:ALA:HA	19:t:601:BCR:H21C	1.95	0.49
12:t:316:GLN:NE2	16:t:508:CLA:O1A	2.46	0.49
16:v:504:CLA:H11	16:v:506:CLA:HAA1	1.95	0.49
1:A:429:MET:HE3	1:A:554:LEU:HD21	1.94	0.49
1:A:508:ALA:HB2	1:A:522:MET:HE2	1.95	0.49
2:G:566:ASP:OD1	2:G:703:ARG:NH1	2.46	0.49
3:N:32:ASP:OD1	3:N:32:ASP:N	2.45	0.49
12:X:148:PHE:HD2	16:X:502:CLA:H3A	1.78	0.49
12:X:267:TYR:O	12:X:300:ARG:NH2	2.45	0.49
12:Z:249:ILE:HG12	16:Z:506:CLA:HAC1	1.94	0.49
12:g:166:LEU:HB2	12:g:200:LEU:HD21	1.95	0.49
12:r:110:HIS:HA	12:r:114:ALA:HB3	1.95	0.49
12:u:110:HIS:HA	12:u:114:ALA:HB3	1.95	0.49
12:u:243:SER:O	12:u:318:HIS:ND1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1104:CLA:HMB2	16:A:1128:CLA:HBB2	1.95	0.49
16:B:1210:CLA:H43	19:B:4005:BCR:H19C	1.95	0.49
5:E:7:ASP:HB2	5:E:70:GLN:HG2	1.95	0.49
12:W:159:LYS:HA	12:W:163:TRP:HB2	1.94	0.49
12:W:305:ASN:HD22	19:W:601:BCR:H393	1.77	0.49
12:Y:145:HIS:ND1	16:Y:510:CLA:OBD	2.38	0.49
1:a:686:LEU:HB3	2:b:662:ILE:HG12	1.95	0.49
12:n:19:ARG:NH1	16:n:512:CLA:OBD	2.40	0.49
12:n:172:GLN:NE2	12:n:270:GLU:OE2	2.42	0.49
2:B:453:ILE:HD13	6:F:53:LEU:HB2	1.95	0.48
2:G:203:ARG:NH2	2:G:253:ALA:O	2.44	0.48
1:H:447:LEU:HB3	1:H:540:PHE:HB2	1.95	0.48
1:H:736:ILE:HG23	16:H:1126:CLA:HAB	1.94	0.48
2:b:126:THR:HG22	2:b:270:LEU:HD21	1.94	0.48
3:c:2:SER:N	3:c:71:ALA:O	2.45	0.48
12:w:34:GLN:HE21	16:w:509:CLA:HMA1	1.78	0.48
1:A:396:ILE:HD12	16:A:1104:CLA:H143	1.95	0.48
1:A:429:MET:HE2	16:A:1119:CLA:H171	1.94	0.48
2:B:15:ASP:OD2	2:B:19:ARG:NH1	2.45	0.48
2:G:264:GLN:HE21	2:G:358:PHE:HZ	1.61	0.48
2:G:339:LEU:HD22	16:G:1225:CLA:HMC1	1.94	0.48
12:W:56:THR:HG22	12:W:82:GLN:HE21	1.78	0.48
1:a:429:MET:HE3	1:a:554:LEU:HD21	1.94	0.48
1:a:641:THR:HG22	1:a:643:ASN:H	1.78	0.48
19:b:4014:BCR:H332	19:j:4012:BCR:HC32	1.95	0.48
12:h:206:GLY:HA3	19:h:603:BCR:H402	1.95	0.48
12:n:34:GLN:HB2	16:n:509:CLA:HMB2	1.96	0.48
12:u:34:GLN:HG2	16:u:509:CLA:HHB	1.95	0.48
12:u:148:PHE:CD2	16:u:502:CLA:H3A	2.48	0.48
12:w:261:ALA:HA	12:w:276:LEU:HD12	1.95	0.48
12:x:166:LEU:HB2	12:x:200:LEU:HD21	1.95	0.48
16:x:511:CLA:H2A	16:x:511:CLA:HED3	1.96	0.48
10:L:53:VAL:O	10:L:57:HIS:ND1	2.43	0.48
12:Z:246:LEU:HD23	16:Z:509:CLA:HED1	1.95	0.48
2:b:44:GLN:OE1	2:b:162:ARG:NH1	2.43	0.48
12:g:148:PHE:HD2	16:g:502:CLA:H3A	1.77	0.48
16:r:505:CLA:H192	16:r:510:CLA:H151	1.95	0.48
12:t:326:LEU:HD21	12:u:113:ARG:HH21	1.78	0.48
12:w:243:SER:O	12:w:318:HIS:ND1	2.42	0.48
2:G:704:LEU:HD11	14:G:848:LMG:H341	1.94	0.48
16:W:515:CLA:H41	16:W:515:CLA:H92	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:110:HIS:HA	12:Z:114:ALA:HB3	1.94	0.48
2:b:339:LEU:HB3	2:b:380:LEU:HD13	1.95	0.48
16:b:1203:CLA:H41	16:b:1203:CLA:H61	1.62	0.48
12:n:213:LEU:HD21	16:n:510:CLA:H143	1.95	0.48
12:n:260:CYS:O	12:n:300:ARG:NH1	2.46	0.48
16:q:507:CLA:HED3	16:q:511:CLA:H52	1.95	0.48
12:t:267:TYR:O	12:t:300:ARG:NH2	2.43	0.48
16:y:508:CLA:HBA1	16:y:515:CLA:H141	1.96	0.48
19:B:4014:BCR:H332	19:J:4012:BCR:HC32	1.96	0.48
16:H:1139:CLA:H72	8:S:18:LEU:HD12	1.96	0.48
12:W:237:SER:OG	12:W:238:GLY:N	2.46	0.48
12:X:207:HIS:HA	12:X:210:VAL:HG12	1.95	0.48
1:a:381:ILE:HB	1:a:519:LYS:HD2	1.95	0.48
1:a:695:GLU:OE2	2:b:547:LYS:NZ	2.38	0.48
17:a:2001:PQN:H142	19:b:4014:BCR:H271	1.94	0.48
2:b:188:LEU:HD11	19:b:4004:BCR:HC7	1.96	0.48
16:b:1225:CLA:H61	21:b:4006:ECH:H39A	1.95	0.48
3:c:34:CYS:HA	5:e:33:ILE:HG23	1.95	0.48
6:f:135:ASP:HA	6:f:138:ILE:HD12	1.95	0.48
12:g:34:GLN:HG2	16:g:509:CLA:H3A	1.95	0.48
16:r:508:CLA:HBC1	16:r:511:CLA:HMD3	1.96	0.48
16:r:513:CLA:HMA3	19:r:603:BCR:H363	1.95	0.48
12:s:243:SER:O	12:s:318:HIS:ND1	2.45	0.48
12:y:148:PHE:O	12:y:152:GLY:N	2.46	0.48
1:A:305:ILE:O	1:A:309:HIS:ND1	2.46	0.48
2:B:94:PRO:O	10:U:157:ASN:ND2	2.47	0.48
2:B:708:ALA:HA	14:B:848:LMG:H391	1.96	0.48
2:G:66:PHE:HZ	11:V:8:ILE:HG23	1.79	0.48
16:H:1101:CLA:H171	19:H:4011:BCR:H401	1.96	0.48
12:X:20:PHE:HA	12:X:23:GLN:HG3	1.96	0.48
1:a:204:LEU:HD11	16:a:1111:CLA:H42	1.96	0.48
1:a:207:LEU:HD21	16:a:1118:CLA:HMC1	1.96	0.48
2:b:53:HIS:HB2	16:b:1202:CLA:HMB2	1.95	0.48
16:g:515:CLA:HBB2	19:h:604:BCR:H351	1.94	0.48
12:n:70:LEU:HD22	12:n:92:ILE:HD13	1.96	0.48
12:p:243:SER:O	12:p:318:HIS:ND1	2.45	0.48
16:q:508:CLA:HBC1	16:q:511:CLA:HMD3	1.95	0.48
16:q:513:CLA:H3A	16:q:513:CLA:HBA2	1.69	0.48
12:s:37:LEU:HD21	16:u:517:CLA:H62	1.95	0.48
12:v:310:LEU:HD11	16:v:514:CLA:HBB2	1.95	0.48
12:Y:34:GLN:HB2	16:Y:509:CLA:HMB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:1132:CLA:HMA2	10:l:68:LEU:HB3	1.96	0.48
2:b:234:ALA:HB2	16:b:1213:CLA:HMA2	1.95	0.48
2:b:413:LYS:HA	2:b:416:LEU:HD12	1.96	0.48
16:b:1207:CLA:H151	19:l:4022:BCR:H362	1.95	0.48
16:h:508:CLA:HBA2	16:h:508:CLA:H3A	1.65	0.48
16:q:505:CLA:H122	16:q:510:CLA:H8	1.96	0.48
12:t:66:LEU:HB3	16:t:504:CLA:HED1	1.96	0.48
12:u:121:LEU:HD11	16:u:503:CLA:HED2	1.96	0.48
12:u:207:HIS:HA	12:u:210:VAL:HG12	1.96	0.48
2:G:665:ARG:H	1:H:583:CYS:HB2	1.79	0.48
16:G:1235:CLA:HBC2	19:S:4015:BCR:HC7	1.95	0.48
16:H:1133:CLA:HMD2	16:H:1134:CLA:HBB1	1.96	0.48
16:n:511:CLA:HMD2	19:n:601:BCR:HC7	1.96	0.48
12:q:243:SER:O	12:q:318:HIS:ND1	2.46	0.48
12:u:260:CYS:O	12:u:300:ARG:NH1	2.46	0.48
16:v:506:CLA:HMB1	16:v:507:CLA:HMC3	1.94	0.48
16:v:510:CLA:H122	19:v:603:BCR:H16C	1.96	0.48
16:A:1112:CLA:HAB	19:A:4002:BCR:H14C	1.96	0.48
2:B:239:THR:HG23	2:B:241:GLY:H	1.79	0.48
14:Q:4017:LMG:HC72	8:S:5:LYS:HB3	1.96	0.48
10:U:46:PRO:HB2	10:U:122:GLN:HB2	1.95	0.48
12:Z:272:TYR:HB3	12:Z:300:ARG:HB3	1.95	0.48
1:a:358:LEU:HD11	16:a:1119:CLA:H51	1.96	0.48
2:b:66:PHE:HZ	11:m:8:ILE:HG23	1.79	0.48
16:b:1235:CLA:H152	19:f:4016:BCR:H402	1.95	0.48
6:f:89:GLU:HG2	6:f:107:LEU:HD11	1.95	0.48
12:r:12:GLU:HG3	12:r:14:TRP:CE2	2.49	0.48
12:s:254:PHE:HE2	12:s:315:LEU:HD22	1.79	0.48
12:u:30:ALA:HB1	16:u:509:CLA:HBB1	1.96	0.48
16:v:509:CLA:HED1	16:v:511:CLA:HBB2	1.95	0.48
2:B:435:TYR:HD2	16:B:1021:CLA:H203	1.78	0.48
2:G:382:VAL:HG13	2:G:531:LEU:HD21	1.95	0.48
16:G:1207:CLA:H193	16:l:1501:CLA:H12	1.96	0.48
14:H:852:LMG:H292	7:R:29:LEU:HB3	1.96	0.48
19:L:4022:BCR:H15C	10:U:56:ALA:HA	1.95	0.48
16:Z:504:CLA:H172	16:Z:507:CLA:HBB2	1.96	0.48
1:a:192:ASN:HD22	16:a:1110:CLA:HED3	1.78	0.48
17:a:2001:PQN:H162	19:b:4014:BCR:H382	1.96	0.48
2:b:684:LEU:HD11	10:l:37:LEU:HD13	1.96	0.48
16:p:508:CLA:H3A	16:p:508:CLA:H43	1.96	0.48
19:s:604:BCR:H313	12:u:258:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:t:42:ALA:O	12:t:46:THR:OG1	2.31	0.48
12:v:251:LEU:HG	16:v:505:CLA:H91	1.96	0.48
12:x:129:HIS:O	12:x:137:GLN:NE2	2.47	0.48
12:x:226:PRO:O	12:x:231:LYS:NZ	2.47	0.48
16:x:511:CLA:HMD2	19:x:601:BCR:HC7	1.95	0.48
16:y:511:CLA:H43	16:y:512:CLA:HAC1	1.96	0.48
16:y:512:CLA:H2	16:y:512:CLA:H102	1.95	0.48
1:A:358:LEU:HD21	16:A:1119:CLA:H71	1.96	0.47
2:G:141:PHE:HZ	16:G:1211:CLA:H101	1.79	0.47
16:G:1219:CLA:HMA1	16:G:1240:CLA:HBB2	1.96	0.47
1:H:355:ASN:ND2	16:H:1103:CLA:OBD	2.43	0.47
9:K:64:ALA:O	9:K:68:HIS:ND1	2.47	0.47
9:T:30:ILE:HG23	16:T:4003:CLA:HMD3	1.96	0.47
12:W:214:LEU:HD11	16:W:510:CLA:H71	1.96	0.47
16:Y:511:CLA:HMD2	19:Y:601:BCR:HC7	1.96	0.47
16:Y:515:CLA:H122	12:Z:98:ILE:HG23	1.96	0.47
12:Z:194:PHE:HZ	19:g:602:BCR:H312	1.79	0.47
1:a:539:ALA:O	1:a:543:HIS:ND1	2.46	0.47
12:n:73:LEU:HD11	16:n:504:CLA:HAA2	1.96	0.47
12:p:239:GLU:OE2	12:p:321:HIS:ND1	2.47	0.47
12:q:233:VAL:HG23	12:q:234:LEU:HG	1.96	0.47
12:t:298:THR:HG23	12:t:301:ALA:H	1.78	0.47
16:t:511:CLA:H172	19:t:601:BCR:H362	1.96	0.47
16:u:504:CLA:H2	16:u:506:CLA:H11	1.96	0.47
16:w:513:CLA:HBB2	16:w:515:CLA:H101	1.96	0.47
2:B:393:VAL:HG21	2:B:552:TYR:HB2	1.95	0.47
16:G:1021:CLA:HMB1	15:H:1011:CL0:H7	1.96	0.47
1:H:539:ALA:HB1	16:H:1136:CLA:HMB3	1.95	0.47
9:K:66:PHE:HB2	19:K:4001:BCR:H23C	1.95	0.47
12:X:156:LEU:HB2	16:X:505:CLA:HMD3	1.96	0.47
12:Y:45:PHE:HA	12:Y:48:PHE:HB3	1.95	0.47
2:b:375:TYR:HA	2:b:584:LEU:HD13	1.96	0.47
16:n:508:CLA:HED1	19:o:604:BCR:H23C	1.96	0.47
12:o:110:HIS:HA	12:o:114:ALA:HB3	1.95	0.47
12:o:267:TYR:O	12:o:300:ARG:NH2	2.42	0.47
16:w:505:CLA:HMB2	19:w:603:BCR:H23C	1.96	0.47
12:x:19:ARG:NH1	16:x:512:CLA:OBD	2.40	0.47
2:G:53:HIS:HB2	16:G:1202:CLA:HMB2	1.96	0.47
2:G:443:ALA:HB1	1:H:666:SER:HB2	1.95	0.47
16:G:1239:CLA:H72	16:H:1131:CLA:H101	1.96	0.47
10:U:38:PRO:O	10:U:49:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:73:ASP:OD1	10:U:73:ASP:N	2.44	0.47
12:X:159:LYS:HD2	12:X:164:GLY:HA3	1.95	0.47
16:Z:505:CLA:H172	16:Z:516:CLA:HBB1	1.96	0.47
1:a:76:HIS:ND1	16:a:1111:CLA:OBD	2.38	0.47
1:a:305:ILE:O	1:a:309:HIS:ND1	2.41	0.47
1:a:396:ILE:HD12	16:a:1104:CLA:H143	1.95	0.47
2:b:70:TRP:NE1	7:i:6:ALA:O	2.35	0.47
16:n:510:CLA:HED2	16:n:516:CLA:HBB1	1.96	0.47
12:o:260:CYS:O	12:o:300:ARG:NH1	2.47	0.47
12:p:146:LEU:HG	16:p:510:CLA:HED1	1.97	0.47
16:r:515:CLA:H2A	12:v:113:ARG:NH2	2.30	0.47
2:B:408:ARG:O	2:B:412:HIS:ND1	2.41	0.47
10:L:56:ALA:HA	19:l:4022:BCR:H15C	1.96	0.47
3:N:34:CYS:HA	5:O:33:ILE:HG23	1.97	0.47
5:O:27:SER:HB3	5:O:38:ILE:HD12	1.95	0.47
19:W:604:BCR:H15C	16:y:515:CLA:H91	1.95	0.47
16:a:1116:CLA:HBA2	16:a:1116:CLA:H3A	1.56	0.47
12:g:79:ASP:OD1	12:g:79:ASP:N	2.45	0.47
12:o:34:GLN:HG2	16:o:509:CLA:H3A	1.95	0.47
12:w:280:LEU:HD13	12:x:47:LEU:HB2	1.95	0.47
1:H:238:LEU:HB2	1:H:241:GLU:HG3	1.96	0.47
1:H:586:SER:OG	1:H:589:ASP:OD2	2.29	0.47
16:H:1121:CLA:HAB	16:H:1801:CLA:HAB	1.97	0.47
13:X:605:LHG:HC91	13:X:605:LHG:H241	1.96	0.47
1:a:447:LEU:HB3	1:a:540:PHE:HB2	1.95	0.47
16:a:1112:CLA:HAB	19:a:4002:BCR:H14C	1.95	0.47
2:b:182:LEU:HD13	16:b:1210:CLA:HHB	1.95	0.47
8:j:1:MET:HB3	12:p:334:GLU:HG3	1.97	0.47
12:o:210:VAL:HG21	16:o:505:CLA:HAB	1.95	0.47
12:p:323:LEU:HD22	12:q:112:LEU:HD12	1.97	0.47
12:u:65:ILE:O	12:u:69:HIS:ND1	2.47	0.47
1:A:288:LEU:HD13	16:A:1116:CLA:HMA2	1.96	0.47
16:G:1216:CLA:HMC2	16:G:1221:CLA:H172	1.97	0.47
12:h:267:TYR:O	12:h:300:ARG:NH2	2.48	0.47
12:o:323:LEU:HD11	12:p:108:LEU:HD22	1.95	0.47
16:w:508:CLA:HBC1	16:w:511:CLA:HMD3	1.97	0.47
16:y:502:CLA:HMD2	16:y:509:CLA:H203	1.96	0.47
1:A:216:GLN:NE2	16:A:1117:CLA:O1D	2.47	0.47
1:A:412:MET:O	1:A:557:ARG:NH1	2.46	0.47
16:A:1022:CLA:H91	16:B:1023:CLA:H112	1.95	0.47
2:B:346:VAL:HG21	16:B:1225:CLA:HHD	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:1211:CLA:H2	16:B:1211:CLA:H61	1.74	0.47
16:B:1211:CLA:HAB	16:B:1225:CLA:H162	1.96	0.47
16:B:1225:CLA:H171	21:B:4006:ECH:H17	1.96	0.47
2:G:408:ARG:O	2:G:412:HIS:ND1	2.43	0.47
1:H:641:THR:HG22	1:H:643:ASN:H	1.79	0.47
3:N:29:VAL:HG12	4:P:112:ARG:HB3	1.97	0.47
10:U:36:ASN:HB3	16:U:1501:CLA:HBC2	1.95	0.47
12:X:150:GLY:HA3	12:X:215:ILE:HG13	1.97	0.47
16:Y:505:CLA:H111	16:Y:510:CLA:H62	1.97	0.47
1:a:148:ARG:HD3	1:a:377:PRO:HB2	1.97	0.47
16:a:1237:CLA:H203	10:l:61:LEU:HD11	1.96	0.47
12:g:280:LEU:H	12:h:51:SER:HB2	1.80	0.47
16:h:510:CLA:HHC	16:h:516:CLA:H3A	1.95	0.47
12:p:19:ARG:NH1	16:p:512:CLA:OBD	2.46	0.47
12:q:226:PRO:O	12:q:231:LYS:NZ	2.45	0.47
12:r:45:PHE:HA	12:r:48:PHE:HB3	1.97	0.47
16:r:505:CLA:H172	16:r:516:CLA:HBB1	1.96	0.47
16:s:505:CLA:H72	16:s:505:CLA:HBB1	1.97	0.47
12:t:254:PHE:HE2	12:t:315:LEU:HD22	1.79	0.47
12:x:243:SER:O	12:x:318:HIS:ND1	2.45	0.47
1:A:373:MET:HE2	16:A:1125:CLA:HMC2	1.96	0.47
1:A:395:TRP:HB3	16:A:1126:CLA:HMC3	1.95	0.47
1:A:412:MET:HE1	1:A:430:LEU:HD11	1.96	0.47
1:A:482:PHE:HB3	16:A:1135:CLA:H12	1.97	0.47
2:B:126:THR:HG22	2:B:270:LEU:HD21	1.97	0.47
2:G:339:LEU:HB3	2:G:380:LEU:HD13	1.97	0.47
2:G:524:LEU:HD12	16:G:1236:CLA:HED3	1.95	0.47
16:G:1023:CLA:H102	1:H:449:PHE:HE1	1.80	0.47
12:Y:227:LEU:HD12	12:Y:229:TRP:HE1	1.80	0.47
16:Z:505:CLA:H201	16:Z:510:CLA:HBB1	1.97	0.47
2:b:436:VAL:HG12	16:b:1230:CLA:HAC1	1.97	0.47
16:g:513:CLA:HMA3	19:g:603:BCR:H363	1.96	0.47
12:r:38:THR:HG23	16:r:507:CLA:HMC1	1.97	0.47
12:x:146:LEU:HD22	12:x:214:LEU:HD22	1.96	0.47
16:y:505:CLA:H201	16:y:510:CLA:HBB1	1.97	0.47
2:G:436:VAL:HG22	16:G:1012:CLA:H43	1.96	0.47
2:G:632:TYR:OH	1:H:459:ASP:OD1	2.29	0.47
16:G:1202:CLA:HBC2	16:G:1226:CLA:HMA1	1.96	0.47
1:H:573:PRO:HB3	1:H:720:ILE:HB	1.97	0.47
7:I:1:MET:N	10:U:153:ARG:O	2.43	0.47
12:X:260:CYS:O	12:X:300:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:1124:CLA:C3D	16:a:1135:CLA:HBB1	2.45	0.47
16:b:1239:CLA:H12	17:b:2002:PQN:H293	1.97	0.47
12:n:30:ALA:HB1	16:n:509:CLA:HBB1	1.96	0.47
16:w:503:CLA:HAC2	19:w:602:BCR:H402	1.96	0.47
16:B:1229:CLA:H72	19:F:4016:BCR:HC32	1.97	0.47
3:C:21:CYS:HG	3:C:25:VAL:H	1.61	0.47
5:E:3:LEU:HD22	5:E:68:LEU:HD13	1.96	0.47
2:G:584:LEU:HD23	2:G:587:LEU:HD21	1.97	0.47
16:H:1103:CLA:H62	16:H:1103:CLA:H2	1.66	0.47
12:X:124:GLN:NE2	16:X:501:CLA:OBD	2.47	0.47
16:a:1122:CLA:H121	16:a:1137:CLA:HAA2	1.96	0.47
12:p:45:PHE:HA	12:p:48:PHE:HB3	1.96	0.47
12:r:146:LEU:HD22	12:r:214:LEU:HD22	1.96	0.47
16:r:502:CLA:HMD2	16:r:509:CLA:H193	1.96	0.47
1:A:242:PHE:HB3	1:A:249:MET:HE2	1.97	0.46
1:A:564:ASP:N	1:A:564:ASP:OD1	2.49	0.46
1:H:564:ASP:OD1	1:H:564:ASP:N	2.47	0.46
1:a:437:ILE:O	1:a:441:ASN:N	2.43	0.46
16:b:1216:CLA:HMC2	16:b:1221:CLA:H172	1.96	0.46
4:d:32:TRP:NE1	4:d:50:MET:SD	2.78	0.46
12:g:57:GLN:HB3	12:g:62:GLN:HE21	1.80	0.46
16:k:4002:CLA:H3A	16:k:4002:CLA:HBA2	1.49	0.46
12:n:316:GLN:NE2	16:n:508:CLA:O1A	2.46	0.46
16:p:515:CLA:H11	16:p:515:CLA:HBA2	1.74	0.46
16:u:511:CLA:HMD2	19:u:601:BCR:HC7	1.97	0.46
19:y:603:BCR:H20C	19:y:603:BCR:H361	1.81	0.46
2:B:436:VAL:HG22	16:B:1012:CLA:H43	1.97	0.46
16:B:1023:CLA:H152	19:I:4018:BCR:H23C	1.97	0.46
16:G:1203:CLA:H62	16:G:1226:CLA:H8	1.96	0.46
12:W:38:THR:HG23	16:W:507:CLA:HMC2	1.97	0.46
12:Z:324:ARG:NH1	16:Z:511:CLA:O1D	2.48	0.46
16:Z:503:CLA:HMC3	19:Z:602:BCR:H23C	1.98	0.46
16:g:505:CLA:H102	16:g:505:CLA:H62	1.76	0.46
16:n:511:CLA:H172	19:n:601:BCR:H362	1.97	0.46
16:q:502:CLA:HAA2	16:q:509:CLA:H102	1.96	0.46
12:s:110:HIS:HA	12:s:114:ALA:HB3	1.96	0.46
16:t:505:CLA:H62	16:t:505:CLA:H102	1.78	0.46
12:w:303:LEU:HD13	16:w:506:CLA:HED2	1.96	0.46
16:A:1122:CLA:H121	16:A:1137:CLA:HAA2	1.96	0.46
2:B:647:PHE:O	2:B:651:HIS:ND1	2.41	0.46
16:G:1228:CLA:HED3	1:H:702:TRP:HH2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:4101:LMG:H171	14:H:4201:LMG:H151	1.96	0.46
16:Z:507:CLA:H102	16:Z:507:CLA:H62	1.57	0.46
12:h:203:LEU:HA	19:h:603:BCR:H401	1.98	0.46
12:n:148:PHE:CD2	16:n:502:CLA:H3A	2.48	0.46
16:n:505:CLA:H171	16:n:510:CLA:H121	1.96	0.46
12:q:308:PHE:HZ	16:q:517:CLA:HBB1	1.81	0.46
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.97	0.46
3:C:2:SER:N	3:C:71:ALA:O	2.48	0.46
4:D:18:LEU:HB2	10:L:17:VAL:HA	1.96	0.46
2:G:243:ILE:HG23	2:G:264:GLN:HE22	1.81	0.46
1:H:192:ASN:HD22	16:H:1110:CLA:HED3	1.80	0.46
1:H:437:ILE:O	1:H:441:ASN:N	2.44	0.46
16:H:1139:CLA:H92	16:H:1139:CLA:H61	1.81	0.46
16:W:511:CLA:HMD2	19:W:601:BCR:HC7	1.96	0.46
1:a:115:GLN:NE2	16:a:1107:CLA:OBD	2.38	0.46
16:a:1101:CLA:H142	16:f:1301:CLA:HMC3	1.98	0.46
16:a:1120:CLA:H43	19:k:4001:BCR:H381	1.98	0.46
7:i:34:ILE:HG13	7:i:35:GLU:HG2	1.96	0.46
12:u:76:GLY:HA2	12:u:85:ASP:HB2	1.97	0.46
16:v:510:CLA:H72	16:v:516:CLA:HBB2	1.97	0.46
16:x:515:CLA:HBB2	19:y:604:BCR:H351	1.97	0.46
2:B:92:TRP:HB3	7:I:15:ILE:HG13	1.96	0.46
2:G:239:THR:HG23	2:G:241:GLY:H	1.80	0.46
2:G:513:ASP:O	2:G:517:HIS:ND1	2.37	0.46
16:G:1218:CLA:HMD2	19:G:4004:BCR:H24C	1.97	0.46
1:H:428:ARG:O	1:H:432:HIS:ND1	2.40	0.46
16:W:501:CLA:H3A	16:W:501:CLA:HBA2	1.52	0.46
1:a:411:PHE:HE2	1:a:426:LEU:HD21	1.80	0.46
1:a:588:TRP:CD1	16:a:1128:CLA:HMD1	2.50	0.46
12:o:27:PHE:O	12:o:31:HIS:ND1	2.49	0.46
12:s:143:GLY:HA3	12:s:222:ILE:HG13	1.97	0.46
12:v:34:GLN:HB2	16:v:509:CLA:HMB2	1.96	0.46
1:A:650:LEU:HD11	15:A:1011:CL0:H43	1.98	0.46
2:G:343:THR:HB	2:G:377:ALA:HB2	1.98	0.46
1:a:484:GLN:NE2	1:a:527:LEU:O	2.44	0.46
16:a:1126:CLA:H61	19:a:4011:BCR:H343	1.98	0.46
12:g:272:TYR:HB3	12:g:300:ARG:HB2	1.98	0.46
16:h:504:CLA:H102	16:h:504:CLA:H41	1.96	0.46
12:n:97:LEU:HD23	19:n:604:BCR:HC7	1.96	0.46
12:o:246:LEU:HD23	16:o:509:CLA:HED1	1.96	0.46
12:t:4:TYR:OH	12:t:328:PHE:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:t:515:CLA:H92	16:t:515:CLA:H41	1.97	0.46
12:x:49:GLU:HB3	12:x:64:LEU:HG	1.98	0.46
1:A:707:LEU:HD11	19:F:4016:BCR:H342	1.97	0.46
16:A:1138:CLA:H203	16:A:1139:CLA:H52	1.97	0.46
2:G:586:TRP:NE1	25:G:901:HOH:O	2.47	0.46
1:H:310:MET:HA	16:H:1120:CLA:HHD	1.97	0.46
12:W:105:ALA:HA	16:y:515:CLA:H11	1.97	0.46
12:X:145:HIS:ND1	16:X:510:CLA:OBD	2.39	0.46
12:Y:254:PHE:HE2	12:Y:315:LEU:HD22	1.81	0.46
12:Z:17:ASN:ND2	16:Z:507:CLA:O1A	2.48	0.46
2:b:557:ASP:OD2	2:b:561:ARG:NH2	2.43	0.46
2:b:586:TRP:NE1	25:b:901:HOH:O	2.47	0.46
2:b:667:TYR:OH	16:b:1023:CLA:OBD	2.27	0.46
12:g:33:ALA:HB1	19:g:604:BCR:H373	1.97	0.46
16:q:513:CLA:HBB2	16:q:515:CLA:H101	1.97	0.46
16:t:515:CLA:H43	12:u:102:VAL:HG13	1.97	0.46
16:A:1237:CLA:H203	10:L:61:LEU:HD11	1.98	0.46
2:B:465:SER:O	2:B:494:TRP:NE1	2.41	0.46
16:B:1215:CLA:H92	16:B:1221:CLA:H41	1.98	0.46
4:D:41:GLU:H	4:D:71:GLN:HE22	1.64	0.46
4:D:101:ASP:OD1	4:D:101:ASP:N	2.46	0.46
2:G:92:TRP:HB3	7:R:15:ILE:HG13	1.97	0.46
2:G:465:SER:O	2:G:494:TRP:NE1	2.40	0.46
1:H:324:ILE:O	1:H:328:HIS:ND1	2.44	0.46
16:H:1132:CLA:HMA2	10:U:68:LEU:HB3	1.97	0.46
19:L:4019:BCR:H20C	19:L:4019:BCR:H361	1.79	0.46
12:Y:143:GLY:HA3	12:Y:222:ILE:HG13	1.97	0.46
12:Z:226:PRO:HA	16:Z:516:CLA:HED3	1.98	0.46
16:Z:515:CLA:H141	19:g:604:BCR:H11C	1.96	0.46
2:b:118:SER:HA	16:b:1224:CLA:HMA2	1.98	0.46
19:b:4014:BCR:HC21	19:j:4015:BCR:H363	1.98	0.46
4:d:34:SER:OG	4:d:51:ASN:O	2.33	0.46
10:l:32:THR:O	10:l:36:ASN:ND2	2.49	0.46
12:n:110:HIS:HA	12:n:114:ALA:HB3	1.96	0.46
16:q:508:CLA:HBC3	16:q:511:CLA:HAC2	1.98	0.46
12:t:310:LEU:HD22	16:t:506:CLA:HMC3	1.98	0.46
1:A:579:ARG:NH2	4:D:63:GLU:OE2	2.49	0.46
1:A:736:ILE:HG23	16:A:1126:CLA:HAB	1.97	0.46
19:A:4002:BCR:H19C	19:A:4003:BCR:H311	1.97	0.46
2:B:114:ASN:ND2	16:B:1206:CLA:OBD	2.49	0.46
3:C:54:CYS:SG	3:C:55:GLU:N	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:LEU:HD23	1:H:233:PRO:HB3	1.98	0.46
14:H:852:LMG:H142	16:l:1501:CLA:H92	1.97	0.46
10:L:94:ALA:HB1	16:U:1501:CLA:H141	1.98	0.46
10:U:67:LEU:HD12	16:U:1503:CLA:HHB	1.96	0.46
12:W:243:SER:O	12:W:318:HIS:ND1	2.48	0.46
12:X:159:LYS:NZ	12:X:165:GLY:O	2.43	0.46
12:Z:30:ALA:HA	16:Z:512:CLA:HMB3	1.98	0.46
16:a:1101:CLA:H172	16:a:1140:CLA:H162	1.98	0.46
16:a:1129:CLA:HAB	16:a:1137:CLA:HBB2	1.97	0.46
19:g:602:BCR:H322	19:g:604:BCR:H333	1.98	0.46
12:r:243:SER:O	12:r:318:HIS:ND1	2.44	0.46
12:w:27:PHE:O	12:w:31:HIS:ND1	2.48	0.46
12:x:32:VAL:HG11	16:x:503:CLA:HMC3	1.97	0.46
16:x:512:CLA:HMC2	23:x:606:LMU:H102	1.97	0.46
2:B:123:TRP:NE1	16:B:1215:CLA:OBD	2.39	0.46
16:H:1131:CLA:HMC2	16:U:1503:CLA:HBB2	1.97	0.46
19:Y:603:BCR:H20C	19:Y:603:BCR:H361	1.83	0.46
1:a:71:LYS:NZ	16:a:1109:CLA:OBD	2.47	0.46
1:a:335:GLU:HG3	1:a:423:ASN:HB3	1.98	0.46
1:a:362:LEU:HD21	16:a:1117:CLA:H93	1.97	0.46
1:a:428:ARG:O	1:a:432:HIS:ND1	2.43	0.46
1:a:576:GLY:HA2	2:b:559:PRO:HD3	1.98	0.46
1:a:685:PHE:HA	17:a:2001:PQN:H9	1.98	0.46
16:g:502:CLA:HMD2	16:g:509:CLA:H193	1.98	0.46
16:h:504:CLA:H41	16:h:504:CLA:H62	1.69	0.46
12:o:198:SER:HA	12:o:265:LEU:HB2	1.98	0.46
16:p:508:CLA:HMA2	16:p:517:CLA:H93	1.97	0.46
12:q:234:LEU:HD13	16:q:510:CLA:HMC3	1.98	0.46
16:u:505:CLA:HBB2	16:u:510:CLA:H92	1.98	0.46
16:u:506:CLA:C2B	16:u:514:CLA:HAB	2.45	0.46
1:A:223:ILE:HG23	1:A:236:ILE:HG21	1.97	0.45
16:A:1134:CLA:HMB1	19:A:4008:BCR:H281	1.98	0.45
16:B:1225:CLA:H61	21:B:4006:ECH:H39A	1.96	0.45
2:G:50:HIS:HE1	16:G:1202:CLA:H171	1.81	0.45
1:H:332:PHE:O	1:H:428:ARG:NH2	2.46	0.45
12:X:148:PHE:CD2	16:X:502:CLA:H3A	2.51	0.45
12:Z:243:SER:O	12:Z:318:HIS:ND1	2.45	0.45
16:g:504:CLA:H41	16:g:505:CLA:HBA2	1.97	0.45
19:h:603:BCR:HC21	12:n:105:ALA:HB1	1.96	0.45
12:n:190:TYR:HD2	19:n:603:BCR:H401	1.81	0.45
12:p:320:TRP:HZ3	13:p:605:LHG:H282	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:503:CLA:HMC2	19:p:602:BCR:H372	1.97	0.45
12:q:110:HIS:HA	12:q:114:ALA:HB3	1.98	0.45
12:s:227:LEU:HD12	12:s:229:TRP:HE1	1.81	0.45
12:t:58:ALA:O	12:t:62:GLN:NE2	2.44	0.45
12:w:177:VAL:HG21	12:w:204:VAL:HG21	1.98	0.45
12:y:54:ASP:HB3	12:y:57:GLN:HB3	1.97	0.45
1:A:13:LYS:HG3	1:A:314:ASN:HD21	1.80	0.45
1:A:265:THR:HB	9:K:14:TRP:HB2	1.97	0.45
1:A:333:THR:HG21	13:A:851:LHG:HC11	1.99	0.45
1:A:561:LEU:O	4:D:61:ARG:NH2	2.49	0.45
1:A:666:SER:HB2	2:B:443:ALA:HB1	1.97	0.45
16:A:1101:CLA:H171	19:A:4011:BCR:H401	1.98	0.45
16:A:1130:CLA:H2	16:L:1502:CLA:H43	1.98	0.45
2:G:324:ILE:HG12	2:G:330:PHE:CE2	2.50	0.45
16:G:1221:CLA:H143	16:G:1221:CLA:H111	1.82	0.45
1:H:86:TRP:HA	16:H:1105:CLA:HBB2	1.99	0.45
1:H:265:THR:HB	9:T:14:TRP:HB2	1.98	0.45
16:Q:1302:CLA:HMB2	19:Q:4016:BCR:H24C	1.99	0.45
2:b:343:THR:HB	2:b:377:ALA:HB2	1.98	0.45
16:b:1211:CLA:HAB	16:b:1225:CLA:H162	1.98	0.45
12:h:20:PHE:HZ	16:h:509:CLA:HAB	1.81	0.45
12:o:207:HIS:HA	12:o:210:VAL:HG12	1.98	0.45
12:q:34:GLN:HG2	16:q:509:CLA:HHB	1.98	0.45
12:r:73:LEU:HB3	12:r:159:LYS:HE2	1.97	0.45
16:x:515:CLA:HAB	12:y:101:ALA:HB1	1.97	0.45
12:y:198:SER:HA	12:y:265:LEU:HD22	1.98	0.45
14:A:4101:LMG:HC61	20:L:4101:LMT:H4B	1.97	0.45
2:B:580:MET:HE3	2:B:580:MET:HB3	1.72	0.45
1:H:76:HIS:CD2	16:H:1103:CLA:HAA1	2.52	0.45
16:a:1124:CLA:C2B	16:a:1137:CLA:H3A	2.47	0.45
19:a:4002:BCR:H20C	19:a:4002:BCR:H361	1.80	0.45
2:b:411:GLU:O	6:f:143:ARG:NH2	2.49	0.45
2:b:582:ASN:HB2	16:b:1012:CLA:HBC2	1.98	0.45
12:g:175:ARG:HH12	12:g:201:GLU:HG3	1.81	0.45
12:g:272:TYR:O	12:g:298:THR:OG1	2.33	0.45
12:h:245:SER:HB2	16:h:510:CLA:HAA1	1.97	0.45
16:h:509:CLA:H202	16:h:509:CLA:H162	1.85	0.45
7:i:17:MET:HG3	7:i:21:LEU:HD23	1.97	0.45
12:n:315:LEU:HD11	16:n:515:CLA:HHC	1.98	0.45
12:t:315:LEU:HD11	16:t:515:CLA:HHC	1.99	0.45
12:u:261:ALA:HB1	12:u:276:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:w:323:LEU:HD22	16:w:508:CLA:HMD1	1.98	0.45
12:y:194:PHE:HB2	19:y:603:BCR:H271	1.98	0.45
2:G:70:TRP:NE1	7:R:6:ALA:O	2.37	0.45
6:Q:125:GLU:HG3	6:Q:130:LYS:HB2	1.98	0.45
12:X:246:LEU:HD23	16:X:509:CLA:HED1	1.99	0.45
12:Y:99:ALA:HA	19:Y:602:BCR:H16C	1.98	0.45
1:a:707:LEU:HD13	19:f:4016:BCR:H321	1.97	0.45
2:b:659:MET:O	2:b:663:SER:OG	2.26	0.45
4:d:38:GLN:HB2	4:d:50:MET:HE3	1.98	0.45
16:h:511:CLA:H12	16:h:512:CLA:HAC1	1.97	0.45
12:p:78:GLY:N	12:p:82:GLN:O	2.40	0.45
12:q:146:LEU:HD22	12:q:214:LEU:HD22	1.98	0.45
12:t:267:TYR:OH	16:t:506:CLA:O1D	2.31	0.45
12:w:226:PRO:O	12:w:231:LYS:NZ	2.50	0.45
12:y:37:LEU:HD11	19:y:604:BCR:H373	1.97	0.45
12:y:251:LEU:HD23	16:y:505:CLA:H121	1.97	0.45
1:A:437:ILE:O	1:A:441:ASN:N	2.45	0.45
16:A:1116:CLA:H93	16:A:1116:CLA:HMC2	1.99	0.45
2:G:118:SER:HA	16:G:1224:CLA:HMA2	1.99	0.45
2:G:181:GLY:HA3	16:G:1210:CLA:HBB1	1.99	0.45
16:G:1223:CLA:H152	19:G:4010:BCR:H14C	1.99	0.45
1:H:500:ASN:HB2	16:H:1134:CLA:HED2	1.99	0.45
3:N:56:THR:HG21	5:O:49:PHE:HD1	1.81	0.45
6:Q:8:THR:HG1	6:Q:13:ASN:HD22	1.61	0.45
6:Q:59:PHE:HA	6:Q:62:ALA:HB2	1.99	0.45
1:a:56:HIS:ND1	16:a:1104:CLA:O1A	2.41	0.45
16:h:509:CLA:HED1	16:h:511:CLA:HBB2	1.98	0.45
16:w:507:CLA:HMA2	16:w:507:CLA:H11	1.98	0.45
12:y:310:LEU:HD13	16:y:506:CLA:HMC3	1.97	0.45
16:y:507:CLA:H61	16:y:511:CLA:HBC3	1.98	0.45
1:A:148:ARG:HD3	1:A:377:PRO:HB2	1.99	0.45
2:B:182:LEU:HD13	16:B:1210:CLA:HHB	1.99	0.45
2:G:453:ILE:HD13	6:Q:53:LEU:HB2	1.97	0.45
16:G:1201:CLA:H11	13:R:103:LHG:H272	1.98	0.45
1:H:433:ARG:HG2	1:H:554:LEU:HB3	1.99	0.45
1:H:478:LEU:HD21	14:H:4101:LMG:H341	1.98	0.45
16:H:1116:CLA:HBA2	16:H:1116:CLA:H3A	1.53	0.45
16:H:1139:CLA:H71	8:S:14:MET:HE3	1.98	0.45
21:I:4020:ECH:H34B	21:I:4020:ECH:H33	1.98	0.45
4:P:25:GLU:HG2	4:P:26:GLU:HG2	1.98	0.45
12:Z:279:LYS:HD3	12:g:51:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:434:ASP:OD1	1:a:555:TYR:OH	2.34	0.45
16:b:1023:CLA:H152	19:i:4018:BCR:H23C	1.98	0.45
4:d:73:ARG:NH1	4:d:106:GLU:OE2	2.49	0.45
12:h:268:PRO:HA	12:h:269:PRO:HD3	1.85	0.45
16:h:508:CLA:HBC1	16:h:511:CLA:HMD3	1.98	0.45
16:p:517:CLA:H3A	16:p:517:CLA:HBA1	1.66	0.45
12:s:246:LEU:HD23	16:s:509:CLA:HED1	1.99	0.45
12:s:267:TYR:OH	16:s:506:CLA:O1D	2.33	0.45
12:t:1:MET:O	12:t:237:SER:OG	2.35	0.45
16:w:515:CLA:HMD2	19:w:603:BCR:H343	1.99	0.45
16:A:1124:CLA:C3D	16:A:1135:CLA:HBB1	2.47	0.45
2:B:234:ALA:HB2	16:B:1213:CLA:HMA2	1.97	0.45
2:B:658:PHE:HB3	16:B:1023:CLA:HMC2	1.98	0.45
16:B:1203:CLA:H151	16:B:1225:CLA:HBB2	1.98	0.45
1:H:207:LEU:HD21	16:H:1118:CLA:HMC1	1.98	0.45
1:H:589:ASP:OD1	1:H:724:ARG:NH1	2.49	0.45
16:H:1124:CLA:H91	19:H:4008:BCR:H23C	1.99	0.45
16:H:1139:CLA:H2	16:H:1139:CLA:H62	1.71	0.45
10:L:132:MET:HG3	19:L:4022:BCR:H23C	1.97	0.45
12:Y:17:ASN:ND2	16:Y:507:CLA:O1A	2.50	0.45
1:a:200:HIS:ND1	16:a:1123:CLA:OBD	2.47	0.45
16:a:1119:CLA:H92	16:a:1119:CLA:H62	1.87	0.45
16:a:1131:CLA:H161	19:l:4019:BCR:H11C	1.99	0.45
2:b:436:VAL:HG22	16:b:1012:CLA:H43	1.99	0.45
12:g:233:VAL:HG23	12:g:234:LEU:HG	1.99	0.45
12:n:34:GLN:HG2	16:n:509:CLA:HHB	1.98	0.45
12:p:169:ALA:HB2	12:p:268:PRO:HB3	1.99	0.45
16:t:507:CLA:HED2	16:t:511:CLA:H72	1.99	0.45
16:u:508:CLA:HMC3	16:u:511:CLA:HBC1	1.99	0.45
16:u:515:CLA:H91	16:u:515:CLA:H111	1.87	0.45
12:v:6:ASN:HD21	12:v:9:VAL:HG22	1.82	0.45
16:A:1130:CLA:HMC2	16:A:1136:CLA:H203	1.98	0.45
6:F:24:LEU:O	6:F:36:ARG:NH2	2.33	0.45
6:F:59:PHE:HA	6:F:62:ALA:HB2	1.98	0.45
16:G:1221:CLA:HMA2	16:G:1221:CLA:H11	1.99	0.45
1:H:200:HIS:ND1	16:H:1123:CLA:OBD	2.50	0.45
1:H:736:ILE:HG21	16:H:1126:CLA:HMC1	1.99	0.45
16:H:1138:CLA:H203	16:H:1139:CLA:H52	1.99	0.45
16:L:1501:CLA:HAA2	19:l:4022:BCR:H363	1.99	0.45
16:X:504:CLA:H3A	16:X:504:CLA:HBA2	1.54	0.45
2:b:56:ILE:HD11	21:m:4021:ECH:H23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:8:THR:O	12:n:10:GLN:NE2	2.50	0.45
16:n:507:CLA:H172	16:n:511:CLA:H193	1.99	0.45
13:o:605:LHG:H241	13:o:605:LHG:HC91	1.98	0.45
12:u:31:HIS:HD2	16:u:509:CLA:H91	1.82	0.45
16:v:512:CLA:HBA1	16:v:512:CLA:H3A	1.73	0.45
16:x:507:CLA:H3A	16:x:511:CLA:HAB	1.99	0.45
16:y:504:CLA:H11	16:y:506:CLA:HAA1	1.98	0.45
16:y:510:CLA:H142	19:y:603:BCR:H362	1.97	0.45
1:A:344:LEU:HB3	16:A:1123:CLA:HBC3	1.99	0.45
2:B:582:ASN:HB2	16:B:1012:CLA:HBC2	1.97	0.45
16:B:1206:CLA:H143	16:B:1206:CLA:H111	1.87	0.45
19:B:4009:BCR:H15C	19:B:4009:BCR:H351	1.87	0.45
2:G:420:LEU:HG	16:G:1236:CLA:HBB1	1.98	0.45
16:H:1105:CLA:HMB1	19:S:4012:BCR:H24C	1.99	0.45
12:W:19:ARG:NH1	16:W:512:CLA:OBD	2.41	0.45
12:X:272:TYR:O	12:X:299:SER:OG	2.34	0.45
16:Y:517:CLA:HBA1	16:Y:517:CLA:H3A	1.65	0.45
16:a:1140:CLA:H171	8:j:23:ALA:HB2	1.98	0.45
2:b:446:THR:HB	2:b:449:LYS:HG3	1.99	0.45
19:n:601:BCR:H20C	19:n:601:BCR:H361	1.84	0.45
12:q:314:PHE:HZ	16:q:507:CLA:HHB	1.82	0.45
16:v:512:CLA:H91	16:v:512:CLA:H111	1.86	0.45
1:A:458:ASN:HD21	1:A:533:MET:HE1	1.82	0.45
15:A:1011:CL0:H7	16:B:1021:CLA:HMB1	1.99	0.45
2:B:449:LYS:NZ	16:B:1230:CLA:OBD	2.46	0.45
1:H:168:MET:HG3	19:H:4002:BCR:H322	1.99	0.45
16:H:1119:CLA:H101	19:H:4008:BCR:H10C	1.99	0.45
12:W:333:VAL:HA	16:X:512:CLA:H8	1.98	0.45
16:W:505:CLA:H171	16:W:510:CLA:H121	1.98	0.45
16:X:517:CLA:HAA1	12:Y:40:PHE:HE2	1.82	0.45
2:b:123:TRP:NE1	16:b:1215:CLA:OBD	2.44	0.45
2:b:393:VAL:HG23	2:b:538:ALA:HB1	1.99	0.45
16:p:513:CLA:H3A	16:p:513:CLA:HBA2	1.57	0.45
16:r:515:CLA:HBB2	19:v:604:BCR:H351	1.98	0.45
16:y:502:CLA:HMD2	16:y:509:CLA:H161	1.98	0.45
1:A:576:GLY:HA2	2:B:559:PRO:HD3	1.99	0.44
19:A:4011:BCR:H20C	2:B:436:VAL:HG11	1.99	0.44
2:B:439:ASP:OD1	2:B:613:LEU:N	2.50	0.44
13:I:103:LHG:H341	21:M:4021:ECH:H29A	1.97	0.44
15:a:1011:CL0:H7	16:b:1021:CLA:HMB1	1.99	0.44
16:b:1211:CLA:H162	19:b:4005:BCR:H14C	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:h:604:BCR:H20C	19:h:604:BCR:H361	1.86	0.44
16:n:504:CLA:H2	16:n:506:CLA:H12	1.99	0.44
12:p:26:LEU:HD13	16:p:512:CLA:HAA2	1.99	0.44
12:w:45:PHE:HA	12:w:48:PHE:HB3	1.99	0.44
1:A:56:HIS:CD2	16:A:1103:CLA:HBB2	2.53	0.44
16:B:1210:CLA:H111	16:B:1210:CLA:H72	1.84	0.44
2:G:415:ALA:HB1	16:G:1227:CLA:HMB3	1.98	0.44
2:G:646:MET:HE2	19:G:4017:BCR:H333	1.99	0.44
21:R:4020:ECH:H31	21:R:4020:ECH:H7	1.74	0.44
12:W:108:LEU:HA	12:W:111:THR:HG22	1.99	0.44
12:Y:301:ALA:O	12:Y:305:ASN:ND2	2.51	0.44
16:Z:515:CLA:H12	19:Z:603:BCR:HC7	1.98	0.44
1:a:581:GLY:O	2:b:665:ARG:NH1	2.44	0.44
19:l:4019:BCR:H20C	19:l:4019:BCR:H361	1.77	0.44
16:s:502:CLA:H43	16:s:504:CLA:HBB2	1.97	0.44
12:v:59:MET:N	12:v:59:MET:SD	2.91	0.44
12:x:246:LEU:HD23	16:x:509:CLA:HED1	1.98	0.44
16:x:503:CLA:HBB1	19:x:602:BCR:H371	1.99	0.44
16:y:508:CLA:H3A	16:y:508:CLA:HBA2	1.62	0.44
16:A:1139:CLA:H92	16:A:1139:CLA:H61	1.81	0.44
2:B:577:MET:HG3	2:B:707:LEU:HD21	2.00	0.44
2:G:339:LEU:HG	16:G:1221:CLA:H12	2.00	0.44
2:G:450:GLN:OE1	2:G:611:THR:OG1	2.35	0.44
16:G:1203:CLA:H151	16:G:1225:CLA:HBB2	1.97	0.44
1:H:223:ILE:HG23	1:H:236:ILE:HG21	1.98	0.44
1:H:433:ARG:NH1	1:H:558:SER:O	2.50	0.44
5:O:36:PRO:HD2	5:O:62:ALA:HA	2.00	0.44
12:Z:1:MET:HG3	12:Z:18:ALA:HB1	1.99	0.44
16:Z:504:CLA:HAB	16:Z:506:CLA:H121	2.00	0.44
2:b:427:LEU:HD11	16:b:1235:CLA:HMB3	2.00	0.44
12:n:298:THR:HG23	12:n:301:ALA:H	1.81	0.44
12:q:91:VAL:HG22	19:q:602:BCR:HC21	1.98	0.44
12:q:128:PHE:CE2	16:q:502:CLA:HBB1	2.52	0.44
12:q:333:VAL:HA	23:r:606:LMU:H21	1.99	0.44
16:r:511:CLA:HMD1	13:r:605:LHG:HC82	1.98	0.44
16:v:509:CLA:H3A	16:v:509:CLA:HBA1	1.62	0.44
16:w:517:CLA:H12	16:w:517:CLA:H51	1.84	0.44
16:A:1103:CLA:H102	19:A:4003:BCR:H21C	2.00	0.44
16:A:1139:CLA:H71	8:J:14:MET:HE3	1.99	0.44
1:H:56:HIS:CD2	16:H:1103:CLA:HBB2	2.52	0.44
1:H:148:ARG:HD3	1:H:377:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:194:GLU:HA	1:H:321:MET:HE3	2.00	0.44
16:X:511:CLA:HMD2	19:X:601:BCR:HC7	1.99	0.44
1:a:332:PHE:O	1:a:428:ARG:NH2	2.47	0.44
1:a:426:LEU:HD22	19:a:4007:BCR:H322	1.99	0.44
1:a:459:ASP:OD1	2:b:632:TYR:OH	2.29	0.44
2:b:177:HIS:CG	16:b:1210:CLA:HMC2	2.53	0.44
2:b:285:ILE:O	2:b:289:HIS:ND1	2.51	0.44
12:h:227:LEU:HD12	12:h:229:TRP:HE1	1.82	0.44
16:h:515:CLA:HMB1	16:h:515:CLA:H122	1.98	0.44
12:o:148:PHE:HD2	16:o:502:CLA:H3A	1.81	0.44
12:r:183:ASP:HB3	12:r:185:LEU:HD23	1.99	0.44
16:x:510:CLA:H72	16:x:516:CLA:HBB2	1.99	0.44
16:y:509:CLA:H91	16:y:509:CLA:H111	1.84	0.44
16:A:1124:CLA:H101	19:A:4008:BCR:H23C	2.00	0.44
2:G:559:PRO:HD3	1:H:576:GLY:HA2	2.00	0.44
16:H:1117:CLA:H72	16:H:1117:CLA:H111	1.88	0.44
12:Y:214:LEU:HD21	16:Y:510:CLA:H72	1.98	0.44
16:Z:508:CLA:HBC3	16:Z:511:CLA:HAC2	1.98	0.44
1:a:56:HIS:CD2	16:a:1103:CLA:HBB2	2.52	0.44
1:a:273:ASP:OD1	1:a:273:ASP:N	2.47	0.44
16:a:1102:CLA:HBA2	16:a:1102:CLA:H3A	1.73	0.44
2:b:22:TRP:CG	2:b:701:GLN:HE22	2.36	0.44
12:p:227:LEU:HD12	12:p:229:TRP:HE1	1.80	0.44
19:p:601:BCR:H20C	19:p:601:BCR:H361	1.82	0.44
16:u:512:CLA:H2	16:u:512:CLA:H61	1.72	0.44
16:v:502:CLA:H11	16:v:504:CLA:HMC2	1.99	0.44
12:x:2:GLN:HG3	12:x:4:TYR:HD2	1.83	0.44
1:A:200:HIS:HB3	16:A:1123:CLA:HED3	1.98	0.44
2:G:339:LEU:O	2:G:343:THR:OG1	2.33	0.44
16:G:1215:CLA:H92	16:G:1221:CLA:H41	1.99	0.44
16:H:1124:CLA:H42	16:H:1136:CLA:HBA1	2.00	0.44
1:a:265:THR:HB	9:k:14:TRP:HB2	2.00	0.44
14:a:4101:LMG:H112	10:l:67:LEU:HD13	1.99	0.44
16:b:1219:CLA:H3A	16:b:1240:CLA:HBB2	1.99	0.44
12:g:177:VAL:HG13	12:g:201:GLU:HG2	1.99	0.44
16:g:508:CLA:H3A	16:g:508:CLA:HBA2	1.73	0.44
12:h:142:LEU:HD11	16:h:516:CLA:HMB3	2.00	0.44
12:p:192:THR:OG1	12:p:193:HIS:N	2.51	0.44
16:p:509:CLA:HBA1	16:p:509:CLA:H11	1.76	0.44
12:s:112:LEU:HD11	12:u:323:LEU:HG	1.99	0.44
1:A:484:GLN:NE2	1:A:527:LEU:O	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1132:CLA:H201	16:L:1502:CLA:HBA1	1.99	0.44
2:B:290:MET:HA	16:B:1218:CLA:HHD	1.99	0.44
16:B:1202:CLA:HBC2	16:B:1226:CLA:HMA1	1.99	0.44
2:G:449:LYS:NZ	16:G:1230:CLA:OBD	2.43	0.44
7:I:36:SER:OG	7:I:37:GLU:N	2.51	0.44
12:X:121:LEU:HD11	16:X:503:CLA:HED2	1.99	0.44
12:X:183:ASP:HB2	12:X:186:VAL:HG22	2.00	0.44
12:X:249:ILE:HG13	16:X:506:CLA:HAC1	2.00	0.44
16:X:505:CLA:H122	16:X:510:CLA:H61	2.00	0.44
16:a:1131:CLA:HMC2	16:l:1503:CLA:HBB2	2.00	0.44
2:b:371:THR:HG23	2:b:588:THR:HG21	2.00	0.44
2:b:386:ALA:HB1	16:b:1226:CLA:HMD3	2.00	0.44
6:f:135:ASP:OD1	6:f:135:ASP:N	2.51	0.44
19:p:602:BCR:H20C	19:p:602:BCR:H361	1.86	0.44
12:r:190:TYR:OH	12:r:202:ASP:OD2	2.34	0.44
12:t:156:LEU:HB2	16:t:505:CLA:HMD3	2.00	0.44
12:x:280:LEU:HD22	12:y:48:PHE:HB2	1.99	0.44
16:x:504:CLA:H41	16:x:505:CLA:HBA2	2.00	0.44
16:x:507:CLA:HED2	16:x:511:CLA:H52	2.00	0.44
16:y:512:CLA:HBA1	19:y:604:BCR:H282	1.99	0.44
16:A:1022:CLA:H172	16:B:1206:CLA:HMB2	2.00	0.44
2:B:85:ARG:HD3	2:B:115:ILE:HD13	1.99	0.44
6:F:67:ILE:HG12	16:J:1303:CLA:HMB3	1.99	0.44
16:H:1101:CLA:HMD1	6:Q:101:VAL:HB	2.00	0.44
16:H:1119:CLA:HMB2	16:H:1123:CLA:HMA3	1.99	0.44
16:K:4004:CLA:H11	16:K:4004:CLA:H51	1.82	0.44
16:U:1502:CLA:H62	16:U:1502:CLA:H41	1.80	0.44
16:W:504:CLA:HAB	16:W:506:CLA:H122	1.99	0.44
16:l:1503:CLA:HBA2	20:l:4101:LMT:H12	2.00	0.44
12:o:305:ASN:HB3	19:o:601:BCR:H382	1.99	0.44
16:r:504:CLA:H13	16:r:504:CLA:H101	1.81	0.44
16:s:515:CLA:H2	19:s:603:BCR:HC7	2.00	0.44
1:A:324:ILE:O	1:A:328:HIS:ND1	2.38	0.44
16:B:1203:CLA:HMC2	19:B:4005:BCR:H401	2.00	0.44
2:G:177:HIS:CG	16:G:1210:CLA:HMC2	2.53	0.44
1:H:199:HIS:CG	16:H:1111:CLA:HMC2	2.53	0.44
1:H:288:LEU:HD13	16:H:1116:CLA:HMA2	2.00	0.44
13:H:851:LHG:HC62	16:H:1801:CLA:HMB3	1.99	0.44
7:I:12:TRP:NE1	10:U:149:ASP:OD1	2.51	0.44
6:f:17:LEU:O	6:f:21:LYS:NZ	2.43	0.44
12:s:51:SER:HB2	12:u:279:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:604:BCR:H20C	19:s:604:BCR:H361	1.88	0.44
12:w:41:TRP:HB2	16:w:507:CLA:HAC2	2.00	0.44
12:w:328:PHE:HZ	12:w:333:VAL:HG23	1.83	0.44
16:x:509:CLA:H161	16:x:509:CLA:H141	1.84	0.44
16:y:509:CLA:H51	16:y:509:CLA:H8	1.66	0.44
16:A:1022:CLA:H151	16:B:1207:CLA:HBC3	2.00	0.43
19:A:4002:BCR:H20C	19:A:4002:BCR:H361	1.82	0.43
2:B:268:LEU:HD22	16:B:1214:CLA:HBA1	1.99	0.43
2:B:697:LEU:HD21	17:B:2002:PQN:H151	1.98	0.43
2:G:393:VAL:HG23	2:G:538:ALA:HB1	2.00	0.43
16:G:1204:CLA:H93	21:V:4021:ECH:H36A	2.00	0.43
16:G:1204:CLA:HHB	16:G:1205:CLA:HHB	2.00	0.43
19:U:4022:BCR:H20C	19:U:4022:BCR:H361	1.80	0.43
20:U:4101:LMT:H5B	20:U:4101:LMT:H6E	2.00	0.43
12:W:144:HIS:CD2	16:W:502:CLA:HAB	2.52	0.43
12:Y:73:LEU:HG	12:Y:159:LYS:HE3	1.98	0.43
12:Y:150:GLY:HA3	12:Y:215:ILE:HG13	1.99	0.43
16:Z:509:CLA:H161	16:Z:509:CLA:H141	1.86	0.43
1:a:285:THR:HB	1:a:377:PRO:HB3	2.00	0.43
1:a:355:ASN:ND2	16:a:1103:CLA:OBD	2.41	0.43
1:a:666:SER:HB2	2:b:443:ALA:HB1	2.00	0.43
16:a:1102:CLA:HBC2	16:a:1128:CLA:H42	1.99	0.43
16:b:1229:CLA:HAB	19:b:4014:BCR:HC8	1.99	0.43
12:g:52:ARG:HE	12:g:52:ARG:HB3	1.61	0.43
12:n:42:ALA:O	12:n:46:THR:OG1	2.34	0.43
12:p:34:GLN:HG2	16:p:509:CLA:HHB	2.00	0.43
12:q:111:THR:HG21	19:q:604:BCR:H391	2.00	0.43
1:A:365:ILE:HG21	16:A:1117:CLA:H191	1.99	0.43
16:B:1207:CLA:H43	16:B:1207:CLA:HED1	2.00	0.43
2:G:22:TRP:CG	2:G:701:GLN:HE22	2.36	0.43
2:G:392:PHE:HB3	2:G:539:ARG:HG3	2.00	0.43
1:H:13:LYS:HA	1:H:13:LYS:HD3	1.81	0.43
12:W:42:ALA:O	12:W:46:THR:OG1	2.31	0.43
12:W:70:LEU:HD11	16:W:504:CLA:HED3	2.00	0.43
12:Y:53:PHE:HB2	12:Y:64:LEU:HD21	2.00	0.43
1:a:120:ILE:HG12	1:a:121:VAL:HG13	1.99	0.43
6:f:91:ARG:HA	6:f:96:PRO:HB3	2.00	0.43
16:o:508:CLA:HMB3	16:o:508:CLA:H71	2.01	0.43
16:o:512:CLA:HBA1	16:o:512:CLA:H3A	1.81	0.43
19:q:604:BCR:H272	23:q:605:LMU:H42	2.00	0.43
16:s:512:CLA:H162	16:s:512:CLA:H202	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:x:30:ALA:HA	16:x:512:CLA:HMB3	2.01	0.43
16:A:1237:CLA:H192	10:L:61:LEU:HD21	1.99	0.43
16:H:1129:CLA:HAB	16:H:1137:CLA:HBB2	1.99	0.43
20:L:4101:LMT:H5B	20:L:4101:LMT:H6E	2.00	0.43
12:W:145:HIS:ND1	16:W:510:CLA:OBD	2.44	0.43
12:X:245:SER:HB3	16:X:510:CLA:HAA1	1.99	0.43
12:s:280:LEU:HD22	12:w:48:PHE:HB2	2.00	0.43
19:s:601:BCR:H312	13:s:605:LHG:HC81	2.00	0.43
12:y:207:HIS:HA	12:y:210:VAL:HG22	2.00	0.43
1:A:332:PHE:O	1:A:428:ARG:NH2	2.48	0.43
1:A:362:LEU:HD22	16:A:1127:CLA:H193	2.00	0.43
1:A:381:ILE:HB	1:A:519:LYS:HD2	2.00	0.43
3:C:32:ASP:OD1	3:C:32:ASP:N	2.49	0.43
16:a:1022:CLA:H172	16:b:1206:CLA:HMB2	2.00	0.43
12:g:45:PHE:HA	12:g:48:PHE:HB3	2.00	0.43
12:p:301:ALA:O	12:p:305:ASN:ND2	2.51	0.43
12:p:305:ASN:HB3	19:p:601:BCR:H23C	2.00	0.43
12:q:226:PRO:HA	16:q:516:CLA:HED3	2.01	0.43
16:q:504:CLA:H93	16:q:510:CLA:H42	1.99	0.43
19:q:602:BCR:H10C	19:q:602:BCR:HC7	1.80	0.43
16:s:505:CLA:H143	16:s:505:CLA:H161	1.88	0.43
16:u:509:CLA:H3A	16:u:509:CLA:HBA1	1.72	0.43
12:v:168:ASP:HB2	12:v:175:ARG:HB2	1.99	0.43
12:y:49:GLU:HB3	12:y:64:LEU:HG	1.99	0.43
2:B:684:LEU:HD11	10:L:37:LEU:HD13	2.00	0.43
16:B:1210:CLA:H141	16:B:1210:CLA:H162	1.88	0.43
17:B:2002:PQN:H252	17:B:2002:PQN:H211	1.72	0.43
16:G:1210:CLA:H111	16:G:1210:CLA:H72	1.82	0.43
1:H:747:SER:HA	1:H:750:ILE:HG12	2.00	0.43
16:H:1103:CLA:H142	19:H:4003:BCR:H372	2.00	0.43
16:X:512:CLA:HMB2	19:X:604:BCR:H24C	2.00	0.43
12:Y:19:ARG:NH1	16:Y:512:CLA:OBD	2.46	0.43
12:Z:335:GLN:NE2	23:g:606:LMU:O3'	2.40	0.43
1:a:111:LYS:HD2	1:a:138:GLN:HE22	1.83	0.43
12:h:245:SER:HA	16:h:510:CLA:H3A	2.00	0.43
16:h:506:CLA:H41	16:h:506:CLA:H93	2.00	0.43
12:n:254:PHE:HE2	12:n:315:LEU:HD22	1.83	0.43
16:n:507:CLA:H112	16:n:511:CLA:H171	1.99	0.43
12:s:239:GLU:OE2	12:s:321:HIS:ND1	2.48	0.43
12:t:237:SER:OG	12:t:238:GLY:N	2.51	0.43
16:w:515:CLA:H121	16:w:515:CLA:HMC2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:HIS:CG	16:B:1210:CLA:HMC2	2.53	0.43
16:B:1202:CLA:H11	16:B:1202:CLA:H51	1.84	0.43
2:G:667:TYR:OH	16:G:1023:CLA:OBD	2.28	0.43
10:L:61:LEU:HD23	10:L:61:LEU:HA	1.91	0.43
9:T:34:LYS:HD3	16:T:4003:CLA:HMD1	2.00	0.43
16:W:502:CLA:H11	16:W:506:CLA:H8	2.00	0.43
12:X:30:ALA:HB1	16:X:509:CLA:HBB1	1.99	0.43
12:X:298:THR:O	12:X:300:ARG:N	2.52	0.43
12:Y:326:LEU:HD13	12:Z:113:ARG:HG3	2.00	0.43
12:Z:310:LEU:HD22	16:Z:506:CLA:HMC3	2.00	0.43
1:a:573:PRO:HB3	1:a:720:ILE:HB	2.00	0.43
16:a:1116:CLA:H41	16:a:1133:CLA:HBA2	2.00	0.43
2:b:315:ALA:O	2:b:318:THR:OG1	2.31	0.43
16:b:1204:CLA:H161	16:b:1205:CLA:H201	2.00	0.43
4:d:87:ARG:NH1	4:d:95:GLN:OE1	2.49	0.43
12:h:65:ILE:O	12:h:69:HIS:ND1	2.49	0.43
12:o:148:PHE:CD2	16:o:502:CLA:H3A	2.53	0.43
12:q:59:MET:HE3	12:q:83:ILE:HG13	2.01	0.43
12:q:161:MET:HE1	12:q:180:PRO:HB3	2.01	0.43
12:q:246:LEU:HD23	16:q:509:CLA:HED1	2.00	0.43
12:q:301:ALA:O	12:q:305:ASN:ND2	2.51	0.43
12:r:210:VAL:HG11	16:r:505:CLA:HHC	2.00	0.43
16:r:512:CLA:HBA2	23:r:606:LMU:H31	2.00	0.43
12:t:30:ALA:HB1	16:t:509:CLA:HBB1	2.00	0.43
12:u:219:ILE:HG12	16:u:501:CLA:HBB2	2.01	0.43
12:x:272:TYR:HB3	12:x:300:ARG:HB2	2.00	0.43
1:A:104:LEU:HD23	1:A:233:PRO:HB3	2.01	0.43
1:A:539:ALA:O	1:A:543:HIS:ND1	2.52	0.43
16:A:1119:CLA:H121	16:A:1124:CLA:HBB1	2.01	0.43
1:H:381:ILE:HG21	1:H:516:VAL:HB	2.00	0.43
19:K:4005:BCR:H20C	19:K:4005:BCR:H361	1.87	0.43
3:N:2:SER:N	3:N:71:ALA:O	2.51	0.43
19:T:4001:BCR:H15C	19:T:4001:BCR:H351	1.89	0.43
19:U:4022:BCR:HC8	16:l:1501:CLA:HBB1	2.01	0.43
12:X:187:ILE:HD11	12:X:206:GLY:HA2	1.99	0.43
12:Z:143:GLY:HA3	12:Z:222:ILE:HG13	2.00	0.43
1:a:13:LYS:HG3	1:a:314:ASN:HD21	1.83	0.43
1:a:257:ALA:HB1	12:r:294:MET:HA	2.01	0.43
12:g:134:ASN:HA	12:g:135:PRO:HD3	1.90	0.43
12:g:298:THR:HG23	12:g:301:ALA:H	1.83	0.43
16:g:505:CLA:H203	19:g:603:BCR:H12C	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:n:504:CLA:HAB	16:n:506:CLA:H111	2.00	0.43
16:t:508:CLA:H3A	16:t:508:CLA:HBA2	1.68	0.43
16:u:509:CLA:H2	16:u:509:CLA:H62	1.79	0.43
4:D:43:PRO:HD3	4:D:68:LEU:HD12	2.01	0.43
4:D:85:ILE:HB	4:D:98:HIS:HB3	2.01	0.43
1:H:118:TRP:HB3	19:S:4013:BCR:HC42	2.01	0.43
16:H:1140:CLA:H151	8:S:19:LEU:HB3	2.01	0.43
8:J:15:ILE:HG23	8:J:16:MET:HE2	1.99	0.43
16:Z:502:CLA:HAA2	16:Z:509:CLA:H102	2.01	0.43
16:Z:515:CLA:H72	16:Z:515:CLA:H112	1.77	0.43
1:a:204:LEU:HD13	16:a:1111:CLA:HHB	1.99	0.43
2:b:73:ASN:HB2	2:b:76:GLN:HB2	2.01	0.43
16:b:1203:CLA:H151	16:b:1225:CLA:HBB2	2.00	0.43
16:o:517:CLA:HAA1	12:p:40:PHE:HE2	1.83	0.43
12:u:156:LEU:HB2	16:u:505:CLA:HMD3	1.99	0.43
12:v:254:PHE:HE2	12:v:315:LEU:HD22	1.84	0.43
16:w:512:CLA:H3A	19:w:604:BCR:H292	1.99	0.43
12:x:205:GLY:HA2	12:x:208:ILE:HD12	2.00	0.43
12:y:37:LEU:HD23	16:y:507:CLA:HAC1	2.01	0.43
12:y:131:THR:HB	12:y:134:ASN:HB2	2.00	0.43
12:y:227:LEU:HD12	12:y:229:TRP:HE1	1.84	0.43
16:A:1117:CLA:H72	16:A:1117:CLA:H111	1.86	0.43
2:B:642:VAL:HG21	16:B:1206:CLA:HMD2	2.01	0.43
16:B:1201:CLA:HMD2	19:L:4019:BCR:HC31	2.01	0.43
16:B:1225:CLA:H161	16:B:1225:CLA:H202	1.85	0.43
2:G:556:CYS:SG	2:G:557:ASP:N	2.90	0.43
1:H:278:LYS:HG2	1:H:502:LEU:HD12	2.00	0.43
19:H:4007:BCR:H15C	19:H:4007:BCR:H351	1.86	0.43
16:T:4002:CLA:HMA3	16:T:4002:CLA:HED2	2.01	0.43
12:W:280:LEU:HD13	12:X:47:LEU:HB2	2.00	0.43
2:b:555:PRO:HB3	2:b:699:ILE:HB	2.01	0.43
16:b:1220:CLA:H61	16:b:1220:CLA:H41	1.83	0.43
12:g:128:PHE:HE2	19:g:602:BCR:H282	1.84	0.43
12:h:146:LEU:HD23	12:h:146:LEU:HA	1.91	0.43
12:o:30:ALA:HB1	16:o:509:CLA:HBB1	2.01	0.43
12:q:148:PHE:CE1	16:q:502:CLA:HHB	2.54	0.43
12:r:246:LEU:HD23	16:r:509:CLA:HED1	2.01	0.43
16:u:504:CLA:H92	16:u:505:CLA:HMC2	2.01	0.43
12:v:31:HIS:HD2	16:v:509:CLA:H141	1.84	0.43
16:v:511:CLA:H43	16:v:512:CLA:HAC1	2.00	0.43
12:w:150:GLY:HA3	12:w:215:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:w:233:VAL:HG21	19:w:603:BCR:HC41	2.01	0.43
12:y:97:LEU:HD13	19:y:604:BCR:H10C	2.01	0.43
16:y:508:CLA:HMC1	16:y:511:CLA:HBC1	2.00	0.43
16:A:1022:CLA:H121	19:B:4017:BCR:H10C	2.01	0.43
2:G:126:THR:HG22	2:G:270:LEU:HD21	2.00	0.43
2:G:371:THR:HG23	2:G:588:THR:HG21	2.01	0.43
1:H:373:MET:HE2	16:H:1125:CLA:HMC2	2.00	0.43
19:K:4005:BCR:H15C	19:K:4005:BCR:H351	1.91	0.43
16:W:507:CLA:H72	19:W:601:BCR:H12C	2.01	0.43
12:X:243:SER:O	12:X:318:HIS:ND1	2.44	0.43
2:b:574:TYR:HD1	2:b:707:LEU:HD22	1.83	0.43
12:n:227:LEU:HD12	12:n:229:TRP:HE1	1.83	0.43
12:r:249:ILE:HG12	16:r:506:CLA:HAC1	2.01	0.43
16:t:509:CLA:H142	16:t:509:CLA:H111	1.92	0.43
12:u:143:GLY:HA3	12:u:222:ILE:HG13	2.01	0.43
12:v:197:ILE:HG23	12:v:265:LEU:HB3	2.01	0.43
12:w:145:HIS:HB3	16:w:509:CLA:H91	2.01	0.43
12:y:11:TYR:O	12:y:19:ARG:NH2	2.52	0.43
2:B:118:SER:HA	16:B:1224:CLA:HMA2	2.01	0.42
2:B:454:GLU:OE1	2:B:459:GLN:NE2	2.42	0.42
16:B:1223:CLA:H193	16:B:1223:CLA:H161	1.89	0.42
2:G:436:VAL:HG12	16:G:1230:CLA:HAC1	2.00	0.42
1:H:366:VAL:HA	16:H:1117:CLA:H42	2.00	0.42
1:H:367:ALA:HB2	1:H:393:HIS:HB2	2.01	0.42
16:H:1101:CLA:H141	19:H:4011:BCR:H292	2.01	0.42
16:H:1110:CLA:H41	16:H:1110:CLA:H62	1.83	0.42
3:N:66:ARG:HD2	3:N:66:ARG:HA	1.81	0.42
10:U:53:VAL:O	10:U:57:HIS:ND1	2.41	0.42
12:W:4:TYR:OH	12:W:328:PHE:O	2.34	0.42
12:X:251:LEU:HB2	16:X:515:CLA:HMC1	2.01	0.42
16:X:515:CLA:H61	16:X:515:CLA:H41	1.80	0.42
12:Y:246:LEU:HD23	16:Y:509:CLA:HED1	2.01	0.42
16:a:1123:CLA:H143	16:a:1123:CLA:HMD2	2.01	0.42
16:a:1129:CLA:H3A	16:a:1130:CLA:OBD	2.19	0.42
16:b:1214:CLA:H3A	16:b:1214:CLA:HBA2	1.68	0.42
16:b:1239:CLA:H112	16:b:1239:CLA:H91	1.80	0.42
16:h:509:CLA:H3A	16:h:509:CLA:HBA1	1.68	0.42
12:n:146:LEU:HG	16:n:510:CLA:HED1	2.01	0.42
12:o:183:ASP:HB2	12:o:186:VAL:HG22	2.01	0.42
12:s:17:ASN:ND2	16:s:507:CLA:O1A	2.52	0.42
12:s:85:ASP:HB3	12:s:86:THR:H	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:w:510:CLA:H91	16:w:510:CLA:H112	1.89	0.42
12:y:245:SER:HA	16:y:510:CLA:H3A	2.01	0.42
1:A:310:MET:HA	16:A:1120:CLA:HHD	2.00	0.42
1:A:362:LEU:HD11	16:A:1117:CLA:H71	2.00	0.42
1:A:588:TRP:CD1	16:A:1128:CLA:HMD1	2.54	0.42
16:A:1107:CLA:HAB	16:B:1230:CLA:HMD2	2.01	0.42
2:B:285:ILE:O	2:B:289:HIS:ND1	2.50	0.42
16:B:1023:CLA:H202	16:B:1023:CLA:H162	1.82	0.42
10:U:5:ASN:HB3	10:U:6:GLN:H	1.63	0.42
12:Y:243:SER:O	12:Y:318:HIS:ND1	2.45	0.42
12:Z:255:VAL:HG21	16:Z:505:CLA:H92	2.00	0.42
1:a:225:LYS:HD3	1:a:252:LEU:HD22	2.01	0.42
2:b:317:HIS:CE1	13:b:4018:LHG:HC11	2.54	0.42
2:b:642:VAL:HG21	16:b:1206:CLA:HMD2	2.00	0.42
20:l:4101:LMT:H5B	20:l:4101:LMT:H6E	2.00	0.42
12:o:17:ASN:HB2	16:o:511:CLA:HAA2	2.00	0.42
16:o:504:CLA:H72	16:o:505:CLA:H43	2.01	0.42
16:q:512:CLA:H3A	19:q:604:BCR:H292	2.00	0.42
19:q:602:BCR:H20C	19:q:602:BCR:H361	1.85	0.42
16:t:510:CLA:H142	19:t:603:BCR:H362	2.00	0.42
12:v:28:ILE:HD11	16:v:502:CLA:HBC3	2.01	0.42
12:y:17:ASN:ND2	16:y:509:CLA:HBB2	2.35	0.42
12:y:242:LEU:HD11	16:y:511:CLA:HBB1	1.99	0.42
16:B:1021:CLA:H101	16:B:1021:CLA:H62	1.81	0.42
16:B:1238:CLA:H201	7:I:20:TRP:HB3	1.99	0.42
19:B:4014:BCR:H11C	19:B:4014:BCR:H341	1.91	0.42
2:G:416:LEU:HD23	16:G:1236:CLA:HBB2	2.01	0.42
2:G:591:TRP:CD1	16:G:1234:CLA:HAC1	2.54	0.42
16:G:1211:CLA:H2	16:G:1211:CLA:H61	1.74	0.42
16:G:1239:CLA:H91	16:G:1239:CLA:H112	1.79	0.42
19:G:4014:BCR:H332	19:S:4012:BCR:HC32	2.01	0.42
4:P:101:ASP:N	4:P:101:ASP:OD1	2.52	0.42
19:X:601:BCR:H20C	19:X:601:BCR:H361	1.88	0.42
1:a:373:MET:HE2	16:a:1125:CLA:HMC2	2.00	0.42
17:b:2002:PQN:H301	19:l:4019:BCR:HC7	2.01	0.42
5:e:10:ARG:HH12	5:e:69:VAL:HG21	1.84	0.42
12:g:110:HIS:HA	12:g:114:ALA:HB3	2.00	0.42
12:h:314:PHE:HZ	16:h:507:CLA:HHB	1.84	0.42
19:s:603:BCR:H24C	19:s:603:BCR:H371	1.89	0.42
16:A:1116:CLA:HBA2	16:A:1116:CLA:H3A	1.56	0.42
2:B:356:TYR:OH	16:B:1225:CLA:OBD	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:VAL:HG12	16:B:1230:CLA:HAC1	2.00	0.42
2:B:586:TRP:NE1	25:B:901:HOH:O	2.48	0.42
16:B:1203:CLA:H192	16:B:1203:CLA:H161	1.84	0.42
2:G:648:LEU:HD21	1:H:646:LEU:HD22	2.02	0.42
21:G:4006:ECH:H15	21:G:4006:ECH:H35	1.85	0.42
16:H:1103:CLA:H3A	16:H:1103:CLA:HBA1	1.76	0.42
16:H:1104:CLA:H151	16:H:1127:CLA:HBB2	2.01	0.42
12:Z:261:ALA:HA	12:Z:276:LEU:HD12	2.01	0.42
16:a:1114:CLA:HBB2	19:a:4002:BCR:H352	2.00	0.42
2:b:180:ALA:HA	2:b:285:ILE:HA	2.01	0.42
2:b:346:VAL:HG21	16:b:1225:CLA:HHD	2.01	0.42
16:b:1203:CLA:HAC1	16:b:1205:CLA:H192	2.02	0.42
16:b:1204:CLA:H102	19:i:4018:BCR:HC41	2.02	0.42
6:f:55:VAL:HG12	6:f:65:PHE:HB2	2.00	0.42
19:p:603:BCR:H15C	19:p:603:BCR:H351	1.88	0.42
12:r:227:LEU:HD12	12:r:229:TRP:HE1	1.83	0.42
12:s:121:LEU:HD11	12:s:125:GLY:HA3	2.01	0.42
16:v:511:CLA:HMD2	19:v:601:BCR:HC7	2.01	0.42
12:w:236:PHE:HE1	16:w:510:CLA:HMC1	1.84	0.42
16:A:1124:CLA:HMB1	16:A:1137:CLA:HAA1	2.01	0.42
16:A:1237:CLA:H91	16:A:1237:CLA:HBB1	2.02	0.42
16:B:1203:CLA:HAA1	16:B:1226:CLA:HMB2	2.02	0.42
16:B:1214:CLA:H43	16:B:1231:CLA:HED3	2.01	0.42
2:G:676:VAL:HG11	3:N:81:TYR:CG	2.54	0.42
1:H:429:MET:HE2	16:H:1119:CLA:H171	2.01	0.42
19:H:4003:BCR:H20C	19:H:4003:BCR:H361	1.86	0.42
7:R:34:ILE:HG13	7:R:35:GLU:HG2	2.01	0.42
10:U:132:MET:HB2	19:U:4022:BCR:H402	2.01	0.42
16:X:505:CLA:H142	16:X:505:CLA:H112	1.84	0.42
12:Z:210:VAL:HG11	16:Z:505:CLA:HHC	2.00	0.42
16:a:1105:CLA:H72	16:a:1105:CLA:H111	1.89	0.42
16:a:1117:CLA:H72	16:a:1117:CLA:H111	1.85	0.42
4:d:118:LYS:NZ	4:d:139:TYR:O	2.50	0.42
12:n:56:THR:OG1	12:n:57:GLN:OE1	2.37	0.42
12:n:143:GLY:HA3	12:n:222:ILE:HG13	2.02	0.42
19:o:603:BCR:H361	19:o:603:BCR:H20C	1.84	0.42
16:p:515:CLA:HMD2	19:p:603:BCR:H343	2.01	0.42
12:q:308:PHE:CZ	16:q:517:CLA:HBB1	2.54	0.42
16:r:512:CLA:HBD	23:r:606:LMU:H11	2.01	0.42
16:u:515:CLA:HBC2	19:u:603:BCR:H341	2.00	0.42
12:v:197:ILE:HD11	12:v:202:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:w:604:BCR:H20C	19:w:604:BCR:H361	1.88	0.42
1:A:485:TRP:HB2	20:A:4202:LMT:H11	2.02	0.42
3:C:81:TYR:HB3	4:D:19:LEU:HD13	2.01	0.42
2:G:315:ALA:O	2:G:318:THR:OG1	2.29	0.42
14:G:848:LMG:H352	16:G:1226:CLA:HBC2	2.02	0.42
16:G:1211:CLA:H93	16:G:1211:CLA:H111	1.92	0.42
4:P:129:VAL:HA	4:P:132:LYS:HG3	2.02	0.42
12:X:34:GLN:HG2	16:X:509:CLA:H3A	2.00	0.42
19:Z:602:BCR:H11C	19:Z:602:BCR:H341	1.91	0.42
1:a:195:SER:OG	16:a:1110:CLA:O1D	2.36	0.42
16:a:1124:CLA:HMA1	19:a:4008:BCR:H15C	2.01	0.42
2:b:524:LEU:HD12	16:b:1236:CLA:HED3	2.02	0.42
2:b:556:CYS:SG	2:b:558:GLY:N	2.82	0.42
2:b:571:ASP:HA	2:b:574:TYR:HB3	2.01	0.42
12:h:24:SER:HB2	12:h:118:LEU:H	1.85	0.42
12:h:194:PHE:HE1	19:n:604:BCR:HC42	1.84	0.42
19:o:603:BCR:H24C	19:o:603:BCR:H371	1.90	0.42
16:p:515:CLA:HAB	12:q:101:ALA:HB1	2.01	0.42
19:q:603:BCR:H15C	19:q:603:BCR:H351	1.88	0.42
12:s:249:ILE:HG12	16:s:506:CLA:HAC1	2.01	0.42
16:u:504:CLA:H42	16:u:506:CLA:HED3	2.02	0.42
16:v:502:CLA:HMD2	16:v:509:CLA:H161	2.01	0.42
16:x:506:CLA:HMB3	16:x:514:CLA:HAB	2.01	0.42
19:x:601:BCR:H11C	19:x:601:BCR:H341	1.92	0.42
19:x:603:BCR:H15C	19:x:603:BCR:H351	1.91	0.42
1:A:381:ILE:HG21	1:A:516:VAL:HB	2.01	0.42
1:A:620:THR:OG1	1:A:628:THR:OG1	2.37	0.42
2:B:568:SER:OG	2:B:571:ASP:OD2	2.36	0.42
16:B:1220:CLA:HHB	16:B:1240:CLA:HAC2	2.02	0.42
16:G:1023:CLA:H52	16:G:1023:CLA:HMB2	2.01	0.42
16:W:506:CLA:HBB2	16:W:507:CLA:H151	2.00	0.42
12:Y:207:HIS:HA	12:Y:210:VAL:HG12	2.01	0.42
16:a:1110:CLA:H62	16:a:1110:CLA:H41	1.75	0.42
16:a:1237:CLA:H192	10:l:61:LEU:HD21	2.02	0.42
19:k:4001:BCR:H15C	19:k:4001:BCR:H351	1.88	0.42
19:l:4019:BCR:H15C	19:l:4019:BCR:H351	1.84	0.42
12:q:144:HIS:CG	16:q:502:CLA:HAB	2.54	0.42
12:q:261:ALA:HA	12:q:276:LEU:HD12	2.01	0.42
12:u:254:PHE:HE2	12:u:315:LEU:HD22	1.84	0.42
1:A:411:PHE:HE2	1:A:426:LEU:HD21	1.85	0.42
1:A:583:CYS:O	2:B:666:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:1105:CLA:H2A	16:A:1107:CLA:HED1	2.01	0.42
1:H:579:ARG:NH2	4:P:63:GLU:OE2	2.48	0.42
19:U:4022:BCR:H353	16:l:1503:CLA:HMD3	2.02	0.42
21:V:4021:ECH:H2A	20:l:4101:LMT:H81	2.01	0.42
12:X:197:ILE:HG22	12:X:263:ASN:HD21	1.84	0.42
12:X:280:LEU:HD13	12:Y:47:LEU:HB2	2.02	0.42
16:X:513:CLA:HBA2	16:X:513:CLA:H3A	1.55	0.42
12:Z:19:ARG:NH1	16:Z:512:CLA:OBD	2.44	0.42
12:Z:280:LEU:HD13	12:g:47:LEU:HB2	2.01	0.42
1:a:293:THR:O	1:a:297:HIS:ND1	2.50	0.42
16:a:1123:CLA:HBA1	16:a:1127:CLA:H203	2.02	0.42
2:b:80:ASP:HB3	2:b:84:ILE:HG12	2.01	0.42
12:g:183:ASP:HB3	12:g:185:LEU:HD23	2.01	0.42
19:g:602:BCR:H20C	19:g:602:BCR:H361	1.91	0.42
16:h:505:CLA:HED2	16:h:505:CLA:HBD	1.93	0.42
12:o:323:LEU:HG	12:p:112:LEU:HD11	2.02	0.42
19:p:603:BCR:H24C	19:p:603:BCR:H371	1.87	0.42
12:q:274:PRO:HA	12:q:275:PRO:HD3	1.93	0.42
16:q:517:CLA:H51	16:q:517:CLA:H12	1.83	0.42
19:v:603:BCR:H15C	19:v:603:BCR:H351	1.92	0.42
12:w:34:GLN:HG2	16:w:509:CLA:H3A	2.00	0.42
12:y:276:LEU:HD22	12:y:286:PHE:HB3	2.02	0.42
1:A:354:ILE:HG12	19:A:4007:BCR:HC7	2.01	0.42
1:A:698:GLU:HA	1:A:701:VAL:HB	2.01	0.42
14:A:4101:LMG:H112	10:L:67:LEU:HD13	2.01	0.42
2:B:80:ASP:HB3	2:B:84:ILE:HG12	2.02	0.42
2:B:719:ALA:HB2	16:B:1224:CLA:HBB1	2.02	0.42
16:G:1205:CLA:H143	16:G:1205:CLA:H161	1.95	0.42
16:G:1207:CLA:H91	16:l:1503:CLA:H91	2.01	0.42
19:G:4014:BCR:H363	16:H:1101:CLA:H112	2.00	0.42
1:H:525:ILE:HD13	1:H:613:MET:HE1	2.02	0.42
16:H:1129:CLA:H3A	16:H:1130:CLA:OBD	2.20	0.42
16:H:1131:CLA:HMC3	14:H:4101:LMG:H352	2.02	0.42
5:O:42:ASP:OD1	5:O:42:ASP:N	2.46	0.42
7:R:17:MET:HE3	7:R:17:MET:HB2	1.84	0.42
19:S:4013:BCR:H15C	19:S:4013:BCR:H351	1.88	0.42
12:X:75:TRP:H	12:X:77:VAL:HG23	1.85	0.42
12:X:121:LEU:HD22	12:X:125:GLY:HA3	2.02	0.42
12:Y:261:ALA:HA	12:Y:276:LEU:HD12	2.01	0.42
12:Z:148:PHE:CD2	16:Z:502:CLA:H3A	2.54	0.42
16:Z:507:CLA:H61	16:Z:507:CLA:H41	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:b:1221:CLA:H143	16:b:1221:CLA:H162	1.95	0.42
12:g:249:ILE:HG12	16:g:506:CLA:HAC1	2.01	0.42
16:g:507:CLA:H72	19:g:601:BCR:H12C	2.01	0.42
16:g:515:CLA:O1D	12:h:113:ARG:NH1	2.53	0.42
16:n:515:CLA:H92	16:n:515:CLA:H41	2.00	0.42
16:o:517:CLA:H91	23:p:606:LMU:H92	2.02	0.42
12:q:118:LEU:HA	12:q:121:LEU:HD13	2.00	0.42
16:q:507:CLA:H112	16:q:507:CLA:H152	1.85	0.42
16:q:515:CLA:HAB	12:r:101:ALA:HB1	2.02	0.42
12:r:213:LEU:HG	16:r:516:CLA:HMC1	2.02	0.42
12:s:150:GLY:HA3	12:s:215:ILE:HG13	2.02	0.42
12:s:199:SER:HB3	12:s:202:ASP:HB2	2.00	0.42
16:s:507:CLA:H93	19:s:601:BCR:H14C	2.02	0.42
16:s:512:CLA:H162	16:s:512:CLA:H141	1.92	0.42
19:u:602:BCR:H15C	19:u:602:BCR:H351	1.95	0.42
12:v:42:ALA:O	12:v:46:THR:OG1	2.32	0.42
12:w:138:LEU:HD23	12:w:141:ILE:HD12	2.01	0.42
16:w:507:CLA:H41	16:w:507:CLA:H61	1.87	0.42
12:y:233:VAL:HG13	12:y:234:LEU:HG	2.01	0.42
1:A:674:ALA:HB2	16:B:1012:CLA:H51	2.02	0.42
16:A:1102:CLA:H3A	16:A:1102:CLA:HBA2	1.73	0.42
16:A:1110:CLA:H62	16:A:1110:CLA:H41	1.80	0.42
16:A:1129:CLA:H3A	16:A:1130:CLA:OBD	2.19	0.42
2:B:524:LEU:HD23	2:B:583:THR:HG21	2.02	0.42
19:L:4022:BCR:H291	10:U:133:GLY:HA3	2.01	0.42
12:X:42:ALA:O	12:X:46:THR:OG1	2.36	0.42
16:Y:509:CLA:H11	16:Y:509:CLA:HBA1	1.77	0.42
16:o:517:CLA:H62	12:p:37:LEU:HD21	2.01	0.42
12:q:41:TRP:HB2	16:q:507:CLA:HAC2	2.02	0.42
12:q:45:PHE:HA	12:q:48:PHE:HB3	2.01	0.42
16:q:515:CLA:HMC2	16:q:515:CLA:H121	2.02	0.42
16:v:507:CLA:H192	16:v:507:CLA:HBC3	2.02	0.42
19:x:601:BCR:H20C	19:x:601:BCR:H361	1.84	0.42
12:y:70:LEU:HD21	12:y:92:ILE:HG21	2.01	0.42
16:A:1128:CLA:H162	16:A:1128:CLA:H192	1.82	0.41
2:B:380:LEU:HD21	16:B:1203:CLA:H142	2.01	0.41
2:B:513:ASP:O	2:B:517:HIS:ND1	2.38	0.41
16:B:1204:CLA:HHB	16:B:1205:CLA:HHB	2.01	0.41
6:F:117:LEU:HD22	6:F:120:LEU:HD12	2.01	0.41
2:G:60:TRP:NE1	16:G:1224:CLA:OBD	2.47	0.41
2:G:290:MET:HA	16:G:1218:CLA:HHD	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:HIS:ND1	16:H:1104:CLA:O1A	2.41	0.41
16:H:1119:CLA:H121	16:H:1124:CLA:HBB1	2.01	0.41
19:U:4019:BCR:H20C	19:U:4019:BCR:H361	1.84	0.41
12:X:187:ILE:HA	12:X:190:TYR:HD2	1.85	0.41
16:Y:506:CLA:HBB2	16:Y:507:CLA:H151	2.01	0.41
16:Y:515:CLA:H92	16:Y:515:CLA:H62	1.89	0.41
1:a:86:TRP:HA	16:a:1105:CLA:HBB2	2.02	0.41
16:a:1105:CLA:HMB1	19:j:4012:BCR:H24C	2.02	0.41
2:b:341:VAL:HG13	16:b:1222:CLA:HED1	2.01	0.41
16:b:1203:CLA:HHB	16:b:1226:CLA:HAB	2.01	0.41
8:j:15:ILE:HG23	8:j:16:MET:HE2	2.01	0.41
16:n:508:CLA:HED2	12:o:108:LEU:HD11	2.02	0.41
16:o:505:CLA:HBB2	16:o:510:CLA:H62	2.02	0.41
16:p:504:CLA:H72	16:p:504:CLA:H112	1.84	0.41
16:r:507:CLA:H72	19:r:601:BCR:H12C	2.01	0.41
16:u:507:CLA:H112	16:u:507:CLA:H152	1.92	0.41
12:w:332:ARG:HG2	23:x:606:LMU:H2'	2.01	0.41
12:x:214:LEU:HD21	16:x:510:CLA:H71	2.01	0.41
19:y:603:BCR:H15C	19:y:603:BCR:H351	1.90	0.41
2:B:452:LEU:O	6:F:53:LEU:N	2.45	0.41
16:H:1118:CLA:H2	16:H:1118:CLA:H62	1.93	0.41
16:H:1131:CLA:H51	16:H:1131:CLA:H12	1.83	0.41
12:X:147:LEU:HD13	16:X:501:CLA:HMC3	2.02	0.41
2:b:65:LEU:HD11	21:b:4006:ECH:H29	2.02	0.41
2:b:556:CYS:SG	2:b:557:ASP:N	2.92	0.41
2:b:676:VAL:HG11	3:c:81:TYR:CG	2.55	0.41
16:b:1238:CLA:H141	16:b:1238:CLA:H162	1.86	0.41
12:g:226:PRO:HA	16:g:516:CLA:HED3	2.03	0.41
12:h:251:LEU:HB2	16:h:515:CLA:HMC1	2.01	0.41
16:h:515:CLA:H11	12:n:105:ALA:HA	2.02	0.41
16:n:501:CLA:HBA2	16:n:501:CLA:H3A	1.53	0.41
16:p:505:CLA:H62	16:p:505:CLA:H41	1.84	0.41
16:p:505:CLA:H111	16:p:510:CLA:H62	2.02	0.41
16:p:511:CLA:H112	16:p:511:CLA:H91	1.88	0.41
12:r:159:LYS:HA	12:r:163:TRP:HB2	2.01	0.41
16:s:513:CLA:HBA2	16:s:513:CLA:H3A	1.58	0.41
19:u:601:BCR:H11C	19:u:601:BCR:H341	1.94	0.41
16:w:502:CLA:H43	19:w:602:BCR:H373	2.01	0.41
1:A:203:GLY:HA3	16:A:1111:CLA:HBB1	2.01	0.41
1:A:573:PRO:HB3	1:A:720:ILE:HB	2.01	0.41
16:B:1012:CLA:HMA3	16:B:1021:CLA:H71	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:1238:CLA:H142	21:I:4020:ECH:H23	2.01	0.41
16:G:1232:CLA:HBA1	16:G:1232:CLA:H3A	1.68	0.41
17:G:2002:PQN:H191	16:H:1131:CLA:H143	2.02	0.41
1:H:362:LEU:HD21	16:H:1117:CLA:H93	2.01	0.41
1:H:708:ASN:HB2	6:Q:133:MET:HE3	2.02	0.41
15:H:1011:CL0:H49	15:H:1011:CL0:H41	1.88	0.41
21:R:4020:ECH:H15	21:R:4020:ECH:H35	1.90	0.41
10:U:72:ARG:HA	10:U:77:GLN:HG3	2.01	0.41
12:W:34:GLN:HG2	16:W:509:CLA:H3A	2.02	0.41
16:Y:515:CLA:HMD2	19:Y:603:BCR:H343	2.02	0.41
16:a:1103:CLA:H142	19:a:4003:BCR:H372	2.02	0.41
16:a:1106:CLA:H62	19:a:4011:BCR:H342	2.03	0.41
2:b:93:ASP:OD1	2:b:95:HIS:ND1	2.42	0.41
2:b:465:SER:O	2:b:494:TRP:NE1	2.45	0.41
16:b:1012:CLA:HMA3	16:b:1021:CLA:H71	2.02	0.41
16:b:1203:CLA:HAA1	16:b:1226:CLA:HMB2	2.02	0.41
12:n:308:PHE:CZ	16:n:517:CLA:HBB1	2.56	0.41
12:q:64:LEU:HD23	12:q:67:LEU:HD12	2.02	0.41
12:r:233:VAL:HG23	12:r:234:LEU:HG	2.02	0.41
19:r:602:BCR:H15C	19:r:602:BCR:H351	1.85	0.41
16:s:512:CLA:HBA1	16:s:512:CLA:H3A	1.74	0.41
16:s:517:CLA:HHB	12:w:44:ALA:HB1	2.02	0.41
12:t:190:TYR:OH	12:t:202:ASP:OD2	2.38	0.41
16:t:512:CLA:H2	16:t:512:CLA:H61	1.76	0.41
12:u:329:ASP:HB3	12:u:332:ARG:HG3	2.02	0.41
12:w:331:LYS:HE2	12:w:331:LYS:HB3	1.87	0.41
16:y:511:CLA:H91	16:y:511:CLA:H112	1.91	0.41
1:A:358:LEU:HD11	16:A:1119:CLA:H51	2.02	0.41
16:H:1119:CLA:H71	19:H:4008:BCR:H12C	2.01	0.41
9:T:18:VAL:HG13	9:T:75:ILE:HD13	2.01	0.41
16:U:1503:CLA:H52	16:U:1503:CLA:HBD	2.02	0.41
12:X:146:LEU:HG	16:X:510:CLA:HED1	2.03	0.41
12:Y:122:LYS:HA	12:Y:126:LYS:HD3	2.03	0.41
1:a:216:GLN:HA	1:a:220:SER:HB2	2.03	0.41
2:b:75:GLU:O	2:b:79:LYS:NZ	2.46	0.41
12:g:213:LEU:HG	16:g:516:CLA:HMC1	2.02	0.41
9:k:18:VAL:HG13	9:k:75:ILE:HD13	2.03	0.41
10:l:132:MET:HB2	19:l:4022:BCR:H402	2.01	0.41
12:n:34:GLN:HG2	16:n:509:CLA:H3A	2.02	0.41
12:n:97:LEU:HG	19:n:604:BCR:H12C	2.03	0.41
12:o:251:LEU:HD21	16:o:513:CLA:HAB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:p:254:PHE:HE2	12:p:315:LEU:HD22	1.85	0.41
16:s:505:CLA:H112	16:s:510:CLA:H41	2.03	0.41
12:u:69:HIS:CD2	16:u:506:CLA:HED2	2.56	0.41
12:v:37:LEU:HD11	19:v:604:BCR:H373	2.01	0.41
12:v:261:ALA:HB1	12:v:276:LEU:HB2	2.03	0.41
12:w:75:TRP:HB3	12:w:88:PRO:HB2	2.02	0.41
2:B:230:TRP:O	16:B:1213:CLA:H3A	2.21	0.41
2:B:413:LYS:HA	2:B:416:LEU:HD12	2.03	0.41
16:B:1203:CLA:H61	16:B:1203:CLA:H41	1.61	0.41
2:G:222:LEU:HD21	19:G:4004:BCR:HC21	2.02	0.41
19:G:4014:BCR:H15C	16:H:1138:CLA:H92	2.02	0.41
16:H:1139:CLA:HED3	6:Q:100:GLU:HA	2.02	0.41
19:H:4002:BCR:H20C	19:H:4002:BCR:H361	1.82	0.41
14:H:4101:LMG:O5	14:H:4101:LMG:O4	2.37	0.41
9:K:26:ASN:HA	9:K:67:GLY:HA3	2.02	0.41
16:L:1503:CLA:H8	16:b:1207:CLA:H202	2.02	0.41
8:S:12:PRO:HB2	19:S:4013:BCR:H292	2.03	0.41
12:W:298:THR:HG23	12:W:301:ALA:H	1.85	0.41
12:Z:118:LEU:HA	12:Z:121:LEU:HD13	2.01	0.41
1:a:482:PHE:HB3	16:a:1135:CLA:H12	2.02	0.41
12:g:42:ALA:O	12:g:46:THR:OG1	2.30	0.41
16:g:505:CLA:H151	16:g:505:CLA:H112	1.90	0.41
16:o:515:CLA:H61	16:o:515:CLA:H41	1.84	0.41
16:p:504:CLA:H203	16:p:504:CLA:H161	1.94	0.41
12:u:145:HIS:ND1	16:u:510:CLA:OBD	2.42	0.41
16:w:507:CLA:H122	16:w:507:CLA:H8	1.94	0.41
12:y:308:PHE:HZ	16:y:517:CLA:HAB	1.85	0.41
19:y:601:BCR:H20C	19:y:601:BCR:H361	1.85	0.41
1:A:300:ILE:HD13	1:A:300:ILE:HA	1.92	0.41
16:A:1132:CLA:H193	16:A:1132:CLA:H162	1.90	0.41
2:G:283:ILE:HD11	16:G:1213:CLA:HBC2	2.02	0.41
16:G:1203:CLA:H191	16:G:1226:CLA:H121	2.02	0.41
19:K:4001:BCR:H15C	19:K:4001:BCR:H351	1.86	0.41
12:W:21:ALA:O	12:W:132:TRP:NE1	2.48	0.41
19:W:601:BCR:H15C	19:W:601:BCR:H351	1.89	0.41
12:X:323:LEU:HD22	16:X:508:CLA:HMD1	2.03	0.41
16:Y:507:CLA:H72	19:Y:601:BCR:H12C	2.02	0.41
16:Z:509:CLA:H72	16:Z:509:CLA:H112	1.89	0.41
1:a:197:MET:HG2	16:a:1123:CLA:HMD3	2.03	0.41
1:a:589:ASP:HA	1:a:592:PHE:HB3	2.02	0.41
16:g:512:CLA:H3A	19:g:604:BCR:H292	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:h:194:PHE:HB2	19:h:603:BCR:H271	2.02	0.41
12:h:255:VAL:HG21	16:h:505:CLA:H92	2.03	0.41
9:k:26:ASN:HA	9:k:67:GLY:HA3	2.02	0.41
10:l:37:LEU:HD21	16:l:1501:CLA:HAB	2.03	0.41
12:o:267:TYR:OH	16:o:505:CLA:O1A	2.34	0.41
16:q:512:CLA:H93	16:q:512:CLA:H111	1.87	0.41
12:u:227:LEU:HD12	12:u:229:TRP:HE1	1.85	0.41
12:v:286:PHE:O	12:v:305:ASN:ND2	2.49	0.41
16:v:515:CLA:H93	16:v:515:CLA:HMB2	2.02	0.41
12:x:110:HIS:HA	12:x:114:ALA:HB3	2.02	0.41
12:y:298:THR:OG1	12:y:299:SER:N	2.52	0.41
1:A:747:SER:HA	1:A:750:ILE:HG12	2.03	0.41
14:A:4101:LMG:H122	14:A:4101:LMG:H291	2.01	0.41
16:B:1213:CLA:H62	16:B:1213:CLA:H41	1.92	0.41
16:B:1229:CLA:H2	6:F:76:ALA:O	2.20	0.41
1:H:359:LEU:HD12	1:H:362:LEU:HD23	2.02	0.41
19:S:4015:BCR:H20C	19:S:4015:BCR:H361	1.86	0.41
12:W:144:HIS:CG	16:W:502:CLA:HAB	2.56	0.41
16:X:510:CLA:H112	19:X:603:BCR:H362	2.02	0.41
12:Y:20:PHE:CD2	16:Y:512:CLA:H2A	2.56	0.41
16:Y:511:CLA:H91	16:Y:511:CLA:H112	1.92	0.41
1:a:120:ILE:HD13	8:j:27:ILE:HG23	2.03	0.41
14:a:852:LMG:H302	13:i:103:LHG:H271	2.02	0.41
16:b:1226:CLA:H11	16:b:1226:CLA:H51	1.89	0.41
19:b:4014:BCR:H20C	19:b:4014:BCR:H361	1.90	0.41
12:n:147:LEU:HD13	16:n:501:CLA:HMC3	2.03	0.41
16:n:504:CLA:H122	16:n:507:CLA:HBB2	2.03	0.41
16:n:507:CLA:H101	16:n:511:CLA:H151	2.03	0.41
12:o:243:SER:O	12:o:318:HIS:ND1	2.45	0.41
16:o:506:CLA:H41	16:o:506:CLA:H8	2.03	0.41
12:r:127:LYS:O	12:r:137:GLN:NE2	2.53	0.41
19:s:603:BCR:H20C	19:s:603:BCR:H361	1.86	0.41
16:v:509:CLA:H51	16:v:509:CLA:H8	1.88	0.41
16:x:507:CLA:H112	16:x:507:CLA:H152	1.89	0.41
1:A:199:HIS:CG	16:A:1111:CLA:HMC2	2.56	0.41
1:A:207:LEU:HD21	16:A:1118:CLA:HMC1	2.01	0.41
1:A:362:LEU:HD11	16:A:1117:CLA:H51	2.03	0.41
17:A:2001:PQN:H211	17:A:2001:PQN:H172	1.89	0.41
2:B:150:LEU:HD22	11:M:22:ALA:HA	2.02	0.41
2:B:369:LEU:HD23	2:B:369:LEU:HA	1.92	0.41
2:B:401:ASN:OD1	2:B:404:ASN:ND2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:333:THR:HG21	13:H:851:LHG:HC11	2.03	0.41
1:H:591:VAL:HG11	16:H:1128:CLA:HMD3	2.02	0.41
14:H:4101:LMG:HC61	20:U:4101:LMT:H4B	2.03	0.41
8:J:12:PRO:HB2	19:J:4013:BCR:H381	2.03	0.41
7:R:1:MET:N	10:l:153:ARG:O	2.47	0.41
16:W:517:CLA:H71	19:X:604:BCR:H372	2.02	0.41
16:a:1105:CLA:H112	19:j:4013:BCR:H21C	2.02	0.41
2:b:167:TRP:CZ2	16:b:1208:CLA:HHB	2.55	0.41
2:b:268:LEU:HD21	2:b:353:LEU:HD22	2.03	0.41
6:f:56:ASP:OD2	6:f:58:ARG:NE	2.50	0.41
10:l:53:VAL:O	10:l:57:HIS:ND1	2.47	0.41
10:l:93:THR:HG21	10:l:128:PHE:HD1	1.86	0.41
12:n:168:ASP:HB3	12:n:171:THR:HG22	2.02	0.41
16:o:502:CLA:HMD2	16:o:509:CLA:H111	2.03	0.41
12:q:150:GLY:HA3	12:q:215:ILE:HG13	2.03	0.41
19:q:603:BCR:H20C	19:q:603:BCR:H361	1.84	0.41
12:r:34:GLN:HG2	16:r:509:CLA:H3A	2.02	0.41
16:r:507:CLA:H112	16:r:507:CLA:H152	1.79	0.41
19:u:601:BCR:H20C	19:u:601:BCR:H361	1.89	0.41
16:v:505:CLA:H151	16:v:505:CLA:H111	1.87	0.41
19:w:602:BCR:HC7	19:w:602:BCR:H10C	1.83	0.41
12:y:110:HIS:HA	12:y:114:ALA:HB3	2.03	0.41
16:y:509:CLA:H3A	16:y:509:CLA:HBA1	1.69	0.41
1:A:49:TRP:HZ2	16:A:1139:CLA:HBB1	1.85	0.41
1:A:387:LEU:HA	1:A:609:PHE:HE2	1.85	0.41
16:A:1102:CLA:HBC2	16:A:1128:CLA:H42	2.03	0.41
2:B:676:VAL:HG11	3:C:81:TYR:CG	2.55	0.41
21:B:4006:ECH:H15	21:B:4006:ECH:H35	1.92	0.41
4:D:41:GLU:HB3	4:D:71:GLN:HE22	1.86	0.41
6:F:56:ASP:OD2	6:F:58:ARG:NE	2.54	0.41
16:G:1216:CLA:HMB2	16:G:1221:CLA:HMA3	2.03	0.41
1:H:685:PHE:HZ	16:H:1140:CLA:HBC3	1.86	0.41
16:H:1139:CLA:HBB2	17:H:2001:PQN:H141	2.03	0.41
7:I:34:ILE:HG13	7:I:35:GLU:HG2	2.03	0.41
9:K:34:LYS:HD3	16:K:4003:CLA:HMD1	2.02	0.41
10:L:65:TRP:HH2	10:L:88:LEU:HD22	1.86	0.41
7:R:12:TRP:NE1	10:l:149:ASP:OD1	2.54	0.41
19:U:4022:BCR:H372	10:l:137:VAL:HG21	2.03	0.41
12:W:68:PRO:HB2	12:W:272:TYR:CZ	2.56	0.41
12:X:17:ASN:ND2	16:X:507:CLA:O1A	2.52	0.41
12:X:143:GLY:HA3	12:X:222:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:504:CLA:H93	16:X:504:CLA:H62	1.92	0.41
16:X:508:CLA:H62	16:X:508:CLA:H41	1.78	0.41
12:Y:54:ASP:O	12:Y:62:GLN:NE2	2.53	0.41
12:Y:267:TYR:OH	16:Y:506:CLA:O1D	2.31	0.41
12:Y:310:LEU:HD22	16:Y:506:CLA:HMC3	2.03	0.41
12:Z:331:LYS:HE2	12:Z:331:LYS:HB3	1.88	0.41
1:a:689:GLY:HA3	2:b:565:CYS:HB2	2.03	0.41
16:a:1102:CLA:H62	16:a:1102:CLA:H102	1.77	0.41
16:a:1124:CLA:H72	16:a:1133:CLA:HBB1	2.03	0.41
2:b:608:GLU:HG3	6:f:48:GLU:HG3	2.03	0.41
12:g:267:TYR:O	12:g:300:ARG:NH2	2.42	0.41
12:g:274:PRO:HA	12:g:275:PRO:HD3	1.97	0.41
12:h:142:LEU:HB2	16:h:510:CLA:HMD3	2.02	0.41
16:h:512:CLA:H102	16:h:512:CLA:H2	2.02	0.41
12:n:70:LEU:HD21	16:n:504:CLA:HED2	2.02	0.41
12:o:323:LEU:HD22	16:o:508:CLA:HMD1	2.03	0.41
12:p:274:PRO:HA	12:p:275:PRO:HD3	1.96	0.41
12:q:21:ALA:O	12:q:132:TRP:NE1	2.44	0.41
16:q:503:CLA:HAC2	19:q:602:BCR:H402	2.01	0.41
19:t:603:BCR:H15C	19:t:603:BCR:H351	1.90	0.41
16:u:510:CLA:H91	16:u:510:CLA:H112	1.87	0.41
12:v:268:PRO:HA	12:v:269:PRO:HD3	1.91	0.41
16:v:505:CLA:H43	16:v:506:CLA:HMD1	2.02	0.41
16:v:505:CLA:H141	16:v:505:CLA:H162	1.78	0.41
16:v:510:CLA:HHC	16:v:516:CLA:H3A	2.03	0.41
12:w:115:PRO:HD2	12:w:121:LEU:HD11	2.03	0.41
16:w:505:CLA:HBB1	16:w:505:CLA:H71	2.03	0.41
16:B:1202:CLA:H3A	16:B:1202:CLA:HBA1	1.78	0.41
2:G:427:LEU:HD11	16:G:1235:CLA:HMB1	2.03	0.41
2:G:507:LEU:HD22	2:G:598:VAL:HG21	2.03	0.41
16:G:1205:CLA:H91	16:G:1205:CLA:H112	1.86	0.41
16:G:1238:CLA:H141	16:G:1238:CLA:H162	1.86	0.41
1:H:16:VAL:HA	1:H:185:PRO:HA	2.03	0.41
1:H:685:PHE:HA	17:H:2001:PQN:H9	2.03	0.41
16:H:1101:CLA:HBB2	16:H:1106:CLA:H172	2.01	0.41
16:H:1119:CLA:H2	16:H:1119:CLA:H61	1.69	0.41
12:X:310:LEU:HD11	16:X:514:CLA:HBB2	2.02	0.41
16:X:504:CLA:H93	16:X:504:CLA:H112	1.97	0.41
12:Z:260:CYS:HB3	12:Z:304:ALA:HB2	2.03	0.41
16:a:1022:CLA:H192	16:a:1022:CLA:H161	1.89	0.41
16:a:1106:CLA:HBB2	16:a:1126:CLA:H142	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:h:168:ASP:HB2	12:h:175:ARG:HD2	2.03	0.41
16:h:512:CLA:H141	16:h:512:CLA:H161	1.84	0.41
16:h:515:CLA:H91	19:n:604:BCR:H15C	2.03	0.41
19:i:4018:BCR:H351	19:i:4018:BCR:H15C	1.93	0.41
21:i:4020:ECH:H11	21:i:4020:ECH:H7	2.03	0.41
12:n:223:LEU:HD21	16:n:501:CLA:HMB3	2.02	0.41
12:o:249:ILE:HG13	16:o:506:CLA:HAC1	2.03	0.41
16:o:508:CLA:H62	16:o:508:CLA:H41	1.82	0.41
12:q:310:LEU:HD23	12:q:310:LEU:HA	1.94	0.41
24:q:601:LUT:H15	24:q:601:LUT:H201	1.96	0.41
12:r:19:ARG:NH1	16:r:512:CLA:OBD	2.41	0.41
12:r:134:ASN:HA	12:r:135:PRO:HD3	1.95	0.41
12:r:146:LEU:HD23	12:r:146:LEU:HA	1.91	0.41
19:s:603:BCR:H15C	19:s:603:BCR:H351	1.90	0.41
19:t:601:BCR:H15C	19:t:601:BCR:H351	1.88	0.41
12:u:34:GLN:HG2	16:u:509:CLA:H3A	2.02	0.41
12:y:44:ALA:O	12:y:48:PHE:N	2.54	0.41
19:y:604:BCR:H361	19:y:604:BCR:H20C	1.81	0.41
3:C:66:ARG:HA	3:C:66:ARG:HD2	1.96	0.40
16:G:1213:CLA:H61	16:G:1213:CLA:H41	1.91	0.40
1:H:485:TRP:HB2	20:H:4202:LMT:H11	2.03	0.40
19:W:601:BCR:H11C	19:W:601:BCR:H341	1.93	0.40
16:Y:504:CLA:H41	16:Y:504:CLA:H61	1.83	0.40
1:a:27:LYS:HD3	1:a:33:HIS:CD2	2.56	0.40
16:a:1119:CLA:HMB2	16:a:1123:CLA:HMA3	2.03	0.40
16:a:1124:CLA:CAD	16:a:1135:CLA:HBB1	2.51	0.40
16:b:1227:CLA:HBB1	13:b:4018:LHG:H142	2.03	0.40
13:i:103:LHG:H341	21:m:4021:ECH:H29A	2.02	0.40
12:o:249:ILE:HD11	16:o:504:CLA:H142	2.03	0.40
16:r:505:CLA:H202	16:r:505:CLA:H162	1.90	0.40
16:s:507:CLA:H152	16:s:507:CLA:H112	1.86	0.40
16:s:509:CLA:H11	16:s:509:CLA:HBA1	1.81	0.40
19:u:603:BCR:H20C	19:u:603:BCR:H361	1.92	0.40
12:v:68:PRO:HB3	12:v:271:PHE:HD1	1.86	0.40
16:w:515:CLA:HBB2	19:x:604:BCR:H351	2.03	0.40
12:x:305:ASN:HD22	19:x:601:BCR:H393	1.86	0.40
16:x:507:CLA:H72	19:x:601:BCR:H12C	2.02	0.40
1:A:202:ALA:HB2	1:A:308:GLY:HA3	2.04	0.40
1:A:278:LYS:HE3	1:A:278:LYS:HB2	1.92	0.40
14:A:4101:LMG:H132	20:L:4101:LMT:H21	2.04	0.40
2:B:378:GLY:HA3	2:B:584:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:1235:CLA:HED3	16:B:1235:CLA:HBD	1.95	0.40
19:I:4018:BCR:H11C	19:I:4018:BCR:H341	1.88	0.40
9:K:30:ILE:HG23	16:K:4003:CLA:HMD3	2.03	0.40
16:Q:1301:CLA:HMB2	8:S:26:LEU:HD11	2.03	0.40
12:W:232:LYS:HE2	12:W:232:LYS:HB3	1.90	0.40
16:W:507:CLA:H122	16:W:507:CLA:H8	1.93	0.40
19:X:602:BCR:H333	19:X:604:BCR:H333	2.03	0.40
16:Z:507:CLA:HMA3	16:Z:507:CLA:H122	2.03	0.40
1:a:324:ILE:O	1:a:328:HIS:ND1	2.43	0.40
1:a:366:VAL:HA	16:a:1117:CLA:H42	2.03	0.40
16:a:1013:CLA:H61	16:a:1013:CLA:H41	1.78	0.40
16:a:1122:CLA:HMD2	16:a:1123:CLA:HAB	2.04	0.40
16:b:1225:CLA:H202	16:b:1225:CLA:H161	1.85	0.40
16:g:515:CLA:H92	16:g:515:CLA:H62	1.91	0.40
12:n:149:LEU:HD12	16:n:510:CLA:HED3	2.02	0.40
12:n:154:LEU:HG	12:n:211:GLY:HA3	2.04	0.40
16:o:506:CLA:C2B	16:o:514:CLA:HAB	2.52	0.40
16:q:512:CLA:H112	16:q:512:CLA:H142	1.89	0.40
19:q:604:BCR:H381	23:q:605:LMU:H62	2.03	0.40
12:r:34:GLN:HG2	16:r:509:CLA:HHB	2.04	0.40
12:r:42:ALA:O	12:r:46:THR:OG1	2.34	0.40
12:s:68:PRO:HB3	12:s:271:PHE:HB3	2.03	0.40
16:w:504:CLA:H112	16:w:504:CLA:H72	1.80	0.40
12:x:1:MET:HE2	12:x:1:MET:HB2	1.90	0.40
16:A:1126:CLA:H193	19:J:4012:BCR:H10C	2.02	0.40
16:A:1131:CLA:HMC2	16:L:1503:CLA:HBB2	2.03	0.40
2:B:167:TRP:CZ2	16:B:1208:CLA:HHB	2.56	0.40
19:B:4009:BCR:H24C	19:B:4009:BCR:H371	1.79	0.40
6:F:73:LEU:HD23	6:F:73:LEU:HA	1.97	0.40
16:G:1202:CLA:H62	16:G:1210:CLA:H92	2.02	0.40
1:H:373:MET:HE3	1:H:373:MET:HB2	1.89	0.40
13:R:103:LHG:H331	21:V:4021:ECH:H29A	2.04	0.40
10:U:90:LEU:HD23	16:l:1503:CLA:H192	2.02	0.40
12:X:34:GLN:HG2	16:X:509:CLA:HHB	2.03	0.40
16:Y:507:CLA:H112	16:Y:511:CLA:H171	2.03	0.40
16:Z:505:CLA:H111	16:Z:510:CLA:H61	2.03	0.40
1:a:671:MET:HA	1:a:674:ALA:HB3	2.03	0.40
16:b:1209:CLA:HMC2	19:b:4005:BCR:H311	2.04	0.40
4:d:85:ILE:HB	4:d:98:HIS:HB3	2.02	0.40
12:h:315:LEU:HD12	12:h:315:LEU:HA	1.93	0.40
12:n:200:LEU:HD13	12:n:265:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:n:505:CLA:H102	16:n:505:CLA:H62	1.74	0.40
12:v:45:PHE:HA	12:v:48:PHE:HB3	2.04	0.40
12:x:234:LEU:HD13	16:x:510:CLA:HMC3	2.02	0.40
16:y:515:CLA:H192	16:y:515:CLA:H162	1.91	0.40
1:A:362:LEU:HD23	16:A:1127:CLA:HBC1	2.03	0.40
1:A:577:PRO:HD3	2:B:558:GLY:HA2	2.04	0.40
2:G:167:TRP:CZ2	16:G:1208:CLA:HHB	2.56	0.40
16:G:1220:CLA:H61	16:G:1220:CLA:H41	1.80	0.40
17:G:2002:PQN:H211	17:G:2002:PQN:H252	1.78	0.40
1:H:71:LYS:NZ	16:H:1109:CLA:OBD	2.52	0.40
1:H:349:HIS:HE1	16:H:1128:CLA:HED1	1.86	0.40
16:X:509:CLA:H142	16:X:509:CLA:H111	1.90	0.40
16:Y:512:CLA:HBD	23:Y:606:LMU:H11	2.04	0.40
1:a:485:TRP:HB2	20:a:4202:LMT:H11	2.04	0.40
15:a:1011:CL0:H49	15:a:1011:CL0:H41	1.86	0.40
16:a:1102:CLA:HAB	16:a:1104:CLA:HBD	2.03	0.40
16:a:1115:CLA:C4C	16:a:1116:CLA:HBB2	2.52	0.40
2:b:122:HIS:O	2:b:126:THR:OG1	2.32	0.40
16:g:517:CLA:H62	16:g:517:CLA:H41	1.83	0.40
12:h:49:GLU:HB2	12:h:67:LEU:HD13	2.03	0.40
16:h:507:CLA:H41	16:h:507:CLA:H61	1.79	0.40
12:o:69:HIS:CE1	12:o:303:LEU:HD21	2.57	0.40
16:p:505:CLA:H18	16:p:510:CLA:H151	2.04	0.40
12:q:310:LEU:HB3	16:q:506:CLA:HMC3	2.02	0.40
16:r:515:CLA:HBC2	19:r:603:BCR:H11C	2.01	0.40
16:s:504:CLA:H112	16:s:504:CLA:H72	1.81	0.40
12:t:276:LEU:HD22	12:t:288:ASP:HA	2.02	0.40
16:x:515:CLA:H162	16:x:515:CLA:H121	1.86	0.40
16:B:1207:CLA:H91	16:U:1503:CLA:H91	2.02	0.40
3:C:15:THR:HG22	3:C:28:MET:HE2	2.03	0.40
2:G:262:HIS:HA	2:G:263:PRO:HD3	1.96	0.40
2:G:596:LEU:HD22	2:G:729:LYS:HD3	2.02	0.40
16:G:1021:CLA:H101	16:G:1021:CLA:H62	1.84	0.40
16:G:1202:CLA:H8	16:G:1221:CLA:HBA1	2.04	0.40
16:G:1210:CLA:H111	16:G:1210:CLA:H152	1.90	0.40
1:H:411:PHE:HE2	1:H:426:LEU:HD21	1.86	0.40
1:H:437:ILE:HG13	1:H:555:TYR:HE2	1.86	0.40
12:Y:183:ASP:HB3	12:Y:186:VAL:HG12	2.03	0.40
1:a:217:ILE:HD11	1:a:275:LEU:HD21	2.02	0.40
1:a:398:GLY:HA3	1:a:602:LEU:HD21	2.02	0.40
16:a:1101:CLA:H151	16:a:1101:CLA:H112	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:4003:BCR:H361	19:a:4003:BCR:H20C	1.82	0.40
16:b:1220:CLA:H51	16:b:1220:CLA:H11	1.86	0.40
12:n:160:ALA:HA	12:n:165:GLY:HA2	2.02	0.40
16:n:508:CLA:H3A	16:n:508:CLA:HBA2	1.65	0.40
16:o:505:CLA:H162	16:o:505:CLA:H121	1.85	0.40
16:q:506:CLA:H143	16:q:506:CLA:H111	1.95	0.40
16:r:505:CLA:H151	16:r:505:CLA:H112	1.96	0.40
16:s:508:CLA:H43	16:s:508:CLA:H3A	2.04	0.40
12:t:272:TYR:O	12:t:298:THR:OG1	2.39	0.40
16:t:515:CLA:H11	12:u:105:ALA:HB1	2.04	0.40
12:v:53:PHE:HE1	12:v:59:MET:HG3	1.87	0.40
12:w:274:PRO:HA	12:w:275:PRO:HD3	1.99	0.40
12:x:52:ARG:HE	12:x:52:ARG:HB3	1.61	0.40
16:x:517:CLA:H41	16:x:517:CLA:H62	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
1	H	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
1	a	737/751 (98%)	711 (96%)	26 (4%)	0	100	100
2	B	728/731 (100%)	713 (98%)	15 (2%)	0	100	100
2	G	728/731 (100%)	712 (98%)	16 (2%)	0	100	100
2	b	728/731 (100%)	711 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	78 (100%)	0	0	100	100
3	N	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	77 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	P	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
4	d	136/141 (96%)	130 (96%)	6 (4%)	0	100	100
5	E	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
5	O	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
5	e	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100	100
6	Q	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
6	f	139/165 (84%)	134 (96%)	5 (4%)	0	100	100
7	I	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	R	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
7	i	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
8	J	37/40 (92%)	37 (100%)	0	0	100	100
8	S	37/40 (92%)	37 (100%)	0	0	100	100
8	j	37/40 (92%)	37 (100%)	0	0	100	100
9	K	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	T	75/86 (87%)	74 (99%)	1 (1%)	0	100	100
9	k	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
10	L	151/157 (96%)	150 (99%)	1 (1%)	0	100	100
10	U	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
10	l	151/157 (96%)	147 (97%)	4 (3%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	W	336/342 (98%)	317 (94%)	18 (5%)	1 (0%)	36	58
12	X	337/342 (98%)	318 (94%)	19 (6%)	0	100	100
12	Y	338/342 (99%)	320 (95%)	17 (5%)	1 (0%)	36	58
12	Z	335/342 (98%)	326 (97%)	8 (2%)	1 (0%)	36	58
12	g	331/342 (97%)	304 (92%)	25 (8%)	2 (1%)	21	42
12	h	328/342 (96%)	308 (94%)	20 (6%)	0	100	100
12	n	336/342 (98%)	322 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	o	337/342 (98%)	318 (94%)	17 (5%)	2 (1%)	21 42
12	p	338/342 (99%)	317 (94%)	21 (6%)	0	100 100
12	q	335/342 (98%)	326 (97%)	9 (3%)	0	100 100
12	r	330/342 (96%)	316 (96%)	12 (4%)	2 (1%)	21 42
12	s	337/342 (98%)	321 (95%)	14 (4%)	2 (1%)	21 42
12	t	336/342 (98%)	319 (95%)	16 (5%)	1 (0%)	36 58
12	u	337/342 (98%)	322 (96%)	14 (4%)	1 (0%)	36 58
12	v	328/342 (96%)	312 (95%)	15 (5%)	1 (0%)	36 58
12	w	335/342 (98%)	322 (96%)	13 (4%)	0	100 100
12	x	330/342 (96%)	311 (94%)	17 (5%)	2 (1%)	21 42
12	y	328/342 (96%)	307 (94%)	21 (6%)	0	100 100
All	All	12645/13047 (97%)	12150 (96%)	479 (4%)	16 (0%)	49 70

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	W	59	MET
12	v	174	VAL
12	s	85	ASP
12	o	11	TYR
12	s	7	ASP
12	u	11	TYR
12	Y	7	ASP
12	g	83	ILE
12	g	177	VAL
12	o	297	HIS
12	t	83	ILE
12	x	83	ILE
12	x	177	VAL
12	Z	178	SER
12	r	83	ILE
12	r	177	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/603 (98%)	593 (100%)	0	100	100
1	H	593/603 (98%)	593 (100%)	0	100	100
1	a	593/603 (98%)	593 (100%)	0	100	100
2	B	582/583 (100%)	582 (100%)	0	100	100
2	G	582/583 (100%)	582 (100%)	0	100	100
2	b	582/583 (100%)	582 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
3	N	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	113/116 (97%)	113 (100%)	0	100	100
4	P	113/116 (97%)	113 (100%)	0	100	100
4	d	113/116 (97%)	113 (100%)	0	100	100
5	E	58/60 (97%)	58 (100%)	0	100	100
5	O	58/60 (97%)	58 (100%)	0	100	100
5	e	58/60 (97%)	58 (100%)	0	100	100
6	F	118/137 (86%)	118 (100%)	0	100	100
6	Q	118/137 (86%)	118 (100%)	0	100	100
6	f	118/137 (86%)	118 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
7	R	31/32 (97%)	31 (100%)	0	100	100
7	i	31/32 (97%)	31 (100%)	0	100	100
8	J	34/35 (97%)	34 (100%)	0	100	100
8	S	34/35 (97%)	34 (100%)	0	100	100
8	j	34/35 (97%)	34 (100%)	0	100	100
9	K	55/62 (89%)	55 (100%)	0	100	100
9	T	55/62 (89%)	55 (100%)	0	100	100
9	k	55/62 (89%)	55 (100%)	0	100	100
10	L	115/118 (98%)	115 (100%)	0	100	100
10	U	115/118 (98%)	115 (100%)	0	100	100
10	l	115/118 (98%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	25/25 (100%)	25 (100%)	0	100	100
11	V	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
12	W	252/260 (97%)	252 (100%)	0	100	100
12	X	256/260 (98%)	256 (100%)	0	100	100
12	Y	255/260 (98%)	255 (100%)	0	100	100
12	Z	253/260 (97%)	253 (100%)	0	100	100
12	g	251/260 (96%)	251 (100%)	0	100	100
12	h	246/260 (95%)	246 (100%)	0	100	100
12	n	252/260 (97%)	252 (100%)	0	100	100
12	o	256/260 (98%)	256 (100%)	0	100	100
12	p	255/260 (98%)	255 (100%)	0	100	100
12	q	253/260 (97%)	253 (100%)	0	100	100
12	r	250/260 (96%)	250 (100%)	0	100	100
12	s	255/260 (98%)	255 (100%)	0	100	100
12	t	252/260 (97%)	252 (100%)	0	100	100
12	u	256/260 (98%)	256 (100%)	0	100	100
12	v	246/260 (95%)	246 (100%)	0	100	100
12	w	253/260 (97%)	253 (100%)	0	100	100
12	x	250/260 (96%)	250 (100%)	0	100	100
12	y	245/260 (94%)	245 (100%)	0	100	100
All	All	9912/10200 (97%)	9912 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	216	GLN
1	A	314	ASN
1	A	368	GLN
1	A	441	ASN
1	A	479	GLN

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Mol	Chain	Res	Type
1	A	484	GLN
1	A	500	ASN
1	A	538	HIS
1	A	705	ASN
2	B	10	GLN
2	B	83	ASN
2	B	158	GLN
2	B	206	HIS
2	B	326	ASN
2	B	348	GLN
2	B	361	GLN
2	B	366	GLN
2	B	419	HIS
2	B	478	ASN
2	B	609	ASN
3	C	16	GLN
4	D	71	GLN
6	F	61	HIS
2	G	10	GLN
2	G	83	ASN
2	G	158	GLN
2	G	170	ASN
2	G	218	HIS
2	G	264	GLN
2	G	294	ASN
2	G	701	GLN
1	H	54	ASN
1	H	135	HIS
1	H	192	ASN
1	H	218	HIS
1	H	441	ASN
1	H	458	ASN
1	H	500	ASN
1	H	538	HIS
1	H	590	HIS
1	H	705	ASN
9	K	26	ASN
10	L	9	GLN
10	L	19	HIS
10	L	144	ASN
4	P	71	GLN
4	P	115	GLN

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Mol	Chain	Res	Type
10	U	108	GLN
10	U	144	ASN
12	W	62	GLN
12	W	82	GLN
12	W	129	HIS
12	W	191	GLN
12	W	207	HIS
12	W	263	ASN
12	W	316	GLN
12	X	10	GLN
12	X	34	GLN
12	X	191	GLN
12	X	295	HIS
12	X	307	HIS
12	Y	129	HIS
12	Y	172	GLN
12	Y	207	HIS
12	Y	297	HIS
12	Y	316	GLN
12	Z	134	ASN
1	a	18	ASN
1	a	138	GLN
1	a	218	HIS
1	a	314	ASN
1	a	500	ASN
1	a	590	HIS
1	a	614	GLN
1	a	705	ASN
2	b	29	HIS
2	b	41	ASN
2	b	83	ASN
2	b	158	GLN
2	b	363	HIS
2	b	701	GLN
3	c	16	GLN
4	d	38	GLN
4	d	71	GLN
4	d	115	GLN
6	f	99	GLN
12	g	57	GLN
12	g	62	GLN
12	g	129	HIS

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Mol	Chain	Res	Type
12	g	191	GLN
12	g	297	HIS
12	g	305	ASN
12	g	316	GLN
12	h	23	GLN
12	h	96	HIS
12	h	134	ASN
12	h	136	GLN
10	l	9	GLN
10	l	19	HIS
10	l	144	ASN
12	n	2	GLN
12	n	31	HIS
12	n	191	GLN
12	n	207	HIS
12	n	297	HIS
12	o	34	GLN
12	o	191	GLN
12	o	335	GLN
12	p	124	GLN
12	p	129	HIS
12	p	136	GLN
12	p	191	GLN
12	q	207	HIS
12	q	297	HIS
12	r	124	GLN
12	r	134	ASN
12	r	191	GLN
12	r	316	GLN
12	s	129	HIS
12	s	136	GLN
12	s	172	GLN
12	s	207	HIS
12	t	69	HIS
12	t	82	GLN
12	t	96	HIS
12	t	124	GLN
12	t	191	GLN
12	t	297	HIS
12	u	10	GLN
12	u	179	GLN
12	u	191	GLN

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Mol	Chain	Res	Type
12	u	321	HIS
12	v	2	GLN
12	v	110	HIS
12	v	124	GLN
12	v	134	ASN
12	v	191	GLN
12	v	316	GLN
12	w	34	GLN
12	w	129	HIS
12	w	335	GLN
12	x	2	GLN
12	x	6	ASN
12	x	62	GLN
12	x	129	HIS
12	x	172	GLN
12	x	191	GLN
12	x	263	ASN
12	y	2	GLN
12	y	17	ASN
12	y	23	GLN
12	y	134	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 798 ligands modelled in this entry, 3 are monoatomic - leaving 795 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	$\#\|Z\| > 2$
16	CLA	a	1122	-	63,67,73	1.04	5 (7%)	74,105,113	1.10	4 (5%)
13	LHG	B	4018	16	37,37,48	0.72	1 (2%)	40,43,54	1.32	5 (12%)
16	CLA	a	1133	-	58,62,73	1.09	5 (8%)	68,99,113	1.10	5 (7%)
14	LMG	A	4201	-	32,32,55	1.00	1 (3%)	40,40,63	1.18	3 (7%)
16	CLA	B	1021	-	69,73,73	1.00	5 (7%)	82,113,113	1.14	6 (7%)
16	CLA	h	506	-	64,68,73	1.05	6 (9%)	76,107,113	1.38	10 (13%)
16	CLA	q	505	-	69,73,73	0.99	6 (8%)	82,113,113	1.16	8 (9%)
16	CLA	p	509	-	64,68,73	1.05	4 (6%)	76,107,113	0.98	3 (3%)
16	CLA	B	1240	13	50,54,73	1.18	5 (10%)	59,90,113	1.21	4 (6%)
16	CLA	B	1205	-	69,73,73	0.99	4 (5%)	82,113,113	1.06	3 (3%)
16	CLA	G	1202	-	69,73,73	0.96	4 (5%)	82,113,113	0.99	5 (6%)
16	CLA	W	506	-	64,68,73	1.03	3 (4%)	76,107,113	1.09	5 (6%)
16	CLA	b	1238	25	69,73,73	0.98	4 (5%)	82,113,113	1.06	8 (9%)
16	CLA	s	511	-	69,73,73	0.98	5 (7%)	82,113,113	1.01	4 (4%)
19	BCR	x	603	-	41,41,41	0.85	0	56,56,56	1.26	6 (10%)
19	BCR	x	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
18	SF4	a	3001	-	0,12,12	-	-	-		
16	CLA	G	1206	2	69,73,73	0.98	5 (7%)	82,113,113	0.95	3 (3%)
23	LMU	w	605	-	36,36,36	0.84	0	47,47,47	1.10	4 (8%)
16	CLA	q	511	-	69,73,73	1.00	4 (5%)	82,113,113	1.05	3 (3%)
16	CLA	p	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.18	5 (6%)
16	CLA	A	1108	-	49,53,73	1.18	5 (10%)	58,89,113	1.10	2 (3%)
16	CLA	b	1215	-	64,68,73	1.00	4 (6%)	76,107,113	1.15	3 (3%)
16	CLA	h	509	-	69,73,73	1.02	6 (8%)	82,113,113	1.07	6 (7%)
16	CLA	X	514	-	54,58,73	1.12	6 (11%)	64,95,113	1.30	6 (9%)
16	CLA	p	502	-	54,58,73	1.10	5 (9%)	64,95,113	1.07	4 (6%)
16	CLA	s	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	X	509	-	64,68,73	1.05	5 (7%)	76,107,113	1.00	6 (7%)
16	CLA	b	1228	-	59,63,73	1.07	4 (6%)	70,101,113	1.07	5 (7%)
16	CLA	B	1234	-	54,58,73	1.13	6 (11%)	64,95,113	1.13	5 (7%)
16	CLA	y	505	-	69,73,73	1.02	5 (7%)	82,113,113	1.21	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	a	1126	-	69,73,73	0.99	5 (7%)	82,113,113	1.08	3 (3%)
16	CLA	p	513	-	50,54,73	1.14	5 (10%)	59,90,113	1.04	4 (6%)
16	CLA	g	509	-	69,73,73	1.01	6 (8%)	82,113,113	1.09	5 (6%)
16	CLA	n	510	-	69,73,73	1.01	3 (4%)	82,113,113	1.04	4 (4%)
16	CLA	H	1101	-	69,73,73	0.98	4 (5%)	82,113,113	1.04	3 (3%)
19	BCR	T	4001	-	41,41,41	0.86	1 (2%)	56,56,56	1.26	6 (10%)
14	LMG	H	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
17	PQN	b	2002	-	34,34,34	0.36	0	43,45,45	1.06	2 (4%)
16	CLA	o	510	-	64,68,73	1.04	4 (6%)	76,107,113	0.98	5 (6%)
16	CLA	T	4003	9	49,53,73	1.18	4 (8%)	58,89,113	1.05	3 (5%)
19	BCR	H	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.30	7 (12%)
19	BCR	y	604	-	41,41,41	0.87	0	56,56,56	1.29	7 (12%)
16	CLA	a	1119	-	69,73,73	1.00	5 (7%)	82,113,113	0.98	4 (4%)
16	CLA	t	504	-	64,68,73	1.04	4 (6%)	76,107,113	1.02	3 (3%)
19	BCR	I	4018	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
16	CLA	n	516	-	50,54,73	1.17	4 (8%)	59,90,113	0.99	3 (5%)
16	CLA	W	516	-	50,54,73	1.16	4 (8%)	59,90,113	1.12	4 (6%)
16	CLA	q	504	-	69,73,73	1.02	5 (7%)	82,113,113	1.11	4 (4%)
16	CLA	G	1228	-	59,63,73	1.07	4 (6%)	70,101,113	1.09	5 (7%)
16	CLA	a	1125	-	69,73,73	0.97	5 (7%)	82,113,113	1.06	3 (3%)
16	CLA	H	1122	-	63,67,73	1.06	5 (7%)	74,105,113	1.09	6 (8%)
16	CLA	o	501	-	50,54,73	1.14	4 (8%)	59,90,113	1.13	4 (6%)
19	BCR	x	604	-	41,41,41	0.88	0	56,56,56	1.29	6 (10%)
16	CLA	H	1120	-	53,57,73	1.09	4 (7%)	61,93,113	1.18	5 (8%)
16	CLA	r	510	-	69,73,73	0.99	4 (5%)	82,113,113	1.00	4 (4%)
16	CLA	v	505	-	69,73,73	1.02	5 (7%)	82,113,113	1.24	5 (6%)
16	CLA	X	517	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	5 (7%)
16	CLA	y	516	-	50,54,73	1.17	5 (10%)	59,90,113	1.18	5 (8%)
17	PQN	G	2002	-	34,34,34	0.38	0	43,45,45	1.04	2 (4%)
16	CLA	A	1114	-	50,54,73	1.12	4 (8%)	59,90,113	1.23	4 (6%)
16	CLA	B	1206	2	69,73,73	0.98	5 (7%)	82,113,113	0.94	4 (4%)
16	CLA	Y	503	-	50,54,73	1.14	4 (8%)	59,90,113	1.19	5 (8%)
19	BCR	k	4001	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
16	CLA	n	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.24	5 (8%)
16	CLA	y	502	-	54,58,73	1.13	5 (9%)	64,95,113	1.01	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	Z	501	-	54,58,73	1.11	5 (9%)	64,95,113	1.18	7 (10%)
16	CLA	x	502	-	54,58,73	1.13	6 (11%)	64,95,113	1.12	3 (4%)
19	BCR	y	601	-	41,41,41	0.83	0	56,56,56	1.24	6 (10%)
16	CLA	G	1012	25	59,63,73	1.13	6 (10%)	70,101,113	1.19	7 (10%)
16	CLA	v	511	-	69,73,73	0.99	4 (5%)	82,113,113	1.08	4 (4%)
16	CLA	A	1127	-	69,73,73	0.99	6 (8%)	82,113,113	1.07	4 (4%)
16	CLA	f	1302	6	50,54,73	1.17	5 (10%)	59,90,113	1.07	4 (6%)
16	CLA	b	1202	-	69,73,73	0.97	4 (5%)	82,113,113	0.97	3 (3%)
16	CLA	A	1121	-	55,59,73	1.11	5 (9%)	64,96,113	1.11	4 (6%)
16	CLA	v	501	-	50,54,73	1.17	5 (10%)	59,90,113	1.26	7 (11%)
21	ECH	I	4020	-	42,42,42	0.88	1 (2%)	55,58,58	1.90	14 (25%)
16	CLA	o	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.09	4 (4%)
16	CLA	b	1205	-	69,73,73	0.98	4 (5%)	82,113,113	1.08	4 (4%)
19	BCR	v	604	-	41,41,41	0.86	0	56,56,56	1.28	8 (14%)
16	CLA	L	1502	-	64,68,73	1.00	5 (7%)	76,107,113	1.12	4 (5%)
13	LHG	s	605	-	31,31,48	0.79	1 (3%)	34,37,54	1.28	4 (11%)
19	BCR	L	4019	-	41,41,41	0.90	0	56,56,56	1.41	6 (10%)
16	CLA	b	1212	-	49,53,73	1.19	5 (10%)	58,89,113	1.19	4 (6%)
19	BCR	w	602	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
16	CLA	n	509	-	64,68,73	1.04	4 (6%)	76,107,113	1.00	6 (7%)
19	BCR	q	602	-	41,41,41	0.85	0	56,56,56	1.24	6 (10%)
16	CLA	G	1211	-	69,73,73	0.98	4 (5%)	82,113,113	1.01	2 (2%)
19	BCR	b	4014	-	41,41,41	0.91	0	56,56,56	1.45	8 (14%)
16	CLA	G	1201	-	58,62,73	1.08	4 (6%)	68,99,113	1.05	4 (5%)
16	CLA	o	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.16	5 (6%)
19	BCR	A	4007	-	41,41,41	0.91	1 (2%)	56,56,56	1.40	9 (16%)
19	BCR	A	4003	-	41,41,41	0.85	0	56,56,56	1.29	7 (12%)
16	CLA	A	1122	-	63,67,73	1.05	5 (7%)	74,105,113	1.09	6 (8%)
16	CLA	A	1123	25	69,73,73	0.99	4 (5%)	82,113,113	1.07	4 (4%)
16	CLA	H	1115	-	58,62,73	1.06	4 (6%)	68,99,113	1.16	2 (2%)
14	LMG	A	4101	-	46,46,55	0.92	2 (4%)	54,54,63	1.23	4 (7%)
16	CLA	a	1103	-	69,73,73	0.97	4 (5%)	82,113,113	0.98	2 (2%)
16	CLA	H	1118	-	59,63,73	1.07	4 (6%)	70,101,113	1.07	7 (10%)
16	CLA	G	1229	-	62,66,73	1.05	4 (6%)	73,104,113	1.03	4 (5%)
16	CLA	y	501	-	50,54,73	1.15	4 (8%)	59,90,113	1.27	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	w	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.05	5 (6%)
16	CLA	a	1138	-	69,73,73	0.98	5 (7%)	82,113,113	1.04	7 (8%)
16	CLA	A	1102	16	60,64,73	1.06	4 (6%)	71,102,113	0.95	3 (4%)
16	CLA	H	1106	1	69,73,73	0.96	4 (5%)	82,113,113	1.11	4 (4%)
16	CLA	B	1202	-	69,73,73	0.99	4 (5%)	82,113,113	0.92	2 (2%)
16	CLA	r	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.11	5 (7%)
16	CLA	b	1012	25	59,63,73	1.13	4 (6%)	70,101,113	1.20	8 (11%)
16	CLA	b	1021	-	69,73,73	1.00	5 (7%)	82,113,113	1.12	6 (7%)
16	CLA	b	1207	-	69,73,73	0.99	4 (5%)	82,113,113	1.17	4 (4%)
16	CLA	o	504	-	64,68,73	1.05	5 (7%)	76,107,113	1.05	4 (5%)
16	CLA	B	1224	-	64,68,73	1.05	6 (9%)	76,107,113	1.07	4 (5%)
16	CLA	G	1239	-	69,73,73	0.96	3 (4%)	82,113,113	1.14	6 (7%)
16	CLA	A	1103	-	69,73,73	0.97	4 (5%)	82,113,113	1.00	1 (1%)
16	CLA	A	1136	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	3 (3%)
16	CLA	q	509	-	69,73,73	1.01	5 (7%)	82,113,113	0.98	6 (7%)
16	CLA	b	1211	-	69,73,73	0.98	5 (7%)	82,113,113	0.98	4 (4%)
16	CLA	b	1208	-	49,53,73	1.16	5 (10%)	58,89,113	1.19	6 (10%)
16	CLA	h	514	-	54,58,73	1.13	4 (7%)	64,95,113	1.14	7 (10%)
16	CLA	a	1114	-	50,54,73	1.15	5 (10%)	59,90,113	1.31	5 (8%)
16	CLA	B	1201	-	58,62,73	1.07	4 (6%)	68,99,113	1.04	4 (5%)
16	CLA	q	506	-	64,68,73	1.03	4 (6%)	76,107,113	1.05	4 (5%)
17	PQN	H	2001	-	34,34,34	0.38	0	43,45,45	1.06	2 (4%)
16	CLA	S	1302	8	49,53,73	1.18	5 (10%)	58,89,113	1.11	5 (8%)
19	BCR	g	604	-	41,41,41	0.88	0	56,56,56	1.28	6 (10%)
16	CLA	W	501	-	54,58,73	1.11	5 (9%)	64,95,113	1.24	5 (7%)
16	CLA	a	1110	-	58,62,73	1.04	4 (6%)	68,99,113	1.01	2 (2%)
16	CLA	k	4004	-	59,63,73	1.07	4 (6%)	70,101,113	0.98	5 (7%)
16	CLA	t	515	-	69,73,73	1.00	4 (5%)	82,113,113	1.15	5 (6%)
16	CLA	u	515	-	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	w	516	-	50,54,73	1.14	4 (8%)	59,90,113	1.01	4 (6%)
16	CLA	H	1237	25	69,73,73	0.99	5 (7%)	82,113,113	1.08	6 (7%)
16	CLA	X	510	-	64,68,73	1.03	4 (6%)	76,107,113	0.97	4 (5%)
16	CLA	A	1109	16	69,73,73	0.98	5 (7%)	82,113,113	1.13	5 (6%)
19	BCR	f	4016	-	41,41,41	0.87	0	56,56,56	1.29	5 (8%)
20	LMT	L	4101	-	36,36,36	1.17	6 (16%)	47,47,47	1.15	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	Y	509	-	64,68,73	1.04	4 (6%)	76,107,113	1.06	6 (7%)
16	CLA	B	1229	-	62,66,73	1.06	4 (6%)	73,104,113	1.05	5 (6%)
16	CLA	H	1121	-	55,59,73	1.12	5 (9%)	64,96,113	1.14	4 (6%)
14	LMG	F	4017	-	27,27,55	1.10	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	Y	506	-	64,68,73	1.01	4 (6%)	76,107,113	1.12	5 (6%)
19	BCR	S	4012	-	41,41,41	0.88	0	56,56,56	1.28	7 (12%)
16	CLA	x	508	12	59,63,73	1.08	4 (6%)	70,101,113	0.99	3 (4%)
16	CLA	q	517	12	59,63,73	1.08	5 (8%)	70,101,113	1.13	6 (8%)
16	CLA	n	507	-	69,73,73	1.00	4 (5%)	82,113,113	1.03	4 (4%)
24	LUT	Z	601	-	42,43,43	0.81	1 (2%)	51,60,60	1.48	6 (11%)
16	CLA	S	1303	-	41,45,73	1.25	5 (12%)	50,78,113	1.03	2 (4%)
19	BCR	K	4005	-	41,41,41	0.86	0	56,56,56	1.28	6 (10%)
19	BCR	o	602	-	41,41,41	0.88	0	56,56,56	1.37	7 (12%)
24	LUT	q	601	-	42,43,43	0.77	0	51,60,60	1.51	9 (17%)
16	CLA	s	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.15	6 (7%)
16	CLA	q	515	-	69,73,73	0.99	5 (7%)	82,113,113	1.20	7 (8%)
16	CLA	B	1239	-	69,73,73	0.95	3 (4%)	82,113,113	1.11	6 (7%)
16	CLA	W	505	-	69,73,73	1.00	4 (5%)	82,113,113	1.15	6 (7%)
16	CLA	A	1106	1	69,73,73	0.98	4 (5%)	82,113,113	1.12	4 (4%)
16	CLA	Y	513	-	50,54,73	1.16	4 (8%)	59,90,113	1.08	5 (8%)
16	CLA	T	4002	-	49,53,73	1.17	4 (8%)	58,89,113	1.03	3 (5%)
16	CLA	B	1012	25	59,63,73	1.12	4 (6%)	70,101,113	1.11	6 (8%)
13	LHG	R	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.24	4 (9%)
16	CLA	G	1213	-	59,63,73	1.08	5 (8%)	70,101,113	1.10	4 (5%)
13	LHG	a	849	-	42,42,48	0.71	1 (2%)	45,48,54	1.22	4 (8%)
16	CLA	s	504	-	69,73,73	0.99	4 (5%)	82,113,113	0.95	3 (3%)
16	CLA	H	1135	-	55,59,73	1.12	4 (7%)	64,96,113	1.26	6 (9%)
18	SF4	H	3001	-	0,12,12	-	-	-		
16	CLA	Y	517	12	59,63,73	1.08	4 (6%)	70,101,113	1.05	3 (4%)
16	CLA	b	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.02	5 (6%)
19	BCR	H	4003	-	41,41,41	0.86	0	56,56,56	1.22	4 (7%)
16	CLA	J	1303	-	41,45,73	1.24	5 (12%)	50,78,113	1.07	3 (6%)
16	CLA	H	1123	-	69,73,73	1.00	4 (5%)	82,113,113	0.96	3 (3%)
16	CLA	t	510	-	69,73,73	1.00	4 (5%)	82,113,113	0.99	5 (6%)
20	LMT	H	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	A	1113	-	49,53,73	1.19	4 (8%)	58,89,113	1.06	2 (3%)
16	CLA	b	1224	-	64,68,73	1.05	6 (9%)	76,107,113	1.20	4 (5%)
16	CLA	Y	515	-	69,73,73	0.98	4 (5%)	82,113,113	1.04	5 (6%)
16	CLA	w	511	-	69,73,73	0.99	5 (7%)	82,113,113	1.04	5 (6%)
16	CLA	B	1238	25	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	a	1135	-	55,59,73	1.14	7 (12%)	64,96,113	1.08	5 (7%)
19	BCR	a	4002	-	41,41,41	0.85	0	56,56,56	1.18	5 (8%)
16	CLA	B	1219	-	49,53,73	1.21	6 (12%)	58,89,113	1.15	4 (6%)
13	LHG	G	4018	16	37,37,48	0.73	1 (2%)	40,43,54	1.32	5 (12%)
16	CLA	G	1224	-	64,68,73	1.05	5 (7%)	76,107,113	1.12	4 (5%)
16	CLA	a	1121	-	55,59,73	1.12	5 (9%)	64,96,113	1.11	5 (7%)
16	CLA	a	1123	-	69,73,73	1.00	4 (5%)	82,113,113	1.01	4 (4%)
16	CLA	w	501	-	54,58,73	1.11	5 (9%)	64,95,113	1.14	6 (9%)
16	CLA	B	1215	-	64,68,73	1.00	5 (7%)	76,107,113	1.11	3 (3%)
16	CLA	a	1105	-	62,66,73	1.07	5 (8%)	73,104,113	1.03	5 (6%)
16	CLA	a	1118	-	59,63,73	1.06	4 (6%)	70,101,113	0.96	2 (2%)
23	LMU	r	606	-	36,36,36	0.87	0	47,47,47	1.10	2 (4%)
16	CLA	A	1119	25	69,73,73	1.00	4 (5%)	82,113,113	0.99	4 (4%)
16	CLA	B	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.01	4 (4%)
16	CLA	p	511	-	69,73,73	0.98	4 (5%)	82,113,113	1.05	5 (6%)
16	CLA	p	515	-	69,73,73	0.98	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	q	507	-	69,73,73	1.00	4 (5%)	82,113,113	1.13	6 (7%)
19	BCR	U	4019	-	41,41,41	0.86	0	56,56,56	1.49	8 (14%)
15	CL0	a	1011	-	58,73,73	1.87	6 (10%)	60,113,113	1.62	11 (18%)
16	CLA	a	1022	-	69,73,73	1.01	5 (7%)	82,113,113	1.04	6 (7%)
16	CLA	p	504	-	69,73,73	1.00	4 (5%)	82,113,113	1.00	3 (3%)
19	BCR	s	601	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	b	1218	-	59,63,73	1.07	4 (6%)	70,101,113	1.10	7 (10%)
16	CLA	Z	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.12	4 (4%)
16	CLA	j	1302	8	49,53,73	1.19	5 (10%)	58,89,113	1.18	6 (10%)
16	CLA	h	515	-	69,73,73	1.01	4 (5%)	82,113,113	1.24	9 (10%)
13	LHG	x	605	-	30,30,48	0.78	1 (3%)	33,36,54	1.28	3 (9%)
16	CLA	Z	502	-	54,58,73	1.11	6 (11%)	64,95,113	1.11	5 (7%)
16	CLA	G	1226	-	64,68,73	1.04	6 (9%)	76,107,113	1.10	5 (6%)
16	CLA	l	1502	-	64,68,73	1.00	5 (7%)	76,107,113	1.16	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	LMU	Y	606	-	36,36,36	0.84	0	47,47,47	1.36	6 (12%)
13	LHG	X	605	-	26,26,48	0.82	0	29,32,54	1.27	2 (6%)
16	CLA	Y	507	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	5 (6%)
16	CLA	g	515	-	69,73,73	1.00	4 (5%)	82,113,113	1.16	6 (7%)
16	CLA	x	514	-	54,58,73	1.11	5 (9%)	64,95,113	1.10	5 (7%)
16	CLA	x	506	-	64,68,73	1.02	6 (9%)	76,107,113	1.12	4 (5%)
16	CLA	h	517	-	59,63,73	1.10	4 (6%)	70,101,113	0.99	5 (7%)
16	CLA	h	504	-	64,68,73	1.05	5 (7%)	76,107,113	1.24	7 (9%)
16	CLA	X	504	-	64,68,73	1.06	6 (9%)	76,107,113	1.16	3 (3%)
16	CLA	A	1135	-	55,59,73	1.13	7 (12%)	64,96,113	1.12	5 (7%)
16	CLA	o	517	12	59,63,73	1.08	4 (6%)	70,101,113	0.98	4 (5%)
16	CLA	H	1140	-	69,73,73	0.97	5 (7%)	82,113,113	1.07	3 (3%)
16	CLA	b	1230	-	49,53,73	1.18	5 (10%)	58,89,113	1.15	4 (6%)
16	CLA	b	1240	13	50,54,73	1.15	4 (8%)	59,90,113	1.16	2 (3%)
19	BCR	B	4005	-	41,41,41	0.85	0	56,56,56	1.17	4 (7%)
16	CLA	o	514	-	54,58,73	1.12	6 (11%)	64,95,113	1.35	4 (6%)
14	LMG	H	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
16	CLA	q	503	-	50,54,73	1.15	6 (12%)	59,90,113	1.26	5 (8%)
16	CLA	L	1503	25	69,73,73	0.99	4 (5%)	82,113,113	0.92	3 (3%)
16	CLA	b	1221	25	69,73,73	1.00	5 (7%)	82,113,113	1.10	5 (6%)
16	CLA	A	1126	-	69,73,73	0.98	5 (7%)	82,113,113	1.13	2 (2%)
16	CLA	b	1220	-	58,62,73	1.10	6 (10%)	68,99,113	1.11	5 (7%)
19	BCR	L	4022	-	41,41,41	0.86	0	56,56,56	1.30	6 (10%)
16	CLA	k	4002	-	49,53,73	1.17	4 (8%)	58,89,113	1.12	4 (6%)
16	CLA	x	511	-	69,73,73	1.00	6 (8%)	82,113,113	0.94	2 (2%)
16	CLA	H	1133	-	58,62,73	1.08	6 (10%)	68,99,113	1.28	6 (8%)
19	BCR	i	4018	-	41,41,41	0.87	0	56,56,56	1.23	8 (14%)
16	CLA	y	512	12	69,73,73	1.00	5 (7%)	82,113,113	1.01	6 (7%)
16	CLA	A	1115	-	58,62,73	1.06	6 (10%)	68,99,113	1.17	3 (4%)
16	CLA	A	1128	-	69,73,73	0.98	5 (7%)	82,113,113	1.08	4 (4%)
19	BCR	b	4004	-	41,41,41	0.84	0	56,56,56	1.26	6 (10%)
16	CLA	H	1105	-	62,66,73	1.05	5 (8%)	73,104,113	1.08	5 (6%)
16	CLA	G	1231	25	49,53,73	1.19	4 (8%)	58,89,113	1.13	4 (6%)
16	CLA	r	516	-	50,54,73	1.15	5 (10%)	59,90,113	1.13	4 (6%)
16	CLA	t	513	-	50,54,73	1.17	5 (10%)	59,90,113	1.15	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	u	513	-	50,54,73	1.15	5 (10%)	59,90,113	1.03	3 (5%)
19	BCR	J	4013	-	41,41,41	0.86	0	56,56,56	1.23	8 (14%)
21	ECH	G	4006	-	42,42,42	0.79	0	55,58,58	1.50	8 (14%)
19	BCR	B	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	G	1210	-	69,73,73	1.00	5 (7%)	82,113,113	1.05	5 (6%)
16	CLA	a	1134	1	49,53,73	1.16	4 (8%)	58,89,113	1.16	4 (6%)
16	CLA	w	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.07	5 (7%)
16	CLA	s	509	-	64,68,73	1.04	4 (6%)	76,107,113	1.04	4 (5%)
16	CLA	B	1221	25	69,73,73	0.99	4 (5%)	82,113,113	1.02	3 (3%)
16	CLA	w	504	-	69,73,73	1.01	5 (7%)	82,113,113	1.02	5 (6%)
19	BCR	g	601	-	41,41,41	0.88	0	56,56,56	1.44	9 (16%)
16	CLA	B	1230	-	49,53,73	1.18	4 (8%)	58,89,113	1.11	4 (6%)
14	LMG	Q	4017	-	27,27,55	1.07	1 (3%)	35,35,63	1.18	3 (8%)
16	CLA	X	506	-	64,68,73	1.02	4 (6%)	76,107,113	1.24	4 (5%)
16	CLA	a	1101	-	69,73,73	0.98	4 (5%)	82,113,113	1.06	4 (4%)
16	CLA	t	516	-	50,54,73	1.16	4 (8%)	59,90,113	1.10	4 (6%)
16	CLA	u	516	-	50,54,73	1.14	5 (10%)	59,90,113	1.15	4 (6%)
16	CLA	p	517	12	59,63,73	1.07	4 (6%)	70,101,113	1.02	4 (5%)
16	CLA	a	1115	-	58,62,73	1.07	5 (8%)	68,99,113	1.14	3 (4%)
16	CLA	A	1133	-	58,62,73	1.08	6 (10%)	68,99,113	1.22	7 (10%)
16	CLA	q	513	-	54,58,73	1.12	4 (7%)	64,95,113	1.08	4 (6%)
16	CLA	g	504	-	69,73,73	1.01	4 (5%)	82,113,113	1.01	6 (7%)
16	CLA	a	1120	-	53,57,73	1.08	4 (7%)	61,93,113	1.21	5 (8%)
16	CLA	B	1231	25	49,53,73	1.19	4 (8%)	58,89,113	1.16	4 (6%)
16	CLA	G	1227	-	53,57,73	1.12	6 (11%)	61,93,113	1.15	5 (8%)
16	CLA	a	1112	-	49,53,73	1.19	5 (10%)	58,89,113	1.00	3 (5%)
16	CLA	K	4002	-	49,53,73	1.17	4 (8%)	58,89,113	1.02	2 (3%)
16	CLA	A	1105	-	62,66,73	1.06	5 (8%)	73,104,113	1.00	4 (5%)
16	CLA	X	516	-	50,54,73	1.13	5 (10%)	59,90,113	1.09	3 (5%)
16	CLA	A	1118	-	59,63,73	1.06	4 (6%)	70,101,113	1.00	3 (4%)
16	CLA	b	1210	-	69,73,73	1.02	5 (7%)	82,113,113	1.05	6 (7%)
16	CLA	s	515	-	69,73,73	0.98	4 (5%)	82,113,113	1.02	6 (7%)
19	BCR	H	4011	-	41,41,41	0.88	0	56,56,56	1.26	6 (10%)
16	CLA	p	510	-	69,73,73	1.01	4 (5%)	82,113,113	1.01	3 (3%)
19	BCR	y	603	-	41,41,41	0.83	0	56,56,56	1.17	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BCR	B	4004	-	41,41,41	0.83	0	56,56,56	1.26	5 (8%)
16	CLA	o	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.10	4 (6%)
13	LHG	r	605	-	30,30,48	0.81	2 (6%)	33,36,54	1.28	3 (9%)
19	BCR	v	601	-	41,41,41	0.83	0	56,56,56	1.30	7 (12%)
16	CLA	Y	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.06	7 (8%)
16	CLA	A	1022	25	69,73,73	1.01	5 (7%)	82,113,113	1.08	9 (10%)
19	BCR	p	604	-	41,41,41	0.87	0	56,56,56	1.23	6 (10%)
16	CLA	q	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.17	5 (7%)
19	BCR	p	602	-	41,41,41	0.87	0	56,56,56	1.31	7 (12%)
16	CLA	h	512	12	69,73,73	1.03	6 (8%)	82,113,113	1.06	7 (8%)
16	CLA	r	515	-	69,73,73	1.00	4 (5%)	82,113,113	1.12	6 (7%)
18	SF4	c	102	-	0,12,12	-	-	-		
16	CLA	W	507	-	69,73,73	1.01	4 (5%)	82,113,113	1.01	4 (4%)
16	CLA	A	1129	-	50,54,73	1.12	4 (8%)	59,90,113	1.15	5 (8%)
16	CLA	B	1023	-	69,73,73	1.01	7 (10%)	82,113,113	1.12	5 (6%)
16	CLA	B	1226	-	64,68,73	1.05	6 (9%)	76,107,113	1.05	3 (3%)
16	CLA	b	1229	-	62,66,73	1.06	4 (6%)	73,104,113	1.04	5 (6%)
16	CLA	g	512	12	69,73,73	1.00	5 (7%)	82,113,113	1.17	4 (4%)
16	CLA	t	507	-	69,73,73	1.01	4 (5%)	82,113,113	0.98	3 (3%)
18	SF4	c	101	-	0,12,12	-	-	-		
16	CLA	v	512	12	69,73,73	1.02	4 (5%)	82,113,113	1.08	7 (8%)
16	CLA	F	1301	25	49,53,73	1.18	4 (8%)	58,89,113	1.13	3 (5%)
13	LHG	I	103	-	39,39,48	0.68	2 (5%)	42,45,54	1.23	4 (9%)
16	CLA	w	507	-	69,73,73	0.99	4 (5%)	82,113,113	0.92	3 (3%)
16	CLA	A	1131	-	69,73,73	1.02	5 (7%)	82,113,113	1.16	5 (6%)
16	CLA	p	516	-	50,54,73	1.14	4 (8%)	59,90,113	1.07	3 (5%)
16	CLA	r	504	-	69,73,73	1.01	4 (5%)	82,113,113	0.99	3 (3%)
16	CLA	v	502	-	54,58,73	1.12	5 (9%)	64,95,113	1.06	5 (7%)
16	CLA	W	502	-	54,58,73	1.14	6 (11%)	64,95,113	1.16	5 (7%)
16	CLA	v	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.24	7 (11%)
16	CLA	o	509	-	64,68,73	1.03	4 (6%)	76,107,113	0.95	5 (6%)
16	CLA	f	1301	25	49,53,73	1.17	4 (8%)	58,89,113	1.06	4 (6%)
16	CLA	x	504	-	69,73,73	1.01	4 (5%)	82,113,113	1.04	6 (7%)
19	BCR	W	601	-	41,41,41	0.86	0	56,56,56	1.27	8 (14%)
19	BCR	W	603	-	41,41,41	0.85	0	56,56,56	1.21	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BCR	v	603	-	41,41,41	0.85	0	56,56,56	1.27	8 (14%)
16	CLA	g	513	-	50,54,73	1.18	4 (8%)	59,90,113	1.00	5 (8%)
16	CLA	B	1227	-	53,57,73	1.13	6 (11%)	61,93,113	1.13	4 (6%)
16	CLA	b	1239	-	69,73,73	0.97	3 (4%)	82,113,113	1.07	7 (8%)
18	SF4	C	101	-	0,12,12	-	-	-		
16	CLA	y	510	-	69,73,73	1.01	4 (5%)	82,113,113	0.95	5 (6%)
16	CLA	x	510	-	69,73,73	0.99	5 (7%)	82,113,113	1.05	4 (4%)
19	BCR	l	4022	-	41,41,41	0.89	1 (2%)	56,56,56	1.41	8 (14%)
16	CLA	h	516	-	50,54,73	1.16	4 (8%)	59,90,113	1.12	4 (6%)
16	CLA	G	1212	-	49,53,73	1.19	5 (10%)	58,89,113	1.20	4 (6%)
16	CLA	H	1102	16	60,64,73	1.05	4 (6%)	71,102,113	0.94	2 (2%)
16	CLA	u	517	12	59,63,73	1.09	4 (6%)	70,101,113	1.04	5 (7%)
16	CLA	W	504	-	64,68,73	1.05	5 (7%)	76,107,113	1.01	3 (3%)
16	CLA	X	515	-	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	Z	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.12	5 (7%)
16	CLA	Y	504	-	69,73,73	1.01	5 (7%)	82,113,113	0.99	3 (3%)
14	LMG	f	4017	-	27,27,55	1.10	2 (7%)	35,35,63	1.16	3 (8%)
16	CLA	g	516	-	50,54,73	1.15	4 (8%)	59,90,113	1.19	3 (5%)
16	CLA	B	1210	-	69,73,73	1.01	5 (7%)	82,113,113	1.09	6 (7%)
16	CLA	o	513	-	50,54,73	1.16	4 (8%)	59,90,113	0.98	1 (1%)
19	BCR	U	4022	-	41,41,41	0.88	0	56,56,56	1.32	6 (10%)
19	BCR	n	603	-	41,41,41	0.83	0	56,56,56	1.20	5 (8%)
24	LUT	w	601	-	42,43,43	0.74	0	51,60,60	1.46	7 (13%)
16	CLA	q	510	-	64,68,73	1.03	4 (6%)	76,107,113	0.96	3 (3%)
16	CLA	b	1216	25	51,55,73	1.16	5 (9%)	60,91,113	1.46	8 (13%)
19	BCR	S	4013	-	41,41,41	0.87	0	56,56,56	1.32	7 (12%)
16	CLA	G	1217	-	49,53,73	1.17	4 (8%)	58,89,113	1.04	2 (3%)
16	CLA	v	514	-	54,58,73	1.13	4 (7%)	64,95,113	1.05	2 (3%)
21	ECH	B	4006	-	42,42,42	0.74	0	55,58,58	1.53	11 (20%)
16	CLA	H	1013	-	69,73,73	1.01	7 (10%)	82,113,113	1.20	9 (10%)
19	BCR	u	604	-	41,41,41	0.89	0	56,56,56	1.35	10 (17%)
16	CLA	H	1130	-	64,68,73	1.03	5 (7%)	76,107,113	1.01	7 (9%)
16	CLA	H	1103	-	69,73,73	0.99	4 (5%)	82,113,113	1.01	4 (4%)
16	CLA	s	510	-	69,73,73	1.01	4 (5%)	82,113,113	0.97	4 (4%)
16	CLA	W	517	12	59,63,73	1.09	5 (8%)	70,101,113	0.98	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	G	1021	-	69,73,73	0.99	5 (7%)	82,113,113	1.16	5 (6%)
16	CLA	o	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	W	514	-	54,58,73	1.11	5 (9%)	64,95,113	1.11	4 (6%)
14	LMG	b	848	-	43,43,55	0.86	1 (2%)	51,51,63	1.28	6 (11%)
19	BCR	j	4012	-	41,41,41	0.88	0	56,56,56	1.29	7 (12%)
16	CLA	L	1501	10	64,68,73	1.02	5 (7%)	76,107,113	0.98	5 (6%)
16	CLA	H	1108	-	49,53,73	1.17	5 (10%)	58,89,113	1.24	4 (6%)
19	BCR	n	604	-	41,41,41	0.86	0	56,56,56	1.33	7 (12%)
19	BCR	t	603	-	41,41,41	0.84	0	56,56,56	1.18	4 (7%)
19	BCR	w	603	-	41,41,41	0.85	0	56,56,56	1.17	6 (10%)
16	CLA	j	1303	-	41,45,73	1.24	5 (12%)	50,78,113	1.10	3 (6%)
19	BCR	Y	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)
16	CLA	Y	501	-	54,58,73	1.10	4 (7%)	64,95,113	1.20	7 (10%)
20	LMT	l	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
16	CLA	a	1136	-	69,73,73	0.99	5 (7%)	82,113,113	1.00	3 (3%)
16	CLA	t	505	-	69,73,73	1.00	5 (7%)	82,113,113	1.19	6 (7%)
16	CLA	u	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.08	5 (6%)
16	CLA	x	509	-	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
16	CLA	y	508	-	59,63,73	1.08	4 (6%)	70,101,113	1.20	6 (8%)
19	BCR	p	603	-	41,41,41	0.86	0	56,56,56	1.21	5 (8%)
16	CLA	b	1234	-	54,58,73	1.14	5 (9%)	64,95,113	1.13	8 (12%)
19	BCR	X	602	-	41,41,41	0.88	0	56,56,56	1.36	7 (12%)
19	BCR	T	4005	-	41,41,41	0.85	0	56,56,56	1.26	7 (12%)
16	CLA	B	1217	-	49,53,73	1.18	4 (8%)	58,89,113	1.11	3 (5%)
16	CLA	H	1801	13	50,54,73	1.13	4 (8%)	59,90,113	1.15	5 (8%)
16	CLA	o	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.06	4 (4%)
19	BCR	F	4016	-	41,41,41	0.86	0	56,56,56	1.31	8 (14%)
16	CLA	G	1234	-	54,58,73	1.13	6 (11%)	64,95,113	1.16	4 (6%)
16	CLA	x	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.11	6 (7%)
16	CLA	b	1219	-	49,53,73	1.21	5 (10%)	58,89,113	1.21	5 (8%)
16	CLA	T	4004	-	59,63,73	1.07	4 (6%)	70,101,113	1.13	4 (5%)
19	BCR	H	4002	-	41,41,41	0.85	0	56,56,56	1.19	5 (8%)
19	BCR	a	4007	-	41,41,41	0.89	1 (2%)	56,56,56	1.30	5 (8%)
15	CL0	A	1011	-	58,73,73	1.91	8 (13%)	60,113,113	1.67	11 (18%)
16	CLA	s	513	-	50,54,73	1.15	4 (8%)	59,90,113	1.16	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BCR	o	601	-	41,41,41	0.88	1 (2%)	56,56,56	1.37	8 (14%)
16	CLA	r	506	-	64,68,73	1.01	3 (4%)	76,107,113	1.07	7 (9%)
16	CLA	A	1110	-	58,62,73	1.05	4 (6%)	68,99,113	1.01	3 (4%)
16	CLA	H	1126	-	69,73,73	0.99	4 (5%)	82,113,113	1.12	5 (6%)
16	CLA	X	505	-	69,73,73	1.00	5 (7%)	82,113,113	1.12	6 (7%)
19	BCR	t	604	-	41,41,41	0.83	0	56,56,56	1.23	4 (7%)
16	CLA	u	511	-	69,73,73	0.97	4 (5%)	82,113,113	1.10	4 (4%)
16	CLA	v	508	-	59,63,73	1.07	5 (8%)	70,101,113	1.31	7 (10%)
16	CLA	W	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.96	3 (4%)
18	SF4	N	102	-	0,12,12	-	-	-		
19	BCR	S	4015	-	41,41,41	0.87	0	56,56,56	1.20	8 (14%)
16	CLA	Z	510	-	64,68,73	1.04	4 (6%)	76,107,113	1.04	3 (3%)
19	BCR	q	604	-	41,41,41	0.87	0	56,56,56	1.26	6 (10%)
16	CLA	u	501	-	50,54,73	1.14	4 (8%)	59,90,113	0.99	3 (5%)
16	CLA	G	1238	25	69,73,73	0.98	4 (5%)	82,113,113	1.04	6 (7%)
16	CLA	x	515	-	69,73,73	0.98	4 (5%)	82,113,113	1.14	6 (7%)
16	CLA	r	513	-	50,54,73	1.18	4 (8%)	59,90,113	1.10	5 (8%)
16	CLA	G	1219	-	49,53,73	1.21	5 (10%)	58,89,113	1.14	5 (8%)
13	LHG	a	851	16	25,25,48	0.88	2 (8%)	28,31,54	1.26	2 (7%)
16	CLA	B	1212	-	49,53,73	1.19	5 (10%)	58,89,113	1.14	4 (6%)
23	LMU	Z	605	-	36,36,36	0.87	0	47,47,47	1.20	4 (8%)
16	CLA	w	517	12	59,63,73	1.09	6 (10%)	70,101,113	1.07	3 (4%)
16	CLA	G	1215	-	64,68,73	1.00	4 (6%)	76,107,113	1.09	2 (2%)
16	CLA	G	1225	-	69,73,73	0.99	6 (8%)	82,113,113	1.14	4 (4%)
16	CLA	W	512	12	64,68,73	1.04	6 (9%)	76,107,113	1.08	4 (5%)
23	LMU	q	605	-	36,36,36	0.83	0	47,47,47	1.13	4 (8%)
21	ECH	R	4020	-	42,42,42	0.99	3 (7%)	55,58,58	1.93	14 (25%)
16	CLA	p	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	A	1101	-	69,73,73	0.98	5 (7%)	82,113,113	1.04	7 (8%)
16	CLA	q	516	-	50,54,73	1.14	5 (10%)	59,90,113	0.99	2 (3%)
16	CLA	w	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.11	5 (6%)
19	BCR	Y	604	-	41,41,41	0.86	0	56,56,56	1.16	6 (10%)
16	CLA	t	503	-	50,54,73	1.16	5 (10%)	59,90,113	1.28	5 (8%)
16	CLA	q	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.03	3 (3%)
16	CLA	w	502	-	54,58,73	1.11	6 (11%)	64,95,113	1.17	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	BCR	r	603	-	41,41,41	0.83	0	56,56,56	1.20	6 (10%)
16	CLA	g	517	12	59,63,73	1.09	4 (6%)	70,101,113	0.99	3 (4%)
16	CLA	p	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.11	6 (7%)
16	CLA	q	502	-	54,58,73	1.13	6 (11%)	64,95,113	1.04	3 (4%)
16	CLA	A	1112	-	49,53,73	1.19	4 (8%)	58,89,113	1.07	4 (6%)
19	BCR	B	4014	-	41,41,41	0.88	0	56,56,56	1.25	7 (12%)
16	CLA	H	1109	16	69,73,73	0.98	4 (5%)	82,113,113	1.12	6 (7%)
16	CLA	Z	503	-	50,54,73	1.15	6 (12%)	59,90,113	1.19	6 (10%)
16	CLA	Y	512	12	69,73,73	1.02	6 (8%)	82,113,113	1.18	8 (9%)
16	CLA	X	513	-	50,54,73	1.14	4 (8%)	59,90,113	1.09	3 (5%)
16	CLA	A	1132	-	69,73,73	0.99	6 (8%)	82,113,113	1.14	6 (7%)
16	CLA	K	4004	-	59,63,73	1.07	4 (6%)	70,101,113	1.10	4 (5%)
16	CLA	H	1129	-	50,54,73	1.13	5 (10%)	59,90,113	1.16	6 (10%)
16	CLA	g	503	-	50,54,73	1.15	4 (8%)	59,90,113	1.13	4 (6%)
19	BCR	g	603	-	41,41,41	0.84	0	56,56,56	1.21	6 (10%)
16	CLA	h	505	-	69,73,73	1.02	5 (7%)	82,113,113	1.15	6 (7%)
16	CLA	A	1134	1	49,53,73	1.19	5 (10%)	58,89,113	1.09	2 (3%)
16	CLA	Y	516	-	50,54,73	1.13	4 (8%)	59,90,113	1.11	4 (6%)
21	ECH	V	4021	-	42,42,42	0.84	1 (2%)	55,58,58	1.55	7 (12%)
16	CLA	G	1209	-	49,53,73	1.18	4 (8%)	58,89,113	1.17	4 (6%)
16	CLA	A	1139	25	64,68,73	1.03	5 (7%)	76,107,113	1.03	4 (5%)
16	CLA	a	1127	-	69,73,73	1.00	6 (8%)	82,113,113	1.08	4 (4%)
19	BCR	a	4011	-	41,41,41	0.89	0	56,56,56	1.26	5 (8%)
16	CLA	g	505	-	69,73,73	0.99	5 (7%)	82,113,113	1.19	7 (8%)
19	BCR	h	604	-	41,41,41	0.86	0	56,56,56	1.25	6 (10%)
16	CLA	t	501	-	54,58,73	1.11	5 (9%)	64,95,113	1.22	5 (7%)
16	CLA	H	1128	-	69,73,73	0.98	5 (7%)	82,113,113	1.04	5 (6%)
16	CLA	w	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.06	5 (7%)
18	SF4	N	101	-	0,12,12	-	-	-		
16	CLA	A	1013	-	69,73,73	0.99	6 (8%)	82,113,113	1.20	10 (12%)
16	CLA	b	1206	2	69,73,73	0.99	5 (7%)	82,113,113	0.94	2 (2%)
16	CLA	n	505	-	69,73,73	1.00	6 (8%)	82,113,113	1.22	6 (7%)
16	CLA	Z	509	-	69,73,73	1.00	5 (7%)	82,113,113	1.01	4 (4%)
16	CLA	x	507	-	69,73,73	1.00	5 (7%)	82,113,113	1.07	6 (7%)
19	BCR	u	601	-	41,41,41	0.91	1 (2%)	56,56,56	1.38	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	o	502	-	54,58,73	1.11	6 (11%)	64,95,113	1.03	4 (6%)
16	CLA	g	511	-	69,73,73	0.99	5 (7%)	82,113,113	0.98	3 (3%)
16	CLA	p	501	-	54,58,73	1.11	5 (9%)	64,95,113	1.16	6 (9%)
19	BCR	G	4010	-	41,41,41	0.94	0	56,56,56	1.39	9 (16%)
16	CLA	y	504	-	64,68,73	1.05	6 (9%)	76,107,113	1.19	8 (10%)
16	CLA	G	1203	-	69,73,73	0.99	5 (7%)	82,113,113	1.14	6 (7%)
16	CLA	g	514	-	54,58,73	1.13	6 (11%)	64,95,113	1.08	5 (7%)
16	CLA	A	1107	1	54,58,73	1.12	4 (7%)	64,95,113	1.15	5 (7%)
16	CLA	l	1503	-	69,73,73	1.00	4 (5%)	82,113,113	0.91	4 (4%)
19	BCR	o	604	-	41,41,41	0.88	0	56,56,56	1.31	10 (17%)
16	CLA	x	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.16	4 (6%)
16	CLA	Z	513	-	54,58,73	1.12	4 (7%)	64,95,113	1.07	5 (7%)
16	CLA	X	501	-	50,54,73	1.14	4 (8%)	59,90,113	1.11	5 (8%)
16	CLA	G	1218	-	59,63,73	1.08	4 (6%)	70,101,113	1.10	4 (5%)
19	BCR	Q	4016	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)
16	CLA	A	1124	25	64,68,73	1.03	4 (6%)	76,107,113	1.05	4 (5%)
16	CLA	W	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.22	5 (8%)
19	BCR	G	4004	-	41,41,41	0.83	0	56,56,56	1.25	6 (10%)
16	CLA	U	1503	-	69,73,73	1.00	4 (5%)	82,113,113	0.87	3 (3%)
16	CLA	b	1227	-	53,57,73	1.11	6 (11%)	61,93,113	1.15	6 (9%)
16	CLA	a	1107	1	54,58,73	1.11	4 (7%)	64,95,113	1.14	3 (4%)
16	CLA	a	1108	-	49,53,73	1.17	5 (10%)	58,89,113	1.25	5 (8%)
16	CLA	b	1231	25	49,53,73	1.18	4 (8%)	58,89,113	1.21	4 (6%)
16	CLA	w	503	-	50,54,73	1.16	6 (12%)	59,90,113	1.18	5 (8%)
16	CLA	Y	511	-	69,73,73	0.98	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	t	502	-	54,58,73	1.14	6 (11%)	64,95,113	1.13	4 (6%)
19	BCR	r	604	-	41,41,41	0.89	0	56,56,56	1.27	6 (10%)
19	BCR	A	4008	-	41,41,41	0.89	0	56,56,56	1.35	8 (14%)
16	CLA	s	507	12	69,73,73	1.01	4 (5%)	82,113,113	1.01	5 (6%)
16	CLA	Y	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.12	5 (7%)
16	CLA	y	511	-	69,73,73	1.00	4 (5%)	82,113,113	1.12	5 (6%)
21	ECH	m	4021	-	42,42,42	0.84	0	55,58,58	1.55	9 (16%)
16	CLA	n	514	-	54,58,73	1.11	6 (11%)	64,95,113	1.10	5 (7%)
19	BCR	B	4010	-	41,41,41	0.91	0	56,56,56	1.35	8 (14%)
16	CLA	H	1110	-	58,62,73	1.05	4 (6%)	68,99,113	1.03	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	B	1203	-	69,73,73	0.99	5 (7%)	82,113,113	1.14	5 (6%)
16	CLA	G	1230	-	49,53,73	1.17	4 (8%)	58,89,113	1.03	2 (3%)
16	CLA	y	514	-	54,58,73	1.13	6 (11%)	64,95,113	1.13	6 (9%)
19	BCR	Y	603	-	41,41,41	0.85	0	56,56,56	1.16	4 (7%)
16	CLA	G	1220	-	58,62,73	1.10	4 (6%)	68,99,113	1.09	5 (7%)
16	CLA	g	510	-	69,73,73	0.99	5 (7%)	82,113,113	1.11	5 (6%)
16	CLA	a	1106	1	69,73,73	0.97	4 (5%)	82,113,113	1.10	3 (3%)
16	CLA	k	4003	9	49,53,73	1.20	4 (8%)	58,89,113	1.14	3 (5%)
16	CLA	h	511	-	69,73,73	1.00	6 (8%)	82,113,113	1.08	8 (9%)
19	BCR	X	603	-	41,41,41	0.85	0	56,56,56	1.15	4 (7%)
16	CLA	x	513	-	50,54,73	1.18	5 (10%)	59,90,113	1.03	2 (3%)
16	CLA	H	1134	1	49,53,73	1.18	4 (8%)	58,89,113	1.09	2 (3%)
16	CLA	h	501	-	50,54,73	1.17	5 (10%)	59,90,113	1.26	6 (10%)
21	ECH	b	4006	-	42,42,42	0.85	2 (4%)	55,58,58	1.52	8 (14%)
19	BCR	a	4003	-	41,41,41	0.87	0	56,56,56	1.22	5 (8%)
16	CLA	H	1104	-	69,73,73	1.00	6 (8%)	82,113,113	1.07	6 (7%)
16	CLA	H	1139	25	64,68,73	1.03	5 (7%)	76,107,113	1.01	4 (5%)
16	CLA	W	511	-	69,73,73	1.01	5 (7%)	82,113,113	1.09	6 (7%)
16	CLA	a	1139	25	59,63,73	1.07	5 (8%)	70,101,113	1.00	5 (7%)
16	CLA	s	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.15	7 (8%)
16	CLA	Z	507	-	69,73,73	1.00	3 (4%)	82,113,113	1.08	5 (6%)
16	CLA	A	1138	-	69,73,73	0.99	4 (5%)	82,113,113	0.98	4 (4%)
16	CLA	G	1221	25	69,73,73	1.00	4 (5%)	82,113,113	1.07	3 (3%)
16	CLA	s	506	-	64,68,73	1.02	6 (9%)	76,107,113	1.12	8 (10%)
16	CLA	g	501	-	54,58,73	1.11	4 (7%)	64,95,113	1.08	5 (7%)
19	BCR	h	601	-	41,41,41	0.84	0	56,56,56	1.28	7 (12%)
16	CLA	H	1111	-	59,63,73	1.09	4 (6%)	70,101,113	1.03	2 (2%)
16	CLA	B	1209	-	49,53,73	1.17	4 (8%)	58,89,113	1.10	3 (5%)
16	CLA	H	1119	25	69,73,73	0.98	5 (7%)	82,113,113	1.02	4 (4%)
16	CLA	H	1113	-	49,53,73	1.20	6 (12%)	58,89,113	1.18	3 (5%)
16	CLA	g	507	-	69,73,73	1.00	4 (5%)	82,113,113	1.01	6 (7%)
19	BCR	G	4005	-	41,41,41	0.85	0	56,56,56	1.14	4 (7%)
16	CLA	b	1222	25	54,58,73	1.14	5 (9%)	64,95,113	1.08	4 (6%)
16	CLA	X	512	12	69,73,73	0.99	5 (7%)	82,113,113	1.00	5 (6%)
16	CLA	r	505	-	69,73,73	0.99	5 (7%)	82,113,113	1.17	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	v	504	-	64,68,73	1.04	5 (7%)	76,107,113	1.09	6 (7%)
19	BCR	A	4011	-	41,41,41	0.88	0	56,56,56	1.29	4 (7%)
16	CLA	n	511	-	69,73,73	1.00	5 (7%)	82,113,113	1.05	5 (6%)
16	CLA	B	1220	-	57,61,73	1.11	4 (7%)	67,98,113	1.11	6 (8%)
16	CLA	s	516	-	50,54,73	1.15	4 (8%)	59,90,113	1.06	3 (5%)
16	CLA	r	511	-	69,73,73	1.01	5 (7%)	82,113,113	0.89	2 (2%)
16	CLA	G	1222	25	54,58,73	1.13	6 (11%)	64,95,113	1.15	8 (12%)
19	BCR	W	604	-	41,41,41	0.86	0	56,56,56	1.37	9 (16%)
16	CLA	h	502	-	54,58,73	1.13	5 (9%)	64,95,113	1.05	5 (7%)
16	CLA	G	1232	25	49,53,73	1.19	5 (10%)	58,89,113	1.29	6 (10%)
16	CLA	r	501	-	54,58,73	1.10	4 (7%)	64,95,113	1.21	6 (9%)
13	LHG	A	851	16	25,25,48	0.87	1 (4%)	28,31,54	1.27	2 (7%)
16	CLA	s	517	12	59,63,73	1.10	5 (8%)	70,101,113	1.09	5 (7%)
16	CLA	A	1137	-	51,55,73	1.14	4 (7%)	60,91,113	1.09	6 (10%)
16	CLA	g	502	-	54,58,73	1.10	5 (9%)	64,95,113	1.07	2 (3%)
16	CLA	v	509	-	69,73,73	1.02	6 (8%)	82,113,113	1.06	7 (8%)
16	CLA	h	510	-	69,73,73	1.01	5 (7%)	82,113,113	1.00	6 (7%)
18	SF4	A	3001	-	0,12,12	-	-	-		
16	CLA	y	507	-	69,73,73	1.02	5 (7%)	82,113,113	0.96	4 (4%)
16	CLA	p	506	-	64,68,73	1.01	4 (6%)	76,107,113	1.12	5 (6%)
16	CLA	a	1013	-	69,73,73	0.99	6 (8%)	82,113,113	1.17	5 (6%)
16	CLA	q	501	-	54,58,73	1.13	5 (9%)	64,95,113	1.19	6 (9%)
16	CLA	a	1140	-	69,73,73	0.97	5 (7%)	82,113,113	1.11	5 (6%)
16	CLA	H	1022	25	69,73,73	1.00	5 (7%)	82,113,113	1.15	8 (9%)
16	CLA	w	506	-	64,68,73	1.03	5 (7%)	76,107,113	1.09	4 (5%)
16	CLA	B	1218	-	59,63,73	1.07	4 (6%)	70,101,113	1.15	5 (7%)
16	CLA	b	1235	-	66,70,73	1.04	6 (9%)	78,109,113	1.15	8 (10%)
19	BCR	J	4012	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
19	BCR	X	604	-	41,41,41	0.88	0	56,56,56	1.31	5 (8%)
16	CLA	u	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.20	6 (9%)
16	CLA	H	1117	-	69,73,73	0.99	5 (7%)	82,113,113	1.15	6 (7%)
16	CLA	b	1201	-	58,62,73	1.07	4 (6%)	68,99,113	1.15	5 (7%)
16	CLA	H	1137	-	51,55,73	1.12	5 (9%)	60,91,113	1.11	5 (8%)
16	CLA	Z	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.13	5 (7%)
16	CLA	h	507	-	69,73,73	0.99	4 (5%)	82,113,113	1.11	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	n	504	-	64,68,73	1.04	4 (6%)	76,107,113	1.10	4 (5%)
16	CLA	b	1217	-	49,53,73	1.16	4 (8%)	58,89,113	1.20	5 (8%)
19	BCR	u	603	-	41,41,41	0.88	0	56,56,56	1.35	8 (14%)
19	BCR	t	601	-	41,41,41	0.83	0	56,56,56	1.18	6 (10%)
16	CLA	Z	515	-	69,73,73	0.99	4 (5%)	82,113,113	1.16	5 (6%)
16	CLA	g	506	-	64,68,73	1.01	4 (6%)	76,107,113	1.01	5 (6%)
16	CLA	X	511	-	69,73,73	0.98	4 (5%)	82,113,113	1.10	6 (7%)
16	CLA	A	1125	-	69,73,73	0.98	4 (5%)	82,113,113	0.97	3 (3%)
16	CLA	B	1222	25	54,58,73	1.13	5 (9%)	64,95,113	1.10	5 (7%)
16	CLA	B	1223	-	69,73,73	0.98	4 (5%)	82,113,113	1.07	3 (3%)
16	CLA	a	1116	-	58,62,73	1.07	5 (8%)	68,99,113	1.02	4 (5%)
16	CLA	n	506	-	64,68,73	1.03	4 (6%)	76,107,113	1.08	5 (6%)
16	CLA	b	1232	25	49,53,73	1.19	5 (10%)	58,89,113	1.35	4 (6%)
16	CLA	n	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.08	4 (4%)
16	CLA	Z	517	12	59,63,73	1.09	5 (8%)	70,101,113	1.03	3 (4%)
16	CLA	v	516	-	50,54,73	1.14	4 (8%)	59,90,113	0.99	3 (5%)
16	CLA	y	509	-	69,73,73	1.00	4 (5%)	82,113,113	0.97	5 (6%)
16	CLA	n	501	-	54,58,73	1.12	4 (7%)	64,95,113	1.21	7 (10%)
19	BCR	s	602	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
16	CLA	B	1214	-	59,63,73	1.06	4 (6%)	70,101,113	1.19	4 (5%)
16	CLA	b	1236	-	54,58,73	1.12	5 (9%)	64,95,113	1.14	6 (9%)
13	LHG	i	103	-	39,39,48	0.69	2 (5%)	42,45,54	1.24	5 (11%)
19	BCR	b	4017	-	41,41,41	0.87	0	56,56,56	1.16	4 (7%)
17	PQN	a	2001	-	34,34,34	0.39	0	43,45,45	1.06	2 (4%)
13	LHG	A	849	-	42,42,48	0.69	1 (2%)	45,48,54	1.23	5 (11%)
19	BCR	j	4013	-	41,41,41	0.86	0	56,56,56	1.26	7 (12%)
14	LMG	G	848	-	43,43,55	0.86	0	51,51,63	1.27	7 (13%)
15	CL0	H	1011	-	58,73,73	1.88	8 (13%)	60,113,113	1.61	11 (18%)
16	CLA	G	1236	-	54,58,73	1.10	4 (7%)	64,95,113	1.14	3 (4%)
16	CLA	b	1209	-	49,53,73	1.17	4 (8%)	58,89,113	1.10	3 (5%)
19	BCR	G	4017	-	41,41,41	0.87	0	56,56,56	1.18	6 (10%)
16	CLA	s	503	-	50,54,73	1.16	6 (12%)	59,90,113	1.25	5 (8%)
16	CLA	B	1207	-	69,73,73	0.99	5 (7%)	82,113,113	1.18	6 (7%)
16	CLA	n	502	-	54,58,73	1.12	6 (11%)	64,95,113	1.13	3 (4%)
19	BCR	r	602	-	41,41,41	0.86	0	56,56,56	1.24	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	u	510	-	64,68,73	1.04	4 (6%)	76,107,113	0.95	5 (6%)
20	LMT	A	4202	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	0
16	CLA	a	1237	25	69,73,73	0.99	4 (5%)	82,113,113	1.12	6 (7%)
16	CLA	B	1235	-	66,70,73	1.03	5 (7%)	78,109,113	1.19	9 (11%)
16	CLA	A	1116	-	58,62,73	1.04	5 (8%)	68,99,113	1.20	7 (10%)
16	CLA	y	517	-	59,63,73	1.11	5 (8%)	70,101,113	1.26	6 (8%)
13	LHG	o	605	-	26,26,48	0.85	0	29,32,54	1.27	2 (6%)
16	CLA	w	510	-	64,68,73	1.04	3 (4%)	76,107,113	0.98	2 (2%)
16	CLA	A	1117	-	69,73,73	0.99	5 (7%)	82,113,113	1.14	4 (4%)
16	CLA	A	1104	-	69,73,73	0.99	5 (7%)	82,113,113	0.98	6 (7%)
21	ECH	i	4020	-	42,42,42	0.84	1 (2%)	55,58,58	1.84	10 (18%)
16	CLA	y	515	-	69,73,73	1.01	4 (5%)	82,113,113	1.14	8 (9%)
19	BCR	J	4015	-	41,41,41	0.87	0	56,56,56	1.26	9 (16%)
19	BCR	k	4005	-	41,41,41	0.85	0	56,56,56	1.26	5 (8%)
16	CLA	Z	511	-	69,73,73	0.99	5 (7%)	82,113,113	1.08	4 (4%)
16	CLA	A	1237	25	69,73,73	0.99	4 (5%)	82,113,113	1.10	6 (7%)
16	CLA	Y	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.04	5 (7%)
16	CLA	G	1216	25	51,55,73	1.13	5 (9%)	60,91,113	1.33	4 (6%)
14	LMG	H	4101	-	46,46,55	0.91	1 (2%)	54,54,63	1.23	4 (7%)
14	LMG	a	4101	-	46,46,55	0.90	2 (4%)	54,54,63	1.22	4 (7%)
19	BCR	p	601	-	41,41,41	0.87	0	56,56,56	1.32	8 (14%)
16	CLA	H	1136	-	69,73,73	0.98	5 (7%)	82,113,113	0.99	3 (3%)
16	CLA	Z	504	-	69,73,73	1.01	6 (8%)	82,113,113	1.09	6 (7%)
16	CLA	u	503	-	50,54,73	1.15	4 (8%)	59,90,113	1.06	3 (5%)
16	CLA	x	505	-	69,73,73	0.99	5 (7%)	82,113,113	1.23	6 (7%)
16	CLA	v	507	12	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
23	LMU	g	606	-	36,36,36	0.86	0	47,47,47	1.32	5 (10%)
16	CLA	l	1501	10	64,68,73	1.03	5 (7%)	76,107,113	0.99	4 (5%)
14	LMG	B	848	-	43,43,55	0.87	1 (2%)	51,51,63	1.28	6 (11%)
16	CLA	b	1023	-	69,73,73	1.01	7 (10%)	82,113,113	1.12	5 (6%)
14	LMG	a	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.24	4 (8%)
19	BCR	q	603	-	41,41,41	0.84	0	56,56,56	1.16	5 (8%)
16	CLA	h	503	-	50,54,73	1.18	5 (10%)	59,90,113	1.26	6 (10%)
19	BCR	h	603	-	41,41,41	0.83	0	56,56,56	1.19	4 (7%)
16	CLA	B	1232	-	49,53,73	1.18	5 (10%)	58,89,113	1.30	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	LMU	s	606	-	36,36,36	0.83	0	47,47,47	1.27	4 (8%)
16	CLA	U	1501	10	64,68,73	1.03	5 (7%)	76,107,113	1.01	4 (5%)
16	CLA	X	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.16	4 (6%)
16	CLA	b	1204	-	69,73,73	0.97	4 (5%)	82,113,113	0.98	3 (3%)
16	CLA	v	515	-	69,73,73	1.02	4 (5%)	82,113,113	1.18	7 (8%)
16	CLA	H	1138	-	69,73,73	0.99	5 (7%)	82,113,113	1.07	4 (4%)
16	CLA	G	1023	-	69,73,73	1.02	8 (11%)	82,113,113	1.13	8 (9%)
16	CLA	U	1502	-	64,68,73	1.01	5 (7%)	76,107,113	1.14	5 (6%)
16	CLA	G	1208	-	49,53,73	1.16	4 (8%)	58,89,113	1.22	6 (10%)
16	CLA	n	517	12	59,63,73	1.08	5 (8%)	70,101,113	1.02	3 (4%)
16	CLA	b	1203	-	69,73,73	1.00	5 (7%)	82,113,113	1.08	6 (7%)
18	SF4	C	102	-	0,12,12	-	-	-		
16	CLA	H	1124	-	64,68,73	1.02	5 (7%)	76,107,113	0.98	3 (3%)
16	CLA	v	517	-	59,63,73	1.11	5 (8%)	70,101,113	1.03	6 (8%)
16	CLA	a	1131	-	69,73,73	1.01	6 (8%)	82,113,113	1.13	3 (3%)
19	BCR	w	604	-	41,41,41	0.87	0	56,56,56	1.27	6 (10%)
16	CLA	H	1125	-	69,73,73	0.98	4 (5%)	82,113,113	0.99	2 (2%)
16	CLA	a	1801	13	50,54,73	1.16	4 (8%)	59,90,113	1.20	4 (6%)
16	CLA	Y	502	-	54,58,73	1.11	4 (7%)	64,95,113	1.03	4 (6%)
19	BCR	A	4002	-	41,41,41	0.84	0	56,56,56	1.15	3 (5%)
16	CLA	x	516	-	50,54,73	1.14	4 (8%)	59,90,113	1.18	5 (8%)
16	CLA	w	509	-	69,73,73	1.00	5 (7%)	82,113,113	1.02	5 (6%)
16	CLA	B	1216	25	51,55,73	1.17	6 (11%)	60,91,113	1.15	4 (6%)
19	BCR	o	603	-	41,41,41	0.87	0	56,56,56	1.31	8 (14%)
16	CLA	a	1109	16	69,73,73	0.98	4 (5%)	82,113,113	1.16	6 (7%)
16	CLA	F	1302	6	50,54,73	1.17	5 (10%)	59,90,113	1.05	3 (5%)
16	CLA	n	515	-	69,73,73	1.00	4 (5%)	82,113,113	1.07	5 (6%)
16	CLA	x	501	-	54,58,73	1.12	5 (9%)	64,95,113	1.34	7 (10%)
16	CLA	o	515	-	69,73,73	0.98	4 (5%)	82,113,113	1.07	6 (7%)
16	CLA	t	514	-	54,58,73	1.12	4 (7%)	64,95,113	1.12	5 (7%)
13	LHG	H	849	-	42,42,48	0.68	0	45,48,54	1.21	4 (8%)
16	CLA	Z	506	-	64,68,73	1.02	3 (4%)	76,107,113	1.03	2 (2%)
19	BCR	G	4014	-	41,41,41	0.90	1 (2%)	56,56,56	1.29	8 (14%)
16	CLA	a	1129	-	50,54,73	1.11	5 (10%)	59,90,113	1.13	5 (8%)
23	LMU	p	606	-	36,36,36	0.83	0	47,47,47	1.33	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	LHG	u	605	-	26,26,48	0.83	0	29,32,54	1.27	2 (6%)
16	CLA	p	514	-	54,58,73	1.13	5 (9%)	64,95,113	1.10	4 (6%)
16	CLA	t	517	12	59,63,73	1.09	5 (8%)	70,101,113	1.00	3 (4%)
19	BCR	b	4005	-	41,41,41	0.85	0	56,56,56	1.15	5 (8%)
14	LMG	a	4201	-	32,32,55	0.98	1 (3%)	40,40,63	1.17	3 (7%)
16	CLA	y	503	-	50,54,73	1.18	6 (12%)	59,90,113	1.21	6 (10%)
16	CLA	s	501	-	54,58,73	1.11	5 (9%)	64,95,113	1.19	6 (9%)
16	CLA	H	1116	-	58,62,73	1.05	5 (8%)	68,99,113	1.08	5 (7%)
16	CLA	J	1302	8	49,53,73	1.19	5 (10%)	58,89,113	1.26	6 (10%)
13	LHG	g	605	-	30,30,48	0.80	2 (6%)	33,36,54	1.26	3 (9%)
16	CLA	W	515	-	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
16	CLA	a	1104	-	69,73,73	1.00	6 (8%)	82,113,113	1.03	4 (4%)
16	CLA	a	1130	-	64,68,73	1.04	5 (7%)	76,107,113	1.01	6 (7%)
16	CLA	H	1107	1	54,58,73	1.11	4 (7%)	64,95,113	1.07	6 (9%)
19	BCR	b	4010	-	41,41,41	0.91	0	56,56,56	1.33	7 (12%)
16	CLA	B	1228	-	59,63,73	1.08	4 (6%)	70,101,113	1.09	4 (5%)
16	CLA	B	1236	-	54,58,73	1.11	6 (11%)	64,95,113	1.14	4 (6%)
16	CLA	Z	516	-	50,54,73	1.13	4 (8%)	59,90,113	1.07	4 (6%)
19	BCR	B	4017	-	41,41,41	0.88	0	56,56,56	1.22	6 (10%)
16	CLA	H	1131	-	69,73,73	1.01	4 (5%)	82,113,113	1.11	4 (4%)
19	BCR	Y	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	B	1211	-	69,73,73	0.98	6 (8%)	82,113,113	1.02	5 (6%)
19	BCR	K	4001	-	41,41,41	0.86	0	56,56,56	1.31	7 (12%)
19	BCR	n	601	-	41,41,41	0.85	0	56,56,56	1.25	6 (10%)
16	CLA	a	1117	-	69,73,73	0.98	5 (7%)	82,113,113	1.14	6 (7%)
16	CLA	t	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.00	4 (5%)
16	CLA	u	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.03	4 (5%)
17	PQN	B	2002	-	34,34,34	0.36	0	43,45,45	1.04	2 (4%)
16	CLA	K	4003	9	49,53,73	1.20	4 (8%)	58,89,113	1.14	4 (6%)
16	CLA	r	507	-	69,73,73	1.00	5 (7%)	82,113,113	0.95	3 (3%)
16	CLA	A	1140	-	69,73,73	0.98	5 (7%)	82,113,113	1.12	5 (6%)
16	CLA	Q	1301	25	49,53,73	1.17	4 (8%)	58,89,113	1.13	4 (6%)
21	ECH	M	4021	-	42,42,42	0.86	0	55,58,58	1.53	9 (16%)
16	CLA	b	1213	-	59,63,73	1.08	6 (10%)	70,101,113	1.09	6 (8%)
19	BCR	r	601	-	41,41,41	0.86	1 (2%)	56,56,56	1.28	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	a	1132	-	69,73,73	0.99	6 (8%)	82,113,113	1.20	5 (6%)
19	BCR	u	602	-	41,41,41	0.88	0	56,56,56	1.36	6 (10%)
23	LMU	x	606	-	36,36,36	0.88	0	47,47,47	1.26	6 (12%)
19	BCR	R	4018	-	41,41,41	0.85	0	56,56,56	1.20	7 (12%)
19	BCR	j	4015	-	41,41,41	0.88	0	56,56,56	1.22	7 (12%)
19	BCR	Z	604	-	41,41,41	0.87	0	56,56,56	1.24	6 (10%)
16	CLA	y	513	-	50,54,73	1.16	4 (8%)	59,90,113	1.01	3 (5%)
16	CLA	q	508	12	59,63,73	1.06	4 (6%)	70,101,113	1.15	5 (7%)
16	CLA	W	510	-	69,73,73	1.01	3 (4%)	82,113,113	1.01	5 (6%)
19	BCR	Z	602	-	41,41,41	0.87	0	56,56,56	1.36	8 (14%)
16	CLA	X	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.97	4 (5%)
16	CLA	a	1128	-	69,73,73	0.97	6 (8%)	82,113,113	1.10	6 (7%)
13	LHG	p	605	-	31,31,48	0.77	1 (3%)	34,37,54	1.29	4 (11%)
16	CLA	x	517	12	59,63,73	1.09	4 (6%)	70,101,113	0.96	2 (2%)
19	BCR	H	4008	-	41,41,41	0.90	1 (2%)	56,56,56	1.37	4 (7%)
19	BCR	b	4009	-	30,30,41	0.85	0	39,39,56	1.35	6 (15%)
20	LMT	a	4202	-	36,36,36	1.17	5 (13%)	47,47,47	0.93	0
16	CLA	a	1111	-	59,63,73	1.09	5 (8%)	70,101,113	1.03	2 (2%)
16	CLA	v	506	-	64,68,73	1.05	5 (7%)	76,107,113	1.33	7 (9%)
16	CLA	a	1113	-	49,53,73	1.21	7 (14%)	58,89,113	1.15	2 (3%)
16	CLA	r	503	-	50,54,73	1.15	5 (10%)	59,90,113	1.13	4 (6%)
16	CLA	u	507	12	69,73,73	1.00	4 (5%)	82,113,113	1.05	6 (7%)
17	PQN	A	2001	-	34,34,34	0.37	0	43,45,45	1.08	2 (4%)
16	CLA	b	1223	-	69,73,73	0.99	4 (5%)	82,113,113	1.09	1 (1%)
19	BCR	l	4019	-	41,41,41	0.88	0	56,56,56	1.44	8 (14%)
16	CLA	G	1240	13	50,54,73	1.18	5 (10%)	59,90,113	1.30	6 (10%)
16	CLA	h	513	-	50,54,73	1.17	4 (8%)	59,90,113	0.99	4 (6%)
16	CLA	G	1205	-	69,73,73	0.99	5 (7%)	82,113,113	1.09	4 (4%)
16	CLA	v	513	-	50,54,73	1.17	4 (8%)	59,90,113	1.01	3 (5%)
19	BCR	G	4009	-	30,30,41	0.84	0	39,39,56	1.32	5 (12%)
16	CLA	H	1112	-	49,53,73	1.19	4 (8%)	58,89,113	0.99	3 (5%)
16	CLA	w	515	-	69,73,73	0.99	5 (7%)	82,113,113	1.12	4 (4%)
16	CLA	o	511	-	69,73,73	0.98	4 (5%)	82,113,113	1.03	5 (6%)
16	CLA	p	508	12	59,63,73	1.07	4 (6%)	70,101,113	1.02	4 (5%)
16	CLA	b	1226	-	64,68,73	1.04	6 (9%)	76,107,113	1.08	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	G	1223	-	69,73,73	0.98	4 (5%)	82,113,113	1.09	4 (4%)
16	CLA	o	506	-	64,68,73	1.04	5 (7%)	76,107,113	1.06	4 (5%)
13	LHG	H	851	16	25,25,48	0.88	1 (4%)	28,31,54	1.27	2 (7%)
16	CLA	H	1132	-	69,73,73	0.99	6 (8%)	82,113,113	1.11	5 (6%)
16	CLA	u	504	-	64,68,73	1.06	6 (9%)	76,107,113	1.05	4 (5%)
16	CLA	v	510	-	69,73,73	1.02	4 (5%)	82,113,113	1.01	7 (8%)
16	CLA	G	1204	-	69,73,73	0.98	4 (5%)	82,113,113	0.98	3 (3%)
16	CLA	t	506	-	64,68,73	1.04	5 (7%)	76,107,113	1.07	5 (6%)
16	CLA	B	1213	-	59,63,73	1.07	6 (10%)	70,101,113	1.08	4 (5%)
13	LHG	b	4018	16	37,37,48	0.71	0	40,43,54	1.31	5 (12%)
16	CLA	s	502	-	54,58,73	1.10	5 (9%)	64,95,113	1.09	3 (4%)
16	CLA	u	506	-	64,68,73	1.08	6 (9%)	76,107,113	1.64	12 (15%)
19	BCR	s	603	-	41,41,41	0.86	0	56,56,56	1.18	6 (10%)
16	CLA	r	509	-	69,73,73	1.01	5 (7%)	82,113,113	1.03	5 (6%)
16	CLA	A	1111	-	59,63,73	1.08	6 (10%)	70,101,113	1.20	5 (7%)
16	CLA	n	513	-	50,54,73	1.16	5 (10%)	59,90,113	1.05	4 (6%)
16	CLA	h	508	-	59,63,73	1.07	4 (6%)	70,101,113	1.15	6 (8%)
16	CLA	y	506	-	64,68,73	1.04	4 (6%)	76,107,113	1.40	9 (11%)
16	CLA	W	509	-	64,68,73	1.04	4 (6%)	76,107,113	1.08	5 (6%)
16	CLA	g	508	12	59,63,73	1.07	4 (6%)	70,101,113	0.98	3 (4%)
16	CLA	r	512	12	69,73,73	1.00	6 (8%)	82,113,113	1.20	4 (4%)
16	CLA	G	1207	-	69,73,73	1.00	4 (5%)	82,113,113	1.15	5 (6%)
16	CLA	r	502	-	54,58,73	1.11	5 (9%)	64,95,113	1.07	3 (4%)
16	CLA	t	509	-	64,68,73	1.06	5 (7%)	76,107,113	1.15	6 (7%)
16	CLA	u	509	-	64,68,73	1.03	5 (7%)	76,107,113	1.07	6 (7%)
16	CLA	n	508	12	59,63,73	1.07	5 (8%)	70,101,113	0.99	2 (2%)
14	LMG	A	852	-	38,38,55	0.94	1 (2%)	46,46,63	1.23	4 (8%)
16	CLA	a	1102	16	60,64,73	1.06	5 (8%)	71,102,113	1.05	3 (4%)
16	CLA	Y	510	-	69,73,73	1.00	4 (5%)	82,113,113	1.02	5 (6%)
16	CLA	o	516	-	50,54,73	1.14	5 (10%)	59,90,113	1.05	2 (3%)
19	BCR	a	4008	-	41,41,41	0.91	1 (2%)	56,56,56	1.35	6 (10%)
16	CLA	G	1235	-	66,70,73	1.02	5 (7%)	78,109,113	1.19	10 (12%)
16	CLA	b	1214	-	59,63,73	1.06	5 (8%)	70,101,113	1.03	4 (5%)
16	CLA	B	1208	-	49,53,73	1.16	4 (8%)	58,89,113	1.16	6 (10%)
16	CLA	X	507	12	69,73,73	1.00	4 (5%)	82,113,113	0.95	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	CLA	H	1114	-	50,54,73	1.13	5 (10%)	59,90,113	1.27	7 (11%)
19	BCR	g	602	-	41,41,41	0.86	0	56,56,56	1.28	7 (12%)
16	CLA	s	514	-	54,58,73	1.12	5 (9%)	64,95,113	1.22	5 (7%)
16	CLA	r	517	12	59,63,73	1.09	4 (6%)	70,101,113	1.01	3 (4%)
16	CLA	t	512	12	69,73,73	1.01	6 (8%)	82,113,113	1.13	5 (6%)
16	CLA	u	512	12	69,73,73	0.98	6 (8%)	82,113,113	1.02	2 (2%)
16	CLA	W	513	-	50,54,73	1.16	5 (10%)	59,90,113	1.14	6 (10%)
19	BCR	s	604	-	41,41,41	0.87	0	56,56,56	1.22	5 (8%)
16	CLA	H	1127	-	69,73,73	1.00	6 (8%)	82,113,113	1.11	5 (6%)
16	CLA	u	502	-	54,58,73	1.12	6 (11%)	64,95,113	1.12	3 (4%)
13	LHG	Y	605	-	31,31,48	0.78	1 (3%)	34,37,54	1.29	4 (11%)
16	CLA	A	1120	-	53,57,73	1.10	4 (7%)	61,93,113	1.12	5 (8%)
16	CLA	B	1204	-	69,73,73	0.97	4 (5%)	82,113,113	0.94	3 (3%)
16	CLA	w	513	-	54,58,73	1.13	4 (7%)	64,95,113	1.15	6 (9%)
19	BCR	X	601	-	41,41,41	0.87	1 (2%)	56,56,56	1.33	6 (10%)
19	BCR	Z	603	-	41,41,41	0.84	0	56,56,56	1.17	4 (7%)
16	CLA	A	1801	13	50,54,73	1.14	4 (8%)	59,90,113	1.22	5 (8%)
16	CLA	X	502	-	54,58,73	1.11	6 (11%)	64,95,113	1.04	3 (4%)
16	CLA	r	508	12	59,63,73	1.08	4 (6%)	70,101,113	1.01	3 (4%)
20	LMT	U	4101	-	36,36,36	1.16	6 (16%)	47,47,47	1.09	1 (2%)
16	CLA	Z	505	-	69,73,73	1.01	5 (7%)	82,113,113	1.03	6 (7%)
16	CLA	G	1214	-	59,63,73	1.06	6 (10%)	70,101,113	1.11	5 (7%)
16	CLA	a	1124	25	64,68,73	1.03	4 (6%)	76,107,113	0.99	2 (2%)
16	CLA	a	1137	-	51,55,73	1.13	4 (7%)	60,91,113	1.14	5 (8%)
16	CLA	p	503	-	50,54,73	1.14	6 (12%)	59,90,113	1.17	6 (10%)
16	CLA	Q	1302	6	50,54,73	1.16	5 (10%)	59,90,113	1.07	4 (6%)
16	CLA	A	1130	-	64,68,73	1.03	5 (7%)	76,107,113	0.94	4 (5%)
16	CLA	t	511	-	69,73,73	1.00	4 (5%)	82,113,113	1.04	5 (6%)
19	BCR	x	602	-	41,41,41	0.86	0	56,56,56	1.29	7 (12%)

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
16	CLA	a	1122	-	-	10/32/108/115	-
13	LHG	B	4018	16	-	17/42/42/53	-
16	CLA	a	1133	-	-	8/26/102/115	-
14	LMG	A	4201	-	-	13/27/47/70	0/1/1/1
16	CLA	B	1021	-	1/1/15/20	13/39/115/115	-
16	CLA	h	506	-	1/1/14/20	11/33/109/115	-
16	CLA	q	505	-	1/1/15/20	13/39/115/115	-
16	CLA	p	509	-	1/1/14/20	20/33/109/115	-
16	CLA	B	1240	13	1/1/11/20	6/17/93/115	-
16	CLA	B	1205	-	1/1/15/20	10/39/115/115	-
16	CLA	G	1202	-	1/1/15/20	18/39/115/115	-
16	CLA	W	506	-	-	11/33/109/115	-
16	CLA	b	1238	25	1/1/15/20	18/39/115/115	-
16	CLA	s	511	-	1/1/15/20	14/39/115/115	-
19	BCR	x	603	-	-	14/29/63/63	0/2/2/2
19	BCR	x	601	-	-	11/29/63/63	0/2/2/2
18	SF4	a	3001	-	-	-	0/6/5/5
16	CLA	G	1206	2	1/1/15/20	12/39/115/115	-
23	LMU	w	605	-	-	5/21/61/61	0/2/2/2
16	CLA	q	511	-	-	5/39/115/115	-
16	CLA	p	512	12	1/1/15/20	10/39/115/115	-
16	CLA	A	1108	-	-	3/15/91/115	-
16	CLA	b	1215	-	-	6/33/109/115	-
16	CLA	h	509	-	1/1/15/20	18/39/115/115	-
16	CLA	X	514	-	1/1/12/20	4/21/97/115	-
16	CLA	p	502	-	1/1/12/20	5/21/97/115	-
16	CLA	s	508	12	1/1/13/20	10/27/103/115	-
16	CLA	X	509	-	1/1/14/20	13/33/109/115	-
16	CLA	b	1228	-	1/1/13/20	12/27/103/115	-
16	CLA	B	1234	-	1/1/12/20	5/21/97/115	-
16	CLA	y	505	-	1/1/15/20	9/39/115/115	-
16	CLA	a	1126	-	1/1/15/20	11/39/115/115	-
16	CLA	p	513	-	-	8/17/93/115	-
16	CLA	g	509	-	1/1/15/20	8/39/115/115	-
16	CLA	n	510	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	1101	-	1/1/15/20	17/39/115/115	-
19	BCR	T	4001	-	-	12/29/63/63	0/2/2/2
14	LMG	H	852	-	-	6/33/53/70	0/1/1/1
17	PQN	b	2002	-	-	8/23/43/43	0/2/2/2
16	CLA	o	510	-	-	5/33/109/115	-
16	CLA	T	4003	9	1/1/11/20	9/15/91/115	-
19	BCR	H	4007	-	-	8/29/63/63	0/2/2/2
19	BCR	y	604	-	-	11/29/63/63	0/2/2/2
16	CLA	a	1119	-	1/1/15/20	8/39/115/115	-
16	CLA	t	504	-	1/1/14/20	6/33/109/115	-
19	BCR	I	4018	-	-	11/29/63/63	0/2/2/2
16	CLA	n	516	-	-	8/17/93/115	-
16	CLA	W	516	-	-	7/17/93/115	-
16	CLA	q	504	-	1/1/15/20	14/39/115/115	-
16	CLA	G	1228	-	1/1/13/20	15/27/103/115	-
16	CLA	a	1125	-	-	10/39/115/115	-
16	CLA	H	1122	-	-	9/32/108/115	-
16	CLA	o	501	-	-	9/17/93/115	-
19	BCR	x	604	-	-	12/29/63/63	0/2/2/2
16	CLA	H	1120	-	-	9/20/96/115	-
16	CLA	r	510	-	-	12/39/115/115	-
16	CLA	v	505	-	-	13/39/115/115	-
16	CLA	X	517	12	-	7/27/103/115	-
16	CLA	y	516	-	1/1/11/20	7/17/93/115	-
17	PQN	G	2002	-	-	10/23/43/43	0/2/2/2
16	CLA	A	1114	-	1/1/11/20	9/17/93/115	-
16	CLA	B	1206	2	1/1/15/20	17/39/115/115	-
16	CLA	Y	503	-	1/1/11/20	7/17/93/115	-
19	BCR	k	4001	-	-	12/29/63/63	0/2/2/2
16	CLA	n	503	-	1/1/11/20	8/17/93/115	-
16	CLA	y	502	-	1/1/12/20	5/21/97/115	-
16	CLA	Z	501	-	1/1/12/20	7/21/97/115	-
16	CLA	x	502	-	1/1/12/20	5/21/97/115	-
19	BCR	y	601	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	G	1012	25	1/1/13/20	7/27/103/115	-
16	CLA	v	511	-	1/1/15/20	11/39/115/115	-
16	CLA	A	1127	-	1/1/15/20	5/39/115/115	-
16	CLA	f	1302	6	1/1/11/20	8/17/93/115	-
16	CLA	b	1202	-	1/1/15/20	16/39/115/115	-
16	CLA	A	1121	-	1/1/12/20	8/23/99/115	-
16	CLA	v	501	-	-	6/17/93/115	-
21	ECH	I	4020	-	-	11/29/66/66	0/2/2/2
16	CLA	o	505	-	1/1/15/20	16/39/115/115	-
16	CLA	b	1205	-	1/1/15/20	12/39/115/115	-
19	BCR	v	604	-	-	12/29/63/63	0/2/2/2
16	CLA	L	1502	-	-	9/33/109/115	-
13	LHG	s	605	-	-	12/36/36/53	-
19	BCR	L	4019	-	-	13/29/63/63	0/2/2/2
16	CLA	b	1212	-	1/1/11/20	4/15/91/115	-
19	BCR	w	602	-	-	11/29/63/63	0/2/2/2
16	CLA	n	509	-	1/1/14/20	9/33/109/115	-
19	BCR	q	602	-	-	12/29/63/63	0/2/2/2
16	CLA	G	1211	-	-	22/39/115/115	-
19	BCR	b	4014	-	-	15/29/63/63	0/2/2/2
16	CLA	G	1201	-	1/1/12/20	4/26/102/115	-
16	CLA	o	512	12	1/1/15/20	8/39/115/115	-
19	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
19	BCR	A	4003	-	-	9/29/63/63	0/2/2/2
16	CLA	A	1122	-	1/1/13/20	9/32/108/115	-
16	CLA	A	1123	25	-	8/39/115/115	-
16	CLA	H	1115	-	-	10/26/102/115	-
14	LMG	A	4101	-	-	24/41/61/70	0/1/1/1
16	CLA	a	1103	-	1/1/15/20	12/39/115/115	-
16	CLA	H	1118	-	-	13/27/103/115	-
16	CLA	G	1229	-	1/1/13/20	10/31/107/115	-
16	CLA	y	501	-	1/1/11/20	8/17/93/115	-
16	CLA	w	505	-	-	9/39/115/115	-
16	CLA	a	1138	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	1102	16	1/1/13/20	6/29/105/115	-
16	CLA	H	1106	1	1/1/15/20	16/39/115/115	-
16	CLA	B	1202	-	1/1/15/20	16/39/115/115	-
16	CLA	r	514	-	1/1/12/20	10/21/97/115	-
16	CLA	b	1012	25	1/1/13/20	10/27/103/115	-
16	CLA	b	1021	-	1/1/15/20	17/39/115/115	-
16	CLA	b	1207	-	-	14/39/115/115	-
16	CLA	o	504	-	-	10/33/109/115	-
16	CLA	B	1224	-	1/1/14/20	10/33/109/115	-
16	CLA	G	1239	-	1/1/15/20	15/39/115/115	-
16	CLA	A	1103	-	1/1/15/20	10/39/115/115	-
16	CLA	A	1136	-	1/1/15/20	7/39/115/115	-
16	CLA	q	509	-	1/1/15/20	12/39/115/115	-
16	CLA	b	1211	-	1/1/15/20	13/39/115/115	-
16	CLA	b	1208	-	1/1/11/20	8/15/91/115	-
16	CLA	h	514	-	-	6/21/97/115	-
16	CLA	a	1114	-	1/1/11/20	10/17/93/115	-
16	CLA	B	1201	-	1/1/12/20	4/26/102/115	-
16	CLA	q	506	-	1/1/14/20	12/33/109/115	-
17	PQN	H	2001	-	-	3/23/43/43	0/2/2/2
16	CLA	S	1302	8	1/1/11/20	7/15/91/115	-
19	BCR	g	604	-	-	16/29/63/63	0/2/2/2
16	CLA	W	501	-	1/1/12/20	8/21/97/115	-
16	CLA	a	1110	-	1/1/12/20	9/26/102/115	-
16	CLA	k	4004	-	1/1/13/20	6/27/103/115	-
16	CLA	t	515	-	1/1/15/20	15/39/115/115	-
16	CLA	w	516	-	1/1/11/20	10/17/93/115	-
16	CLA	u	515	-	-	17/39/115/115	-
16	CLA	H	1237	25	1/1/15/20	11/39/115/115	-
16	CLA	X	510	-	-	8/33/109/115	-
16	CLA	A	1109	16	1/1/15/20	9/39/115/115	-
19	BCR	f	4016	-	-	11/29/63/63	0/2/2/2
20	LMT	L	4101	-	-	9/21/61/61	0/2/2/2
16	CLA	Y	509	-	1/1/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	1229	-	1/1/13/20	9/31/107/115	-
16	CLA	H	1121	-	1/1/12/20	8/23/99/115	-
14	LMG	F	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	Y	506	-	-	14/33/109/115	-
19	BCR	S	4012	-	-	10/29/63/63	0/2/2/2
16	CLA	x	508	12	1/1/13/20	12/27/103/115	-
16	CLA	q	517	12	-	11/27/103/115	-
16	CLA	n	507	-	1/1/15/20	11/39/115/115	-
24	LUT	Z	601	-	-	7/29/67/67	0/2/2/2
16	CLA	S	1303	-	-	2/4/76/115	-
19	BCR	K	4005	-	-	9/29/63/63	0/2/2/2
19	BCR	o	602	-	-	14/29/63/63	0/2/2/2
24	LUT	q	601	-	-	7/29/67/67	0/2/2/2
16	CLA	s	512	12	1/1/15/20	8/39/115/115	-
16	CLA	q	515	-	1/1/15/20	12/39/115/115	-
16	CLA	B	1239	-	-	14/39/115/115	-
16	CLA	W	505	-	1/1/15/20	20/39/115/115	-
16	CLA	A	1106	1	1/1/15/20	15/39/115/115	-
16	CLA	Y	513	-	-	10/17/93/115	-
16	CLA	T	4002	-	1/1/11/20	7/15/91/115	-
16	CLA	B	1012	25	1/1/13/20	11/27/103/115	-
13	LHG	R	103	-	-	23/44/44/53	-
16	CLA	G	1213	-	1/1/13/20	8/27/103/115	-
13	LHG	a	849	-	-	17/47/47/53	-
16	CLA	s	504	-	1/1/15/20	16/39/115/115	-
16	CLA	H	1135	-	-	4/23/99/115	-
19	BCR	H	4003	-	-	10/29/63/63	0/2/2/2
16	CLA	Y	517	12	-	10/27/103/115	-
16	CLA	b	1225	-	-	12/39/115/115	-
18	SF4	H	3001	-	-	-	0/6/5/5
16	CLA	J	1303	-	-	2/4/76/115	-
16	CLA	H	1123	-	-	10/39/115/115	-
16	CLA	t	510	-	-	9/39/115/115	-
20	LMT	H	4202	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	1113	-	1/1/11/20	7/15/91/115	-
16	CLA	b	1224	-	1/1/14/20	9/33/109/115	-
16	CLA	Y	515	-	1/1/15/20	8/39/115/115	-
16	CLA	w	511	-	1/1/15/20	9/39/115/115	-
16	CLA	B	1238	25	1/1/15/20	9/39/115/115	-
16	CLA	a	1135	-	1/1/12/20	3/23/99/115	-
19	BCR	a	4002	-	-	12/29/63/63	0/2/2/2
16	CLA	B	1219	-	-	4/15/91/115	-
13	LHG	G	4018	16	-	12/42/42/53	-
16	CLA	G	1224	-	1/1/14/20	12/33/109/115	-
16	CLA	a	1121	-	1/1/12/20	6/23/99/115	-
16	CLA	a	1123	-	-	13/39/115/115	-
16	CLA	w	501	-	1/1/12/20	10/21/97/115	-
16	CLA	B	1215	-	1/1/14/20	7/33/109/115	-
16	CLA	a	1105	-	1/1/13/20	7/31/107/115	-
16	CLA	a	1118	-	-	11/27/103/115	-
23	LMU	r	606	-	-	6/21/61/61	0/2/2/2
16	CLA	A	1119	25	1/1/15/20	5/39/115/115	-
16	CLA	p	515	-	1/1/15/20	14/39/115/115	-
16	CLA	p	511	-	1/1/15/20	15/39/115/115	-
16	CLA	q	507	-	1/1/15/20	12/39/115/115	-
16	CLA	B	1225	-	-	11/39/115/115	-
19	BCR	U	4019	-	-	10/29/63/63	0/2/2/2
15	CL0	a	1011	-	2/2/20/25	9/37/135/135	-
16	CLA	a	1022	-	1/1/15/20	8/39/115/115	-
16	CLA	p	504	-	-	16/39/115/115	-
19	BCR	s	601	-	-	12/29/63/63	0/2/2/2
16	CLA	b	1218	-	-	9/27/103/115	-
16	CLA	Z	512	12	1/1/15/20	14/39/115/115	-
16	CLA	j	1302	8	-	7/15/91/115	-
16	CLA	h	515	-	1/1/15/20	17/39/115/115	-
13	LHG	x	605	-	-	20/35/35/53	-
16	CLA	Z	502	-	1/1/12/20	7/21/97/115	-
16	CLA	G	1226	-	-	17/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	l	1502	-	-	9/33/109/115	-
23	LMU	Y	606	-	-	6/21/61/61	0/2/2/2
16	CLA	g	515	-	1/1/15/20	9/39/115/115	-
13	LHG	X	605	-	-	12/31/31/53	-
16	CLA	Y	507	12	-	10/39/115/115	-
16	CLA	x	514	-	1/1/12/20	7/21/97/115	-
16	CLA	x	506	-	-	14/33/109/115	-
16	CLA	h	517	-	1/1/13/20	10/27/103/115	-
16	CLA	h	504	-	-	14/33/109/115	-
16	CLA	X	504	-	-	16/33/109/115	-
16	CLA	A	1135	-	1/1/12/20	3/23/99/115	-
16	CLA	o	517	12	-	11/27/103/115	-
16	CLA	H	1140	-	1/1/15/20	15/39/115/115	-
16	CLA	b	1240	13	1/1/11/20	5/17/93/115	-
16	CLA	b	1230	-	-	7/15/91/115	-
19	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
16	CLA	o	514	-	1/1/12/20	8/21/97/115	-
14	LMG	H	4201	-	-	10/27/47/70	0/1/1/1
16	CLA	q	503	-	1/1/11/20	9/17/93/115	-
16	CLA	L	1503	25	1/1/15/20	11/39/115/115	-
16	CLA	b	1221	25	1/1/15/20	19/39/115/115	-
16	CLA	A	1126	-	1/1/15/20	11/39/115/115	-
16	CLA	b	1220	-	-	13/26/102/115	-
19	BCR	L	4022	-	-	14/29/63/63	0/2/2/2
16	CLA	k	4002	-	1/1/11/20	7/15/91/115	-
16	CLA	x	511	-	-	7/39/115/115	-
16	CLA	H	1133	-	-	10/26/102/115	-
19	BCR	i	4018	-	-	13/29/63/63	0/2/2/2
16	CLA	y	512	12	-	12/39/115/115	-
16	CLA	A	1115	-	1/1/12/20	8/26/102/115	-
16	CLA	A	1128	-	1/1/15/20	20/39/115/115	-
19	BCR	b	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1105	-	1/1/13/20	9/31/107/115	-
16	CLA	G	1231	25	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	r	516	-	1/1/11/20	5/17/93/115	-
16	CLA	t	513	-	-	8/17/93/115	-
16	CLA	u	513	-	-	7/17/93/115	-
19	BCR	J	4013	-	-	9/29/63/63	0/2/2/2
21	ECH	G	4006	-	-	10/29/66/66	0/2/2/2
19	BCR	B	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	G	1210	-	-	16/39/115/115	-
16	CLA	w	514	-	1/1/12/20	8/21/97/115	-
16	CLA	a	1134	1	-	6/15/91/115	-
16	CLA	s	509	-	1/1/14/20	15/33/109/115	-
16	CLA	B	1221	25	-	15/39/115/115	-
16	CLA	w	504	-	1/1/15/20	12/39/115/115	-
19	BCR	g	601	-	-	17/29/63/63	0/2/2/2
16	CLA	B	1230	-	1/1/11/20	7/15/91/115	-
14	LMG	Q	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	X	506	-	1/1/14/20	13/33/109/115	-
16	CLA	a	1101	-	1/1/15/20	19/39/115/115	-
16	CLA	t	516	-	1/1/11/20	9/17/93/115	-
16	CLA	u	516	-	1/1/11/20	9/17/93/115	-
16	CLA	p	517	12	-	10/27/103/115	-
16	CLA	a	1115	-	1/1/12/20	8/26/102/115	-
16	CLA	A	1133	-	1/1/12/20	11/26/102/115	-
16	CLA	q	513	-	-	8/21/97/115	-
16	CLA	g	504	-	1/1/15/20	22/39/115/115	-
16	CLA	a	1120	-	-	8/20/96/115	-
16	CLA	B	1231	25	1/1/11/20	9/15/91/115	-
16	CLA	G	1227	-	-	9/20/96/115	-
16	CLA	a	1112	-	-	6/15/91/115	-
16	CLA	K	4002	-	1/1/11/20	4/15/91/115	-
16	CLA	A	1105	-	1/1/13/20	9/31/107/115	-
16	CLA	X	516	-	-	8/17/93/115	-
16	CLA	A	1118	-	-	11/27/103/115	-
16	CLA	b	1210	-	1/1/15/20	12/39/115/115	-
16	CLA	s	515	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	H	4011	-	-	16/29/63/63	0/2/2/2
16	CLA	p	510	-	-	11/39/115/115	-
19	BCR	y	603	-	-	11/29/63/63	0/2/2/2
19	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	o	503	-	-	5/17/93/115	-
13	LHG	r	605	-	-	17/35/35/53	-
19	BCR	v	601	-	-	11/29/63/63	0/2/2/2
16	CLA	Y	505	-	1/1/15/20	15/39/115/115	-
16	CLA	A	1022	25	1/1/15/20	10/39/115/115	-
19	BCR	p	604	-	-	15/29/63/63	0/2/2/2
16	CLA	q	514	-	1/1/12/20	10/21/97/115	-
19	BCR	p	602	-	-	11/29/63/63	0/2/2/2
16	CLA	h	512	12	-	16/39/115/115	-
16	CLA	r	515	-	1/1/15/20	12/39/115/115	-
18	SF4	c	102	-	-	-	0/6/5/5
16	CLA	W	507	-	-	12/39/115/115	-
16	CLA	A	1129	-	-	6/17/93/115	-
16	CLA	B	1023	-	-	9/39/115/115	-
16	CLA	B	1226	-	-	13/33/109/115	-
16	CLA	b	1229	-	1/1/13/20	9/31/107/115	-
16	CLA	g	512	12	1/1/15/20	10/39/115/115	-
16	CLA	t	507	-	1/1/15/20	11/39/115/115	-
18	SF4	c	101	-	-	-	0/6/5/5
16	CLA	v	512	12	-	12/39/115/115	-
16	CLA	F	1301	25	1/1/11/20	3/15/91/115	-
16	CLA	w	507	-	1/1/15/20	10/39/115/115	-
13	LHG	I	103	-	-	20/44/44/53	-
16	CLA	p	516	-	1/1/11/20	9/17/93/115	-
16	CLA	r	504	-	1/1/15/20	17/39/115/115	-
16	CLA	v	502	-	1/1/12/20	6/21/97/115	-
16	CLA	v	503	-	1/1/11/20	7/17/93/115	-
16	CLA	W	502	-	1/1/12/20	10/21/97/115	-
16	CLA	A	1131	-	-	14/39/115/115	-
16	CLA	o	509	-	1/1/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	f	1301	25	1/1/11/20	4/15/91/115	-
16	CLA	x	504	-	1/1/15/20	21/39/115/115	-
19	BCR	W	601	-	-	16/29/63/63	0/2/2/2
19	BCR	W	603	-	-	13/29/63/63	0/2/2/2
19	BCR	v	603	-	-	12/29/63/63	0/2/2/2
16	CLA	g	513	-	-	11/17/93/115	-
16	CLA	B	1227	-	1/1/11/20	11/20/96/115	-
16	CLA	b	1239	-	-	14/39/115/115	-
18	SF4	C	101	-	-	-	0/6/5/5
16	CLA	y	510	-	-	6/39/115/115	-
16	CLA	x	510	-	-	13/39/115/115	-
19	BCR	l	4022	-	-	18/29/63/63	0/2/2/2
16	CLA	h	516	-	1/1/11/20	8/17/93/115	-
16	CLA	G	1212	-	1/1/11/20	8/15/91/115	-
16	CLA	H	1102	16	1/1/13/20	5/29/105/115	-
16	CLA	u	517	12	-	8/27/103/115	-
16	CLA	W	504	-	1/1/14/20	6/33/109/115	-
16	CLA	X	515	-	1/1/15/20	16/39/115/115	-
16	CLA	Z	508	12	1/1/13/20	9/27/103/115	-
16	CLA	Y	504	-	1/1/15/20	16/39/115/115	-
14	LMG	f	4017	-	-	5/22/42/70	0/1/1/1
16	CLA	g	516	-	1/1/11/20	5/17/93/115	-
16	CLA	B	1210	-	-	14/39/115/115	-
16	CLA	o	513	-	-	5/17/93/115	-
19	BCR	U	4022	-	-	16/29/63/63	0/2/2/2
19	BCR	n	603	-	-	12/29/63/63	0/2/2/2
24	LUT	w	601	-	-	7/29/67/67	0/2/2/2
16	CLA	q	510	-	-	10/33/109/115	-
16	CLA	b	1216	25	1/1/11/20	2/18/94/115	-
19	BCR	S	4013	-	-	10/29/63/63	0/2/2/2
16	CLA	G	1217	-	-	9/15/91/115	-
16	CLA	v	514	-	1/1/12/20	7/21/97/115	-
21	ECH	B	4006	-	-	10/29/66/66	0/2/2/2
16	CLA	H	1013	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	u	604	-	-	17/29/63/63	0/2/2/2
16	CLA	H	1130	-	-	10/33/109/115	-
16	CLA	H	1103	-	1/1/15/20	12/39/115/115	-
16	CLA	s	510	-	-	9/39/115/115	-
16	CLA	W	517	12	1/1/13/20	10/27/103/115	-
16	CLA	G	1021	-	1/1/15/20	14/39/115/115	-
16	CLA	o	508	12	1/1/13/20	14/27/103/115	-
16	CLA	W	514	-	1/1/12/20	8/21/97/115	-
14	LMG	b	848	-	-	19/38/58/70	0/1/1/1
19	BCR	j	4012	-	-	9/29/63/63	0/2/2/2
16	CLA	L	1501	10	-	13/33/109/115	-
16	CLA	H	1108	-	-	5/15/91/115	-
19	BCR	n	604	-	-	13/29/63/63	0/2/2/2
19	BCR	t	603	-	-	11/29/63/63	0/2/2/2
19	BCR	w	603	-	-	13/29/63/63	0/2/2/2
16	CLA	j	1303	-	-	2/4/76/115	-
19	BCR	Y	602	-	-	10/29/63/63	0/2/2/2
16	CLA	Y	501	-	1/1/12/20	6/21/97/115	-
20	LMT	l	4101	-	-	7/21/61/61	0/2/2/2
16	CLA	a	1136	-	1/1/15/20	11/39/115/115	-
16	CLA	t	505	-	-	11/39/115/115	-
16	CLA	u	505	-	1/1/15/20	14/39/115/115	-
16	CLA	x	509	-	1/1/15/20	14/39/115/115	-
16	CLA	y	508	-	1/1/13/20	10/27/103/115	-
19	BCR	p	603	-	-	7/29/63/63	0/2/2/2
16	CLA	b	1234	-	1/1/12/20	4/21/97/115	-
19	BCR	X	602	-	-	17/29/63/63	0/2/2/2
19	BCR	T	4005	-	-	9/29/63/63	0/2/2/2
16	CLA	H	1801	13	1/1/11/20	5/17/93/115	-
16	CLA	B	1217	-	-	7/15/91/115	-
16	CLA	o	507	12	-	13/39/115/115	-
19	BCR	F	4016	-	-	9/29/63/63	0/2/2/2
16	CLA	G	1234	-	1/1/12/20	3/21/97/115	-
16	CLA	x	512	12	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	b	1219	-	-	6/15/91/115	-
16	CLA	T	4004	-	-	4/27/103/115	-
19	BCR	H	4002	-	-	11/29/63/63	0/2/2/2
19	BCR	a	4007	-	-	7/29/63/63	0/2/2/2
15	CL0	A	1011	-	2/2/20/25	10/37/135/135	-
16	CLA	s	513	-	-	9/17/93/115	-
19	BCR	o	601	-	-	8/29/63/63	0/2/2/2
16	CLA	r	506	-	-	12/33/109/115	-
16	CLA	A	1110	-	1/1/12/20	10/26/102/115	-
16	CLA	H	1126	-	1/1/15/20	12/39/115/115	-
16	CLA	X	505	-	1/1/15/20	12/39/115/115	-
19	BCR	t	604	-	-	14/29/63/63	0/2/2/2
16	CLA	u	511	-	1/1/15/20	8/39/115/115	-
16	CLA	v	508	-	1/1/13/20	13/27/103/115	-
16	CLA	W	508	12	1/1/13/20	9/27/103/115	-
18	SF4	N	102	-	-	-	0/6/5/5
19	BCR	S	4015	-	-	10/29/63/63	0/2/2/2
16	CLA	Z	510	-	-	11/33/109/115	-
19	BCR	q	604	-	-	16/29/63/63	0/2/2/2
16	CLA	u	501	-	-	6/17/93/115	-
16	CLA	G	1238	25	1/1/15/20	11/39/115/115	-
16	CLA	x	515	-	1/1/15/20	10/39/115/115	-
16	CLA	r	513	-	-	13/17/93/115	-
16	CLA	G	1219	-	-	6/15/91/115	-
13	LHG	a	851	16	-	9/30/30/53	-
16	CLA	B	1212	-	1/1/11/20	6/15/91/115	-
23	LMU	Z	605	-	-	5/21/61/61	0/2/2/2
16	CLA	w	517	12	1/1/13/20	8/27/103/115	-
16	CLA	G	1215	-	1/1/14/20	8/33/109/115	-
16	CLA	G	1225	-	1/1/15/20	11/39/115/115	-
16	CLA	W	512	12	1/1/14/20	18/33/109/115	-
23	LMU	q	605	-	-	5/21/61/61	0/2/2/2
21	ECH	R	4020	-	-	11/29/66/66	0/2/2/2
16	CLA	p	507	12	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	1101	-	1/1/15/20	15/39/115/115	-
16	CLA	q	516	-	1/1/11/20	11/17/93/115	-
16	CLA	w	512	12	1/1/15/20	11/39/115/115	-
19	BCR	Y	604	-	-	14/29/63/63	0/2/2/2
16	CLA	t	503	-	1/1/11/20	7/17/93/115	-
16	CLA	q	512	12	1/1/15/20	15/39/115/115	-
16	CLA	w	502	-	1/1/12/20	8/21/97/115	-
19	BCR	r	603	-	-	11/29/63/63	0/2/2/2
16	CLA	g	517	12	-	10/27/103/115	-
16	CLA	p	505	-	-	14/39/115/115	-
16	CLA	q	502	-	1/1/12/20	7/21/97/115	-
16	CLA	A	1112	-	-	4/15/91/115	-
19	BCR	B	4014	-	-	16/29/63/63	0/2/2/2
16	CLA	H	1109	16	1/1/15/20	11/39/115/115	-
16	CLA	Z	503	-	1/1/11/20	9/17/93/115	-
16	CLA	Y	512	12	1/1/15/20	9/39/115/115	-
16	CLA	X	513	-	-	9/17/93/115	-
16	CLA	A	1132	-	1/1/15/20	15/39/115/115	-
16	CLA	K	4004	-	1/1/13/20	5/27/103/115	-
16	CLA	H	1129	-	-	6/17/93/115	-
16	CLA	g	503	-	-	9/17/93/115	-
19	BCR	g	603	-	-	15/29/63/63	0/2/2/2
16	CLA	h	505	-	-	6/39/115/115	-
16	CLA	A	1134	1	-	6/15/91/115	-
16	CLA	Y	516	-	-	11/17/93/115	-
21	ECH	V	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	G	1209	-	1/1/11/20	5/15/91/115	-
16	CLA	A	1139	25	1/1/14/20	15/33/109/115	-
16	CLA	a	1127	-	1/1/15/20	4/39/115/115	-
19	BCR	a	4011	-	-	16/29/63/63	0/2/2/2
16	CLA	g	505	-	1/1/15/20	11/39/115/115	-
19	BCR	h	604	-	-	13/29/63/63	0/2/2/2
16	CLA	t	501	-	1/1/12/20	7/21/97/115	-
16	CLA	H	1128	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	w	508	12	1/1/13/20	8/27/103/115	-
18	SF4	N	101	-	-	-	0/6/5/5
16	CLA	A	1013	-	1/1/15/20	14/39/115/115	-
16	CLA	b	1206	2	1/1/15/20	15/39/115/115	-
16	CLA	n	505	-	1/1/15/20	22/39/115/115	-
16	CLA	Z	509	-	1/1/15/20	16/39/115/115	-
16	CLA	x	507	-	1/1/15/20	10/39/115/115	-
19	BCR	u	601	-	-	8/29/63/63	0/2/2/2
16	CLA	o	502	-	1/1/12/20	8/21/97/115	-
16	CLA	g	511	-	1/1/15/20	9/39/115/115	-
16	CLA	p	501	-	1/1/12/20	7/21/97/115	-
19	BCR	G	4010	-	-	17/29/63/63	0/2/2/2
16	CLA	y	504	-	-	12/33/109/115	-
16	CLA	G	1203	-	1/1/15/20	16/39/115/115	-
16	CLA	g	514	-	1/1/12/20	7/21/97/115	-
16	CLA	A	1107	1	-	6/21/97/115	-
16	CLA	l	1503	-	1/1/15/20	12/39/115/115	-
19	BCR	o	604	-	-	18/29/63/63	0/2/2/2
16	CLA	x	503	-	-	8/17/93/115	-
16	CLA	Z	513	-	-	8/21/97/115	-
16	CLA	X	501	-	-	9/17/93/115	-
16	CLA	G	1218	-	-	14/27/103/115	-
19	BCR	Q	4016	-	-	11/29/63/63	0/2/2/2
16	CLA	A	1124	25	1/1/14/20	7/33/109/115	-
16	CLA	W	503	-	1/1/11/20	10/17/93/115	-
19	BCR	G	4004	-	-	11/29/63/63	0/2/2/2
16	CLA	U	1503	-	1/1/15/20	9/39/115/115	-
16	CLA	b	1227	-	1/1/11/20	6/20/96/115	-
16	CLA	a	1107	1	-	8/21/97/115	-
16	CLA	a	1108	-	-	7/15/91/115	-
16	CLA	b	1231	25	1/1/11/20	8/15/91/115	-
16	CLA	w	503	-	1/1/11/20	8/17/93/115	-
16	CLA	Y	511	-	1/1/15/20	14/39/115/115	-
16	CLA	t	502	-	1/1/12/20	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	r	604	-	-	15/29/63/63	0/2/2/2
19	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
16	CLA	s	507	12	-	11/39/115/115	-
16	CLA	Y	514	-	1/1/12/20	7/21/97/115	-
16	CLA	y	511	-	1/1/15/20	11/39/115/115	-
21	ECH	m	4021	-	-	14/29/66/66	0/2/2/2
16	CLA	n	514	-	1/1/12/20	7/21/97/115	-
19	BCR	B	4010	-	-	16/29/63/63	0/2/2/2
16	CLA	H	1110	-	1/1/12/20	9/26/102/115	-
16	CLA	B	1203	-	1/1/15/20	15/39/115/115	-
16	CLA	G	1230	-	1/1/11/20	8/15/91/115	-
16	CLA	y	514	-	-	8/21/97/115	-
19	BCR	Y	603	-	-	8/29/63/63	0/2/2/2
16	CLA	G	1220	-	1/1/12/20	15/26/102/115	-
16	CLA	g	510	-	-	12/39/115/115	-
16	CLA	a	1106	1	1/1/15/20	17/39/115/115	-
16	CLA	k	4003	9	1/1/11/20	5/15/91/115	-
16	CLA	h	511	-	1/1/15/20	15/39/115/115	-
19	BCR	X	603	-	-	12/29/63/63	0/2/2/2
16	CLA	x	513	-	-	10/17/93/115	-
16	CLA	H	1134	1	-	4/15/91/115	-
16	CLA	h	501	-	-	9/17/93/115	-
21	ECH	b	4006	-	-	9/29/66/66	0/2/2/2
19	BCR	a	4003	-	-	12/29/63/63	0/2/2/2
16	CLA	H	1104	-	1/1/15/20	17/39/115/115	-
16	CLA	H	1139	25	1/1/14/20	13/33/109/115	-
16	CLA	W	511	-	1/1/15/20	9/39/115/115	-
16	CLA	a	1139	25	1/1/13/20	6/27/103/115	-
16	CLA	s	505	-	1/1/15/20	13/39/115/115	-
16	CLA	Z	507	-	1/1/15/20	15/39/115/115	-
16	CLA	A	1138	-	1/1/15/20	12/39/115/115	-
16	CLA	G	1221	25	1/1/15/20	18/39/115/115	-
16	CLA	s	506	-	-	11/33/109/115	-
16	CLA	g	501	-	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	h	601	-	-	14/29/63/63	0/2/2/2
16	CLA	H	1111	-	1/1/13/20	8/27/103/115	-
16	CLA	B	1209	-	1/1/11/20	7/15/91/115	-
16	CLA	H	1119	25	1/1/15/20	12/39/115/115	-
16	CLA	H	1113	-	1/1/11/20	1/15/91/115	-
16	CLA	g	507	-	1/1/15/20	9/39/115/115	-
19	BCR	G	4005	-	-	11/29/63/63	0/2/2/2
16	CLA	b	1222	25	-	8/21/97/115	-
16	CLA	X	512	12	-	11/39/115/115	-
16	CLA	r	505	-	-	13/39/115/115	-
16	CLA	v	504	-	1/1/14/20	13/33/109/115	-
19	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
16	CLA	n	511	-	-	7/39/115/115	-
16	CLA	B	1220	-	1/1/12/20	12/25/101/115	-
16	CLA	s	516	-	-	10/17/93/115	-
16	CLA	r	511	-	1/1/15/20	6/39/115/115	-
16	CLA	G	1222	25	-	8/21/97/115	-
19	BCR	W	604	-	-	10/29/63/63	0/2/2/2
16	CLA	h	502	-	1/1/12/20	7/21/97/115	-
16	CLA	G	1232	25	1/1/11/20	6/15/91/115	-
16	CLA	r	501	-	1/1/12/20	6/21/97/115	-
13	LHG	A	851	16	-	7/30/30/53	-
16	CLA	s	517	12	-	9/27/103/115	-
16	CLA	A	1137	-	1/1/11/20	7/18/94/115	-
16	CLA	g	502	-	1/1/12/20	6/21/97/115	-
16	CLA	v	509	-	-	16/39/115/115	-
16	CLA	h	510	-	-	9/39/115/115	-
18	SF4	A	3001	-	-	-	0/6/5/5
16	CLA	y	507	-	-	13/39/115/115	-
16	CLA	p	506	-	-	15/33/109/115	-
16	CLA	a	1013	-	1/1/15/20	12/39/115/115	-
16	CLA	q	501	-	1/1/12/20	7/21/97/115	-
16	CLA	a	1140	-	-	13/39/115/115	-
16	CLA	H	1022	25	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	w	506	-	-	7/33/109/115	-
16	CLA	b	1235	-	1/1/14/20	14/36/112/115	-
16	CLA	B	1218	-	-	9/27/103/115	-
19	BCR	J	4012	-	-	12/29/63/63	0/2/2/2
19	BCR	X	604	-	-	19/29/63/63	0/2/2/2
16	CLA	u	514	-	1/1/12/20	6/21/97/115	-
16	CLA	H	1117	-	1/1/15/20	9/39/115/115	-
16	CLA	b	1201	-	1/1/12/20	4/26/102/115	-
16	CLA	H	1137	-	1/1/11/20	6/18/94/115	-
16	CLA	Z	514	-	1/1/12/20	9/21/97/115	-
16	CLA	h	507	-	1/1/15/20	15/39/115/115	-
16	CLA	n	504	-	-	5/33/109/115	-
16	CLA	b	1217	-	-	3/15/91/115	-
19	BCR	u	603	-	-	9/29/63/63	0/2/2/2
19	BCR	t	601	-	-	14/29/63/63	0/2/2/2
16	CLA	Z	515	-	1/1/15/20	11/39/115/115	-
16	CLA	g	506	-	-	11/33/109/115	-
16	CLA	X	511	-	1/1/15/20	10/39/115/115	-
16	CLA	B	1223	-	1/1/15/20	11/39/115/115	-
16	CLA	A	1125	-	-	11/39/115/115	-
16	CLA	B	1222	25	-	8/21/97/115	-
16	CLA	a	1116	-	1/1/12/20	9/26/102/115	-
16	CLA	n	506	-	-	8/33/109/115	-
16	CLA	b	1232	25	1/1/11/20	8/15/91/115	-
16	CLA	n	512	12	1/1/15/20	19/39/115/115	-
16	CLA	Z	517	12	1/1/13/20	6/27/103/115	-
16	CLA	v	516	-	1/1/11/20	6/17/93/115	-
16	CLA	y	509	-	1/1/15/20	19/39/115/115	-
16	CLA	n	501	-	1/1/12/20	10/21/97/115	-
19	BCR	s	602	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1214	-	1/1/13/20	10/27/103/115	-
16	CLA	b	1236	-	-	7/21/97/115	-
13	LHG	i	103	-	-	22/44/44/53	-
19	BCR	b	4017	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PQN	a	2001	-	-	5/23/43/43	0/2/2/2
13	LHG	A	849	-	-	19/47/47/53	-
19	BCR	j	4013	-	-	11/29/63/63	0/2/2/2
15	CL0	H	1011	-	2/2/20/25	7/37/135/135	-
14	LMG	G	848	-	-	18/38/58/70	0/1/1/1
16	CLA	b	1209	-	1/1/11/20	5/15/91/115	-
16	CLA	G	1236	-	-	7/21/97/115	-
19	BCR	G	4017	-	-	13/29/63/63	0/2/2/2
16	CLA	s	503	-	1/1/11/20	10/17/93/115	-
16	CLA	B	1207	-	-	18/39/115/115	-
16	CLA	n	502	-	1/1/12/20	7/21/97/115	-
19	BCR	r	602	-	-	16/29/63/63	0/2/2/2
16	CLA	u	510	-	-	9/33/109/115	-
20	LMT	A	4202	-	-	7/21/61/61	0/2/2/2
16	CLA	a	1237	25	1/1/15/20	13/39/115/115	-
16	CLA	B	1235	-	1/1/14/20	11/36/112/115	-
16	CLA	A	1116	-	1/1/12/20	12/26/102/115	-
16	CLA	y	517	-	1/1/13/20	15/27/103/115	-
13	LHG	o	605	-	-	12/31/31/53	-
16	CLA	w	510	-	-	10/33/109/115	-
16	CLA	A	1117	-	1/1/15/20	7/39/115/115	-
16	CLA	A	1104	-	1/1/15/20	19/39/115/115	-
21	ECH	i	4020	-	-	12/29/66/66	0/2/2/2
16	CLA	y	515	-	1/1/15/20	15/39/115/115	-
19	BCR	J	4015	-	-	7/29/63/63	0/2/2/2
19	BCR	k	4005	-	-	7/29/63/63	0/2/2/2
16	CLA	Z	511	-	1/1/15/20	4/39/115/115	-
16	CLA	A	1237	25	1/1/15/20	11/39/115/115	-
16	CLA	Y	508	12	1/1/13/20	13/27/103/115	-
16	CLA	G	1216	25	1/1/11/20	4/18/94/115	-
14	LMG	H	4101	-	-	23/41/61/70	0/1/1/1
14	LMG	a	4101	-	-	21/41/61/70	0/1/1/1
19	BCR	p	601	-	-	9/29/63/63	0/2/2/2
16	CLA	H	1136	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	Z	504	-	1/1/15/20	14/39/115/115	-
16	CLA	u	503	-	-	9/17/93/115	-
16	CLA	x	505	-	1/1/15/20	10/39/115/115	-
16	CLA	v	507	12	-	9/39/115/115	-
23	LMU	g	606	-	-	5/21/61/61	0/2/2/2
16	CLA	l	1501	10	-	15/33/109/115	-
14	LMG	B	848	-	-	18/38/58/70	0/1/1/1
16	CLA	b	1023	-	-	12/39/115/115	-
14	LMG	a	852	-	-	10/33/53/70	0/1/1/1
19	BCR	q	603	-	-	6/29/63/63	0/2/2/2
16	CLA	h	503	-	1/1/11/20	5/17/93/115	-
19	BCR	h	603	-	-	11/29/63/63	0/2/2/2
16	CLA	B	1232	-	1/1/11/20	8/15/91/115	-
23	LMU	s	606	-	-	6/21/61/61	0/2/2/2
16	CLA	b	1204	-	1/1/15/20	13/39/115/115	-
16	CLA	U	1501	10	-	13/33/109/115	-
16	CLA	v	515	-	1/1/15/20	17/39/115/115	-
16	CLA	X	503	-	-	11/17/93/115	-
16	CLA	H	1138	-	1/1/15/20	11/39/115/115	-
16	CLA	G	1023	-	-	8/39/115/115	-
16	CLA	U	1502	-	-	9/33/109/115	-
16	CLA	G	1208	-	1/1/11/20	8/15/91/115	-
16	CLA	n	517	12	1/1/13/20	11/27/103/115	-
16	CLA	b	1203	-	1/1/15/20	16/39/115/115	-
18	SF4	C	102	-	-	-	0/6/5/5
16	CLA	H	1124	-	1/1/14/20	6/33/109/115	-
16	CLA	v	517	-	1/1/13/20	15/27/103/115	-
16	CLA	a	1131	-	-	13/39/115/115	-
19	BCR	w	604	-	-	17/29/63/63	0/2/2/2
16	CLA	H	1125	-	-	11/39/115/115	-
16	CLA	a	1801	13	1/1/11/20	7/17/93/115	-
16	CLA	Y	502	-	1/1/12/20	6/21/97/115	-
19	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
16	CLA	x	516	-	1/1/11/20	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	w	509	-	1/1/15/20	12/39/115/115	-
16	CLA	B	1216	25	-	5/18/94/115	-
19	BCR	o	603	-	-	9/29/63/63	0/2/2/2
16	CLA	a	1109	16	1/1/15/20	9/39/115/115	-
16	CLA	F	1302	6	1/1/11/20	8/17/93/115	-
16	CLA	n	515	-	1/1/15/20	15/39/115/115	-
16	CLA	x	501	-	-	6/21/97/115	-
16	CLA	o	515	-	1/1/15/20	16/39/115/115	-
16	CLA	t	514	-	1/1/12/20	8/21/97/115	-
13	LHG	H	849	-	-	17/47/47/53	-
16	CLA	Z	506	-	-	8/33/109/115	-
19	BCR	G	4014	-	-	16/29/63/63	0/2/2/2
16	CLA	a	1129	-	-	3/17/93/115	-
23	LMU	p	606	-	-	9/21/61/61	0/2/2/2
13	LHG	u	605	-	-	12/31/31/53	-
16	CLA	p	514	-	1/1/12/20	8/21/97/115	-
16	CLA	t	517	12	1/1/13/20	8/27/103/115	-
19	BCR	b	4005	-	-	12/29/63/63	0/2/2/2
14	LMG	a	4201	-	-	11/27/47/70	0/1/1/1
16	CLA	y	503	-	1/1/11/20	4/17/93/115	-
16	CLA	s	501	-	1/1/12/20	9/21/97/115	-
16	CLA	H	1116	-	1/1/12/20	10/26/102/115	-
16	CLA	J	1302	8	1/1/11/20	6/15/91/115	-
16	CLA	W	515	-	1/1/15/20	16/39/115/115	-
16	CLA	a	1104	-	1/1/15/20	18/39/115/115	-
13	LHG	g	605	-	-	16/35/35/53	-
16	CLA	a	1130	-	-	10/33/109/115	-
16	CLA	H	1107	1	-	5/21/97/115	-
19	BCR	b	4010	-	-	15/29/63/63	0/2/2/2
16	CLA	B	1228	-	-	14/27/103/115	-
16	CLA	B	1236	-	1/1/12/20	11/21/97/115	-
16	CLA	Z	516	-	1/1/11/20	11/17/93/115	-
19	BCR	B	4017	-	-	11/29/63/63	0/2/2/2
16	CLA	H	1131	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	Y	601	-	-	12/29/63/63	0/2/2/2
16	CLA	B	1211	-	1/1/15/20	17/39/115/115	-
19	BCR	K	4001	-	-	11/29/63/63	0/2/2/2
19	BCR	n	601	-	-	12/29/63/63	0/2/2/2
16	CLA	a	1117	-	1/1/15/20	10/39/115/115	-
16	CLA	t	508	12	1/1/13/20	9/27/103/115	-
16	CLA	u	508	12	1/1/13/20	12/27/103/115	-
17	PQN	B	2002	-	-	9/23/43/43	0/2/2/2
16	CLA	K	4003	9	1/1/11/20	8/15/91/115	-
16	CLA	r	507	-	1/1/15/20	11/39/115/115	-
16	CLA	A	1140	-	1/1/15/20	12/39/115/115	-
16	CLA	Q	1301	25	1/1/11/20	2/15/91/115	-
21	ECH	M	4021	-	-	15/29/66/66	0/2/2/2
16	CLA	b	1213	-	1/1/13/20	6/27/103/115	-
19	BCR	r	601	-	-	15/29/63/63	0/2/2/2
16	CLA	a	1132	-	1/1/15/20	14/39/115/115	-
19	BCR	u	602	-	-	13/29/63/63	0/2/2/2
23	LMU	x	606	-	-	14/21/61/61	0/2/2/2
19	BCR	R	4018	-	-	13/29/63/63	0/2/2/2
19	BCR	j	4015	-	-	14/29/63/63	0/2/2/2
19	BCR	Z	604	-	-	19/29/63/63	0/2/2/2
16	CLA	y	513	-	1/1/11/20	7/17/93/115	-
16	CLA	q	508	12	1/1/13/20	10/27/103/115	-
16	CLA	W	510	-	-	14/39/115/115	-
19	BCR	Z	602	-	-	11/29/63/63	0/2/2/2
16	CLA	X	508	12	1/1/13/20	15/27/103/115	-
16	CLA	a	1128	-	1/1/15/20	18/39/115/115	-
13	LHG	p	605	-	-	13/36/36/53	-
16	CLA	x	517	12	-	9/27/103/115	-
19	BCR	H	4008	-	-	13/29/63/63	0/2/2/2
19	BCR	b	4009	-	-	7/24/41/63	0/1/1/2
20	LMT	a	4202	-	-	8/21/61/61	0/2/2/2
16	CLA	a	1111	-	1/1/13/20	8/27/103/115	-
16	CLA	v	506	-	1/1/14/20	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	a	1113	-	1/1/11/20	3/15/91/115	-
16	CLA	u	507	12	1/1/15/20	12/39/115/115	-
16	CLA	r	503	-	-	9/17/93/115	-
17	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
16	CLA	b	1223	-	1/1/15/20	11/39/115/115	-
19	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
16	CLA	G	1240	13	1/1/11/20	5/17/93/115	-
16	CLA	h	513	-	1/1/11/20	6/17/93/115	-
16	CLA	G	1205	-	1/1/15/20	10/39/115/115	-
16	CLA	v	513	-	1/1/11/20	4/17/93/115	-
19	BCR	G	4009	-	-	7/24/41/63	0/1/1/2
16	CLA	H	1112	-	-	2/15/91/115	-
16	CLA	w	515	-	1/1/15/20	13/39/115/115	-
16	CLA	o	511	-	1/1/15/20	10/39/115/115	-
16	CLA	p	508	12	1/1/13/20	10/27/103/115	-
16	CLA	b	1226	-	1/1/14/20	16/33/109/115	-
16	CLA	G	1223	-	1/1/15/20	6/39/115/115	-
16	CLA	o	506	-	1/1/14/20	16/33/109/115	-
13	LHG	H	851	16	-	7/30/30/53	-
16	CLA	H	1132	-	1/1/15/20	16/39/115/115	-
16	CLA	u	504	-	-	18/33/109/115	-
16	CLA	v	510	-	-	6/39/115/115	-
16	CLA	G	1204	-	1/1/15/20	9/39/115/115	-
16	CLA	t	506	-	1/1/14/20	13/33/109/115	-
16	CLA	B	1213	-	1/1/13/20	8/27/103/115	-
16	CLA	s	502	-	1/1/12/20	6/21/97/115	-
16	CLA	u	506	-	1/1/14/20	11/33/109/115	-
13	LHG	b	4018	16	-	16/42/42/53	-
19	BCR	s	603	-	-	7/29/63/63	0/2/2/2
16	CLA	r	509	-	-	10/39/115/115	-
16	CLA	A	1111	-	1/1/13/20	7/27/103/115	-
16	CLA	n	513	-	-	9/17/93/115	-
16	CLA	h	508	-	1/1/13/20	12/27/103/115	-
16	CLA	y	506	-	1/1/14/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	W	509	-	1/1/14/20	5/33/109/115	-
16	CLA	g	508	12	1/1/13/20	7/27/103/115	-
16	CLA	r	512	12	1/1/15/20	11/39/115/115	-
16	CLA	G	1207	-	-	14/39/115/115	-
16	CLA	r	502	-	1/1/12/20	6/21/97/115	-
16	CLA	t	509	-	1/1/14/20	6/33/109/115	-
16	CLA	u	509	-	1/1/14/20	8/33/109/115	-
16	CLA	n	508	12	1/1/13/20	9/27/103/115	-
14	LMG	A	852	-	-	10/33/53/70	0/1/1/1
16	CLA	a	1102	16	1/1/13/20	7/29/105/115	-
16	CLA	Y	510	-	-	11/39/115/115	-
16	CLA	o	516	-	-	11/17/93/115	-
19	BCR	a	4008	-	-	10/29/63/63	0/2/2/2
16	CLA	G	1235	-	1/1/14/20	11/36/112/115	-
16	CLA	b	1214	-	1/1/13/20	7/27/103/115	-
16	CLA	B	1208	-	1/1/11/20	6/15/91/115	-
16	CLA	X	507	12	-	10/39/115/115	-
16	CLA	H	1114	-	1/1/11/20	9/17/93/115	-
19	BCR	g	602	-	-	14/29/63/63	0/2/2/2
16	CLA	s	514	-	1/1/12/20	7/21/97/115	-
16	CLA	r	517	12	-	12/27/103/115	-
16	CLA	t	512	12	1/1/15/20	11/39/115/115	-
16	CLA	u	512	12	-	11/39/115/115	-
16	CLA	W	513	-	-	10/17/93/115	-
19	BCR	s	604	-	-	16/29/63/63	0/2/2/2
16	CLA	H	1127	-	1/1/15/20	7/39/115/115	-
16	CLA	u	502	-	1/1/12/20	7/21/97/115	-
13	LHG	Y	605	-	-	16/36/36/53	-
16	CLA	A	1120	-	-	7/20/96/115	-
16	CLA	B	1204	-	1/1/15/20	9/39/115/115	-
16	CLA	w	513	-	-	8/21/97/115	-
19	BCR	X	601	-	-	10/29/63/63	0/2/2/2
19	BCR	Z	603	-	-	8/29/63/63	0/2/2/2
16	CLA	A	1801	13	1/1/11/20	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	X	502	-	1/1/12/20	6/21/97/115	-
16	CLA	r	508	12	1/1/13/20	9/27/103/115	-
20	LMT	U	4101	-	-	8/21/61/61	0/2/2/2
16	CLA	Z	505	-	1/1/15/20	14/39/115/115	-
16	CLA	G	1214	-	1/1/13/20	13/27/103/115	-
16	CLA	a	1124	25	1/1/14/20	7/33/109/115	-
16	CLA	a	1137	-	1/1/11/20	6/18/94/115	-
16	CLA	p	503	-	1/1/11/20	6/17/93/115	-
16	CLA	Q	1302	6	1/1/11/20	6/17/93/115	-
16	CLA	A	1130	-	1/1/14/20	10/33/109/115	-
16	CLA	t	511	-	1/1/15/20	9/39/115/115	-
19	BCR	x	602	-	-	17/29/63/63	0/2/2/2

All (2895) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1011	CL0	C1B-C2B	8.84	1.49	1.39
15	a	1011	CL0	C1B-C2B	8.67	1.49	1.39
15	H	1011	CL0	C1B-C2B	8.48	1.49	1.39
15	H	1011	CL0	C3B-C4B	8.15	1.49	1.41
15	A	1011	CL0	C3B-C4B	8.03	1.49	1.41
15	a	1011	CL0	C3B-C4B	8.01	1.49	1.41
15	a	1011	CL0	C3D-C4D	3.89	1.47	1.41
15	H	1011	CL0	C3D-C4D	3.88	1.47	1.41
15	A	1011	CL0	C3D-C4D	3.78	1.47	1.41
16	G	1012	CLA	C1D-ND	3.66	1.42	1.37
16	G	1218	CLA	C1D-ND	3.63	1.42	1.37
16	n	510	CLA	C1D-ND	3.61	1.42	1.37
16	g	504	CLA	C1D-ND	3.56	1.42	1.37
16	p	510	CLA	C1D-ND	3.56	1.42	1.37
16	y	510	CLA	C1D-ND	3.56	1.42	1.37
16	B	1218	CLA	C1D-ND	3.56	1.42	1.37
16	W	504	CLA	C1D-ND	3.54	1.42	1.37
16	h	510	CLA	C1D-ND	3.54	1.42	1.37
16	t	510	CLA	C1D-ND	3.54	1.42	1.37
16	y	513	CLA	C1D-ND	3.53	1.42	1.37
16	b	1218	CLA	C1D-ND	3.53	1.42	1.37
16	v	515	CLA	C1D-ND	3.52	1.42	1.37
16	g	517	CLA	C1D-ND	3.52	1.42	1.37
16	W	510	CLA	C1D-ND	3.51	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	y	517	CLA	C1D-ND	3.51	1.42	1.37
16	Y	507	CLA	C1D-ND	3.50	1.42	1.37
16	u	504	CLA	C1D-ND	3.48	1.42	1.37
16	J	1303	CLA	C1D-ND	3.48	1.42	1.37
16	p	507	CLA	C1D-ND	3.48	1.42	1.37
16	g	513	CLA	C1D-ND	3.48	1.42	1.37
16	Y	510	CLA	C1D-ND	3.48	1.42	1.37
16	v	517	CLA	C1D-ND	3.48	1.42	1.37
16	r	517	CLA	C1D-ND	3.47	1.42	1.37
16	s	510	CLA	C1D-ND	3.47	1.42	1.37
16	s	507	CLA	C1D-ND	3.47	1.42	1.37
16	B	1205	CLA	C1D-ND	3.46	1.42	1.37
16	h	517	CLA	C1D-ND	3.46	1.42	1.37
16	G	1231	CLA	C1D-ND	3.46	1.42	1.37
16	q	504	CLA	C1D-ND	3.46	1.42	1.37
16	n	516	CLA	C1D-ND	3.46	1.42	1.37
16	j	1303	CLA	C1D-ND	3.46	1.42	1.37
16	X	504	CLA	C1D-ND	3.46	1.42	1.37
16	W	515	CLA	C1D-ND	3.45	1.42	1.37
16	n	515	CLA	C1D-ND	3.45	1.42	1.37
16	t	503	CLA	C1D-ND	3.45	1.42	1.37
16	X	510	CLA	C1D-ND	3.44	1.42	1.37
16	S	1303	CLA	C1D-ND	3.44	1.42	1.37
16	x	517	CLA	C1D-ND	3.44	1.42	1.37
16	o	513	CLA	C1D-ND	3.44	1.42	1.37
16	k	4003	CLA	C1D-ND	3.44	1.42	1.37
16	h	507	CLA	C1D-ND	3.43	1.42	1.37
16	B	1012	CLA	C1D-ND	3.43	1.42	1.37
16	o	510	CLA	C1D-ND	3.43	1.42	1.37
16	v	512	CLA	C1D-ND	3.43	1.42	1.37
16	A	1134	CLA	C1D-ND	3.42	1.42	1.37
16	v	514	CLA	C1D-ND	3.42	1.42	1.37
16	H	1135	CLA	C1D-ND	3.42	1.42	1.37
16	W	516	CLA	C1D-ND	3.42	1.42	1.37
16	t	507	CLA	C1D-ND	3.42	1.42	1.37
16	t	515	CLA	C1D-ND	3.41	1.42	1.37
16	u	517	CLA	C1D-ND	3.41	1.42	1.37
16	U	1503	CLA	C1D-ND	3.41	1.42	1.37
16	v	510	CLA	C1D-ND	3.41	1.42	1.37
16	h	515	CLA	C1D-ND	3.41	1.42	1.37
16	w	504	CLA	C1D-ND	3.41	1.42	1.37
16	r	510	CLA	C1D-ND	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	u	510	CLA	C1D-ND	3.41	1.42	1.37
16	F	1301	CLA	C1D-ND	3.40	1.42	1.37
16	H	1134	CLA	C1D-ND	3.40	1.42	1.37
16	Y	517	CLA	C1D-ND	3.40	1.42	1.37
16	v	506	CLA	C1D-ND	3.40	1.42	1.37
16	K	4003	CLA	C1D-ND	3.40	1.42	1.37
16	u	513	CLA	C1D-ND	3.40	1.42	1.37
16	b	1234	CLA	C1D-ND	3.40	1.42	1.37
16	B	1231	CLA	C1D-ND	3.40	1.42	1.37
16	f	1301	CLA	C1D-ND	3.40	1.42	1.37
16	q	510	CLA	C1D-ND	3.40	1.42	1.37
16	X	507	CLA	C1D-ND	3.39	1.42	1.37
16	h	501	CLA	C1D-ND	3.39	1.42	1.37
16	y	515	CLA	C1D-ND	3.39	1.42	1.37
16	b	1230	CLA	C1D-ND	3.39	1.42	1.37
16	B	1223	CLA	C1D-ND	3.39	1.42	1.37
16	q	517	CLA	C1D-ND	3.39	1.42	1.37
16	W	507	CLA	C1D-ND	3.39	1.42	1.37
16	w	516	CLA	C1D-ND	3.39	1.42	1.37
16	s	517	CLA	C1D-ND	3.39	1.42	1.37
16	x	501	CLA	C1D-ND	3.38	1.42	1.37
16	B	1217	CLA	C1D-ND	3.38	1.42	1.37
16	o	517	CLA	C1D-ND	3.38	1.42	1.37
16	r	513	CLA	C1D-ND	3.38	1.42	1.37
16	v	505	CLA	C1D-ND	3.38	1.42	1.37
16	y	507	CLA	C1D-ND	3.38	1.42	1.37
16	n	507	CLA	C1D-ND	3.37	1.42	1.37
16	Z	510	CLA	C1D-ND	3.37	1.42	1.37
16	H	1122	CLA	C1D-ND	3.37	1.42	1.37
16	G	1219	CLA	C1D-ND	3.37	1.42	1.37
16	t	513	CLA	C1D-ND	3.37	1.42	1.37
16	h	514	CLA	C1D-ND	3.37	1.42	1.37
16	v	501	CLA	C1D-ND	3.37	1.42	1.37
16	G	1240	CLA	C1D-ND	3.37	1.42	1.37
16	G	1232	CLA	C1D-ND	3.37	1.42	1.37
16	b	1224	CLA	C1D-ND	3.37	1.42	1.37
16	A	1137	CLA	C1D-ND	3.36	1.42	1.37
16	l	1503	CLA	C1D-ND	3.36	1.42	1.37
16	K	4004	CLA	C1D-ND	3.36	1.42	1.37
16	h	513	CLA	C1D-ND	3.36	1.42	1.37
16	F	1302	CLA	C1D-ND	3.36	1.42	1.37
16	Q	1301	CLA	C1D-ND	3.36	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	w	507	CLA	C1D-ND	3.36	1.42	1.37
16	x	513	CLA	C1D-ND	3.36	1.42	1.37
16	B	1209	CLA	C1D-ND	3.36	1.42	1.37
16	b	1229	CLA	C1D-ND	3.36	1.42	1.37
16	b	1231	CLA	C1D-ND	3.36	1.42	1.37
16	t	516	CLA	C1D-ND	3.36	1.42	1.37
16	b	1240	CLA	C1D-ND	3.36	1.42	1.37
16	j	1302	CLA	C1D-ND	3.36	1.42	1.37
16	t	511	CLA	C1D-ND	3.36	1.42	1.37
16	q	513	CLA	C1D-ND	3.35	1.42	1.37
16	W	509	CLA	C1D-ND	3.35	1.42	1.37
16	G	1217	CLA	C1D-ND	3.35	1.42	1.37
16	o	507	CLA	C1D-ND	3.35	1.42	1.37
16	g	501	CLA	C1D-ND	3.35	1.42	1.37
16	o	504	CLA	C1D-ND	3.35	1.42	1.37
16	H	1103	CLA	C1D-ND	3.35	1.42	1.37
16	g	516	CLA	C1D-ND	3.35	1.42	1.37
16	b	1205	CLA	C1D-ND	3.35	1.42	1.37
16	L	1503	CLA	C1D-ND	3.34	1.42	1.37
16	J	1302	CLA	C1D-ND	3.34	1.42	1.37
16	b	1012	CLA	C1D-ND	3.34	1.42	1.37
16	h	516	CLA	C1D-ND	3.34	1.42	1.37
16	B	1240	CLA	C1D-ND	3.34	1.42	1.37
16	u	501	CLA	C1D-ND	3.34	1.42	1.37
16	H	1118	CLA	C1D-ND	3.34	1.42	1.37
16	G	1230	CLA	C1D-ND	3.34	1.42	1.37
16	b	1238	CLA	C1D-ND	3.34	1.42	1.37
16	v	513	CLA	C1D-ND	3.34	1.42	1.37
16	h	505	CLA	C1D-ND	3.33	1.42	1.37
16	A	1122	CLA	C1D-ND	3.33	1.42	1.37
16	W	513	CLA	C1D-ND	3.33	1.42	1.37
16	T	4003	CLA	C1D-ND	3.33	1.42	1.37
16	X	513	CLA	C1D-ND	3.33	1.42	1.37
16	Z	506	CLA	C1D-ND	3.33	1.42	1.37
16	y	505	CLA	C1D-ND	3.33	1.42	1.37
16	B	1224	CLA	C1D-ND	3.33	1.42	1.37
16	x	510	CLA	C1D-ND	3.32	1.42	1.37
16	y	506	CLA	C1D-ND	3.32	1.42	1.37
16	A	1112	CLA	C1D-ND	3.32	1.42	1.37
16	w	505	CLA	C1D-ND	3.32	1.42	1.37
16	A	1113	CLA	C1D-ND	3.32	1.42	1.37
16	B	1212	CLA	C1D-ND	3.32	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	1209	CLA	C1D-ND	3.32	1.42	1.37
16	K	4002	CLA	C1D-ND	3.32	1.42	1.37
16	W	503	CLA	C1D-ND	3.32	1.42	1.37
16	o	501	CLA	C1D-ND	3.32	1.42	1.37
16	o	505	CLA	C1D-ND	3.32	1.42	1.37
16	w	510	CLA	C1D-ND	3.32	1.42	1.37
16	S	1302	CLA	C1D-ND	3.32	1.42	1.37
16	G	1209	CLA	C1D-ND	3.32	1.42	1.37
16	t	506	CLA	C1D-ND	3.31	1.42	1.37
16	b	1223	CLA	C1D-ND	3.31	1.42	1.37
16	v	503	CLA	C1D-ND	3.31	1.42	1.37
16	a	1114	CLA	C1D-ND	3.31	1.42	1.37
16	A	1118	CLA	C1D-ND	3.31	1.42	1.37
16	b	1228	CLA	C1D-ND	3.31	1.42	1.37
16	u	503	CLA	C1D-ND	3.31	1.42	1.37
16	B	1202	CLA	C1D-ND	3.31	1.42	1.37
16	k	4002	CLA	C1D-ND	3.31	1.42	1.37
16	H	1101	CLA	C1D-ND	3.31	1.42	1.37
16	H	1111	CLA	C1D-ND	3.31	1.42	1.37
16	Y	501	CLA	C1D-ND	3.31	1.42	1.37
16	a	1113	CLA	C1D-ND	3.31	1.42	1.37
16	X	501	CLA	C1D-ND	3.31	1.42	1.37
16	y	501	CLA	C1D-ND	3.30	1.42	1.37
16	n	503	CLA	C1D-ND	3.30	1.42	1.37
16	H	1112	CLA	C1D-ND	3.30	1.42	1.37
16	a	1111	CLA	C1D-ND	3.30	1.42	1.37
16	k	4004	CLA	C1D-ND	3.30	1.42	1.37
16	v	516	CLA	C1D-ND	3.30	1.42	1.37
16	a	1022	CLA	C1D-ND	3.30	1.42	1.37
16	a	1112	CLA	C1D-ND	3.30	1.42	1.37
16	q	501	CLA	C1D-ND	3.30	1.42	1.37
16	r	511	CLA	C1D-ND	3.29	1.42	1.37
16	T	4004	CLA	C1D-ND	3.29	1.42	1.37
16	Z	504	CLA	C1D-ND	3.29	1.42	1.37
16	B	1219	CLA	C1D-ND	3.29	1.42	1.37
16	r	515	CLA	C1D-ND	3.29	1.42	1.37
16	x	504	CLA	C1D-ND	3.29	1.42	1.37
16	r	501	CLA	C1D-ND	3.29	1.42	1.37
16	B	1228	CLA	C1D-ND	3.29	1.42	1.37
16	r	508	CLA	C1D-ND	3.29	1.42	1.37
16	y	508	CLA	C1D-ND	3.29	1.42	1.37
16	H	1113	CLA	C1D-ND	3.29	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1210	CLA	C1D-ND	3.28	1.42	1.37
16	r	516	CLA	C1D-ND	3.28	1.42	1.37
16	r	504	CLA	C1D-ND	3.28	1.42	1.37
16	h	503	CLA	C1D-ND	3.28	1.42	1.37
16	Z	505	CLA	C1D-ND	3.28	1.42	1.37
16	b	1204	CLA	C1D-ND	3.28	1.42	1.37
16	g	510	CLA	C1D-ND	3.28	1.42	1.37
16	A	1101	CLA	C1D-ND	3.28	1.42	1.37
16	U	1501	CLA	C1D-ND	3.28	1.42	1.37
16	n	504	CLA	C1D-ND	3.28	1.42	1.37
16	p	517	CLA	C1D-ND	3.28	1.42	1.37
16	y	514	CLA	C1D-ND	3.28	1.42	1.37
16	x	507	CLA	C1D-ND	3.28	1.42	1.37
16	q	507	CLA	C1D-ND	3.27	1.42	1.37
16	t	509	CLA	C1D-ND	3.27	1.42	1.37
16	A	1123	CLA	C1D-ND	3.27	1.42	1.37
16	A	1132	CLA	C1D-ND	3.27	1.42	1.37
16	a	1122	CLA	C1D-ND	3.27	1.42	1.37
16	B	1230	CLA	C1D-ND	3.27	1.42	1.37
16	Z	512	CLA	C1D-ND	3.27	1.42	1.37
16	n	512	CLA	C1D-ND	3.27	1.42	1.37
16	r	505	CLA	C1D-ND	3.27	1.42	1.37
16	A	1130	CLA	C1D-ND	3.26	1.42	1.37
16	p	514	CLA	C1D-ND	3.26	1.42	1.37
16	u	507	CLA	C1D-ND	3.26	1.42	1.37
16	b	1219	CLA	C1D-ND	3.26	1.42	1.37
16	B	1201	CLA	C1D-ND	3.26	1.42	1.37
16	h	512	CLA	C1D-ND	3.26	1.42	1.37
16	r	512	CLA	C1D-ND	3.26	1.42	1.37
16	s	512	CLA	C1D-ND	3.26	1.42	1.37
16	Z	508	CLA	C1D-ND	3.26	1.42	1.37
16	b	1201	CLA	C1D-ND	3.26	1.42	1.37
16	A	1107	CLA	C1D-ND	3.26	1.42	1.37
16	X	505	CLA	C1D-ND	3.26	1.42	1.37
16	G	1238	CLA	C1D-ND	3.26	1.42	1.37
16	W	517	CLA	C1D-ND	3.26	1.42	1.37
16	B	1238	CLA	C1D-ND	3.26	1.42	1.37
16	G	1201	CLA	C1D-ND	3.26	1.42	1.37
16	G	1224	CLA	C1D-ND	3.26	1.42	1.37
16	Z	515	CLA	C1D-ND	3.26	1.42	1.37
16	a	1130	CLA	C1D-ND	3.26	1.42	1.37
16	Z	507	CLA	C1D-ND	3.25	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	501	CLA	C1D-ND	3.25	1.42	1.37
16	Z	513	CLA	C1D-ND	3.25	1.42	1.37
16	n	501	CLA	C1D-ND	3.25	1.42	1.37
16	a	1123	CLA	C1D-ND	3.25	1.42	1.37
16	g	507	CLA	C1D-ND	3.25	1.42	1.37
16	s	513	CLA	C1D-ND	3.25	1.42	1.37
16	p	505	CLA	C1D-ND	3.25	1.42	1.37
16	W	506	CLA	C1D-ND	3.25	1.42	1.37
16	b	1217	CLA	C1D-ND	3.25	1.42	1.37
16	G	1213	CLA	C1D-ND	3.25	1.42	1.37
16	y	503	CLA	C1D-ND	3.25	1.42	1.37
16	h	508	CLA	C1D-ND	3.25	1.42	1.37
16	B	1232	CLA	C1D-ND	3.25	1.42	1.37
16	Y	508	CLA	C1D-ND	3.25	1.42	1.37
16	b	1216	CLA	C1D-ND	3.25	1.42	1.37
16	v	507	CLA	C1D-ND	3.25	1.42	1.37
16	T	4002	CLA	C1D-ND	3.25	1.42	1.37
16	L	1501	CLA	C1D-ND	3.25	1.42	1.37
16	u	505	CLA	C1D-ND	3.25	1.42	1.37
16	G	1235	CLA	C1D-ND	3.24	1.42	1.37
16	a	1137	CLA	C1D-ND	3.24	1.42	1.37
16	r	506	CLA	C1D-ND	3.24	1.42	1.37
16	G	1228	CLA	C1D-ND	3.24	1.42	1.37
16	a	1118	CLA	C1D-ND	3.24	1.42	1.37
16	s	503	CLA	C1D-ND	3.24	1.42	1.37
16	B	1204	CLA	C1D-ND	3.24	1.42	1.37
16	p	515	CLA	C1D-ND	3.24	1.42	1.37
16	v	511	CLA	C1D-ND	3.24	1.42	1.37
16	b	1210	CLA	C1D-ND	3.24	1.42	1.37
16	b	1235	CLA	C1D-ND	3.24	1.42	1.37
16	n	517	CLA	C1D-ND	3.24	1.42	1.37
16	t	501	CLA	C1D-ND	3.24	1.42	1.37
16	w	514	CLA	C1D-ND	3.24	1.42	1.37
16	G	1207	CLA	C1D-ND	3.23	1.42	1.37
16	H	1130	CLA	C1D-ND	3.23	1.42	1.37
16	W	512	CLA	C1D-ND	3.23	1.42	1.37
16	n	506	CLA	C1D-ND	3.23	1.42	1.37
16	n	509	CLA	C1D-ND	3.23	1.42	1.37
16	a	1132	CLA	C1D-ND	3.23	1.42	1.37
16	t	517	CLA	C1D-ND	3.23	1.42	1.37
16	p	513	CLA	C1D-ND	3.23	1.42	1.37
16	p	508	CLA	C1D-ND	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	q	511	CLA	C1D-ND	3.23	1.42	1.37
16	q	516	CLA	C1D-ND	3.23	1.42	1.37
16	A	1138	CLA	C1D-ND	3.23	1.42	1.37
16	a	1801	CLA	C1D-ND	3.23	1.42	1.37
16	r	507	CLA	C1D-ND	3.23	1.42	1.37
16	y	512	CLA	C1D-ND	3.23	1.42	1.37
16	n	505	CLA	C1D-ND	3.23	1.42	1.37
16	p	512	CLA	C1D-ND	3.22	1.42	1.37
16	H	1132	CLA	C1D-ND	3.22	1.42	1.37
16	Z	517	CLA	C1D-ND	3.22	1.42	1.37
16	B	1220	CLA	C1D-ND	3.22	1.42	1.37
16	x	508	CLA	C1D-ND	3.22	1.42	1.37
16	p	509	CLA	C1D-ND	3.22	1.42	1.37
16	W	505	CLA	C1D-ND	3.22	1.42	1.37
16	A	1114	CLA	C1D-ND	3.22	1.42	1.37
16	h	509	CLA	C1D-ND	3.21	1.42	1.37
16	n	511	CLA	C1D-ND	3.21	1.42	1.37
16	t	504	CLA	C1D-ND	3.21	1.42	1.37
16	G	1208	CLA	C1D-ND	3.21	1.42	1.37
16	s	516	CLA	C1D-ND	3.21	1.42	1.37
16	A	1129	CLA	C1D-ND	3.21	1.42	1.37
16	a	1133	CLA	C1D-ND	3.21	1.42	1.37
16	p	516	CLA	C1D-ND	3.21	1.42	1.37
16	y	504	CLA	C1D-ND	3.21	1.42	1.37
16	b	1212	CLA	C1D-ND	3.21	1.42	1.37
16	X	517	CLA	C1D-ND	3.21	1.42	1.37
16	b	1232	CLA	C1D-ND	3.21	1.42	1.37
16	l	1501	CLA	C1D-ND	3.21	1.42	1.37
16	g	515	CLA	C1D-ND	3.21	1.42	1.37
16	X	516	CLA	C1D-ND	3.20	1.42	1.37
16	u	514	CLA	C1D-ND	3.20	1.42	1.37
16	y	516	CLA	C1D-ND	3.20	1.42	1.37
16	q	508	CLA	C1D-ND	3.20	1.42	1.37
16	Y	516	CLA	C1D-ND	3.20	1.42	1.37
16	b	1207	CLA	C1D-ND	3.20	1.42	1.37
16	q	506	CLA	C1D-ND	3.20	1.42	1.37
16	A	1103	CLA	C1D-ND	3.20	1.42	1.37
16	w	517	CLA	C1D-ND	3.20	1.42	1.37
16	A	1120	CLA	C1D-ND	3.20	1.42	1.37
16	t	514	CLA	C1D-ND	3.20	1.42	1.37
16	A	1136	CLA	C1D-ND	3.20	1.42	1.37
16	b	1239	CLA	C1D-ND	3.20	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	o	516	CLA	C1D-ND	3.19	1.42	1.37
16	q	515	CLA	C1D-ND	3.19	1.42	1.37
16	y	511	CLA	C1D-ND	3.19	1.42	1.37
16	Z	501	CLA	C1D-ND	3.19	1.42	1.37
16	b	1214	CLA	C1D-ND	3.19	1.42	1.37
16	s	505	CLA	C1D-ND	3.19	1.42	1.37
16	a	1120	CLA	C1D-ND	3.19	1.42	1.37
16	B	1235	CLA	C1D-ND	3.19	1.42	1.37
16	H	1120	CLA	C1D-ND	3.19	1.42	1.37
16	a	1134	CLA	C1D-ND	3.19	1.42	1.37
16	f	1302	CLA	C1D-ND	3.19	1.42	1.37
16	g	506	CLA	C1D-ND	3.18	1.42	1.37
16	w	503	CLA	C1D-ND	3.18	1.42	1.37
16	a	1108	CLA	C1D-ND	3.18	1.42	1.37
16	A	1108	CLA	C1D-ND	3.18	1.42	1.37
16	B	1239	CLA	C1D-ND	3.18	1.42	1.37
16	Y	505	CLA	C1D-ND	3.18	1.42	1.37
16	n	513	CLA	C1D-ND	3.18	1.42	1.37
16	o	506	CLA	C1D-ND	3.18	1.42	1.37
16	x	516	CLA	C1D-ND	3.18	1.42	1.37
16	G	1204	CLA	C1D-ND	3.18	1.42	1.37
16	G	1215	CLA	C1D-ND	3.18	1.42	1.37
16	G	1205	CLA	C1D-ND	3.18	1.42	1.37
16	w	513	CLA	C1D-ND	3.18	1.42	1.37
16	a	1103	CLA	C1D-ND	3.18	1.42	1.37
16	H	1801	CLA	C1D-ND	3.18	1.42	1.37
16	A	1105	CLA	C1D-ND	3.18	1.42	1.37
16	G	1210	CLA	C1D-ND	3.18	1.42	1.37
16	Y	513	CLA	C1D-ND	3.18	1.42	1.37
16	h	502	CLA	C1D-ND	3.18	1.42	1.37
16	A	1801	CLA	C1D-ND	3.17	1.42	1.37
16	b	1203	CLA	C1D-ND	3.17	1.42	1.37
16	Y	509	CLA	C1D-ND	3.17	1.42	1.37
16	G	1202	CLA	C1D-ND	3.17	1.42	1.37
16	h	504	CLA	C1D-ND	3.17	1.42	1.37
16	g	511	CLA	C1D-ND	3.17	1.42	1.37
16	B	1234	CLA	C1D-ND	3.17	1.42	1.37
16	b	1222	CLA	C1D-ND	3.17	1.42	1.37
16	W	511	CLA	C1D-ND	3.17	1.42	1.37
16	s	501	CLA	C1D-ND	3.17	1.42	1.37
16	G	1223	CLA	C1D-ND	3.16	1.42	1.37
16	G	1234	CLA	C1D-ND	3.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	o	503	CLA	C1D-ND	3.16	1.42	1.37
16	o	508	CLA	C1D-ND	3.16	1.42	1.37
16	a	1119	CLA	C1D-ND	3.16	1.42	1.37
16	a	1107	CLA	C1D-ND	3.16	1.42	1.37
16	t	512	CLA	C1D-ND	3.16	1.42	1.37
16	X	511	CLA	C1D-ND	3.16	1.42	1.37
16	Y	514	CLA	C1D-ND	3.16	1.42	1.37
16	a	1121	CLA	C1D-ND	3.16	1.42	1.37
16	G	1229	CLA	C1D-ND	3.15	1.42	1.37
16	Z	514	CLA	C1D-ND	3.15	1.42	1.37
16	B	1222	CLA	C1D-ND	3.15	1.42	1.37
16	h	506	CLA	C1D-ND	3.15	1.42	1.37
16	H	1136	CLA	C1D-ND	3.15	1.42	1.37
16	o	509	CLA	C1D-ND	3.15	1.42	1.37
16	t	505	CLA	C1D-ND	3.15	1.42	1.37
16	o	515	CLA	C1D-ND	3.15	1.42	1.37
16	X	506	CLA	C1D-ND	3.15	1.42	1.37
16	G	1212	CLA	C1D-ND	3.15	1.42	1.37
16	Q	1302	CLA	C1D-ND	3.15	1.42	1.37
16	v	508	CLA	C1D-ND	3.15	1.42	1.37
16	x	514	CLA	C1D-ND	3.15	1.42	1.37
16	G	1220	CLA	C1D-ND	3.15	1.42	1.37
16	a	1136	CLA	C1D-ND	3.15	1.42	1.37
16	W	514	CLA	C1D-ND	3.15	1.42	1.37
16	t	508	CLA	C1D-ND	3.15	1.42	1.37
16	A	1121	CLA	C1D-ND	3.14	1.42	1.37
16	H	1109	CLA	C1D-ND	3.14	1.42	1.37
16	p	504	CLA	C1D-ND	3.14	1.42	1.37
16	H	1123	CLA	C1D-ND	3.14	1.42	1.37
16	G	1239	CLA	C1D-ND	3.14	1.42	1.37
16	X	515	CLA	C1D-ND	3.14	1.42	1.37
16	H	1137	CLA	C1D-ND	3.14	1.42	1.37
16	b	1202	CLA	C1D-ND	3.14	1.42	1.37
16	s	508	CLA	C1D-ND	3.14	1.42	1.37
16	s	514	CLA	C1D-ND	3.14	1.42	1.37
16	X	508	CLA	C1D-ND	3.14	1.42	1.37
16	r	503	CLA	C1D-ND	3.14	1.42	1.37
16	x	515	CLA	C1D-ND	3.14	1.42	1.37
16	s	504	CLA	C1D-ND	3.14	1.42	1.37
16	w	511	CLA	C1D-ND	3.14	1.42	1.37
16	H	1133	CLA	C1D-ND	3.13	1.42	1.37
16	G	1216	CLA	C1D-ND	3.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	s	515	CLA	C1D-ND	3.13	1.42	1.37
16	B	1229	CLA	C1D-ND	3.13	1.42	1.37
16	s	509	CLA	C1D-ND	3.13	1.42	1.37
16	y	509	CLA	C1D-ND	3.13	1.42	1.37
16	B	1207	CLA	C1D-ND	3.13	1.42	1.37
16	q	514	CLA	C1D-ND	3.13	1.42	1.37
16	Y	511	CLA	C1D-ND	3.13	1.42	1.37
16	a	1104	CLA	C1D-ND	3.13	1.42	1.37
16	X	509	CLA	C1D-ND	3.12	1.42	1.37
16	a	1101	CLA	C1D-ND	3.12	1.42	1.37
16	A	1124	CLA	C1D-ND	3.12	1.42	1.37
16	a	1109	CLA	C1D-ND	3.12	1.42	1.37
16	g	508	CLA	C1D-ND	3.12	1.42	1.37
16	H	1114	CLA	C1D-ND	3.12	1.42	1.37
16	n	514	CLA	C1D-ND	3.12	1.42	1.37
16	B	1227	CLA	C1D-ND	3.12	1.42	1.37
16	G	1222	CLA	C1D-ND	3.12	1.42	1.37
16	H	1138	CLA	C1D-ND	3.12	1.42	1.37
16	X	503	CLA	C1D-ND	3.12	1.42	1.37
16	Z	503	CLA	C1D-ND	3.12	1.42	1.37
16	a	1135	CLA	C1D-ND	3.12	1.42	1.37
16	B	1203	CLA	C1D-ND	3.12	1.42	1.37
16	w	508	CLA	C1D-ND	3.12	1.42	1.37
16	n	508	CLA	C1D-ND	3.12	1.42	1.37
16	y	502	CLA	C1D-ND	3.11	1.42	1.37
16	H	1102	CLA	C1D-ND	3.11	1.41	1.37
16	Z	516	CLA	C1D-ND	3.11	1.41	1.37
16	H	1107	CLA	C1D-ND	3.11	1.41	1.37
16	H	1119	CLA	C1D-ND	3.11	1.41	1.37
16	a	1105	CLA	C1D-ND	3.11	1.41	1.37
16	q	512	CLA	C1D-ND	3.11	1.41	1.37
16	A	1133	CLA	C1D-ND	3.11	1.41	1.37
16	u	516	CLA	C1D-ND	3.11	1.41	1.37
16	A	1135	CLA	C1D-ND	3.10	1.41	1.37
16	B	1214	CLA	C1D-ND	3.10	1.41	1.37
16	o	514	CLA	C1D-ND	3.10	1.41	1.37
16	H	1125	CLA	C1D-ND	3.10	1.41	1.37
16	G	1211	CLA	C1D-ND	3.10	1.41	1.37
16	X	514	CLA	C1D-ND	3.10	1.41	1.37
16	v	502	CLA	C1D-ND	3.10	1.41	1.37
16	w	501	CLA	C1D-ND	3.10	1.41	1.37
16	x	512	CLA	C1D-ND	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1121	CLA	C1D-ND	3.09	1.41	1.37
16	A	1131	CLA	C1D-ND	3.09	1.41	1.37
16	b	1213	CLA	C1D-ND	3.09	1.41	1.37
16	A	1237	CLA	C1D-ND	3.09	1.41	1.37
16	A	1106	CLA	C1D-ND	3.09	1.41	1.37
16	B	1208	CLA	C1D-ND	3.09	1.41	1.37
16	b	1215	CLA	C1D-ND	3.09	1.41	1.37
16	B	1206	CLA	C1D-ND	3.09	1.41	1.37
16	A	1110	CLA	C1D-ND	3.09	1.41	1.37
16	X	512	CLA	C1D-ND	3.09	1.41	1.37
16	u	508	CLA	C1D-ND	3.09	1.41	1.37
16	v	504	CLA	C1D-ND	3.08	1.41	1.37
16	w	506	CLA	C1D-ND	3.08	1.41	1.37
16	Y	504	CLA	C1D-ND	3.08	1.41	1.37
16	p	501	CLA	C1D-ND	3.08	1.41	1.37
16	H	1108	CLA	C1D-ND	3.08	1.41	1.37
16	Y	512	CLA	C1D-ND	3.08	1.41	1.37
16	x	505	CLA	C1D-ND	3.08	1.41	1.37
16	x	509	CLA	C1D-ND	3.08	1.41	1.37
16	p	511	CLA	C1D-ND	3.08	1.41	1.37
16	g	512	CLA	C1D-ND	3.08	1.41	1.37
16	A	1117	CLA	C1D-ND	3.07	1.41	1.37
16	b	1236	CLA	C1D-ND	3.07	1.41	1.37
16	x	503	CLA	C1D-ND	3.07	1.41	1.37
16	b	1208	CLA	C1D-ND	3.07	1.41	1.37
16	H	1131	CLA	C1D-ND	3.07	1.41	1.37
16	a	1124	CLA	C1D-ND	3.07	1.41	1.37
16	g	503	CLA	C1D-ND	3.07	1.41	1.37
16	A	1104	CLA	C1D-ND	3.07	1.41	1.37
16	x	506	CLA	C1D-ND	3.07	1.41	1.37
16	a	1106	CLA	C1D-ND	3.06	1.41	1.37
16	u	512	CLA	C1D-ND	3.06	1.41	1.37
16	H	1129	CLA	C1D-ND	3.06	1.41	1.37
16	H	1106	CLA	C1D-ND	3.06	1.41	1.37
16	a	1116	CLA	C1D-ND	3.06	1.41	1.37
16	v	509	CLA	C1D-ND	3.06	1.41	1.37
16	B	1216	CLA	C1D-ND	3.06	1.41	1.37
16	a	1117	CLA	C1D-ND	3.06	1.41	1.37
16	r	502	CLA	C1D-ND	3.06	1.41	1.37
16	H	1110	CLA	C1D-ND	3.06	1.41	1.37
16	r	509	CLA	C1D-ND	3.06	1.41	1.37
16	G	1203	CLA	C1D-ND	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1139	CLA	C1D-ND	3.05	1.41	1.37
16	b	1226	CLA	C1D-ND	3.05	1.41	1.37
16	G	1236	CLA	C1D-ND	3.05	1.41	1.37
16	W	508	CLA	C1D-ND	3.05	1.41	1.37
16	A	1102	CLA	C1D-ND	3.05	1.41	1.37
16	G	1214	CLA	C1D-ND	3.05	1.41	1.37
16	g	505	CLA	C1D-ND	3.04	1.41	1.37
16	H	1022	CLA	C1D-ND	3.04	1.41	1.37
16	u	509	CLA	C1D-ND	3.04	1.41	1.37
16	u	515	CLA	C1D-ND	3.04	1.41	1.37
16	G	1221	CLA	C1D-ND	3.04	1.41	1.37
16	A	1139	CLA	C1D-ND	3.04	1.41	1.37
16	H	1105	CLA	C1D-ND	3.04	1.41	1.37
16	Z	511	CLA	C1D-ND	3.04	1.41	1.37
16	A	1109	CLA	C1D-ND	3.04	1.41	1.37
16	g	509	CLA	C1D-ND	3.04	1.41	1.37
16	s	511	CLA	C1D-ND	3.04	1.41	1.37
16	a	1138	CLA	C1D-ND	3.03	1.41	1.37
16	A	1022	CLA	C1D-ND	3.03	1.41	1.37
16	x	511	CLA	C1D-ND	3.03	1.41	1.37
16	a	1115	CLA	C1D-ND	3.03	1.41	1.37
16	B	1215	CLA	C1D-ND	3.03	1.41	1.37
16	b	1220	CLA	C1D-ND	3.03	1.41	1.37
16	Z	509	CLA	C1D-ND	3.03	1.41	1.37
16	W	502	CLA	C1D-ND	3.03	1.41	1.37
16	h	511	CLA	C1D-ND	3.03	1.41	1.37
16	o	511	CLA	C1D-ND	3.02	1.41	1.37
16	g	502	CLA	C1D-ND	3.02	1.41	1.37
16	r	514	CLA	C1D-ND	3.01	1.41	1.37
16	u	506	CLA	C1D-ND	3.01	1.41	1.37
16	Y	506	CLA	C1D-ND	3.01	1.41	1.37
16	B	1221	CLA	C1D-ND	3.01	1.41	1.37
16	a	1110	CLA	C1D-ND	3.01	1.41	1.37
16	q	509	CLA	C1D-ND	3.01	1.41	1.37
16	B	1236	CLA	C1D-ND	3.01	1.41	1.37
16	o	502	CLA	C1D-ND	3.01	1.41	1.37
16	H	1104	CLA	C1D-ND	3.00	1.41	1.37
16	g	514	CLA	C1D-ND	3.00	1.41	1.37
16	w	512	CLA	C1D-ND	3.00	1.41	1.37
16	b	1211	CLA	C1D-ND	3.00	1.41	1.37
16	A	1111	CLA	C1D-ND	3.00	1.41	1.37
16	b	1221	CLA	C1D-ND	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	515	CLA	C1D-ND	3.00	1.41	1.37
16	A	1125	CLA	C1D-ND	3.00	1.41	1.37
16	q	505	CLA	C1D-ND	3.00	1.41	1.37
16	G	1226	CLA	C1D-ND	2.99	1.41	1.37
21	i	4020	ECH	C1-C6	2.99	1.57	1.53
16	a	1129	CLA	C1D-ND	2.99	1.41	1.37
16	G	1206	CLA	C1D-ND	2.99	1.41	1.37
16	A	1119	CLA	C1D-ND	2.99	1.41	1.37
16	p	506	CLA	C1D-ND	2.99	1.41	1.37
16	w	509	CLA	C1D-ND	2.99	1.41	1.37
16	p	502	CLA	C1D-ND	2.99	1.41	1.37
16	A	1126	CLA	C1D-ND	2.98	1.41	1.37
16	a	1237	CLA	C1D-ND	2.98	1.41	1.37
16	Y	503	CLA	C1D-ND	2.98	1.41	1.37
16	a	1102	CLA	C1D-ND	2.98	1.41	1.37
16	b	1206	CLA	C1D-ND	2.98	1.41	1.37
16	G	1227	CLA	C1D-ND	2.97	1.41	1.37
16	b	1227	CLA	C1D-ND	2.97	1.41	1.37
16	B	1213	CLA	C1D-ND	2.97	1.41	1.37
16	B	1021	CLA	C1D-ND	2.96	1.41	1.37
16	a	1131	CLA	C1D-ND	2.96	1.41	1.37
16	o	512	CLA	C1D-ND	2.96	1.41	1.37
16	A	1127	CLA	C1D-ND	2.96	1.41	1.37
16	Z	502	CLA	C1D-ND	2.96	1.41	1.37
16	G	1021	CLA	C1D-ND	2.96	1.41	1.37
16	B	1226	CLA	C1D-ND	2.95	1.41	1.37
16	X	502	CLA	C1D-ND	2.95	1.41	1.37
16	H	1126	CLA	C1D-ND	2.95	1.41	1.37
16	A	1140	CLA	C1D-ND	2.94	1.41	1.37
16	a	1140	CLA	C1D-ND	2.94	1.41	1.37
16	w	515	CLA	C1D-ND	2.94	1.41	1.37
16	a	1139	CLA	C1D-ND	2.94	1.41	1.37
16	H	1124	CLA	C1D-ND	2.94	1.41	1.37
16	x	502	CLA	C1D-ND	2.94	1.41	1.37
16	p	503	CLA	C1D-ND	2.93	1.41	1.37
21	R	4020	ECH	C1-C6	2.93	1.57	1.53
16	a	1126	CLA	C1D-ND	2.93	1.41	1.37
16	t	502	CLA	C1D-ND	2.93	1.41	1.37
16	H	1117	CLA	C1D-ND	2.92	1.41	1.37
16	s	506	CLA	C1D-ND	2.92	1.41	1.37
16	u	511	CLA	C1D-ND	2.92	1.41	1.37
16	q	502	CLA	C1D-ND	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	502	CLA	C1D-ND	2.91	1.41	1.37
16	W	507	CLA	C1B-C2B	2.91	1.50	1.43
16	n	502	CLA	C1D-ND	2.91	1.41	1.37
16	w	502	CLA	C1D-ND	2.90	1.41	1.37
16	l	1502	CLA	C1D-ND	2.90	1.41	1.37
16	B	1211	CLA	C1D-ND	2.90	1.41	1.37
16	b	1021	CLA	C1D-ND	2.90	1.41	1.37
16	a	1125	CLA	C1D-ND	2.90	1.41	1.37
14	A	4101	LMG	C4-C5	2.89	1.59	1.53
16	H	1237	CLA	C1D-ND	2.89	1.41	1.37
14	H	4101	LMG	C4-C5	2.88	1.59	1.53
16	u	502	CLA	C1D-ND	2.88	1.41	1.37
16	H	1116	CLA	C1D-ND	2.88	1.41	1.37
16	a	1127	CLA	C1D-ND	2.87	1.41	1.37
16	A	1115	CLA	C1D-ND	2.86	1.41	1.37
21	I	4020	ECH	C1-C6	2.85	1.57	1.53
16	H	1127	CLA	C1D-ND	2.84	1.41	1.37
16	U	1502	CLA	C1D-ND	2.84	1.41	1.37
16	A	1116	CLA	C1D-ND	2.83	1.41	1.37
16	H	1128	CLA	C1D-ND	2.81	1.41	1.37
16	H	1115	CLA	C1D-ND	2.81	1.41	1.37
14	a	4101	LMG	C4-C5	2.81	1.59	1.53
16	s	502	CLA	C1D-ND	2.79	1.41	1.37
16	H	1140	CLA	C1D-ND	2.78	1.41	1.37
16	G	1225	CLA	C1D-ND	2.78	1.41	1.37
16	q	503	CLA	C1D-ND	2.77	1.41	1.37
16	b	1225	CLA	C1D-ND	2.77	1.41	1.37
16	L	1502	CLA	C1D-ND	2.76	1.41	1.37
16	A	1128	CLA	C1D-ND	2.74	1.41	1.37
16	o	507	CLA	C1B-C2B	2.74	1.49	1.43
16	a	1128	CLA	C1D-ND	2.73	1.41	1.37
16	t	507	CLA	C1B-C2B	2.73	1.49	1.43
16	b	1216	CLA	C1B-C2B	2.72	1.49	1.43
16	v	507	CLA	C1B-C2B	2.72	1.49	1.43
16	o	514	CLA	C1B-C2B	2.72	1.49	1.43
16	B	1225	CLA	C1D-ND	2.71	1.41	1.37
16	w	503	CLA	C1B-C2B	2.71	1.49	1.43
16	g	507	CLA	C1B-C2B	2.70	1.49	1.43
16	u	506	CLA	C1B-C2B	2.70	1.49	1.43
16	v	517	CLA	C1B-C2B	2.70	1.49	1.43
16	B	1023	CLA	C1D-ND	2.70	1.41	1.37
16	u	517	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	y	517	CLA	C1B-C2B	2.69	1.49	1.43
16	n	516	CLA	C1B-C2B	2.69	1.49	1.43
16	B	1220	CLA	C1B-C2B	2.69	1.49	1.43
16	y	507	CLA	C1B-C2B	2.69	1.49	1.43
16	n	501	CLA	C1B-C2B	2.69	1.49	1.43
16	W	510	CLA	C1B-C2B	2.68	1.49	1.43
16	u	507	CLA	C1B-C2B	2.68	1.49	1.43
16	b	1012	CLA	C3B-C4B	2.68	1.50	1.42
16	Z	507	CLA	C1B-C2B	2.68	1.49	1.43
16	t	516	CLA	C1B-C2B	2.68	1.49	1.43
16	v	513	CLA	C1B-C2B	2.68	1.49	1.43
16	t	515	CLA	C1B-C2B	2.67	1.49	1.43
16	n	504	CLA	C1B-C2B	2.67	1.49	1.43
16	b	1023	CLA	C1D-ND	2.67	1.41	1.37
16	B	1217	CLA	C1B-C2B	2.67	1.49	1.43
16	h	512	CLA	C1B-C2B	2.66	1.49	1.43
15	A	1011	CL0	C1A-CHA	-2.66	1.37	1.40
16	n	507	CLA	C1B-C2B	2.66	1.49	1.43
16	n	510	CLA	C1B-C2B	2.66	1.49	1.43
16	q	501	CLA	C1B-C2B	2.65	1.49	1.43
16	s	507	CLA	C1B-C2B	2.65	1.49	1.43
16	r	513	CLA	C1B-C2B	2.65	1.49	1.43
16	x	507	CLA	C1B-C2B	2.65	1.49	1.43
16	o	517	CLA	C1B-C2B	2.65	1.49	1.43
16	A	1113	CLA	C1B-C2B	2.65	1.49	1.43
16	G	1217	CLA	C1B-C2B	2.64	1.49	1.43
16	y	516	CLA	C1B-C2B	2.64	1.49	1.43
16	a	1113	CLA	C1B-C2B	2.64	1.49	1.43
16	W	516	CLA	C1B-C2B	2.64	1.49	1.43
16	y	508	CLA	C1B-C2B	2.64	1.49	1.43
16	v	515	CLA	C1B-C2B	2.63	1.49	1.43
16	Z	503	CLA	C1B-C2B	2.63	1.49	1.43
16	T	4004	CLA	C1B-C2B	2.63	1.49	1.43
16	X	504	CLA	C1B-C2B	2.63	1.49	1.43
16	k	4004	CLA	C1B-C2B	2.63	1.49	1.43
16	G	1021	CLA	C3B-C4B	2.63	1.50	1.42
16	w	507	CLA	C1B-C2B	2.63	1.49	1.43
16	u	504	CLA	C1B-C2B	2.63	1.49	1.43
16	A	1107	CLA	C1B-C2B	2.62	1.49	1.43
16	b	1219	CLA	C1B-C2B	2.62	1.49	1.43
16	Y	501	CLA	C1B-C2B	2.62	1.49	1.43
16	p	501	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1113	CLA	C1B-C2B	2.62	1.49	1.43
16	h	507	CLA	C1B-C2B	2.62	1.49	1.43
16	t	506	CLA	C1B-C2B	2.62	1.49	1.43
16	B	1218	CLA	C1B-C2B	2.62	1.49	1.43
16	x	508	CLA	C1B-C2B	2.62	1.49	1.43
16	q	515	CLA	C1B-C2B	2.62	1.49	1.43
16	H	1107	CLA	C1B-C2B	2.62	1.49	1.43
16	Z	515	CLA	C1B-C2B	2.62	1.49	1.43
16	a	1107	CLA	C1B-C2B	2.62	1.49	1.43
16	t	501	CLA	C1B-C2B	2.62	1.49	1.43
16	b	1217	CLA	C1B-C2B	2.62	1.49	1.43
16	r	507	CLA	C1B-C2B	2.62	1.49	1.43
16	h	516	CLA	C1B-C2B	2.62	1.49	1.43
16	h	502	CLA	C1B-C2B	2.62	1.49	1.43
16	t	513	CLA	C1B-C2B	2.62	1.49	1.43
16	H	1118	CLA	C1B-C2B	2.61	1.49	1.43
16	b	1023	CLA	C1B-C2B	2.61	1.49	1.43
16	K	4004	CLA	C1B-C2B	2.61	1.49	1.43
16	h	513	CLA	C1B-C2B	2.61	1.49	1.43
16	W	504	CLA	C1B-C2B	2.61	1.49	1.43
16	y	513	CLA	C1B-C2B	2.61	1.49	1.43
16	a	1125	CLA	C1B-C2B	2.61	1.49	1.43
16	y	503	CLA	C1B-C2B	2.61	1.49	1.43
16	n	513	CLA	C1B-C2B	2.61	1.49	1.43
16	s	501	CLA	C1B-C2B	2.61	1.49	1.43
16	b	1218	CLA	C1B-C2B	2.61	1.49	1.43
16	a	1114	CLA	C1B-C2B	2.61	1.49	1.43
16	B	1219	CLA	C1B-C2B	2.61	1.49	1.43
16	F	1302	CLA	C1B-C2B	2.61	1.49	1.43
16	H	1121	CLA	C1B-C2B	2.60	1.49	1.43
16	h	517	CLA	C1B-C2B	2.60	1.49	1.43
16	G	1218	CLA	C1B-C2B	2.60	1.49	1.43
16	x	504	CLA	C1B-C2B	2.60	1.49	1.43
16	n	515	CLA	C1B-C2B	2.60	1.49	1.43
16	T	4003	CLA	C1B-C2B	2.60	1.49	1.43
16	v	501	CLA	C1B-C2B	2.60	1.49	1.43
16	x	513	CLA	C1B-C2B	2.60	1.49	1.43
16	W	513	CLA	C1B-C2B	2.60	1.49	1.43
16	b	1220	CLA	C1B-C2B	2.60	1.49	1.43
16	g	515	CLA	C1B-C2B	2.60	1.49	1.43
16	Y	507	CLA	C1B-C2B	2.60	1.49	1.43
16	B	1012	CLA	C3B-C4B	2.60	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	v	512	CLA	C1B-C2B	2.60	1.49	1.43
16	w	501	CLA	C1B-C2B	2.60	1.49	1.43
16	k	4003	CLA	C1B-C2B	2.59	1.49	1.43
16	B	1228	CLA	C1B-C2B	2.59	1.49	1.43
16	Y	517	CLA	C1B-C2B	2.59	1.49	1.43
16	W	515	CLA	C1B-C2B	2.59	1.49	1.43
16	b	1012	CLA	CHC-C1C	2.59	1.43	1.38
16	H	1125	CLA	C1B-C2B	2.59	1.49	1.43
16	B	1239	CLA	C1B-C2B	2.59	1.49	1.43
16	X	517	CLA	C1B-C2B	2.59	1.49	1.43
16	h	503	CLA	C1B-C2B	2.59	1.49	1.43
16	q	503	CLA	C1B-C2B	2.59	1.49	1.43
16	q	507	CLA	C1B-C2B	2.59	1.49	1.43
16	r	514	CLA	C1B-C2B	2.59	1.49	1.43
16	H	1114	CLA	C1B-C2B	2.59	1.49	1.43
16	y	505	CLA	C1B-C2B	2.59	1.49	1.43
16	w	514	CLA	C1B-C2B	2.59	1.49	1.43
16	S	1303	CLA	C1B-C2B	2.59	1.49	1.43
16	X	514	CLA	C1B-C2B	2.59	1.49	1.43
16	r	508	CLA	C1B-C2B	2.59	1.49	1.43
16	J	1303	CLA	C1B-C2B	2.58	1.49	1.43
16	Y	513	CLA	C1B-C2B	2.58	1.49	1.43
16	s	513	CLA	C1B-C2B	2.58	1.49	1.43
16	b	1201	CLA	C1B-C2B	2.58	1.49	1.43
16	h	504	CLA	C1B-C2B	2.58	1.49	1.43
16	Z	514	CLA	C1B-C2B	2.58	1.49	1.43
16	g	513	CLA	C1B-C2B	2.58	1.49	1.43
16	h	501	CLA	C1B-C2B	2.58	1.49	1.43
16	p	507	CLA	C1B-C2B	2.58	1.49	1.43
16	y	514	CLA	C1B-C2B	2.58	1.49	1.43
16	u	501	CLA	C1B-C2B	2.58	1.49	1.43
16	r	515	CLA	C1B-C2B	2.58	1.49	1.43
16	T	4002	CLA	C1B-C2B	2.58	1.49	1.43
16	p	506	CLA	C1B-C2B	2.58	1.49	1.43
16	H	1126	CLA	CHC-C1C	2.58	1.43	1.38
16	H	1115	CLA	C1B-C2B	2.58	1.49	1.43
16	Q	1302	CLA	C1B-C2B	2.58	1.49	1.43
16	r	517	CLA	C1B-C2B	2.58	1.49	1.43
16	Z	501	CLA	C1B-C2B	2.58	1.49	1.43
16	g	517	CLA	C1B-C2B	2.58	1.49	1.43
16	v	508	CLA	C1B-C2B	2.58	1.49	1.43
16	t	504	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	s	506	CLA	C1B-C2B	2.58	1.49	1.43
16	x	514	CLA	C1B-C2B	2.58	1.49	1.43
16	o	504	CLA	C1B-C2B	2.57	1.49	1.43
16	h	509	CLA	C1B-C2B	2.57	1.49	1.43
16	y	511	CLA	C1B-C2B	2.57	1.49	1.43
16	G	1220	CLA	C1B-C2B	2.57	1.49	1.43
16	h	505	CLA	C1B-C2B	2.57	1.49	1.43
16	X	501	CLA	C1B-C2B	2.57	1.49	1.43
16	b	1230	CLA	C1B-C2B	2.57	1.49	1.43
16	x	515	CLA	C1B-C2B	2.57	1.49	1.43
16	B	1240	CLA	C1B-C2B	2.57	1.49	1.43
16	p	513	CLA	C1B-C2B	2.57	1.49	1.43
16	a	1102	CLA	CHC-C1C	2.57	1.43	1.38
16	K	4003	CLA	C1B-C2B	2.57	1.49	1.43
16	B	1021	CLA	C1B-C2B	2.57	1.49	1.43
16	B	1201	CLA	C1B-C2B	2.57	1.49	1.43
16	B	1216	CLA	MG-NB	-2.57	2.00	2.05
16	a	1121	CLA	C1B-C2B	2.56	1.49	1.43
16	j	1303	CLA	C1B-C2B	2.56	1.49	1.43
16	B	1012	CLA	CHC-C1C	2.56	1.43	1.38
16	r	504	CLA	C1B-C2B	2.56	1.49	1.43
16	W	506	CLA	C1B-C2B	2.56	1.49	1.43
16	u	511	CLA	C3B-C4B	2.56	1.50	1.42
16	a	1115	CLA	C1B-C2B	2.56	1.49	1.43
16	v	502	CLA	C3B-C4B	2.56	1.50	1.42
16	n	503	CLA	C1B-C2B	2.56	1.49	1.43
16	v	516	CLA	C1B-C2B	2.56	1.49	1.43
16	r	501	CLA	C1B-C2B	2.56	1.49	1.43
16	a	1118	CLA	C1B-C2B	2.56	1.49	1.43
16	a	1126	CLA	C3B-C4B	2.56	1.50	1.42
16	G	1219	CLA	C1B-C2B	2.56	1.49	1.43
16	X	507	CLA	C1B-C2B	2.56	1.49	1.43
16	g	508	CLA	C1B-C2B	2.56	1.49	1.43
16	G	1240	CLA	C1B-C2B	2.56	1.49	1.43
16	W	501	CLA	C1B-C2B	2.55	1.49	1.43
16	w	513	CLA	C1B-C2B	2.55	1.49	1.43
16	u	508	CLA	C1B-C2B	2.55	1.49	1.43
16	o	501	CLA	C1B-C2B	2.55	1.49	1.43
16	K	4002	CLA	C1B-C2B	2.55	1.49	1.43
16	A	1119	CLA	C3B-C4B	2.55	1.50	1.42
16	f	1302	CLA	C1B-C2B	2.55	1.49	1.43
16	s	517	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	y	515	CLA	C1B-C2B	2.55	1.49	1.43
16	G	1239	CLA	C1B-C2B	2.55	1.49	1.43
16	x	517	CLA	C1B-C2B	2.55	1.49	1.43
16	W	503	CLA	C1B-C2B	2.55	1.49	1.43
16	a	1122	CLA	C1B-C2B	2.55	1.49	1.43
16	o	508	CLA	C1B-C2B	2.55	1.49	1.43
16	p	517	CLA	C1B-C2B	2.54	1.49	1.43
16	t	503	CLA	C1B-C2B	2.54	1.49	1.43
16	q	514	CLA	C1B-C2B	2.54	1.49	1.43
16	G	1204	CLA	C1B-C2B	2.54	1.49	1.43
16	H	1119	CLA	C3B-C4B	2.54	1.50	1.42
16	h	508	CLA	C1B-C2B	2.54	1.49	1.43
16	Z	506	CLA	C1B-C2B	2.54	1.49	1.43
16	W	502	CLA	C1B-C2B	2.54	1.49	1.43
16	s	516	CLA	C1B-C2B	2.54	1.49	1.43
16	G	1213	CLA	C1B-C2B	2.54	1.49	1.43
16	k	4002	CLA	C1B-C2B	2.54	1.49	1.43
16	X	513	CLA	C1B-C2B	2.54	1.49	1.43
16	Z	517	CLA	C1B-C2B	2.54	1.49	1.43
16	Y	506	CLA	C1B-C2B	2.54	1.49	1.43
16	t	502	CLA	C1B-C2B	2.54	1.49	1.43
16	b	1228	CLA	C1B-C2B	2.54	1.49	1.43
16	a	1102	CLA	C3B-C4B	2.54	1.50	1.42
16	v	510	CLA	C1B-C2B	2.54	1.49	1.43
16	A	1115	CLA	C1B-C2B	2.54	1.49	1.43
16	x	501	CLA	C1B-C2B	2.54	1.49	1.43
16	b	1240	CLA	C1B-C2B	2.53	1.49	1.43
16	w	515	CLA	C1B-C2B	2.53	1.49	1.43
16	H	1126	CLA	C3B-C4B	2.53	1.50	1.42
16	G	1023	CLA	C1B-C2B	2.53	1.49	1.43
16	v	514	CLA	C1B-C2B	2.53	1.49	1.43
16	y	501	CLA	C1B-C2B	2.53	1.49	1.43
16	n	506	CLA	C1B-C2B	2.53	1.49	1.43
16	b	1204	CLA	C1B-C2B	2.53	1.49	1.43
16	Y	510	CLA	C1B-C2B	2.53	1.49	1.43
15	H	1011	CL0	C1A-CHA	-2.53	1.37	1.40
16	G	1209	CLA	C1B-C2B	2.53	1.49	1.43
16	h	510	CLA	C1B-C2B	2.53	1.49	1.43
16	B	1023	CLA	C1B-C2B	2.53	1.49	1.43
16	w	510	CLA	C1B-C2B	2.53	1.49	1.43
16	F	1301	CLA	C3B-C4B	2.53	1.50	1.42
16	g	504	CLA	C1B-C2B	2.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	q	513	CLA	C1B-C2B	2.53	1.49	1.43
16	Z	513	CLA	C1B-C2B	2.53	1.49	1.43
16	G	1201	CLA	C1B-C2B	2.53	1.49	1.43
16	u	514	CLA	C1B-C2B	2.52	1.49	1.43
16	r	503	CLA	C3B-C4B	2.52	1.50	1.42
16	A	1116	CLA	C3B-C4B	2.52	1.50	1.42
16	A	1121	CLA	C1B-C2B	2.52	1.49	1.43
16	n	508	CLA	C1B-C2B	2.52	1.49	1.43
16	y	504	CLA	C1B-C2B	2.52	1.49	1.43
16	p	510	CLA	C1B-C2B	2.52	1.49	1.43
16	a	1108	CLA	C1B-C2B	2.51	1.49	1.43
16	x	503	CLA	C3B-C4B	2.51	1.50	1.42
16	A	1104	CLA	C1B-C2B	2.51	1.49	1.43
16	A	1237	CLA	C1B-C2B	2.51	1.49	1.43
16	b	1223	CLA	C1B-C2B	2.51	1.49	1.43
16	A	1125	CLA	C1B-C2B	2.51	1.49	1.43
16	t	510	CLA	C1B-C2B	2.51	1.49	1.43
16	J	1302	CLA	C1B-C2B	2.51	1.49	1.43
16	j	1302	CLA	C1B-C2B	2.51	1.49	1.43
16	g	503	CLA	C3B-C4B	2.51	1.50	1.42
16	b	1021	CLA	C3B-C4B	2.51	1.50	1.42
16	v	505	CLA	C1B-C2B	2.51	1.49	1.43
16	X	510	CLA	C1B-C2B	2.51	1.49	1.43
16	a	1109	CLA	C1B-C2B	2.51	1.49	1.43
16	u	510	CLA	C1B-C2B	2.51	1.49	1.43
16	v	504	CLA	C1B-C2B	2.51	1.49	1.43
16	A	1123	CLA	C1B-C2B	2.51	1.49	1.43
16	o	516	CLA	C1B-C2B	2.51	1.49	1.43
16	n	502	CLA	C1B-C2B	2.51	1.49	1.43
16	G	1211	CLA	C1B-C2B	2.51	1.49	1.43
16	a	1134	CLA	C1B-C2B	2.51	1.49	1.43
16	q	504	CLA	C1B-C2B	2.51	1.49	1.43
16	a	1103	CLA	C1B-C2B	2.51	1.49	1.43
16	x	510	CLA	C1B-C2B	2.51	1.49	1.43
16	G	1228	CLA	C1B-C2B	2.51	1.49	1.43
16	S	1302	CLA	C1B-C2B	2.51	1.49	1.43
16	n	517	CLA	C1B-C2B	2.51	1.49	1.43
16	x	506	CLA	C1B-C2B	2.51	1.49	1.43
16	a	1124	CLA	C1B-C2B	2.50	1.49	1.43
16	h	514	CLA	C1B-C2B	2.50	1.49	1.43
16	G	1023	CLA	C1D-ND	2.50	1.41	1.37
16	W	508	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1225	CLA	C1B-C2B	2.50	1.49	1.43
16	g	516	CLA	C1B-C2B	2.50	1.49	1.43
16	a	1119	CLA	C3B-C4B	2.50	1.50	1.42
16	b	1208	CLA	C1B-C2B	2.50	1.49	1.43
16	o	510	CLA	C1B-C2B	2.50	1.49	1.43
16	B	1207	CLA	C1B-C2B	2.50	1.49	1.43
16	B	1208	CLA	C1B-C2B	2.50	1.49	1.43
16	s	502	CLA	C1B-C2B	2.50	1.49	1.43
16	g	514	CLA	C1B-C2B	2.50	1.49	1.43
16	b	1207	CLA	C1B-C2B	2.50	1.49	1.43
16	t	514	CLA	C1B-C2B	2.50	1.49	1.43
16	a	1126	CLA	CHC-C1C	2.50	1.43	1.38
16	G	1223	CLA	C1B-C2B	2.50	1.49	1.43
16	Z	509	CLA	CHC-C1C	2.50	1.43	1.38
16	g	505	CLA	C1B-C2B	2.50	1.49	1.43
16	q	509	CLA	CHC-C1C	2.50	1.43	1.38
16	B	1202	CLA	C1B-C2B	2.50	1.49	1.43
16	a	1131	CLA	C1B-C2B	2.50	1.49	1.43
16	v	503	CLA	C1B-C2B	2.50	1.49	1.43
16	t	509	CLA	C3B-C4B	2.49	1.50	1.42
16	G	1236	CLA	C1B-C2B	2.49	1.49	1.43
16	v	509	CLA	C1B-C2B	2.49	1.49	1.43
16	H	1106	CLA	C1B-C2B	2.49	1.49	1.43
16	o	513	CLA	C1B-C2B	2.49	1.49	1.43
16	r	510	CLA	C1B-C2B	2.49	1.49	1.43
16	v	511	CLA	C1B-C2B	2.49	1.49	1.43
16	o	503	CLA	C1B-C2B	2.49	1.49	1.43
16	A	1122	CLA	C1B-C2B	2.49	1.49	1.43
16	H	1109	CLA	C1B-C2B	2.49	1.49	1.43
16	t	508	CLA	C1B-C2B	2.49	1.49	1.43
16	A	1103	CLA	C1B-C2B	2.49	1.49	1.43
16	X	508	CLA	C1B-C2B	2.49	1.49	1.43
16	b	1229	CLA	C1B-C2B	2.49	1.49	1.43
16	A	1129	CLA	C3B-C4B	2.49	1.50	1.42
16	p	516	CLA	C1B-C2B	2.49	1.49	1.43
16	y	512	CLA	C1B-C2B	2.49	1.49	1.43
16	B	1209	CLA	C1B-C2B	2.49	1.49	1.43
16	g	501	CLA	C1B-C2B	2.49	1.49	1.43
16	t	517	CLA	C1B-C2B	2.48	1.49	1.43
16	H	1134	CLA	C3B-C4B	2.48	1.50	1.42
16	q	502	CLA	C3B-C4B	2.48	1.50	1.42
16	u	503	CLA	C1B-C2B	2.48	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X	503	CLA	CHC-C1C	2.48	1.43	1.38
16	H	1122	CLA	C1B-C2B	2.48	1.49	1.43
16	p	514	CLA	C1B-C2B	2.48	1.49	1.43
16	l	1503	CLA	C3B-C4B	2.48	1.50	1.42
16	A	1109	CLA	C1B-C2B	2.48	1.49	1.43
16	B	1204	CLA	C1B-C2B	2.48	1.49	1.43
16	s	514	CLA	C1B-C2B	2.48	1.49	1.43
16	X	503	CLA	C3B-C4B	2.48	1.50	1.42
16	p	511	CLA	C3B-C4B	2.48	1.50	1.42
16	f	1301	CLA	C3B-C4B	2.48	1.50	1.42
16	Y	504	CLA	C1B-C2B	2.48	1.48	1.43
16	y	511	CLA	C3B-C4B	2.48	1.50	1.42
16	A	1114	CLA	C1B-C2B	2.48	1.48	1.43
16	g	510	CLA	C1B-C2B	2.48	1.48	1.43
16	r	516	CLA	C1B-C2B	2.48	1.48	1.43
16	g	503	CLA	C1B-C2B	2.48	1.48	1.43
16	s	504	CLA	C1B-C2B	2.48	1.48	1.43
16	y	509	CLA	C1B-C2B	2.48	1.48	1.43
16	Y	516	CLA	C1B-C2B	2.48	1.48	1.43
16	a	1111	CLA	C1B-C2B	2.48	1.48	1.43
16	x	516	CLA	C1B-C2B	2.48	1.48	1.43
20	a	4202	LMT	O3'-C3'	-2.48	1.36	1.43
16	n	512	CLA	C1B-C2B	2.48	1.48	1.43
16	W	517	CLA	C1B-C2B	2.48	1.48	1.43
16	Y	514	CLA	C1B-C2B	2.48	1.48	1.43
16	q	511	CLA	C3B-C4B	2.48	1.49	1.42
16	r	509	CLA	C3B-C4B	2.48	1.49	1.42
16	X	515	CLA	C1B-C2B	2.48	1.48	1.43
16	r	505	CLA	C1B-C2B	2.48	1.48	1.43
16	X	516	CLA	C1B-C2B	2.48	1.48	1.43
16	G	1208	CLA	C1B-C2B	2.47	1.48	1.43
16	G	1229	CLA	C1B-C2B	2.47	1.48	1.43
16	Z	504	CLA	C1B-C2B	2.47	1.48	1.43
16	G	1222	CLA	C1B-C2B	2.47	1.48	1.43
16	H	1013	CLA	C3B-C4B	2.47	1.49	1.42
16	H	1102	CLA	C3B-C4B	2.47	1.49	1.42
16	o	511	CLA	C3B-C4B	2.47	1.49	1.42
16	a	1116	CLA	C3B-C4B	2.47	1.49	1.42
16	G	1231	CLA	C1B-C2B	2.47	1.48	1.43
16	p	504	CLA	C1B-C2B	2.47	1.48	1.43
16	h	511	CLA	C3B-C4B	2.47	1.49	1.42
16	u	516	CLA	C1B-C2B	2.47	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1212	CLA	C1B-C2B	2.47	1.48	1.43
16	H	1123	CLA	C1B-C2B	2.47	1.48	1.43
16	u	515	CLA	C1B-C2B	2.47	1.48	1.43
16	B	1222	CLA	C1B-C2B	2.47	1.48	1.43
16	X	506	CLA	C1B-C2B	2.47	1.48	1.43
16	a	1106	CLA	C1B-C2B	2.47	1.48	1.43
16	a	1110	CLA	C3B-C4B	2.47	1.49	1.42
16	A	1108	CLA	C1B-C2B	2.47	1.48	1.43
16	o	506	CLA	C1B-C2B	2.47	1.48	1.43
16	y	502	CLA	C1B-C2B	2.47	1.48	1.43
16	q	517	CLA	C1B-C2B	2.47	1.48	1.43
16	J	1302	CLA	C3B-C4B	2.47	1.49	1.42
16	j	1302	CLA	C3B-C4B	2.47	1.49	1.42
16	B	1213	CLA	C1B-C2B	2.47	1.48	1.43
16	A	1137	CLA	C1B-C2B	2.47	1.48	1.43
16	A	1134	CLA	C3B-C4B	2.47	1.49	1.42
16	Z	509	CLA	C3B-C4B	2.47	1.49	1.42
16	h	506	CLA	C1B-C2B	2.46	1.48	1.43
16	n	514	CLA	C1B-C2B	2.46	1.48	1.43
15	a	1011	CL0	C1A-CHA	-2.46	1.37	1.40
16	H	1111	CLA	C1B-C2B	2.46	1.48	1.43
16	s	511	CLA	C3B-C4B	2.46	1.49	1.42
16	A	1119	CLA	CHC-C1C	2.46	1.43	1.38
16	G	1230	CLA	C1B-C2B	2.46	1.48	1.43
16	b	1231	CLA	C1B-C2B	2.46	1.48	1.43
16	G	1023	CLA	MG-NB	-2.46	2.00	2.05
16	B	1203	CLA	C1B-C2B	2.46	1.48	1.43
16	q	506	CLA	C1B-C2B	2.46	1.48	1.43
16	u	513	CLA	C1B-C2B	2.46	1.48	1.43
16	G	1207	CLA	C1B-C2B	2.46	1.48	1.43
16	W	514	CLA	C1B-C2B	2.46	1.48	1.43
16	A	1102	CLA	C3B-C4B	2.46	1.49	1.42
16	H	1131	CLA	C1B-C2B	2.46	1.48	1.43
16	X	503	CLA	C1B-C2B	2.46	1.48	1.43
16	b	1225	CLA	C1B-C2B	2.46	1.48	1.43
16	q	510	CLA	C1B-C2B	2.46	1.48	1.43
16	g	517	CLA	C3B-C4B	2.46	1.49	1.42
16	u	506	CLA	MG-NB	-2.46	2.00	2.05
16	b	1205	CLA	C1B-C2B	2.46	1.48	1.43
16	H	1013	CLA	CHC-C1C	2.46	1.43	1.38
16	a	1134	CLA	C3B-C4B	2.46	1.49	1.42
16	B	1021	CLA	C3B-C4B	2.46	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	g	506	CLA	C1B-C2B	2.45	1.48	1.43
16	b	1222	CLA	C1B-C2B	2.45	1.48	1.43
16	b	1227	CLA	C3B-C4B	2.45	1.49	1.42
16	a	1013	CLA	C3B-C4B	2.45	1.49	1.42
20	A	4202	LMT	O3'-C3'	-2.45	1.36	1.43
16	A	1112	CLA	C1B-C2B	2.45	1.48	1.43
16	n	509	CLA	C3B-C4B	2.45	1.49	1.42
16	H	1108	CLA	C1B-C2B	2.45	1.48	1.43
16	W	505	CLA	C3B-C4B	2.45	1.49	1.42
16	y	501	CLA	C3B-C4B	2.45	1.49	1.42
16	w	506	CLA	C1B-C2B	2.45	1.48	1.43
16	S	1303	CLA	C3B-C4B	2.45	1.49	1.42
16	w	513	CLA	C3B-C4B	2.45	1.49	1.42
16	G	1231	CLA	C3B-C4B	2.45	1.49	1.42
20	a	4202	LMT	O2'-C2'	-2.45	1.36	1.43
16	Z	516	CLA	C1B-C2B	2.45	1.48	1.43
16	w	509	CLA	C3B-C4B	2.45	1.49	1.42
16	t	511	CLA	C3B-C4B	2.45	1.49	1.42
16	x	502	CLA	C1B-C2B	2.45	1.48	1.43
16	B	1235	CLA	C3B-C4B	2.45	1.49	1.42
16	a	1137	CLA	C1B-C2B	2.45	1.48	1.43
16	W	509	CLA	C3B-C4B	2.45	1.49	1.42
16	H	1013	CLA	MG-NB	-2.45	2.00	2.05
16	A	1106	CLA	C3B-C4B	2.45	1.49	1.42
16	G	1240	CLA	C3B-C4B	2.45	1.49	1.42
16	A	1124	CLA	C1B-C2B	2.45	1.48	1.43
16	A	1138	CLA	C3B-C4B	2.45	1.49	1.42
16	Y	511	CLA	C3B-C4B	2.45	1.49	1.42
16	A	1110	CLA	C1B-C2B	2.45	1.48	1.43
16	x	512	CLA	C1B-C2B	2.45	1.48	1.43
16	X	511	CLA	C3B-C4B	2.45	1.49	1.42
16	u	505	CLA	C3B-C4B	2.44	1.49	1.42
16	p	502	CLA	C1B-C2B	2.44	1.48	1.43
16	t	512	CLA	C1B-C2B	2.44	1.48	1.43
20	H	4202	LMT	O3'-C3'	-2.44	1.36	1.43
16	G	1023	CLA	CHC-C1C	2.44	1.43	1.38
16	v	506	CLA	C1B-C2B	2.44	1.48	1.43
16	n	505	CLA	C1B-C2B	2.44	1.48	1.43
16	r	509	CLA	CHC-C1C	2.44	1.43	1.38
16	H	1237	CLA	C1B-C2B	2.44	1.48	1.43
16	L	1503	CLA	C3B-C4B	2.44	1.49	1.42
16	b	1222	CLA	C3B-C4B	2.44	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1237	CLA	C1B-C2B	2.44	1.48	1.43
16	H	1129	CLA	C3B-C4B	2.44	1.49	1.42
16	r	513	CLA	C3B-C4B	2.44	1.49	1.42
16	b	1209	CLA	C1B-C2B	2.44	1.48	1.43
16	A	1126	CLA	CHC-C1C	2.44	1.43	1.38
20	L	4101	LMT	O3'-C3'	-2.44	1.36	1.43
16	B	1230	CLA	C1B-C2B	2.44	1.48	1.43
16	b	1221	CLA	C1B-C2B	2.44	1.48	1.43
16	A	1140	CLA	C3B-C4B	2.44	1.49	1.42
16	B	1210	CLA	C3B-C4B	2.44	1.49	1.42
16	t	508	CLA	C3B-C4B	2.44	1.49	1.42
16	t	505	CLA	C1B-C2B	2.44	1.48	1.43
16	H	1110	CLA	C3B-C4B	2.44	1.49	1.42
16	A	1102	CLA	CHC-C1C	2.44	1.43	1.38
16	s	510	CLA	C1B-C2B	2.44	1.48	1.43
16	a	1104	CLA	C1B-C2B	2.44	1.48	1.43
16	w	509	CLA	CHC-C1C	2.44	1.43	1.38
16	A	1110	CLA	C3B-C4B	2.44	1.49	1.42
16	x	517	CLA	C3B-C4B	2.44	1.49	1.42
16	o	515	CLA	C1B-C2B	2.44	1.48	1.43
16	a	1120	CLA	C1B-C2B	2.44	1.48	1.43
16	b	1202	CLA	C1B-C2B	2.44	1.48	1.43
16	x	503	CLA	C1B-C2B	2.44	1.48	1.43
16	g	509	CLA	C3B-C4B	2.44	1.49	1.42
16	a	1106	CLA	C3B-C4B	2.44	1.49	1.42
16	A	1013	CLA	MG-NB	-2.44	2.01	2.05
16	G	1235	CLA	C3B-C4B	2.44	1.49	1.42
16	G	1021	CLA	C1B-C2B	2.44	1.48	1.43
16	u	511	CLA	CHC-C1C	2.44	1.43	1.38
16	g	511	CLA	C3B-C4B	2.43	1.49	1.42
16	b	1021	CLA	C1B-C2B	2.43	1.48	1.43
16	q	508	CLA	C1B-C2B	2.43	1.48	1.43
16	n	511	CLA	C1B-C2B	2.43	1.48	1.43
16	s	515	CLA	C1B-C2B	2.43	1.48	1.43
16	L	1501	CLA	C3B-C4B	2.43	1.49	1.42
16	b	1236	CLA	C1B-C2B	2.43	1.48	1.43
16	b	1231	CLA	C3B-C4B	2.43	1.49	1.42
16	A	1106	CLA	C1B-C2B	2.43	1.48	1.43
16	B	1223	CLA	C1B-C2B	2.43	1.48	1.43
16	A	1118	CLA	C1B-C2B	2.43	1.48	1.43
16	H	1127	CLA	C1B-C2B	2.43	1.48	1.43
16	H	1110	CLA	C1B-C2B	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	t	511	CLA	C1B-C2B	2.43	1.48	1.43
16	A	1126	CLA	C3B-C4B	2.43	1.49	1.42
16	U	1502	CLA	C3B-C4B	2.43	1.49	1.42
16	a	1129	CLA	C3B-C4B	2.43	1.49	1.42
16	B	1229	CLA	C1B-C2B	2.43	1.48	1.43
16	n	508	CLA	C3B-C4B	2.43	1.49	1.42
16	H	1101	CLA	C3B-C4B	2.43	1.49	1.42
16	H	1801	CLA	C3B-C4B	2.43	1.49	1.42
16	H	1120	CLA	C1B-C2B	2.43	1.48	1.43
16	G	1012	CLA	C3B-C4B	2.43	1.49	1.42
16	r	511	CLA	C3B-C4B	2.43	1.49	1.42
16	b	1239	CLA	C1B-C2B	2.43	1.48	1.43
16	r	503	CLA	C1B-C2B	2.43	1.48	1.43
16	B	1210	CLA	CHC-C1C	2.43	1.43	1.38
16	g	512	CLA	C1B-C2B	2.43	1.48	1.43
16	W	511	CLA	C3B-C4B	2.43	1.49	1.42
16	q	509	CLA	C3B-C4B	2.43	1.49	1.42
16	h	501	CLA	C3B-C4B	2.43	1.49	1.42
16	H	1135	CLA	C1B-C2B	2.43	1.48	1.43
16	b	1221	CLA	C3B-C4B	2.43	1.49	1.42
16	b	1212	CLA	CHC-C1C	2.43	1.43	1.38
16	G	1222	CLA	CHC-C1C	2.43	1.43	1.38
16	u	503	CLA	C3B-C4B	2.43	1.49	1.42
16	H	1140	CLA	C3B-C4B	2.43	1.49	1.42
16	u	513	CLA	C3B-C4B	2.43	1.49	1.42
16	p	515	CLA	C1B-C2B	2.42	1.48	1.43
16	H	1131	CLA	C3B-C4B	2.42	1.49	1.42
16	Y	515	CLA	C1B-C2B	2.42	1.48	1.43
16	Y	503	CLA	CHC-C1C	2.42	1.43	1.38
16	r	506	CLA	C1B-C2B	2.42	1.48	1.43
16	A	1101	CLA	C3B-C4B	2.42	1.49	1.42
16	G	1202	CLA	C3B-C4B	2.42	1.49	1.42
16	Z	511	CLA	C3B-C4B	2.42	1.49	1.42
16	a	1101	CLA	C1B-C2B	2.42	1.48	1.43
16	b	1213	CLA	C1B-C2B	2.42	1.48	1.43
16	B	1221	CLA	C3B-C4B	2.42	1.49	1.42
16	v	511	CLA	C3B-C4B	2.42	1.49	1.42
16	H	1116	CLA	C3B-C4B	2.42	1.49	1.42
16	H	1102	CLA	CHC-C1C	2.42	1.43	1.38
16	h	511	CLA	C1B-C2B	2.42	1.48	1.43
16	y	510	CLA	C1B-C2B	2.42	1.48	1.43
16	w	502	CLA	C1B-C2B	2.42	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	y	506	CLA	C1B-C2B	2.42	1.48	1.43
16	v	501	CLA	C3B-C4B	2.42	1.49	1.42
16	B	1211	CLA	C1B-C2B	2.42	1.48	1.43
16	H	1103	CLA	C1B-C2B	2.42	1.48	1.43
16	W	512	CLA	C1B-C2B	2.42	1.48	1.43
16	r	502	CLA	C1B-C2B	2.42	1.48	1.43
16	W	508	CLA	C3B-C4B	2.42	1.49	1.42
16	A	1106	CLA	CHC-C1C	2.42	1.43	1.38
16	p	508	CLA	C1B-C2B	2.41	1.48	1.43
16	Q	1301	CLA	C1B-C2B	2.41	1.48	1.43
16	A	1121	CLA	C3B-C4B	2.41	1.49	1.42
16	S	1302	CLA	C3B-C4B	2.41	1.49	1.42
16	h	515	CLA	C3B-C4B	2.41	1.49	1.42
16	o	502	CLA	C3B-C4B	2.41	1.49	1.42
16	W	511	CLA	C1B-C2B	2.41	1.48	1.43
16	r	512	CLA	C1B-C2B	2.41	1.48	1.43
16	y	511	CLA	CHC-C1C	2.41	1.43	1.38
16	B	1221	CLA	C1B-C2B	2.41	1.48	1.43
16	A	1120	CLA	C3B-C4B	2.41	1.49	1.42
16	X	505	CLA	C3B-C4B	2.41	1.49	1.42
16	u	502	CLA	C3B-C4B	2.41	1.49	1.42
16	h	511	CLA	CHC-C1C	2.41	1.43	1.38
16	o	513	CLA	C3B-C4B	2.41	1.49	1.42
16	G	1224	CLA	C1B-C2B	2.41	1.48	1.43
16	W	505	CLA	C1B-C2B	2.41	1.48	1.43
16	Y	503	CLA	C1B-C2B	2.41	1.48	1.43
16	G	1201	CLA	C3B-C4B	2.41	1.49	1.42
16	G	1210	CLA	C3B-C4B	2.41	1.49	1.42
16	H	1121	CLA	C3B-C4B	2.41	1.49	1.42
16	p	508	CLA	C3B-C4B	2.41	1.49	1.42
16	B	1231	CLA	C1B-C2B	2.41	1.48	1.43
16	B	1202	CLA	CHC-C1C	2.41	1.43	1.38
16	a	1127	CLA	C1B-C2B	2.41	1.48	1.43
16	b	1215	CLA	C1B-C2B	2.41	1.48	1.43
16	J	1303	CLA	C3B-C4B	2.41	1.49	1.42
16	w	511	CLA	C3B-C4B	2.41	1.49	1.42
16	A	1131	CLA	C1B-C2B	2.41	1.48	1.43
16	o	505	CLA	C1B-C2B	2.41	1.48	1.43
16	H	1134	CLA	C1B-C2B	2.41	1.48	1.43
16	A	1140	CLA	C1B-C2B	2.41	1.48	1.43
16	a	1013	CLA	MG-NB	-2.41	2.01	2.05
16	H	1105	CLA	CHC-C1C	2.41	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	u	516	CLA	CHC-C1C	2.41	1.43	1.38
16	G	1234	CLA	C3B-C4B	2.41	1.49	1.42
16	w	517	CLA	C1B-C2B	2.41	1.48	1.43
16	Z	513	CLA	C3B-C4B	2.41	1.49	1.42
16	k	4002	CLA	C3B-C4B	2.41	1.49	1.42
16	a	1117	CLA	CHC-C1C	2.41	1.43	1.38
16	B	1240	CLA	C3B-C4B	2.41	1.49	1.42
16	a	1136	CLA	C3B-C4B	2.41	1.49	1.42
16	B	1230	CLA	C3B-C4B	2.41	1.49	1.42
16	h	517	CLA	C3B-C4B	2.41	1.49	1.42
16	j	1303	CLA	C3B-C4B	2.41	1.49	1.42
20	U	4101	LMT	O3'-C3'	-2.40	1.37	1.43
16	A	1131	CLA	C3B-C4B	2.40	1.49	1.42
16	B	1212	CLA	C1B-C2B	2.40	1.48	1.43
16	n	511	CLA	C3B-C4B	2.40	1.49	1.42
16	B	1205	CLA	C1B-C2B	2.40	1.48	1.43
16	G	1212	CLA	CHC-C1C	2.40	1.43	1.38
16	x	503	CLA	CHC-C1C	2.40	1.43	1.38
16	b	1211	CLA	C1B-C2B	2.40	1.48	1.43
16	u	505	CLA	C1B-C2B	2.40	1.48	1.43
16	a	1139	CLA	C3B-C4B	2.40	1.49	1.42
16	G	1221	CLA	C1B-C2B	2.40	1.48	1.43
16	g	513	CLA	C3B-C4B	2.40	1.49	1.42
16	p	513	CLA	C3B-C4B	2.40	1.49	1.42
16	A	1111	CLA	C1B-C2B	2.40	1.48	1.43
16	b	1220	CLA	CHC-C1C	2.40	1.43	1.38
16	w	508	CLA	C1B-C2B	2.40	1.48	1.43
16	b	1211	CLA	CHC-C1C	2.40	1.43	1.38
16	n	514	CLA	C3B-C4B	2.40	1.49	1.42
16	Y	502	CLA	C1B-C2B	2.40	1.48	1.43
21	b	4006	ECH	C2-C1	2.40	1.59	1.54
16	t	502	CLA	C3B-C4B	2.40	1.49	1.42
16	a	1117	CLA	C3B-C4B	2.40	1.49	1.42
16	x	505	CLA	C1B-C2B	2.40	1.48	1.43
21	R	4020	ECH	C5-C6	2.40	1.38	1.34
16	H	1104	CLA	C1B-C2B	2.40	1.48	1.43
16	G	1219	CLA	C3B-C4B	2.40	1.49	1.42
16	x	505	CLA	C3B-C4B	2.40	1.49	1.42
16	B	1214	CLA	C3B-C4B	2.40	1.49	1.42
16	s	508	CLA	C1B-C2B	2.40	1.48	1.43
16	A	1130	CLA	C3B-C4B	2.40	1.49	1.42
16	U	1503	CLA	C1B-C2B	2.40	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	x	516	CLA	C3B-C4B	2.40	1.49	1.42
16	G	1203	CLA	C1B-C2B	2.40	1.48	1.43
16	Y	513	CLA	C3B-C4B	2.40	1.49	1.42
16	A	1134	CLA	CHC-C1C	2.40	1.43	1.38
16	B	1211	CLA	CHC-C1C	2.40	1.43	1.38
16	a	1121	CLA	C3B-C4B	2.40	1.49	1.42
16	H	1137	CLA	C1B-C2B	2.40	1.48	1.43
16	H	1129	CLA	CHC-C1C	2.40	1.43	1.38
16	q	516	CLA	C1B-C2B	2.39	1.48	1.43
16	a	1801	CLA	C1B-C2B	2.39	1.48	1.43
20	A	4202	LMT	O2'-C2'	-2.39	1.37	1.43
16	U	1501	CLA	C3B-C4B	2.39	1.49	1.42
13	a	849	LHG	O7-C5	-2.39	1.41	1.46
16	Z	505	CLA	C1B-C2B	2.39	1.48	1.43
16	B	1231	CLA	C3B-C4B	2.39	1.49	1.42
16	U	1503	CLA	C3B-C4B	2.39	1.49	1.42
16	g	501	CLA	C3B-C4B	2.39	1.49	1.42
16	a	1126	CLA	C1B-C2B	2.39	1.48	1.43
16	o	517	CLA	C3B-C4B	2.39	1.49	1.42
16	b	1212	CLA	C3B-C4B	2.39	1.49	1.42
16	G	1023	CLA	MG-ND	-2.39	2.01	2.05
16	Y	508	CLA	C3B-C4B	2.39	1.49	1.42
16	y	510	CLA	C3B-C4B	2.39	1.49	1.42
16	A	1129	CLA	CHC-C1C	2.39	1.43	1.38
16	B	1236	CLA	C1B-C2B	2.39	1.48	1.43
16	Y	503	CLA	C3B-C4B	2.39	1.49	1.42
16	l	1501	CLA	C3B-C4B	2.39	1.49	1.42
16	s	505	CLA	C1B-C2B	2.39	1.48	1.43
16	x	502	CLA	C3B-C4B	2.39	1.49	1.42
16	H	1117	CLA	C3B-C4B	2.39	1.49	1.42
16	X	502	CLA	C3B-C4B	2.39	1.49	1.42
16	o	502	CLA	C1B-C2B	2.39	1.48	1.43
16	b	1227	CLA	CHC-C1C	2.39	1.43	1.38
16	v	503	CLA	C3B-C4B	2.39	1.49	1.42
16	H	1138	CLA	C1B-C2B	2.39	1.48	1.43
16	Y	508	CLA	C1B-C2B	2.39	1.48	1.43
20	H	4202	LMT	O2'-C2'	-2.39	1.37	1.43
16	a	1101	CLA	C3B-C4B	2.39	1.49	1.42
16	b	1202	CLA	CHC-C1C	2.39	1.43	1.38
16	p	503	CLA	C1B-C2B	2.39	1.48	1.43
16	T	4002	CLA	C3B-C4B	2.39	1.49	1.42
16	y	513	CLA	C3B-C4B	2.39	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	f	1302	CLA	C3B-C4B	2.39	1.49	1.42
16	x	511	CLA	C3B-C4B	2.39	1.49	1.42
16	B	1216	CLA	CHC-C1C	2.39	1.43	1.38
16	x	513	CLA	C3B-C4B	2.39	1.49	1.42
16	s	508	CLA	C3B-C4B	2.39	1.49	1.42
16	H	1117	CLA	CHC-C1C	2.39	1.43	1.38
16	u	506	CLA	MG-ND	-2.39	2.01	2.05
16	h	507	CLA	C3B-C4B	2.39	1.49	1.42
16	y	515	CLA	C3B-C4B	2.39	1.49	1.42
16	Z	508	CLA	C1B-C2B	2.39	1.48	1.43
16	w	517	CLA	CHC-C1C	2.39	1.43	1.38
16	q	503	CLA	MG-ND	-2.39	2.01	2.05
16	B	1236	CLA	C3B-C4B	2.39	1.49	1.42
16	b	1210	CLA	CHC-C1C	2.39	1.43	1.38
16	a	1105	CLA	C3B-C4B	2.39	1.49	1.42
16	Z	502	CLA	C3B-C4B	2.38	1.49	1.42
16	a	1131	CLA	C3B-C4B	2.38	1.49	1.42
16	p	509	CLA	C3B-C4B	2.38	1.49	1.42
16	h	503	CLA	C3B-C4B	2.38	1.49	1.42
16	G	1202	CLA	C1B-C2B	2.38	1.48	1.43
16	a	1110	CLA	C1B-C2B	2.38	1.48	1.43
16	Y	509	CLA	C3B-C4B	2.38	1.49	1.42
16	u	509	CLA	C3B-C4B	2.38	1.49	1.42
16	v	513	CLA	C3B-C4B	2.38	1.49	1.42
16	B	1212	CLA	CHC-C1C	2.38	1.43	1.38
16	B	1212	CLA	C3B-C4B	2.38	1.49	1.42
16	b	1221	CLA	CHC-C1C	2.38	1.43	1.38
16	G	1203	CLA	C3B-C4B	2.38	1.49	1.42
16	G	1212	CLA	C3B-C4B	2.38	1.49	1.42
20	l	4101	LMT	O3'-C3'	-2.38	1.37	1.43
16	Y	515	CLA	C3B-C4B	2.38	1.49	1.42
16	b	1212	CLA	C1B-C2B	2.38	1.48	1.43
16	H	1130	CLA	C3B-C4B	2.38	1.49	1.42
16	a	1123	CLA	C1B-C2B	2.38	1.48	1.43
16	A	1801	CLA	C3B-C4B	2.38	1.49	1.42
16	q	516	CLA	C3B-C4B	2.38	1.49	1.42
16	H	1124	CLA	C1B-C2B	2.38	1.48	1.43
16	b	1210	CLA	C3B-C4B	2.38	1.49	1.42
16	A	1105	CLA	C1B-C2B	2.38	1.48	1.43
16	a	1129	CLA	CHC-C1C	2.38	1.43	1.38
16	w	504	CLA	C3B-C4B	2.38	1.49	1.42
16	y	507	CLA	C3B-C4B	2.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	u	502	CLA	C1B-C2B	2.38	1.48	1.43
16	h	501	CLA	CHC-C1C	2.38	1.43	1.38
16	v	504	CLA	C3B-C4B	2.38	1.49	1.42
16	x	509	CLA	CHC-C1C	2.38	1.43	1.38
16	W	513	CLA	C3B-C4B	2.38	1.49	1.42
16	o	516	CLA	CHC-C1C	2.38	1.43	1.38
16	A	1135	CLA	C1B-C2B	2.38	1.48	1.43
16	y	503	CLA	C3B-C4B	2.38	1.49	1.42
16	H	1132	CLA	C1B-C2B	2.38	1.48	1.43
16	W	511	CLA	CHC-C1C	2.38	1.43	1.38
16	g	502	CLA	C3B-C4B	2.37	1.49	1.42
16	Y	505	CLA	C3B-C4B	2.37	1.49	1.42
16	x	511	CLA	C1B-C2B	2.37	1.48	1.43
16	A	1125	CLA	C3B-C4B	2.37	1.49	1.42
16	g	509	CLA	CHC-C1C	2.37	1.43	1.38
16	a	1140	CLA	C3B-C4B	2.37	1.49	1.42
16	s	513	CLA	C3B-C4B	2.37	1.49	1.42
16	G	1202	CLA	CHC-C1C	2.37	1.43	1.38
16	H	1126	CLA	C1B-C2B	2.37	1.48	1.43
16	Q	1301	CLA	C3B-C4B	2.37	1.49	1.42
16	g	508	CLA	C3B-C4B	2.37	1.49	1.42
16	B	1213	CLA	CHC-C1C	2.37	1.43	1.38
16	A	1013	CLA	C3B-C4B	2.37	1.49	1.42
16	B	1234	CLA	C3B-C4B	2.37	1.49	1.42
16	Y	502	CLA	C3B-C4B	2.37	1.49	1.42
16	g	516	CLA	C3B-C4B	2.37	1.49	1.42
16	K	4002	CLA	C3B-C4B	2.37	1.49	1.42
16	l	1502	CLA	C3B-C4B	2.37	1.49	1.42
16	u	503	CLA	CHC-C1C	2.37	1.43	1.38
16	T	4003	CLA	C3B-C4B	2.37	1.49	1.42
16	x	501	CLA	C3B-C4B	2.37	1.49	1.42
16	v	503	CLA	CHC-C1C	2.37	1.43	1.38
16	b	1211	CLA	C3B-C4B	2.37	1.49	1.42
16	r	502	CLA	C3B-C4B	2.37	1.49	1.42
16	q	513	CLA	C3B-C4B	2.37	1.49	1.42
16	X	509	CLA	C1B-C2B	2.37	1.48	1.43
16	b	1222	CLA	CHC-C1C	2.37	1.43	1.38
16	p	503	CLA	C3B-C4B	2.37	1.49	1.42
16	v	505	CLA	C3B-C4B	2.37	1.49	1.42
16	g	502	CLA	C1B-C2B	2.37	1.48	1.43
16	B	1219	CLA	C3B-C4B	2.37	1.49	1.42
16	q	512	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	r	501	CLA	C3B-C4B	2.37	1.49	1.42
16	b	1202	CLA	C3B-C4B	2.37	1.49	1.42
16	Z	505	CLA	C3B-C4B	2.37	1.49	1.42
16	b	1235	CLA	C3B-C4B	2.37	1.49	1.42
16	A	1120	CLA	C1B-C2B	2.37	1.48	1.43
16	s	503	CLA	C1B-C2B	2.37	1.48	1.43
16	B	1209	CLA	C3B-C4B	2.37	1.49	1.42
16	x	509	CLA	C3B-C4B	2.37	1.49	1.42
16	H	1112	CLA	C1B-C2B	2.37	1.48	1.43
16	w	504	CLA	C1B-C2B	2.37	1.48	1.43
16	B	1201	CLA	C3B-C4B	2.37	1.49	1.42
16	b	1203	CLA	C3B-C4B	2.37	1.49	1.42
16	h	502	CLA	C3B-C4B	2.37	1.49	1.42
16	H	1237	CLA	C3B-C4B	2.37	1.49	1.42
16	A	1139	CLA	C1B-C2B	2.37	1.48	1.43
16	H	1111	CLA	C3B-C4B	2.37	1.49	1.42
16	y	517	CLA	C3B-C4B	2.37	1.49	1.42
16	B	1227	CLA	C3B-C4B	2.36	1.49	1.42
16	y	504	CLA	C3B-C4B	2.36	1.49	1.42
16	k	4003	CLA	C3B-C4B	2.36	1.49	1.42
16	r	505	CLA	C3B-C4B	2.36	1.49	1.42
16	H	1139	CLA	CHC-C1C	2.36	1.43	1.38
16	o	510	CLA	C3B-C4B	2.36	1.49	1.42
16	s	509	CLA	C3B-C4B	2.36	1.49	1.42
16	s	517	CLA	C3B-C4B	2.36	1.49	1.42
16	w	508	CLA	C3B-C4B	2.36	1.49	1.42
16	w	516	CLA	C1B-C2B	2.36	1.48	1.43
16	H	1120	CLA	C3B-C4B	2.36	1.49	1.42
16	Z	508	CLA	C3B-C4B	2.36	1.49	1.42
16	v	507	CLA	C3B-C4B	2.36	1.49	1.42
16	A	1117	CLA	C3B-C4B	2.36	1.49	1.42
16	p	503	CLA	CHC-C1C	2.36	1.43	1.38
16	s	503	CLA	C3B-C4B	2.36	1.49	1.42
16	u	516	CLA	C3B-C4B	2.36	1.49	1.42
16	n	505	CLA	C3B-C4B	2.36	1.49	1.42
16	o	509	CLA	C3B-C4B	2.36	1.49	1.42
16	o	503	CLA	CHC-C1C	2.36	1.43	1.38
16	A	1105	CLA	C3B-C4B	2.36	1.49	1.42
16	Z	510	CLA	C3B-C4B	2.36	1.49	1.42
16	B	1235	CLA	CHC-C1C	2.36	1.43	1.38
16	X	508	CLA	C3B-C4B	2.36	1.49	1.42
16	a	1106	CLA	CHC-C1C	2.36	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	h	513	CLA	C3B-C4B	2.36	1.49	1.42
16	n	511	CLA	CHC-C1C	2.36	1.43	1.38
16	B	1023	CLA	CHC-C1C	2.36	1.43	1.38
16	A	1114	CLA	C3B-C4B	2.36	1.49	1.42
16	B	1225	CLA	C3B-C4B	2.36	1.49	1.42
16	r	508	CLA	C3B-C4B	2.36	1.49	1.42
16	X	513	CLA	C3B-C4B	2.36	1.49	1.42
16	b	1224	CLA	C1B-C2B	2.36	1.48	1.43
16	h	505	CLA	CHC-C1C	2.36	1.43	1.38
16	x	505	CLA	CHC-C1C	2.36	1.43	1.38
16	y	516	CLA	CHC-C1C	2.36	1.43	1.38
16	A	1101	CLA	C1B-C2B	2.36	1.48	1.43
16	a	1135	CLA	C1B-C2B	2.36	1.48	1.43
16	b	1203	CLA	C1B-C2B	2.36	1.48	1.43
16	v	505	CLA	CHC-C1C	2.36	1.43	1.38
16	s	505	CLA	C3B-C4B	2.36	1.49	1.42
16	H	1105	CLA	C3B-C4B	2.35	1.49	1.42
16	t	514	CLA	C3B-C4B	2.35	1.49	1.42
16	v	514	CLA	C3B-C4B	2.35	1.49	1.42
16	A	1116	CLA	CHC-C1C	2.35	1.43	1.38
16	a	1013	CLA	CHC-C1C	2.35	1.43	1.38
16	h	503	CLA	CHC-C1C	2.35	1.43	1.38
16	t	509	CLA	CHC-C1C	2.35	1.43	1.38
16	Z	502	CLA	C1B-C2B	2.35	1.48	1.43
16	f	1301	CLA	C1B-C2B	2.35	1.48	1.43
16	t	503	CLA	C3B-C4B	2.35	1.49	1.42
16	u	508	CLA	C3B-C4B	2.35	1.49	1.42
16	v	517	CLA	C3B-C4B	2.35	1.49	1.42
16	W	514	CLA	C3B-C4B	2.35	1.49	1.42
16	v	508	CLA	CHC-C1C	2.35	1.43	1.38
16	b	1023	CLA	MG-NB	-2.35	2.01	2.05
16	Z	510	CLA	C1B-C2B	2.35	1.48	1.43
16	Q	1302	CLA	C3B-C4B	2.35	1.49	1.42
16	Z	516	CLA	C3B-C4B	2.35	1.49	1.42
16	q	508	CLA	CHC-C1C	2.35	1.43	1.38
16	A	1127	CLA	C1B-C2B	2.35	1.48	1.43
16	X	517	CLA	C3B-C4B	2.35	1.49	1.42
16	b	1209	CLA	C3B-C4B	2.35	1.49	1.42
16	n	502	CLA	C3B-C4B	2.35	1.49	1.42
16	y	509	CLA	C3B-C4B	2.35	1.49	1.42
16	H	1139	CLA	C1B-C2B	2.35	1.48	1.43
16	b	1236	CLA	C3B-C4B	2.35	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1101	CLA	C1B-C2B	2.35	1.48	1.43
16	K	4003	CLA	C3B-C4B	2.35	1.49	1.42
16	W	501	CLA	C3B-C4B	2.35	1.49	1.42
16	y	503	CLA	CHC-C1C	2.35	1.43	1.38
16	X	505	CLA	C1B-C2B	2.35	1.48	1.43
16	B	1023	CLA	C3B-C4B	2.35	1.49	1.42
16	B	1202	CLA	C3B-C4B	2.35	1.49	1.42
16	b	1234	CLA	CHC-C1C	2.35	1.43	1.38
16	x	511	CLA	CHC-C1C	2.35	1.43	1.38
16	W	502	CLA	C3B-C4B	2.35	1.49	1.42
16	H	1123	CLA	C3B-C4B	2.35	1.49	1.42
16	g	514	CLA	C3B-C4B	2.35	1.49	1.42
16	w	517	CLA	C3B-C4B	2.35	1.49	1.42
16	o	505	CLA	C3B-C4B	2.35	1.49	1.42
16	s	515	CLA	C3B-C4B	2.35	1.49	1.42
16	o	511	CLA	CHC-C1C	2.35	1.43	1.38
16	X	509	CLA	C3B-C4B	2.35	1.49	1.42
16	a	1120	CLA	C3B-C4B	2.35	1.49	1.42
16	v	511	CLA	CHC-C1C	2.35	1.43	1.38
16	A	1127	CLA	C3B-C4B	2.35	1.49	1.42
16	a	1109	CLA	C3B-C4B	2.35	1.49	1.42
16	r	517	CLA	C3B-C4B	2.35	1.49	1.42
16	s	504	CLA	C3B-C4B	2.35	1.49	1.42
16	h	515	CLA	C1B-C2B	2.35	1.48	1.43
16	u	517	CLA	C3B-C4B	2.35	1.49	1.42
16	A	1136	CLA	C3B-C4B	2.35	1.49	1.42
16	b	1023	CLA	MG-ND	-2.35	2.01	2.05
16	b	1234	CLA	C1B-C2B	2.35	1.48	1.43
16	v	502	CLA	C1B-C2B	2.35	1.48	1.43
16	o	503	CLA	C3B-C4B	2.35	1.49	1.42
16	r	516	CLA	C3B-C4B	2.35	1.49	1.42
16	G	1219	CLA	CHC-C1C	2.35	1.43	1.38
16	x	508	CLA	C3B-C4B	2.34	1.49	1.42
16	h	505	CLA	C3B-C4B	2.34	1.49	1.42
16	G	1210	CLA	CHC-C1C	2.34	1.43	1.38
16	b	1232	CLA	C1B-C2B	2.34	1.48	1.43
16	A	1123	CLA	C3B-C4B	2.34	1.49	1.42
16	t	504	CLA	C3B-C4B	2.34	1.49	1.42
16	p	505	CLA	C1B-C2B	2.34	1.48	1.43
16	w	516	CLA	C3B-C4B	2.34	1.49	1.42
16	B	1213	CLA	C3B-C4B	2.34	1.49	1.42
16	B	1222	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1215	CLA	C1B-C2B	2.34	1.48	1.43
16	H	1106	CLA	C3B-C4B	2.34	1.49	1.42
16	t	517	CLA	C3B-C4B	2.34	1.49	1.42
16	A	1134	CLA	C1B-C2B	2.34	1.48	1.43
16	b	1210	CLA	C1B-C2B	2.34	1.48	1.43
16	G	1203	CLA	CHC-C1C	2.34	1.43	1.38
16	H	1134	CLA	CHC-C1C	2.34	1.43	1.38
16	A	1126	CLA	C1B-C2B	2.34	1.48	1.43
16	B	1229	CLA	C3B-C4B	2.34	1.49	1.42
16	W	503	CLA	C3B-C4B	2.34	1.49	1.42
16	H	1136	CLA	C3B-C4B	2.34	1.49	1.42
16	A	1130	CLA	CHC-C1C	2.34	1.43	1.38
16	A	1013	CLA	MG-ND	-2.34	2.01	2.05
16	G	1238	CLA	C1B-C2B	2.34	1.48	1.43
16	w	505	CLA	C1B-C2B	2.34	1.48	1.43
16	A	1124	CLA	C3B-C4B	2.34	1.49	1.42
16	a	1112	CLA	C1B-C2B	2.34	1.48	1.43
16	a	1237	CLA	C3B-C4B	2.34	1.49	1.42
16	b	1234	CLA	C3B-C4B	2.34	1.49	1.42
16	G	1227	CLA	C3B-C4B	2.34	1.49	1.42
16	a	1112	CLA	C3B-C4B	2.34	1.49	1.42
16	B	1225	CLA	CHC-C1C	2.34	1.43	1.38
16	o	509	CLA	C1B-C2B	2.34	1.48	1.43
16	s	512	CLA	C1B-C2B	2.34	1.48	1.43
16	v	509	CLA	C3B-C4B	2.34	1.49	1.42
16	A	1111	CLA	MG-ND	-2.34	2.01	2.05
16	t	509	CLA	C1B-C2B	2.34	1.48	1.43
16	G	1214	CLA	C3B-C4B	2.34	1.49	1.42
16	X	512	CLA	C3B-C4B	2.34	1.49	1.42
16	H	1119	CLA	CHC-C1C	2.34	1.43	1.38
16	X	505	CLA	CHC-C1C	2.34	1.43	1.38
16	G	1229	CLA	C3B-C4B	2.34	1.49	1.42
16	W	517	CLA	C3B-C4B	2.34	1.49	1.42
16	o	515	CLA	C3B-C4B	2.34	1.49	1.42
16	a	1105	CLA	C1B-C2B	2.34	1.48	1.43
16	p	516	CLA	C3B-C4B	2.34	1.49	1.42
16	r	504	CLA	C3B-C4B	2.34	1.49	1.42
16	h	508	CLA	C3B-C4B	2.34	1.49	1.42
16	a	1105	CLA	CHC-C1C	2.34	1.43	1.38
16	g	511	CLA	C1B-C2B	2.33	1.48	1.43
16	b	1239	CLA	C3B-C4B	2.33	1.49	1.42
16	n	503	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	512	CLA	C1B-C2B	2.33	1.48	1.43
16	G	1218	CLA	C3B-C4B	2.33	1.49	1.42
16	s	516	CLA	C3B-C4B	2.33	1.49	1.42
16	H	1127	CLA	CHC-C1C	2.33	1.43	1.38
16	r	503	CLA	CHC-C1C	2.33	1.43	1.38
19	A	4007	BCR	C33-C5	-2.33	1.47	1.50
16	A	1103	CLA	C3B-C4B	2.33	1.49	1.42
16	b	1213	CLA	C3B-C4B	2.33	1.49	1.42
16	p	505	CLA	C3B-C4B	2.33	1.49	1.42
16	A	1139	CLA	C3B-C4B	2.33	1.49	1.42
16	B	1216	CLA	C3B-C4B	2.33	1.49	1.42
16	G	1012	CLA	CHC-C1C	2.33	1.43	1.38
16	n	509	CLA	C1B-C2B	2.33	1.48	1.43
16	q	508	CLA	C3B-C4B	2.33	1.49	1.42
16	s	503	CLA	CHC-C1C	2.33	1.43	1.38
16	B	1225	CLA	C1B-C2B	2.33	1.48	1.43
16	G	1232	CLA	C1B-C2B	2.33	1.48	1.43
16	Y	515	CLA	CHC-C1C	2.33	1.43	1.38
16	t	513	CLA	CHC-C1C	2.33	1.43	1.38
16	b	1232	CLA	C3B-C4B	2.33	1.49	1.42
16	G	1205	CLA	C1B-C2B	2.33	1.48	1.43
16	G	1221	CLA	C3B-C4B	2.33	1.49	1.42
13	g	605	LHG	P-O6	2.33	1.68	1.59
16	L	1502	CLA	C1B-C2B	2.33	1.48	1.43
16	B	1222	CLA	C3B-C4B	2.33	1.49	1.42
16	h	514	CLA	C3B-C4B	2.33	1.49	1.42
16	y	501	CLA	CHC-C1C	2.33	1.43	1.38
16	g	504	CLA	C3B-C4B	2.33	1.49	1.42
16	v	515	CLA	C3B-C4B	2.33	1.49	1.42
16	G	1220	CLA	C3B-C4B	2.33	1.49	1.42
16	t	503	CLA	CHC-C1C	2.33	1.43	1.38
16	H	1122	CLA	C3B-C4B	2.33	1.49	1.42
16	G	1216	CLA	C1B-C2B	2.33	1.48	1.43
16	Y	505	CLA	C1B-C2B	2.33	1.48	1.43
16	A	1117	CLA	CHC-C1C	2.33	1.43	1.38
16	G	1211	CLA	C3B-C4B	2.33	1.49	1.42
16	A	1127	CLA	CHC-C1C	2.33	1.43	1.38
16	y	516	CLA	C3B-C4B	2.33	1.49	1.42
16	G	1235	CLA	CHC-C1C	2.33	1.43	1.38
16	g	511	CLA	CHC-C1C	2.33	1.43	1.38
16	b	1240	CLA	C3B-C4B	2.33	1.49	1.42
16	y	502	CLA	C3B-C4B	2.33	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1101	CLA	CHC-C1C	2.33	1.43	1.38
16	A	1118	CLA	C3B-C4B	2.33	1.49	1.42
16	f	1302	CLA	CHC-C1C	2.33	1.43	1.38
16	h	512	CLA	C3B-C4B	2.33	1.49	1.42
16	s	502	CLA	C3B-C4B	2.33	1.49	1.42
16	t	513	CLA	C3B-C4B	2.33	1.49	1.42
16	G	1230	CLA	C3B-C4B	2.33	1.49	1.42
16	X	502	CLA	C1B-C2B	2.33	1.48	1.43
16	s	515	CLA	CHC-C1C	2.33	1.43	1.38
16	o	512	CLA	C3B-C4B	2.33	1.49	1.42
16	s	517	CLA	CHC-C1C	2.33	1.43	1.38
16	G	1238	CLA	C3B-C4B	2.32	1.49	1.42
16	b	1214	CLA	C3B-C4B	2.32	1.49	1.42
16	G	1229	CLA	CHC-C1C	2.32	1.43	1.38
16	a	1132	CLA	C3B-C4B	2.32	1.49	1.42
16	p	512	CLA	C1B-C2B	2.32	1.48	1.43
16	q	502	CLA	C1B-C2B	2.32	1.48	1.43
16	o	508	CLA	C3B-C4B	2.32	1.49	1.42
16	y	505	CLA	C3B-C4B	2.32	1.49	1.42
16	w	511	CLA	C1B-C2B	2.32	1.48	1.43
16	F	1302	CLA	C3B-C4B	2.32	1.49	1.42
16	h	516	CLA	C3B-C4B	2.32	1.49	1.42
16	W	513	CLA	CHC-C1C	2.32	1.43	1.38
16	n	509	CLA	CHC-C1C	2.32	1.43	1.38
16	y	505	CLA	CHC-C1C	2.32	1.43	1.38
16	B	1228	CLA	C3B-C4B	2.32	1.49	1.42
16	X	514	CLA	C3B-C4B	2.32	1.49	1.42
16	a	1103	CLA	C3B-C4B	2.32	1.49	1.42
16	b	1219	CLA	C3B-C4B	2.32	1.49	1.42
16	G	1222	CLA	C3B-C4B	2.32	1.49	1.42
16	b	1228	CLA	C3B-C4B	2.32	1.49	1.42
16	y	512	CLA	C3B-C4B	2.32	1.49	1.42
16	L	1501	CLA	CHC-C1C	2.32	1.43	1.38
16	p	514	CLA	CHC-C1C	2.32	1.43	1.38
16	a	1115	CLA	C3B-C4B	2.32	1.49	1.42
16	r	511	CLA	CHC-C1C	2.32	1.43	1.38
16	v	504	CLA	CHC-C1C	2.32	1.43	1.38
16	L	1503	CLA	CHC-C1C	2.32	1.43	1.38
16	B	1211	CLA	C3B-C4B	2.32	1.49	1.42
16	t	511	CLA	CHC-C1C	2.32	1.43	1.38
16	A	1102	CLA	C1B-C2B	2.32	1.48	1.43
16	a	1801	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1125	CLA	CHC-C1C	2.32	1.43	1.38
16	B	1238	CLA	C3B-C4B	2.32	1.49	1.42
16	r	515	CLA	C3B-C4B	2.32	1.49	1.42
16	B	1224	CLA	C1B-C2B	2.32	1.48	1.43
16	l	1501	CLA	C1B-C2B	2.32	1.48	1.43
16	w	505	CLA	C3B-C4B	2.32	1.49	1.42
16	y	514	CLA	C3B-C4B	2.32	1.49	1.42
16	H	1105	CLA	C1B-C2B	2.32	1.48	1.43
16	p	514	CLA	C3B-C4B	2.32	1.49	1.42
16	l	1503	CLA	C1B-C2B	2.32	1.48	1.43
16	H	1103	CLA	C3B-C4B	2.32	1.49	1.42
16	H	1112	CLA	C3B-C4B	2.32	1.49	1.42
16	Y	517	CLA	C3B-C4B	2.32	1.49	1.42
16	q	517	CLA	C3B-C4B	2.32	1.49	1.42
16	W	504	CLA	C3B-C4B	2.32	1.49	1.42
16	w	515	CLA	C3B-C4B	2.32	1.49	1.42
16	W	503	CLA	CHC-C1C	2.32	1.43	1.38
16	o	516	CLA	C3B-C4B	2.31	1.49	1.42
16	a	1138	CLA	C1B-C2B	2.31	1.48	1.43
16	B	1219	CLA	CHC-C1C	2.31	1.43	1.38
16	H	1109	CLA	C3B-C4B	2.31	1.49	1.42
16	h	504	CLA	C3B-C4B	2.31	1.49	1.42
16	a	1130	CLA	C3B-C4B	2.31	1.49	1.42
16	B	1221	CLA	CHC-C1C	2.31	1.43	1.38
16	g	503	CLA	CHC-C1C	2.31	1.43	1.38
16	G	1227	CLA	CHC-C1C	2.31	1.43	1.38
16	y	504	CLA	CHC-C1C	2.31	1.43	1.38
15	A	1011	CL0	C1D-C2D	2.31	1.42	1.39
16	a	1101	CLA	CHC-C1C	2.31	1.43	1.38
16	A	1112	CLA	C3B-C4B	2.31	1.49	1.42
16	v	516	CLA	C3B-C4B	2.31	1.49	1.42
16	F	1302	CLA	CHC-C1C	2.31	1.43	1.38
16	a	1139	CLA	CHC-C1C	2.31	1.43	1.38
16	t	505	CLA	C3B-C4B	2.31	1.49	1.42
16	v	508	CLA	C3B-C4B	2.31	1.49	1.42
16	b	1201	CLA	C3B-C4B	2.31	1.49	1.42
16	A	1109	CLA	C3B-C4B	2.31	1.49	1.42
16	y	506	CLA	C3B-C4B	2.31	1.49	1.42
16	G	1225	CLA	CHC-C1C	2.31	1.43	1.38
16	a	1132	CLA	C1B-C2B	2.31	1.48	1.43
16	t	512	CLA	C3B-C4B	2.31	1.49	1.42
16	u	505	CLA	CHC-C1C	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	w	511	CLA	CHC-C1C	2.31	1.43	1.38
16	q	514	CLA	C3B-C4B	2.31	1.49	1.42
16	a	1130	CLA	C1B-C2B	2.31	1.48	1.43
16	X	514	CLA	CHC-C1C	2.31	1.43	1.38
16	v	509	CLA	CHC-C1C	2.31	1.43	1.38
16	b	1235	CLA	CHC-C1C	2.31	1.43	1.38
16	p	502	CLA	C3B-C4B	2.31	1.49	1.42
16	L	1502	CLA	C3B-C4B	2.31	1.49	1.42
16	Y	511	CLA	CHC-C1C	2.31	1.43	1.38
16	H	1139	CLA	C3B-C4B	2.31	1.49	1.42
16	r	514	CLA	C3B-C4B	2.31	1.49	1.42
16	Z	516	CLA	CHC-C1C	2.31	1.43	1.38
16	G	1023	CLA	C3B-C4B	2.31	1.49	1.42
16	G	1209	CLA	C3B-C4B	2.30	1.49	1.42
16	G	1236	CLA	C3B-C4B	2.30	1.49	1.42
16	G	1234	CLA	CHC-C1C	2.30	1.43	1.38
16	Y	504	CLA	C3B-C4B	2.30	1.49	1.42
16	b	1218	CLA	C3B-C4B	2.30	1.49	1.42
16	w	512	CLA	C1B-C2B	2.30	1.48	1.43
16	a	1123	CLA	C3B-C4B	2.30	1.49	1.42
16	G	1213	CLA	C3B-C4B	2.30	1.49	1.42
16	H	1106	CLA	CHC-C1C	2.30	1.43	1.38
16	Z	517	CLA	CHC-C1C	2.30	1.43	1.38
16	u	513	CLA	CHC-C1C	2.30	1.43	1.38
16	X	515	CLA	C3B-C4B	2.30	1.49	1.42
16	p	501	CLA	C3B-C4B	2.30	1.49	1.42
16	x	504	CLA	C3B-C4B	2.30	1.49	1.42
16	p	504	CLA	C3B-C4B	2.30	1.49	1.42
16	n	514	CLA	CHC-C1C	2.30	1.43	1.38
16	G	1216	CLA	CHC-C1C	2.30	1.43	1.38
16	b	1203	CLA	CHC-C1C	2.30	1.43	1.38
16	u	514	CLA	C3B-C4B	2.30	1.49	1.42
16	U	1502	CLA	C1B-C2B	2.30	1.48	1.43
16	a	1139	CLA	C1B-C2B	2.30	1.48	1.43
16	p	512	CLA	C3B-C4B	2.30	1.49	1.42
16	x	515	CLA	C3B-C4B	2.30	1.49	1.42
16	H	1104	CLA	C3B-C4B	2.30	1.49	1.42
16	a	1138	CLA	C3B-C4B	2.30	1.49	1.42
16	g	515	CLA	C3B-C4B	2.30	1.49	1.42
16	A	1132	CLA	C1B-C2B	2.30	1.48	1.43
16	B	1210	CLA	C1B-C2B	2.30	1.48	1.43
16	A	1111	CLA	CHC-C1C	2.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	o	505	CLA	CHC-C1C	2.30	1.43	1.38
16	t	501	CLA	C3B-C4B	2.30	1.49	1.42
16	B	1234	CLA	CHC-C1C	2.30	1.43	1.38
16	s	514	CLA	CHC-C1C	2.30	1.43	1.38
16	q	516	CLA	CHC-C1C	2.30	1.43	1.38
16	G	1228	CLA	C3B-C4B	2.30	1.49	1.42
16	h	508	CLA	CHC-C1C	2.30	1.43	1.38
16	B	1227	CLA	C1B-C2B	2.30	1.48	1.43
16	s	501	CLA	C3B-C4B	2.30	1.49	1.42
16	q	509	CLA	C1B-C2B	2.30	1.48	1.43
16	G	1232	CLA	C3B-C4B	2.30	1.49	1.42
16	H	1127	CLA	C3B-C4B	2.30	1.49	1.42
16	U	1501	CLA	C1B-C2B	2.30	1.48	1.43
16	J	1303	CLA	CHC-C1C	2.30	1.43	1.38
16	x	516	CLA	CHC-C1C	2.30	1.43	1.38
16	A	1133	CLA	C3B-C4B	2.30	1.49	1.42
16	H	1113	CLA	C3B-C4B	2.30	1.49	1.42
16	B	1232	CLA	C3B-C4B	2.30	1.49	1.42
16	A	1121	CLA	CHC-C1C	2.30	1.43	1.38
16	W	514	CLA	CHC-C1C	2.30	1.43	1.38
16	Z	504	CLA	CHC-C1C	2.30	1.43	1.38
16	B	1226	CLA	MG-NB	-2.30	2.01	2.05
16	n	513	CLA	C3B-C4B	2.30	1.49	1.42
16	t	510	CLA	C3B-C4B	2.30	1.49	1.42
16	n	503	CLA	CHC-C1C	2.30	1.43	1.38
16	Z	504	CLA	C3B-C4B	2.30	1.49	1.42
16	J	1302	CLA	CHC-C1C	2.30	1.43	1.38
16	b	1224	CLA	CHC-C1C	2.30	1.43	1.38
16	b	1217	CLA	C3B-C4B	2.30	1.49	1.42
16	H	1104	CLA	CHC-C1C	2.30	1.43	1.38
16	h	516	CLA	CHC-C1C	2.30	1.43	1.38
16	H	1102	CLA	C1B-C2B	2.29	1.48	1.43
16	Z	514	CLA	C3B-C4B	2.29	1.49	1.42
16	G	1215	CLA	C1B-C2B	2.29	1.48	1.43
16	A	1111	CLA	C3B-C4B	2.29	1.49	1.42
16	p	515	CLA	C3B-C4B	2.29	1.49	1.42
16	s	514	CLA	C3B-C4B	2.29	1.49	1.42
16	B	1231	CLA	CHC-C1C	2.29	1.43	1.38
16	n	504	CLA	C3B-C4B	2.29	1.49	1.42
16	q	505	CLA	C3B-C4B	2.29	1.49	1.42
16	u	501	CLA	C3B-C4B	2.29	1.49	1.42
16	g	517	CLA	CHC-C1C	2.29	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	4004	CLA	C3B-C4B	2.29	1.49	1.42
16	W	505	CLA	CHC-C1C	2.29	1.43	1.38
16	H	1104	CLA	MG-NB	-2.29	2.01	2.05
16	y	503	CLA	MG-NB	-2.29	2.01	2.05
16	G	1205	CLA	C3B-C4B	2.29	1.49	1.42
16	X	511	CLA	CHC-C1C	2.29	1.43	1.38
16	Y	516	CLA	C3B-C4B	2.29	1.49	1.42
16	B	1218	CLA	C3B-C4B	2.29	1.49	1.42
16	u	515	CLA	C3B-C4B	2.29	1.49	1.42
16	X	515	CLA	CHC-C1C	2.29	1.43	1.38
16	n	505	CLA	CHC-C1C	2.29	1.43	1.38
16	s	509	CLA	C1B-C2B	2.29	1.48	1.43
16	W	517	CLA	CHC-C1C	2.29	1.43	1.38
16	p	511	CLA	CHC-C1C	2.29	1.43	1.38
16	x	501	CLA	CHC-C1C	2.29	1.43	1.38
16	b	1206	CLA	C3B-C4B	2.29	1.49	1.42
16	n	517	CLA	CHC-C1C	2.29	1.43	1.38
16	b	1238	CLA	C3B-C4B	2.29	1.49	1.42
16	t	516	CLA	C3B-C4B	2.29	1.49	1.42
16	u	517	CLA	CHC-C1C	2.29	1.43	1.38
16	W	512	CLA	C3B-C4B	2.29	1.49	1.42
16	p	517	CLA	C3B-C4B	2.29	1.49	1.42
16	H	1108	CLA	CHC-C1C	2.29	1.43	1.38
16	a	1125	CLA	C3B-C4B	2.29	1.49	1.42
16	H	1124	CLA	C3B-C4B	2.29	1.49	1.42
16	s	511	CLA	CHC-C1C	2.28	1.43	1.38
16	w	508	CLA	CHC-C1C	2.28	1.43	1.38
16	A	1115	CLA	C3B-C4B	2.28	1.49	1.42
16	G	1231	CLA	CHC-C1C	2.28	1.43	1.38
16	W	509	CLA	CHC-C1C	2.28	1.43	1.38
16	L	1503	CLA	C1B-C2B	2.28	1.48	1.43
13	A	849	LHG	O7-C5	-2.28	1.41	1.46
16	q	511	CLA	CHC-C1C	2.28	1.43	1.38
19	H	4007	BCR	C33-C5	-2.28	1.47	1.50
16	q	511	CLA	C1B-C2B	2.28	1.48	1.43
16	Y	509	CLA	C1B-C2B	2.28	1.48	1.43
16	n	517	CLA	C3B-C4B	2.28	1.49	1.42
16	j	1303	CLA	CHC-C1C	2.28	1.43	1.38
16	u	514	CLA	CHC-C1C	2.28	1.43	1.38
16	H	1115	CLA	C3B-C4B	2.28	1.49	1.42
16	q	505	CLA	C1B-C2B	2.28	1.48	1.43
16	a	1119	CLA	CHC-C1C	2.28	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	q	517	CLA	CHC-C1C	2.28	1.43	1.38
16	Y	514	CLA	C3B-C4B	2.28	1.49	1.42
16	a	1104	CLA	C3B-C4B	2.28	1.49	1.42
16	h	513	CLA	CHC-C1C	2.28	1.43	1.38
16	H	1133	CLA	C3B-C4B	2.28	1.49	1.42
16	r	510	CLA	C3B-C4B	2.28	1.49	1.42
16	t	505	CLA	CHC-C1C	2.28	1.43	1.38
16	n	501	CLA	C3B-C4B	2.28	1.49	1.42
16	b	1213	CLA	CHC-C1C	2.28	1.43	1.38
16	y	513	CLA	CHC-C1C	2.28	1.43	1.38
16	B	1023	CLA	MG-NB	-2.28	2.01	2.05
16	Z	508	CLA	CHC-C1C	2.28	1.43	1.38
16	H	1138	CLA	C3B-C4B	2.28	1.49	1.42
16	r	504	CLA	CHC-C1C	2.28	1.43	1.38
16	y	517	CLA	CHC-C1C	2.28	1.43	1.38
16	B	1232	CLA	C1B-C2B	2.28	1.48	1.43
16	T	4004	CLA	C3B-C4B	2.28	1.49	1.42
16	S	1303	CLA	CHC-C1C	2.28	1.43	1.38
16	G	1215	CLA	C3B-C4B	2.28	1.49	1.42
16	y	508	CLA	C3B-C4B	2.28	1.49	1.42
16	t	514	CLA	CHC-C1C	2.28	1.43	1.38
16	t	517	CLA	CHC-C1C	2.28	1.43	1.38
16	H	1128	CLA	C3B-C4B	2.28	1.49	1.42
16	b	1214	CLA	CHC-C1C	2.28	1.43	1.38
16	X	507	CLA	C3B-C4B	2.27	1.49	1.42
16	H	1111	CLA	CHC-C1C	2.27	1.43	1.38
16	r	511	CLA	C1B-C2B	2.27	1.48	1.43
16	B	1217	CLA	C3B-C4B	2.27	1.49	1.42
16	a	1111	CLA	C3B-C4B	2.27	1.49	1.42
16	b	1231	CLA	CHC-C1C	2.27	1.43	1.38
16	U	1501	CLA	CHC-C1C	2.27	1.43	1.38
16	W	515	CLA	C3B-C4B	2.27	1.49	1.42
16	G	1210	CLA	C1B-C2B	2.27	1.48	1.43
16	G	1214	CLA	CHC-C1C	2.27	1.43	1.38
16	B	1204	CLA	C3B-C4B	2.27	1.49	1.42
16	X	509	CLA	CHC-C1C	2.27	1.43	1.38
16	A	1104	CLA	C3B-C4B	2.27	1.49	1.42
16	k	4004	CLA	C3B-C4B	2.27	1.49	1.42
16	A	1801	CLA	C1B-C2B	2.27	1.48	1.43
16	v	512	CLA	C3B-C4B	2.27	1.49	1.42
16	G	1216	CLA	MG-NB	-2.27	2.01	2.05
16	b	1023	CLA	CHC-C1C	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1801	CLA	CHC-C1C	2.27	1.43	1.38
16	b	1208	CLA	CHC-C1C	2.27	1.43	1.38
16	v	501	CLA	CHC-C1C	2.27	1.43	1.38
16	G	1208	CLA	C3B-C4B	2.27	1.49	1.42
16	Z	517	CLA	C3B-C4B	2.27	1.49	1.42
16	b	1232	CLA	MG-NB	-2.27	2.01	2.05
16	A	1101	CLA	CHC-C1C	2.27	1.43	1.38
16	a	1104	CLA	CHC-C1C	2.27	1.43	1.38
16	a	1127	CLA	CHC-C1C	2.27	1.43	1.38
16	a	1134	CLA	CHC-C1C	2.27	1.43	1.38
16	H	1137	CLA	C3B-C4B	2.27	1.49	1.42
16	A	1108	CLA	CHC-C1C	2.27	1.43	1.38
16	s	505	CLA	CHC-C1C	2.27	1.43	1.38
16	h	510	CLA	C3B-C4B	2.27	1.49	1.42
16	H	1013	CLA	MG-ND	-2.27	2.01	2.05
16	X	516	CLA	C3B-C4B	2.27	1.49	1.42
16	q	504	CLA	C3B-C4B	2.27	1.49	1.42
16	h	506	CLA	MG-NB	-2.27	2.01	2.05
16	a	1124	CLA	C3B-C4B	2.27	1.49	1.42
16	o	504	CLA	C3B-C4B	2.27	1.49	1.42
16	Y	509	CLA	CHC-C1C	2.27	1.43	1.38
16	Y	512	CLA	MG-ND	-2.27	2.01	2.05
16	Y	514	CLA	CHC-C1C	2.27	1.43	1.38
16	x	514	CLA	C3B-C4B	2.27	1.49	1.42
16	W	516	CLA	C3B-C4B	2.27	1.49	1.42
16	G	1221	CLA	CHC-C1C	2.27	1.43	1.38
16	w	514	CLA	C3B-C4B	2.27	1.49	1.42
16	Y	511	CLA	C1B-C2B	2.27	1.48	1.43
16	a	1130	CLA	CHC-C1C	2.27	1.43	1.38
16	g	515	CLA	CHC-C1C	2.27	1.43	1.38
16	r	513	CLA	CHC-C1C	2.27	1.43	1.38
16	G	1239	CLA	C3B-C4B	2.27	1.49	1.42
16	p	507	CLA	C3B-C4B	2.27	1.49	1.42
16	G	1211	CLA	CHC-C1C	2.26	1.43	1.38
16	q	505	CLA	CHC-C1C	2.26	1.43	1.38
16	F	1301	CLA	C1B-C2B	2.26	1.48	1.43
16	b	1227	CLA	C1B-C2B	2.26	1.48	1.43
16	j	1302	CLA	CHC-C1C	2.26	1.43	1.38
16	n	515	CLA	C3B-C4B	2.26	1.49	1.42
16	t	507	CLA	C3B-C4B	2.26	1.49	1.42
16	A	1013	CLA	CHC-C1C	2.26	1.43	1.38
16	w	502	CLA	C3B-C4B	2.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1133	CLA	C1B-C2B	2.26	1.48	1.43
16	t	504	CLA	CHC-C1C	2.26	1.43	1.38
16	H	1125	CLA	C3B-C4B	2.26	1.49	1.42
16	X	510	CLA	C3B-C4B	2.26	1.49	1.42
16	a	1133	CLA	C3B-C4B	2.26	1.49	1.42
16	n	508	CLA	CHC-C1C	2.26	1.43	1.38
16	n	516	CLA	CHC-C1C	2.26	1.43	1.38
20	H	4202	LMT	O2B-C2B	-2.26	1.37	1.43
16	u	512	CLA	C1B-C2B	2.26	1.48	1.43
16	B	1239	CLA	C3B-C4B	2.26	1.49	1.42
16	b	1220	CLA	C3B-C4B	2.26	1.49	1.42
16	n	507	CLA	C3B-C4B	2.26	1.49	1.42
13	H	851	LHG	O7-C5	-2.26	1.41	1.46
16	a	1136	CLA	CHC-C1C	2.26	1.43	1.38
16	l	1501	CLA	CHC-C1C	2.26	1.43	1.38
20	A	4202	LMT	O2B-C2B	-2.26	1.37	1.43
16	H	1130	CLA	CHC-C1C	2.26	1.43	1.38
20	L	4101	LMT	O2B-C2B	-2.26	1.37	1.43
16	G	1225	CLA	MG-NB	-2.26	2.01	2.05
16	H	1118	CLA	C3B-C4B	2.26	1.49	1.42
16	G	1201	CLA	CHC-C1C	2.26	1.43	1.38
16	g	501	CLA	CHC-C1C	2.26	1.43	1.38
16	H	1121	CLA	CHC-C1C	2.26	1.43	1.38
16	w	504	CLA	CHC-C1C	2.26	1.43	1.38
16	b	1238	CLA	C1B-C2B	2.26	1.48	1.43
16	u	510	CLA	C3B-C4B	2.26	1.49	1.42
16	a	1013	CLA	MG-ND	-2.26	2.01	2.05
16	Z	505	CLA	CHC-C1C	2.26	1.43	1.38
16	h	504	CLA	CHC-C1C	2.26	1.43	1.38
16	t	508	CLA	CHC-C1C	2.26	1.43	1.38
16	a	1118	CLA	C3B-C4B	2.26	1.49	1.42
16	B	1236	CLA	CHC-C1C	2.26	1.43	1.38
16	H	1140	CLA	C1B-C2B	2.26	1.48	1.43
16	G	1217	CLA	C3B-C4B	2.26	1.49	1.42
16	g	516	CLA	CHC-C1C	2.26	1.43	1.38
16	p	515	CLA	CHC-C1C	2.26	1.43	1.38
16	y	514	CLA	CHC-C1C	2.26	1.43	1.38
16	G	1023	CLA	C4B-NB	-2.26	1.34	1.37
16	l	1503	CLA	CHC-C1C	2.26	1.43	1.38
16	o	501	CLA	C3B-C4B	2.26	1.49	1.42
16	Y	501	CLA	C3B-C4B	2.25	1.49	1.42
16	b	1208	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1137	CLA	C3B-C4B	2.25	1.49	1.42
16	G	1216	CLA	C3B-C4B	2.25	1.49	1.42
16	p	516	CLA	CHC-C1C	2.25	1.43	1.38
16	A	1138	CLA	C1B-C2B	2.25	1.48	1.43
16	H	1132	CLA	C3B-C4B	2.25	1.49	1.42
16	a	1128	CLA	C3B-C4B	2.25	1.49	1.42
16	B	1228	CLA	CHC-C1C	2.25	1.43	1.38
16	G	1228	CLA	CHC-C1C	2.25	1.43	1.38
16	u	504	CLA	C3B-C4B	2.25	1.49	1.42
16	a	1132	CLA	C4B-NB	-2.25	1.34	1.37
16	G	1227	CLA	C1B-C2B	2.25	1.48	1.43
16	o	512	CLA	C1B-C2B	2.25	1.48	1.43
16	h	509	CLA	C3B-C4B	2.25	1.49	1.42
20	a	4202	LMT	O2B-C2B	-2.25	1.37	1.43
16	B	1023	CLA	C4B-NB	-2.25	1.34	1.37
16	G	1204	CLA	C3B-C4B	2.25	1.49	1.42
16	H	1110	CLA	CHC-C1C	2.25	1.43	1.38
16	Z	514	CLA	CHC-C1C	2.25	1.43	1.38
16	o	515	CLA	CHC-C1C	2.25	1.43	1.38
16	v	506	CLA	C3B-C4B	2.25	1.49	1.42
16	y	502	CLA	CHC-C1C	2.25	1.43	1.38
16	A	1139	CLA	CHC-C1C	2.25	1.43	1.38
16	B	1227	CLA	CHC-C1C	2.25	1.43	1.38
16	s	516	CLA	CHC-C1C	2.25	1.43	1.38
16	v	513	CLA	CHC-C1C	2.25	1.43	1.38
16	G	1208	CLA	CHC-C1C	2.25	1.43	1.38
16	h	509	CLA	CHC-C1C	2.25	1.43	1.38
16	B	1238	CLA	C1B-C2B	2.25	1.48	1.43
16	s	512	CLA	C3B-C4B	2.25	1.49	1.42
16	W	508	CLA	CHC-C1C	2.25	1.43	1.38
16	u	509	CLA	CHC-C1C	2.25	1.43	1.38
16	y	515	CLA	CHC-C1C	2.25	1.43	1.38
16	B	1225	CLA	MG-NB	-2.25	2.01	2.05
16	j	1303	CLA	CBD-CAD	2.25	1.56	1.51
16	b	1224	CLA	C3B-C4B	2.25	1.49	1.42
16	g	510	CLA	C3B-C4B	2.25	1.49	1.42
16	b	1023	CLA	C4B-NB	-2.25	1.34	1.37
16	A	1119	CLA	MG-NB	-2.25	2.01	2.05
16	W	509	CLA	C1B-C2B	2.25	1.48	1.43
16	v	510	CLA	C3B-C4B	2.25	1.49	1.42
16	A	1130	CLA	C1B-C2B	2.25	1.48	1.43
16	A	1136	CLA	C1B-C2B	2.25	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1205	CLA	MG-NB	-2.25	2.01	2.05
16	Y	512	CLA	C3B-C4B	2.25	1.49	1.42
16	n	516	CLA	C3B-C4B	2.25	1.49	1.42
16	A	1109	CLA	CHC-C1C	2.25	1.43	1.38
16	Z	511	CLA	CHC-C1C	2.25	1.43	1.38
16	t	501	CLA	CHC-C1C	2.25	1.43	1.38
16	Z	512	CLA	C3B-C4B	2.25	1.49	1.42
16	b	1225	CLA	MG-NB	-2.25	2.01	2.05
16	b	1226	CLA	MG-NB	-2.25	2.01	2.05
16	a	1140	CLA	CHC-C1C	2.25	1.43	1.38
16	r	516	CLA	CHC-C1C	2.25	1.43	1.38
16	b	1235	CLA	MG-NB	-2.25	2.01	2.05
20	L	4101	LMT	O3B-C3B	-2.25	1.37	1.43
16	Z	503	CLA	CHC-C1C	2.25	1.43	1.38
16	A	1105	CLA	CHC-C1C	2.24	1.43	1.38
16	H	1140	CLA	CHC-C1C	2.24	1.43	1.38
16	b	1219	CLA	CHC-C1C	2.24	1.43	1.38
16	v	517	CLA	CHC-C1C	2.24	1.43	1.38
16	w	501	CLA	C3B-C4B	2.24	1.49	1.42
16	o	512	CLA	MG-ND	-2.24	2.01	2.05
16	A	1117	CLA	MG-NB	-2.24	2.01	2.05
16	L	1501	CLA	C1B-C2B	2.24	1.48	1.43
16	p	509	CLA	C1B-C2B	2.24	1.48	1.43
16	a	1137	CLA	C3B-C4B	2.24	1.49	1.42
16	g	504	CLA	CHC-C1C	2.24	1.43	1.38
16	Z	501	CLA	C3B-C4B	2.24	1.49	1.42
20	L	4101	LMT	O2'-C2'	-2.24	1.37	1.43
16	o	514	CLA	C3B-C4B	2.24	1.49	1.42
16	b	1207	CLA	C3B-C4B	2.24	1.49	1.42
16	B	1226	CLA	C1B-C2B	2.24	1.48	1.43
16	Z	512	CLA	C1B-C2B	2.24	1.48	1.43
16	x	509	CLA	C1B-C2B	2.24	1.48	1.43
16	S	1302	CLA	CHC-C1C	2.24	1.43	1.38
16	n	512	CLA	C3B-C4B	2.24	1.49	1.42
16	H	1801	CLA	C1B-C2B	2.24	1.48	1.43
20	l	4101	LMT	O2B-C2B	-2.24	1.37	1.43
16	B	1208	CLA	C3B-C4B	2.24	1.49	1.42
16	a	1103	CLA	CHC-C1C	2.24	1.43	1.38
16	u	515	CLA	CHC-C1C	2.24	1.43	1.38
16	h	515	CLA	CHC-C1C	2.24	1.43	1.38
16	t	515	CLA	C3B-C4B	2.24	1.49	1.42
16	x	517	CLA	CHC-C1C	2.24	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	s	506	CLA	MG-NB	-2.24	2.01	2.05
16	A	1132	CLA	C3B-C4B	2.24	1.49	1.42
16	a	1117	CLA	C1B-C2B	2.24	1.48	1.43
16	o	511	CLA	C1B-C2B	2.24	1.48	1.43
16	B	1215	CLA	C3B-C4B	2.24	1.49	1.42
16	B	1234	CLA	C1B-C2B	2.24	1.48	1.43
16	B	1214	CLA	C1B-C2B	2.24	1.48	1.43
16	t	502	CLA	MG-NB	-2.24	2.01	2.05
16	b	1230	CLA	C3B-C4B	2.24	1.49	1.42
16	o	514	CLA	CHC-C1C	2.24	1.43	1.38
16	a	1109	CLA	CHC-C1C	2.24	1.43	1.38
16	w	514	CLA	CHC-C1C	2.24	1.43	1.38
16	A	1124	CLA	CHC-C1C	2.23	1.43	1.38
16	A	1237	CLA	C3B-C4B	2.23	1.49	1.42
16	v	514	CLA	CHC-C1C	2.23	1.43	1.38
16	B	1220	CLA	C3B-C4B	2.23	1.49	1.42
16	Z	511	CLA	C1B-C2B	2.23	1.48	1.43
16	q	503	CLA	MG-NB	-2.23	2.01	2.05
16	A	1122	CLA	C3B-C4B	2.23	1.49	1.42
16	x	512	CLA	C3B-C4B	2.23	1.49	1.42
16	u	511	CLA	C1B-C2B	2.23	1.48	1.43
16	q	510	CLA	C3B-C4B	2.23	1.49	1.42
16	r	514	CLA	CHC-C1C	2.23	1.43	1.38
16	H	1116	CLA	CHC-C1C	2.23	1.43	1.38
16	n	504	CLA	CHC-C1C	2.23	1.43	1.38
16	B	1224	CLA	C3B-C4B	2.23	1.49	1.42
16	H	1127	CLA	MG-NB	-2.23	2.01	2.05
16	u	507	CLA	C3B-C4B	2.23	1.49	1.42
16	X	516	CLA	CHC-C1C	2.23	1.43	1.38
13	x	605	LHG	P-O6	2.23	1.68	1.59
16	G	1234	CLA	MG-NB	-2.23	2.01	2.05
16	b	1220	CLA	MG-NB	-2.23	2.01	2.05
16	u	512	CLA	C3B-C4B	2.23	1.49	1.42
16	b	1236	CLA	CHC-C1C	2.23	1.43	1.38
16	q	504	CLA	CHC-C1C	2.23	1.43	1.38
16	x	504	CLA	CHC-C1C	2.23	1.43	1.38
16	h	514	CLA	CHC-C1C	2.23	1.43	1.38
16	p	509	CLA	CHC-C1C	2.23	1.43	1.38
16	w	515	CLA	CHC-C1C	2.23	1.43	1.38
16	J	1303	CLA	CBD-CAD	2.23	1.56	1.51
16	A	1110	CLA	CHC-C1C	2.23	1.43	1.38
16	q	512	CLA	CHC-C1C	2.23	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1122	CLA	C3B-C4B	2.23	1.49	1.42
16	A	1111	CLA	MG-NB	-2.23	2.01	2.05
16	B	1229	CLA	CHC-C1C	2.23	1.42	1.38
16	W	502	CLA	MG-NB	-2.23	2.01	2.05
16	H	1108	CLA	C3B-C4B	2.23	1.49	1.42
16	w	507	CLA	C3B-C4B	2.23	1.49	1.42
16	Z	509	CLA	C1B-C2B	2.23	1.48	1.43
16	r	517	CLA	CHC-C1C	2.23	1.42	1.38
16	h	506	CLA	C3B-C4B	2.23	1.49	1.42
16	B	1023	CLA	MG-ND	-2.23	2.01	2.05
16	Z	503	CLA	C3B-C4B	2.23	1.49	1.42
16	G	1213	CLA	CHC-C1C	2.23	1.42	1.38
16	b	1206	CLA	MG-NB	-2.23	2.01	2.05
16	h	512	CLA	CHC-C1C	2.23	1.42	1.38
13	r	605	LHG	P-O6	2.23	1.68	1.59
16	o	509	CLA	CHC-C1C	2.23	1.42	1.38
16	r	501	CLA	CHC-C1C	2.23	1.42	1.38
16	u	509	CLA	C1B-C2B	2.23	1.48	1.43
13	s	605	LHG	O7-C5	-2.23	1.41	1.46
16	h	517	CLA	CHC-C1C	2.22	1.42	1.38
16	h	507	CLA	CHC-C1C	2.22	1.42	1.38
16	W	516	CLA	CHC-C1C	2.22	1.42	1.38
16	o	517	CLA	CHC-C1C	2.22	1.42	1.38
16	v	502	CLA	CHC-C1C	2.22	1.42	1.38
16	y	502	CLA	MG-NB	-2.22	2.01	2.05
16	r	505	CLA	CHC-C1C	2.22	1.42	1.38
16	q	514	CLA	CHC-C1C	2.22	1.42	1.38
16	b	1023	CLA	C3B-C4B	2.22	1.49	1.42
16	p	511	CLA	C1B-C2B	2.22	1.48	1.43
20	U	4101	LMT	O3B-C3B	-2.22	1.37	1.43
16	a	1108	CLA	CHC-C1C	2.22	1.42	1.38
16	Y	507	CLA	C3B-C4B	2.22	1.49	1.42
16	H	1133	CLA	MG-NB	-2.22	2.01	2.05
16	q	507	CLA	C3B-C4B	2.22	1.49	1.42
16	H	1103	CLA	CHC-C1C	2.22	1.42	1.38
16	H	1136	CLA	CHC-C1C	2.22	1.42	1.38
16	X	512	CLA	CHC-C1C	2.22	1.42	1.38
16	h	502	CLA	CHC-C1C	2.22	1.42	1.38
16	r	512	CLA	C3B-C4B	2.22	1.49	1.42
16	B	1216	CLA	MG-ND	-2.22	2.01	2.05
20	U	4101	LMT	O2B-C2B	-2.22	1.37	1.43
16	s	504	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	501	CLA	CHC-C1C	2.22	1.42	1.38
16	w	512	CLA	C3B-C4B	2.22	1.49	1.42
16	A	1122	CLA	CHC-C1C	2.22	1.42	1.38
16	b	1209	CLA	CHC-C1C	2.22	1.42	1.38
16	p	508	CLA	CHC-C1C	2.22	1.42	1.38
16	G	1226	CLA	MG-NB	-2.22	2.01	2.05
16	G	1206	CLA	C1B-C2B	2.22	1.48	1.43
16	B	1230	CLA	CHC-C1C	2.22	1.42	1.38
16	a	1115	CLA	CHC-C1C	2.22	1.42	1.38
16	b	1232	CLA	CHC-C1C	2.22	1.42	1.38
16	l	1502	CLA	C1B-C2B	2.22	1.48	1.43
16	G	1222	CLA	MG-NB	-2.22	2.01	2.05
16	Q	1302	CLA	CHC-C1C	2.22	1.42	1.38
16	r	515	CLA	CHC-C1C	2.22	1.42	1.38
16	b	1205	CLA	C3B-C4B	2.22	1.49	1.42
16	S	1303	CLA	CBD-CAD	2.22	1.56	1.51
16	B	1220	CLA	CHC-C1C	2.22	1.42	1.38
16	q	501	CLA	C3B-C4B	2.22	1.49	1.42
16	X	511	CLA	C1B-C2B	2.22	1.48	1.43
16	h	512	CLA	MG-NB	-2.22	2.01	2.05
16	Y	505	CLA	CHC-C1C	2.22	1.42	1.38
16	n	501	CLA	CHC-C1C	2.22	1.42	1.38
16	y	507	CLA	CHC-C1C	2.22	1.42	1.38
16	G	1207	CLA	C3B-C4B	2.21	1.49	1.42
16	B	1232	CLA	MG-NB	-2.21	2.01	2.05
16	X	504	CLA	C3B-C4B	2.21	1.49	1.42
16	o	510	CLA	CHC-C1C	2.21	1.42	1.38
16	x	506	CLA	MG-NB	-2.21	2.01	2.05
16	H	1109	CLA	CHC-C1C	2.21	1.42	1.38
16	p	510	CLA	C3B-C4B	2.21	1.49	1.42
16	q	501	CLA	CHC-C1C	2.21	1.42	1.38
16	v	507	CLA	CHC-C1C	2.21	1.42	1.38
16	x	513	CLA	CHC-C1C	2.21	1.42	1.38
16	y	504	CLA	MG-NB	-2.21	2.01	2.05
16	H	1123	CLA	CHC-C1C	2.21	1.42	1.38
16	a	1127	CLA	C3B-C4B	2.21	1.49	1.42
16	b	1229	CLA	C3B-C4B	2.21	1.49	1.42
16	b	1225	CLA	CHC-C1C	2.21	1.42	1.38
16	b	1229	CLA	CHC-C1C	2.21	1.42	1.38
16	q	503	CLA	C3B-C4B	2.21	1.49	1.42
16	a	1128	CLA	MG-NB	-2.21	2.01	2.05
16	t	516	CLA	CHC-C1C	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1232	CLA	MG-NB	-2.21	2.01	2.05
16	b	1206	CLA	CHC-C1C	2.21	1.42	1.38
16	g	512	CLA	C3B-C4B	2.21	1.49	1.42
16	a	1121	CLA	CHC-C1C	2.21	1.42	1.38
16	X	501	CLA	C3B-C4B	2.21	1.49	1.42
16	p	513	CLA	CHC-C1C	2.21	1.42	1.38
16	Y	510	CLA	C3B-C4B	2.21	1.49	1.42
16	b	1204	CLA	C3B-C4B	2.21	1.49	1.42
16	Z	502	CLA	MG-NB	-2.21	2.01	2.05
16	W	504	CLA	CHC-C1C	2.21	1.42	1.38
16	g	514	CLA	CHC-C1C	2.21	1.42	1.38
16	A	1117	CLA	C1B-C2B	2.21	1.48	1.43
16	B	1205	CLA	C3B-C4B	2.21	1.49	1.42
16	B	1206	CLA	C3B-C4B	2.21	1.49	1.42
20	U	4101	LMT	O2'-C2'	-2.21	1.37	1.43
16	w	517	CLA	MG-NB	-2.21	2.01	2.05
16	w	505	CLA	CHC-C1C	2.21	1.42	1.38
16	r	509	CLA	C1B-C2B	2.21	1.48	1.43
16	H	1137	CLA	CHC-C1C	2.20	1.42	1.38
16	a	1110	CLA	CHC-C1C	2.20	1.42	1.38
20	l	4101	LMT	O2'-C2'	-2.20	1.37	1.43
19	u	601	BCR	C33-C5	-2.20	1.47	1.50
16	v	516	CLA	CHC-C1C	2.20	1.42	1.38
16	Z	515	CLA	C3B-C4B	2.20	1.49	1.42
16	A	1131	CLA	CHC-C1C	2.20	1.42	1.38
16	b	1217	CLA	CHC-C1C	2.20	1.42	1.38
16	g	510	CLA	CHC-C1C	2.20	1.42	1.38
16	a	1140	CLA	C1B-C2B	2.20	1.48	1.43
14	A	4201	LMG	O7-C8	-2.20	1.41	1.46
16	g	505	CLA	C3B-C4B	2.20	1.49	1.42
16	H	1133	CLA	C1B-C2B	2.20	1.48	1.43
16	a	1137	CLA	CHC-C1C	2.20	1.42	1.38
16	b	1214	CLA	C1B-C2B	2.20	1.48	1.43
16	A	1128	CLA	MG-NB	-2.20	2.01	2.05
16	Z	501	CLA	CHC-C1C	2.20	1.42	1.38
16	a	1125	CLA	CHC-C1C	2.20	1.42	1.38
16	b	1228	CLA	CHC-C1C	2.20	1.42	1.38
16	q	502	CLA	MG-NB	-2.20	2.01	2.05
16	a	1132	CLA	CHC-C1C	2.20	1.42	1.38
16	a	1127	CLA	MG-NB	-2.20	2.01	2.05
16	f	1301	CLA	CHC-C1C	2.20	1.42	1.38
16	x	515	CLA	CHC-C1C	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1138	CLA	CHC-C1C	2.20	1.42	1.38
16	B	1226	CLA	MG-ND	-2.20	2.01	2.05
16	a	1135	CLA	MG-ND	-2.20	2.01	2.05
16	a	1108	CLA	C3B-C4B	2.20	1.49	1.42
16	w	516	CLA	CHC-C1C	2.20	1.42	1.38
16	G	1226	CLA	C1B-C2B	2.20	1.48	1.43
16	H	1022	CLA	MG-NB	-2.20	2.01	2.05
16	h	503	CLA	MG-NB	-2.20	2.01	2.05
14	H	852	LMG	C4-C5	2.20	1.57	1.53
16	n	513	CLA	CHC-C1C	2.20	1.42	1.38
16	p	505	CLA	CHC-C1C	2.20	1.42	1.38
16	x	502	CLA	MG-NB	-2.20	2.01	2.05
16	g	508	CLA	CHC-C1C	2.20	1.42	1.38
16	u	508	CLA	CHC-C1C	2.20	1.42	1.38
15	a	1011	CL0	MG-NB	-2.19	2.01	2.05
16	A	1104	CLA	CHC-C1C	2.19	1.42	1.38
16	a	1128	CLA	MG-ND	-2.19	2.01	2.05
20	l	4101	LMT	O3B-C3B	-2.19	1.37	1.43
16	X	508	CLA	CHC-C1C	2.19	1.42	1.38
16	A	1022	CLA	MG-NB	-2.19	2.01	2.05
16	Z	512	CLA	MG-NB	-2.19	2.01	2.05
16	A	1140	CLA	CHC-C1C	2.19	1.42	1.38
16	s	508	CLA	CHC-C1C	2.19	1.42	1.38
16	X	512	CLA	C1B-C2B	2.19	1.48	1.43
16	y	505	CLA	MG-NB	-2.19	2.01	2.05
16	x	510	CLA	C3B-C4B	2.19	1.49	1.42
16	n	515	CLA	CHC-C1C	2.19	1.42	1.38
16	o	508	CLA	CHC-C1C	2.19	1.42	1.38
16	p	512	CLA	MG-ND	-2.19	2.01	2.05
16	y	512	CLA	CHC-C1C	2.19	1.42	1.38
16	w	503	CLA	MG-ND	-2.19	2.01	2.05
16	H	1117	CLA	C1B-C2B	2.19	1.48	1.43
16	r	511	CLA	MG-NB	-2.19	2.01	2.05
16	b	1226	CLA	MG-ND	-2.19	2.01	2.05
16	n	510	CLA	C3B-C4B	2.19	1.49	1.42
16	B	1208	CLA	CHC-C1C	2.19	1.42	1.38
16	s	511	CLA	C1B-C2B	2.19	1.48	1.43
16	H	1117	CLA	MG-NB	-2.19	2.01	2.05
16	r	506	CLA	C3B-C4B	2.19	1.49	1.42
16	H	1122	CLA	CHC-C1C	2.19	1.42	1.38
16	a	1116	CLA	CHC-C1C	2.19	1.42	1.38
16	s	509	CLA	CHC-C1C	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	x	508	CLA	CHC-C1C	2.19	1.42	1.38
16	A	1113	CLA	C3B-C4B	2.19	1.49	1.42
16	B	1203	CLA	C3B-C4B	2.19	1.49	1.42
16	Y	504	CLA	CHC-C1C	2.19	1.42	1.38
16	q	503	CLA	CHC-C1C	2.19	1.42	1.38
16	w	509	CLA	C1B-C2B	2.19	1.48	1.43
16	Z	510	CLA	CHC-C1C	2.19	1.42	1.38
16	B	1206	CLA	MG-NB	-2.19	2.01	2.05
16	x	512	CLA	MG-NB	-2.19	2.01	2.05
16	B	1217	CLA	CHC-C1C	2.18	1.42	1.38
16	X	517	CLA	CHC-C1C	2.18	1.42	1.38
16	a	1122	CLA	CHC-C1C	2.18	1.42	1.38
16	y	508	CLA	CHC-C1C	2.18	1.42	1.38
16	H	1127	CLA	MG-ND	-2.18	2.01	2.05
16	G	1240	CLA	CHC-C1C	2.18	1.42	1.38
16	v	515	CLA	CHC-C1C	2.18	1.42	1.38
16	r	507	CLA	C3B-C4B	2.18	1.49	1.42
16	v	509	CLA	MG-NB	-2.18	2.01	2.05
16	H	1125	CLA	CHC-C1C	2.18	1.42	1.38
16	b	1226	CLA	C3B-C4B	2.18	1.49	1.42
21	R	4020	ECH	C2-C3	-2.18	1.47	1.52
16	H	1139	CLA	MG-NB	-2.18	2.01	2.05
16	g	509	CLA	MG-NB	-2.18	2.01	2.05
16	x	502	CLA	CHC-C1C	2.18	1.42	1.38
16	B	1206	CLA	C1B-C2B	2.18	1.48	1.43
16	b	1213	CLA	MG-NB	-2.18	2.01	2.05
14	f	4017	LMG	C4-C5	2.18	1.57	1.53
16	a	1022	CLA	C1B-C2B	2.18	1.48	1.43
16	H	1105	CLA	MG-NB	-2.18	2.01	2.05
16	G	1214	CLA	C1B-C2B	2.18	1.48	1.43
16	X	512	CLA	MG-NB	-2.18	2.01	2.05
16	a	1102	CLA	C1B-C2B	2.18	1.48	1.43
16	a	1111	CLA	CHC-C1C	2.18	1.42	1.38
16	w	513	CLA	CHC-C1C	2.18	1.42	1.38
13	Y	605	LHG	O7-C5	-2.18	1.41	1.46
16	B	1222	CLA	MG-NB	-2.18	2.01	2.05
16	A	1115	CLA	CHC-C1C	2.18	1.42	1.38
16	G	1209	CLA	CHC-C1C	2.18	1.42	1.38
16	G	1220	CLA	CHC-C1C	2.18	1.42	1.38
16	H	1022	CLA	C1B-C2B	2.18	1.48	1.43
16	b	1226	CLA	C1B-C2B	2.18	1.48	1.43
16	T	4003	CLA	CHC-C1C	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Z	507	CLA	C3B-C4B	2.18	1.49	1.42
16	A	1103	CLA	CHC-C1C	2.18	1.42	1.38
16	s	513	CLA	CHC-C1C	2.18	1.42	1.38
16	x	514	CLA	CHC-C1C	2.18	1.42	1.38
16	p	504	CLA	CHC-C1C	2.18	1.42	1.38
16	g	509	CLA	C1B-C2B	2.18	1.48	1.43
14	A	852	LMG	C4-C5	2.18	1.57	1.53
16	G	1226	CLA	MG-ND	-2.18	2.01	2.05
16	H	1114	CLA	C3B-C4B	2.18	1.49	1.42
16	B	1214	CLA	CHC-C1C	2.18	1.42	1.38
16	o	513	CLA	CHC-C1C	2.18	1.42	1.38
16	u	506	CLA	C4B-NB	-2.18	1.35	1.37
16	A	1128	CLA	C3B-C4B	2.18	1.49	1.42
16	a	1113	CLA	C3B-C4B	2.18	1.49	1.42
16	H	1136	CLA	C1B-C2B	2.18	1.48	1.43
16	G	1225	CLA	C3B-C4B	2.17	1.49	1.42
16	B	1207	CLA	C3B-C4B	2.17	1.49	1.42
15	A	1011	CL0	MG-NB	-2.17	2.01	2.05
16	w	503	CLA	MG-NB	-2.17	2.01	2.05
16	H	1131	CLA	CHC-C1C	2.17	1.42	1.38
16	q	512	CLA	MG-NB	-2.17	2.01	2.05
16	B	1206	CLA	CHC-C1C	2.17	1.42	1.38
13	A	851	LHG	O7-C5	-2.17	1.41	1.46
16	a	1136	CLA	C1B-C2B	2.17	1.48	1.43
16	t	515	CLA	CHC-C1C	2.17	1.42	1.38
16	A	1132	CLA	C4B-NB	-2.17	1.35	1.37
16	u	504	CLA	CHC-C1C	2.17	1.42	1.38
16	Z	512	CLA	CHC-C1C	2.17	1.42	1.38
16	Y	508	CLA	CHC-C1C	2.17	1.42	1.38
16	p	517	CLA	CHC-C1C	2.17	1.42	1.38
13	a	851	LHG	O7-C5	-2.17	1.41	1.46
16	X	514	CLA	MG-ND	-2.17	2.01	2.05
16	Y	516	CLA	CHC-C1C	2.17	1.42	1.38
24	Z	601	LUT	C1-C6	-2.17	1.51	1.53
16	H	1113	CLA	CHC-C1C	2.17	1.42	1.38
16	K	4003	CLA	CHC-C1C	2.17	1.42	1.38
16	q	502	CLA	CHC-C1C	2.17	1.42	1.38
16	u	501	CLA	CHC-C1C	2.17	1.42	1.38
16	G	1227	CLA	MG-NB	-2.17	2.01	2.05
16	w	502	CLA	MG-NB	-2.17	2.01	2.05
16	A	1137	CLA	CHC-C1C	2.17	1.42	1.38
16	w	512	CLA	MG-ND	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	s	510	CLA	C3B-C4B	2.17	1.49	1.42
16	q	504	CLA	MG-NB	-2.17	2.01	2.05
15	H	1011	CL0	CBD-CGD	-2.17	1.49	1.52
20	H	4202	LMT	O3B-C3B	-2.17	1.37	1.43
16	A	1108	CLA	C3B-C4B	2.17	1.49	1.42
16	B	1204	CLA	CHC-C1C	2.17	1.42	1.38
16	r	508	CLA	CHC-C1C	2.17	1.42	1.38
16	h	504	CLA	MG-NB	-2.17	2.01	2.05
16	Y	512	CLA	CHC-C1C	2.17	1.42	1.38
16	Z	504	CLA	MG-NB	-2.17	2.01	2.05
16	s	517	CLA	MG-NB	-2.17	2.01	2.05
16	B	1201	CLA	CHC-C1C	2.17	1.42	1.38
16	s	512	CLA	MG-ND	-2.17	2.01	2.05
16	u	502	CLA	MG-NB	-2.17	2.01	2.05
20	a	4202	LMT	O3B-C3B	-2.16	1.37	1.43
16	Y	513	CLA	CHC-C1C	2.16	1.42	1.38
16	a	1123	CLA	CHC-C1C	2.16	1.42	1.38
16	s	501	CLA	CHC-C1C	2.16	1.42	1.38
16	w	512	CLA	CHC-C1C	2.16	1.42	1.38
16	A	1133	CLA	C1B-C2B	2.16	1.48	1.43
16	x	506	CLA	C3B-C4B	2.16	1.49	1.42
16	a	1104	CLA	MG-NB	-2.16	2.01	2.05
16	t	512	CLA	CHC-C1C	2.16	1.42	1.38
16	W	507	CLA	C3B-C4B	2.16	1.49	1.42
16	b	1224	CLA	MG-ND	-2.16	2.01	2.05
16	A	1123	CLA	CHC-C1C	2.16	1.42	1.38
16	B	1209	CLA	CHC-C1C	2.16	1.42	1.38
16	o	501	CLA	CHC-C1C	2.16	1.42	1.38
16	g	506	CLA	C3B-C4B	2.16	1.49	1.42
16	W	512	CLA	CHC-C1C	2.16	1.42	1.38
16	g	505	CLA	CHC-C1C	2.16	1.42	1.38
16	Z	502	CLA	CHC-C1C	2.16	1.42	1.38
16	v	512	CLA	CHC-C1C	2.16	1.42	1.38
16	Y	517	CLA	CHC-C1C	2.16	1.42	1.38
16	a	1133	CLA	MG-NB	-2.16	2.01	2.05
16	H	1114	CLA	CHC-C1C	2.16	1.42	1.38
16	Z	513	CLA	CHC-C1C	2.16	1.42	1.38
16	y	509	CLA	CHC-C1C	2.16	1.42	1.38
16	q	512	CLA	MG-ND	-2.16	2.01	2.05
16	b	1223	CLA	C3B-C4B	2.16	1.49	1.42
16	H	1132	CLA	CHC-C1C	2.16	1.42	1.38
16	A	1801	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	1216	CLA	C3B-C4B	2.16	1.49	1.42
16	A	1122	CLA	MG-NB	-2.16	2.01	2.05
16	G	1206	CLA	MG-NB	-2.16	2.01	2.05
16	p	507	CLA	CHC-C1C	2.16	1.42	1.38
16	G	1214	CLA	MG-NB	-2.16	2.01	2.05
16	b	1240	CLA	CHC-C1C	2.16	1.42	1.38
16	w	501	CLA	CHC-C1C	2.15	1.42	1.38
15	H	1011	CL0	MG-NB	-2.15	2.01	2.05
16	U	1502	CLA	CHC-C1C	2.15	1.42	1.38
16	n	506	CLA	C3B-C4B	2.15	1.49	1.42
16	G	1204	CLA	CHC-C1C	2.15	1.42	1.38
14	a	852	LMG	C4-C5	2.15	1.57	1.53
16	A	1133	CLA	MG-NB	-2.15	2.01	2.05
16	Y	512	CLA	MG-NB	-2.15	2.01	2.05
16	A	1114	CLA	CHC-C1C	2.15	1.42	1.38
16	Z	515	CLA	CHC-C1C	2.15	1.42	1.38
16	H	1122	CLA	MG-NB	-2.15	2.01	2.05
16	H	1138	CLA	CHC-C1C	2.15	1.42	1.38
16	l	1502	CLA	CHC-C1C	2.15	1.42	1.38
16	w	503	CLA	C3B-C4B	2.15	1.49	1.42
16	o	512	CLA	MG-NB	-2.15	2.01	2.05
16	k	4003	CLA	CHC-C1C	2.15	1.42	1.38
16	G	1206	CLA	C3B-C4B	2.15	1.49	1.42
16	G	1223	CLA	C3B-C4B	2.15	1.49	1.42
16	y	516	CLA	MG-NB	-2.15	2.01	2.05
16	a	1133	CLA	CHC-C1C	2.15	1.42	1.38
16	b	1021	CLA	CHC-C1C	2.15	1.42	1.38
16	X	507	CLA	CHC-C1C	2.15	1.42	1.38
16	p	501	CLA	CHC-C1C	2.15	1.42	1.38
16	A	1120	CLA	CHC-C1C	2.15	1.42	1.38
16	W	502	CLA	MG-ND	-2.15	2.01	2.05
16	a	1112	CLA	CHC-C1C	2.15	1.42	1.38
16	y	510	CLA	CHC-C1C	2.15	1.42	1.38
16	A	1107	CLA	CHC-C1C	2.15	1.42	1.38
16	u	507	CLA	CHC-C1C	2.15	1.42	1.38
16	t	506	CLA	C3B-C4B	2.15	1.49	1.42
16	G	1236	CLA	CHC-C1C	2.15	1.42	1.38
16	w	509	CLA	MG-NB	-2.15	2.01	2.05
16	A	1107	CLA	C3B-C4B	2.15	1.49	1.42
16	H	1107	CLA	C3B-C4B	2.15	1.49	1.42
14	F	4017	LMG	O7-C8	-2.15	1.41	1.46
16	W	506	CLA	C3B-C4B	2.15	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1135	CLA	MG-NB	-2.15	2.01	2.05
16	b	1225	CLA	C3B-C4B	2.15	1.49	1.42
16	H	1112	CLA	CHC-C1C	2.15	1.42	1.38
16	b	1224	CLA	MG-NB	-2.15	2.01	2.05
16	h	509	CLA	MG-NB	-2.15	2.01	2.05
16	s	507	CLA	C3B-C4B	2.15	1.49	1.42
16	s	506	CLA	MG-ND	-2.14	2.01	2.05
16	G	1226	CLA	C3B-C4B	2.14	1.49	1.42
16	x	512	CLA	CHC-C1C	2.14	1.42	1.38
16	B	1218	CLA	CHC-C1C	2.14	1.42	1.38
13	p	605	LHG	O7-C5	-2.14	1.41	1.46
16	L	1502	CLA	CHC-C1C	2.14	1.42	1.38
16	H	1135	CLA	MG-NB	-2.14	2.01	2.05
16	g	505	CLA	MG-NB	-2.14	2.01	2.05
16	t	503	CLA	MG-NB	-2.14	2.01	2.05
20	A	4202	LMT	O3B-C3B	-2.14	1.37	1.43
16	W	515	CLA	CHC-C1C	2.14	1.42	1.38
16	B	1224	CLA	CHC-C1C	2.14	1.42	1.38
16	A	1127	CLA	MG-NB	-2.14	2.01	2.05
16	H	1104	CLA	MG-ND	-2.14	2.01	2.05
16	a	1131	CLA	CHC-C1C	2.14	1.42	1.38
16	q	513	CLA	CHC-C1C	2.14	1.42	1.38
15	A	1011	CL0	CBD-CGD	-2.14	1.49	1.52
16	H	1130	CLA	C1B-C2B	2.14	1.48	1.43
16	a	1138	CLA	CHC-C1C	2.14	1.42	1.38
16	A	1133	CLA	CHC-C1C	2.14	1.42	1.38
13	G	4018	LHG	O7-C5	-2.14	1.41	1.46
16	B	1223	CLA	C3B-C4B	2.14	1.49	1.42
16	g	513	CLA	CHC-C1C	2.14	1.42	1.38
16	v	506	CLA	CHC-C1C	2.14	1.42	1.38
16	W	510	CLA	C3B-C4B	2.14	1.49	1.42
16	B	1213	CLA	MG-NB	-2.14	2.01	2.05
16	W	511	CLA	MG-NB	-2.14	2.01	2.05
16	q	515	CLA	CHC-C1C	2.14	1.42	1.38
16	A	1128	CLA	MG-ND	-2.14	2.01	2.05
16	b	1234	CLA	MG-NB	-2.14	2.01	2.05
16	b	1215	CLA	C3B-C4B	2.14	1.49	1.42
16	b	1210	CLA	MG-NB	-2.14	2.01	2.05
16	A	1112	CLA	CHC-C1C	2.14	1.42	1.38
16	F	1301	CLA	CHC-C1C	2.14	1.42	1.38
16	K	4004	CLA	CHC-C1C	2.14	1.42	1.38
16	g	502	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	4002	CLA	CHC-C1C	2.14	1.42	1.38
16	Z	503	CLA	MG-ND	-2.14	2.01	2.05
16	y	512	CLA	MG-NB	-2.14	2.01	2.05
16	H	1128	CLA	C1B-C2B	2.13	1.48	1.43
16	o	506	CLA	MG-NB	-2.13	2.01	2.05
16	H	1128	CLA	MG-NB	-2.13	2.01	2.05
16	H	1124	CLA	CHC-C1C	2.13	1.42	1.38
16	G	1203	CLA	MG-NB	-2.13	2.01	2.05
16	x	511	CLA	MG-NB	-2.13	2.01	2.05
16	a	1127	CLA	MG-ND	-2.13	2.01	2.05
20	U	4101	LMT	O1'-C1'	-2.13	1.36	1.40
16	G	1218	CLA	CHC-C1C	2.13	1.42	1.38
16	H	1115	CLA	CHC-C1C	2.13	1.42	1.38
16	U	1503	CLA	CHC-C1C	2.13	1.42	1.38
16	H	1013	CLA	C1D-ND	2.13	1.40	1.37
16	A	1135	CLA	MG-NB	-2.13	2.01	2.05
16	H	1129	CLA	MG-NB	-2.13	2.01	2.05
13	i	103	LHG	P-O6	2.13	1.67	1.59
16	b	1203	CLA	MG-NB	-2.13	2.01	2.05
16	x	512	CLA	MG-ND	-2.13	2.01	2.05
14	F	4017	LMG	C4-C5	2.13	1.57	1.53
16	w	510	CLA	C3B-C4B	2.13	1.48	1.42
16	h	506	CLA	CHC-C1C	2.13	1.42	1.38
16	A	1139	CLA	MG-NB	-2.13	2.01	2.05
16	B	1234	CLA	MG-NB	-2.13	2.01	2.05
16	s	512	CLA	MG-NB	-2.13	2.01	2.05
16	w	504	CLA	MG-NB	-2.13	2.01	2.05
16	n	502	CLA	MG-NB	-2.13	2.01	2.05
16	A	1135	CLA	MG-ND	-2.13	2.01	2.05
16	Z	512	CLA	MG-ND	-2.13	2.01	2.05
16	t	513	CLA	MG-NB	-2.13	2.01	2.05
16	t	512	CLA	MG-NB	-2.12	2.01	2.05
16	q	501	CLA	MG-NB	-2.12	2.01	2.05
16	a	1107	CLA	C3B-C4B	2.12	1.48	1.42
16	q	512	CLA	C1B-C2B	2.12	1.48	1.43
16	B	1238	CLA	CHC-C1C	2.12	1.42	1.38
16	y	506	CLA	CHC-C1C	2.12	1.42	1.38
16	b	1201	CLA	CHC-C1C	2.12	1.42	1.38
16	o	512	CLA	CHC-C1C	2.12	1.42	1.38
16	b	1235	CLA	C1B-C2B	2.12	1.48	1.43
16	a	1135	CLA	C3B-C4B	2.12	1.48	1.42
16	G	1212	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	1021	CLA	MG-NB	-2.12	2.01	2.05
16	t	517	CLA	MG-NB	-2.12	2.01	2.05
16	n	507	CLA	CHC-C1C	2.12	1.42	1.38
16	A	1022	CLA	C1B-C2B	2.12	1.48	1.43
16	A	1132	CLA	CHC-C1C	2.12	1.42	1.38
16	h	506	CLA	MG-ND	-2.12	2.01	2.05
16	a	1013	CLA	C1D-ND	2.12	1.40	1.37
16	Y	504	CLA	MG-NB	-2.12	2.01	2.05
16	w	502	CLA	CHC-C1C	2.12	1.42	1.38
16	h	511	CLA	MG-NB	-2.12	2.01	2.05
16	A	1113	CLA	CHC-C1C	2.11	1.42	1.38
16	o	502	CLA	MG-NB	-2.11	2.01	2.05
19	a	4007	BCR	C33-C5	-2.11	1.47	1.50
16	p	506	CLA	C3B-C4B	2.11	1.48	1.42
16	A	1116	CLA	C1B-C2B	2.11	1.48	1.43
16	o	506	CLA	MG-ND	-2.11	2.01	2.05
16	G	1230	CLA	CHC-C1C	2.11	1.42	1.38
16	a	1113	CLA	MG-NB	-2.11	2.01	2.05
16	b	1227	CLA	MG-NB	-2.11	2.01	2.05
16	T	4004	CLA	CHC-C1C	2.11	1.42	1.38
16	r	502	CLA	CHC-C1C	2.11	1.42	1.38
16	p	512	CLA	MG-NB	-2.11	2.01	2.05
16	b	1207	CLA	CHC-C1C	2.11	1.42	1.38
16	Y	507	CLA	CHC-C1C	2.11	1.42	1.38
16	q	515	CLA	C3B-C4B	2.11	1.48	1.42
16	r	510	CLA	CHC-C1C	2.11	1.42	1.38
16	t	507	CLA	CHC-C1C	2.11	1.42	1.38
16	x	510	CLA	CHC-C1C	2.11	1.42	1.38
16	b	1206	CLA	C1B-C2B	2.11	1.48	1.43
16	Z	517	CLA	MG-NB	-2.11	2.01	2.05
16	u	512	CLA	MG-NB	-2.11	2.01	2.05
16	w	507	CLA	CHC-C1C	2.11	1.42	1.38
16	B	1240	CLA	MG-NB	-2.11	2.01	2.05
16	v	504	CLA	MG-NB	-2.11	2.01	2.05
16	a	1114	CLA	C3B-C4B	2.11	1.48	1.42
16	B	1224	CLA	MG-NB	-2.11	2.01	2.05
16	b	1212	CLA	MG-NB	-2.11	2.01	2.05
16	b	1223	CLA	CHC-C1C	2.11	1.42	1.38
16	o	504	CLA	CHC-C1C	2.11	1.42	1.38
16	G	1213	CLA	MG-NB	-2.11	2.01	2.05
13	B	4018	LHG	P-O6	2.11	1.67	1.59
16	Y	501	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	1224	CLA	C3B-C4B	2.10	1.48	1.42
16	X	501	CLA	CHC-C1C	2.10	1.42	1.38
16	A	1127	CLA	MG-ND	-2.10	2.01	2.05
16	h	501	CLA	MG-NB	-2.10	2.01	2.05
16	u	516	CLA	MG-NB	-2.10	2.01	2.05
16	W	507	CLA	CHC-C1C	2.10	1.42	1.38
16	a	1120	CLA	CHC-C1C	2.10	1.42	1.38
16	u	510	CLA	CHC-C1C	2.10	1.42	1.38
16	a	1801	CLA	CHC-C1C	2.10	1.42	1.38
16	H	1108	CLA	MG-NB	-2.10	2.01	2.05
13	r	605	LHG	O7-C5	-2.10	1.41	1.46
16	a	1113	CLA	CHC-C1C	2.10	1.42	1.38
16	b	1218	CLA	CHC-C1C	2.10	1.42	1.38
16	u	502	CLA	CHC-C1C	2.10	1.42	1.38
16	a	1139	CLA	MG-NB	-2.10	2.01	2.05
16	h	510	CLA	CHC-C1C	2.10	1.42	1.38
15	A	1011	CL0	MG-ND	-2.10	2.01	2.05
16	w	512	CLA	MG-NB	-2.10	2.01	2.05
16	X	513	CLA	CHC-C1C	2.10	1.42	1.38
16	A	1013	CLA	C1D-ND	2.10	1.40	1.37
16	o	507	CLA	C3B-C4B	2.10	1.48	1.42
16	b	1204	CLA	CHC-C1C	2.10	1.42	1.38
16	b	1012	CLA	MG-NB	-2.10	2.01	2.05
16	g	514	CLA	MG-NB	-2.10	2.01	2.05
16	r	507	CLA	CHC-C1C	2.10	1.42	1.38
16	q	505	CLA	MG-NB	-2.10	2.01	2.05
13	I	103	LHG	P-O6	2.10	1.67	1.59
16	B	1210	CLA	MG-NB	-2.10	2.01	2.05
16	X	503	CLA	MG-NB	-2.10	2.01	2.05
16	b	1222	CLA	MG-NB	-2.10	2.01	2.05
16	o	516	CLA	MG-NB	-2.10	2.01	2.05
16	s	512	CLA	CHC-C1C	2.10	1.42	1.38
16	B	1235	CLA	MG-NB	-2.10	2.01	2.05
16	K	4002	CLA	CHC-C1C	2.10	1.42	1.38
16	n	505	CLA	MG-NB	-2.10	2.01	2.05
16	u	502	CLA	MG-ND	-2.10	2.01	2.05
16	q	507	CLA	CHC-C1C	2.09	1.42	1.38
16	x	506	CLA	CHC-C1C	2.09	1.42	1.38
16	a	1107	CLA	CHC-C1C	2.09	1.42	1.38
16	J	1302	CLA	MG-NB	-2.09	2.01	2.05
16	b	1216	CLA	MG-NB	-2.09	2.01	2.05
16	G	1012	CLA	C1B-C2B	2.09	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	v	509	CLA	MG-ND	-2.09	2.01	2.05
16	w	501	CLA	MG-NB	-2.09	2.01	2.05
16	y	517	CLA	MG-NB	-2.09	2.01	2.05
16	a	1113	CLA	C4B-NB	-2.09	1.35	1.37
16	k	4004	CLA	CHC-C1C	2.09	1.42	1.38
16	B	1240	CLA	CHC-C1C	2.09	1.42	1.38
16	x	505	CLA	MG-NB	-2.09	2.01	2.05
16	B	1216	CLA	C1B-C2B	2.09	1.48	1.43
16	H	1120	CLA	CHC-C1C	2.09	1.42	1.38
16	s	506	CLA	C3B-C4B	2.09	1.48	1.42
16	x	507	CLA	C3B-C4B	2.09	1.48	1.42
16	A	1115	CLA	MG-ND	-2.09	2.01	2.05
16	X	505	CLA	MG-NB	-2.09	2.01	2.05
16	r	502	CLA	MG-NB	-2.09	2.01	2.05
16	B	1203	CLA	CHC-C1C	2.09	1.42	1.38
16	Q	1301	CLA	CHC-C1C	2.09	1.42	1.38
16	B	1232	CLA	CHC-C1C	2.09	1.42	1.38
16	q	509	CLA	MG-NB	-2.09	2.01	2.05
16	H	1133	CLA	CHC-C1C	2.09	1.42	1.38
16	H	1237	CLA	MG-ND	-2.09	2.01	2.05
16	a	1122	CLA	MG-NB	-2.09	2.01	2.05
16	b	1221	CLA	MG-NB	-2.09	2.01	2.05
16	X	506	CLA	C3B-C4B	2.09	1.48	1.42
16	a	1115	CLA	MG-NB	-2.09	2.01	2.05
16	t	512	CLA	MG-ND	-2.09	2.01	2.05
16	A	1135	CLA	C3B-C4B	2.08	1.48	1.42
16	G	1214	CLA	MG-ND	-2.08	2.01	2.05
15	H	1011	CL0	C1D-C2D	2.08	1.41	1.39
16	a	1129	CLA	C1B-C2B	2.08	1.48	1.43
16	B	1212	CLA	MG-NB	-2.08	2.01	2.05
16	a	1105	CLA	MG-NB	-2.08	2.01	2.05
16	k	4002	CLA	CHC-C1C	2.08	1.42	1.38
16	b	1215	CLA	MG-NB	-2.08	2.01	2.05
16	H	1132	CLA	MG-NB	-2.08	2.01	2.05
16	Y	506	CLA	C3B-C4B	2.08	1.48	1.42
16	q	517	CLA	MG-NB	-2.08	2.01	2.05
16	o	506	CLA	C3B-C4B	2.08	1.48	1.42
16	Z	506	CLA	C3B-C4B	2.08	1.48	1.42
16	A	1118	CLA	CHC-C1C	2.08	1.42	1.38
16	r	512	CLA	CHC-C1C	2.08	1.42	1.38
16	g	506	CLA	MG-NB	-2.08	2.01	2.05
16	r	512	CLA	MG-NB	-2.08	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Z	509	CLA	MG-NB	-2.08	2.01	2.05
16	a	1112	CLA	MG-NB	-2.08	2.01	2.05
16	X	510	CLA	CHC-C1C	2.08	1.42	1.38
16	a	1124	CLA	CHC-C1C	2.08	1.42	1.38
16	Z	503	CLA	MG-NB	-2.08	2.01	2.05
16	o	503	CLA	MG-NB	-2.08	2.01	2.05
16	F	1302	CLA	MG-NB	-2.08	2.01	2.05
16	q	510	CLA	CHC-C1C	2.08	1.42	1.38
16	B	1203	CLA	MG-NB	-2.08	2.01	2.05
16	q	505	CLA	MG-ND	-2.08	2.01	2.05
16	v	505	CLA	MG-NB	-2.08	2.01	2.05
16	A	1136	CLA	CHC-C1C	2.08	1.42	1.38
16	a	1130	CLA	MG-NB	-2.08	2.01	2.05
16	a	1114	CLA	CHC-C1C	2.08	1.42	1.38
16	n	512	CLA	CHC-C1C	2.08	1.42	1.38
16	q	506	CLA	C3B-C4B	2.08	1.48	1.42
16	X	514	CLA	MG-NB	-2.08	2.01	2.05
16	a	1131	CLA	MG-NB	-2.08	2.01	2.05
16	v	510	CLA	CHC-C1C	2.08	1.42	1.38
16	H	1121	CLA	MG-NB	-2.08	2.01	2.05
16	U	1502	CLA	MG-NB	-2.08	2.01	2.05
16	G	1223	CLA	CHC-C1C	2.08	1.42	1.38
16	G	1232	CLA	CHC-C1C	2.08	1.42	1.38
16	s	507	CLA	CHC-C1C	2.08	1.42	1.38
16	A	1108	CLA	MG-NB	-2.08	2.01	2.05
13	R	103	LHG	O7-C5	-2.08	1.41	1.46
16	a	1116	CLA	C1B-C2B	2.08	1.48	1.43
16	H	1132	CLA	C4B-NB	-2.08	1.35	1.37
16	G	1235	CLA	MG-NB	-2.07	2.01	2.05
20	L	4101	LMT	O4'-C4B	-2.07	1.37	1.43
16	n	502	CLA	CHC-C1C	2.07	1.42	1.38
16	A	1132	CLA	MG-NB	-2.07	2.01	2.05
16	G	1224	CLA	MG-NB	-2.07	2.01	2.05
16	G	1234	CLA	MG-ND	-2.07	2.01	2.05
16	W	513	CLA	MG-NB	-2.07	2.01	2.05
16	r	512	CLA	MG-ND	-2.07	2.01	2.05
16	q	515	CLA	MG-NB	-2.07	2.01	2.05
16	r	514	CLA	MG-NB	-2.07	2.01	2.05
19	a	4008	BCR	C33-C5	-2.07	1.47	1.50
16	X	509	CLA	MG-NB	-2.07	2.01	2.05
16	a	1117	CLA	MG-NB	-2.07	2.01	2.05
16	t	506	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1013	CLA	C4B-NB	-2.07	1.35	1.37
16	B	1226	CLA	C3B-C4B	2.07	1.48	1.42
16	H	1116	CLA	C1B-C2B	2.07	1.48	1.43
16	G	1238	CLA	CHC-C1C	2.07	1.42	1.38
16	B	1225	CLA	MG-ND	-2.07	2.01	2.05
16	j	1302	CLA	MG-NB	-2.07	2.01	2.05
16	l	1502	CLA	MG-NB	-2.07	2.01	2.05
16	w	506	CLA	MG-NB	-2.07	2.01	2.05
16	n	511	CLA	MG-NB	-2.07	2.01	2.05
16	B	1215	CLA	MG-NB	-2.07	2.01	2.05
14	a	4201	LMG	O7-C8	-2.07	1.41	1.46
16	G	1217	CLA	CHC-C1C	2.07	1.42	1.38
16	B	1205	CLA	MG-NB	-2.07	2.01	2.05
16	G	1012	CLA	C4B-NB	-2.07	1.35	1.37
16	B	1012	CLA	C1B-C2B	2.07	1.48	1.43
16	W	517	CLA	MG-NB	-2.07	2.01	2.05
16	a	1022	CLA	MG-NB	-2.07	2.01	2.05
16	n	503	CLA	MG-NB	-2.07	2.01	2.05
16	w	515	CLA	MG-NB	-2.07	2.01	2.05
16	p	512	CLA	CHC-C1C	2.07	1.42	1.38
16	l	1501	CLA	MG-NB	-2.07	2.01	2.05
16	b	1205	CLA	MG-NB	-2.07	2.01	2.05
16	p	505	CLA	MG-NB	-2.07	2.01	2.05
16	r	505	CLA	MG-NB	-2.07	2.01	2.05
16	B	1021	CLA	CHC-C1C	2.06	1.42	1.38
16	a	1125	CLA	MG-ND	-2.06	2.01	2.05
16	Y	502	CLA	MG-NB	-2.06	2.01	2.05
16	w	506	CLA	C3B-C4B	2.06	1.48	1.42
16	a	1108	CLA	MG-NB	-2.06	2.01	2.05
16	h	502	CLA	MG-NB	-2.06	2.01	2.05
16	G	1240	CLA	MG-NB	-2.06	2.01	2.05
16	v	517	CLA	MG-NB	-2.06	2.01	2.05
13	g	605	LHG	O7-C5	-2.06	1.41	1.46
16	Z	501	CLA	MG-NB	-2.06	2.01	2.05
16	v	506	CLA	MG-NB	-2.06	2.01	2.05
20	l	4101	LMT	O1'-C1'	-2.06	1.36	1.40
16	b	1219	CLA	MG-NB	-2.06	2.01	2.05
16	p	503	CLA	MG-ND	-2.06	2.01	2.05
16	s	503	CLA	MG-ND	-2.06	2.01	2.05
16	g	507	CLA	C3B-C4B	2.06	1.48	1.42
16	a	1116	CLA	MG-NB	-2.06	2.01	2.05
16	A	1237	CLA	MG-ND	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	1138	CLA	MG-NB	-2.06	2.01	2.05
16	H	1136	CLA	MG-NB	-2.06	2.01	2.05
16	X	504	CLA	CHC-C1C	2.06	1.42	1.38
16	b	1230	CLA	CHC-C1C	2.06	1.42	1.38
16	u	512	CLA	CHC-C1C	2.06	1.42	1.38
16	B	1227	CLA	MG-NB	-2.06	2.01	2.05
16	H	1124	CLA	MG-NB	-2.06	2.01	2.05
16	G	1205	CLA	MG-ND	-2.06	2.01	2.05
16	g	511	CLA	MG-NB	-2.06	2.01	2.05
16	G	1227	CLA	MG-ND	-2.06	2.01	2.05
16	v	507	CLA	MG-NB	-2.06	2.01	2.05
16	G	1021	CLA	CHC-C1C	2.06	1.42	1.38
16	a	1128	CLA	CHC-C1C	2.06	1.42	1.38
16	H	1022	CLA	C3B-C4B	2.06	1.48	1.42
16	g	512	CLA	MG-ND	-2.06	2.01	2.05
16	g	514	CLA	MG-ND	-2.06	2.01	2.05
16	B	1207	CLA	CHC-C1C	2.06	1.42	1.38
14	A	4101	LMG	C3-C2	2.06	1.57	1.52
16	a	1140	CLA	MG-NB	-2.06	2.01	2.05
16	s	505	CLA	MG-NB	-2.06	2.01	2.05
16	A	1022	CLA	C3B-C4B	2.06	1.48	1.42
16	H	1022	CLA	CHC-C1C	2.06	1.42	1.38
16	A	1129	CLA	C1B-C2B	2.06	1.48	1.43
19	G	4014	BCR	C38-C26	-2.06	1.47	1.50
16	n	517	CLA	MG-NB	-2.06	2.01	2.05
16	B	1021	CLA	MG-NB	-2.05	2.01	2.05
16	a	1118	CLA	CHC-C1C	2.05	1.42	1.38
16	W	512	CLA	MG-NB	-2.05	2.01	2.05
16	a	1119	CLA	MG-NB	-2.05	2.01	2.05
16	G	1215	CLA	CHC-C1C	2.05	1.42	1.38
16	a	1022	CLA	CHC-C1C	2.05	1.42	1.38
16	A	1105	CLA	MG-NB	-2.05	2.01	2.05
16	t	505	CLA	MG-NB	-2.05	2.01	2.05
16	a	1135	CLA	C4B-NB	-2.05	1.35	1.37
16	a	1022	CLA	C3B-C4B	2.05	1.48	1.42
16	x	513	CLA	MG-NB	-2.05	2.01	2.05
13	i	103	LHG	O7-C5	-2.05	1.41	1.46
16	h	511	CLA	MG-ND	-2.05	2.01	2.05
16	y	514	CLA	MG-NB	-2.05	2.01	2.05
13	I	103	LHG	O7-C5	-2.05	1.41	1.46
16	W	502	CLA	CHC-C1C	2.05	1.42	1.38
16	W	514	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	1237	CLA	MG-ND	-2.05	2.01	2.05
16	x	503	CLA	MG-NB	-2.05	2.01	2.05
16	a	1104	CLA	MG-ND	-2.05	2.01	2.05
16	n	514	CLA	MG-NB	-2.05	2.01	2.05
20	A	4202	LMT	O1'-C1'	-2.05	1.36	1.40
16	A	1101	CLA	MG-NB	-2.05	2.01	2.05
16	A	1130	CLA	MG-NB	-2.05	2.01	2.05
16	U	1501	CLA	MG-NB	-2.05	2.01	2.05
16	x	509	CLA	MG-NB	-2.05	2.01	2.05
16	b	1238	CLA	CHC-C1C	2.05	1.42	1.38
16	p	510	CLA	CHC-C1C	2.05	1.42	1.38
16	a	1119	CLA	C1B-C2B	2.05	1.47	1.43
16	A	1104	CLA	MG-NB	-2.05	2.01	2.05
16	s	502	CLA	MG-NB	-2.05	2.01	2.05
16	B	1226	CLA	C4B-NB	-2.05	1.35	1.37
16	B	1219	CLA	MG-NB	-2.05	2.01	2.05
16	G	1225	CLA	MG-ND	-2.05	2.01	2.05
16	H	1113	CLA	MG-NB	-2.05	2.01	2.05
16	s	502	CLA	MG-ND	-2.05	2.01	2.05
16	t	502	CLA	CHC-C1C	2.05	1.42	1.38
16	a	1102	CLA	MG-NB	-2.05	2.01	2.05
16	h	505	CLA	MG-NB	-2.05	2.01	2.05
16	B	1215	CLA	CHC-C1C	2.05	1.42	1.38
16	t	509	CLA	MG-NB	-2.05	2.01	2.05
16	x	514	CLA	MG-NB	-2.05	2.01	2.05
16	G	1235	CLA	C1B-C2B	2.05	1.47	1.43
16	H	1107	CLA	CHC-C1C	2.05	1.42	1.38
16	w	511	CLA	MG-NB	-2.05	2.01	2.05
16	q	506	CLA	MG-NB	-2.04	2.01	2.05
20	a	4202	LMT	O4'-C4B	-2.04	1.37	1.43
16	H	1114	CLA	MG-NB	-2.04	2.01	2.05
16	Z	505	CLA	MG-NB	-2.04	2.01	2.05
14	a	4101	LMG	C1-C2	2.04	1.58	1.52
16	Z	502	CLA	MG-ND	-2.04	2.01	2.05
16	y	504	CLA	MG-ND	-2.04	2.01	2.05
13	R	103	LHG	P-O6	2.04	1.67	1.59
16	a	1126	CLA	MG-NB	-2.04	2.01	2.05
16	n	512	CLA	MG-NB	-2.04	2.01	2.05
16	v	503	CLA	MG-NB	-2.04	2.01	2.05
16	A	1135	CLA	C4B-NB	-2.04	1.35	1.37
16	s	501	CLA	MG-NB	-2.04	2.01	2.05
16	b	1236	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	w	517	CLA	MG-ND	-2.04	2.01	2.05
16	Y	510	CLA	CHC-C1C	2.04	1.42	1.38
16	A	1109	CLA	MG-NB	-2.04	2.01	2.05
16	B	1211	CLA	MG-ND	-2.04	2.01	2.05
16	H	1137	CLA	MG-NB	-2.04	2.01	2.05
16	a	1013	CLA	C1B-C2B	2.04	1.47	1.43
16	b	1235	CLA	MG-ND	-2.04	2.01	2.05
16	B	1211	CLA	MG-NB	-2.04	2.01	2.05
16	W	512	CLA	MG-ND	-2.04	2.01	2.05
16	X	516	CLA	MG-NB	-2.04	2.01	2.05
16	p	503	CLA	MG-NB	-2.04	2.01	2.05
16	B	1227	CLA	MG-ND	-2.04	2.01	2.05
19	H	4008	BCR	C33-C5	-2.04	1.47	1.50
16	H	1113	CLA	C4B-NB	-2.04	1.35	1.37
16	x	501	CLA	MG-NB	-2.04	2.01	2.05
20	U	4101	LMT	O4'-C4B	-2.04	1.37	1.43
16	S	1302	CLA	MG-NB	-2.04	2.01	2.05
16	r	507	CLA	MG-NB	-2.04	2.01	2.05
16	o	502	CLA	CHC-C1C	2.04	1.42	1.38
16	r	516	CLA	MG-NB	-2.04	2.01	2.05
16	y	514	CLA	MG-ND	-2.04	2.01	2.05
16	W	503	CLA	MG-NB	-2.04	2.01	2.05
16	g	510	CLA	MG-NB	-2.04	2.01	2.05
16	g	512	CLA	MG-NB	-2.04	2.01	2.05
16	o	514	CLA	MG-ND	-2.04	2.01	2.05
16	w	503	CLA	CHC-C1C	2.04	1.42	1.38
16	A	1115	CLA	MG-NB	-2.04	2.01	2.05
16	A	1131	CLA	MG-NB	-2.04	2.01	2.05
16	a	1129	CLA	MG-NB	-2.04	2.01	2.05
16	p	502	CLA	MG-NB	-2.04	2.01	2.05
19	T	4001	BCR	C33-C5	-2.04	1.47	1.50
16	B	1236	CLA	MG-ND	-2.04	2.01	2.05
16	a	1114	CLA	MG-NB	-2.04	2.01	2.05
16	b	1213	CLA	MG-ND	-2.04	2.01	2.05
20	L	4101	LMT	O1'-C1'	-2.03	1.36	1.40
16	X	502	CLA	MG-NB	-2.03	2.01	2.05
16	a	1131	CLA	C4B-NB	-2.03	1.35	1.37
16	f	1302	CLA	MG-NB	-2.03	2.01	2.05
16	x	511	CLA	MG-ND	-2.03	2.01	2.05
16	b	1214	CLA	MG-NB	-2.03	2.01	2.05
14	H	4201	LMG	O7-C8	-2.03	1.41	1.46
16	A	1135	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	u	513	CLA	MG-NB	-2.03	2.01	2.05
16	H	1119	CLA	C1B-C2B	2.03	1.47	1.43
16	w	506	CLA	MG-ND	-2.03	2.01	2.05
16	H	1140	CLA	MG-ND	-2.03	2.01	2.05
16	G	1226	CLA	CHC-C1C	2.03	1.42	1.38
16	B	1234	CLA	MG-ND	-2.03	2.01	2.05
16	H	1237	CLA	MG-NB	-2.03	2.01	2.05
16	a	1111	CLA	MG-NB	-2.03	2.01	2.05
16	X	504	CLA	C4B-NB	-2.03	1.35	1.37
16	a	1135	CLA	CHC-C1C	2.03	1.42	1.38
16	H	1133	CLA	MG-ND	-2.03	2.01	2.05
16	A	1133	CLA	MG-ND	-2.03	2.01	2.05
16	H	1116	CLA	MG-ND	-2.03	2.01	2.05
16	a	1132	CLA	MG-NB	-2.03	2.01	2.05
16	b	1226	CLA	CHC-C1C	2.03	1.42	1.38
16	p	502	CLA	CHC-C1C	2.03	1.42	1.38
16	H	1119	CLA	MG-NB	-2.03	2.01	2.05
16	B	1219	CLA	C4B-NB	-2.03	1.35	1.37
16	H	1135	CLA	MG-ND	-2.03	2.01	2.05
16	t	502	CLA	MG-ND	-2.03	2.01	2.05
16	x	510	CLA	MG-NB	-2.03	2.01	2.05
19	r	601	BCR	C33-C5	-2.03	1.47	1.50
16	G	1234	CLA	C1B-C2B	2.03	1.47	1.43
16	B	1236	CLA	MG-NB	-2.03	2.01	2.05
16	n	506	CLA	MG-NB	-2.03	2.01	2.05
16	u	506	CLA	CHC-C1C	2.03	1.42	1.38
16	H	1129	CLA	C1B-C2B	2.03	1.47	1.43
16	L	1501	CLA	MG-NB	-2.03	2.01	2.05
16	G	1207	CLA	CHC-C1C	2.03	1.42	1.38
16	G	1021	CLA	MG-NB	-2.03	2.01	2.05
16	g	502	CLA	MG-NB	-2.03	2.01	2.05
16	q	514	CLA	MG-NB	-2.03	2.01	2.05
16	G	1023	CLA	C1D-C2D	-2.03	1.41	1.45
16	G	1222	CLA	MG-ND	-2.02	2.01	2.05
16	a	1113	CLA	MG-ND	-2.02	2.01	2.05
16	h	512	CLA	MG-ND	-2.02	2.01	2.05
16	r	509	CLA	MG-NB	-2.02	2.01	2.05
16	o	507	CLA	CHC-C1C	2.02	1.42	1.38
16	x	507	CLA	MG-NB	-2.02	2.01	2.05
16	b	1230	CLA	MG-NB	-2.02	2.01	2.05
16	B	1235	CLA	C1B-C2B	2.02	1.47	1.43
16	v	502	CLA	MG-NB	-2.02	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	1216	CLA	CHC-C1C	2.02	1.42	1.38
16	H	1013	CLA	C1B-C2B	2.02	1.47	1.43
16	H	1128	CLA	MG-ND	-2.02	2.01	2.05
16	Y	506	CLA	MG-NB	-2.02	2.01	2.05
16	X	502	CLA	CHC-C1C	2.02	1.42	1.38
16	Y	505	CLA	MG-NB	-2.02	2.01	2.05
16	o	514	CLA	MG-NB	-2.02	2.01	2.05
14	B	848	LMG	O7-C8	-2.02	1.41	1.46
14	f	4017	LMG	O7-C8	-2.02	1.41	1.46
15	H	1011	CL0	MG-ND	-2.02	2.01	2.05
16	u	504	CLA	C4B-NB	-2.02	1.35	1.37
16	x	507	CLA	CHC-C1C	2.02	1.42	1.38
16	G	1012	CLA	MG-NB	-2.02	2.01	2.05
16	b	1227	CLA	MG-ND	-2.02	2.01	2.05
16	g	509	CLA	MG-ND	-2.02	2.01	2.05
16	h	510	CLA	MG-NB	-2.02	2.01	2.05
16	Y	514	CLA	MG-NB	-2.02	2.01	2.05
16	Z	504	CLA	MG-ND	-2.02	2.01	2.05
20	H	4202	LMT	O1'-C1'	-2.02	1.36	1.40
20	l	4101	LMT	O4'-C4B	-2.02	1.38	1.43
16	A	1134	CLA	MG-NB	-2.02	2.01	2.05
16	a	1121	CLA	MG-NB	-2.02	2.01	2.05
16	o	502	CLA	MG-ND	-2.02	2.01	2.05
16	w	502	CLA	MG-ND	-2.02	2.01	2.05
16	s	506	CLA	CHC-C1C	2.02	1.42	1.38
16	H	1118	CLA	CHC-C1C	2.02	1.42	1.38
16	A	1140	CLA	MG-ND	-2.02	2.01	2.05
16	X	506	CLA	MG-ND	-2.02	2.01	2.05
21	V	4021	ECH	C11-C10	2.02	1.49	1.43
16	h	509	CLA	MG-ND	-2.02	2.01	2.05
16	r	503	CLA	MG-NB	-2.02	2.01	2.05
16	B	1213	CLA	MG-ND	-2.02	2.01	2.05
16	o	504	CLA	MG-NB	-2.02	2.01	2.05
16	y	503	CLA	MG-ND	-2.02	2.01	2.05
16	B	1223	CLA	CHC-C1C	2.02	1.42	1.38
16	t	506	CLA	CHC-C1C	2.02	1.42	1.38
16	x	502	CLA	MG-ND	-2.01	2.01	2.05
16	b	1220	CLA	MG-ND	-2.01	2.01	2.05
16	p	501	CLA	MG-NB	-2.01	2.01	2.05
16	u	504	CLA	MG-NB	-2.01	2.01	2.05
16	q	516	CLA	MG-NB	-2.01	2.01	2.05
16	w	514	CLA	MG-NB	-2.01	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	1211	CLA	MG-NB	-2.01	2.01	2.05
16	u	509	CLA	MG-NB	-2.01	2.01	2.05
21	b	4006	ECH	C1-C6	2.01	1.56	1.53
19	o	601	BCR	C33-C5	-2.01	1.47	1.50
16	q	502	CLA	MG-ND	-2.01	2.01	2.05
16	s	511	CLA	MG-NB	-2.01	2.01	2.05
16	A	1022	CLA	CHC-C1C	2.01	1.42	1.38
16	Q	1302	CLA	MG-NB	-2.01	2.01	2.05
16	p	513	CLA	MG-NB	-2.01	2.01	2.05
13	a	851	LHG	P-O6	2.01	1.67	1.59
16	A	1126	CLA	MG-NB	-2.01	2.01	2.05
16	Z	511	CLA	MG-ND	-2.01	2.01	2.05
16	v	501	CLA	MG-NB	-2.01	2.01	2.05
16	s	510	CLA	CHC-C1C	2.01	1.42	1.38
16	t	510	CLA	CHC-C1C	2.01	1.42	1.38
16	s	514	CLA	MG-NB	-2.01	2.01	2.05
16	t	501	CLA	MG-NB	-2.01	2.01	2.05
16	A	1116	CLA	MG-NB	-2.01	2.01	2.05
16	n	505	CLA	MG-ND	-2.01	2.01	2.05
16	n	513	CLA	MG-NB	-2.01	2.01	2.05
16	v	508	CLA	MG-ND	-2.01	2.01	2.05
16	p	514	CLA	MG-NB	-2.01	2.01	2.05
16	n	502	CLA	MG-ND	-2.01	2.01	2.05
14	Q	4017	LMG	O7-C8	-2.01	1.41	1.46
15	a	1011	CL0	MG-ND	-2.01	2.01	2.05
16	a	1138	CLA	MG-NB	-2.01	2.01	2.05
16	s	503	CLA	MG-NB	-2.01	2.01	2.05
14	b	848	LMG	C3-C2	2.01	1.57	1.52
16	p	506	CLA	MG-NB	-2.01	2.01	2.05
16	B	1207	CLA	MG-ND	-2.01	2.01	2.05
16	G	1210	CLA	MG-NB	-2.01	2.01	2.05
16	X	502	CLA	MG-ND	-2.01	2.01	2.05
16	a	1136	CLA	MG-NB	-2.01	2.01	2.05
16	b	1208	CLA	MG-NB	-2.01	2.01	2.05
16	x	506	CLA	MG-ND	-2.01	2.01	2.05
16	W	504	CLA	MG-NB	-2.01	2.01	2.05
16	b	1225	CLA	MG-ND	-2.01	2.01	2.05
16	a	1128	CLA	C1B-C2B	2.01	1.47	1.43
16	n	512	CLA	MG-ND	-2.01	2.01	2.05
16	g	507	CLA	CHC-C1C	2.00	1.42	1.38
16	n	508	CLA	MG-NB	-2.00	2.01	2.05
19	l	4022	BCR	C27-C26	-2.00	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1121	CLA	MG-NB	-2.00	2.01	2.05
16	G	1219	CLA	MG-NB	-2.00	2.01	2.05
16	n	514	CLA	MG-ND	-2.00	2.01	2.05
16	y	507	CLA	MG-NB	-2.00	2.01	2.05
16	X	504	CLA	MG-NB	-2.00	2.01	2.05
16	A	1013	CLA	C1B-NB	-2.00	1.35	1.37
16	W	501	CLA	MG-NB	-2.00	2.01	2.05
16	A	1128	CLA	C1B-C2B	2.00	1.47	1.43
16	H	1130	CLA	MG-NB	-2.00	2.01	2.05
16	L	1502	CLA	MG-NB	-2.00	2.01	2.05
16	B	1224	CLA	MG-ND	-2.00	2.01	2.05
16	u	512	CLA	MG-ND	-2.00	2.01	2.05
19	X	601	BCR	C33-C5	-2.00	1.47	1.50
16	G	1224	CLA	MG-ND	-2.00	2.01	2.05
16	G	1206	CLA	CHC-C1C	2.00	1.42	1.38

All (3868) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	506	CLA	C4A-NA-C1A	8.41	110.52	106.68
15	a	1011	CL0	C1B-CHB-C4A	7.74	126.30	121.32
15	A	1011	CL0	C1B-CHB-C4A	7.67	126.26	121.32
15	H	1011	CL0	C1B-CHB-C4A	6.98	125.81	121.32
21	i	4020	ECH	C8-C9-C10	6.94	129.93	119.01
16	x	505	CLA	C4A-NA-C1A	6.63	109.70	106.68
16	v	505	CLA	C4A-NA-C1A	6.59	109.69	106.68
16	b	1216	CLA	C4A-NA-C1A	6.57	109.68	106.68
16	o	514	CLA	C4A-NA-C1A	6.54	109.66	106.68
16	X	506	CLA	C4A-NA-C1A	6.37	109.58	106.68
16	n	505	CLA	C4A-NA-C1A	6.27	109.54	106.68
16	v	508	CLA	C4A-NA-C1A	6.22	109.52	106.68
16	t	505	CLA	C4A-NA-C1A	6.15	109.48	106.68
16	b	1224	CLA	C4A-NA-C1A	6.14	109.48	106.68
16	g	505	CLA	C4A-NA-C1A	6.10	109.46	106.68
16	q	515	CLA	C4A-NA-C1A	6.05	109.44	106.68
16	A	1106	CLA	C4A-NA-C1A	6.03	109.43	106.68
16	y	517	CLA	C4A-NA-C1A	5.99	109.41	106.68
16	Z	515	CLA	C4A-NA-C1A	5.90	109.37	106.68
16	a	1106	CLA	C4A-NA-C1A	5.85	109.35	106.68
16	y	508	CLA	C4A-NA-C1A	5.83	109.34	106.68
16	b	1212	CLA	C4A-NA-C1A	5.81	109.33	106.68
16	A	1126	CLA	C4A-NA-C1A	5.78	109.32	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	r	512	CLA	C4A-NA-C1A	5.78	109.32	106.68
16	g	515	CLA	C4A-NA-C1A	5.78	109.32	106.68
16	B	1207	CLA	C4A-NA-C1A	5.77	109.31	106.68
16	h	505	CLA	C4A-NA-C1A	5.77	109.31	106.68
16	x	501	CLA	C4A-NA-C1A	5.71	109.29	106.68
16	b	1232	CLA	C4A-NA-C1A	5.71	109.28	106.68
21	R	4020	ECH	C8-C7-C6	5.67	142.13	127.00
16	t	515	CLA	C4A-NA-C1A	5.64	109.25	106.68
16	w	515	CLA	C4A-NA-C1A	5.60	109.23	106.68
16	b	1215	CLA	C4A-NA-C1A	5.59	109.23	106.68
16	X	504	CLA	C4A-NA-C1A	5.56	109.21	106.68
16	t	512	CLA	C4A-NA-C1A	5.55	109.21	106.68
16	r	505	CLA	C4A-NA-C1A	5.54	109.21	106.68
16	y	505	CLA	C4A-NA-C1A	5.53	109.20	106.68
16	H	1106	CLA	C4A-NA-C1A	5.52	109.20	106.68
16	X	514	CLA	C4A-NA-C1A	5.51	109.19	106.68
16	b	1207	CLA	C4A-NA-C1A	5.50	109.19	106.68
16	a	1114	CLA	C4A-NA-C1A	5.49	109.18	106.68
16	q	508	CLA	C4A-NA-C1A	5.46	109.17	106.68
16	y	506	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
16	s	501	CLA	C4A-NA-C1A	5.42	109.15	106.68
16	H	1133	CLA	C4A-NA-C1A	5.41	109.15	106.68
16	y	511	CLA	C4A-NA-C1A	5.40	109.14	106.68
16	x	515	CLA	C4A-NA-C1A	5.39	109.14	106.68
16	b	1223	CLA	C4A-NA-C1A	5.37	109.13	106.68
16	v	515	CLA	C4A-NA-C1A	5.37	109.13	106.68
16	Z	508	CLA	C4A-NA-C1A	5.37	109.13	106.68
21	R	4020	ECH	C7-C8-C9	5.37	134.17	126.23
16	W	505	CLA	C4A-NA-C1A	5.36	109.12	106.68
16	X	515	CLA	C4A-NA-C1A	5.32	109.11	106.68
21	I	4020	ECH	C7-C8-C9	5.30	134.07	126.23
16	g	510	CLA	C4A-NA-C1A	5.30	109.09	106.68
16	G	1216	CLA	C4A-NA-C1A	5.26	109.08	106.68
16	a	1126	CLA	C4A-NA-C1A	5.26	109.08	106.68
16	G	1212	CLA	C4A-NA-C1A	5.25	109.07	106.68
16	y	501	CLA	C4A-NA-C1A	5.24	109.07	106.68
16	G	1207	CLA	C4A-NA-C1A	5.23	109.07	106.68
16	u	515	CLA	C4A-NA-C1A	5.22	109.06	106.68
16	v	511	CLA	C4A-NA-C1A	5.20	109.05	106.68
16	h	506	CLA	C4A-NA-C1A	5.20	109.05	106.68
16	T	4004	CLA	C4A-NA-C1A	5.18	109.04	106.68
16	s	514	CLA	C4A-NA-C1A	5.18	109.04	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	U	4019	BCR	C24-C23-C22	-5.15	118.61	126.23
16	G	1232	CLA	C4A-NA-C1A	5.14	109.02	106.68
16	G	1224	CLA	C4A-NA-C1A	5.14	109.02	106.68
16	a	1801	CLA	C4A-NA-C1A	5.12	109.02	106.68
16	r	515	CLA	C4A-NA-C1A	5.12	109.02	106.68
16	G	1205	CLA	C4A-NA-C1A	5.10	109.01	106.68
19	l	4019	BCR	C24-C23-C22	-5.10	118.69	126.23
16	h	507	CLA	C4A-NA-C1A	5.08	109.00	106.68
16	H	1108	CLA	C4A-NA-C1A	5.06	108.99	106.68
16	Z	512	CLA	C4A-NA-C1A	5.06	108.99	106.68
16	A	1115	CLA	C4A-NA-C1A	5.05	108.98	106.68
16	A	1140	CLA	C4A-NA-C1A	5.05	108.98	106.68
16	B	1215	CLA	C4A-NA-C1A	5.03	108.98	106.68
16	u	511	CLA	C4A-NA-C1A	5.02	108.97	106.68
16	B	1212	CLA	C4A-NA-C1A	5.02	108.97	106.68
16	B	1205	CLA	C4A-NA-C1A	5.01	108.97	106.68
21	I	4020	ECH	C8-C7-C6	5.00	140.34	127.00
16	p	512	CLA	C4A-NA-C1A	4.98	108.95	106.68
16	g	516	CLA	C4A-NA-C1A	4.96	108.94	106.68
16	h	504	CLA	C4A-NA-C1A	4.96	108.94	106.68
16	A	1801	CLA	C4A-NA-C1A	4.94	108.93	106.68
16	n	504	CLA	C4A-NA-C1A	4.94	108.93	106.68
16	A	1117	CLA	C4A-NA-C1A	4.93	108.93	106.68
16	B	1232	CLA	C4A-NA-C1A	4.93	108.93	106.68
16	q	505	CLA	C4A-NA-C1A	4.91	108.92	106.68
16	A	1131	CLA	C4A-NA-C1A	4.91	108.92	106.68
16	p	501	CLA	C4A-NA-C1A	4.90	108.92	106.68
16	n	515	CLA	C4A-NA-C1A	4.89	108.91	106.68
16	H	1126	CLA	C4A-NA-C1A	4.89	108.91	106.68
16	b	1205	CLA	C4A-NA-C1A	4.89	108.91	106.68
16	n	503	CLA	C4A-NA-C1A	4.89	108.91	106.68
21	i	4020	ECH	C34-C9-C10	-4.87	114.93	122.82
16	G	1215	CLA	C4A-NA-C1A	4.84	108.89	106.68
16	G	1021	CLA	C4A-NA-C1A	4.81	108.88	106.68
16	n	510	CLA	C4A-NA-C1A	4.81	108.87	106.68
16	r	501	CLA	C4A-NA-C1A	4.81	108.87	106.68
16	H	1115	CLA	C4A-NA-C1A	4.81	108.87	106.68
16	A	1111	CLA	C4A-NA-C1A	4.80	108.87	106.68
16	Z	507	CLA	C4A-NA-C1A	4.80	108.87	106.68
16	a	1108	CLA	C4A-NA-C1A	4.78	108.86	106.68
16	X	511	CLA	C4A-NA-C1A	4.78	108.86	106.68
16	t	509	CLA	C4A-NA-C1A	4.78	108.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	1225	CLA	C4A-NA-C1A	4.78	108.86	106.68
16	W	515	CLA	C4A-NA-C1A	4.78	108.86	106.68
16	b	1231	CLA	C4A-NA-C1A	4.77	108.86	106.68
16	K	4004	CLA	C4A-NA-C1A	4.77	108.85	106.68
16	h	503	CLA	C4A-NA-C1A	4.77	108.85	106.68
24	w	601	LUT	C21-C26-C27	4.76	118.30	112.83
16	Z	511	CLA	C4A-NA-C1A	4.76	108.85	106.68
16	H	1127	CLA	C4A-NA-C1A	4.75	108.84	106.68
16	A	1114	CLA	C4A-NA-C1A	4.74	108.84	106.68
16	G	1223	CLA	C4A-NA-C1A	4.73	108.84	106.68
16	B	1218	CLA	C4A-NA-C1A	4.73	108.84	106.68
16	b	1221	CLA	C4A-NA-C1A	4.73	108.84	106.68
16	a	1117	CLA	C4A-NA-C1A	4.73	108.83	106.68
16	Y	501	CLA	C4A-NA-C1A	4.72	108.83	106.68
16	q	507	CLA	C4A-NA-C1A	4.71	108.83	106.68
16	A	1109	CLA	C4A-NA-C1A	4.70	108.83	106.68
16	a	1131	CLA	C4A-NA-C1A	4.70	108.82	106.68
16	B	1231	CLA	C4A-NA-C1A	4.69	108.82	106.68
16	h	501	CLA	C4A-NA-C1A	4.67	108.81	106.68
16	s	512	CLA	C4A-NA-C1A	4.66	108.80	106.68
16	b	1023	CLA	C4A-NA-C1A	4.66	108.80	106.68
16	w	512	CLA	C4A-NA-C1A	4.64	108.80	106.68
16	B	1240	CLA	C4A-NA-C1A	4.63	108.79	106.68
16	G	1203	CLA	C4A-NA-C1A	4.62	108.79	106.68
16	a	1120	CLA	C4A-NA-C1A	4.62	108.78	106.68
16	W	511	CLA	C4A-NA-C1A	4.61	108.78	106.68
16	n	512	CLA	C4A-NA-C1A	4.59	108.78	106.68
16	n	501	CLA	C4A-NA-C1A	4.59	108.77	106.68
16	H	1111	CLA	C4A-NA-C1A	4.57	108.76	106.68
16	H	1117	CLA	C4A-NA-C1A	4.57	108.76	106.68
16	H	1140	CLA	C4A-NA-C1A	4.57	108.76	106.68
16	B	1214	CLA	C4A-NA-C1A	4.56	108.76	106.68
16	H	1131	CLA	C4A-NA-C1A	4.56	108.76	106.68
24	Z	601	LUT	C21-C26-C27	4.56	118.07	112.83
16	A	1139	CLA	C4A-NA-C1A	4.55	108.75	106.68
16	b	1217	CLA	C4A-NA-C1A	4.55	108.75	106.68
16	u	514	CLA	C4A-NA-C1A	4.54	108.75	106.68
16	G	1211	CLA	C4A-NA-C1A	4.54	108.75	106.68
16	b	1201	CLA	C4A-NA-C1A	4.54	108.75	106.68
16	v	503	CLA	C4A-NA-C1A	4.54	108.75	106.68
16	y	506	CLA	C2B-C1B-NB	-4.52	105.64	110.33
16	G	1208	CLA	C4A-NA-C1A	4.52	108.74	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	v	506	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
16	Z	510	CLA	C4A-NA-C1A	4.51	108.74	106.68
16	B	1203	CLA	C4A-NA-C1A	4.50	108.73	106.68
16	B	1208	CLA	C4A-NA-C1A	4.50	108.73	106.68
16	g	512	CLA	C4A-NA-C1A	4.50	108.73	106.68
16	q	511	CLA	C4A-NA-C1A	4.49	108.73	106.68
16	a	1111	CLA	C4A-NA-C1A	4.49	108.73	106.68
16	H	1113	CLA	C4A-NA-C1A	4.49	108.73	106.68
16	B	1227	CLA	C4A-NA-C1A	4.48	108.72	106.68
16	U	1502	CLA	C4A-NA-C1A	4.47	108.72	106.68
16	H	1114	CLA	C4A-NA-C1A	4.46	108.71	106.68
13	X	605	LHG	O4-P-O5	4.46	133.18	112.44
16	B	1225	CLA	C4A-NA-C1A	4.45	108.71	106.68
16	G	1240	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	v	512	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	a	1132	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	t	506	CLA	C4A-NA-C1A	4.43	108.70	106.68
16	W	510	CLA	C4A-NA-C1A	4.43	108.70	106.68
16	B	1228	CLA	C4A-NA-C1A	4.43	108.70	106.68
16	x	510	CLA	C4A-NA-C1A	4.43	108.70	106.68
16	Y	511	CLA	C4A-NA-C1A	4.42	108.70	106.68
16	h	506	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
16	h	515	CLA	C4A-NA-C1A	4.41	108.69	106.68
16	Y	512	CLA	C4A-NA-C1A	4.41	108.69	106.68
16	l	1502	CLA	C4A-NA-C1A	4.41	108.69	106.68
16	v	506	CLA	C2B-C1B-NB	-4.41	105.75	110.33
13	p	605	LHG	O4-P-O5	4.41	132.94	112.44
16	A	1123	CLA	C4A-NA-C1A	4.41	108.69	106.68
13	R	103	LHG	O4-P-O5	4.41	132.94	112.44
16	A	1133	CLA	C4A-NA-C1A	4.40	108.69	106.68
16	a	1237	CLA	C4A-NA-C1A	4.40	108.69	106.68
13	u	605	LHG	O4-P-O5	4.40	132.91	112.44
16	h	508	CLA	C4A-NA-C1A	4.40	108.69	106.68
13	A	849	LHG	O4-P-O5	4.39	132.89	112.44
13	I	103	LHG	O4-P-O5	4.39	132.88	112.44
13	a	849	LHG	O4-P-O5	4.39	132.87	112.44
16	o	511	CLA	C4A-NA-C1A	4.39	108.68	106.68
16	b	1240	CLA	C4A-NA-C1A	4.39	108.68	106.68
13	H	849	LHG	O4-P-O5	4.38	132.84	112.44
13	o	605	LHG	O4-P-O5	4.38	132.83	112.44
13	i	103	LHG	O4-P-O5	4.38	132.83	112.44
16	X	505	CLA	C4A-NA-C1A	4.38	108.67	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1224	CLA	C4A-NA-C1A	4.37	108.67	106.68
13	s	605	LHG	O4-P-O5	4.37	132.75	112.44
13	Y	605	LHG	O4-P-O5	4.36	132.75	112.44
13	G	4018	LHG	O4-P-O5	4.36	132.73	112.44
16	B	1021	CLA	C4A-NA-C1A	4.35	108.66	106.68
13	x	605	LHG	O4-P-O5	4.34	132.66	112.44
13	B	4018	LHG	O4-P-O5	4.34	132.64	112.44
16	B	1211	CLA	C4A-NA-C1A	4.34	108.66	106.68
13	r	605	LHG	O4-P-O5	4.33	132.60	112.44
16	W	503	CLA	C4A-NA-C1A	4.33	108.66	106.68
16	W	509	CLA	C4A-NA-C1A	4.32	108.65	106.68
16	o	512	CLA	C4A-NA-C1A	4.32	108.65	106.68
16	a	1127	CLA	C4A-NA-C1A	4.31	108.65	106.68
21	I	4020	ECH	C33-C5-C6	-4.31	119.78	124.48
16	a	1140	CLA	C4A-NA-C1A	4.31	108.64	106.68
16	x	512	CLA	C4A-NA-C1A	4.31	108.64	106.68
16	x	516	CLA	C4A-NA-C1A	4.31	108.64	106.68
13	g	605	LHG	O4-P-O5	4.30	132.45	112.44
16	b	1228	CLA	C4A-NA-C1A	4.30	108.64	106.68
16	J	1302	CLA	C4A-NA-C1A	4.29	108.64	106.68
13	b	4018	LHG	O4-P-O5	4.29	132.39	112.44
16	t	501	CLA	C4A-NA-C1A	4.28	108.63	106.68
16	A	1237	CLA	C4A-NA-C1A	4.28	108.63	106.68
16	H	1120	CLA	C4A-NA-C1A	4.27	108.63	106.68
16	w	506	CLA	C4A-NA-C1A	4.27	108.63	106.68
16	o	515	CLA	C4A-NA-C1A	4.27	108.63	106.68
16	v	510	CLA	C4A-NA-C1A	4.27	108.62	106.68
16	a	1128	CLA	C4A-NA-C1A	4.26	108.62	106.68
16	p	511	CLA	C4A-NA-C1A	4.26	108.62	106.68
16	t	511	CLA	C4A-NA-C1A	4.25	108.62	106.68
16	H	1128	CLA	C4A-NA-C1A	4.24	108.61	106.68
16	b	1208	CLA	C4A-NA-C1A	4.24	108.61	106.68
16	y	503	CLA	C4A-NA-C1A	4.24	108.61	106.68
16	H	1135	CLA	C4A-NA-C1A	4.24	108.61	106.68
16	q	514	CLA	C4A-NA-C1A	4.23	108.61	106.68
16	a	1113	CLA	C4A-NA-C1A	4.23	108.61	106.68
16	W	512	CLA	C4A-NA-C1A	4.23	108.61	106.68
16	y	515	CLA	C4A-NA-C1A	4.22	108.60	106.68
13	a	851	LHG	O4-P-O5	4.22	132.06	112.44
13	H	851	LHG	O4-P-O5	4.21	132.01	112.44
13	A	851	LHG	O4-P-O5	4.20	131.98	112.44
21	i	4020	ECH	C11-C10-C9	4.20	133.17	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1023	CLA	C4A-NA-C1A	4.20	108.59	106.68
16	o	507	CLA	C4A-NA-C1A	4.18	108.59	106.68
16	A	1128	CLA	C4A-NA-C1A	4.18	108.59	106.68
16	k	4002	CLA	C4A-NA-C1A	4.18	108.59	106.68
16	a	1122	CLA	C4A-NA-C1A	4.18	108.58	106.68
16	W	501	CLA	C4A-NA-C1A	4.16	108.58	106.68
16	G	1210	CLA	C4A-NA-C1A	4.16	108.58	106.68
16	a	1109	CLA	C4A-NA-C1A	4.16	108.58	106.68
16	n	506	CLA	C4A-NA-C1A	4.15	108.57	106.68
16	w	508	CLA	C4A-NA-C1A	4.14	108.57	106.68
16	s	511	CLA	C4A-NA-C1A	4.13	108.56	106.68
16	r	516	CLA	C4A-NA-C1A	4.12	108.56	106.68
16	w	513	CLA	C4A-NA-C1A	4.12	108.56	106.68
16	Q	1301	CLA	C4A-NA-C1A	4.11	108.55	106.68
16	H	1237	CLA	C4A-NA-C1A	4.10	108.55	106.68
16	G	1209	CLA	C4A-NA-C1A	4.09	108.54	106.68
16	A	1127	CLA	C4A-NA-C1A	4.08	108.54	106.68
16	G	1228	CLA	C4A-NA-C1A	4.07	108.54	106.68
16	B	1239	CLA	C4A-NA-C1A	4.07	108.54	106.68
16	H	1109	CLA	C4A-NA-C1A	4.06	108.53	106.68
16	Y	515	CLA	C4A-NA-C1A	4.05	108.53	106.68
16	W	504	CLA	C4A-NA-C1A	4.05	108.53	106.68
16	Y	506	CLA	C4A-NA-C1A	4.04	108.52	106.68
16	p	510	CLA	C4A-NA-C1A	4.04	108.52	106.68
16	o	505	CLA	C4A-NA-C1A	4.03	108.52	106.68
16	v	509	CLA	C4A-NA-C1A	4.03	108.52	106.68
16	L	1502	CLA	C4A-NA-C1A	4.02	108.51	106.68
16	o	501	CLA	C4A-NA-C1A	4.02	108.51	106.68
16	v	506	CLA	C4A-NA-C1A	4.02	108.51	106.68
24	q	601	LUT	C21-C26-C27	4.00	117.42	112.83
16	b	1227	CLA	C4A-NA-C1A	3.99	108.50	106.68
16	G	1227	CLA	C4A-NA-C1A	3.99	108.50	106.68
16	u	516	CLA	C4A-NA-C1A	3.98	108.50	106.68
16	w	502	CLA	C4A-NA-C1A	3.98	108.50	106.68
16	h	512	CLA	C4A-NA-C1A	3.97	108.49	106.68
16	x	507	CLA	C4A-NA-C1A	3.97	108.49	106.68
16	t	510	CLA	C4A-NA-C1A	3.96	108.48	106.68
19	A	4007	BCR	C3-C4-C5	-3.95	107.01	114.06
16	l	1502	CLA	CHD-C1D-ND	-3.93	119.27	124.80
16	F	1301	CLA	C4A-NA-C1A	3.93	108.47	106.68
16	B	1216	CLA	C3B-C4B-NB	-3.92	107.03	110.53
16	H	1121	CLA	C4A-NA-C1A	3.92	108.47	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	4020	ECH	C1-C6-C5	-3.92	117.28	122.64
16	A	1131	CLA	C3B-C4B-NB	-3.91	107.04	110.53
16	G	1239	CLA	CHD-C1D-ND	-3.90	119.31	124.80
16	t	502	CLA	C3B-C4B-NB	-3.90	107.05	110.53
16	a	1104	CLA	C4A-NA-C1A	3.90	108.46	106.68
19	L	4019	BCR	C24-C23-C22	-3.89	120.48	126.23
16	a	1134	CLA	C4A-NA-C1A	3.88	108.45	106.68
16	w	505	CLA	C4A-NA-C1A	3.88	108.45	106.68
16	t	516	CLA	C4A-NA-C1A	3.88	108.45	106.68
16	a	1125	CLA	C4A-NA-C1A	3.87	108.44	106.68
19	l	4022	BCR	C28-C27-C26	-3.87	107.16	114.06
23	Z	605	LMU	C1'-O5'-C5'	3.87	121.28	113.72
16	H	1135	CLA	C3B-C4B-NB	-3.87	107.08	110.53
16	G	1231	CLA	C4A-NA-C1A	3.86	108.44	106.68
16	G	1225	CLA	C3B-C4B-NB	-3.86	107.09	110.53
16	s	505	CLA	C4A-NA-C1A	3.85	108.44	106.68
16	b	1211	CLA	C4A-NA-C1A	3.84	108.43	106.68
16	G	1234	CLA	C4A-NA-C1A	3.84	108.43	106.68
23	g	606	LMU	C1B-O1B-C4'	-3.83	108.90	117.98
21	V	4021	ECH	C33-C5-C6	-3.83	120.31	124.48
16	W	506	CLA	C4A-NA-C1A	3.82	108.42	106.68
16	H	1138	CLA	C3B-C4B-NB	-3.82	107.12	110.53
16	X	503	CLA	C3B-C4B-NB	-3.81	107.13	110.53
16	o	506	CLA	C4A-NA-C1A	3.81	108.42	106.68
21	I	4020	ECH	C1-C6-C5	-3.81	117.43	122.64
21	m	4021	ECH	C33-C5-C6	-3.80	120.34	124.48
16	u	512	CLA	C4A-NA-C1A	3.80	108.41	106.68
24	Z	601	LUT	C7-C8-C9	-3.79	120.62	126.23
16	s	515	CLA	C4A-NA-C1A	3.79	108.41	106.68
19	I	4018	BCR	C2-C1-C6	3.79	115.94	110.44
16	s	513	CLA	C4A-NA-C1A	3.79	108.41	106.68
16	v	515	CLA	C3B-C4B-NB	-3.78	107.15	110.53
16	y	504	CLA	C3B-C2B-C1B	-3.78	102.71	107.17
16	u	506	CLA	CMC-C2C-C1C	-3.78	119.13	125.03
24	q	601	LUT	C38-C25-C24	-3.77	114.43	123.36
16	H	1801	CLA	C4A-NA-C1A	3.77	108.40	106.68
16	W	516	CLA	C4A-NA-C1A	3.77	108.40	106.68
16	Y	509	CLA	C4A-NA-C1A	3.77	108.40	106.68
23	p	606	LMU	C2'-C3'-C4'	3.77	118.24	109.68
16	H	1013	CLA	C3B-C4B-NB	-3.76	107.17	110.53
16	v	501	CLA	C3B-C2B-C1B	-3.76	102.74	107.17
16	b	1225	CLA	C4A-NA-C1A	3.75	108.39	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	t	503	CLA	C4A-NA-C1A	3.75	108.39	106.68
16	x	506	CLA	C4A-NA-C1A	3.75	108.39	106.68
16	B	1239	CLA	CHD-C1D-ND	-3.75	119.53	124.80
16	G	1221	CLA	C4A-NA-C1A	3.74	108.39	106.68
19	g	601	BCR	C24-C23-C22	-3.74	120.71	126.23
16	h	509	CLA	C4A-NA-C1A	3.73	108.38	106.68
16	x	501	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
16	H	1139	CLA	C4A-NA-C1A	3.72	108.38	106.68
16	s	502	CLA	C4A-NA-C1A	3.72	108.38	106.68
16	q	503	CLA	CHD-C1D-ND	-3.72	119.56	124.80
21	I	4020	ECH	C34-C9-C10	-3.72	116.80	122.82
16	u	505	CLA	C4A-NA-C1A	3.71	108.37	106.68
24	Z	601	LUT	C38-C25-C24	-3.71	114.59	123.36
23	x	606	LMU	C4B-C3B-C2B	3.71	117.33	110.83
16	a	1131	CLA	C3B-C4B-NB	-3.70	107.22	110.53
16	b	1021	CLA	C4A-NA-C1A	3.70	108.37	106.68
16	Y	510	CLA	C4A-NA-C1A	3.70	108.37	106.68
21	V	4021	ECH	C1-C6-C5	-3.70	117.59	122.64
19	T	4005	BCR	C2-C1-C6	3.69	115.79	110.44
21	b	4006	ECH	C2-C1-C6	3.68	115.79	110.44
16	A	1124	CLA	C4A-NA-C1A	3.68	108.36	106.68
16	H	1125	CLA	C4A-NA-C1A	3.67	108.36	106.68
16	v	501	CLA	C4A-NA-C1A	3.66	108.35	106.68
16	a	1107	CLA	C4A-NA-C1A	3.66	108.35	106.68
16	q	504	CLA	C4A-NA-C1A	3.66	108.35	106.68
16	x	502	CLA	C3B-C4B-NB	-3.65	107.27	110.53
16	a	1121	CLA	C4A-NA-C1A	3.65	108.35	106.68
16	h	510	CLA	C4A-NA-C1A	3.65	108.35	106.68
16	G	1216	CLA	C3B-C4B-NB	-3.65	107.27	110.53
16	H	1104	CLA	C4A-NA-C1A	3.65	108.34	106.68
16	w	511	CLA	C4A-NA-C1A	3.65	108.34	106.68
23	s	606	LMU	C2'-C3'-C4'	3.65	117.96	109.68
16	X	512	CLA	C4A-NA-C1A	3.64	108.34	106.68
16	s	506	CLA	C4A-NA-C1A	3.64	108.34	106.68
19	K	4005	BCR	C2-C1-C6	3.64	115.72	110.44
19	k	4005	BCR	C2-C1-C6	3.63	115.72	110.44
16	U	1501	CLA	C4A-NA-C1A	3.63	108.33	106.68
16	q	513	CLA	C4A-NA-C1A	3.62	108.33	106.68
15	A	1011	CL0	C4D-CHA-CBD	-3.62	105.32	108.97
16	W	502	CLA	C4A-NA-C1A	3.61	108.33	106.68
16	q	512	CLA	C4A-NA-C1A	3.61	108.33	106.68
16	A	1111	CLA	OBD-CAD-C3D	-3.61	119.98	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	v	504	CLA	C4A-NA-C1A	3.61	108.33	106.68
23	Y	606	LMU	C4B-C3B-C2B	3.61	117.16	110.83
16	b	1203	CLA	C4A-NA-C1A	3.61	108.32	106.68
16	H	1105	CLA	C3B-C4B-NB	-3.60	107.31	110.53
24	w	601	LUT	C38-C25-C24	-3.60	114.83	123.36
16	a	1102	CLA	C4A-NA-C1A	3.60	108.32	106.68
21	R	4020	ECH	C12-C13-C14	3.60	124.67	119.01
16	u	507	CLA	C3B-C4B-NB	-3.60	107.32	110.53
16	a	1132	CLA	C3B-C4B-NB	-3.59	107.33	110.53
16	B	1209	CLA	C4A-NA-C1A	3.58	108.31	106.68
16	q	501	CLA	C3B-C4B-NB	-3.57	107.34	110.53
16	H	1132	CLA	C3B-C4B-NB	-3.56	107.35	110.53
16	H	1122	CLA	C3B-C4B-NB	-3.56	107.35	110.53
16	A	1135	CLA	C4A-NA-C1A	3.56	108.30	106.68
16	H	1131	CLA	C3B-C4B-NB	-3.56	107.35	110.53
16	F	1302	CLA	C4A-NA-C1A	3.56	108.30	106.68
16	Y	507	CLA	C4A-NA-C1A	3.56	108.30	106.68
16	H	1101	CLA	CHD-C1D-ND	-3.56	119.80	124.80
16	G	1219	CLA	C3B-C4B-NB	-3.55	107.36	110.53
21	M	4021	ECH	C1-C6-C5	-3.55	117.78	122.64
21	B	4006	ECH	C33-C5-C6	-3.54	120.62	124.48
16	n	502	CLA	C4A-NA-C1A	3.54	108.30	106.68
16	b	1213	CLA	C4A-NA-C1A	3.54	108.30	106.68
19	v	601	BCR	C2-C1-C6	3.54	115.58	110.44
16	b	1218	CLA	C4A-NA-C1A	3.54	108.29	106.68
16	b	1210	CLA	C4A-NA-C1A	3.53	108.29	106.68
19	a	4007	BCR	C15-C16-C17	-3.53	116.30	123.52
16	A	1122	CLA	C3B-C4B-NB	-3.53	107.38	110.53
16	p	515	CLA	C4A-NA-C1A	3.52	108.29	106.68
16	r	510	CLA	C4A-NA-C1A	3.52	108.29	106.68
16	u	509	CLA	C4A-NA-C1A	3.52	108.29	106.68
16	A	1132	CLA	C4A-NA-C1A	3.52	108.28	106.68
16	Z	501	CLA	C3B-C4B-NB	-3.52	107.39	110.53
16	u	502	CLA	C4A-NA-C1A	3.51	108.28	106.68
16	a	1105	CLA	C3B-C4B-NB	-3.50	107.40	110.53
19	g	601	BCR	C15-C16-C17	-3.50	116.35	123.52
19	b	4014	BCR	C15-C16-C17	-3.50	116.35	123.52
16	s	514	CLA	CHD-C1D-ND	-3.50	119.87	124.80
16	a	1115	CLA	CHD-C1D-ND	-3.50	119.88	124.80
16	L	1502	CLA	CHD-C1D-ND	-3.50	119.88	124.80
16	x	503	CLA	C3B-C4B-NB	-3.50	107.41	110.53
23	g	606	LMU	C2'-C3'-C4'	3.50	117.62	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	m	4021	ECH	C8-C9-C10	3.49	124.50	119.01
16	y	504	CLA	C4A-NA-C1A	3.49	108.27	106.68
16	A	1129	CLA	C4A-NA-C1A	3.49	108.27	106.68
16	X	501	CLA	C4A-NA-C1A	3.49	108.27	106.68
16	f	1302	CLA	C4A-NA-C1A	3.49	108.27	106.68
16	a	1129	CLA	C4A-NA-C1A	3.48	108.27	106.68
16	H	1133	CLA	C3B-C2B-C1B	-3.48	103.06	107.17
19	Z	602	BCR	C2-C1-C6	3.48	115.50	110.44
16	b	1219	CLA	C3B-C4B-NB	-3.48	107.42	110.53
16	A	1108	CLA	C3B-C4B-NB	-3.48	107.43	110.53
16	H	1118	CLA	C4A-NA-C1A	3.47	108.26	106.68
16	B	1210	CLA	C4A-NA-C1A	3.46	108.26	106.68
16	h	506	CLA	C3B-C4B-NB	-3.46	107.44	110.53
16	A	1132	CLA	C3B-C4B-NB	-3.46	107.44	110.53
19	u	601	BCR	C2-C1-C6	3.46	115.46	110.44
21	R	4020	ECH	C11-C10-C9	-3.45	122.44	127.28
16	b	1208	CLA	C3B-C4B-NB	-3.45	107.45	110.53
21	b	4006	ECH	C33-C5-C6	-3.45	120.72	124.48
16	Q	1302	CLA	C4A-NA-C1A	3.45	108.25	106.68
16	n	511	CLA	C4A-NA-C1A	3.44	108.25	106.68
19	x	604	BCR	C24-C23-C22	-3.44	121.14	126.23
16	G	1208	CLA	C3B-C4B-NB	-3.44	107.46	110.53
21	M	4021	ECH	C33-C5-C6	-3.44	120.73	124.48
16	o	502	CLA	C4A-NA-C1A	3.44	108.25	106.68
19	U	4022	BCR	C28-C27-C26	-3.43	107.94	114.06
16	t	514	CLA	CHD-C1D-ND	-3.43	119.97	124.80
16	l	1501	CLA	C4A-NA-C1A	3.43	108.24	106.68
19	o	601	BCR	C2-C1-C6	3.43	115.42	110.44
16	G	1239	CLA	C4A-NA-C1A	3.42	108.24	106.68
16	H	1022	CLA	C3B-C4B-NB	-3.42	107.48	110.53
16	p	507	CLA	C4A-NA-C1A	3.42	108.24	106.68
16	o	503	CLA	C3B-C4B-NB	-3.42	107.48	110.53
23	p	606	LMU	C4B-C3B-C2B	3.41	116.82	110.83
23	Y	606	LMU	C2'-C3'-C4'	3.41	117.42	109.68
16	t	504	CLA	C4A-NA-C1A	3.41	108.23	106.68
21	m	4021	ECH	C1-C6-C5	-3.41	117.98	122.64
16	G	1235	CLA	C2A-C1A-CHA	3.40	129.78	123.87
19	H	4007	BCR	C15-C16-C17	-3.40	116.55	123.52
19	H	4008	BCR	C15-C14-C13	-3.40	122.50	127.28
16	t	503	CLA	C3B-C4B-NB	-3.40	107.49	110.53
16	B	1234	CLA	C4A-NA-C1A	3.40	108.23	106.68
16	G	1218	CLA	C4A-NA-C1A	3.40	108.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	n	507	CLA	CMB-C2B-C1B	3.40	130.59	125.42
16	B	1236	CLA	C3B-C4B-NB	-3.40	107.50	110.53
19	p	601	BCR	C2-C1-C6	3.39	115.37	110.44
16	h	504	CLA	C3B-C2B-C1B	-3.39	103.17	107.17
19	L	4022	BCR	C2-C1-C6	3.39	115.37	110.44
16	y	516	CLA	C3B-C4B-NB	-3.39	107.50	110.53
21	G	4006	ECH	C35-C13-C14	-3.39	117.32	122.82
16	n	514	CLA	CHD-C1D-ND	-3.39	120.03	124.80
21	B	4006	ECH	C1-C6-C5	-3.39	118.01	122.64
16	G	1229	CLA	CHD-C1D-ND	-3.39	120.04	124.80
21	R	4020	ECH	C35-C13-C14	-3.39	117.33	122.82
16	g	509	CLA	C4A-NA-C1A	3.39	108.22	106.68
16	Y	503	CLA	C3B-C4B-NB	-3.39	107.51	110.53
21	V	4021	ECH	C8-C9-C10	3.38	124.33	119.01
16	H	1126	CLA	CHD-C1D-ND	-3.38	120.05	124.80
16	A	1116	CLA	C4A-NA-C1A	3.37	108.22	106.68
21	b	4006	ECH	C35-C13-C14	-3.37	117.35	122.82
16	u	504	CLA	C3B-C4B-NB	-3.37	107.52	110.53
19	G	4010	BCR	C15-C16-C17	-3.37	116.62	123.52
19	w	602	BCR	C15-C16-C17	-3.37	116.62	123.52
16	b	1235	CLA	CAA-C2A-C3A	-3.37	103.89	113.00
16	B	1219	CLA	C3B-C4B-NB	-3.36	107.53	110.53
23	g	606	LMU	O5'-C5'-C4'	3.36	116.67	109.72
19	X	601	BCR	C15-C16-C17	-3.36	116.65	123.52
16	X	513	CLA	C4A-NA-C1A	3.36	108.21	106.68
19	X	604	BCR	C15-C14-C13	-3.35	122.58	127.28
19	g	604	BCR	C24-C23-C22	-3.35	121.28	126.23
16	y	510	CLA	C4A-NA-C1A	3.34	108.20	106.68
16	B	1203	CLA	C3B-C4B-NB	-3.34	107.55	110.53
16	g	501	CLA	C4A-NA-C1A	3.34	108.20	106.68
19	X	601	BCR	C24-C23-C22	-3.33	121.31	126.23
16	o	516	CLA	C3B-C4B-NB	-3.33	107.56	110.53
23	Y	606	LMU	C1B-O1B-C4'	-3.33	110.09	117.98
19	i	4018	BCR	C2-C1-C6	3.33	115.27	110.44
16	B	1201	CLA	C4A-NA-C1A	3.32	108.19	106.68
16	g	503	CLA	C3B-C4B-NB	-3.32	107.56	110.53
19	u	603	BCR	C3-C4-C5	-3.32	108.14	114.06
16	a	1013	CLA	CHD-C1D-ND	-3.32	120.14	124.80
16	A	1113	CLA	C4A-NA-C1A	3.32	108.19	106.68
16	H	1132	CLA	C4A-NA-C1A	3.32	108.19	106.68
16	X	514	CLA	CHD-C1D-ND	-3.31	120.14	124.80
19	q	602	BCR	C15-C16-C17	-3.31	116.75	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	W	501	CLA	C3B-C2B-C1B	-3.31	103.27	107.17
16	u	505	CLA	CHD-C1D-ND	-3.31	120.15	124.80
19	r	601	BCR	C15-C16-C17	-3.30	116.76	123.52
16	q	506	CLA	C4A-NA-C1A	3.30	108.19	106.68
21	i	4020	ECH	C33-C5-C6	-3.30	120.88	124.48
19	Z	602	BCR	C15-C16-C17	-3.30	116.77	123.52
21	B	4006	ECH	C35-C13-C14	-3.30	117.47	122.82
21	R	4020	ECH	C24-C23-C22	3.30	131.11	126.23
19	s	601	BCR	C15-C16-C17	-3.29	116.79	123.52
19	h	603	BCR	C24-C23-C22	-3.29	121.37	126.23
16	x	514	CLA	C4A-NA-C1A	3.29	108.18	106.68
21	G	4006	ECH	C1-C6-C5	-3.28	118.15	122.64
19	r	604	BCR	C24-C23-C22	-3.28	121.38	126.23
16	v	507	CLA	C4A-NA-C1A	3.28	108.17	106.68
16	n	503	CLA	C3B-C4B-NB	-3.28	107.60	110.53
16	A	1013	CLA	C3B-C4B-NB	-3.28	107.60	110.53
19	o	603	BCR	C2-C1-C6	3.28	115.20	110.44
16	a	1013	CLA	C3B-C4B-NB	-3.27	107.61	110.53
21	i	4020	ECH	C7-C8-C9	3.27	131.07	126.23
16	r	503	CLA	C3B-C4B-NB	-3.27	107.61	110.53
16	v	506	CLA	C3B-C4B-NB	-3.27	107.61	110.53
19	y	604	BCR	C3-C4-C5	-3.27	108.23	114.06
21	M	4021	ECH	C8-C9-C10	3.26	124.14	119.01
16	A	1111	CLA	CHD-C1D-ND	-3.26	120.21	124.80
21	M	4021	ECH	C35-C13-C14	-3.26	117.54	122.82
16	G	1226	CLA	C3B-C4B-NB	-3.25	107.63	110.53
16	H	1119	CLA	C3B-C2B-C1B	-3.25	103.33	107.17
16	H	1135	CLA	C3B-C2B-C1B	-3.25	103.34	107.17
16	a	1130	CLA	C3B-C4B-NB	-3.25	107.63	110.53
23	r	606	LMU	C1B-O1B-C4'	-3.25	110.27	117.98
16	G	1212	CLA	CHD-C1D-ND	-3.25	120.23	124.80
16	B	1023	CLA	CHD-C1D-ND	-3.25	120.23	124.80
16	h	506	CLA	C2B-C1B-NB	-3.24	106.96	110.33
16	B	1235	CLA	C2A-C1A-CHA	3.24	129.49	123.87
16	s	517	CLA	C3B-C4B-NB	-3.24	107.64	110.53
23	x	606	LMU	C1B-O1B-C4'	-3.24	110.30	117.98
16	s	507	CLA	C4A-NA-C1A	3.24	108.16	106.68
16	H	1105	CLA	CHD-C1D-ND	-3.24	120.25	124.80
16	G	1235	CLA	CAA-C2A-C3A	-3.24	104.25	113.00
16	u	514	CLA	CHD-C1D-ND	-3.23	120.25	124.80
16	p	503	CLA	C3B-C4B-NB	-3.23	107.64	110.53
21	m	4021	ECH	C34-C9-C10	-3.23	117.58	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	n	507	CLA	C4A-NA-C1A	3.23	108.15	106.68
19	b	4014	BCR	C11-C10-C9	-3.23	122.75	127.28
16	w	501	CLA	C3B-C4B-NB	-3.23	107.65	110.53
19	B	4004	BCR	C24-C23-C22	-3.22	121.47	126.23
16	B	1223	CLA	C4A-NA-C1A	3.22	108.15	106.68
21	V	4021	ECH	C35-C13-C14	-3.22	117.60	122.82
16	y	509	CLA	C4A-NA-C1A	3.22	108.15	106.68
19	A	4008	BCR	C15-C14-C13	-3.22	122.77	127.28
21	V	4021	ECH	C34-C9-C10	-3.22	117.61	122.82
19	o	601	BCR	C15-C16-C17	-3.22	116.94	123.52
16	G	1023	CLA	C3B-C4B-NB	-3.22	107.66	110.53
16	t	507	CLA	CMB-C2B-C1B	3.22	130.31	125.42
16	H	1129	CLA	C3B-C4B-NB	-3.21	107.66	110.53
16	B	1238	CLA	C4A-NA-C1A	3.21	108.14	106.68
19	u	601	BCR	C15-C16-C17	-3.21	116.96	123.52
16	G	1201	CLA	C4A-NA-C1A	3.21	108.14	106.68
16	g	507	CLA	C4A-NA-C1A	3.21	108.14	106.68
16	h	515	CLA	C2B-C1B-NB	-3.21	107.00	110.33
16	W	507	CLA	CMB-C2B-C1B	3.21	130.30	125.42
16	A	1105	CLA	C3B-C4B-NB	-3.21	107.67	110.53
20	L	4101	LMT	C3'-C4'-C5'	-3.21	103.82	110.93
16	g	514	CLA	CHD-C1D-ND	-3.20	120.29	124.80
16	a	1119	CLA	C3B-C2B-C1B	-3.20	103.40	107.17
16	A	1107	CLA	C4A-NA-C1A	3.20	108.14	106.68
16	b	1209	CLA	C4A-NA-C1A	3.20	108.14	106.68
16	G	1214	CLA	C4A-NA-C1A	3.19	108.14	106.68
15	H	1011	CL0	C4D-CHA-CBD	-3.19	105.75	108.97
19	s	602	BCR	C2-C1-C6	3.19	115.08	110.44
15	H	1011	CL0	CHA-C1A-C2A	-3.19	125.81	133.31
16	A	1120	CLA	C4A-NA-C1A	3.19	108.13	106.68
21	m	4021	ECH	C35-C13-C14	-3.19	117.65	122.82
21	G	4006	ECH	C12-C13-C14	3.19	124.02	119.01
23	p	606	LMU	C1B-O1B-C4'	-3.19	110.43	117.98
16	g	502	CLA	C3B-C4B-NB	-3.18	107.69	110.53
19	o	602	BCR	C2-C1-C6	3.18	115.06	110.44
19	o	603	BCR	C3-C4-C5	-3.18	108.38	114.06
16	Z	513	CLA	C4A-NA-C1A	3.18	108.13	106.68
21	B	4006	ECH	C8-C9-C10	3.18	124.02	119.01
16	g	504	CLA	C4A-NA-C1A	3.18	108.13	106.68
16	G	1012	CLA	C3B-C2B-C1B	-3.17	103.43	107.17
16	a	1132	CLA	CAA-CBA-CGA	-3.17	104.20	113.21
24	w	601	LUT	C22-C23-C24	-3.17	106.48	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	I	4020	ECH	C24-C23-C22	3.17	130.92	126.23
16	G	1023	CLA	C4A-NA-C1A	3.17	108.12	106.68
23	s	606	LMU	C1B-O1B-C4'	-3.16	110.48	117.98
19	u	602	BCR	C2-C1-C6	3.16	115.03	110.44
19	v	601	BCR	C15-C16-C17	-3.16	117.06	123.52
19	H	4008	BCR	C15-C16-C17	-3.16	117.06	123.52
19	b	4004	BCR	C24-C23-C22	-3.16	121.56	126.23
16	A	1136	CLA	C4A-NA-C1A	3.16	108.12	106.68
19	A	4007	BCR	C11-C10-C9	-3.15	122.85	127.28
16	o	514	CLA	CHD-C1D-ND	-3.15	120.36	124.80
19	u	603	BCR	C2-C1-C6	3.15	115.02	110.44
16	u	503	CLA	C3B-C4B-NB	-3.15	107.72	110.53
16	Z	504	CLA	C4A-NA-C1A	3.15	108.11	106.68
19	w	604	BCR	C24-C23-C22	-3.14	121.58	126.23
24	q	601	LUT	C31-C32-C33	-3.14	117.74	126.36
16	B	1217	CLA	C3B-C4B-NB	-3.14	107.72	110.53
21	b	4006	ECH	C12-C13-C14	3.14	123.95	119.01
16	A	1116	CLA	C3B-C4B-NB	-3.14	107.72	110.53
16	W	514	CLA	CHD-C1D-ND	-3.14	120.38	124.80
16	A	1101	CLA	CHD-C1D-ND	-3.14	120.38	124.80
16	x	509	CLA	C3B-C2B-C1B	-3.14	103.47	107.17
16	B	1213	CLA	C3B-C4B-NB	-3.14	107.73	110.53
16	A	1107	CLA	C3B-C4B-NB	-3.14	107.73	110.53
21	G	4006	ECH	C33-C5-C6	-3.14	121.06	124.48
19	h	601	BCR	C27-C26-C25	3.13	126.94	122.70
16	y	502	CLA	C4A-NA-C1A	3.13	108.11	106.68
21	i	4020	ECH	C24-C23-C22	3.13	130.87	126.23
16	G	1023	CLA	CHD-C1D-ND	-3.13	120.40	124.80
16	b	1226	CLA	C3B-C4B-NB	-3.13	107.74	110.53
19	U	4019	BCR	C15-C16-C17	-3.13	117.12	123.52
16	H	1115	CLA	CHD-C1D-ND	-3.13	120.40	124.80
16	H	1133	CLA	C3B-C4B-NB	-3.13	107.74	110.53
16	y	506	CLA	C3B-C4B-NB	-3.13	107.74	110.53
19	Y	602	BCR	C2-C1-C6	3.12	114.97	110.44
16	H	1108	CLA	C3B-C4B-NB	-3.12	107.75	110.53
16	s	503	CLA	C3C-C4C-NC	-3.12	106.43	110.43
16	A	1121	CLA	C4A-NA-C1A	3.12	108.10	106.68
16	x	509	CLA	C4A-NA-C1A	3.12	108.10	106.68
19	y	604	BCR	C2-C1-C6	3.12	114.97	110.44
16	t	513	CLA	C4A-NA-C1A	3.12	108.10	106.68
16	p	506	CLA	C4A-NA-C1A	3.11	108.10	106.68
16	G	1238	CLA	C4A-NA-C1A	3.11	108.10	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	1116	CLA	C4A-NA-C1A	3.11	108.10	106.68
16	a	1124	CLA	C4A-NA-C1A	3.11	108.10	106.68
24	w	601	LUT	C7-C8-C9	-3.11	121.64	126.23
21	M	4021	ECH	C34-C9-C10	-3.10	117.80	122.82
16	a	1137	CLA	C3B-C4B-NB	-3.10	107.77	110.53
13	a	851	LHG	O8-C23-C24	3.10	120.55	111.15
19	y	603	BCR	C24-C23-C22	-3.10	121.65	126.23
16	G	1213	CLA	C4A-NA-C1A	3.09	108.09	106.68
16	B	1229	CLA	CHD-C1D-ND	-3.09	120.45	124.80
19	n	604	BCR	C2-C1-C6	3.09	114.92	110.44
19	B	4004	BCR	C15-C16-C17	-3.09	117.21	123.52
16	a	1132	CLA	CHD-C1D-ND	-3.08	120.46	124.80
19	b	4014	BCR	C29-C30-C25	3.08	114.92	110.44
16	x	516	CLA	CHD-C1D-ND	-3.08	120.46	124.80
16	s	509	CLA	C4A-NA-C1A	3.08	108.08	106.68
19	G	4009	BCR	C15-C16-C17	-3.08	117.22	123.52
16	a	1133	CLA	C3B-C4B-NB	-3.08	107.78	110.53
16	j	1302	CLA	C2B-C1B-NB	-3.08	107.13	110.33
16	G	1228	CLA	C3B-C4B-NB	-3.08	107.78	110.53
16	u	502	CLA	C3B-C4B-NB	-3.07	107.78	110.53
16	u	506	CLA	C3B-C4B-NB	-3.07	107.79	110.53
19	p	602	BCR	C2-C1-C6	3.07	114.90	110.44
21	R	4020	ECH	C2-C1-C6	3.07	114.90	110.44
19	x	601	BCR	C24-C23-C22	-3.07	121.70	126.23
19	A	4011	BCR	C28-C27-C26	-3.06	108.59	114.06
15	A	1011	CL0	CHA-C1A-C2A	-3.06	126.11	133.31
16	Z	516	CLA	CHD-C1D-ND	-3.06	120.49	124.80
15	a	1011	CL0	CHA-C1A-C2A	-3.06	126.11	133.31
16	H	1130	CLA	C3B-C2B-C1B	-3.06	103.56	107.17
16	r	514	CLA	CHD-C1D-ND	-3.06	120.49	124.80
19	X	602	BCR	C2-C1-C6	3.06	114.89	110.44
19	W	604	BCR	C2-C1-C6	3.06	114.88	110.44
16	q	504	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
16	A	1132	CLA	CHD-C1D-ND	-3.06	120.50	124.80
16	v	505	CLA	C3B-C4B-NB	-3.06	107.80	110.53
16	t	513	CLA	C3B-C4B-NB	-3.05	107.80	110.53
16	n	511	CLA	C3B-C4B-NB	-3.05	107.81	110.53
16	h	514	CLA	C3B-C2B-C1B	-3.05	103.57	107.17
16	x	513	CLA	CHA-C1A-NA	-3.05	119.48	126.39
16	W	503	CLA	CHD-C1D-ND	-3.05	120.51	124.80
16	p	514	CLA	CHD-C1D-ND	-3.05	120.51	124.80
19	b	4009	BCR	C15-C16-C17	-3.05	117.28	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	v	603	BCR	C39-C30-C25	3.05	115.02	110.24
16	G	1220	CLA	C4A-NA-C1A	3.05	108.07	106.68
16	s	506	CLA	CHD-C1D-ND	-3.05	120.52	124.80
16	A	1133	CLA	C3B-C4B-NB	-3.04	107.81	110.53
16	G	1236	CLA	C4A-NA-C1A	3.04	108.07	106.68
19	u	602	BCR	C3-C4-C5	-3.04	108.63	114.06
16	h	512	CLA	C3B-C4B-NB	-3.04	107.81	110.53
16	X	507	CLA	C4A-NA-C1A	3.04	108.07	106.68
16	a	1101	CLA	C4A-NA-C1A	3.04	108.07	106.68
19	W	603	BCR	C15-C16-C17	-3.04	117.30	123.52
19	A	4008	BCR	C15-C16-C17	-3.04	117.31	123.52
19	u	601	BCR	C24-C23-C22	-3.04	121.74	126.23
19	s	602	BCR	C15-C16-C17	-3.03	117.31	123.52
16	p	508	CLA	C4A-NA-C1A	3.03	108.06	106.68
16	U	1502	CLA	CHD-C1D-ND	-3.03	120.54	124.80
17	A	2001	PQN	C14-C13-C15	3.03	120.48	115.23
13	A	851	LHG	O8-C23-C24	3.03	120.34	111.15
19	Z	604	BCR	C24-C23-C22	-3.03	121.76	126.23
16	q	503	CLA	C4A-NA-C1A	3.02	108.06	106.68
16	H	1103	CLA	CHD-C1D-ND	-3.02	120.55	124.80
16	W	503	CLA	C3B-C4B-NB	-3.02	107.83	110.53
16	H	1022	CLA	C4A-NA-C1A	3.02	108.06	106.68
16	r	507	CLA	C4A-NA-C1A	3.02	108.06	106.68
21	I	4020	ECH	C35-C13-C14	-3.02	117.92	122.82
15	H	1011	CL0	C1C-CHC-C4B	3.02	126.88	116.07
16	v	501	CLA	C3B-C4B-NB	-3.02	107.83	110.53
16	b	1222	CLA	C3B-C4B-NB	-3.02	107.83	110.53
16	Y	504	CLA	CHD-C1D-ND	-3.02	120.55	124.80
16	B	1235	CLA	CAA-C2A-C3A	-3.02	104.84	113.00
16	A	1123	CLA	CHD-C1D-ND	-3.02	120.56	124.80
19	A	4007	BCR	C15-C16-C17	-3.02	117.34	123.52
24	w	601	LUT	C31-C32-C33	-3.02	118.09	126.36
19	F	4016	BCR	C11-C10-C9	-3.02	123.05	127.28
16	G	1222	CLA	C3B-C4B-NB	-3.02	107.84	110.53
19	b	4010	BCR	C24-C23-C22	-3.01	121.78	126.23
16	A	1103	CLA	CHD-C1D-ND	-3.01	120.57	124.80
19	X	604	BCR	C11-C10-C9	-3.01	123.06	127.28
16	a	1108	CLA	C3B-C4B-NB	-3.01	107.84	110.53
16	K	4003	CLA	C4A-NA-C1A	3.01	108.05	106.68
19	W	604	BCR	C15-C16-C17	-3.01	117.37	123.52
16	b	1220	CLA	C3B-C4B-NB	-3.01	107.85	110.53
19	X	604	BCR	C15-C16-C17	-3.01	117.37	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	J	1302	CLA	C2B-C1B-NB	-3.00	107.21	110.33
16	o	512	CLA	CAA-CBA-CGA	-3.00	104.68	113.21
16	H	1111	CLA	CHD-C1D-ND	-3.00	120.58	124.80
16	h	504	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	o	602	BCR	C3-C4-C5	-3.00	108.71	114.06
19	x	603	BCR	C11-C10-C9	-3.00	123.07	127.28
16	p	511	CLA	CHD-C1D-ND	-3.00	120.58	124.80
16	q	503	CLA	C2D-C1D-ND	-2.99	107.16	110.13
16	H	1104	CLA	C3B-C2B-C1B	-2.99	103.64	107.17
16	H	1136	CLA	C4A-NA-C1A	2.99	108.04	106.68
16	A	1132	CLA	CAA-CBA-CGA	-2.99	104.72	113.21
16	W	513	CLA	C3B-C4B-NB	-2.99	107.86	110.53
16	v	517	CLA	C4A-NA-C1A	2.99	108.04	106.68
16	n	512	CLA	CHA-C1A-NA	-2.99	119.63	126.39
16	b	1202	CLA	CHD-C1D-ND	-2.99	120.60	124.80
16	B	1228	CLA	C3B-C4B-NB	-2.99	107.86	110.53
16	Z	504	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	G	1207	CLA	CHA-C1A-NA	-2.98	119.63	126.39
16	A	1134	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	a	1138	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	Y	516	CLA	C4A-NA-C1A	2.98	108.04	106.68
19	H	4007	BCR	C11-C10-C9	-2.98	123.10	127.28
16	X	502	CLA	C3B-C4B-NB	-2.98	107.87	110.53
19	p	601	BCR	C27-C26-C25	2.98	126.73	122.70
16	A	1137	CLA	C3B-C4B-NB	-2.98	107.87	110.53
16	H	1022	CLA	C2B-C1B-NB	-2.98	107.24	110.33
16	u	504	CLA	C4A-NA-C1A	2.98	108.04	106.68
16	Z	509	CLA	CHD-C1D-ND	-2.98	120.61	124.80
16	W	511	CLA	C3B-C4B-NB	-2.98	107.87	110.53
19	S	4013	BCR	C27-C26-C25	2.97	126.72	122.70
16	r	512	CLA	CHA-C1A-NA	-2.97	119.66	126.39
19	Y	601	BCR	C27-C26-C25	2.97	126.72	122.70
16	J	1302	CLA	C3B-C4B-NB	-2.97	107.88	110.53
13	H	851	LHG	O8-C23-C24	2.97	120.16	111.15
16	t	501	CLA	C3B-C2B-C1B	-2.97	103.67	107.17
16	A	1128	CLA	CHD-C1D-ND	-2.97	120.62	124.80
16	G	1236	CLA	C3B-C4B-NB	-2.97	107.88	110.53
16	u	506	CLA	C1C-C2C-C3C	-2.97	103.86	106.98
15	A	1011	CL0	C1C-CHC-C4B	2.96	126.68	116.07
16	H	1132	CLA	CAA-CBA-CGA	-2.96	104.79	113.21
16	u	507	CLA	C4A-NA-C1A	2.96	108.03	106.68
19	q	604	BCR	C24-C23-C22	-2.96	121.85	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	1101	CLA	CHD-C1D-ND	-2.96	120.64	124.80
23	s	606	LMU	C4B-C3B-C2B	2.96	116.03	110.83
16	g	509	CLA	C3B-C4B-NB	-2.96	107.89	110.53
16	B	1207	CLA	CHA-C1A-NA	-2.96	119.69	126.39
16	U	1502	CLA	C3B-C2B-C1B	-2.96	103.68	107.17
19	b	4009	BCR	C24-C23-C22	-2.96	121.86	126.23
16	A	1129	CLA	C3B-C4B-NB	-2.96	107.89	110.53
16	h	509	CLA	C3B-C4B-NB	-2.96	107.89	110.53
16	v	508	CLA	CHD-C1D-ND	-2.96	120.64	124.80
16	h	515	CLA	C3B-C4B-NB	-2.95	107.89	110.53
16	r	509	CLA	C4A-NA-C1A	2.95	108.03	106.68
19	a	4008	BCR	C15-C14-C13	-2.95	123.14	127.28
19	j	4015	BCR	C11-C10-C9	-2.95	123.14	127.28
16	b	1207	CLA	CHA-C1A-NA	-2.95	119.71	126.39
16	G	1229	CLA	C4A-NA-C1A	2.95	108.02	106.68
19	g	604	BCR	C15-C16-C17	-2.95	117.49	123.52
16	Z	509	CLA	C3B-C2B-C1B	-2.95	103.69	107.17
24	q	601	LUT	C22-C23-C24	-2.95	106.81	111.18
16	a	1122	CLA	C3B-C4B-NB	-2.95	107.90	110.53
16	T	4003	CLA	C4A-NA-C1A	2.95	108.02	106.68
16	r	513	CLA	C4A-NA-C1A	2.95	108.02	106.68
16	s	508	CLA	C4A-NA-C1A	2.95	108.02	106.68
16	H	1134	CLA	C3B-C4B-NB	-2.95	107.90	110.53
16	o	505	CLA	C3B-C4B-NB	-2.95	107.90	110.53
19	r	604	BCR	C15-C16-C17	-2.94	117.49	123.52
19	Q	4016	BCR	C11-C10-C9	-2.94	123.15	127.28
16	H	1129	CLA	C4A-NA-C1A	2.94	108.02	106.68
14	H	4201	LMG	O6-C1-O1	-2.94	103.09	110.04
16	G	1231	CLA	CHA-C1A-NA	-2.94	119.73	126.39
16	w	503	CLA	CHD-C1D-ND	-2.94	120.67	124.80
16	p	514	CLA	C3B-C4B-NB	-2.94	107.91	110.53
16	Z	514	CLA	C4A-NA-C1A	2.94	108.02	106.68
16	a	1137	CLA	C4A-NA-C1A	2.94	108.02	106.68
19	n	604	BCR	C3-C4-C5	-2.94	108.81	114.06
16	x	515	CLA	CHD-C1D-ND	-2.94	120.67	124.80
19	a	4008	BCR	C28-C27-C26	-2.94	108.82	114.06
16	A	1125	CLA	C4A-NA-C1A	2.94	108.02	106.68
16	A	1133	CLA	C3B-C2B-C1B	-2.94	103.71	107.17
19	A	4011	BCR	C24-C23-C22	-2.94	121.89	126.23
19	s	601	BCR	C24-C23-C22	-2.94	121.89	126.23
19	s	602	BCR	C15-C14-C13	-2.94	123.16	127.28
16	x	511	CLA	C3B-C4B-NB	-2.93	107.91	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	506	CLA	CHA-C1A-NA	-2.93	119.75	126.39
16	h	511	CLA	CHD-C1D-ND	-2.93	120.67	124.80
19	n	603	BCR	C15-C16-C17	-2.93	117.52	123.52
16	o	509	CLA	C4A-NA-C1A	2.93	108.02	106.68
16	a	1136	CLA	C4A-NA-C1A	2.93	108.02	106.68
16	r	502	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	B	4010	BCR	C15-C16-C17	-2.93	117.52	123.52
16	b	1227	CLA	CHD-C1D-ND	-2.93	120.68	124.80
19	y	601	BCR	C15-C16-C17	-2.93	117.53	123.52
16	b	1012	CLA	C3B-C2B-C1B	-2.93	103.72	107.17
19	l	4019	BCR	C15-C16-C17	-2.93	117.53	123.52
14	A	4201	LMG	O6-C1-O1	-2.93	103.13	110.04
19	a	4011	BCR	C31-C1-C6	2.93	114.83	110.24
16	Z	504	CLA	CHD-C1D-ND	-2.93	120.69	124.80
16	v	508	CLA	C2D-C1D-ND	-2.92	107.23	110.13
19	S	4012	BCR	C27-C26-C25	2.92	126.65	122.70
16	x	501	CLA	C3B-C4B-NB	-2.92	107.92	110.53
16	l	1502	CLA	C3B-C2B-C1B	-2.92	103.73	107.17
19	h	601	BCR	C15-C16-C17	-2.92	117.54	123.52
16	q	501	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
19	A	4003	BCR	C30-C25-C26	-2.92	118.65	122.64
24	Z	601	LUT	C22-C23-C24	-2.92	106.85	111.18
16	B	1210	CLA	OBD-CAD-C3D	-2.92	121.60	128.42
16	y	504	CLA	C3B-C4B-NB	-2.92	107.93	110.53
16	y	503	CLA	C3B-C2B-C1B	-2.92	103.73	107.17
16	W	502	CLA	CHD-C1D-ND	-2.92	120.70	124.80
16	H	1104	CLA	C3B-C4B-NB	-2.91	107.93	110.53
15	a	1011	CL0	C1C-CHC-C4B	2.91	126.49	116.07
19	p	602	BCR	C15-C16-C17	-2.91	117.56	123.52
16	v	501	CLA	C2B-C1B-NB	-2.91	107.31	110.33
16	v	504	CLA	C3B-C2B-C1B	-2.91	103.74	107.17
16	Z	502	CLA	C4A-NA-C1A	2.91	108.01	106.68
16	H	1103	CLA	C4A-NA-C1A	2.91	108.00	106.68
16	Y	512	CLA	CAA-C2A-C3A	-2.91	105.15	113.00
19	K	4001	BCR	C24-C23-C22	-2.91	121.94	126.23
16	Z	505	CLA	C3B-C4B-NB	-2.90	107.94	110.53
16	t	514	CLA	C4A-NA-C1A	2.90	108.00	106.68
16	p	512	CLA	CHA-C1A-NA	-2.90	119.82	126.39
16	G	1227	CLA	CHD-C1D-ND	-2.90	120.72	124.80
20	U	4101	LMT	C3'-C4'-C5'	-2.90	104.50	110.93
19	p	601	BCR	C15-C16-C17	-2.90	117.58	123.52
16	a	1129	CLA	C3B-C4B-NB	-2.90	107.94	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	1130	CLA	CHD-C1D-ND	-2.90	120.72	124.80
16	A	1022	CLA	C3B-C4B-NB	-2.90	107.94	110.53
16	H	1124	CLA	CHD-C1D-ND	-2.90	120.73	124.80
16	Y	514	CLA	CHD-C1D-ND	-2.90	120.73	124.80
16	K	4003	CLA	C3B-C2B-C1B	-2.90	103.75	107.17
16	G	1203	CLA	C3B-C4B-NB	-2.90	107.94	110.53
19	G	4014	BCR	C20-C21-C22	-2.89	123.22	127.28
16	B	1222	CLA	C3B-C4B-NB	-2.89	107.95	110.53
16	j	1303	CLA	C4A-NA-C1A	2.89	108.00	106.68
19	g	601	BCR	C15-C14-C13	-2.89	123.22	127.28
19	A	4007	BCR	C2-C1-C6	2.89	114.64	110.44
16	B	1021	CLA	CHD-C1D-ND	-2.89	120.73	124.80
16	Y	514	CLA	C3B-C4B-NB	-2.89	107.95	110.53
19	a	4008	BCR	C15-C16-C17	-2.89	117.60	123.52
16	o	501	CLA	C3B-C4B-NB	-2.89	107.95	110.53
16	H	1132	CLA	CHD-C1D-ND	-2.89	120.74	124.80
19	b	4004	BCR	C15-C16-C17	-2.89	117.61	123.52
16	p	512	CLA	C1-C2-C3	-2.89	121.47	126.20
16	Z	514	CLA	CHD-C1D-ND	-2.89	120.74	124.80
19	G	4004	BCR	C24-C23-C22	-2.89	121.96	126.23
16	n	502	CLA	C3B-C4B-NB	-2.89	107.95	110.53
16	s	512	CLA	CHA-C1A-NA	-2.89	119.86	126.39
16	b	1216	CLA	CMB-C2B-C3B	-2.89	119.77	126.55
16	B	1226	CLA	C3B-C4B-NB	-2.88	107.96	110.53
16	q	515	CLA	C3B-C4B-NB	-2.88	107.96	110.53
16	W	502	CLA	C3B-C4B-NB	-2.88	107.96	110.53
16	x	507	CLA	C3B-C4B-NB	-2.88	107.96	110.53
16	G	1225	CLA	CHD-C1D-ND	-2.88	120.75	124.80
16	G	1235	CLA	CHD-C1D-ND	-2.88	120.75	124.80
19	G	4010	BCR	C24-C23-C22	-2.88	121.98	126.23
16	u	517	CLA	C2A-C1A-CHA	2.88	128.86	123.87
16	a	1104	CLA	CHD-C1D-ND	-2.87	120.76	124.80
19	A	4003	BCR	C27-C26-C25	2.87	126.59	122.70
16	B	1023	CLA	C3B-C4B-NB	-2.87	107.97	110.53
19	b	4009	BCR	C27-C26-C25	2.87	126.58	122.70
23	g	606	LMU	C3'-C4'-C5'	2.87	117.29	110.93
16	B	1222	CLA	C2A-C1A-CHA	2.87	128.85	123.87
16	h	515	CLA	C3B-C2B-C1B	-2.87	103.79	107.17
14	a	4201	LMG	O6-C1-O1	-2.87	103.27	110.04
16	A	1122	CLA	C4A-NA-C1A	2.87	107.99	106.68
16	q	517	CLA	C4A-NA-C1A	2.87	107.99	106.68
16	n	517	CLA	C3B-C4B-NB	-2.87	107.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	1125	CLA	CHD-C1D-ND	-2.87	120.77	124.80
17	b	2002	PQN	C11-C12-C13	-2.87	121.89	126.83
13	G	4018	LHG	O8-C23-C24	2.86	120.57	111.83
16	h	508	CLA	C3B-C2B-C1B	-2.86	103.79	107.17
16	w	511	CLA	CHD-C1D-ND	-2.86	120.77	124.80
16	o	507	CLA	CMB-C2B-C1B	2.86	129.78	125.42
15	a	1011	CL0	C4D-CHA-CBD	-2.86	106.08	108.97
21	B	4006	ECH	C12-C13-C14	2.86	123.51	119.01
19	Z	602	BCR	C27-C26-C25	2.86	126.57	122.70
16	a	1116	CLA	C3B-C4B-NB	-2.86	107.98	110.53
16	x	509	CLA	C3B-C4B-NB	-2.86	107.98	110.53
21	I	4020	ECH	C2-C1-C6	2.86	114.59	110.44
16	H	1137	CLA	C3B-C4B-NB	-2.86	107.98	110.53
16	w	502	CLA	C3B-C4B-NB	-2.86	107.98	110.53
16	A	1136	CLA	CHD-C1D-ND	-2.86	120.78	124.80
16	a	1117	CLA	CHD-C1D-ND	-2.86	120.78	124.80
19	l	4019	BCR	C15-C14-C13	-2.86	123.27	127.28
16	r	501	CLA	CHD-C1D-ND	-2.85	120.79	124.80
16	t	515	CLA	C3B-C4B-NB	-2.85	107.98	110.53
19	Y	601	BCR	C15-C16-C17	-2.85	117.68	123.52
16	x	506	CLA	CHD-C1D-ND	-2.85	120.79	124.80
16	B	1229	CLA	C4A-NA-C1A	2.85	107.98	106.68
16	u	516	CLA	C3B-C4B-NB	-2.85	107.99	110.53
19	S	4013	BCR	C15-C16-C17	-2.85	117.69	123.52
19	o	604	BCR	C15-C14-C13	-2.85	123.29	127.28
19	u	603	BCR	C15-C16-C17	-2.85	117.70	123.52
16	a	1140	CLA	C3B-C4B-NB	-2.84	107.99	110.53
16	G	1220	CLA	CHD-C1D-ND	-2.84	120.80	124.80
16	a	1133	CLA	C2B-C1B-NB	-2.84	107.38	110.33
16	v	509	CLA	C3B-C2B-C1B	-2.84	103.82	107.17
16	B	1235	CLA	CHD-C1D-ND	-2.84	120.80	124.80
16	g	515	CLA	C3B-C4B-NB	-2.84	107.99	110.53
16	b	1222	CLA	C2A-C1A-CHA	2.84	128.79	123.87
16	t	512	CLA	CHA-C1A-NA	-2.84	119.96	126.39
19	J	4012	BCR	C15-C16-C17	-2.84	117.71	123.52
16	x	504	CLA	C1-C2-C3	-2.84	121.55	126.20
16	v	509	CLA	C3B-C4B-NB	-2.84	108.00	110.53
16	q	505	CLA	C3C-C4C-NC	-2.84	106.80	110.43
16	Y	513	CLA	C4A-NA-C1A	2.83	107.97	106.68
19	G	4009	BCR	C27-C26-C25	2.83	126.53	122.70
16	a	1136	CLA	CHD-C1D-ND	-2.83	120.82	124.80
19	B	4009	BCR	C15-C16-C17	-2.83	117.73	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	4014	BCR	C24-C23-C22	-2.82	122.06	126.23
19	r	602	BCR	C24-C23-C22	-2.82	122.06	126.23
16	A	1137	CLA	C4A-NA-C1A	2.82	107.97	106.68
16	a	1124	CLA	CHD-C1D-ND	-2.82	120.83	124.80
16	u	513	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	L	4019	BCR	C15-C16-C17	-2.82	117.75	123.52
19	x	604	BCR	C15-C16-C17	-2.82	117.75	123.52
19	a	4007	BCR	C15-C14-C13	-2.82	123.32	127.28
16	y	504	CLA	C2B-C1B-NB	-2.82	107.40	110.33
16	Z	503	CLA	C3B-C4B-NB	-2.82	108.01	110.53
16	a	1114	CLA	C3B-C4B-NB	-2.82	108.01	110.53
16	v	507	CLA	CMB-C2B-C1B	2.82	129.71	125.42
16	b	1225	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	g	602	BCR	C24-C23-C22	-2.82	122.07	126.23
19	r	602	BCR	C15-C16-C17	-2.82	117.75	123.52
19	s	602	BCR	C3-C4-C5	-2.82	109.03	114.06
19	H	4011	BCR	C28-C27-C26	-2.82	109.03	114.06
19	R	4018	BCR	C15-C16-C17	-2.81	117.76	123.52
16	g	512	CLA	CHA-C1A-NA	-2.81	120.02	126.39
16	h	507	CLA	CHD-C1D-ND	-2.81	120.84	124.80
16	L	1502	CLA	C3B-C2B-C1B	-2.81	103.85	107.17
16	H	1117	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	X	604	BCR	C24-C23-C22	-2.81	122.07	126.23
16	B	1213	CLA	CHD-C1D-ND	-2.81	120.84	124.80
16	g	511	CLA	C4A-NA-C1A	2.81	107.96	106.68
16	v	507	CLA	CHD-C1D-ND	-2.81	120.84	124.80
16	A	1102	CLA	C3B-C4B-NB	-2.81	108.02	110.53
16	q	517	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	B	4009	BCR	C27-C26-C25	2.81	126.50	122.70
16	X	506	CLA	CHA-C1A-NA	-2.81	120.03	126.39
16	W	512	CLA	CHA-C1A-NA	-2.81	120.03	126.39
19	v	603	BCR	C27-C26-C25	2.81	126.50	122.70
16	a	1102	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	H	4007	BCR	C15-C14-C13	-2.81	123.34	127.28
16	A	1118	CLA	CHD-C1D-ND	-2.81	120.85	124.80
16	b	1234	CLA	CHA-C1A-NA	-2.81	120.03	126.39
16	H	1138	CLA	CHD-C1D-ND	-2.81	120.85	124.80
19	b	4010	BCR	C15-C16-C17	-2.81	117.78	123.52
16	a	1135	CLA	C4A-NA-C1A	2.81	107.96	106.68
16	H	1112	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	X	505	CLA	CHD-C1D-ND	-2.80	120.86	124.80
16	q	515	CLA	CHD-C1D-ND	-2.80	120.86	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	p	504	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	B	1210	CLA	CHD-C1D-ND	-2.80	120.86	124.80
16	a	1119	CLA	CHA-C1A-NA	-2.80	120.05	126.39
13	b	4018	LHG	O8-C23-C24	2.80	120.38	111.83
16	B	1204	CLA	CHD-C1D-ND	-2.80	120.86	124.80
16	H	1013	CLA	CHD-C1D-ND	-2.80	120.86	124.80
21	M	4021	ECH	C12-C13-C14	2.80	123.42	119.01
19	j	4012	BCR	C27-C26-C25	2.80	126.49	122.70
14	G	848	LMG	O6-C1-O1	-2.80	103.43	110.04
16	A	1121	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	Y	514	CLA	CHA-C1A-NA	-2.80	120.05	126.39
13	s	605	LHG	O8-C23-C24	2.80	120.37	111.83
19	Z	602	BCR	C24-C23-C22	-2.80	122.09	126.23
19	v	604	BCR	C27-C26-C25	2.80	126.49	122.70
16	r	513	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	p	602	BCR	C15-C14-C13	-2.80	123.36	127.28
16	G	1213	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	A	1112	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	b	1239	CLA	CHD-C1D-ND	-2.79	120.87	124.80
16	h	506	CLA	C2D-C1D-ND	-2.79	107.36	110.13
16	o	515	CLA	CHA-C1A-NA	-2.79	120.07	126.39
16	h	501	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	B	1220	CLA	CHD-C1D-ND	-2.79	120.88	124.80
16	Y	509	CLA	CHA-C1A-NA	-2.79	120.08	126.39
16	r	517	CLA	C4A-NA-C1A	2.79	107.95	106.68
19	L	4019	BCR	C15-C14-C13	-2.78	123.37	127.28
19	S	4015	BCR	C15-C14-C13	-2.78	123.37	127.28
16	L	1501	CLA	C4A-NA-C1A	2.78	107.95	106.68
16	w	509	CLA	C3B-C4B-NB	-2.78	108.05	110.53
21	G	4006	ECH	C8-C9-C10	2.78	123.39	119.01
16	y	515	CLA	C3B-C4B-NB	-2.78	108.05	110.53
16	Z	506	CLA	C4A-NA-C1A	2.78	107.95	106.68
16	w	517	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	Z	602	BCR	C3-C4-C5	-2.78	109.10	114.06
19	W	604	BCR	C15-C14-C13	-2.78	123.38	127.28
16	H	1114	CLA	CHA-C1A-NA	-2.78	120.10	126.39
19	o	604	BCR	C15-C16-C17	-2.78	117.83	123.52
19	h	604	BCR	C27-C26-C25	2.78	126.46	122.70
16	o	505	CLA	CHD-C1D-ND	-2.78	120.89	124.80
16	X	501	CLA	C3B-C4B-NB	-2.78	108.05	110.53
16	r	514	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	o	601	BCR	C24-C23-C22	-2.78	122.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	1219	CLA	C3B-C2B-C1B	-2.78	103.90	107.17
16	A	1120	CLA	C3C-C4C-NC	-2.77	106.88	110.43
19	w	602	BCR	C15-C14-C13	-2.77	123.39	127.28
16	h	509	CLA	CHD-C1D-ND	-2.77	120.90	124.80
16	y	506	CLA	CMC-C2C-C1C	-2.77	120.71	125.03
16	h	502	CLA	C3B-C4B-NB	-2.77	108.06	110.53
16	A	1124	CLA	CHD-C1D-ND	-2.77	120.91	124.80
19	Y	602	BCR	C15-C16-C17	-2.77	117.86	123.52
16	B	1238	CLA	C3B-C4B-NB	-2.77	108.06	110.53
16	x	514	CLA	CHD-C1D-ND	-2.77	120.91	124.80
19	v	601	BCR	C15-C14-C13	-2.77	123.40	127.28
19	i	4018	BCR	C11-C10-C9	-2.77	123.40	127.28
19	h	601	BCR	C15-C14-C13	-2.77	123.40	127.28
19	Y	602	BCR	C15-C14-C13	-2.77	123.40	127.28
16	n	517	CLA	CMB-C2B-C1B	2.76	129.63	125.42
19	U	4019	BCR	C15-C14-C13	-2.76	123.40	127.28
16	G	1012	CLA	CHD-C1D-ND	-2.76	120.91	124.80
16	r	509	CLA	C3B-C2B-C1B	-2.76	103.91	107.17
16	X	516	CLA	C3B-C4B-NB	-2.76	108.06	110.53
16	b	1023	CLA	CHD-C1D-ND	-2.76	120.92	124.80
16	u	506	CLA	C2C-C1C-NC	-2.76	107.08	109.98
16	r	515	CLA	CHD-C1D-ND	-2.76	120.92	124.80
16	v	502	CLA	C4A-NA-C1A	2.76	107.94	106.68
13	x	605	LHG	O8-C23-C24	2.76	120.25	111.83
19	L	4019	BCR	C29-C30-C25	2.76	114.45	110.44
16	q	511	CLA	CHD-C1D-ND	-2.76	120.92	124.80
19	T	4001	BCR	C27-C26-C25	2.76	126.43	122.70
16	A	1129	CLA	CHD-C1D-ND	-2.76	120.92	124.80
21	V	4021	ECH	C12-C13-C14	2.76	123.34	119.01
16	Z	512	CLA	CHA-C1A-NA	-2.76	120.15	126.39
16	h	515	CLA	C2A-C1A-CHA	2.76	128.65	123.87
16	a	1129	CLA	CHD-C1D-ND	-2.76	120.92	124.80
19	x	604	BCR	C7-C8-C9	-2.76	122.16	126.23
15	H	1011	CL0	CMB-C2B-C3B	2.76	130.19	124.68
16	w	514	CLA	C3B-C4B-NB	-2.76	108.07	110.53
19	o	601	BCR	C15-C14-C13	-2.76	123.41	127.28
19	y	601	BCR	C15-C14-C13	-2.75	123.42	127.28
16	H	1114	CLA	CHD-C1D-ND	-2.75	120.93	124.80
16	b	1204	CLA	CHD-C1D-ND	-2.75	120.93	124.80
19	j	4013	BCR	C15-C16-C17	-2.75	117.89	123.52
16	t	503	CLA	CHD-C1D-ND	-2.75	120.93	124.80
16	w	504	CLA	CHD-C1D-ND	-2.75	120.93	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	x	504	CLA	C3B-C4B-NB	-2.75	108.07	110.53
21	B	4006	ECH	C34-C9-C10	-2.75	118.36	122.82
16	Y	504	CLA	C4A-NA-C1A	2.75	107.93	106.68
16	b	1220	CLA	C4A-NA-C1A	2.75	107.93	106.68
16	A	1105	CLA	CHD-C1D-ND	-2.75	120.93	124.80
16	p	514	CLA	CHA-C1A-NA	-2.75	120.17	126.39
19	Z	602	BCR	C15-C14-C13	-2.75	123.42	127.28
16	v	503	CLA	CHD-C1D-ND	-2.75	120.94	124.80
16	X	509	CLA	CHA-C1A-NA	-2.75	120.17	126.39
16	s	512	CLA	C1-C2-C3	-2.75	121.70	126.20
19	u	604	BCR	C15-C16-C17	-2.75	117.90	123.52
16	x	507	CLA	CMB-C2B-C1B	2.74	129.60	125.42
16	q	514	CLA	CHD-C1D-ND	-2.74	120.94	124.80
19	n	603	BCR	C15-C14-C13	-2.74	123.43	127.28
19	B	4009	BCR	C24-C23-C22	-2.74	122.18	126.23
16	h	512	CLA	C2B-C1B-NB	-2.74	107.48	110.33
16	q	504	CLA	C3B-C4B-NB	-2.74	108.08	110.53
16	H	1110	CLA	C4A-NA-C1A	2.74	107.93	106.68
19	j	4012	BCR	C15-C16-C17	-2.74	117.91	123.52
16	B	1202	CLA	CHD-C1D-ND	-2.74	120.94	124.80
16	H	1119	CLA	CHD-C1D-ND	-2.74	120.94	124.80
19	J	4012	BCR	C11-C10-C9	-2.74	123.43	127.28
19	a	4011	BCR	C15-C16-C17	-2.74	117.91	123.52
16	p	509	CLA	CHA-C1A-NA	-2.74	120.19	126.39
16	A	1127	CLA	CHD-C1D-ND	-2.74	120.95	124.80
16	A	1115	CLA	CHD-C1D-ND	-2.74	120.95	124.80
16	y	515	CLA	C3B-C2B-C1B	-2.74	103.94	107.17
19	j	4015	BCR	C15-C14-C13	-2.74	123.44	127.28
16	B	1215	CLA	CHD-C1D-ND	-2.74	120.95	124.80
19	x	601	BCR	C15-C16-C17	-2.74	117.92	123.52
16	y	506	CLA	C4A-NA-C1A	2.74	107.93	106.68
16	y	505	CLA	CHD-C1D-ND	-2.74	120.95	124.80
16	q	516	CLA	C3B-C4B-NB	-2.74	108.09	110.53
19	g	601	BCR	C27-C26-C25	2.74	126.40	122.70
16	B	1218	CLA	CHD-C1D-ND	-2.73	120.95	124.80
16	b	1203	CLA	CHD-C1D-ND	-2.73	120.95	124.80
16	b	1213	CLA	CHD-C1D-ND	-2.73	120.95	124.80
19	l	4019	BCR	C27-C26-C25	2.73	126.40	122.70
16	X	509	CLA	C3B-C4B-NB	-2.73	108.09	110.53
16	b	1230	CLA	CMC-C2C-C1C	-2.73	120.77	125.03
19	G	4004	BCR	C15-C16-C17	-2.73	117.93	123.52
19	k	4001	BCR	C15-C16-C17	-2.73	117.93	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	p	602	BCR	C3-C4-C5	-2.73	109.19	114.06
20	l	4101	LMT	C3'-C4'-C5'	-2.73	104.88	110.93
16	t	509	CLA	C3B-C4B-NB	-2.73	108.09	110.53
16	G	1216	CLA	CHA-C1A-NA	-2.73	120.21	126.39
16	b	1235	CLA	CHD-C1D-ND	-2.73	120.96	124.80
16	b	1012	CLA	C3B-C4B-NB	-2.73	108.09	110.53
19	U	4019	BCR	C27-C26-C25	2.73	126.39	122.70
19	W	603	BCR	C15-C14-C13	-2.73	123.45	127.28
19	f	4016	BCR	C11-C10-C9	-2.73	123.45	127.28
13	p	605	LHG	O8-C23-C24	2.73	120.15	111.83
23	Z	605	LMU	O5'-C5'-C4'	2.73	115.36	109.72
23	x	606	LMU	C1'-O5'-C5'	2.73	119.05	113.72
16	G	1224	CLA	C3B-C4B-NB	-2.73	108.09	110.53
16	n	509	CLA	C3B-C2B-C1B	-2.73	103.95	107.17
16	a	1103	CLA	CHD-C1D-ND	-2.73	120.97	124.80
13	B	4018	LHG	O8-C23-C24	2.72	120.14	111.83
16	s	517	CLA	CHA-C1A-NA	-2.72	120.22	126.39
16	w	514	CLA	CHD-C1D-ND	-2.72	120.97	124.80
16	A	1138	CLA	C3B-C4B-NB	-2.72	108.10	110.53
16	s	507	CLA	CMB-C2B-C1B	2.72	129.57	125.42
16	y	506	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
21	m	4021	ECH	C12-C13-C14	2.72	123.29	119.01
14	B	848	LMG	O6-C1-O1	-2.72	103.61	110.04
19	y	604	BCR	C27-C26-C25	2.72	126.38	122.70
16	n	517	CLA	CHD-C1D-ND	-2.72	120.97	124.80
16	s	509	CLA	CHA-C1A-NA	-2.72	120.23	126.39
16	p	507	CLA	CMB-C2B-C1B	2.72	129.56	125.42
16	A	1101	CLA	C4A-NA-C1A	2.72	107.92	106.68
16	p	505	CLA	C4A-NA-C1A	2.72	107.92	106.68
16	B	1221	CLA	CHD-C1D-ND	-2.72	120.98	124.80
16	B	1227	CLA	CHD-C1D-ND	-2.72	120.98	124.80
16	h	517	CLA	CHD-C1D-ND	-2.72	120.98	124.80
16	p	505	CLA	C3B-C2B-C1B	-2.72	103.97	107.17
13	r	605	LHG	O8-C23-C24	2.72	120.12	111.83
16	G	1238	CLA	C3B-C4B-NB	-2.72	108.11	110.53
16	W	517	CLA	CHD-C1D-ND	-2.72	120.98	124.80
19	t	604	BCR	C15-C16-C17	-2.72	117.96	123.52
15	A	1011	CL0	C4C-CHD-C1D	2.72	125.78	116.07
16	a	1133	CLA	C3B-C2B-C1B	-2.71	103.97	107.17
16	h	514	CLA	CHA-C1A-NA	-2.71	120.25	126.39
16	b	1235	CLA	C2A-C1A-CHA	2.71	128.57	123.87
16	v	508	CLA	C3B-C4B-NB	-2.71	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1012	CLA	C4A-NA-C1A	2.71	107.92	106.68
16	H	1117	CLA	CHD-C1D-ND	-2.71	120.99	124.80
16	v	508	CLA	C3B-C2B-C1B	-2.71	103.98	107.17
16	Y	503	CLA	CHD-C1D-ND	-2.71	120.99	124.80
19	a	4007	BCR	C11-C10-C9	-2.71	123.48	127.28
16	b	1228	CLA	C3B-C4B-NB	-2.71	108.11	110.53
16	g	514	CLA	C3B-C4B-NB	-2.71	108.11	110.53
16	q	502	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	h	603	BCR	C27-C26-C25	2.71	126.36	122.70
16	g	509	CLA	C2B-C1B-NB	-2.71	107.52	110.33
19	B	4014	BCR	C20-C21-C22	-2.71	123.48	127.28
19	x	603	BCR	C24-C23-C22	-2.71	122.23	126.23
16	G	1202	CLA	C3B-C2B-C1B	-2.71	103.98	107.17
19	y	601	BCR	C27-C26-C25	2.71	126.36	122.70
19	s	604	BCR	C24-C23-C22	-2.71	122.23	126.23
19	x	602	BCR	C15-C16-C17	-2.71	117.98	123.52
16	X	506	CLA	CHD-C1D-ND	-2.71	121.00	124.80
19	G	4010	BCR	C15-C14-C13	-2.71	123.48	127.28
16	s	511	CLA	CHD-C1D-ND	-2.70	121.00	124.80
19	Y	602	BCR	C3-C4-C5	-2.70	109.23	114.06
24	q	601	LUT	C1-C6-C5	-2.70	118.94	122.64
16	x	514	CLA	C3B-C4B-NB	-2.70	108.12	110.53
16	Z	501	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
16	B	1222	CLA	CMB-C2B-C1B	2.70	129.53	125.42
16	j	1302	CLA	C3B-C4B-NB	-2.70	108.12	110.53
16	g	507	CLA	CMB-C2B-C1B	2.70	129.53	125.42
19	W	604	BCR	C3-C4-C5	-2.70	109.24	114.06
19	L	4022	BCR	C27-C26-C25	2.70	126.35	122.70
19	o	603	BCR	C27-C26-C25	2.70	126.35	122.70
16	f	1301	CLA	C4A-NA-C1A	2.70	107.91	106.68
16	x	502	CLA	C4A-NA-C1A	2.70	107.91	106.68
16	q	517	CLA	C2A-C1A-CHA	2.70	128.55	123.87
19	k	4001	BCR	C24-C23-C22	-2.70	122.24	126.23
19	s	604	BCR	C27-C26-C25	2.70	126.35	122.70
16	o	512	CLA	CHA-C1A-NA	-2.70	120.28	126.39
16	r	505	CLA	CHA-C1A-NA	-2.70	120.28	126.39
19	x	604	BCR	C15-C14-C13	-2.70	123.49	127.28
23	Y	606	LMU	O5B-C5B-C4B	2.70	114.56	109.70
13	Y	605	LHG	O8-C23-C24	2.70	120.06	111.83
16	y	509	CLA	C3B-C2B-C1B	-2.70	103.99	107.17
19	b	4005	BCR	C15-C16-C17	-2.70	118.00	123.52
16	q	509	CLA	CHD-C1D-ND	-2.70	121.01	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	o	508	CLA	C3B-C4B-NB	-2.70	108.12	110.53
17	B	2002	PQN	C14-C13-C15	2.70	119.91	115.23
16	q	501	CLA	C3B-C2B-C1B	-2.70	103.99	107.17
19	W	601	BCR	C28-C27-C26	-2.70	109.25	114.06
16	Y	507	CLA	CMB-C2B-C1B	2.70	129.52	125.42
16	b	1236	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	H	4101	LMG	O6-C1-O1	-2.69	103.68	110.04
16	A	1022	CLA	C2B-C1B-NB	-2.69	107.53	110.33
15	H	1011	CL0	C4C-CHD-C1D	2.69	125.70	116.07
16	y	501	CLA	CHD-C1D-ND	-2.69	121.01	124.80
19	k	4001	BCR	C15-C14-C13	-2.69	123.50	127.28
16	a	1139	CLA	C4A-NA-C1A	2.69	107.91	106.68
16	b	1236	CLA	C4A-NA-C1A	2.69	107.91	106.68
16	G	1213	CLA	CHD-C1D-ND	-2.69	121.02	124.80
16	q	504	CLA	CHD-C1D-ND	-2.69	121.02	124.80
16	k	4003	CLA	CHD-C1D-ND	-2.69	121.02	124.80
16	q	512	CLA	CHA-C1A-NA	-2.69	120.30	126.39
21	b	4006	ECH	C8-C9-C10	2.69	123.24	119.01
16	Y	501	CLA	C3B-C4B-NB	-2.69	108.13	110.53
16	v	511	CLA	CHD-C1D-ND	-2.69	121.02	124.80
16	y	514	CLA	CHD-C1D-ND	-2.69	121.02	124.80
19	u	601	BCR	C3-C4-C5	-2.69	109.26	114.06
19	v	601	BCR	C27-C26-C25	2.69	126.34	122.70
16	Z	503	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
16	G	1235	CLA	C1-C2-C3	-2.69	121.79	126.20
16	H	1129	CLA	C3B-C2B-C1B	-2.69	104.00	107.17
21	i	4020	ECH	C35-C13-C14	-2.69	118.46	122.82
16	o	507	CLA	CHD-C1D-ND	-2.69	121.02	124.80
19	B	4004	BCR	C15-C14-C13	-2.69	123.51	127.28
16	b	1230	CLA	C4A-NA-C1A	2.69	107.90	106.68
19	X	603	BCR	C27-C26-C25	2.68	126.33	122.70
16	q	509	CLA	C3B-C4B-NB	-2.68	108.13	110.53
19	i	4018	BCR	C15-C16-C17	-2.68	118.03	123.52
16	t	517	CLA	C3B-C4B-NB	-2.68	108.14	110.53
19	q	602	BCR	C15-C14-C13	-2.68	123.52	127.28
16	n	514	CLA	CHA-C1A-NA	-2.68	120.32	126.39
16	X	511	CLA	C3B-C4B-NB	-2.68	108.14	110.53
19	B	4014	BCR	C11-C10-C9	-2.68	123.52	127.28
16	t	514	CLA	CHA-C1A-NA	-2.68	120.32	126.39
16	b	1218	CLA	C3B-C4B-NB	-2.68	108.14	110.53
16	v	512	CLA	CHA-C1A-NA	-2.68	120.33	126.39
16	J	1302	CLA	C3B-C2B-C1B	-2.68	104.01	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	1107	CLA	C3B-C4B-NB	-2.68	108.14	110.53
16	u	511	CLA	C3B-C4B-NB	-2.68	108.14	110.53
19	q	604	BCR	C11-C10-C9	-2.67	123.53	127.28
21	G	4006	ECH	C34-C9-C10	-2.67	118.48	122.82
16	x	505	CLA	CHD-C1D-ND	-2.67	121.04	124.80
19	r	601	BCR	C15-C14-C13	-2.67	123.53	127.28
14	a	4101	LMG	O6-C1-O1	-2.67	103.73	110.04
16	x	504	CLA	CHD-C1D-ND	-2.67	121.04	124.80
16	W	509	CLA	CHA-C1A-NA	-2.67	120.34	126.39
19	p	604	BCR	C27-C26-C25	2.67	126.32	122.70
19	u	604	BCR	C15-C14-C13	-2.67	123.53	127.28
16	A	1117	CLA	CHD-C1D-ND	-2.67	121.05	124.80
19	g	601	BCR	C11-C10-C9	-2.67	123.53	127.28
16	y	514	CLA	C4A-NA-C1A	2.67	107.90	106.68
16	H	1102	CLA	CHD-C1D-ND	-2.67	121.05	124.80
16	a	1105	CLA	CHD-C1D-ND	-2.67	121.05	124.80
16	w	504	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
17	H	2001	PQN	C11-C12-C13	-2.67	122.24	126.83
16	y	512	CLA	C3B-C2B-C1B	-2.66	104.03	107.17
16	w	512	CLA	CHA-C1A-NA	-2.66	120.36	126.39
16	H	1106	CLA	CHD-C1D-ND	-2.66	121.05	124.80
16	a	1110	CLA	CHD-C1D-ND	-2.66	121.05	124.80
16	B	1212	CLA	CHD-C1D-ND	-2.66	121.05	124.80
19	I	4018	BCR	C11-C10-C9	-2.66	123.54	127.28
16	Q	1301	CLA	CHA-C1A-NA	-2.66	120.36	126.39
19	v	601	BCR	C24-C23-C22	-2.66	122.30	126.23
16	G	1235	CLA	C3B-C4B-NB	-2.66	108.15	110.53
16	g	504	CLA	CHD-C1D-ND	-2.66	121.06	124.80
16	Y	517	CLA	C3B-C4B-NB	-2.66	108.16	110.53
16	n	516	CLA	C3B-C4B-NB	-2.66	108.16	110.53
16	G	1205	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	k	4001	BCR	C27-C26-C25	2.66	126.30	122.70
16	H	1101	CLA	C3B-C4B-NB	-2.66	108.16	110.53
16	g	516	CLA	C3B-C4B-NB	-2.66	108.16	110.53
16	y	511	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	g	603	BCR	C11-C10-C9	-2.66	123.55	127.28
16	H	1125	CLA	CHD-C1D-ND	-2.66	121.06	124.80
16	w	501	CLA	CHD-C1D-ND	-2.66	121.06	124.80
16	B	1012	CLA	C4A-NA-C1A	2.66	107.89	106.68
16	B	1208	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	p	604	BCR	C24-C23-C22	-2.66	122.31	126.23
16	H	1121	CLA	CHD-C1D-ND	-2.66	121.06	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1203	CLA	CHD-C1D-ND	-2.66	121.07	124.80
16	a	1136	CLA	C3B-C4B-NB	-2.65	108.16	110.53
16	b	1227	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	G	4014	BCR	C27-C26-C25	2.65	126.29	122.70
16	x	512	CLA	CHA-C1A-NA	-2.65	120.38	126.39
17	G	2002	PQN	C11-C12-C13	-2.65	122.26	126.83
19	b	4010	BCR	C40-C30-C25	2.65	114.41	110.24
19	s	603	BCR	C15-C16-C17	-2.65	118.09	123.52
16	b	1229	CLA	CHD-C1D-ND	-2.65	121.07	124.80
16	A	1114	CLA	CHA-C1A-NA	-2.65	120.38	126.39
19	G	4017	BCR	C27-C26-C25	2.65	126.29	122.70
19	Y	604	BCR	C27-C26-C25	2.65	126.29	122.70
19	w	602	BCR	C27-C26-C25	2.65	126.29	122.70
16	G	1238	CLA	C3B-C2B-C1B	-2.65	104.04	107.17
16	w	506	CLA	CHD-C1D-ND	-2.65	121.07	124.80
16	r	509	CLA	C3B-C4B-NB	-2.65	108.16	110.53
16	n	508	CLA	CHD-C1D-ND	-2.65	121.07	124.80
16	o	516	CLA	CHD-C1D-ND	-2.65	121.07	124.80
16	u	501	CLA	C4A-NA-C1A	2.65	107.89	106.68
16	Z	502	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	U	4019	BCR	C11-C10-C9	-2.65	123.56	127.28
16	h	503	CLA	C3B-C2B-C1B	-2.65	104.05	107.17
16	n	510	CLA	C3B-C2B-C1B	-2.65	104.05	107.17
16	n	513	CLA	C3B-C4B-NB	-2.65	108.17	110.53
16	t	509	CLA	C3B-C2B-C1B	-2.65	104.05	107.17
16	Z	503	CLA	CHD-C1D-ND	-2.65	121.08	124.80
19	r	603	BCR	C27-C26-C25	2.65	126.28	122.70
19	J	4015	BCR	C15-C14-C13	-2.65	123.56	127.28
16	W	507	CLA	C3B-C4B-NB	-2.65	108.17	110.53
21	I	4020	ECH	C12-C13-C14	2.65	123.17	119.01
16	G	1240	CLA	C2C-C1C-NC	-2.65	107.20	109.98
16	h	503	CLA	CHD-C1D-ND	-2.65	121.08	124.80
13	g	605	LHG	O8-C23-C24	2.65	119.91	111.83
19	S	4013	BCR	C31-C1-C6	2.65	114.39	110.24
19	W	601	BCR	C15-C16-C17	-2.65	118.11	123.52
16	Y	502	CLA	CHD-C1D-ND	-2.65	121.08	124.80
19	G	4004	BCR	C27-C26-C25	2.64	126.28	122.70
19	g	603	BCR	C27-C26-C25	2.64	126.28	122.70
16	x	501	CLA	C2B-C1B-NB	-2.64	107.58	110.33
19	I	4018	BCR	C15-C16-C17	-2.64	118.11	123.52
23	Z	605	LMU	O5'-C1'-C2'	2.64	115.80	110.37
16	t	511	CLA	C3B-C4B-NB	-2.64	108.17	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	1111	CLA	CHD-C1D-ND	-2.64	121.08	124.80
19	B	4010	BCR	C40-C30-C25	2.64	114.39	110.24
16	B	1235	CLA	C1-C2-C3	-2.64	121.87	126.20
14	b	848	LMG	O6-C1-O1	-2.64	103.80	110.04
16	b	1221	CLA	CHD-C1D-ND	-2.64	121.09	124.80
16	q	507	CLA	C3B-C4B-NB	-2.64	108.17	110.53
16	Z	509	CLA	C4A-NA-C1A	2.64	107.88	106.68
16	x	505	CLA	CHA-C1A-NA	-2.64	120.42	126.39
19	B	4010	BCR	C24-C23-C22	-2.64	122.33	126.23
19	o	604	BCR	C31-C1-C6	2.64	114.38	110.24
19	W	603	BCR	C27-C26-C25	2.64	126.27	122.70
16	j	1302	CLA	C4A-NA-C1A	2.64	107.88	106.68
19	b	4004	BCR	C27-C26-C25	2.64	126.27	122.70
19	b	4010	BCR	C27-C26-C25	2.64	126.27	122.70
16	t	504	CLA	CHD-C1D-ND	-2.64	121.09	124.80
16	p	517	CLA	C3B-C4B-NB	-2.64	108.18	110.53
19	X	602	BCR	C15-C16-C17	-2.64	118.13	123.52
19	T	4001	BCR	C24-C23-C22	-2.64	122.34	126.23
16	A	1116	CLA	CHD-C1D-ND	-2.64	121.09	124.80
16	F	1301	CLA	CHA-C1A-NA	-2.63	120.42	126.39
16	g	511	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	w	515	CLA	CHD-C1D-ND	-2.63	121.10	124.80
19	j	4013	BCR	C24-C23-C22	-2.63	122.34	126.23
16	h	502	CLA	C4A-NA-C1A	2.63	107.88	106.68
16	H	1102	CLA	C3B-C4B-NB	-2.63	108.18	110.53
16	a	1127	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	p	506	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	H	1127	CLA	CHD-C1D-ND	-2.63	121.10	124.80
16	w	504	CLA	C3B-C4B-NB	-2.63	108.18	110.53
16	p	516	CLA	C3B-C4B-NB	-2.63	108.18	110.53
16	q	506	CLA	CHD-C1D-ND	-2.63	121.10	124.80
19	B	4017	BCR	C27-C26-C25	2.63	126.26	122.70
16	X	510	CLA	C3B-C2B-C1B	-2.63	104.07	107.17
16	b	1218	CLA	CHD-C1D-ND	-2.63	121.11	124.80
16	w	517	CLA	CHD-C1D-ND	-2.63	121.11	124.80
16	h	512	CLA	C3B-C2B-C1B	-2.62	104.08	107.17
16	g	506	CLA	CHD-C1D-ND	-2.62	121.11	124.80
16	q	514	CLA	CHA-C1A-NA	-2.62	120.45	126.39
16	p	505	CLA	C3B-C4B-NB	-2.62	108.19	110.53
19	h	604	BCR	C31-C1-C6	2.62	114.36	110.24
16	a	1123	CLA	C2A-C1A-CHA	2.62	128.42	123.87
19	J	4015	BCR	C27-C26-C25	2.62	126.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	X	517	CLA	CHD-C1D-ND	-2.62	121.11	124.80
16	B	1221	CLA	C3B-C4B-NB	-2.62	108.19	110.53
16	A	1135	CLA	CHA-C1A-NA	-2.62	120.46	126.39
19	t	601	BCR	C27-C26-C25	2.62	126.24	122.70
19	B	4004	BCR	C27-C26-C25	2.62	126.24	122.70
19	u	603	BCR	C27-C26-C25	2.62	126.24	122.70
16	x	508	CLA	CHD-C1D-ND	-2.62	121.12	124.80
19	X	601	BCR	C15-C14-C13	-2.62	123.61	127.28
16	G	1232	CLA	C3B-C4B-NB	-2.62	108.19	110.53
16	B	1012	CLA	CHD-C1D-ND	-2.62	121.12	124.80
16	q	505	CLA	CHD-C1D-ND	-2.62	121.12	124.80
16	g	503	CLA	C3C-C4C-NC	-2.62	107.08	110.43
19	p	604	BCR	C15-C16-C17	-2.62	118.17	123.52
16	Z	515	CLA	C3B-C4B-NB	-2.62	108.19	110.53
19	u	603	BCR	C15-C14-C13	-2.61	123.61	127.28
15	A	1011	CL0	C3D-C4D-CHA	2.61	112.51	108.54
16	H	1119	CLA	CHA-C1A-NA	-2.61	120.47	126.39
16	Z	505	CLA	CHD-C1D-ND	-2.61	121.12	124.80
19	s	602	BCR	C27-C26-C25	2.61	126.23	122.70
16	o	510	CLA	C4A-NA-C1A	2.61	107.87	106.68
16	q	508	CLA	CHA-C1A-NA	-2.61	120.47	126.39
16	A	1136	CLA	C3B-C4B-NB	-2.61	108.20	110.53
16	k	4003	CLA	C3B-C2B-C1B	-2.61	104.09	107.17
19	J	4015	BCR	C2-C1-C6	2.61	114.23	110.44
19	v	604	BCR	C31-C1-C6	2.61	114.34	110.24
16	h	514	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	G	1228	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	w	505	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	H	1136	CLA	CHD-C1D-ND	-2.61	121.13	124.80
16	W	514	CLA	CHA-C1A-NA	-2.61	120.49	126.39
16	s	505	CLA	C3B-C2B-C1B	-2.61	104.10	107.17
16	s	516	CLA	C4A-NA-C1A	2.61	107.87	106.68
16	X	503	CLA	CMB-C2B-C1B	2.61	129.39	125.42
19	Z	604	BCR	C27-C26-C25	2.61	126.22	122.70
16	y	503	CLA	C3B-C4B-NB	-2.61	108.20	110.53
16	u	506	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
19	o	601	BCR	C3-C4-C5	-2.60	109.41	114.06
16	H	1123	CLA	CHD-C1D-ND	-2.60	121.14	124.80
19	r	601	BCR	C24-C23-C22	-2.60	122.38	126.23
19	x	601	BCR	C27-C26-C25	2.60	126.22	122.70
19	p	602	BCR	C27-C26-C25	2.60	126.22	122.70
16	a	1022	CLA	C3C-C4C-NC	-2.60	107.09	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	1138	CLA	CHD-C1D-ND	-2.60	121.14	124.80
16	A	1101	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
19	S	4015	BCR	C27-C26-C25	2.60	126.22	122.70
16	n	509	CLA	CHA-C1A-NA	-2.60	120.50	126.39
16	A	1101	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	Q	1302	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	r	504	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	A	1022	CLA	C4A-NA-C1A	2.60	107.86	106.68
19	u	601	BCR	C15-C14-C13	-2.60	123.63	127.28
16	g	515	CLA	CHD-C1D-ND	-2.60	121.14	124.80
16	F	1302	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	p	502	CLA	C3B-C4B-NB	-2.60	108.21	110.53
16	s	516	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	u	604	BCR	C11-C10-C9	-2.60	123.64	127.28
16	u	511	CLA	CHD-C1D-ND	-2.60	121.15	124.80
19	y	603	BCR	C27-C26-C25	2.60	126.21	122.70
16	p	501	CLA	CHD-C1D-ND	-2.60	121.15	124.80
16	h	508	CLA	C3B-C4B-NB	-2.59	108.21	110.53
16	Z	508	CLA	CHA-C1A-NA	-2.59	120.52	126.39
16	w	509	CLA	C4A-NA-C1A	2.59	107.86	106.68
16	H	1129	CLA	CHD-C1D-ND	-2.59	121.15	124.80
16	a	1109	CLA	CHD-C1D-ND	-2.59	121.15	124.80
19	B	4014	BCR	C27-C26-C25	2.59	126.21	122.70
19	G	4010	BCR	C40-C30-C25	2.59	114.31	110.24
16	x	506	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
16	h	510	CLA	C3B-C4B-NB	-2.59	108.22	110.53
13	o	605	LHG	O8-C23-C24	2.59	119.74	111.83
16	Z	507	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
16	b	1214	CLA	C3B-C4B-NB	-2.59	108.22	110.53
16	w	511	CLA	C3B-C4B-NB	-2.59	108.22	110.53
19	q	603	BCR	C11-C10-C9	-2.59	123.64	127.28
16	H	1135	CLA	CHA-C1A-NA	-2.59	120.53	126.39
19	x	604	BCR	C27-C26-C25	2.59	126.20	122.70
16	u	508	CLA	CHD-C1D-ND	-2.59	121.16	124.80
16	o	511	CLA	C3B-C4B-NB	-2.59	108.22	110.53
16	a	1130	CLA	C4A-NA-C1A	2.59	107.86	106.68
16	o	512	CLA	O2A-CGA-O1A	-2.59	117.16	123.63
16	g	511	CLA	C3B-C4B-NB	-2.59	108.22	110.53
16	b	1231	CLA	CHA-C1A-NA	-2.59	120.53	126.39
16	w	508	CLA	CHA-C1A-NA	-2.59	120.53	126.39
16	t	503	CLA	C3C-C4C-NC	-2.59	107.12	110.43
16	A	1119	CLA	CHD-C1D-ND	-2.59	121.16	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	513	CLA	C3B-C4B-NB	-2.59	108.22	110.53
19	X	602	BCR	C3-C4-C5	-2.59	109.44	114.06
16	a	1123	CLA	CHA-C1A-NA	-2.59	120.53	126.39
16	u	508	CLA	CMB-C2B-C1B	2.59	129.36	125.42
16	b	1229	CLA	C1D-ND-C4D	-2.59	104.50	106.31
19	G	4009	BCR	C15-C14-C13	-2.58	123.65	127.28
19	Q	4016	BCR	C27-C26-C25	2.58	126.20	122.70
16	b	1232	CLA	C3B-C4B-NB	-2.58	108.22	110.53
19	p	603	BCR	C15-C16-C17	-2.58	118.23	123.52
16	W	514	CLA	C3B-C4B-NB	-2.58	108.22	110.53
19	H	4003	BCR	C27-C26-C25	2.58	126.19	122.70
16	A	1106	CLA	CHD-C1D-ND	-2.58	121.17	124.80
16	A	1137	CLA	CHD-C1D-ND	-2.58	121.17	124.80
19	H	4002	BCR	C27-C26-C25	2.58	126.19	122.70
19	Y	602	BCR	C27-C26-C25	2.58	126.19	122.70
16	g	517	CLA	C3B-C4B-NB	-2.58	108.23	110.53
19	n	603	BCR	C27-C26-C25	2.58	126.19	122.70
16	a	1138	CLA	CHD-C1D-ND	-2.58	121.17	124.80
16	Z	516	CLA	C3B-C4B-NB	-2.58	108.23	110.53
19	x	603	BCR	C15-C16-C17	-2.58	118.24	123.52
16	a	1132	CLA	C3B-C2B-C1B	-2.58	104.13	107.17
19	t	601	BCR	C24-C23-C22	-2.58	122.42	126.23
19	w	604	BCR	C27-C26-C25	2.58	126.19	122.70
13	X	605	LHG	O8-C23-C24	2.58	119.69	111.83
19	q	602	BCR	C27-C26-C25	2.58	126.19	122.70
19	g	601	BCR	C31-C1-C6	2.58	114.28	110.24
16	p	517	CLA	CMB-C2B-C1B	2.58	129.34	125.42
16	y	505	CLA	CHA-C1A-NA	-2.57	120.56	126.39
16	a	1130	CLA	CHD-C1D-ND	-2.57	121.18	124.80
19	w	604	BCR	C11-C10-C9	-2.57	123.67	127.28
19	x	603	BCR	C27-C26-C25	2.57	126.18	122.70
16	p	512	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
16	w	509	CLA	C3B-C2B-C1B	-2.57	104.14	107.17
16	a	1115	CLA	C3B-C4B-NB	-2.57	108.23	110.53
16	A	1122	CLA	CHD-C1D-ND	-2.57	121.18	124.80
16	f	1301	CLA	CHA-C1A-NA	-2.57	120.57	126.39
16	b	1227	CLA	C3B-C2B-C1B	-2.57	104.14	107.17
16	H	1103	CLA	CAA-CBA-CGA	-2.57	105.91	113.21
16	B	1230	CLA	CHD-C1D-ND	-2.57	121.18	124.80
16	B	1208	CLA	C3B-C4B-NB	-2.57	108.23	110.53
16	p	515	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
19	b	4014	BCR	C15-C14-C13	-2.57	123.68	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	501	CLA	CHD-C1D-ND	-2.57	121.19	124.80
21	b	4006	ECH	C34-C9-C10	-2.57	118.66	122.82
19	w	603	BCR	C27-C26-C25	2.57	126.17	122.70
13	a	849	LHG	O8-C23-C24	2.57	119.66	111.83
19	L	4019	BCR	C11-C10-C9	-2.57	123.68	127.28
16	s	501	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	s	507	CLA	C3B-C4B-NB	-2.57	108.24	110.53
16	B	1238	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	b	1230	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	B	1236	CLA	C4A-NA-C1A	2.57	107.85	106.68
16	o	508	CLA	CHD-C1D-ND	-2.57	121.19	124.80
16	B	1235	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
16	B	1238	CLA	CHA-C1A-NA	-2.57	120.58	126.39
19	l	4022	BCR	C24-C23-C22	-2.57	122.44	126.23
19	X	604	BCR	C27-C26-C25	2.57	126.17	122.70
19	q	603	BCR	C27-C26-C25	2.57	126.17	122.70
16	h	503	CLA	C3B-C4B-NB	-2.57	108.24	110.53
16	g	514	CLA	CHA-C1A-NA	-2.56	120.58	126.39
16	b	1203	CLA	C3B-C4B-NB	-2.56	108.24	110.53
16	o	504	CLA	C3B-C4B-NB	-2.56	108.24	110.53
19	s	604	BCR	C15-C14-C13	-2.56	123.68	127.28
16	u	509	CLA	C3B-C2B-C1B	-2.56	104.15	107.17
16	b	1231	CLA	CHD-C1D-ND	-2.56	121.20	124.80
19	r	602	BCR	C15-C14-C13	-2.56	123.68	127.28
16	Z	509	CLA	C3B-C4B-NB	-2.56	108.24	110.53
17	a	2001	PQN	C14-C13-C15	2.56	119.67	115.23
19	a	4002	BCR	C27-C26-C25	2.56	126.17	122.70
19	B	4010	BCR	C15-C14-C13	-2.56	123.69	127.28
19	r	604	BCR	C15-C14-C13	-2.56	123.69	127.28
16	s	503	CLA	C3B-C4B-NB	-2.56	108.24	110.53
16	s	515	CLA	CHD-C1D-ND	-2.56	121.20	124.80
16	B	1220	CLA	C3B-C4B-NB	-2.56	108.25	110.53
16	H	1139	CLA	C3B-C4B-NB	-2.56	108.25	110.53
16	Y	517	CLA	CMB-C2B-C1B	2.56	129.32	125.42
16	X	511	CLA	C2C-C1C-NC	-2.56	107.29	109.98
16	b	1210	CLA	OBD-CAD-C3D	-2.56	122.44	128.42
16	A	1127	CLA	CHA-C1A-NA	-2.56	120.60	126.39
16	a	1139	CLA	CHA-C1A-NA	-2.56	120.60	126.39
16	B	1225	CLA	CHD-C1D-ND	-2.56	121.20	124.80
16	G	1201	CLA	C3B-C4B-NB	-2.56	108.25	110.53
16	g	512	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
16	o	510	CLA	C3B-C2B-C1B	-2.56	104.16	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	j	4012	BCR	C11-C10-C9	-2.56	123.69	127.28
16	o	502	CLA	CHD-C1D-ND	-2.56	121.20	124.80
16	v	514	CLA	CHD-C1D-ND	-2.56	121.20	124.80
21	I	4020	ECH	C4-C5-C6	-2.56	119.25	122.70
16	a	1120	CLA	C3C-C4C-NC	-2.56	107.16	110.43
16	h	505	CLA	CHD-C1D-ND	-2.56	121.21	124.80
19	a	4003	BCR	C27-C26-C25	2.56	126.16	122.70
16	n	504	CLA	C3B-C4B-NB	-2.56	108.25	110.53
16	b	1210	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	B	1231	CLA	CHA-C1A-NA	-2.55	120.61	126.39
16	a	1119	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	h	501	CLA	C3B-C2B-C1B	-2.55	104.16	107.17
16	X	509	CLA	C4A-NA-C1A	2.55	107.84	106.68
16	W	511	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	X	507	CLA	CMB-C2B-C1B	2.55	129.31	125.42
19	t	603	BCR	C27-C26-C25	2.55	126.15	122.70
16	Y	508	CLA	CHA-C1A-NA	-2.55	120.61	126.39
16	b	1202	CLA	C3B-C2B-C1B	-2.55	104.16	107.17
19	B	4014	BCR	C7-C8-C9	-2.55	122.46	126.23
16	G	1216	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	X	505	CLA	C3B-C4B-NB	-2.55	108.25	110.53
19	A	4007	BCR	C7-C8-C9	-2.55	122.46	126.23
16	G	1208	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	r	504	CLA	CHD-C1D-ND	-2.55	121.21	124.80
16	r	516	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	R	4018	BCR	C11-C10-C9	-2.55	123.70	127.28
16	B	1012	CLA	CHA-C1A-NA	-2.55	120.61	126.39
19	y	601	BCR	C24-C23-C22	-2.55	122.46	126.23
14	a	852	LMG	O6-C1-O1	-2.55	104.02	110.04
16	x	514	CLA	CHA-C1A-NA	-2.55	120.62	126.39
16	Z	505	CLA	C3B-C2B-C1B	-2.55	104.17	107.17
19	p	603	BCR	C11-C10-C9	-2.55	123.70	127.28
19	K	4001	BCR	C15-C16-C17	-2.55	118.31	123.52
19	T	4005	BCR	C27-C26-C25	2.55	126.15	122.70
16	q	508	CLA	CHD-C1D-ND	-2.55	121.22	124.80
16	u	512	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
19	Z	603	BCR	C27-C26-C25	2.55	126.14	122.70
19	j	4015	BCR	C27-C26-C25	2.55	126.14	122.70
19	k	4005	BCR	C27-C26-C25	2.55	126.14	122.70
19	G	4004	BCR	C15-C14-C13	-2.55	123.71	127.28
19	G	4014	BCR	C7-C8-C9	-2.55	122.47	126.23
16	l	1503	CLA	C3B-C2B-C1B	-2.55	104.17	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	u	511	CLA	C2C-C1C-NC	-2.54	107.31	109.98
16	K	4002	CLA	C4A-NA-C1A	2.54	107.84	106.68
16	t	508	CLA	CHD-C1D-ND	-2.54	121.22	124.80
16	w	508	CLA	CHD-C1D-ND	-2.54	121.22	124.80
16	Y	512	CLA	CHA-C1A-NA	-2.54	120.63	126.39
16	b	1225	CLA	CHD-C1D-ND	-2.54	121.22	124.80
16	a	1127	CLA	CHA-C1A-NA	-2.54	120.63	126.39
19	A	4002	BCR	C27-C26-C25	2.54	126.14	122.70
16	G	1235	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
19	p	604	BCR	C15-C14-C13	-2.54	123.71	127.28
16	B	1224	CLA	CHA-C1A-NA	-2.54	120.64	126.39
16	n	515	CLA	C3B-C4B-NB	-2.54	108.26	110.53
16	G	1202	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	H	1127	CLA	CHA-C1A-NA	-2.54	120.64	126.39
16	u	503	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	v	501	CLA	CHD-C1D-ND	-2.54	121.23	124.80
19	g	604	BCR	C27-C26-C25	2.54	126.14	122.70
16	g	506	CLA	C1-C2-C3	-2.54	122.03	126.20
19	w	602	BCR	C24-C23-C22	-2.54	122.48	126.23
16	w	512	CLA	C3B-C4B-NB	-2.54	108.26	110.53
16	b	1219	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	H	1130	CLA	C4A-NA-C1A	2.54	107.84	106.68
19	B	4010	BCR	C27-C26-C25	2.54	126.13	122.70
16	b	1226	CLA	CHD-C1D-ND	-2.54	121.23	124.80
19	S	4012	BCR	C15-C16-C17	-2.54	118.33	123.52
16	H	1109	CLA	CHD-C1D-ND	-2.54	121.23	124.80
19	r	603	BCR	C11-C10-C9	-2.54	123.72	127.28
19	b	4017	BCR	C27-C26-C25	2.53	126.13	122.70
16	A	1129	CLA	CHA-C1A-NA	-2.53	120.65	126.39
16	W	516	CLA	C3B-C4B-NB	-2.53	108.27	110.53
16	q	514	CLA	C3B-C4B-NB	-2.53	108.27	110.53
16	G	1202	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
16	G	1201	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	y	502	CLA	CHD-C1D-ND	-2.53	121.24	124.80
19	K	4005	BCR	C27-C26-C25	2.53	126.13	122.70
16	f	1302	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	b	1236	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	t	511	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	y	517	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	q	516	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	a	1013	CLA	CMD-C2D-C1D	-2.53	120.27	124.73
13	i	103	LHG	O8-C23-C24	2.53	119.55	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	r	514	CLA	C4A-NA-C1A	2.53	107.83	106.68
23	q	605	LMU	O5'-C1'-C2'	2.53	115.57	110.37
16	s	509	CLA	CHD-C1D-ND	-2.53	121.24	124.80
16	t	517	CLA	CMB-C2B-C1B	2.53	129.27	125.42
19	G	4010	BCR	C27-C26-C25	2.53	126.12	122.70
19	j	4013	BCR	C27-C26-C25	2.53	126.12	122.70
16	b	1229	CLA	CHA-C1A-NA	-2.53	120.67	126.39
19	u	604	BCR	C2-C1-C6	2.53	114.11	110.44
16	a	1101	CLA	CMD-C2D-C1D	-2.53	120.28	124.73
16	h	505	CLA	C3B-C4B-NB	-2.53	108.28	110.53
16	h	504	CLA	CHD-C1D-ND	-2.53	121.25	124.80
16	G	1227	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	b	1217	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	G	1204	CLA	CHD-C1D-ND	-2.52	121.25	124.80
19	Z	602	BCR	C11-C10-C9	-2.52	123.74	127.28
16	H	1124	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	x	513	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	g	505	CLA	CHD-C1D-ND	-2.52	121.25	124.80
16	g	516	CLA	CHD-C1D-ND	-2.52	121.25	124.80
16	H	1122	CLA	C4A-NA-C1A	2.52	107.83	106.68
16	t	501	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	u	508	CLA	C3B-C4B-NB	-2.52	108.28	110.53
19	B	4017	BCR	C16-C15-C14	-2.52	118.36	123.52
16	a	1101	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
14	B	848	LMG	O2-C2-C1	-2.52	104.07	110.08
13	u	605	LHG	O8-C23-C24	2.52	119.52	111.83
16	r	506	CLA	C1-C2-C3	-2.52	122.07	126.20
16	Y	515	CLA	CHD-C1D-ND	-2.52	121.26	124.80
19	K	4001	BCR	C15-C14-C13	-2.52	123.75	127.28
16	A	1133	CLA	C2B-C1B-NB	-2.52	107.72	110.33
16	v	502	CLA	CHD-C1D-ND	-2.52	121.26	124.80
16	B	1210	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	H	1118	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	H	1119	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	b	1229	CLA	C3B-C4B-NB	-2.52	108.28	110.53
16	b	1224	CLA	CHA-C1A-NA	-2.52	120.69	126.39
14	b	848	LMG	O2-C2-C1	-2.52	104.08	110.08
16	h	505	CLA	CHA-C1A-NA	-2.51	120.70	126.39
16	b	1021	CLA	C3B-C4B-NB	-2.51	108.28	110.53
16	W	501	CLA	C3B-C4B-NB	-2.51	108.29	110.53
19	g	604	BCR	C15-C14-C13	-2.51	123.75	127.28
16	b	1236	CLA	C1C-C2C-C3C	-2.51	104.34	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	F	4016	BCR	C27-C26-C25	2.51	126.10	122.70
19	p	603	BCR	C27-C26-C25	2.51	126.10	122.70
19	j	4013	BCR	C31-C1-C6	2.51	114.18	110.24
19	G	4014	BCR	C11-C10-C9	-2.51	123.76	127.28
16	p	502	CLA	C4A-NA-C1A	2.51	107.82	106.68
14	Q	4017	LMG	O6-C1-O1	-2.51	104.11	110.04
19	I	4018	BCR	C27-C26-C25	2.51	126.09	122.70
19	H	4011	BCR	C15-C16-C17	-2.51	118.39	123.52
16	A	1110	CLA	CHD-C1D-ND	-2.51	121.27	124.80
16	A	1013	CLA	CHD-C1D-ND	-2.51	121.27	124.80
16	A	1134	CLA	CHD-C1D-ND	-2.51	121.27	124.80
16	t	517	CLA	CHD-C1D-ND	-2.51	121.27	124.80
16	p	513	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	s	515	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	y	507	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	g	506	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
16	Q	1302	CLA	CHD-C1D-ND	-2.51	121.28	124.80
16	B	1219	CLA	C3B-C2B-C1B	-2.51	104.22	107.17
16	y	504	CLA	CHA-C1A-NA	-2.51	120.72	126.39
19	B	4017	BCR	C10-C11-C12	-2.51	115.94	123.20
16	b	1023	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	a	1106	CLA	CHD-C1D-ND	-2.51	121.28	124.80
16	H	1138	CLA	C1-C2-C3	-2.51	122.09	126.20
16	B	1238	CLA	C3B-C2B-C1B	-2.51	104.22	107.17
19	g	602	BCR	C15-C16-C17	-2.50	118.39	123.52
16	a	1135	CLA	CHA-C1A-NA	-2.50	120.72	126.39
16	A	1104	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	o	603	BCR	C15-C16-C17	-2.50	118.40	123.52
16	b	1220	CLA	CHD-C1D-ND	-2.50	121.28	124.80
16	w	503	CLA	C3B-C4B-NB	-2.50	108.30	110.53
16	a	1115	CLA	C2A-C1A-CHA	2.50	128.21	123.87
16	X	516	CLA	C4A-NA-C1A	2.50	107.82	106.68
19	W	604	BCR	C27-C26-C25	2.50	126.08	122.70
16	A	1109	CLA	C3B-C4B-NB	-2.50	108.30	110.53
13	G	4018	LHG	C11-C10-C9	-2.50	101.73	114.37
19	R	4018	BCR	C15-C14-C13	-2.50	123.77	127.28
16	B	1201	CLA	C3B-C4B-NB	-2.50	108.30	110.53
16	o	514	CLA	CHA-C1A-NA	-2.50	120.73	126.39
23	x	606	LMU	O5B-C5B-C4B	2.50	114.20	109.70
16	v	516	CLA	CHD-C1D-ND	-2.50	121.29	124.80
16	G	1215	CLA	CHD-C1D-ND	-2.50	121.29	124.80
16	b	1212	CLA	CHD-C1D-ND	-2.50	121.29	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1234	CLA	CHA-C1A-NA	-2.50	120.74	126.39
19	u	603	BCR	C11-C10-C9	-2.50	123.78	127.28
21	R	4020	ECH	C34-C9-C10	-2.50	118.77	122.82
19	I	4018	BCR	C3-C4-C5	-2.50	109.61	114.06
16	n	515	CLA	CHD-C1D-ND	-2.50	121.29	124.80
16	Z	501	CLA	C3B-C2B-C1B	-2.50	104.23	107.17
13	H	849	LHG	O8-C23-C24	2.49	119.44	111.83
16	b	1205	CLA	CHD-C1D-ND	-2.49	121.29	124.80
16	b	1211	CLA	CHD-C1D-ND	-2.49	121.29	124.80
19	J	4015	BCR	C15-C16-C17	-2.49	118.42	123.52
16	v	515	CLA	C3B-C2B-C1B	-2.49	104.23	107.17
19	U	4022	BCR	C2-C1-C6	2.49	114.06	110.44
16	b	1221	CLA	C3B-C4B-NB	-2.49	108.30	110.53
16	h	516	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	G	4004	BCR	C11-C10-C9	-2.49	123.78	127.28
16	p	515	CLA	CHD-C1D-ND	-2.49	121.30	124.80
19	l	4019	BCR	C11-C10-C9	-2.49	123.78	127.28
16	b	1202	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
19	r	604	BCR	C27-C26-C25	2.49	126.07	122.70
16	A	1121	CLA	CHD-C1D-ND	-2.49	121.30	124.80
16	B	1214	CLA	C3C-C4C-NC	-2.49	107.24	110.43
19	t	604	BCR	C15-C14-C13	-2.49	123.79	127.28
19	w	604	BCR	C15-C16-C17	-2.49	118.42	123.52
16	b	1228	CLA	CHD-C1D-ND	-2.49	121.30	124.80
16	v	517	CLA	CHD-C1D-ND	-2.49	121.30	124.80
15	a	1011	CL0	CMD-C2D-C3D	2.49	129.66	124.68
19	o	604	BCR	C27-C26-C25	2.49	126.07	122.70
16	s	514	CLA	CHA-C1A-NA	-2.49	120.76	126.39
16	y	517	CLA	CHA-C1A-NA	-2.49	120.76	126.39
16	b	1234	CLA	CHD-C1D-ND	-2.49	121.30	124.80
16	h	501	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
16	y	514	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	B	4014	BCR	C15-C16-C17	-2.48	118.44	123.52
16	q	517	CLA	CMB-C2B-C1B	2.48	129.20	125.42
16	G	1221	CLA	CHD-C1D-ND	-2.48	121.31	124.80
16	Y	505	CLA	C4A-NA-C1A	2.48	107.81	106.68
16	u	510	CLA	C4A-NA-C1A	2.48	107.81	106.68
16	y	507	CLA	CHD-C1D-ND	-2.48	121.31	124.80
21	I	4020	ECH	C8-C9-C10	2.48	122.91	119.01
16	x	508	CLA	C3B-C4B-NB	-2.48	108.32	110.53
23	q	605	LMU	C1B-O1B-C4'	-2.48	112.10	117.98
16	Z	515	CLA	CHD-C1D-ND	-2.48	121.31	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	1022	CLA	C3C-C4C-NC	-2.48	107.25	110.43
16	b	1230	CLA	CMB-C2B-C1B	2.48	129.19	125.42
16	a	1129	CLA	CHA-C1A-NA	-2.48	120.78	126.39
19	u	602	BCR	C15-C16-C17	-2.48	118.45	123.52
16	T	4002	CLA	CHD-C1D-ND	-2.48	121.31	124.80
16	A	1123	CLA	CHA-C1A-NA	-2.48	120.78	126.39
16	X	514	CLA	CHA-C1A-NA	-2.48	120.78	126.39
19	A	4008	BCR	C28-C27-C26	-2.48	109.64	114.06
16	h	514	CLA	C4A-NA-C1A	2.48	107.81	106.68
16	h	511	CLA	C3B-C4B-NB	-2.48	108.32	110.53
16	G	1232	CLA	CHA-C1A-NA	-2.48	120.78	126.39
16	h	510	CLA	C3B-C2B-C1B	-2.48	104.25	107.17
16	n	501	CLA	CHD-C1D-ND	-2.48	121.32	124.80
19	A	4011	BCR	C15-C16-C17	-2.48	118.45	123.52
16	Y	506	CLA	CHD-C1D-ND	-2.48	121.32	124.80
16	G	1240	CLA	CMC-C2C-C1C	-2.48	121.17	125.03
19	k	4005	BCR	C24-C23-C22	-2.47	122.57	126.23
16	h	517	CLA	C4A-NA-C1A	2.47	107.81	106.68
16	Y	515	CLA	C3B-C4B-NB	-2.47	108.32	110.53
19	b	4014	BCR	C7-C8-C9	-2.47	122.58	126.23
16	H	1121	CLA	C3B-C4B-NB	-2.47	108.32	110.53
13	R	103	LHG	O8-C23-C24	2.47	119.38	111.83
16	a	1122	CLA	CHD-C1D-ND	-2.47	121.32	124.80
16	g	509	CLA	CHD-C1D-ND	-2.47	121.32	124.80
16	y	514	CLA	CHA-C1A-NA	-2.47	120.79	126.39
16	b	1201	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
16	A	1114	CLA	CHD-C1D-ND	-2.47	121.32	124.80
16	G	1238	CLA	CHD-C1D-ND	-2.47	121.32	124.80
19	A	4003	BCR	C15-C16-C17	-2.47	118.46	123.52
19	A	4007	BCR	C15-C14-C13	-2.47	123.81	127.28
19	g	604	BCR	C11-C10-C9	-2.47	123.81	127.28
16	t	503	CLA	CHA-C1A-NA	-2.47	120.80	126.39
16	u	509	CLA	C3B-C4B-NB	-2.47	108.32	110.53
16	b	1232	CLA	CHD-C1D-ND	-2.47	121.33	124.80
19	J	4013	BCR	C27-C26-C25	2.47	126.04	122.70
14	H	852	LMG	O6-C1-O1	-2.47	104.20	110.04
16	H	1132	CLA	C3B-C2B-C1B	-2.47	104.26	107.17
16	s	508	CLA	CHA-C1A-NA	-2.47	120.80	126.39
16	A	1125	CLA	CHD-C1D-ND	-2.47	121.33	124.80
16	b	1235	CLA	C3B-C4B-NB	-2.47	108.33	110.53
13	s	605	LHG	C11-C10-C9	-2.47	101.89	114.37
16	r	507	CLA	CHD-C1D-ND	-2.47	121.33	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	1227	CLA	CHA-C1A-NA	-2.47	120.80	126.39
16	t	502	CLA	C4A-NA-C1A	2.47	107.81	106.68
17	G	2002	PQN	C14-C13-C15	2.47	119.51	115.23
16	A	1102	CLA	CHD-C1D-ND	-2.47	121.33	124.80
16	k	4002	CLA	CHD-C1D-ND	-2.47	121.33	124.80
14	G	848	LMG	O2-C2-C1	-2.47	104.20	110.08
16	v	506	CLA	CHA-C1A-NA	-2.47	120.81	126.39
16	g	505	CLA	CHA-C1A-NA	-2.46	120.81	126.39
16	g	509	CLA	C3B-C2B-C1B	-2.46	104.26	107.17
16	o	507	CLA	C3B-C4B-NB	-2.46	108.33	110.53
16	r	515	CLA	C3B-C4B-NB	-2.46	108.33	110.53
16	x	512	CLA	C3B-C4B-NB	-2.46	108.33	110.53
13	b	4018	LHG	C11-C10-C9	-2.46	101.91	114.37
16	a	1114	CLA	CHA-C1A-NA	-2.46	120.81	126.39
16	H	1110	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	H	1139	CLA	CHA-C1A-NA	-2.46	120.81	126.39
16	t	509	CLA	CHA-C1A-NA	-2.46	120.81	126.39
16	A	1122	CLA	CMB-C2B-C1B	2.46	129.17	125.42
19	u	604	BCR	C24-C23-C22	-2.46	122.59	126.23
13	x	605	LHG	C11-C10-C9	-2.46	101.93	114.37
16	h	511	CLA	C2C-C1C-NC	-2.46	107.40	109.98
16	l	1502	CLA	C3B-C4B-NB	-2.46	108.33	110.53
16	y	508	CLA	CHA-C1A-NA	-2.46	120.82	126.39
16	h	516	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	s	505	CLA	CHD-C1D-ND	-2.46	121.34	124.80
19	n	601	BCR	C7-C8-C9	-2.46	122.60	126.23
16	o	515	CLA	C3B-C4B-NB	-2.46	108.34	110.53
16	x	505	CLA	C3B-C4B-NB	-2.46	108.34	110.53
13	B	4018	LHG	C11-C10-C9	-2.46	101.95	114.37
14	A	852	LMG	O6-C1-O1	-2.46	104.24	110.04
16	u	516	CLA	CHD-C1D-ND	-2.46	121.34	124.80
16	G	1218	CLA	CHA-C1A-NA	-2.46	120.83	126.39
16	a	1102	CLA	CHD-C1D-ND	-2.46	121.35	124.80
16	H	1129	CLA	CHA-C1A-NA	-2.46	120.83	126.39
19	v	604	BCR	C2-C1-C6	2.46	114.01	110.44
16	p	506	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
16	h	512	CLA	CHA-C1A-NA	-2.46	120.83	126.39
16	y	512	CLA	C2B-C1B-NB	-2.46	107.78	110.33
16	r	512	CLA	O2A-CGA-O1A	-2.46	117.49	123.63
16	Z	514	CLA	CHA-C1A-NA	-2.45	120.83	126.39
16	y	515	CLA	CHD-C1D-ND	-2.45	121.35	124.80
19	S	4013	BCR	C24-C23-C22	-2.45	122.60	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	1127	CLA	C3B-C4B-NB	-2.45	108.34	110.53
16	b	1234	CLA	C3B-C4B-NB	-2.45	108.34	110.53
16	H	1104	CLA	CHD-C1D-ND	-2.45	121.35	124.80
16	n	505	CLA	C3B-C2B-C1B	-2.45	104.28	107.17
16	Z	512	CLA	C3B-C4B-NB	-2.45	108.34	110.53
16	H	1105	CLA	C4A-NA-C1A	2.45	107.80	106.68
16	X	501	CLA	CHD-C1D-ND	-2.45	121.35	124.80
16	G	1226	CLA	C3C-C4C-NC	-2.45	107.29	110.43
16	v	507	CLA	C3B-C4B-NB	-2.45	108.34	110.53
16	w	516	CLA	C4A-NA-C1A	2.45	107.80	106.68
19	q	604	BCR	C27-C26-C25	2.45	126.02	122.70
19	r	604	BCR	C11-C10-C9	-2.45	123.84	127.28
16	b	1238	CLA	C3B-C4B-NB	-2.45	108.34	110.53
16	o	515	CLA	CHD-C1D-ND	-2.45	121.36	124.80
19	t	601	BCR	C15-C16-C17	-2.45	118.51	123.52
16	W	515	CLA	C3B-C4B-NB	-2.45	108.34	110.53
16	Z	514	CLA	C3B-C4B-NB	-2.45	108.34	110.53
13	A	849	LHG	O8-C23-C24	2.45	119.30	111.83
24	q	601	LUT	C1-C6-C7	2.45	122.29	115.65
19	W	601	BCR	C11-C10-C9	-2.45	123.84	127.28
19	s	601	BCR	C15-C14-C13	-2.45	123.84	127.28
24	Z	601	LUT	C1-C6-C5	-2.45	119.29	122.64
16	b	1238	CLA	C3B-C2B-C1B	-2.45	104.28	107.17
17	a	2001	PQN	C11-C12-C13	-2.45	122.61	126.83
16	v	505	CLA	CHA-C1A-NA	-2.45	120.85	126.39
16	q	508	CLA	C3B-C4B-NB	-2.45	108.35	110.53
19	b	4004	BCR	C15-C14-C13	-2.45	123.85	127.28
16	u	507	CLA	CHD-C1D-ND	-2.45	121.36	124.80
16	v	504	CLA	CHD-C1D-ND	-2.45	121.36	124.80
16	v	511	CLA	CHA-C1A-NA	-2.45	120.85	126.39
16	g	501	CLA	C3B-C2B-C1B	-2.45	104.29	107.17
19	x	602	BCR	C15-C14-C13	-2.45	123.85	127.28
16	y	503	CLA	CHD-C1D-ND	-2.45	121.36	124.80
16	H	1130	CLA	C3B-C4B-NB	-2.45	108.35	110.53
16	q	515	CLA	C2D-C1D-ND	-2.45	107.71	110.13
16	r	508	CLA	CHD-C1D-ND	-2.44	121.36	124.80
16	w	501	CLA	C4B-C3B-C2B	-2.44	104.26	107.30
16	y	515	CLA	C2B-C1B-NB	-2.44	107.79	110.33
16	B	1216	CLA	CHD-C1D-ND	-2.44	121.36	124.80
16	S	1302	CLA	CHD-C1D-ND	-2.44	121.36	124.80
16	S	1303	CLA	CHD-C1D-ND	-2.44	121.36	124.80
15	A	1011	CL0	O2A-CGA-O1A	-2.44	117.52	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	1214	CLA	C3C-C4C-NC	-2.44	107.30	110.43
16	X	508	CLA	C3B-C4B-NB	-2.44	108.35	110.53
16	S	1302	CLA	C4A-NA-C1A	2.44	107.79	106.68
16	B	1216	CLA	C2B-C1B-NB	-2.44	107.79	110.33
16	X	503	CLA	C2B-C1B-NB	-2.44	107.79	110.33
19	B	4009	BCR	C15-C14-C13	-2.44	123.85	127.28
16	G	1218	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	Y	512	CLA	C3B-C4B-NB	-2.44	108.35	110.53
19	A	4007	BCR	C28-C27-C26	-2.44	109.70	114.06
16	X	516	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	b	4017	BCR	C16-C15-C14	-2.44	118.53	123.52
19	J	4013	BCR	C2-C1-C6	2.44	113.98	110.44
13	g	605	LHG	C11-C10-C9	-2.44	102.04	114.37
16	B	1219	CLA	CHD-C1D-ND	-2.44	121.37	124.80
13	r	605	LHG	C11-C10-C9	-2.44	102.04	114.37
19	K	4001	BCR	C40-C30-C25	2.44	114.07	110.24
16	W	513	CLA	C2B-C1B-NB	-2.44	107.80	110.33
15	a	1011	CL0	C4C-CHD-C1D	2.44	124.79	116.07
15	H	1011	CL0	C4D-ND-C1D	2.44	107.07	105.22
16	b	1204	CLA	C3B-C4B-NB	-2.44	108.35	110.53
23	w	605	LMU	O5'-C1'-C2'	2.44	115.38	110.37
16	s	503	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	t	507	CLA	CHD-C1D-ND	-2.44	121.37	124.80
16	B	1218	CLA	C3B-C4B-NB	-2.44	108.36	110.53
16	H	1109	CLA	C3B-C4B-NB	-2.44	108.36	110.53
16	a	1128	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	t	604	BCR	C24-C23-C22	-2.44	122.63	126.23
21	i	4020	ECH	C1-C6-C5	-2.43	119.31	122.64
19	t	603	BCR	C15-C16-C17	-2.43	118.54	123.52
16	a	1137	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	b	1012	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	H	1124	CLA	C3B-C2B-C1B	-2.43	104.30	107.17
16	n	509	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	p	507	CLA	CHD-C1D-ND	-2.43	121.38	124.80
19	n	601	BCR	C11-C10-C9	-2.43	123.87	127.28
14	H	852	LMG	C1-C2-C3	-2.43	104.89	110.01
19	u	604	BCR	C31-C1-C6	2.43	114.06	110.24
19	s	604	BCR	C15-C16-C17	-2.43	118.54	123.52
19	a	4011	BCR	C1-C6-C5	-2.43	119.31	122.64
15	H	1011	CL0	O2A-CGA-O1A	-2.43	117.54	123.63
16	p	507	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	a	1123	CLA	CHD-C1D-ND	-2.43	121.38	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1021	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	w	516	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	x	509	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	B	1023	CLA	C2A-C1A-CHA	2.43	128.09	123.87
16	q	515	CLA	CHA-C1A-NA	-2.43	120.89	126.39
19	p	604	BCR	C33-C5-C6	-2.43	121.83	124.48
16	A	1109	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	H	1022	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	X	510	CLA	C4A-NA-C1A	2.43	107.79	106.68
19	G	4014	BCR	C24-C23-C22	-2.43	122.64	126.23
16	B	1202	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
14	a	852	LMG	C38-C37-C36	-2.43	102.08	114.37
16	W	512	CLA	CHD-C1D-ND	-2.43	121.38	124.80
16	H	1114	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	G	1238	CLA	CHA-C1A-NA	-2.43	120.89	126.39
19	s	603	BCR	C27-C26-C25	2.43	125.99	122.70
16	b	1208	CLA	CHD-C1D-ND	-2.43	121.38	124.80
17	H	2001	PQN	C14-C13-C15	2.43	119.44	115.23
16	B	1213	CLA	C4A-NA-C1A	2.43	107.79	106.68
16	k	4003	CLA	C4A-NA-C1A	2.43	107.79	106.68
16	k	4004	CLA	C4A-NA-C1A	2.43	107.79	106.68
16	G	1226	CLA	CHD-C1D-ND	-2.43	121.39	124.80
19	J	4013	BCR	C15-C16-C17	-2.43	118.55	123.52
16	y	510	CLA	CHA-C1A-NA	-2.43	120.89	126.39
16	G	1214	CLA	C3B-C4B-NB	-2.43	108.36	110.53
16	X	509	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
16	A	1126	CLA	CHD-C1D-ND	-2.43	121.39	124.80
16	B	1232	CLA	CHA-C1A-NA	-2.43	120.90	126.39
16	A	1109	CLA	CHA-C1A-NA	-2.42	120.90	126.39
16	H	1133	CLA	CHA-C1A-NA	-2.42	120.90	126.39
16	J	1303	CLA	CHD-C1D-ND	-2.42	121.39	124.80
16	t	505	CLA	CHA-C1A-NA	-2.42	120.90	126.39
16	y	512	CLA	C3B-C4B-NB	-2.42	108.37	110.53
19	Y	603	BCR	C27-C26-C25	2.42	125.98	122.70
19	o	602	BCR	C15-C16-C17	-2.42	118.56	123.52
16	U	1503	CLA	CHA-C1A-NA	-2.42	120.91	126.39
16	b	1238	CLA	CHA-C1A-NA	-2.42	120.91	126.39
16	a	1121	CLA	CHD-C1D-ND	-2.42	121.39	124.80
16	A	1119	CLA	CHA-C1A-NA	-2.42	120.91	126.39
19	a	4007	BCR	C28-C27-C26	-2.42	109.74	114.06
14	H	852	LMG	C38-C37-C36	-2.42	102.13	114.37
16	s	513	CLA	C1C-C2C-C3C	-2.42	104.44	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	516	CLA	CHD-C1D-ND	-2.42	121.40	124.80
16	w	509	CLA	CHD-C1D-ND	-2.42	121.40	124.80
13	p	605	LHG	C11-C10-C9	-2.42	102.14	114.37
16	y	506	CLA	CHA-C1A-NA	-2.42	120.91	126.39
16	a	1114	CLA	CHD-C1D-ND	-2.42	121.40	124.80
16	H	1013	CLA	CAA-C2A-C1A	-2.42	104.05	111.97
16	v	502	CLA	C3B-C2B-C1B	-2.42	104.32	107.17
21	R	4020	ECH	C10-C11-C12	2.42	130.20	123.20
19	H	4008	BCR	C7-C8-C9	-2.42	122.66	126.23
16	G	1023	CLA	C4D-C3D-CAD	-2.41	105.48	108.11
16	q	513	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	B	1220	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
16	k	4004	CLA	CHA-C1A-NA	-2.41	120.93	126.39
19	I	4018	BCR	C15-C14-C13	-2.41	123.89	127.28
16	o	511	CLA	CHD-C1D-ND	-2.41	121.41	124.80
19	S	4015	BCR	C11-C10-C9	-2.41	123.89	127.28
16	Z	503	CLA	CHA-C1A-NA	-2.41	120.93	126.39
16	Z	515	CLA	CHA-C1A-NA	-2.41	120.93	126.39
16	H	1128	CLA	CMD-C2D-C1D	-2.41	120.48	124.73
16	A	1123	CLA	C2A-C1A-CHA	2.41	128.05	123.87
16	r	505	CLA	CHD-C1D-ND	-2.41	121.41	124.80
16	g	507	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	s	506	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
16	u	506	CLA	CHD-C1D-ND	-2.41	121.41	124.80
13	I	103	LHG	O8-C23-C24	2.41	119.18	111.83
19	W	601	BCR	C7-C8-C9	-2.41	122.67	126.23
19	l	4022	BCR	C2-C1-C6	2.41	113.94	110.44
16	b	1214	CLA	C3C-C4C-NC	-2.41	107.34	110.43
16	W	504	CLA	CHD-C1D-ND	-2.41	121.41	124.80
16	b	1215	CLA	CHD-C1D-ND	-2.41	121.41	124.80
16	G	1021	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	Y	605	LHG	C11-C10-C9	-2.41	102.19	114.37
19	r	603	BCR	C15-C16-C17	-2.41	118.59	123.52
16	H	1109	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
19	H	4011	BCR	C24-C23-C22	-2.41	122.67	126.23
16	u	509	CLA	CHA-C1A-NA	-2.41	120.94	126.39
19	h	604	BCR	C2-C1-C6	2.41	113.94	110.44
15	A	1011	CL0	CMB-C2B-C3B	2.41	129.49	124.68
16	h	514	CLA	C3B-C4B-NB	-2.41	108.38	110.53
16	A	1135	CLA	C2D-C1D-ND	-2.41	107.75	110.13
16	r	512	CLA	CHD-C1D-ND	-2.41	121.42	124.80
19	G	4010	BCR	C7-C8-C9	-2.41	122.68	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	s	505	CLA	C3B-C4B-NB	-2.40	108.38	110.53
16	W	509	CLA	CHD-C1D-ND	-2.40	121.42	124.80
14	A	852	LMG	C1-C2-C3	-2.40	104.95	110.01
16	r	514	CLA	CHA-C1A-NA	-2.40	120.95	126.39
15	a	1011	CL0	CMB-C2B-C3B	2.40	129.48	124.68
16	s	510	CLA	C4A-NA-C1A	2.40	107.78	106.68
16	y	507	CLA	C4A-NA-C1A	2.40	107.78	106.68
16	f	1302	CLA	C3B-C4B-NB	-2.40	108.39	110.53
19	G	4017	BCR	C30-C25-C26	-2.40	119.35	122.64
16	B	1214	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	v	516	CLA	CMB-C2B-C1B	2.40	129.07	125.42
16	W	513	CLA	C4A-NA-C1A	2.40	107.77	106.68
16	b	1209	CLA	CHD-C1D-ND	-2.40	121.42	124.80
16	J	1302	CLA	CHD-C1D-ND	-2.40	121.43	124.80
16	j	1302	CLA	C3B-C2B-C1B	-2.40	104.34	107.17
16	n	512	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	w	603	BCR	C2-C1-C6	2.40	113.92	110.44
19	R	4018	BCR	C27-C26-C25	2.40	125.94	122.70
16	B	1232	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	X	513	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	n	505	CLA	CHA-C1A-NA	-2.40	120.96	126.39
16	A	1237	CLA	CHD-C1D-ND	-2.40	121.43	124.80
16	v	509	CLA	CHA-C1A-NA	-2.40	120.96	126.39
16	A	1013	CLA	C2B-C1B-NB	-2.40	107.84	110.33
16	s	513	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	y	505	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	x	503	CLA	CHD-C1D-ND	-2.40	121.43	124.80
16	w	515	CLA	CHA-C1A-NA	-2.40	120.96	126.39
19	J	4013	BCR	C24-C23-C22	-2.40	122.69	126.23
19	s	604	BCR	C33-C5-C6	-2.40	121.87	124.48
16	x	517	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	F	4016	BCR	C40-C30-C25	2.40	114.00	110.24
19	a	4011	BCR	C27-C26-C25	2.40	125.94	122.70
16	A	1237	CLA	CMB-C2B-C3B	-2.40	120.92	126.55
17	B	2002	PQN	C11-C12-C13	-2.40	122.70	126.83
16	B	1210	CLA	CHA-C1A-NA	-2.40	120.97	126.39
16	r	515	CLA	CHA-C1A-NA	-2.40	120.97	126.39
19	a	4008	BCR	C30-C25-C26	-2.40	119.36	122.64
16	g	517	CLA	CHD-C1D-ND	-2.40	121.43	124.80
14	A	4101	LMG	C38-C37-C36	-2.39	102.26	114.37
19	p	601	BCR	C15-C14-C13	-2.39	123.92	127.28
16	H	1137	CLA	CHD-C1D-ND	-2.39	121.43	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1236	CLA	C3B-C2B-C1B	-2.39	104.35	107.17
16	a	1125	CLA	C4D-C3D-CAD	-2.39	105.51	108.11
14	a	852	LMG	C1-C2-C3	-2.39	104.97	110.01
16	k	4004	CLA	CHD-C1D-ND	-2.39	121.43	124.80
16	A	1133	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	G	1240	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	X	507	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	b	1239	CLA	CHA-C1A-NA	-2.39	120.97	126.39
16	B	1201	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	s	509	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
16	s	501	CLA	CHA-C1A-NA	-2.39	120.98	126.39
16	G	1210	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	g	515	CLA	CHA-C1A-NA	-2.39	120.98	126.39
16	x	512	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
16	W	505	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	b	1206	CLA	CHA-C1A-NA	-2.39	120.98	126.39
16	G	1234	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
14	A	852	LMG	C38-C37-C36	-2.39	102.30	114.37
16	Y	512	CLA	C1-C2-C3	-2.39	122.28	126.20
19	j	4012	BCR	C15-C14-C13	-2.39	123.93	127.28
16	W	502	CLA	CMD-C2D-C1D	-2.39	120.53	124.73
16	y	501	CLA	CMB-C2B-C1B	2.39	129.05	125.42
16	v	503	CLA	C3B-C4B-NB	-2.39	108.40	110.53
16	Y	511	CLA	CHD-C1D-ND	-2.39	121.44	124.80
16	K	4004	CLA	CHA-C1A-NA	-2.39	120.99	126.39
16	K	4004	CLA	CHD-C1D-ND	-2.39	121.45	124.80
16	t	506	CLA	CHD-C1D-ND	-2.39	121.45	124.80
16	y	515	CLA	C2A-C1A-CHA	2.38	128.01	123.87
16	w	508	CLA	C3B-C4B-NB	-2.38	108.40	110.53
16	b	1219	CLA	C2B-C1B-NB	-2.38	107.85	110.33
19	Z	604	BCR	C11-C10-C9	-2.38	123.93	127.28
16	j	1303	CLA	CHD-C1D-ND	-2.38	121.45	124.80
16	n	501	CLA	C3B-C2B-C1B	-2.38	104.36	107.17
16	p	508	CLA	CHD-C1D-ND	-2.38	121.45	124.80
16	B	1239	CLA	C1C-C2C-C3C	-2.38	104.47	106.98
19	b	4009	BCR	C15-C14-C13	-2.38	123.94	127.28
19	o	601	BCR	C11-C10-C9	-2.38	123.94	127.28
16	a	1138	CLA	C2B-C1B-NB	-2.38	107.86	110.33
16	h	510	CLA	CHA-C1A-NA	-2.38	121.00	126.39
16	a	1134	CLA	CHD-C1D-ND	-2.38	121.45	124.80
19	S	4012	BCR	C11-C10-C9	-2.38	123.94	127.28
16	b	1210	CLA	C3B-C4B-NB	-2.38	108.40	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	r	501	CLA	C3B-C2B-C1B	-2.38	104.36	107.17
15	a	1011	CL0	O2A-CGA-O1A	-2.38	117.67	123.63
19	b	4010	BCR	C15-C14-C13	-2.38	123.94	127.28
23	p	606	LMU	O5B-C5B-C4B	2.38	113.99	109.70
19	v	603	BCR	C30-C25-C26	-2.38	119.38	122.64
16	G	1222	CLA	C3C-C4C-NC	-2.38	107.38	110.43
13	b	4018	LHG	C20-C19-C18	-2.38	102.34	114.37
19	T	4001	BCR	C15-C14-C13	-2.38	123.94	127.28
16	b	1213	CLA	C3B-C4B-NB	-2.38	108.41	110.53
16	p	509	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
16	J	1303	CLA	C4A-NA-C1A	2.38	107.76	106.68
19	j	4012	BCR	C33-C5-C6	-2.38	121.89	124.48
19	h	601	BCR	C11-C10-C9	-2.38	123.94	127.28
19	S	4012	BCR	C7-C8-C9	-2.38	122.72	126.23
16	H	1118	CLA	CHD-C1D-ND	-2.38	121.46	124.80
16	X	511	CLA	CHD-C1D-ND	-2.38	121.46	124.80
14	f	4017	LMG	O6-C1-O1	-2.38	104.43	110.04
16	s	510	CLA	C3B-C2B-C1B	-2.38	104.37	107.17
16	H	1123	CLA	CHA-C1A-NA	-2.38	121.01	126.39
16	x	515	CLA	CHA-C1A-NA	-2.38	121.01	126.39
16	Y	508	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
16	b	1021	CLA	C3B-C2B-C1B	-2.38	104.37	107.17
16	n	515	CLA	CHA-C1A-NA	-2.38	121.01	126.39
19	J	4012	BCR	C15-C14-C13	-2.38	123.95	127.28
16	g	513	CLA	C3B-C4B-NB	-2.37	108.41	110.53
16	a	1135	CLA	C3B-C2B-C1B	-2.37	104.37	107.17
16	H	1120	CLA	C3C-C4C-NC	-2.37	107.39	110.43
16	G	1217	CLA	C1D-ND-C4D	-2.37	104.65	106.31
16	h	508	CLA	CHD-C1D-ND	-2.37	121.46	124.80
16	b	1216	CLA	CHA-C1A-NA	-2.37	121.02	126.39
19	i	4018	BCR	C27-C26-C25	2.37	125.91	122.70
16	G	1239	CLA	CMB-C2B-C3B	-2.37	120.97	126.55
16	Y	503	CLA	C3C-C4C-NC	-2.37	107.39	110.43
16	p	511	CLA	CHA-C1A-NA	-2.37	121.02	126.39
16	Z	503	CLA	CMB-C2B-C1B	2.37	129.03	125.42
16	t	510	CLA	C3B-C2B-C1B	-2.37	104.38	107.17
19	J	4015	BCR	C11-C10-C9	-2.37	123.95	127.28
16	p	508	CLA	CHA-C1A-NA	-2.37	121.02	126.39
16	L	1503	CLA	CHD-C1D-ND	-2.37	121.47	124.80
16	X	504	CLA	CHA-C1A-NA	-2.37	121.03	126.39
19	A	4003	BCR	C40-C30-C25	2.37	113.96	110.24
15	H	1011	CL0	C3D-C4D-CHA	2.37	112.14	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1206	CLA	C3B-C4B-NB	-2.37	108.42	110.53
16	B	1228	CLA	CHD-C1D-ND	-2.37	121.47	124.80
16	v	517	CLA	CHA-C1A-NA	-2.37	121.03	126.39
16	b	1203	CLA	O2A-CGA-O1A	-2.37	117.71	123.63
19	X	602	BCR	C15-C14-C13	-2.37	123.96	127.28
16	A	1117	CLA	C1-C2-C3	-2.37	122.32	126.20
16	s	512	CLA	CHD-C1D-ND	-2.37	121.47	124.80
16	Y	507	CLA	CHD-C1D-ND	-2.37	121.47	124.80
16	A	1118	CLA	C4A-NA-C1A	2.37	107.76	106.68
19	B	4014	BCR	C24-C23-C22	-2.36	122.74	126.23
16	y	501	CLA	C3B-C4B-NB	-2.36	108.42	110.53
19	K	4001	BCR	C27-C26-C25	2.36	125.90	122.70
16	g	510	CLA	CHA-C1A-NA	-2.36	121.04	126.39
16	G	1234	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	W	510	CLA	CHA-C1A-NA	-2.36	121.04	126.39
16	n	505	CLA	CHD-C1D-ND	-2.36	121.48	124.80
13	B	4018	LHG	C20-C19-C18	-2.36	102.44	114.37
16	s	512	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
16	y	511	CLA	C3B-C4B-NB	-2.36	108.42	110.53
16	A	1104	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
16	n	511	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	G	1222	CLA	C2A-C1A-CHA	2.36	127.96	123.87
16	r	517	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	W	501	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	a	1116	CLA	CHD-C1D-ND	-2.36	121.48	124.80
16	Z	507	CLA	CMB-C2B-C1B	2.36	129.01	125.42
16	G	1228	CLA	CHA-C1A-NA	-2.36	121.05	126.39
16	B	1221	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
16	G	1222	CLA	C3B-C2B-C1B	-2.36	104.39	107.17
16	H	1116	CLA	CHD-C1D-ND	-2.36	121.48	124.80
19	f	4016	BCR	C27-C26-C25	2.36	125.89	122.70
14	b	848	LMG	C38-C37-C36	-2.36	102.45	114.37
16	F	1302	CLA	CHD-C1D-ND	-2.36	121.49	124.80
16	G	1240	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	o	510	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	B	1211	CLA	CHA-C1A-NA	-2.35	121.06	126.39
19	K	4001	BCR	C11-C10-C9	-2.35	123.98	127.28
19	n	604	BCR	C15-C16-C17	-2.35	118.70	123.52
19	j	4013	BCR	C1-C6-C5	-2.35	119.42	122.64
19	Z	603	BCR	C11-C10-C9	-2.35	123.98	127.28
16	W	517	CLA	C3B-C4B-NB	-2.35	108.43	110.53
16	a	1109	CLA	O2A-CGA-O1A	-2.35	117.74	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	504	CLA	CHA-C1A-NA	-2.35	121.06	126.39
19	J	4013	BCR	C31-C1-C6	2.35	113.93	110.24
16	B	1218	CLA	CHA-C1A-NA	-2.35	121.06	126.39
16	p	503	CLA	C3C-C4C-NC	-2.35	107.42	110.43
16	o	515	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
16	W	517	CLA	C4A-NA-C1A	2.35	107.75	106.68
16	Y	517	CLA	C4A-NA-C1A	2.35	107.75	106.68
19	Z	603	BCR	C15-C16-C17	-2.35	118.71	123.52
23	w	605	LMU	C1B-O1B-C4'	-2.35	112.41	117.98
16	r	511	CLA	CHD-C1D-ND	-2.35	121.49	124.80
16	a	1237	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	T	4001	BCR	C11-C10-C9	-2.35	123.98	127.28
16	w	505	CLA	C1-C2-C3	-2.35	122.35	126.20
16	v	510	CLA	CHA-C1A-NA	-2.35	121.07	126.39
16	H	1120	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	n	513	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	g	508	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	h	506	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	q	509	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
16	g	503	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	B	4017	BCR	C30-C25-C26	-2.35	119.43	122.64
19	X	601	BCR	C11-C10-C9	-2.35	123.98	127.28
19	R	4018	BCR	C33-C5-C6	-2.35	121.92	124.48
13	H	849	LHG	C11-C10-C9	-2.35	102.50	114.37
19	H	4002	BCR	C24-C23-C22	-2.35	122.76	126.23
16	B	1012	CLA	C3B-C2B-C1B	-2.35	104.40	107.17
16	G	1230	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	b	1222	CLA	CHD-C1D-ND	-2.35	121.50	124.80
16	x	505	CLA	C3C-C4C-NC	-2.35	107.42	110.43
16	r	506	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
16	G	1229	CLA	CHA-C1A-NA	-2.35	121.08	126.39
16	n	510	CLA	CHA-C1A-NA	-2.35	121.08	126.39
16	s	511	CLA	CHA-C1A-NA	-2.35	121.08	126.39
19	h	601	BCR	C33-C5-C6	-2.35	121.92	124.48
16	r	509	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	l	4022	BCR	C31-C1-C6	2.35	113.92	110.24
19	s	602	BCR	C11-C10-C9	-2.35	123.99	127.28
16	Y	505	CLA	C3B-C2B-C1B	-2.34	104.41	107.17
16	b	1234	CLA	O2A-CGA-O1A	-2.34	117.76	123.63
16	H	1136	CLA	C3B-C4B-NB	-2.34	108.44	110.53
19	p	602	BCR	C11-C10-C9	-2.34	123.99	127.28
16	H	1108	CLA	CHA-C1A-NA	-2.34	121.08	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	q	604	BCR	C15-C16-C17	-2.34	118.72	123.52
16	A	1133	CLA	CHA-C1A-NA	-2.34	121.08	126.39
16	A	1132	CLA	C3B-C2B-C1B	-2.34	104.41	107.17
16	o	517	CLA	CHD-C1D-ND	-2.34	121.50	124.80
16	p	503	CLA	CHD-C1D-ND	-2.34	121.50	124.80
16	t	515	CLA	CHD-C1D-ND	-2.34	121.50	124.80
16	v	513	CLA	CHD-C1D-ND	-2.34	121.50	124.80
16	p	508	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
19	y	601	BCR	C33-C5-C6	-2.34	121.93	124.48
16	Z	517	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	Y	501	CLA	CHA-C1A-NA	-2.34	121.09	126.39
16	Y	509	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
16	a	1135	CLA	C3B-C4B-NB	-2.34	108.44	110.53
16	r	508	CLA	C3B-C4B-NB	-2.34	108.44	110.53
16	y	504	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	b	1238	CLA	C1-C2-C3	-2.34	122.36	126.20
16	a	1140	CLA	CMB-C2B-C1B	2.34	128.98	125.42
16	B	1229	CLA	CHA-C1A-NA	-2.34	121.09	126.39
14	B	848	LMG	O3-C3-C2	-2.34	104.86	110.38
16	o	501	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	h	503	CLA	CHA-C1A-NA	-2.34	121.09	126.39
23	Z	605	LMU	C1B-O1B-C4'	-2.34	112.44	117.98
19	v	601	BCR	C3-C4-C5	-2.34	109.89	114.06
16	H	1113	CLA	CHD-C1D-ND	-2.34	121.51	124.80
16	U	1501	CLA	CHD-C1D-ND	-2.34	121.51	124.80
19	Y	602	BCR	C11-C10-C9	-2.34	124.00	127.28
16	G	1211	CLA	CHA-C1A-NA	-2.34	121.10	126.39
16	v	512	CLA	C3B-C4B-NB	-2.34	108.44	110.53
16	W	515	CLA	CHA-C1A-NA	-2.34	121.10	126.39
16	b	1235	CLA	CHA-C1A-NA	-2.34	121.10	126.39
16	n	503	CLA	CHD-C1D-ND	-2.34	121.52	124.80
16	L	1503	CLA	C2A-C1A-CHA	2.34	127.92	123.87
19	K	4005	BCR	C24-C23-C22	-2.34	122.78	126.23
19	b	4004	BCR	C11-C10-C9	-2.34	124.00	127.28
16	b	1220	CLA	O2A-CGA-O1A	-2.34	117.79	123.63
16	H	1109	CLA	CHA-C1A-NA	-2.33	121.10	126.39
16	t	510	CLA	CHA-C1A-NA	-2.33	121.10	126.39
16	H	1133	CLA	C2B-C1B-NB	-2.33	107.91	110.33
16	A	1013	CLA	C2A-C3A-C4A	-2.33	98.10	101.87
16	p	516	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	G	1012	CLA	CHA-C1A-NA	-2.33	121.11	126.39
21	I	4020	ECH	O27-C27-C26	2.33	123.07	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1239	CLA	C4A-NA-C1A	2.33	107.74	106.68
16	q	509	CLA	C4A-NA-C1A	2.33	107.74	106.68
16	G	1239	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
16	T	4004	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	v	503	CLA	C3B-C2B-C1B	-2.33	104.42	107.17
16	v	504	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	Z	511	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	o	504	CLA	CHD-C1D-ND	-2.33	121.52	124.80
16	q	507	CLA	CHD-C1D-ND	-2.33	121.52	124.80
19	o	602	BCR	C15-C14-C13	-2.33	124.01	127.28
16	y	516	CLA	CHA-C1A-NA	-2.33	121.11	126.39
13	G	4018	LHG	C20-C19-C18	-2.33	102.59	114.37
16	B	1021	CLA	CMB-C2B-C1B	2.33	128.97	125.42
16	Z	508	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	n	505	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	Z	508	CLA	CHD-C1D-ND	-2.33	121.52	124.80
14	A	4101	LMG	O6-C1-O1	-2.33	104.54	110.04
19	L	4022	BCR	C24-C23-C22	-2.33	122.79	126.23
16	a	1138	CLA	C1-C2-C3	-2.33	122.38	126.20
16	X	515	CLA	C3B-C4B-NB	-2.33	108.45	110.53
19	s	601	BCR	C27-C26-C25	2.33	125.85	122.70
19	g	602	BCR	C15-C14-C13	-2.33	124.01	127.28
16	b	1216	CLA	CHD-C1D-ND	-2.33	121.53	124.80
19	G	4014	BCR	C30-C25-C26	-2.33	119.45	122.64
19	o	604	BCR	C1-C6-C5	-2.33	119.45	122.64
16	G	1232	CLA	CHD-C1D-ND	-2.33	121.53	124.80
14	H	4101	LMG	C38-C37-C36	-2.33	102.60	114.37
16	A	1112	CLA	C2A-C1A-CHA	2.33	127.91	123.87
16	b	1220	CLA	CHA-C1A-NA	-2.33	121.12	126.39
16	a	1138	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
16	H	1127	CLA	C3B-C4B-NB	-2.33	108.45	110.53
16	g	501	CLA	C3B-C4B-NB	-2.33	108.45	110.53
19	Y	601	BCR	C15-C14-C13	-2.33	124.02	127.28
16	B	1206	CLA	CHA-C1A-NA	-2.33	121.12	126.39
16	h	508	CLA	CHA-C1A-NA	-2.33	121.12	126.39
16	n	507	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	p	502	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	q	517	CLA	CHD-C1D-ND	-2.33	121.53	124.80
16	Y	513	CLA	CMB-C2B-C1B	2.32	128.96	125.42
16	h	515	CLA	C1-C2-C3	-2.32	122.39	126.20
19	j	4015	BCR	C1-C6-C5	-2.32	119.46	122.64
16	u	506	CLA	C3C-C4C-NC	-2.32	107.45	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	t	603	BCR	C15-C14-C13	-2.32	124.02	127.28
16	h	504	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
16	a	1134	CLA	CHA-C1A-NA	-2.32	121.13	126.39
16	a	1139	CLA	C3B-C4B-NB	-2.32	108.46	110.53
16	h	513	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	B	1235	CLA	CHA-C1A-NA	-2.32	121.14	126.39
16	b	1224	CLA	CMC-C2C-C1C	-2.32	121.41	125.03
19	L	4022	BCR	C3-C4-C5	-2.32	109.92	114.06
16	S	1302	CLA	C3B-C4B-NB	-2.32	108.46	110.53
19	G	4005	BCR	C15-C16-C17	-2.32	118.77	123.52
16	A	1104	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	b	1023	CLA	C2A-C1A-CHA	2.32	127.89	123.87
21	G	4006	ECH	C24-C23-C22	2.32	129.66	126.23
16	h	501	CLA	CHD-C1D-ND	-2.32	121.54	124.80
19	g	601	BCR	C2-C1-C6	2.32	113.81	110.44
16	A	1119	CLA	C3B-C4B-NB	-2.32	108.46	110.53
19	x	601	BCR	C7-C8-C9	-2.32	122.81	126.23
16	G	1023	CLA	C2A-C1A-CHA	2.32	127.89	123.87
19	T	4005	BCR	C3-C4-C5	-2.32	109.92	114.06
16	B	1234	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	u	509	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
16	H	1801	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	p	512	CLA	CHD-C1D-ND	-2.32	121.54	124.80
16	G	1240	CLA	C2B-C1B-NB	-2.32	107.92	110.33
19	B	4005	BCR	C15-C16-C17	-2.32	118.78	123.52
16	G	1204	CLA	C4A-NA-C1A	2.31	107.73	106.68
16	n	509	CLA	C4A-NA-C1A	2.31	107.73	106.68
16	s	517	CLA	CMB-C2B-C1B	2.31	128.94	125.42
16	A	1113	CLA	CHD-C1D-ND	-2.31	121.55	124.80
15	A	1011	CL0	C4D-ND-C1D	2.31	106.97	105.22
16	y	504	CLA	C2D-C1D-ND	-2.31	107.84	110.13
16	t	515	CLA	CHA-C1A-NA	-2.31	121.15	126.39
16	y	513	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	r	501	CLA	C3B-C4B-NB	-2.31	108.47	110.53
19	W	601	BCR	C15-C14-C13	-2.31	124.03	127.28
19	k	4001	BCR	C11-C10-C9	-2.31	124.03	127.28
16	r	502	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	G	1220	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
16	W	503	CLA	CHA-C1A-NA	-2.31	121.16	126.39
16	r	513	CLA	C1C-C2C-C3C	-2.31	104.55	106.98
19	h	601	BCR	C24-C23-C22	-2.31	122.82	126.23
19	n	601	BCR	C24-C23-C22	-2.31	122.82	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	848	LMG	O1-C7-C8	-2.31	105.20	110.82
16	a	1117	CLA	C3B-C4B-NB	-2.31	108.47	110.53
16	G	1231	CLA	CHD-C1D-ND	-2.31	121.55	124.80
19	a	4011	BCR	C24-C23-C22	-2.31	122.82	126.23
16	n	501	CLA	C3B-C4B-NB	-2.31	108.47	110.53
16	w	504	CLA	C1-C2-C3	-2.31	122.42	126.20
16	Z	507	CLA	CHD-C1D-ND	-2.31	121.55	124.80
16	T	4004	CLA	CHA-C1A-NA	-2.31	121.17	126.39
16	w	513	CLA	CMB-C2B-C1B	2.31	128.93	125.42
16	B	1207	CLA	CHD-C1D-ND	-2.31	121.56	124.80
16	h	517	CLA	CHA-C1A-NA	-2.31	121.17	126.39
16	q	509	CLA	CHA-C1A-NA	-2.31	121.17	126.39
16	y	512	CLA	CHA-C1A-NA	-2.31	121.17	126.39
19	w	604	BCR	C16-C15-C14	-2.31	118.80	123.52
19	H	4003	BCR	C11-C10-C9	-2.31	124.04	127.28
16	s	504	CLA	CHD-C1D-ND	-2.31	121.56	124.80
19	n	604	BCR	C15-C14-C13	-2.31	124.04	127.28
16	p	516	CLA	C4A-NA-C1A	2.31	107.73	106.68
16	t	507	CLA	C4A-NA-C1A	2.31	107.73	106.68
16	r	502	CLA	CMB-C2B-C1B	2.31	128.93	125.42
16	b	1232	CLA	CHA-C1A-NA	-2.31	121.17	126.39
16	x	504	CLA	C3B-C2B-C1B	-2.31	104.45	107.17
16	B	1220	CLA	C2C-C1C-NC	-2.31	107.56	109.98
16	H	1122	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	v	507	CLA	CHA-C1A-NA	-2.30	121.17	126.39
16	Z	505	CLA	C1-C2-C3	-2.30	122.42	126.20
16	L	1501	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	B	1227	CLA	CHA-C1A-NA	-2.30	121.17	126.39
16	H	1105	CLA	CHA-C1A-NA	-2.30	121.17	126.39
16	B	1021	CLA	C2A-C1A-CHA	2.30	127.86	123.87
19	a	4003	BCR	C33-C5-C6	-2.30	121.97	124.48
16	A	1112	CLA	CHD-C1D-ND	-2.30	121.56	124.80
19	Z	603	BCR	C15-C14-C13	-2.30	124.05	127.28
19	A	4003	BCR	C33-C5-C6	-2.30	121.97	124.48
16	H	1013	CLA	C2A-C3A-C4A	-2.30	98.15	101.87
19	g	602	BCR	C7-C8-C9	-2.30	122.83	126.23
16	y	513	CLA	C4A-NA-C1A	2.30	107.73	106.68
16	g	507	CLA	CHD-C1D-ND	-2.30	121.56	124.80
16	G	1023	CLA	C2C-C1C-NC	-2.30	107.56	109.98
16	p	515	CLA	C3B-C4B-NB	-2.30	108.48	110.53
16	g	503	CLA	C2B-C1B-NB	-2.30	107.94	110.33
16	G	1208	CLA	C3B-C2B-C1B	-2.30	104.46	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	4101	LMG	C38-C37-C36	-2.30	102.75	114.37
14	F	4017	LMG	O6-C1-O1	-2.30	104.61	110.04
16	Y	513	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
16	G	1218	CLA	C3B-C4B-NB	-2.30	108.48	110.53
16	Y	508	CLA	C3B-C4B-NB	-2.30	108.48	110.53
16	s	504	CLA	C1-C2-C3	-2.30	122.43	126.20
16	h	515	CLA	CHA-C1A-NA	-2.30	121.19	126.39
19	q	604	BCR	C16-C15-C14	-2.30	118.82	123.52
16	b	1239	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
16	q	507	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
16	G	1224	CLA	CHA-C1A-NA	-2.30	121.19	126.39
16	B	1224	CLA	CHD-C1D-ND	-2.30	121.57	124.80
19	p	603	BCR	C7-C8-C9	-2.30	122.84	126.23
19	B	4005	BCR	C30-C25-C26	-2.30	119.50	122.64
16	H	1127	CLA	C1-C2-C3	-2.30	122.44	126.20
16	a	1120	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
16	B	1012	CLA	C3B-C4B-NB	-2.30	108.48	110.53
16	b	1204	CLA	C4A-NA-C1A	2.29	107.73	106.68
16	T	4003	CLA	C3B-C2B-C1B	-2.29	104.46	107.17
16	n	511	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
14	G	848	LMG	O3-C3-C2	-2.29	104.97	110.38
16	s	508	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
14	B	848	LMG	O1-C7-C8	-2.29	105.24	110.82
16	a	1237	CLA	C1C-C2C-C3C	-2.29	104.57	106.98
16	G	1235	CLA	CHA-C1A-NA	-2.29	121.20	126.39
16	H	1013	CLA	C3A-C2A-C1A	-2.29	97.90	101.34
19	o	603	BCR	C15-C14-C13	-2.29	124.06	127.28
16	t	516	CLA	CHD-C1D-ND	-2.29	121.58	124.80
16	a	1130	CLA	C1-C2-C3	-2.29	122.44	126.20
17	A	2001	PQN	C11-C12-C13	-2.29	122.88	126.83
16	t	504	CLA	CHA-C1A-NA	-2.29	121.20	126.39
16	G	1217	CLA	CHD-C1D-ND	-2.29	121.58	124.80
16	u	513	CLA	C2A-C1A-CHA	2.29	127.84	123.87
19	W	604	BCR	C24-C23-C22	-2.29	122.85	126.23
16	Z	513	CLA	C3B-C4B-NB	-2.29	108.48	110.53
19	p	601	BCR	C3-C4-C5	-2.29	109.97	114.06
19	b	4005	BCR	C15-C14-C13	-2.29	124.07	127.28
16	G	1225	CLA	CHA-C1A-NA	-2.29	121.20	126.39
16	y	511	CLA	CHA-C1A-NA	-2.29	121.20	126.39
16	Y	510	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
19	A	4003	BCR	C15-C14-C13	-2.29	124.07	127.28
16	Q	1302	CLA	C3B-C2B-C1B	-2.29	104.47	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	1301	CLA	CHD-C1D-ND	-2.29	121.58	124.80
16	a	1130	CLA	C3B-C2B-C1B	-2.29	104.47	107.17
16	Z	501	CLA	CHA-C1A-NA	-2.29	121.21	126.39
16	K	4002	CLA	CHD-C1D-ND	-2.29	121.58	124.80
16	b	1216	CLA	CMB-C2B-C1B	2.29	128.90	125.42
19	x	601	BCR	C15-C14-C13	-2.29	124.07	127.28
19	J	4015	BCR	C1-C6-C5	-2.29	119.51	122.64
16	Y	505	CLA	C2A-C1A-CHA	2.29	127.83	123.87
16	a	1013	CLA	C2B-C1B-NB	-2.29	107.95	110.33
16	Y	505	CLA	CHD-C1D-ND	-2.29	121.58	124.80
16	s	503	CLA	C4A-NA-C1A	2.29	107.72	106.68
16	h	507	CLA	CHA-C1A-NA	-2.29	121.22	126.39
16	x	509	CLA	CHA-C1A-NA	-2.29	121.22	126.39
16	h	516	CLA	C1C-C2C-C3C	-2.29	104.58	106.98
16	Y	516	CLA	C3B-C4B-NB	-2.29	108.49	110.53
16	n	502	CLA	CHD-C1D-ND	-2.28	121.59	124.80
16	n	516	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
19	G	4017	BCR	C15-C16-C17	-2.28	118.84	123.52
19	G	4017	BCR	C10-C11-C12	-2.28	116.58	123.20
19	G	4005	BCR	C27-C26-C25	2.28	125.79	122.70
19	s	603	BCR	C15-C14-C13	-2.28	124.08	127.28
16	n	511	CLA	CHA-C1A-NA	-2.28	121.22	126.39
24	Z	601	LUT	C31-C32-C33	-2.28	120.10	126.36
16	a	1119	CLA	C3B-C4B-NB	-2.28	108.49	110.53
16	W	513	CLA	CHA-C1A-NA	-2.28	121.22	126.39
16	t	502	CLA	CHA-C1A-NA	-2.28	121.22	126.39
16	b	1226	CLA	C3C-C4C-NC	-2.28	107.51	110.43
19	y	601	BCR	C11-C10-C9	-2.28	124.08	127.28
16	H	1122	CLA	CHA-C1A-NA	-2.28	121.22	126.39
16	v	501	CLA	CHA-C1A-NA	-2.28	121.23	126.39
19	S	4012	BCR	C24-C23-C22	-2.28	122.86	126.23
16	B	1214	CLA	CHD-C1D-ND	-2.28	121.59	124.80
16	w	501	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
16	B	1239	CLA	C3C-C4C-NC	-2.28	107.51	110.43
16	v	503	CLA	CHA-C1A-NA	-2.28	121.23	126.39
16	G	1012	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
16	q	515	CLA	C3B-C2B-C1B	-2.28	104.48	107.17
16	o	513	CLA	C3B-C4B-NB	-2.28	108.50	110.53
16	r	513	CLA	CHA-C1A-NA	-2.28	121.23	126.39
14	H	4101	LMG	O2-C2-C1	-2.28	104.64	110.08
13	i	103	LHG	C11-C10-C9	-2.28	102.85	114.37
24	w	601	LUT	C3-C4-C5	-2.28	106.50	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	p	505	CLA	CHD-C1D-ND	-2.28	121.60	124.80
16	t	509	CLA	CHD-C1D-ND	-2.28	121.60	124.80
16	B	1230	CLA	C4A-NA-C1A	2.28	107.72	106.68
16	S	1303	CLA	C4A-NA-C1A	2.28	107.72	106.68
16	Z	517	CLA	C4A-NA-C1A	2.28	107.72	106.68
16	A	1127	CLA	C3B-C4B-NB	-2.28	108.50	110.53
16	H	1126	CLA	C3B-C4B-NB	-2.28	108.50	110.53
16	Z	504	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
19	G	4010	BCR	C10-C11-C12	-2.28	116.60	123.20
16	Y	511	CLA	CHA-C1A-NA	-2.28	121.23	126.39
16	u	504	CLA	CHA-C1A-NA	-2.28	121.23	126.39
16	G	1236	CLA	CHA-C1A-NA	-2.28	121.24	126.39
16	w	514	CLA	CHA-C1A-NA	-2.28	121.24	126.39
16	Z	516	CLA	C3B-C2B-C1B	-2.28	104.49	107.17
19	F	4016	BCR	C15-C16-C17	-2.28	118.86	123.52
16	X	509	CLA	C3B-C2B-C1B	-2.27	104.49	107.17
16	p	505	CLA	C2D-C1D-ND	-2.27	107.88	110.13
16	y	505	CLA	C4D-C3D-CAD	-2.27	105.64	108.11
19	S	4013	BCR	C1-C6-C5	-2.27	119.53	122.64
16	a	1112	CLA	C3B-C4B-NB	-2.27	108.50	110.53
16	u	515	CLA	C3B-C4B-NB	-2.27	108.50	110.53
16	H	1801	CLA	C3C-C4C-NC	-2.27	107.52	110.43
16	t	513	CLA	C2B-C1B-NB	-2.27	107.97	110.33
16	X	510	CLA	CHD-C1D-ND	-2.27	121.60	124.80
16	t	512	CLA	CHD-C1D-ND	-2.27	121.60	124.80
19	o	602	BCR	C20-C21-C22	-2.27	124.09	127.28
16	Y	504	CLA	C3B-C4B-NB	-2.27	108.50	110.53
16	W	510	CLA	C3B-C2B-C1B	-2.27	104.49	107.17
16	Z	515	CLA	C3B-C2B-C1B	-2.27	104.49	107.17
19	n	604	BCR	C27-C26-C25	2.27	125.78	122.70
19	q	602	BCR	C7-C8-C9	-2.27	122.87	126.23
16	o	509	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
19	J	4012	BCR	C33-C5-C6	-2.27	122.00	124.48
14	b	848	LMG	O3-C3-C2	-2.27	105.02	110.38
16	o	506	CLA	CHA-C1A-NA	-2.27	121.25	126.39
16	s	513	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	v	603	BCR	C11-C10-C9	-2.27	124.09	127.28
16	G	1203	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	H	1114	CLA	C3B-C2B-C1B	-2.27	104.49	107.17
24	q	601	LUT	C15-C35-C34	-2.27	118.87	123.52
19	g	603	BCR	C33-C5-C6	-2.27	122.01	124.48
19	x	603	BCR	C33-C5-C6	-2.27	122.01	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	1108	CLA	CHD-C1D-ND	-2.27	121.61	124.80
16	h	509	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
16	x	510	CLA	CHA-C1A-NA	-2.27	121.25	126.39
16	v	510	CLA	C3B-C2B-C1B	-2.27	104.49	107.17
19	J	4015	BCR	C7-C8-C9	-2.27	122.88	126.23
16	v	503	CLA	C2B-C1B-NB	-2.27	107.97	110.33
16	B	1235	CLA	C3B-C4B-NB	-2.27	108.50	110.53
16	b	1236	CLA	CHA-C1A-NA	-2.27	121.25	126.39
16	B	1231	CLA	CHD-C1D-ND	-2.27	121.61	124.80
13	Y	605	LHG	C27-C26-C25	-2.27	102.91	114.37
19	B	4005	BCR	C15-C14-C13	-2.27	124.10	127.28
16	K	4003	CLA	C3B-C4B-NB	-2.27	108.51	110.53
15	H	1011	CL0	CMD-C2D-C3D	2.27	129.21	124.68
19	g	604	BCR	C7-C8-C9	-2.27	122.88	126.23
16	X	508	CLA	CMB-C2B-C1B	2.27	128.87	125.42
16	G	1221	CLA	CHA-C1A-NA	-2.27	121.26	126.39
16	Y	515	CLA	C3B-C2B-C1B	-2.27	104.50	107.17
16	b	1228	CLA	CHA-C1A-NA	-2.27	121.26	126.39
19	l	4022	BCR	C15-C16-C17	-2.27	118.88	123.52
16	s	517	CLA	C2B-C1B-NB	-2.27	107.98	110.33
16	w	513	CLA	C3B-C4B-NB	-2.27	108.51	110.53
16	x	511	CLA	CHD-C1D-ND	-2.26	121.61	124.80
13	R	103	LHG	C11-C10-C9	-2.26	102.92	114.37
16	p	511	CLA	C3B-C4B-NB	-2.26	108.51	110.53
19	j	4012	BCR	C7-C8-C9	-2.26	122.89	126.23
16	b	1217	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	Z	511	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	t	511	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
19	B	4010	BCR	C7-C8-C9	-2.26	122.89	126.23
16	H	1013	CLA	CHB-C1B-C2B	-2.26	120.86	127.43
16	X	505	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	A	1107	CLA	C1-C2-C3	-2.26	123.10	126.76
16	v	501	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
19	W	601	BCR	C29-C30-C25	2.26	113.72	110.44
16	K	4003	CLA	CHD-C1D-ND	-2.26	121.62	124.80
16	r	503	CLA	C3C-C4C-NC	-2.26	107.53	110.43
13	A	849	LHG	C11-C10-C9	-2.26	102.94	114.37
19	r	601	BCR	C11-C10-C9	-2.26	124.11	127.28
16	o	501	CLA	CHA-C1A-NA	-2.26	121.27	126.39
16	r	511	CLA	C3B-C4B-NB	-2.26	108.51	110.53
19	R	4018	BCR	C7-C8-C9	-2.26	122.89	126.23
19	T	4001	BCR	C15-C16-C17	-2.26	118.89	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1235	CLA	CHD-C1D-C2D	2.26	130.19	125.49
16	x	503	CLA	C2B-C1B-NB	-2.26	107.98	110.33
16	A	1116	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
16	G	1203	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
16	r	503	CLA	CHD-C1D-ND	-2.26	121.62	124.80
16	B	1201	CLA	C3B-C2B-C1B	-2.26	104.51	107.17
16	h	514	CLA	C2B-C1B-NB	-2.26	107.98	110.33
19	b	4010	BCR	C30-C25-C26	-2.26	119.55	122.64
16	B	1216	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	A	1106	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	y	515	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	a	1104	CLA	C3B-C4B-NB	-2.26	108.52	110.53
16	B	1212	CLA	CHA-C1A-NA	-2.26	121.28	126.39
19	q	602	BCR	C24-C23-C22	-2.26	122.90	126.23
19	K	4005	BCR	C3-C4-C5	-2.26	110.03	114.06
19	H	4008	BCR	C33-C5-C6	-2.26	122.02	124.48
16	G	1235	CLA	C3B-C2B-C1B	-2.26	104.51	107.17
16	h	509	CLA	C3B-C2B-C1B	-2.26	104.51	107.17
16	H	1130	CLA	C1-C2-C3	-2.26	122.50	126.20
16	o	510	CLA	CHD-C1D-ND	-2.26	121.63	124.80
16	A	1109	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
16	H	1137	CLA	C4A-NA-C1A	2.26	107.71	106.68
16	b	1208	CLA	CHA-C1A-NA	-2.26	121.28	126.39
16	H	1130	CLA	CHD-C1D-ND	-2.26	121.63	124.80
23	Y	606	LMU	C1'-C2'-C3'	2.26	114.75	110.01
16	A	1116	CLA	C2D-C1D-ND	-2.25	107.89	110.13
17	b	2002	PQN	C14-C13-C15	2.25	119.14	115.23
16	b	1238	CLA	CHD-C1D-ND	-2.25	121.63	124.80
16	x	503	CLA	C3C-C4C-NC	-2.25	107.54	110.43
16	Y	515	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
16	a	1107	CLA	C1-C2-C3	-2.25	123.12	126.76
16	b	1239	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
16	h	511	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
19	J	4012	BCR	C7-C8-C9	-2.25	122.90	126.23
19	U	4022	BCR	C31-C1-C6	2.25	113.78	110.24
16	x	507	CLA	CHD-C1D-ND	-2.25	121.63	124.80
19	t	603	BCR	C33-C5-C6	-2.25	122.03	124.48
13	I	103	LHG	C11-C10-C9	-2.25	102.99	114.37
16	b	1201	CLA	C3B-C2B-C1B	-2.25	104.52	107.17
16	B	1223	CLA	CHD-C1D-ND	-2.25	121.63	124.80
16	n	503	CLA	C3C-C4C-NC	-2.25	107.55	110.43
24	w	601	LUT	C15-C35-C34	-2.25	118.91	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	p	604	BCR	C11-C10-C9	-2.25	124.12	127.28
16	B	1230	CLA	C3B-C2B-C1B	-2.25	104.52	107.17
16	A	1131	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	p	602	BCR	C24-C23-C22	-2.25	122.91	126.23
19	b	4014	BCR	C30-C25-C26	-2.25	119.56	122.64
23	x	606	LMU	C1B-C2B-C3B	2.25	114.74	110.01
16	r	517	CLA	C3B-C4B-NB	-2.25	108.52	110.53
16	v	517	CLA	C3B-C4B-NB	-2.25	108.52	110.53
16	A	1135	CLA	CHD-C1D-ND	-2.25	121.64	124.80
19	A	4008	BCR	C33-C5-C6	-2.25	122.03	124.48
19	t	601	BCR	C15-C14-C13	-2.25	124.12	127.28
16	y	516	CLA	C4A-NA-C1A	2.25	107.70	106.68
16	W	507	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	t	505	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	y	517	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
16	n	509	CLA	C3B-C4B-NB	-2.25	108.52	110.53
19	i	4018	BCR	C15-C14-C13	-2.25	124.12	127.28
16	t	511	CLA	CHA-C1A-NA	-2.25	121.30	126.39
16	s	506	CLA	CMB-C2B-C1B	2.25	128.84	125.42
16	H	1129	CLA	C2B-C1B-NB	-2.25	108.00	110.33
16	b	1217	CLA	C1D-ND-C4D	-2.25	104.73	106.31
16	H	1107	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	Y	514	CLA	C4A-NA-C1A	2.25	107.70	106.68
16	B	1209	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	Z	501	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	A	1116	CLA	CHA-C1A-NA	-2.25	121.30	126.39
16	A	1013	CLA	CAA-CBA-CGA	-2.25	106.83	113.21
19	x	603	BCR	C15-C14-C13	-2.25	124.13	127.28
16	B	1234	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
16	y	506	CLA	C3C-C4C-NC	-2.25	107.55	110.43
16	W	505	CLA	CHA-C1A-NA	-2.24	121.31	126.39
19	x	601	BCR	C11-C10-C9	-2.24	124.13	127.28
16	A	1022	CLA	CHD-C1D-ND	-2.24	121.64	124.80
19	s	602	BCR	C24-C23-C22	-2.24	122.92	126.23
16	b	1208	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
19	s	603	BCR	C7-C8-C9	-2.24	122.92	126.23
16	H	1116	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	a	1116	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	u	505	CLA	C3B-C4B-NB	-2.24	108.53	110.53
19	h	603	BCR	C11-C10-C9	-2.24	124.13	127.28
16	h	515	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	r	505	CLA	O2A-CGA-O1A	-2.24	118.02	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	4008	BCR	C33-C5-C6	-2.24	122.04	124.48
16	G	1207	CLA	C1-O2A-CGA	2.24	122.08	116.65
16	b	1235	CLA	C1-C2-C3	-2.24	122.53	126.20
16	H	1123	CLA	C2A-C1A-CHA	2.24	127.76	123.87
16	G	1201	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
16	a	1114	CLA	C3B-C2B-C1B	-2.24	104.53	107.17
16	W	505	CLA	C3B-C4B-NB	-2.24	108.53	110.53
16	u	510	CLA	CHD-C1D-ND	-2.24	121.65	124.80
16	G	1222	CLA	CHD-C1D-ND	-2.24	121.65	124.80
16	r	501	CLA	CHA-C1A-NA	-2.24	121.32	126.39
16	G	1220	CLA	C3B-C4B-NB	-2.24	108.53	110.53
19	J	4013	BCR	C1-C6-C5	-2.24	119.58	122.64
19	l	4022	BCR	C20-C21-C22	-2.24	124.14	127.28
16	n	513	CLA	C1C-C2C-C3C	-2.24	104.63	106.98
16	s	516	CLA	CHD-C1D-ND	-2.24	121.65	124.80
16	g	513	CLA	C4A-NA-C1A	2.24	107.70	106.68
19	q	603	BCR	C15-C16-C17	-2.24	118.94	123.52
16	b	1213	CLA	CHA-C1A-NA	-2.24	121.33	126.39
19	u	602	BCR	C20-C21-C22	-2.24	124.14	127.28
16	A	1801	CLA	CHD-C1D-ND	-2.24	121.66	124.80
14	H	4201	LMG	O3-C3-C2	-2.24	105.10	110.38
19	t	601	BCR	C11-C10-C9	-2.24	124.14	127.28
16	p	503	CLA	C2D-C1D-ND	-2.24	107.91	110.13
21	M	4021	ECH	C2-C1-C6	2.24	113.69	110.44
16	H	1110	CLA	C3B-C4B-NB	-2.24	108.53	110.53
16	A	1107	CLA	CHD-C1D-ND	-2.24	121.66	124.80
16	G	1234	CLA	CHA-C1A-NA	-2.24	121.33	126.39
16	q	510	CLA	C4A-NA-C1A	2.24	107.70	106.68
19	b	4017	BCR	C10-C11-C12	-2.24	116.72	123.20
19	H	4007	BCR	C28-C27-C26	-2.24	110.07	114.06
16	A	1138	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
19	S	4015	BCR	C24-C23-C22	-2.23	122.93	126.23
19	B	4004	BCR	C11-C10-C9	-2.23	124.14	127.28
16	W	513	CLA	C3B-C2B-C1B	-2.23	104.53	107.17
23	Y	606	LMU	C1B-C2B-C3B	2.23	114.71	110.01
16	v	509	CLA	C2D-C1D-ND	-2.23	107.92	110.13
16	G	1214	CLA	CHD-C1D-ND	-2.23	121.66	124.80
16	u	504	CLA	CHD-C1D-ND	-2.23	121.66	124.80
16	w	503	CLA	C2C-C1C-NC	-2.23	107.64	109.98
19	G	4014	BCR	C15-C16-C17	-2.23	118.95	123.52
19	Q	4016	BCR	C15-C16-C17	-2.23	118.95	123.52
19	F	4016	BCR	C7-C8-C9	-2.23	122.93	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	o	508	CLA	CMB-C2B-C1B	2.23	128.82	125.42
16	A	1022	CLA	C4D-C3D-CAD	-2.23	105.68	108.11
16	W	509	CLA	C3B-C4B-NB	-2.23	108.54	110.53
13	R	103	LHG	C27-C26-C25	-2.23	103.08	114.37
16	G	1219	CLA	C2B-C1B-NB	-2.23	108.01	110.33
16	a	1117	CLA	CHD-C1D-C2D	2.23	130.13	125.49
16	b	1211	CLA	CHA-C1A-NA	-2.23	121.34	126.39
16	u	517	CLA	CMB-C2B-C1B	2.23	128.82	125.42
14	a	4201	LMG	O3-C3-C2	-2.23	105.11	110.38
16	r	506	CLA	CMB-C2B-C1B	2.23	128.82	125.42
16	X	508	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	K	4005	BCR	C15-C16-C17	-2.23	118.95	123.52
14	b	848	LMG	O1-C7-C8	-2.23	105.39	110.82
19	b	4005	BCR	C27-C26-C25	2.23	125.72	122.70
19	n	604	BCR	C24-C23-C22	-2.23	122.94	126.23
16	H	1109	CLA	C3B-C2B-C1B	-2.23	104.54	107.17
16	W	510	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
19	Z	602	BCR	C1-C6-C5	-2.23	119.59	122.64
16	U	1503	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
15	A	1011	CL0	C3C-C4C-NC	-2.23	109.20	114.65
16	r	506	CLA	C4A-NA-C1A	2.23	107.70	106.68
13	a	849	LHG	C11-C10-C9	-2.23	103.10	114.37
13	b	4018	LHG	C18-C17-C16	-2.23	103.10	114.37
13	G	4018	LHG	C18-C17-C16	-2.23	103.11	114.37
16	t	513	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	v	603	BCR	C15-C14-C13	-2.23	124.15	127.28
16	o	506	CLA	CHD-C1D-ND	-2.23	121.67	124.80
16	a	1129	CLA	C3B-C2B-C1B	-2.23	104.54	107.17
16	b	1238	CLA	C4A-NA-C1A	2.23	107.69	106.68
16	r	506	CLA	CHD-C1D-ND	-2.23	121.67	124.80
16	W	501	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
16	A	1117	CLA	C3B-C4B-NB	-2.23	108.54	110.53
23	w	605	LMU	C1'-O5'-C5'	2.22	118.06	113.72
16	X	502	CLA	CHA-C1A-NA	-2.22	121.35	126.39
16	h	508	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
16	x	516	CLA	C3B-C4B-NB	-2.22	108.54	110.53
21	B	4006	ECH	C15-C16-C17	2.22	128.07	123.52
14	A	4201	LMG	O3-C3-C2	-2.22	105.13	110.38
16	p	515	CLA	CHA-C1A-NA	-2.22	121.35	126.39
16	a	1128	CLA	CHA-C1A-NA	-2.22	121.36	126.39
16	F	1301	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	h	515	CLA	CHD-C1D-ND	-2.22	121.67	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	s	513	CLA	CMB-C2B-C1B	2.22	128.81	125.42
16	H	1103	CLA	C3B-C2B-C1B	-2.22	104.55	107.17
19	q	603	BCR	C15-C14-C13	-2.22	124.16	127.28
16	q	511	CLA	CHA-C1A-NA	-2.22	121.36	126.39
16	h	516	CLA	CHA-C1A-NA	-2.22	121.36	126.39
16	t	514	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
16	A	1108	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	a	1126	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	v	509	CLA	CHD-C1D-ND	-2.22	121.67	124.80
16	H	1120	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
16	a	1121	CLA	C3B-C4B-NB	-2.22	108.55	110.53
16	s	506	CLA	C3B-C4B-NB	-2.22	108.55	110.53
16	y	516	CLA	CHD-C1D-ND	-2.22	121.68	124.80
16	G	1232	CLA	C2A-C1A-CHA	2.22	127.72	123.87
16	H	1138	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
16	W	511	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
16	A	1140	CLA	C3B-C4B-NB	-2.22	108.55	110.53
16	T	4003	CLA	CHD-C1D-ND	-2.22	121.68	124.80
16	B	1203	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
16	A	1013	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
16	T	4002	CLA	CMB-C2B-C1B	2.22	128.80	125.42
16	l	1501	CLA	C3B-C4B-NB	-2.22	108.55	110.53
23	p	606	LMU	C1'-C2'-C3'	2.22	114.68	110.01
19	G	4017	BCR	C16-C15-C14	-2.22	118.98	123.52
19	S	4013	BCR	C2-C1-C6	2.22	113.66	110.44
16	Y	501	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
19	X	603	BCR	C30-C25-C26	-2.22	119.61	122.64
16	b	1212	CLA	CHA-C1A-NA	-2.22	121.37	126.39
21	R	4020	ECH	C2-C3-C4	-2.22	106.40	111.28
16	Y	505	CLA	C3B-C4B-NB	-2.22	108.55	110.53
16	b	1216	CLA	C3B-C4B-NB	-2.22	108.55	110.53
19	p	603	BCR	C15-C14-C13	-2.22	124.17	127.28
16	n	501	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
16	X	505	CLA	C2A-C1A-CHA	2.22	127.71	123.87
16	u	509	CLA	CHD-C1D-ND	-2.22	121.68	124.80
16	G	1220	CLA	C3B-C2B-C1B	-2.22	104.56	107.17
16	H	1104	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
19	w	603	BCR	C16-C15-C14	-2.22	118.98	123.52
16	W	506	CLA	CHD-C1D-ND	-2.22	121.69	124.80
16	q	501	CLA	CHD-C1D-ND	-2.22	121.69	124.80
16	y	507	CLA	CMB-C2B-C1B	2.22	128.79	125.42
16	v	516	CLA	CHA-C1A-NA	-2.22	121.38	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	S	4012	BCR	C33-C5-C6	-2.22	122.07	124.48
19	G	4014	BCR	C16-C15-C14	-2.21	118.99	123.52
16	X	515	CLA	CHA-C1A-NA	-2.21	121.38	126.39
16	w	507	CLA	CHA-C1A-NA	-2.21	121.38	126.39
16	A	1013	CLA	CAA-C2A-C1A	-2.21	104.72	111.97
16	H	1118	CLA	C3B-C2B-C1B	-2.21	104.56	107.17
16	a	1131	CLA	CHD-C1D-ND	-2.21	121.69	124.80
16	U	1502	CLA	C3B-C4B-NB	-2.21	108.55	110.53
16	s	515	CLA	C3B-C2B-C1B	-2.21	104.56	107.17
16	s	515	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
16	h	502	CLA	CHD-C1D-ND	-2.21	121.69	124.80
16	Y	507	CLA	C3B-C4B-NB	-2.21	108.56	110.53
19	Y	603	BCR	C15-C16-C17	-2.21	119.00	123.52
21	b	4006	ECH	C24-C23-C22	2.21	129.50	126.23
14	A	4101	LMG	O2-C2-C1	-2.21	104.81	110.08
16	x	516	CLA	CHA-C1A-NA	-2.21	121.39	126.39
16	q	507	CLA	C3B-C2B-C1B	-2.21	104.56	107.17
16	H	1120	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
16	G	1206	CLA	CHA-C1A-NA	-2.21	121.39	126.39
19	u	601	BCR	C11-C10-C9	-2.21	124.18	127.28
16	B	1239	CLA	CMB-C2B-C3B	-2.21	121.36	126.55
16	g	506	CLA	C4A-NA-C1A	2.21	107.69	106.68
16	H	1122	CLA	CMB-C2B-C1B	2.21	128.78	125.42
16	Z	505	CLA	C2B-C1B-NB	-2.21	108.03	110.33
19	A	4007	BCR	C1-C6-C5	-2.21	119.62	122.64
19	r	603	BCR	C15-C14-C13	-2.21	124.18	127.28
16	A	1237	CLA	CHA-C1A-NA	-2.21	121.39	126.39
14	G	848	LMG	C38-C37-C36	-2.21	103.20	114.37
16	t	515	CLA	C3B-C2B-C1B	-2.21	104.57	107.17
16	b	1201	CLA	CHD-C1D-ND	-2.21	121.70	124.80
16	u	517	CLA	C3B-C4B-NB	-2.21	108.56	110.53
16	v	514	CLA	CHA-C1A-NA	-2.21	121.39	126.39
16	v	512	CLA	CAA-CBA-CGA	-2.21	106.94	113.21
19	f	4016	BCR	C16-C15-C14	-2.21	119.01	123.52
16	b	1235	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
16	X	503	CLA	CHD-C1D-ND	-2.20	121.70	124.80
16	W	504	CLA	CHA-C1A-NA	-2.20	121.40	126.39
16	Y	505	CLA	CHA-C1A-NA	-2.20	121.40	126.39
16	n	506	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
19	r	603	BCR	C33-C5-C6	-2.20	122.08	124.48
19	o	603	BCR	C30-C25-C26	-2.20	119.62	122.64
13	B	4018	LHG	C18-C17-C16	-2.20	103.23	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	a	1109	CLA	C3B-C4B-NB	-2.20	108.56	110.53
16	Y	508	CLA	CMB-C2B-C1B	2.20	128.77	125.42
16	B	1232	CLA	CHD-C1D-ND	-2.20	121.70	124.80
16	p	517	CLA	CHD-C1D-ND	-2.20	121.70	124.80
19	W	604	BCR	C40-C30-C25	2.20	113.70	110.24
19	s	601	BCR	C33-C5-C6	-2.20	122.08	124.48
16	A	1013	CLA	C4A-NA-C1A	2.20	107.68	106.68
16	B	1220	CLA	C4A-NA-C1A	2.20	107.68	106.68
16	a	1108	CLA	CHA-C1A-NA	-2.20	121.40	126.39
14	B	848	LMG	C38-C37-C36	-2.20	103.23	114.37
16	r	510	CLA	C3B-C2B-C1B	-2.20	104.57	107.17
16	p	501	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	t	505	CLA	C3B-C4B-NB	-2.20	108.56	110.53
19	A	4007	BCR	C29-C30-C25	2.20	113.64	110.44
16	B	1236	CLA	CHA-C1A-NA	-2.20	121.41	126.39
16	X	509	CLA	CHD-C1D-ND	-2.20	121.70	124.80
19	J	4012	BCR	C27-C26-C25	2.20	125.68	122.70
19	x	602	BCR	C24-C23-C22	-2.20	122.98	126.23
16	h	507	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	b	1207	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	t	505	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
16	H	1108	CLA	CHD-C1D-ND	-2.20	121.70	124.80
16	W	515	CLA	CHD-C1D-ND	-2.20	121.70	124.80
16	A	1139	CLA	CHA-C1A-NA	-2.20	121.41	126.39
16	x	507	CLA	C3B-C2B-C1B	-2.20	104.58	107.17
16	s	505	CLA	C2A-C1A-CHA	2.20	127.69	123.87
16	w	507	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	b	4004	BCR	C7-C8-C9	-2.20	122.98	126.23
16	H	1801	CLA	C1C-C2C-C3C	-2.20	104.67	106.98
16	n	508	CLA	C3B-C4B-NB	-2.20	108.57	110.53
16	s	505	CLA	C2D-C1D-ND	-2.20	107.95	110.13
16	b	1214	CLA	CHD-C1D-ND	-2.20	121.71	124.80
16	Y	506	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
16	Y	509	CLA	C3B-C4B-NB	-2.20	108.57	110.53
19	w	602	BCR	C7-C8-C9	-2.20	122.98	126.23
16	B	1217	CLA	C3B-C2B-C1B	-2.20	104.58	107.17
16	y	508	CLA	C3B-C2B-C1B	-2.20	104.58	107.17
16	B	1235	CLA	CHB-C1B-C2B	-2.20	121.05	127.43
16	Z	513	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	Y	601	BCR	C33-C5-C6	-2.20	122.09	124.48
14	A	852	LMG	O2-C2-C1	-2.20	104.84	110.08
19	v	603	BCR	C15-C16-C17	-2.20	119.03	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1229	CLA	C1D-ND-C4D	-2.20	104.77	106.31
16	H	1134	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	a	4007	BCR	C29-C30-C25	2.20	113.63	110.44
16	H	1117	CLA	C1-C2-C3	-2.20	122.60	126.20
16	L	1502	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
19	B	4014	BCR	C30-C25-C26	-2.20	119.64	122.64
16	k	4004	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
19	t	601	BCR	C7-C8-C9	-2.20	122.99	126.23
16	n	516	CLA	CHD-C1D-ND	-2.20	121.71	124.80
16	o	503	CLA	CHA-C1A-NA	-2.20	121.42	126.39
16	A	1120	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
16	q	503	CLA	CMD-C2D-C1D	-2.19	120.86	124.73
16	b	1240	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	v	510	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
16	B	1211	CLA	C3B-C4B-NB	-2.19	108.57	110.53
16	A	1013	CLA	CMD-C2D-C1D	-2.19	120.87	124.73
16	G	1208	CLA	CHA-C1A-NA	-2.19	121.43	126.39
16	n	510	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
16	G	1209	CLA	C3B-C4B-NB	-2.19	108.57	110.53
19	p	601	BCR	C24-C23-C22	-2.19	122.99	126.23
19	l	4022	BCR	C1-C6-C5	-2.19	119.64	122.64
16	b	1225	CLA	CHA-C1A-NA	-2.19	121.43	126.39
16	o	504	CLA	CHA-C1A-NA	-2.19	121.43	126.39
16	t	516	CLA	C3B-C4B-NB	-2.19	108.57	110.53
19	Q	4016	BCR	C15-C14-C13	-2.19	124.21	127.28
16	o	511	CLA	CHA-C1A-NA	-2.19	121.43	126.39
16	J	1303	CLA	C3B-C4B-NB	-2.19	108.58	110.53
16	H	1139	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
19	Z	604	BCR	C15-C14-C13	-2.19	124.21	127.28
16	Z	512	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	Y	511	CLA	C3B-C4B-NB	-2.19	108.58	110.53
16	H	1237	CLA	C1C-C2C-C3C	-2.19	104.68	106.98
16	a	1138	CLA	CMB-C2B-C1B	2.19	128.75	125.42
16	B	1205	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	n	506	CLA	CHD-C1D-ND	-2.19	121.72	124.80
16	s	508	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	h	604	BCR	C30-C25-C26	-2.19	119.65	122.64
16	B	1204	CLA	C3B-C4B-NB	-2.19	108.58	110.53
16	W	508	CLA	C3B-C4B-NB	-2.19	108.58	110.53
16	h	506	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
19	S	4015	BCR	C15-C16-C17	-2.19	119.05	123.52
16	a	1801	CLA	CHA-C1A-NA	-2.19	121.44	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	p	510	CLA	C3B-C2B-C1B	-2.19	104.59	107.17
16	v	515	CLA	C2A-C1A-CHA	2.19	127.66	123.87
16	A	1140	CLA	CHD-C1D-ND	-2.19	121.73	124.80
16	j	1302	CLA	CHD-C1D-ND	-2.19	121.73	124.80
16	x	501	CLA	CHD-C1D-ND	-2.19	121.73	124.80
19	o	601	BCR	C27-C26-C25	2.19	125.66	122.70
16	r	508	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	Y	511	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	q	508	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	B	1218	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
16	h	507	CLA	CMB-C2B-C1B	2.18	128.75	125.42
16	g	508	CLA	C3B-C4B-NB	-2.18	108.58	110.53
16	Z	508	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
19	j	4012	BCR	C24-C23-C22	-2.18	123.00	126.23
19	A	4008	BCR	C7-C8-C9	-2.18	123.00	126.23
16	p	501	CLA	C3B-C4B-NB	-2.18	108.58	110.53
16	Z	514	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
19	s	601	BCR	C7-C8-C9	-2.18	123.01	126.23
16	v	505	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	G	1210	CLA	C3B-C4B-NB	-2.18	108.58	110.53
19	X	601	BCR	C7-C8-C9	-2.18	123.01	126.23
16	n	514	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	n	501	CLA	CHA-C1A-NA	-2.18	121.45	126.39
19	v	604	BCR	C30-C25-C26	-2.18	119.65	122.64
16	W	506	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	v	509	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	a	4101	LMG	O2-C2-C1	-2.18	104.88	110.08
23	r	606	LMU	C4B-C3B-C2B	2.18	114.66	110.83
16	s	510	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	B	1228	CLA	CHA-C1A-NA	-2.18	121.45	126.39
19	Y	601	BCR	C24-C23-C22	-2.18	123.01	126.23
16	G	1229	CLA	C1D-ND-C4D	-2.18	104.78	106.31
14	G	848	LMG	O7-C10-O9	-2.18	118.61	123.70
16	G	1224	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	x	512	CLA	CHD-C1D-ND	-2.18	121.73	124.80
16	p	511	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	X	512	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
16	a	1022	CLA	C2C-C1C-NC	-2.18	107.69	109.98
16	w	514	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
16	A	1121	CLA	CMB-C2B-C1B	2.18	128.74	125.42
16	b	1224	CLA	CHD-C1D-ND	-2.18	121.74	124.80
16	o	514	CLA	CHD-C1D-C2D	2.18	130.02	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1219	CLA	C2D-C1D-ND	-2.18	107.97	110.13
19	S	4013	BCR	C15-C14-C13	-2.18	124.22	127.28
23	q	605	LMU	C1'-O5'-C5'	2.18	117.97	113.72
19	u	602	BCR	C15-C14-C13	-2.18	124.22	127.28
16	W	511	CLA	CHA-C1A-NA	-2.18	121.46	126.39
16	a	1123	CLA	C3B-C2B-C1B	-2.18	104.60	107.17
16	a	1128	CLA	C4B-C3B-C2B	-2.18	104.59	107.30
16	y	506	CLA	CHD-C1D-ND	-2.18	121.74	124.80
16	g	507	CLA	C1-C2-C3	-2.17	122.63	126.20
13	I	103	LHG	C27-C26-C25	-2.17	103.38	114.37
19	l	4019	BCR	C37-C22-C21	-2.17	119.29	122.82
16	p	502	CLA	C1-C2-C3	-2.17	123.24	126.76
16	h	504	CLA	CHA-C1A-NA	-2.17	121.47	126.39
16	h	513	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
16	W	507	CLA	C4A-NA-C1A	2.17	107.67	106.68
19	G	4005	BCR	C15-C14-C13	-2.17	124.23	127.28
19	w	602	BCR	C11-C10-C9	-2.17	124.23	127.28
16	v	515	CLA	CHD-C1D-ND	-2.17	121.74	124.80
16	t	513	CLA	CHA-C1A-NA	-2.17	121.47	126.39
19	Z	604	BCR	C15-C16-C17	-2.17	119.07	123.52
16	a	1140	CLA	C2B-C1B-NB	-2.17	108.07	110.33
16	H	1101	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
16	n	514	CLA	C3B-C4B-NB	-2.17	108.59	110.53
14	A	4201	LMG	O2-C2-C1	-2.17	104.90	110.08
16	p	514	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
19	b	4017	BCR	C30-C25-C26	-2.17	119.67	122.64
16	y	517	CLA	C3B-C4B-NB	-2.17	108.59	110.53
16	p	506	CLA	C1D-ND-C4D	-2.17	104.79	106.31
16	B	1203	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
19	a	4003	BCR	C29-C30-C25	2.17	113.59	110.44
16	u	515	CLA	CHA-C1A-NA	-2.17	121.47	126.39
13	A	849	LHG	C27-C26-C25	-2.17	103.39	114.37
16	B	1208	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
16	r	509	CLA	CHA-C1A-NA	-2.17	121.48	126.39
16	w	501	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	o	517	CLA	C3B-C4B-NB	-2.17	108.59	110.53
16	v	502	CLA	C3B-C4B-NB	-2.17	108.59	110.53
19	o	603	BCR	C7-C8-C9	-2.17	123.03	126.23
16	b	1218	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	q	501	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	G	1205	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
16	A	1128	CLA	O2A-CGA-O1A	-2.17	118.20	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	4011	BCR	C10-C11-C12	-2.17	116.92	123.20
16	h	506	CLA	CHA-C1A-NA	-2.17	121.48	126.39
16	b	1207	CLA	CHD-C1D-ND	-2.17	121.75	124.80
16	a	1022	CLA	C4A-NA-C1A	2.17	107.67	106.68
16	s	502	CLA	C3B-C4B-NB	-2.17	108.59	110.53
16	x	507	CLA	C1-C2-C3	-2.17	122.65	126.20
19	A	4008	BCR	C24-C23-C22	-2.17	123.03	126.23
19	W	604	BCR	C11-C10-C9	-2.17	124.24	127.28
16	B	1021	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
16	s	511	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
16	g	515	CLA	C3B-C2B-C1B	-2.17	104.61	107.17
14	F	4017	LMG	O2-C2-C1	-2.17	104.91	110.08
19	f	4016	BCR	C40-C30-C25	2.17	113.64	110.24
16	W	516	CLA	CHD-C1D-ND	-2.17	121.75	124.80
16	a	1140	CLA	CHD-C1D-ND	-2.17	121.75	124.80
16	y	513	CLA	C3B-C4B-NB	-2.17	108.60	110.53
16	X	511	CLA	CHA-C1A-NA	-2.17	121.49	126.39
16	o	505	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
16	w	516	CLA	CHA-C1A-NA	-2.16	121.49	126.39
16	s	506	CLA	C2D-C1D-ND	-2.16	107.98	110.13
16	s	504	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
19	o	603	BCR	C11-C10-C9	-2.16	124.24	127.28
16	s	514	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
19	y	604	BCR	C16-C15-C14	-2.16	119.09	123.52
16	h	511	CLA	CHA-C1A-NA	-2.16	121.49	126.39
16	v	510	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	b	1205	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	A	1115	CLA	C2A-C1A-CHA	2.16	127.62	123.87
14	Q	4017	LMG	O2-C2-C1	-2.16	104.92	110.08
16	l	1501	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	y	516	CLA	CHD-C1D-C2D	2.16	129.99	125.49
16	G	1226	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	G	1012	CLA	C1-C2-C3	-2.16	122.66	126.20
16	b	1012	CLA	C1-C2-C3	-2.16	122.66	126.20
19	X	602	BCR	C20-C21-C22	-2.16	124.25	127.28
16	h	517	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
19	Z	604	BCR	C33-C5-C6	-2.16	122.13	124.48
21	m	4021	ECH	C19-C18-C17	2.16	122.41	119.01
16	a	1104	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	B	1226	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	Z	501	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
16	x	515	CLA	O2A-CGA-O1A	-2.16	118.22	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	1107	CLA	C1-C2-C3	-2.16	123.27	126.76
16	a	1120	CLA	C1C-C2C-C3C	-2.16	104.71	106.98
16	o	503	CLA	CHD-C1D-ND	-2.16	121.76	124.80
16	X	510	CLA	C3B-C4B-NB	-2.16	108.60	110.53
16	X	515	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	j	4013	BCR	C2-C1-C6	2.16	113.58	110.44
16	H	1121	CLA	CMB-C2B-C1B	2.16	128.71	125.42
19	H	4003	BCR	C15-C16-C17	-2.16	119.10	123.52
16	h	509	CLA	CHA-C1A-NA	-2.16	121.50	126.39
19	x	604	BCR	C11-C10-C9	-2.16	124.25	127.28
21	I	4020	ECH	C2-C3-C4	-2.16	106.53	111.28
16	y	503	CLA	CHA-C1A-NA	-2.16	121.50	126.39
16	Z	502	CLA	CHD-C1D-ND	-2.16	121.77	124.80
14	Q	4017	LMG	O3-C3-C2	-2.16	105.29	110.38
16	t	510	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
19	W	604	BCR	C30-C25-C26	-2.16	119.69	122.64
19	w	604	BCR	C33-C5-C6	-2.16	122.13	124.48
16	a	1128	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
16	g	505	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
16	a	1109	CLA	CHA-C1A-NA	-2.16	121.51	126.39
16	s	506	CLA	CHA-C1A-NA	-2.16	121.51	126.39
16	t	506	CLA	CHA-C1A-NA	-2.16	121.51	126.39
16	y	501	CLA	CHA-C1A-NA	-2.16	121.51	126.39
16	p	515	CLA	C3B-C2B-C1B	-2.16	104.63	107.17
16	y	509	CLA	CHD-C1D-ND	-2.16	121.77	124.80
16	G	1239	CLA	CHA-C1A-NA	-2.16	121.51	126.39
19	o	604	BCR	C2-C1-C6	2.16	113.57	110.44
16	s	501	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
16	u	502	CLA	CHD-C1D-ND	-2.15	121.77	124.80
16	H	1107	CLA	C4A-NA-C1A	2.15	107.66	106.68
16	b	1214	CLA	CHA-C1A-NA	-2.15	121.51	126.39
19	G	4005	BCR	C30-C25-C26	-2.15	119.69	122.64
16	a	1121	CLA	CMB-C2B-C1B	2.15	128.70	125.42
16	Y	503	CLA	C3B-C2B-C1B	-2.15	104.63	107.17
19	f	4016	BCR	C15-C16-C17	-2.15	119.11	123.52
13	i	103	LHG	C27-C26-C25	-2.15	103.48	114.37
16	g	514	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
19	u	604	BCR	C27-C26-C25	2.15	125.61	122.70
16	Y	510	CLA	CHD-C1D-ND	-2.15	121.77	124.80
16	A	1137	CLA	C3B-C2B-C1B	-2.15	104.63	107.17
16	X	501	CLA	C3B-C2B-C1B	-2.15	104.63	107.17
16	l	1502	CLA	O2A-CGA-O1A	-2.15	118.24	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	517	CLA	C3B-C4B-NB	-2.15	108.61	110.53
19	b	4014	BCR	C16-C15-C14	-2.15	119.11	123.52
16	h	505	CLA	C2A-C1A-CHA	2.15	127.60	123.87
16	G	1238	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
16	H	1237	CLA	CHA-C1A-NA	-2.15	121.52	126.39
19	A	4002	BCR	C15-C16-C17	-2.15	119.11	123.52
19	T	4005	BCR	C24-C23-C22	-2.15	123.05	126.23
16	A	1110	CLA	C3B-C4B-NB	-2.15	108.61	110.53
16	s	512	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
19	j	4015	BCR	C7-C8-C9	-2.15	123.05	126.23
16	W	505	CLA	C3C-C4C-NC	-2.15	107.67	110.43
16	X	504	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	Y	512	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	p	513	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	a	1013	CLA	C3A-C2A-C1A	-2.15	98.12	101.34
16	B	1225	CLA	CHA-C1A-NA	-2.15	121.52	126.39
19	v	604	BCR	C15-C16-C17	-2.15	119.12	123.52
16	B	1240	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	a	1113	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	a	1110	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
16	B	1207	CLA	C1-O2A-CGA	2.15	121.86	116.65
16	g	501	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	x	516	CLA	C3B-C2B-C1B	-2.15	104.64	107.17
16	h	510	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
16	q	507	CLA	CMB-C2B-C1B	2.15	128.69	125.42
16	n	505	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
19	o	604	BCR	C40-C30-C25	2.15	113.61	110.24
16	w	517	CLA	CMB-C2B-C1B	2.15	128.69	125.42
16	a	1237	CLA	CHA-C1A-NA	-2.15	121.53	126.39
21	i	4020	ECH	C2-C1-C6	2.15	113.56	110.44
16	Y	506	CLA	C3B-C4B-NB	-2.15	108.61	110.53
16	b	1206	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	a	1133	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
16	b	1216	CLA	C4B-C3B-C2B	-2.15	104.63	107.30
16	Z	502	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	A	1102	CLA	C3B-C2B-C1B	-2.15	104.64	107.17
16	Z	503	CLA	C3B-C2B-C1B	-2.15	104.64	107.17
19	F	4016	BCR	C15-C14-C13	-2.15	124.27	127.28
19	h	604	BCR	C1-C6-C5	-2.15	119.70	122.64
16	l	1503	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	o	506	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	n	506	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	h	514	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
16	h	511	CLA	C4A-NA-C1A	2.15	107.66	106.68
16	G	1219	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	H	1140	CLA	CMB-C2B-C1B	2.15	128.69	125.42
16	G	1223	CLA	C7-C6-C5	-2.15	107.54	113.26
16	B	1208	CLA	CHA-C1A-NA	-2.15	121.53	126.39
16	b	1234	CLA	CHB-C1B-C2B	-2.15	121.20	127.43
15	a	1011	CL0	C3C-C4C-NC	-2.14	109.41	114.65
16	a	1118	CLA	C3B-C4B-NB	-2.14	108.62	110.53
16	Y	512	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	q	514	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	B	1023	CLA	C4D-C3D-CAD	-2.14	105.78	108.11
16	b	1021	CLA	C2A-C1A-CHA	2.14	127.59	123.87
16	h	513	CLA	C3B-C4B-NB	-2.14	108.62	110.53
16	r	516	CLA	C3B-C4B-NB	-2.14	108.62	110.53
16	U	1502	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	y	512	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	a	4002	BCR	C15-C16-C17	-2.14	119.14	123.52
16	v	504	CLA	C2D-C1D-ND	-2.14	108.01	110.13
16	G	1207	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
16	b	1012	CLA	C2A-C1A-CHA	2.14	127.58	123.87
16	t	508	CLA	CMB-C2B-C1B	2.14	128.68	125.42
19	u	601	BCR	C1-C6-C5	-2.14	119.71	122.64
21	b	4006	ECH	C1-C6-C5	-2.14	119.71	122.64
16	u	506	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
16	X	502	CLA	CHD-C1D-ND	-2.14	121.79	124.80
20	L	4101	LMT	C3B-C4B-C5B	-2.14	106.35	110.23
16	y	508	CLA	CHD-C1D-ND	-2.14	121.79	124.80
16	K	4004	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	Y	514	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	t	512	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	b	1234	CLA	C4A-NA-C1A	2.14	107.66	106.68
16	A	1112	CLA	O2A-CGA-O1A	-2.14	117.83	123.33
19	u	604	BCR	C1-C6-C5	-2.14	119.71	122.64
16	b	1215	CLA	CHA-C1A-NA	-2.14	121.55	126.39
16	H	1128	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
16	v	506	CLA	CHD-C1D-ND	-2.14	121.79	124.80
19	q	604	BCR	C33-C5-C6	-2.14	122.15	124.48
16	u	515	CLA	CHD-C1D-ND	-2.14	121.80	124.80
16	Y	503	CLA	C4D-C3D-CAD	-2.14	105.78	108.11
16	A	1013	CLA	CHA-C1A-NA	-2.14	121.55	126.39
16	B	1222	CLA	CHD-C1D-ND	-2.14	121.80	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	501	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
19	n	603	BCR	C11-C10-C9	-2.14	124.28	127.28
14	a	4101	LMG	O3-C3-C2	-2.14	105.34	110.38
16	X	512	CLA	C2A-C1A-CHA	2.14	127.57	123.87
19	u	601	BCR	C28-C27-C26	-2.14	110.25	114.06
16	b	1211	CLA	C3B-C4B-NB	-2.14	108.62	110.53
16	A	1104	CLA	C4A-NA-C1A	2.13	107.65	106.68
16	x	504	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
16	p	513	CLA	C1C-C2C-C3C	-2.13	104.73	106.98
16	l	1503	CLA	CHD-C1D-ND	-2.13	121.80	124.80
16	G	1012	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
16	t	501	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
19	H	4002	BCR	C16-C15-C14	-2.13	119.15	123.52
19	x	602	BCR	C7-C8-C9	-2.13	123.08	126.23
16	n	501	CLA	C1C-C2C-C3C	-2.13	104.74	106.98
21	B	4006	ECH	O27-C27-C26	2.13	122.89	120.98
16	A	1105	CLA	CHA-C1A-NA	-2.13	121.56	126.39
13	H	849	LHG	C27-C26-C25	-2.13	103.59	114.37
16	g	504	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	r	515	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
19	s	603	BCR	C11-C10-C9	-2.13	124.29	127.28
16	Y	516	CLA	CMB-C2B-C1B	2.13	128.66	125.42
16	y	512	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	H	1137	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	X	506	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
19	u	602	BCR	C28-C27-C26	-2.13	110.26	114.06
16	L	1501	CLA	C3B-C4B-NB	-2.13	108.63	110.53
16	b	1229	CLA	C4A-NA-C1A	2.13	107.65	106.68
16	y	510	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
16	a	1105	CLA	CHA-C1A-NA	-2.13	121.57	126.39
16	p	501	CLA	CHA-C1A-NA	-2.13	121.57	126.39
16	u	510	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	G	1209	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	t	501	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	G	1023	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
16	g	513	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
16	u	507	CLA	CMB-C2B-C1B	2.13	128.66	125.42
16	g	515	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
16	H	1116	CLA	C3B-C4B-NB	-2.13	108.63	110.53
16	b	1239	CLA	C3B-C4B-NB	-2.13	108.63	110.53
16	Y	508	CLA	C4A-NA-C1A	2.13	107.65	106.68
19	n	601	BCR	C15-C16-C17	-2.13	119.17	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	506	CLA	C3B-C2B-C1B	-2.13	104.66	107.17
16	n	514	CLA	CHD-C1D-C2D	2.13	129.91	125.49
16	o	515	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
16	q	505	CLA	CHA-C1A-NA	-2.13	121.57	126.39
16	B	1206	CLA	CHD-C1D-ND	-2.13	121.81	124.80
19	U	4022	BCR	C20-C21-C22	-2.13	124.30	127.28
16	G	1202	CLA	CHA-C1A-NA	-2.13	121.58	126.39
16	B	1225	CLA	C3B-C4B-NB	-2.13	108.63	110.53
24	q	601	LUT	C7-C8-C9	-2.13	123.09	126.23
16	a	1118	CLA	CHD-C1D-ND	-2.13	121.81	124.80
16	B	1232	CLA	C2A-C1A-CHA	2.13	127.56	123.87
19	w	603	BCR	C10-C11-C12	-2.13	117.04	123.20
16	H	1105	CLA	CHD-C1D-C2D	2.13	129.91	125.49
16	a	1022	CLA	CAA-CBA-CGA	-2.13	107.17	113.21
16	v	508	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
19	T	4005	BCR	C16-C15-C14	-2.12	119.17	123.52
16	h	512	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
19	Y	603	BCR	C16-C15-C14	-2.12	119.17	123.52
16	w	513	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
16	A	1140	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
16	b	1218	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
16	n	504	CLA	CHD-C1D-ND	-2.12	121.81	124.80
16	G	1231	CLA	CMB-C2B-C1B	2.12	128.65	125.42
19	Y	601	BCR	C7-C8-C9	-2.12	123.09	126.23
16	a	1022	CLA	CHD-C1D-ND	-2.12	121.81	124.80
16	v	515	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
16	y	504	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
16	H	1112	CLA	O2A-CGA-O1A	-2.12	117.87	123.33
16	H	1128	CLA	CHA-C1A-NA	-2.12	121.58	126.39
16	x	501	CLA	CHA-C1A-NA	-2.12	121.58	126.39
16	A	1118	CLA	C3B-C4B-NB	-2.12	108.64	110.53
19	J	4012	BCR	C24-C23-C22	-2.12	123.09	126.23
19	r	604	BCR	C7-C8-C9	-2.12	123.09	126.23
14	F	4017	LMG	O3-C3-C2	-2.12	105.37	110.38
16	f	1301	CLA	CHD-C1D-ND	-2.12	121.82	124.80
14	f	4017	LMG	O2-C2-C1	-2.12	105.02	110.08
16	n	515	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
16	B	1224	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	o	509	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	b	1021	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	K	4001	BCR	C30-C25-C26	-2.12	119.74	122.64
16	A	1124	CLA	C1C-C2C-C3C	-2.12	104.75	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	s	606	LMU	C1'-C2'-C3'	2.12	114.47	110.01
16	B	1204	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
16	A	1139	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
16	B	1238	CLA	CHB-C1B-C2B	-2.12	121.27	127.43
16	a	1134	CLA	C3B-C4B-NB	-2.12	108.64	110.53
19	Y	604	BCR	C24-C23-C22	-2.12	123.10	126.23
19	Q	4016	BCR	C16-C15-C14	-2.12	119.18	123.52
16	w	510	CLA	CHD-C1D-ND	-2.12	121.82	124.80
19	r	603	BCR	C30-C25-C26	-2.12	119.74	122.64
16	a	1116	CLA	CHA-C1A-NA	-2.12	121.59	126.39
16	v	508	CLA	CHA-C1A-NA	-2.12	121.59	126.39
16	v	513	CLA	C4A-NA-C1A	2.12	107.65	106.68
16	H	1013	CLA	CAA-CBA-CGA	-2.12	107.19	113.21
16	q	503	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	A	1120	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	q	506	CLA	CMB-C2B-C1B	2.12	128.65	125.42
16	Z	513	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
15	H	1011	CL0	C3C-C4C-NC	-2.12	109.47	114.65
19	k	4005	BCR	C16-C15-C14	-2.12	119.19	123.52
16	b	1239	CLA	C3C-C4C-NC	-2.12	107.72	110.43
19	F	4016	BCR	C16-C15-C14	-2.12	119.19	123.52
16	Z	506	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	x	502	CLA	CHD-C1D-ND	-2.12	121.82	124.80
16	H	1801	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	v	515	CLA	CHA-C1A-NA	-2.12	121.60	126.39
16	Y	507	CLA	C1-C2-C3	-2.12	122.73	126.20
16	q	505	CLA	C1-C2-C3	-2.12	122.73	126.20
14	A	4101	LMG	O3-C3-C2	-2.12	105.39	110.38
16	X	517	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
16	A	1107	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
16	g	505	CLA	C3B-C2B-C1B	-2.12	104.67	107.17
19	X	603	BCR	C15-C16-C17	-2.12	119.19	123.52
16	p	504	CLA	CHD-C1D-ND	-2.12	121.83	124.80
16	W	515	CLA	C3B-C2B-C1B	-2.12	104.68	107.17
16	B	1211	CLA	CMB-C2B-C1B	2.11	128.64	125.42
16	Y	506	CLA	CHA-C1A-NA	-2.11	121.60	126.39
19	J	4015	BCR	C24-C23-C22	-2.11	123.11	126.23
16	B	1217	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	H	1131	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	s	505	CLA	CHA-C1A-NA	-2.11	121.60	126.39
16	x	510	CLA	C3B-C4B-NB	-2.11	108.64	110.53
19	W	601	BCR	C24-C23-C22	-2.11	123.11	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	x	508	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
16	B	1210	CLA	C3B-C2B-C1B	-2.11	104.68	107.17
16	A	1138	CLA	C1-C2-C3	-2.11	122.73	126.20
19	k	4005	BCR	C3-C4-C5	-2.11	110.29	114.06
16	s	514	CLA	C3B-C4B-NB	-2.11	108.64	110.53
16	w	503	CLA	C4B-C3B-C2B	-2.11	104.67	107.30
19	S	4015	BCR	C1-C6-C5	-2.11	119.75	122.64
19	U	4022	BCR	C1-C6-C5	-2.11	119.75	122.64
19	H	4002	BCR	C16-C17-C18	-2.11	124.32	127.28
19	A	4003	BCR	C38-C26-C27	-2.11	109.09	113.60
16	X	501	CLA	CHA-C1A-NA	-2.11	121.61	126.39
16	v	510	CLA	C3B-C4B-NB	-2.11	108.64	110.53
19	X	602	BCR	C27-C26-C25	2.11	125.56	122.70
16	Y	505	CLA	C1-C2-C3	-2.11	122.74	126.20
16	g	513	CLA	CHA-C1A-NA	-2.11	121.61	126.39
16	A	1132	CLA	C2B-C1B-NB	-2.11	108.14	110.33
16	H	1128	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	f	1302	CLA	C3B-C2B-C1B	-2.11	104.68	107.17
16	H	1116	CLA	CHA-C1A-NA	-2.11	121.61	126.39
16	b	1234	CLA	C1-C2-C3	-2.11	123.35	126.76
19	v	604	BCR	C1-C6-C5	-2.11	119.75	122.64
19	u	604	BCR	C40-C30-C25	2.11	113.55	110.24
16	A	1801	CLA	C3B-C4B-NB	-2.11	108.65	110.53
16	h	506	CLA	C3C-C4C-NC	-2.11	107.73	110.43
16	b	1227	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
16	a	1120	CLA	CHD-C1D-ND	-2.11	121.83	124.80
16	t	509	CLA	C7-C6-C5	-2.11	107.64	113.26
16	B	1231	CLA	C3B-C4B-NB	-2.11	108.65	110.53
16	x	515	CLA	C3B-C4B-NB	-2.11	108.65	110.53
16	p	504	CLA	C1-C2-C3	-2.11	122.74	126.20
16	x	514	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
14	H	4101	LMG	O3-C3-C2	-2.11	105.41	110.38
21	R	4020	ECH	C32-C1-C6	-2.11	106.94	110.24
16	B	1215	CLA	CHA-C1A-NA	-2.11	121.62	126.39
16	a	1105	CLA	CHD-C1D-C2D	2.11	129.87	125.49
16	v	505	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
19	H	4011	BCR	C29-C30-C25	2.11	113.50	110.44
16	o	508	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
16	H	1237	CLA	CMB-C2B-C3B	-2.11	121.60	126.55
16	A	1114	CLA	C4D-CHA-C1A	-2.11	118.73	121.24
16	y	510	CLA	C3B-C4B-NB	-2.11	108.65	110.53
13	a	849	LHG	C27-C26-C25	-2.11	103.72	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	1117	CLA	CHD-C1D-C2D	2.10	129.87	125.49
16	A	1104	CLA	C11-C12-C13	-2.10	108.97	115.97
16	u	517	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
19	n	601	BCR	C28-C27-C26	-2.10	110.30	114.06
16	h	513	CLA	CHA-C1A-NA	-2.10	121.63	126.39
16	B	1206	CLA	C4A-NA-C1A	2.10	107.64	106.68
16	A	1110	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
16	r	515	CLA	O2A-CGA-O1A	-2.10	118.36	123.63
19	g	603	BCR	C16-C15-C14	-2.10	119.21	123.52
16	W	506	CLA	CHA-C1A-NA	-2.10	121.63	126.39
16	v	517	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	Z	513	CLA	CMB-C2B-C1B	2.10	128.62	125.42
16	s	501	CLA	CMB-C2B-C1B	2.10	128.62	125.42
16	A	1137	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
23	w	605	LMU	C4B-C3B-C2B	2.10	114.52	110.83
16	B	1236	CLA	CHD-C1D-ND	-2.10	121.84	124.80
16	r	503	CLA	C2B-C1B-NB	-2.10	108.15	110.33
16	g	506	CLA	CHA-C1A-NA	-2.10	121.63	126.39
16	l	1503	CLA	C4A-NA-C1A	2.10	107.64	106.68
16	X	508	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	W	509	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
16	A	1104	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
16	s	507	CLA	CHD-C1D-ND	-2.10	121.84	124.80
16	G	1230	CLA	C3B-C4B-NB	-2.10	108.65	110.53
15	a	1011	CL0	C3D-C4D-CHA	2.10	111.73	108.54
16	X	505	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
19	u	603	BCR	C7-C8-C9	-2.10	123.13	126.23
19	x	602	BCR	C11-C10-C9	-2.10	124.33	127.28
16	y	503	CLA	C3C-C4C-NC	-2.10	107.74	110.43
16	a	1137	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
19	j	4015	BCR	C30-C25-C26	-2.10	119.77	122.64
16	H	1133	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	W	508	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	a	1139	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	t	510	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	Z	502	CLA	CMB-C2B-C1B	2.10	128.61	125.42
16	G	1202	CLA	C3B-C4B-NB	-2.10	108.66	110.53
16	Z	507	CLA	C3B-C4B-NB	-2.10	108.66	110.53
19	T	4005	BCR	C15-C16-C17	-2.10	119.23	123.52
16	G	1203	CLA	C3B-C2B-C1B	-2.10	104.70	107.17
16	x	506	CLA	CHA-C1A-NA	-2.10	121.64	126.39
16	G	1021	CLA	C2A-C1A-CHA	2.10	127.51	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1222	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	H	1126	CLA	CHA-C1A-NA	-2.10	121.64	126.39
16	w	502	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	W	505	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	H	1122	CLA	C3B-C2B-C1B	-2.10	104.70	107.17
16	G	1208	CLA	O2A-CGA-O1A	-2.10	117.94	123.33
16	r	510	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
16	A	1022	CLA	CAA-CBA-CGA	-2.10	107.26	113.21
16	b	1226	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
19	Y	604	BCR	C33-C5-C6	-2.10	122.20	124.48
19	x	602	BCR	C33-C5-C6	-2.10	122.20	124.48
16	G	1206	CLA	C3B-C4B-NB	-2.10	108.66	110.53
16	H	1013	CLA	CHA-C1A-NA	-2.10	121.64	126.39
16	g	510	CLA	O2A-CGA-O1A	-2.10	118.39	123.63
13	s	605	LHG	C27-C26-C25	-2.10	103.78	114.37
19	b	4009	BCR	C30-C25-C26	-2.09	119.77	122.64
16	A	1130	CLA	C3B-C4B-NB	-2.09	108.66	110.53
16	a	1126	CLA	CHA-C1A-NA	-2.09	121.65	126.39
16	b	1012	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
16	w	504	CLA	CHA-C1A-NA	-2.09	121.65	126.39
16	y	508	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
16	G	1213	CLA	CHA-C1A-NA	-2.09	121.65	126.39
16	b	1012	CLA	CHA-C1A-NA	-2.09	121.65	126.39
16	y	508	CLA	C3B-C4B-NB	-2.09	108.66	110.53
19	r	601	BCR	C7-C8-C9	-2.09	123.14	126.23
19	b	4005	BCR	C30-C25-C26	-2.09	119.78	122.64
16	g	510	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	u	506	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
16	Y	502	CLA	C3B-C4B-NB	-2.09	108.66	110.53
16	q	505	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
19	S	4015	BCR	C7-C8-C9	-2.09	123.14	126.23
21	G	4006	ECH	C2-C1-C6	2.09	113.48	110.44
19	K	4005	BCR	C11-C10-C9	-2.09	124.35	127.28
23	g	606	LMU	C4B-C3B-C2B	2.09	114.50	110.83
16	G	1212	CLA	CHA-C1A-NA	-2.09	121.66	126.39
16	B	1213	CLA	CHD-C1D-C2D	2.09	129.84	125.49
16	a	1117	CLA	C1-C2-C3	-2.09	122.77	126.20
16	H	1237	CLA	CHD-C1D-ND	-2.09	121.86	124.80
24	q	601	LUT	C11-C10-C9	2.09	130.21	127.28
16	B	1227	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
16	B	1205	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
16	t	506	CLA	O2A-CGA-O1A	-2.09	118.40	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	1137	CLA	CHA-C1A-NA	-2.09	121.66	126.39
16	u	505	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
13	i	103	LHG	C5-O7-C7	-2.09	112.80	117.80
16	h	503	CLA	C2B-C1B-NB	-2.09	108.16	110.33
16	w	505	CLA	CHA-C1A-NA	-2.09	121.66	126.39
19	J	4012	BCR	C30-C25-C26	-2.09	119.78	122.64
19	w	602	BCR	C30-C25-C26	-2.09	119.78	122.64
16	X	513	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	Y	513	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	v	512	CLA	CHD-C1D-ND	-2.09	121.86	124.80
16	b	1228	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
16	H	1106	CLA	CHA-C1A-NA	-2.09	121.66	126.39
16	W	512	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	r	516	CLA	CHA-C1A-NA	-2.09	121.67	126.39
16	B	1223	CLA	C3B-C4B-NB	-2.09	108.67	110.53
19	i	4018	BCR	C30-C25-C26	-2.09	119.78	122.64
19	j	4015	BCR	C2-C1-C6	2.09	113.47	110.44
16	o	503	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
16	G	1021	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	B	1229	CLA	C3B-C2B-C1B	-2.09	104.71	107.17
16	y	514	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
16	a	1109	CLA	CMB-C2B-C1B	2.08	128.59	125.42
16	W	517	CLA	C3B-C2B-C1B	-2.08	104.71	107.17
16	u	507	CLA	C3B-C2B-C1B	-2.08	104.71	107.17
19	g	601	BCR	C1-C6-C5	-2.08	119.79	122.64
16	u	510	CLA	C3B-C4B-NB	-2.08	108.67	110.53
16	o	502	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	H	1140	CLA	CHD-C1D-ND	-2.08	121.87	124.80
16	n	513	CLA	C4A-NA-C1A	2.08	107.63	106.68
19	o	604	BCR	C11-C10-C9	-2.08	124.36	127.28
16	a	1130	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	A	1101	CLA	C11-C10-C8	-2.08	109.05	115.97
16	v	507	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	Y	510	CLA	C3B-C4B-NB	-2.08	108.67	110.53
16	B	1220	CLA	CHA-C1A-NA	-2.08	121.68	126.39
16	Y	502	CLA	CHA-C1A-NA	-2.08	121.68	126.39
16	G	1223	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
16	k	4004	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
19	A	4008	BCR	C29-C30-C25	2.08	113.46	110.44
16	r	506	CLA	C1C-C2C-C3C	-2.08	104.79	106.98
16	g	504	CLA	C3B-C4B-NB	-2.08	108.67	110.53
19	o	604	BCR	C30-C25-C26	-2.08	119.79	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Z	501	CLA	C4A-NA-C1A	2.08	107.63	106.68
16	w	511	CLA	CHA-C1A-NA	-2.08	121.68	126.39
16	G	1239	CLA	C3C-C4C-NC	-2.08	107.77	110.43
19	y	603	BCR	C16-C15-C14	-2.08	119.26	123.52
16	A	1122	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	h	603	BCR	C1-C6-C5	-2.08	119.79	122.64
16	H	1114	CLA	CHD-C1D-C2D	2.08	129.81	125.49
16	w	502	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
16	A	1124	CLA	C3B-C4B-NB	-2.08	108.67	110.53
16	g	510	CLA	C3B-C4B-NB	-2.08	108.67	110.53
16	Y	510	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	H	1131	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	G	4004	BCR	C7-C8-C9	-2.08	123.16	126.23
16	T	4004	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
16	X	515	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	W	514	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	r	507	CLA	C1-C2-C3	-2.08	122.79	126.20
16	H	1110	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
16	H	1135	CLA	CHC-C4B-NB	2.08	127.16	124.05
16	p	510	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
19	S	4012	BCR	C15-C14-C13	-2.08	124.37	127.28
19	o	602	BCR	C11-C10-C9	-2.08	124.37	127.28
16	G	1204	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
16	Y	512	CLA	CHA-C4D-ND	2.08	136.83	132.55
16	n	506	CLA	CHA-C1A-NA	-2.08	121.69	126.39
16	B	1219	CLA	O2A-CGA-O1A	-2.08	117.99	123.33
19	g	601	BCR	C7-C8-C9	-2.08	123.16	126.23
14	a	852	LMG	O2-C2-C1	-2.08	105.13	110.08
16	L	1503	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
19	o	602	BCR	C28-C27-C26	-2.08	110.36	114.06
16	w	506	CLA	C3B-C2B-C1B	-2.08	104.72	107.17
19	I	4018	BCR	C30-C25-C26	-2.08	119.80	122.64
16	B	1222	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
19	y	604	BCR	C24-C23-C22	-2.07	123.17	126.23
16	G	1219	CLA	O2A-CGA-O1A	-2.07	118.00	123.33
19	x	602	BCR	C27-C26-C25	2.07	125.51	122.70
16	b	1219	CLA	O2A-CGA-O1A	-2.07	118.00	123.33
16	H	1022	CLA	CAA-CBA-CGA	-2.07	107.32	113.21
16	x	510	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
16	w	507	CLA	CMB-C2B-C1B	2.07	128.57	125.42
19	Y	602	BCR	C24-C23-C22	-2.07	123.17	126.23
16	a	1121	CLA	CHA-C1A-NA	-2.07	121.70	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1210	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	o	502	CLA	C3B-C4B-NB	-2.07	108.68	110.53
16	h	501	CLA	CHA-C1A-NA	-2.07	121.70	126.39
19	G	4010	BCR	C8-C7-C6	-2.07	121.46	127.00
19	g	602	BCR	C33-C5-C6	-2.07	122.22	124.48
16	G	1021	CLA	CHD-C1D-ND	-2.07	121.89	124.80
19	Y	604	BCR	C15-C16-C17	-2.07	119.28	123.52
16	W	506	CLA	CMB-C2B-C1B	2.07	128.57	125.42
16	w	506	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	p	507	CLA	C1-C2-C3	-2.07	122.81	126.20
21	B	4006	ECH	C37-C22-C21	-2.07	119.46	122.82
14	B	848	LMG	O7-C10-O9	-2.07	118.86	123.70
16	w	509	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
16	v	504	CLA	CHA-C1A-NA	-2.07	121.70	126.39
16	b	1238	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
16	b	1203	CLA	C4-C3-C5	2.07	118.82	115.23
16	a	1105	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
14	f	4017	LMG	O3-C3-C2	-2.07	105.50	110.38
16	g	513	CLA	CHD-C1D-ND	-2.07	121.89	124.80
16	A	1131	CLA	CHA-C1A-NA	-2.07	121.71	126.39
16	H	1104	CLA	CHA-C4D-ND	2.07	136.82	132.55
16	v	506	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
20	L	4101	LMT	O5B-C1B-C2B	2.07	114.62	110.37
16	A	1116	CLA	C4D-C3D-CAD	-2.07	105.86	108.11
16	A	1801	CLA	C1C-C2C-C3C	-2.07	104.81	106.98
16	s	506	CLA	CMD-C2D-C1D	-2.07	121.09	124.73
16	w	514	CLA	C4A-NA-C1A	2.07	107.62	106.68
16	H	1107	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
16	w	505	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	B	1208	CLA	O2A-CGA-O1A	-2.07	118.02	123.33
16	p	517	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
16	G	1235	CLA	CHD-C1D-C2D	2.07	129.78	125.49
19	X	603	BCR	C15-C14-C13	-2.07	124.38	127.28
16	w	513	CLA	C2B-C1B-NB	-2.07	108.18	110.33
16	A	1130	CLA	C1-C2-C3	-2.07	122.81	126.20
16	Z	510	CLA	C3B-C2B-C1B	-2.06	104.73	107.17
16	x	512	CLA	C3B-C2B-C1B	-2.06	104.73	107.17
19	B	4017	BCR	C16-C17-C18	-2.06	124.38	127.28
23	q	605	LMU	C4B-C3B-C2B	2.06	114.45	110.83
16	q	515	CLA	CMB-C2B-C1B	2.06	128.56	125.42
19	u	601	BCR	C27-C26-C25	2.06	125.49	122.70
19	G	4009	BCR	C21-C20-C19	-2.06	117.22	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	X	511	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
21	B	4006	ECH	C24-C23-C22	2.06	129.29	126.23
16	X	507	CLA	C1-C2-C3	-2.06	122.81	126.20
16	g	505	CLA	C1-C2-C3	-2.06	122.81	126.20
19	y	604	BCR	C30-C25-C26	-2.06	119.81	122.64
16	H	1107	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	u	501	CLA	CHD-C1D-ND	-2.06	121.90	124.80
16	T	4002	CLA	O2A-CGA-O1A	-2.06	118.02	123.33
16	a	1237	CLA	CMB-C2B-C3B	-2.06	121.70	126.55
16	G	1214	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
19	n	601	BCR	C29-C30-C25	2.06	113.44	110.44
16	X	517	CLA	CHA-C1A-NA	-2.06	121.72	126.39
16	G	1227	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	u	514	CLA	CHA-C1A-NA	-2.06	121.72	126.39
16	g	502	CLA	CMB-C2B-C1B	2.06	128.56	125.42
16	A	1140	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	A	1237	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
19	Q	4016	BCR	C24-C23-C22	-2.06	123.19	126.23
16	G	1222	CLA	CMB-C2B-C1B	2.06	128.56	125.42
16	J	1302	CLA	O2A-CGA-O1A	-2.06	118.03	123.33
19	U	4019	BCR	C37-C22-C21	-2.06	119.48	122.82
16	v	502	CLA	C1-C2-C3	-2.06	123.43	126.76
16	h	511	CLA	C3C-C4C-NC	-2.06	107.79	110.43
19	v	604	BCR	C3-C4-C5	-2.06	110.38	114.06
19	y	604	BCR	C1-C6-C5	-2.06	119.82	122.64
16	G	1222	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
16	b	1205	CLA	C1C-C2C-C3C	-2.06	104.81	106.98
16	G	1226	CLA	C3B-C2B-C1B	-2.06	104.74	107.17
19	G	4010	BCR	C30-C25-C26	-2.06	119.82	122.64
16	p	509	CLA	CHD-C1D-ND	-2.06	121.91	124.80
19	r	601	BCR	C27-C26-C25	2.06	125.49	122.70
16	A	1237	CLA	C1-C2-C3	-2.06	122.82	126.20
19	p	601	BCR	C20-C21-C22	-2.06	124.39	127.28
19	A	4008	BCR	C35-C13-C14	-2.06	119.48	122.82
16	A	1120	CLA	C1C-C2C-C3C	-2.06	104.81	106.98
19	r	601	BCR	C33-C5-C6	-2.06	122.24	124.48
16	a	1112	CLA	CHD-C1D-ND	-2.06	121.91	124.80
16	h	517	CLA	C3B-C2B-C1B	-2.06	104.74	107.17
19	U	4022	BCR	C15-C16-C17	-2.06	119.31	123.52
16	b	1227	CLA	CHA-C1A-NA	-2.06	121.73	126.39
16	S	1302	CLA	C2B-C1B-NB	-2.06	108.19	110.33
16	r	501	CLA	O2A-CGA-O1A	-2.06	118.48	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	501	CLA	CMB-C2B-C1B	2.06	128.55	125.42
19	I	4018	BCR	C1-C6-C5	-2.06	119.82	122.64
19	g	603	BCR	C30-C25-C26	-2.06	119.82	122.64
19	T	4001	BCR	C33-C5-C6	-2.06	122.24	124.48
16	Y	509	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
16	q	517	CLA	CHA-C1A-NA	-2.06	121.73	126.39
16	w	508	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
16	u	517	CLA	CHD-C1D-ND	-2.06	121.91	124.80
16	A	1139	CLA	C3B-C4B-NB	-2.06	108.69	110.53
16	y	509	CLA	C3B-C4B-NB	-2.06	108.69	110.53
21	V	4021	ECH	C19-C18-C17	2.06	122.24	119.01
21	I	4020	ECH	C38-C26-C25	-2.06	120.80	124.11
19	H	4007	BCR	C29-C30-C25	2.06	113.43	110.44
16	H	1135	CLA	CHD-C1D-ND	-2.06	121.91	124.80
16	a	1137	CLA	CHA-C1A-NA	-2.06	121.73	126.39
16	k	4002	CLA	CHA-C1A-NA	-2.06	121.73	126.39
16	n	503	CLA	CHA-C1A-NA	-2.06	121.73	126.39
16	H	1237	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
19	t	604	BCR	C27-C26-C25	2.06	125.48	122.70
16	t	508	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
16	t	513	CLA	C2A-C1A-CHA	2.06	127.43	123.87
16	b	1213	CLA	CHD-C1D-C2D	2.06	129.76	125.49
16	w	512	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	G	1209	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
16	w	510	CLA	C3B-C2B-C1B	-2.05	104.75	107.17
16	A	1111	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	b	1217	CLA	O2A-CGA-O1A	-2.05	118.05	123.33
16	b	1209	CLA	C3B-C4B-NB	-2.05	108.70	110.53
16	a	1106	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	G	1207	CLA	C2A-C1A-CHA	2.05	127.43	123.87
16	H	1112	CLA	CHD-C1D-ND	-2.05	121.91	124.80
16	q	513	CLA	CHD-C1D-ND	-2.05	121.91	124.80
16	H	1137	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	u	503	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	b	1221	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
19	U	4019	BCR	C20-C21-C22	-2.05	124.40	127.28
19	Y	604	BCR	C15-C14-C13	-2.05	124.40	127.28
16	G	1012	CLA	O2D-CGD-CBD	2.05	114.82	111.23
16	r	514	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
16	B	1012	CLA	C1-C2-C3	-2.05	122.83	126.20
19	R	4018	BCR	C30-C25-C26	-2.05	119.83	122.64
16	b	1218	CLA	CHA-C1A-NA	-2.05	121.74	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1218	CLA	C1C-C2C-C3C	-2.05	104.82	106.98
16	g	504	CLA	C1-C2-C3	-2.05	122.83	126.20
16	b	1238	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
16	s	517	CLA	CHD-C1D-ND	-2.05	121.91	124.80
19	H	4011	BCR	C7-C8-C9	-2.05	123.20	126.23
16	y	502	CLA	C3B-C4B-NB	-2.05	108.70	110.53
16	W	515	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	q	603	BCR	C30-C25-C26	-2.05	119.83	122.64
19	s	602	BCR	C30-C25-C26	-2.05	119.83	122.64
16	n	512	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	F	4016	BCR	C30-C25-C26	-2.05	119.83	122.64
16	a	1103	CLA	CAA-CBA-CGA	-2.05	107.39	113.21
16	o	510	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
16	o	517	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	p	605	LHG	C27-C26-C25	-2.05	104.01	114.37
16	G	1206	CLA	C4A-NA-C1A	2.05	107.61	106.68
16	b	1213	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
16	h	512	CLA	CHD-C1D-ND	-2.05	121.92	124.80
16	a	1133	CLA	CHD-C1D-ND	-2.05	121.92	124.80
19	k	4001	BCR	C40-C30-C25	2.05	113.45	110.24
16	B	1021	CLA	C2B-C1B-NB	-2.05	108.20	110.33
16	a	1112	CLA	O2A-CGA-O1A	-2.05	118.06	123.33
16	U	1501	CLA	C3B-C4B-NB	-2.05	108.70	110.53
16	G	1232	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
16	b	1208	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
19	g	603	BCR	C15-C16-C17	-2.05	119.33	123.52
16	u	516	CLA	CHA-C1A-NA	-2.05	121.76	126.39
16	H	1113	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
19	W	601	BCR	C30-C25-C26	-2.05	119.84	122.64
16	S	1302	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
21	R	4020	ECH	C34-C9-C8	2.05	121.21	118.09
16	u	514	CLA	CMB-C2B-C1B	2.05	128.53	125.42
16	g	504	CLA	C3B-C2B-C1B	-2.05	104.76	107.17
15	A	1011	CL0	CMD-C2D-C3D	2.05	128.77	124.68
16	W	510	CLA	CHD-C1D-ND	-2.04	121.92	124.80
16	u	513	CLA	CHA-C1A-NA	-2.04	121.76	126.39
16	a	1122	CLA	CMB-C2B-C1B	2.04	128.53	125.42
16	r	506	CLA	CHA-C1A-NA	-2.04	121.76	126.39
19	X	601	BCR	C27-C26-C25	2.04	125.47	122.70
14	a	4201	LMG	O2-C2-C1	-2.04	105.20	110.08
16	t	502	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	y	501	CLA	C3B-C2B-C1B	-2.04	104.76	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1210	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	L	4019	BCR	C27-C26-C25	2.04	125.46	122.70
16	L	1501	CLA	CHA-C1A-NA	-2.04	121.77	126.39
16	H	1117	CLA	C3C-C4C-NC	-2.04	107.81	110.43
16	x	515	CLA	C2D-C1D-ND	-2.04	108.11	110.13
19	b	4009	BCR	C11-C10-C9	-2.04	124.36	127.48
16	n	509	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	G	1205	CLA	CHA-C1A-NA	-2.04	121.77	126.39
19	J	4015	BCR	C30-C25-C26	-2.04	119.85	122.64
16	q	510	CLA	CHD-C1D-ND	-2.04	121.93	124.80
16	A	1022	CLA	C1-C2-C3	-2.04	122.85	126.20
16	A	1101	CLA	C1-C2-C3	-2.04	122.85	126.20
16	H	1130	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	h	506	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
16	u	515	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	v	604	BCR	C16-C15-C14	-2.04	119.34	123.52
16	u	507	CLA	C1-C2-C3	-2.04	122.85	126.20
16	H	1022	CLA	C3B-C2B-C1B	-2.04	104.76	107.17
16	s	502	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	o	601	BCR	C1-C6-C5	-2.04	119.85	122.64
16	B	1240	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	r	510	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	A	1131	CLA	CMB-C2B-C1B	2.04	128.53	125.42
16	H	1126	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	W	502	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	L	4022	BCR	C15-C16-C17	-2.04	119.35	123.52
19	v	603	BCR	C24-C23-C22	-2.04	123.22	126.23
16	g	501	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	q	509	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	j	1303	CLA	CMB-C2B-C1B	2.04	128.52	125.42
19	B	4009	BCR	C11-C10-C9	-2.04	124.36	127.48
16	B	1226	CLA	C3C-C4C-NC	-2.04	107.82	110.43
16	v	511	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	g	505	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	p	503	CLA	C4D-C3D-CAD	-2.04	105.89	108.11
16	p	501	CLA	CMB-C2B-C1B	2.04	128.52	125.42
16	A	1111	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	b	1201	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	A	1119	CLA	CHD-C1D-C2D	2.04	129.72	125.49
16	s	515	CLA	CHA-C1A-NA	-2.04	121.78	126.39
19	l	4019	BCR	C20-C21-C22	-2.04	124.42	127.28
16	A	1128	CLA	CHA-C1A-NA	-2.04	121.78	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	1129	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
16	a	1139	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	A	4002	BCR	C24-C23-C22	-2.04	123.22	126.23
16	B	1209	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	H	1107	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	b	1231	CLA	C3B-C4B-NB	-2.04	108.71	110.53
16	r	504	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
16	B	1207	CLA	C2A-C1A-CHA	2.04	127.40	123.87
19	j	4013	BCR	C30-C25-C26	-2.04	119.85	122.64
16	B	1211	CLA	CHD-C1D-ND	-2.04	121.94	124.80
16	o	509	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
16	o	511	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
19	Q	4016	BCR	C7-C8-C9	-2.04	123.22	126.23
16	H	1118	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
16	t	508	CLA	C3B-C4B-NB	-2.04	108.71	110.53
19	u	604	BCR	C3-C4-C5	-2.04	110.43	114.06
16	a	1138	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
16	a	1801	CLA	C3B-C2B-C1B	-2.04	104.77	107.17
16	v	512	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
19	a	4008	BCR	C29-C30-C25	2.03	113.39	110.44
16	H	1022	CLA	C2D-C1D-ND	-2.03	108.11	110.13
16	s	507	CLA	C1-C2-C3	-2.03	122.86	126.20
16	w	511	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	a	1022	CLA	CHA-C1A-NA	-2.03	121.78	126.39
16	u	515	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
16	t	505	CLA	C3C-C4C-NC	-2.03	107.82	110.43
16	Y	502	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	o	509	CLA	CHA-C1A-NA	-2.03	121.78	126.39
16	o	517	CLA	CMB-C2B-C1B	2.03	128.52	125.42
16	y	502	CLA	C1-C2-C3	-2.03	123.47	126.76
16	a	1117	CLA	C3C-C4C-NC	-2.03	107.83	110.43
19	H	4002	BCR	C30-C25-C26	-2.03	119.86	122.64
19	Y	603	BCR	C30-C25-C26	-2.03	119.86	122.64
16	b	1212	CLA	C3B-C4B-NB	-2.03	108.72	110.53
16	t	516	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
16	r	513	CLA	C2B-C1B-NB	-2.03	108.22	110.33
16	a	1801	CLA	CHD-C1D-ND	-2.03	121.94	124.80
16	y	511	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
16	H	1118	CLA	C1D-ND-C4D	-2.03	104.89	106.31
16	H	1013	CLA	C1-O2A-CGA	2.03	121.57	116.65
16	n	504	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	y	515	CLA	O2A-CGA-O1A	-2.03	118.55	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	b	1234	CLA	C4D-C3D-CAD	-2.03	105.90	108.11
19	u	603	BCR	C30-C25-C26	-2.03	119.86	122.64
16	b	1235	CLA	C3A-C2A-C1A	-2.03	98.30	101.34
19	o	604	BCR	C24-C23-C22	-2.03	123.23	126.23
16	A	1105	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
16	G	1223	CLA	CHA-C1A-NA	-2.03	121.79	126.39
14	b	848	LMG	O7-C10-O9	-2.03	118.96	123.70
16	B	1234	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
19	J	4013	BCR	C30-C25-C26	-2.03	119.86	122.64
19	v	601	BCR	C1-C6-C5	-2.03	119.86	122.64
16	x	517	CLA	C4A-NA-C1A	2.03	107.61	106.68
21	i	4020	ECH	O27-C27-C28	-2.03	117.54	120.87
16	u	510	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
19	h	601	BCR	C38-C26-C25	-2.03	122.27	124.48
16	Z	504	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
16	a	1128	CLA	C1-C2-C3	-2.03	122.87	126.20
16	W	513	CLA	CMB-C2B-C1B	2.03	128.51	125.42
16	j	1302	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
16	X	517	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	s	503	CLA	CHA-C1A-NA	-2.03	121.80	126.39
16	W	503	CLA	C3C-C4C-NC	-2.03	107.83	110.43
19	T	4005	BCR	C11-C10-C9	-2.03	124.43	127.28
19	S	4015	BCR	C30-C25-C26	-2.03	119.86	122.64
19	w	603	BCR	C30-C25-C26	-2.03	119.86	122.64
14	H	852	LMG	O2-C2-C1	-2.03	105.24	110.08
16	x	504	CLA	C2A-C1A-CHA	2.03	127.39	123.87
16	y	517	CLA	C1C-C2C-C3C	-2.03	104.85	106.98
19	r	602	BCR	C27-C26-C25	2.03	125.44	122.70
16	H	1106	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
19	a	4002	BCR	C30-C25-C26	-2.03	119.87	122.64
21	M	4021	ECH	C19-C18-C17	2.03	122.20	119.01
21	m	4021	ECH	C15-C16-C17	2.03	127.67	123.52
16	A	1101	CLA	CHA-C1A-NA	-2.03	121.80	126.39
16	h	502	CLA	C1-C2-C3	-2.03	123.48	126.76
16	x	501	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	s	603	BCR	C21-C20-C19	-2.03	117.33	123.20
16	a	1237	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
16	y	509	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	n	604	BCR	C7-C8-C9	-2.03	123.24	126.23
16	A	1135	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
16	a	1108	CLA	C3B-C2B-C1B	-2.03	104.78	107.17
19	B	4010	BCR	C30-C25-C26	-2.02	119.87	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	q	505	CLA	CHD-C1D-C2D	2.02	129.70	125.49
16	G	1210	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	X	514	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	g	508	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	G	1235	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
16	g	514	CLA	C1-C2-C3	-2.02	123.49	126.76
16	X	514	CLA	C3B-C4B-NB	-2.02	108.72	110.53
16	W	511	CLA	C2D-C1D-ND	-2.02	108.12	110.13
16	G	1228	CLA	C3B-C2B-C1B	-2.02	104.78	107.17
19	g	602	BCR	C28-C27-C26	-2.02	110.45	114.06
19	a	4003	BCR	C15-C14-C13	-2.02	124.44	127.28
16	x	505	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
16	X	512	CLA	CHD-C1D-ND	-2.02	121.96	124.80
16	q	505	CLA	C3B-C4B-NB	-2.02	108.72	110.53
16	q	512	CLA	C3B-C4B-NB	-2.02	108.72	110.53
21	B	4006	ECH	C23-C22-C21	2.02	122.19	119.01
16	G	1023	CLA	CMD-C2D-C1D	-2.02	121.17	124.73
19	B	4010	BCR	C10-C11-C12	-2.02	117.34	123.20
19	i	4018	BCR	C1-C6-C5	-2.02	119.87	122.64
19	G	4009	BCR	C11-C10-C9	-2.02	124.39	127.48
16	y	514	CLA	C1C-C2C-C3C	-2.02	104.86	106.98
16	Z	510	CLA	CHA-C1A-NA	-2.02	121.82	126.39
16	n	507	CLA	C1-C2-C3	-2.02	122.89	126.20
16	G	1212	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
16	U	1501	CLA	CHA-C1A-NA	-2.02	121.82	126.39
16	u	514	CLA	C3B-C4B-NB	-2.02	108.73	110.53
16	w	515	CLA	C3B-C4B-NB	-2.02	108.73	110.53
16	A	1022	CLA	CHA-C1A-NA	-2.02	121.82	126.39
16	w	513	CLA	CHD-C1D-ND	-2.02	121.96	124.80
16	A	1106	CLA	C1-C2-C3	-2.02	122.89	126.20
16	b	1023	CLA	C3B-C2B-C1B	-2.02	104.79	107.17
16	W	516	CLA	CMB-C2B-C1B	2.02	128.49	125.42
19	J	4013	BCR	C16-C15-C14	-2.02	119.39	123.52
19	Y	604	BCR	C11-C10-C9	-2.02	124.45	127.28
19	a	4002	BCR	C15-C14-C13	-2.02	124.45	127.28
16	H	1118	CLA	C3C-C4C-NC	-2.02	107.84	110.43
16	q	510	CLA	CHA-C1A-NA	-2.02	121.82	126.39
16	b	1216	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
16	B	1240	CLA	CHA-C1A-NA	-2.02	121.82	126.39
16	h	510	CLA	CHD-C1D-ND	-2.02	121.96	124.80
16	G	1222	CLA	CHD-C1D-C2D	2.02	129.68	125.49
19	h	604	BCR	C15-C16-C17	-2.02	119.39	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	h	502	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
16	B	1230	CLA	C3B-C4B-NB	-2.02	108.73	110.53
16	p	513	CLA	C2B-C1B-NB	-2.02	108.23	110.33
16	v	503	CLA	CMB-C2B-C1B	2.02	128.49	125.42
16	s	510	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
16	h	504	CLA	CHD-C1D-C2D	2.02	129.68	125.49
19	X	602	BCR	C1-C6-C5	-2.02	119.88	122.64
19	n	603	BCR	C7-C8-C9	-2.02	123.25	126.23
16	u	508	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
16	A	1133	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
19	g	602	BCR	C27-C26-C25	2.02	125.43	122.70
19	p	601	BCR	C1-C6-C5	-2.02	119.88	122.64
16	Y	509	CLA	C3B-C2B-C1B	-2.01	104.79	107.17
16	v	517	CLA	C3B-C2B-C1B	-2.01	104.79	107.17
16	b	1203	CLA	C2D-C1D-ND	-2.01	108.13	110.13
16	u	505	CLA	CHA-C1A-NA	-2.01	121.83	126.39
16	Q	1301	CLA	O2A-CGA-O1A	-2.01	118.15	123.33
16	A	1130	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	x	509	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	y	501	CLA	C2B-C1B-NB	-2.01	108.24	110.33
16	G	1210	CLA	CHA-C1A-NA	-2.01	121.83	126.39
19	H	4011	BCR	C10-C11-C12	-2.01	117.36	123.20
16	w	502	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	G	1203	CLA	C4-C3-C5	2.01	118.72	115.23
19	l	4022	BCR	C16-C15-C14	-2.01	119.40	123.52
19	y	603	BCR	C11-C10-C9	-2.01	124.45	127.28
16	g	517	CLA	CMB-C2B-C1B	2.01	128.49	125.42
16	h	511	CLA	CHD-C1D-C2D	2.01	129.68	125.49
16	w	503	CLA	CHA-C1A-NA	-2.01	121.83	126.39
16	b	1221	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
16	f	1301	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
19	G	4017	BCR	C15-C14-C13	-2.01	124.45	127.28
14	H	4201	LMG	O2-C2-C1	-2.01	105.28	110.08
16	q	501	CLA	C1-C2-C3	-2.01	123.51	126.76
16	w	501	CLA	C1-C2-C3	-2.01	123.51	126.76
16	Z	516	CLA	C4A-NA-C1A	2.01	107.60	106.68
16	k	4002	CLA	CMB-C2B-C1B	2.01	128.48	125.42
19	v	603	BCR	C1-C6-C5	-2.01	119.89	122.64
16	B	1207	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
16	H	1114	CLA	C2A-C1A-CHA	2.01	127.36	123.87
16	X	517	CLA	C3B-C4B-NB	-2.01	108.73	110.53
16	t	512	CLA	C3B-C4B-NB	-2.01	108.73	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	t	514	CLA	C3B-C4B-NB	-2.01	108.73	110.53
21	R	4020	ECH	O27-C27-C28	-2.01	117.57	120.87
19	l	4019	BCR	C31-C1-C6	2.01	113.40	110.24
16	q	502	CLA	C2B-C1B-NB	-2.01	108.24	110.33
16	Z	511	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
16	B	1212	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
16	Z	505	CLA	CHA-C1A-NA	-2.01	121.84	126.39
16	X	514	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
19	s	601	BCR	C30-C25-C26	-2.01	119.89	122.64
16	v	512	CLA	C2A-C1A-CHA	2.01	127.35	123.87
16	A	1125	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
14	G	848	LMG	O1-C1-C2	-2.01	105.22	108.27
21	M	4021	ECH	C10-C11-C12	2.01	129.02	123.20
16	p	505	CLA	CHA-C1A-NA	-2.01	121.84	126.39
19	B	4017	BCR	C15-C14-C13	-2.01	124.46	127.28
19	H	4007	BCR	C7-C8-C9	-2.01	123.26	126.23
16	X	515	CLA	C3B-C2B-C1B	-2.01	104.80	107.17
16	A	1801	CLA	CHA-C1A-NA	-2.01	121.84	126.39
16	p	506	CLA	CHA-C1A-NA	-2.01	121.84	126.39
19	H	4003	BCR	C15-C14-C13	-2.01	124.46	127.28
16	g	512	CLA	CHD-C1D-ND	-2.01	121.98	124.80
16	X	512	CLA	C3B-C4B-NB	-2.01	108.74	110.53
16	p	503	CLA	CHD-C1D-C2D	2.01	129.66	125.49
16	A	1122	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	A	1022	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
19	b	4005	BCR	C24-C23-C22	-2.01	123.27	126.23
16	a	1135	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
19	b	4010	BCR	C10-C11-C12	-2.01	117.39	123.20
21	m	4021	ECH	O27-C27-C26	2.01	122.78	120.98
16	l	1501	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	w	516	CLA	C3B-C4B-NB	-2.01	108.74	110.53
16	y	510	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
16	u	506	CLA	C2B-C1B-NB	-2.01	108.25	110.33
16	B	1239	CLA	CMB-C2B-C1B	2.01	128.47	125.42
16	v	513	CLA	CMB-C2B-C1B	2.01	128.47	125.42
16	U	1503	CLA	CHD-C1D-ND	-2.01	121.98	124.80
16	q	502	CLA	C4A-NA-C1A	2.01	107.59	106.68
19	H	4007	BCR	C1-C6-C5	-2.01	119.89	122.64
16	W	508	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
16	q	513	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
19	B	4005	BCR	C28-C27-C26	-2.00	110.48	114.06
19	L	4022	BCR	C20-C21-C22	-2.00	124.47	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	x	606	LMU	O5'-C1'-C2'	2.00	114.49	110.37
16	v	510	CLA	C1C-C2C-C3C	-2.00	104.87	106.98
16	t	506	CLA	C3B-C4B-NB	-2.00	108.74	110.53
16	H	1130	CLA	CHA-C1A-NA	-2.00	121.85	126.39
16	L	1501	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
16	b	1225	CLA	C2D-C1D-ND	-2.00	108.14	110.13
19	w	603	BCR	C31-C1-C6	2.00	113.39	110.24
16	u	501	CLA	CHA-C1A-NA	-2.00	121.85	126.39
16	w	512	CLA	CHD-C1D-ND	-2.00	121.98	124.80
19	y	603	BCR	C1-C6-C5	-2.00	119.90	122.64
16	o	504	CLA	C2D-C1D-ND	-2.00	108.14	110.13
19	q	602	BCR	C33-C5-C6	-2.00	122.30	124.48
16	s	501	CLA	C3B-C4B-NB	-2.00	108.74	110.53
19	i	4018	BCR	C3-C4-C5	-2.00	110.49	114.06
16	g	507	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
15	a	1011	CL0	C4D-ND-C1D	2.00	106.74	105.22
19	U	4019	BCR	C7-C8-C9	-2.00	123.27	126.23
16	h	505	CLA	C3B-C2B-C1B	-2.00	104.81	107.17
13	A	849	LHG	O8-C23-O10	-2.00	118.62	123.63
19	a	4003	BCR	C16-C15-C14	-2.00	119.42	123.52
19	a	4002	BCR	C24-C23-C22	-2.00	123.28	126.23
16	u	514	CLA	CHD-C1D-C2D	2.00	129.65	125.49
16	o	512	CLA	C2A-C1A-CHA	2.00	127.34	123.87

All (405) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	1011	CL0	NC
15	A	1011	CL0	ND
15	H	1011	CL0	NC
15	H	1011	CL0	ND
15	a	1011	CL0	NC
15	a	1011	CL0	ND
16	A	1013	CLA	ND
16	A	1022	CLA	ND
16	A	1101	CLA	ND
16	A	1102	CLA	ND
16	A	1103	CLA	ND
16	A	1104	CLA	ND
16	A	1105	CLA	ND
16	A	1106	CLA	ND
16	A	1109	CLA	ND

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Mol	Chain	Res	Type	Atom
16	A	1110	CLA	ND
16	A	1111	CLA	ND
16	A	1113	CLA	ND
16	A	1114	CLA	ND
16	A	1115	CLA	ND
16	A	1116	CLA	ND
16	A	1117	CLA	ND
16	A	1119	CLA	ND
16	A	1121	CLA	ND
16	A	1122	CLA	ND
16	A	1124	CLA	ND
16	A	1126	CLA	ND
16	A	1127	CLA	ND
16	A	1128	CLA	ND
16	A	1130	CLA	ND
16	A	1132	CLA	ND
16	A	1133	CLA	ND
16	A	1135	CLA	ND
16	A	1136	CLA	ND
16	A	1137	CLA	ND
16	A	1138	CLA	ND
16	A	1139	CLA	ND
16	A	1140	CLA	ND
16	A	1237	CLA	ND
16	A	1801	CLA	ND
16	B	1012	CLA	ND
16	B	1021	CLA	ND
16	B	1201	CLA	ND
16	B	1202	CLA	ND
16	B	1203	CLA	ND
16	B	1204	CLA	ND
16	B	1205	CLA	ND
16	B	1206	CLA	ND
16	B	1208	CLA	ND
16	B	1209	CLA	ND
16	B	1211	CLA	ND
16	B	1212	CLA	ND
16	B	1213	CLA	ND
16	B	1214	CLA	ND
16	B	1215	CLA	ND
16	B	1220	CLA	ND
16	B	1223	CLA	ND

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Mol	Chain	Res	Type	Atom
16	B	1224	CLA	ND
16	B	1227	CLA	ND
16	B	1229	CLA	ND
16	B	1230	CLA	ND
16	B	1231	CLA	ND
16	B	1232	CLA	ND
16	B	1234	CLA	ND
16	B	1235	CLA	ND
16	B	1236	CLA	ND
16	B	1238	CLA	ND
16	B	1240	CLA	ND
16	F	1301	CLA	ND
16	F	1302	CLA	ND
16	G	1012	CLA	ND
16	G	1021	CLA	ND
16	G	1201	CLA	ND
16	G	1202	CLA	ND
16	G	1203	CLA	ND
16	G	1204	CLA	ND
16	G	1205	CLA	ND
16	G	1206	CLA	ND
16	G	1208	CLA	ND
16	G	1209	CLA	ND
16	G	1212	CLA	ND
16	G	1213	CLA	ND
16	G	1214	CLA	ND
16	G	1215	CLA	ND
16	G	1216	CLA	ND
16	G	1220	CLA	ND
16	G	1221	CLA	ND
16	G	1223	CLA	ND
16	G	1224	CLA	ND
16	G	1225	CLA	ND
16	G	1228	CLA	ND
16	G	1229	CLA	ND
16	G	1230	CLA	ND
16	G	1231	CLA	ND
16	G	1232	CLA	ND
16	G	1234	CLA	ND
16	G	1235	CLA	ND
16	G	1238	CLA	ND
16	G	1239	CLA	ND

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Mol	Chain	Res	Type	Atom
16	G	1240	CLA	ND
16	H	1013	CLA	ND
16	H	1022	CLA	ND
16	H	1101	CLA	ND
16	H	1102	CLA	ND
16	H	1103	CLA	ND
16	H	1104	CLA	ND
16	H	1105	CLA	ND
16	H	1106	CLA	ND
16	H	1109	CLA	ND
16	H	1110	CLA	ND
16	H	1111	CLA	ND
16	H	1113	CLA	ND
16	H	1114	CLA	ND
16	H	1116	CLA	ND
16	H	1117	CLA	ND
16	H	1119	CLA	ND
16	H	1121	CLA	ND
16	H	1124	CLA	ND
16	H	1126	CLA	ND
16	H	1127	CLA	ND
16	H	1128	CLA	ND
16	H	1131	CLA	ND
16	H	1132	CLA	ND
16	H	1136	CLA	ND
16	H	1137	CLA	ND
16	H	1138	CLA	ND
16	H	1139	CLA	ND
16	H	1140	CLA	ND
16	H	1237	CLA	ND
16	H	1801	CLA	ND
16	J	1302	CLA	ND
16	K	4002	CLA	ND
16	K	4003	CLA	ND
16	K	4004	CLA	ND
16	L	1503	CLA	ND
16	Q	1301	CLA	ND
16	Q	1302	CLA	ND
16	S	1302	CLA	ND
16	T	4002	CLA	ND
16	T	4003	CLA	ND
16	U	1503	CLA	ND

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Mol	Chain	Res	Type	Atom
16	W	501	CLA	ND
16	W	502	CLA	ND
16	W	503	CLA	ND
16	W	504	CLA	ND
16	W	505	CLA	ND
16	W	508	CLA	ND
16	W	509	CLA	ND
16	W	511	CLA	ND
16	W	512	CLA	ND
16	W	514	CLA	ND
16	W	515	CLA	ND
16	W	517	CLA	ND
16	X	502	CLA	ND
16	X	505	CLA	ND
16	X	506	CLA	ND
16	X	508	CLA	ND
16	X	509	CLA	ND
16	X	511	CLA	ND
16	X	514	CLA	ND
16	X	515	CLA	ND
16	Y	501	CLA	ND
16	Y	502	CLA	ND
16	Y	503	CLA	ND
16	Y	504	CLA	ND
16	Y	505	CLA	ND
16	Y	508	CLA	ND
16	Y	509	CLA	ND
16	Y	511	CLA	ND
16	Y	512	CLA	ND
16	Y	514	CLA	ND
16	Y	515	CLA	ND
16	Z	501	CLA	ND
16	Z	502	CLA	ND
16	Z	503	CLA	ND
16	Z	504	CLA	ND
16	Z	505	CLA	ND
16	Z	507	CLA	ND
16	Z	508	CLA	ND
16	Z	509	CLA	ND
16	Z	511	CLA	ND
16	Z	512	CLA	ND
16	Z	514	CLA	ND

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Mol	Chain	Res	Type	Atom
16	Z	515	CLA	ND
16	Z	516	CLA	ND
16	Z	517	CLA	ND
16	a	1013	CLA	ND
16	a	1022	CLA	ND
16	a	1101	CLA	ND
16	a	1102	CLA	ND
16	a	1103	CLA	ND
16	a	1104	CLA	ND
16	a	1105	CLA	ND
16	a	1106	CLA	ND
16	a	1109	CLA	ND
16	a	1110	CLA	ND
16	a	1111	CLA	ND
16	a	1113	CLA	ND
16	a	1114	CLA	ND
16	a	1115	CLA	ND
16	a	1116	CLA	ND
16	a	1117	CLA	ND
16	a	1119	CLA	ND
16	a	1121	CLA	ND
16	a	1124	CLA	ND
16	a	1126	CLA	ND
16	a	1127	CLA	ND
16	a	1128	CLA	ND
16	a	1132	CLA	ND
16	a	1135	CLA	ND
16	a	1136	CLA	ND
16	a	1137	CLA	ND
16	a	1138	CLA	ND
16	a	1139	CLA	ND
16	a	1237	CLA	ND
16	a	1801	CLA	ND
16	b	1012	CLA	ND
16	b	1021	CLA	ND
16	b	1201	CLA	ND
16	b	1202	CLA	ND
16	b	1203	CLA	ND
16	b	1204	CLA	ND
16	b	1205	CLA	ND
16	b	1206	CLA	ND
16	b	1208	CLA	ND

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Mol	Chain	Res	Type	Atom
16	b	1209	CLA	ND
16	b	1210	CLA	ND
16	b	1211	CLA	ND
16	b	1212	CLA	ND
16	b	1213	CLA	ND
16	b	1214	CLA	ND
16	b	1216	CLA	ND
16	b	1221	CLA	ND
16	b	1223	CLA	ND
16	b	1224	CLA	ND
16	b	1226	CLA	ND
16	b	1227	CLA	ND
16	b	1228	CLA	ND
16	b	1229	CLA	ND
16	b	1231	CLA	ND
16	b	1232	CLA	ND
16	b	1234	CLA	ND
16	b	1235	CLA	ND
16	b	1238	CLA	ND
16	b	1240	CLA	ND
16	f	1301	CLA	ND
16	f	1302	CLA	ND
16	g	502	CLA	ND
16	g	504	CLA	ND
16	g	505	CLA	ND
16	g	507	CLA	ND
16	g	508	CLA	ND
16	g	509	CLA	ND
16	g	511	CLA	ND
16	g	512	CLA	ND
16	g	514	CLA	ND
16	g	515	CLA	ND
16	g	516	CLA	ND
16	h	502	CLA	ND
16	h	503	CLA	ND
16	h	506	CLA	ND
16	h	507	CLA	ND
16	h	508	CLA	ND
16	h	509	CLA	ND
16	h	511	CLA	ND
16	h	513	CLA	ND
16	h	515	CLA	ND

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Mol	Chain	Res	Type	Atom
16	h	516	CLA	ND
16	h	517	CLA	ND
16	k	4002	CLA	ND
16	k	4003	CLA	ND
16	k	4004	CLA	ND
16	l	1503	CLA	ND
16	n	501	CLA	ND
16	n	502	CLA	ND
16	n	503	CLA	ND
16	n	505	CLA	ND
16	n	507	CLA	ND
16	n	508	CLA	ND
16	n	509	CLA	ND
16	n	512	CLA	ND
16	n	514	CLA	ND
16	n	515	CLA	ND
16	n	517	CLA	ND
16	o	502	CLA	ND
16	o	505	CLA	ND
16	o	506	CLA	ND
16	o	508	CLA	ND
16	o	509	CLA	ND
16	o	511	CLA	ND
16	o	512	CLA	ND
16	o	514	CLA	ND
16	o	515	CLA	ND
16	p	501	CLA	ND
16	p	502	CLA	ND
16	p	503	CLA	ND
16	p	508	CLA	ND
16	p	509	CLA	ND
16	p	511	CLA	ND
16	p	512	CLA	ND
16	p	514	CLA	ND
16	p	515	CLA	ND
16	p	516	CLA	ND
16	q	501	CLA	ND
16	q	502	CLA	ND
16	q	503	CLA	ND
16	q	504	CLA	ND
16	q	505	CLA	ND
16	q	506	CLA	ND

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Mol	Chain	Res	Type	Atom
16	q	507	CLA	ND
16	q	508	CLA	ND
16	q	509	CLA	ND
16	q	512	CLA	ND
16	q	514	CLA	ND
16	q	515	CLA	ND
16	q	516	CLA	ND
16	r	501	CLA	ND
16	r	502	CLA	ND
16	r	504	CLA	ND
16	r	507	CLA	ND
16	r	508	CLA	ND
16	r	511	CLA	ND
16	r	512	CLA	ND
16	r	514	CLA	ND
16	r	515	CLA	ND
16	r	516	CLA	ND
16	s	501	CLA	ND
16	s	502	CLA	ND
16	s	503	CLA	ND
16	s	504	CLA	ND
16	s	505	CLA	ND
16	s	508	CLA	ND
16	s	509	CLA	ND
16	s	511	CLA	ND
16	s	512	CLA	ND
16	s	514	CLA	ND
16	s	515	CLA	ND
16	t	501	CLA	ND
16	t	502	CLA	ND
16	t	503	CLA	ND
16	t	504	CLA	ND
16	t	506	CLA	ND
16	t	507	CLA	ND
16	t	508	CLA	ND
16	t	509	CLA	ND
16	t	511	CLA	ND
16	t	512	CLA	ND
16	t	514	CLA	ND
16	t	515	CLA	ND
16	t	516	CLA	ND
16	t	517	CLA	ND

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Mol	Chain	Res	Type	Atom
16	u	502	CLA	ND
16	u	505	CLA	ND
16	u	506	CLA	ND
16	u	507	CLA	ND
16	u	508	CLA	ND
16	u	509	CLA	ND
16	u	511	CLA	ND
16	u	514	CLA	ND
16	u	516	CLA	ND
16	v	502	CLA	ND
16	v	503	CLA	ND
16	v	504	CLA	ND
16	v	506	CLA	ND
16	v	508	CLA	ND
16	v	511	CLA	ND
16	v	513	CLA	ND
16	v	514	CLA	ND
16	v	515	CLA	ND
16	v	516	CLA	ND
16	v	517	CLA	ND
16	w	501	CLA	ND
16	w	502	CLA	ND
16	w	503	CLA	ND
16	w	504	CLA	ND
16	w	507	CLA	ND
16	w	508	CLA	ND
16	w	509	CLA	ND
16	w	511	CLA	ND
16	w	512	CLA	ND
16	w	514	CLA	ND
16	w	515	CLA	ND
16	w	516	CLA	ND
16	w	517	CLA	ND
16	x	502	CLA	ND
16	x	504	CLA	ND
16	x	505	CLA	ND
16	x	507	CLA	ND
16	x	508	CLA	ND
16	x	509	CLA	ND
16	x	514	CLA	ND
16	x	515	CLA	ND
16	x	516	CLA	ND

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Mol	Chain	Res	Type	Atom
16	y	501	CLA	ND
16	y	502	CLA	ND
16	y	503	CLA	ND
16	y	505	CLA	ND
16	y	506	CLA	ND
16	y	508	CLA	ND
16	y	509	CLA	ND
16	y	511	CLA	ND
16	y	513	CLA	ND
16	y	515	CLA	ND
16	y	516	CLA	ND
16	y	517	CLA	ND

All (8161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	849	LHG	O1-C1-C2-O2
13	A	849	LHG	O1-C1-C2-C3
13	A	849	LHG	C3-O3-P-O5
13	A	851	LHG	C3-O3-P-O5
13	B	4018	LHG	O1-C1-C2-O2
13	B	4018	LHG	O1-C1-C2-C3
13	B	4018	LHG	C3-O3-P-O5
13	G	4018	LHG	O1-C1-C2-C3
13	G	4018	LHG	C3-O3-P-O5
13	H	851	LHG	C3-O3-P-O5
13	I	103	LHG	C3-O3-P-O5
13	I	103	LHG	C4-O6-P-O3
13	I	103	LHG	C4-O6-P-O4
13	R	103	LHG	C3-O3-P-O6
13	R	103	LHG	C4-O6-P-O4
13	X	605	LHG	C3-O3-P-O5
13	Y	605	LHG	C3-O3-P-O4
13	Y	605	LHG	C3-O3-P-O6
13	Y	605	LHG	C4-O6-P-O3
13	a	849	LHG	O1-C1-C2-C3
13	a	851	LHG	C3-O3-P-O5
13	a	851	LHG	O9-C7-O7-C5
13	a	851	LHG	C8-C7-O7-C5
13	b	4018	LHG	O1-C1-C2-C3
13	b	4018	LHG	C3-O3-P-O5
13	g	605	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
13	g	605	LHG	C4-O6-P-O3
13	g	605	LHG	C4-O6-P-O5
13	i	103	LHG	C3-O3-P-O6
13	i	103	LHG	C4-O6-P-O4
13	o	605	LHG	O1-C1-C2-C3
13	p	605	LHG	C4-O6-P-O3
13	p	605	LHG	O7-C5-C6-O8
13	r	605	LHG	C1-C2-C3-O3
13	r	605	LHG	C3-O3-P-O4
13	r	605	LHG	C3-O3-P-O5
13	r	605	LHG	C4-O6-P-O3
13	r	605	LHG	C4-O6-P-O4
13	r	605	LHG	C5-C4-O6-P
13	s	605	LHG	C3-O3-P-O4
13	s	605	LHG	C3-O3-P-O5
13	s	605	LHG	C3-O3-P-O6
13	s	605	LHG	C4-O6-P-O3
13	s	605	LHG	O7-C5-C6-O8
13	u	605	LHG	O1-C1-C2-O2
13	u	605	LHG	O1-C1-C2-C3
13	u	605	LHG	C3-O3-P-O4
13	x	605	LHG	C3-O3-P-O5
13	x	605	LHG	C4-O6-P-O3
13	x	605	LHG	C4-O6-P-O4
13	x	605	LHG	C5-C4-O6-P
14	A	852	LMG	O7-C8-C9-O8
14	A	4101	LMG	O6-C1-O1-C7
14	A	4101	LMG	O1-C7-C8-O7
14	A	4101	LMG	O9-C10-O7-C8
14	A	4101	LMG	C11-C10-O7-C8
14	H	4101	LMG	O6-C1-O1-C7
14	H	4101	LMG	O1-C7-C8-O7
14	H	4101	LMG	O9-C10-O7-C8
14	H	4201	LMG	O7-C8-C9-O8
14	a	852	LMG	O7-C8-C9-O8
14	a	4101	LMG	O6-C1-O1-C7
14	a	4101	LMG	O1-C7-C8-O7
14	a	4101	LMG	O9-C10-O7-C8
16	A	1022	CLA	C1A-C2A-CAA-CBA
16	A	1101	CLA	C1A-C2A-CAA-CBA
16	A	1103	CLA	CAD-CBD-CGD-O1D
16	A	1103	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	A	1104	CLA	CBD-CGD-O2D-CED
16	A	1106	CLA	CHA-CBD-CGD-O1D
16	A	1106	CLA	CHA-CBD-CGD-O2D
16	A	1107	CLA	C1A-C2A-CAA-CBA
16	A	1110	CLA	C4B-C3B-CAB-CBB
16	A	1111	CLA	C1A-C2A-CAA-CBA
16	A	1111	CLA	C3A-C2A-CAA-CBA
16	A	1112	CLA	C1A-C2A-CAA-CBA
16	A	1112	CLA	CBD-CGD-O2D-CED
16	A	1113	CLA	CBD-CGD-O2D-CED
16	A	1114	CLA	C1A-C2A-CAA-CBA
16	A	1114	CLA	C4B-C3B-CAB-CBB
16	A	1114	CLA	CHA-CBD-CGD-O1D
16	A	1114	CLA	CHA-CBD-CGD-O2D
16	A	1115	CLA	C1A-C2A-CAA-CBA
16	A	1116	CLA	C3A-C2A-CAA-CBA
16	A	1116	CLA	CBD-CGD-O2D-CED
16	A	1117	CLA	CBD-CGD-O2D-CED
16	A	1118	CLA	C1A-C2A-CAA-CBA
16	A	1118	CLA	C2B-C3B-CAB-CBB
16	A	1120	CLA	CBD-CGD-O2D-CED
16	A	1121	CLA	C1A-C2A-CAA-CBA
16	A	1121	CLA	C4B-C3B-CAB-CBB
16	A	1122	CLA	C2B-C3B-CAB-CBB
16	A	1122	CLA	C4B-C3B-CAB-CBB
16	A	1128	CLA	CHA-CBD-CGD-O1D
16	A	1128	CLA	CHA-CBD-CGD-O2D
16	A	1130	CLA	C1A-C2A-CAA-CBA
16	A	1131	CLA	C4B-C3B-CAB-CBB
16	A	1131	CLA	CBD-CGD-O2D-CED
16	A	1132	CLA	CHA-CBD-CGD-O1D
16	A	1132	CLA	CHA-CBD-CGD-O2D
16	A	1133	CLA	C4B-C3B-CAB-CBB
16	A	1134	CLA	C4B-C3B-CAB-CBB
16	A	1135	CLA	C1A-C2A-CAA-CBA
16	A	1135	CLA	C3A-C2A-CAA-CBA
16	A	1136	CLA	C4B-C3B-CAB-CBB
16	A	1137	CLA	C1A-C2A-CAA-CBA
16	A	1137	CLA	C2B-C3B-CAB-CBB
16	A	1137	CLA	C4B-C3B-CAB-CBB
16	A	1137	CLA	CBD-CGD-O2D-CED
16	A	1138	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	A	1138	CLA	C4B-C3B-CAB-CBB
16	A	1140	CLA	C1A-C2A-CAA-CBA
16	A	1140	CLA	C4B-C3B-CAB-CBB
16	A	1237	CLA	C4B-C3B-CAB-CBB
16	B	1012	CLA	C1A-C2A-CAA-CBA
16	B	1012	CLA	C3A-C2A-CAA-CBA
16	B	1202	CLA	C1A-C2A-CAA-CBA
16	B	1202	CLA	C3A-C2A-CAA-CBA
16	B	1203	CLA	C1A-C2A-CAA-CBA
16	B	1203	CLA	C3A-C2A-CAA-CBA
16	B	1203	CLA	CBD-CGD-O2D-CED
16	B	1205	CLA	C4B-C3B-CAB-CBB
16	B	1205	CLA	CHA-CBD-CGD-O1D
16	B	1205	CLA	CHA-CBD-CGD-O2D
16	B	1206	CLA	C1A-C2A-CAA-CBA
16	B	1206	CLA	C3A-C2A-CAA-CBA
16	B	1207	CLA	C2B-C3B-CAB-CBB
16	B	1207	CLA	CHA-CBD-CGD-O1D
16	B	1207	CLA	CHA-CBD-CGD-O2D
16	B	1207	CLA	CBD-CGD-O2D-CED
16	B	1209	CLA	C1A-C2A-CAA-CBA
16	B	1209	CLA	C2B-C3B-CAB-CBB
16	B	1210	CLA	C1A-C2A-CAA-CBA
16	B	1211	CLA	C1A-C2A-CAA-CBA
16	B	1211	CLA	CBD-CGD-O2D-CED
16	B	1214	CLA	C1A-C2A-CAA-CBA
16	B	1214	CLA	C3A-C2A-CAA-CBA
16	B	1215	CLA	CBD-CGD-O2D-CED
16	B	1217	CLA	C1A-C2A-CAA-CBA
16	B	1217	CLA	C2B-C3B-CAB-CBB
16	B	1217	CLA	C4B-C3B-CAB-CBB
16	B	1219	CLA	CBD-CGD-O2D-CED
16	B	1220	CLA	C1A-C2A-CAA-CBA
16	B	1221	CLA	C1A-C2A-CAA-CBA
16	B	1221	CLA	C3A-C2A-CAA-CBA
16	B	1221	CLA	C14-C13-C15-C16
16	B	1222	CLA	C2B-C3B-CAB-CBB
16	B	1222	CLA	CHA-CBD-CGD-O1D
16	B	1222	CLA	CHA-CBD-CGD-O2D
16	B	1227	CLA	CHA-CBD-CGD-O2D
16	B	1228	CLA	C1A-C2A-CAA-CBA
16	B	1230	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	B	1230	CLA	C3A-C2A-CAA-CBA
16	B	1231	CLA	C1A-C2A-CAA-CBA
16	B	1231	CLA	C3A-C2A-CAA-CBA
16	B	1231	CLA	C2B-C3B-CAB-CBB
16	B	1232	CLA	C4B-C3B-CAB-CBB
16	B	1232	CLA	CAD-CBD-CGD-O1D
16	B	1232	CLA	CAD-CBD-CGD-O2D
16	B	1234	CLA	C1A-C2A-CAA-CBA
16	B	1235	CLA	CBD-CGD-O2D-CED
16	B	1235	CLA	O1D-CGD-O2D-CED
16	B	1236	CLA	C1A-C2A-CAA-CBA
16	B	1238	CLA	C4B-C3B-CAB-CBB
16	B	1239	CLA	C1A-C2A-CAA-CBA
16	B	1239	CLA	C3A-C2A-CAA-CBA
16	B	1239	CLA	C4B-C3B-CAB-CBB
16	B	1240	CLA	C4B-C3B-CAB-CBB
16	F	1301	CLA	C4B-C3B-CAB-CBB
16	F	1301	CLA	CBD-CGD-O2D-CED
16	F	1302	CLA	CBD-CGD-O2D-CED
16	G	1012	CLA	C1A-C2A-CAA-CBA
16	G	1012	CLA	C3A-C2A-CAA-CBA
16	G	1021	CLA	CBD-CGD-O2D-CED
16	G	1202	CLA	C1A-C2A-CAA-CBA
16	G	1202	CLA	C3A-C2A-CAA-CBA
16	G	1203	CLA	C4B-C3B-CAB-CBB
16	G	1205	CLA	C4B-C3B-CAB-CBB
16	G	1207	CLA	C2B-C3B-CAB-CBB
16	G	1207	CLA	CBD-CGD-O2D-CED
16	G	1209	CLA	C1A-C2A-CAA-CBA
16	G	1210	CLA	C1A-C2A-CAA-CBA
16	G	1211	CLA	C1A-C2A-CAA-CBA
16	G	1211	CLA	CBD-CGD-O2D-CED
16	G	1212	CLA	CHA-CBD-CGD-O1D
16	G	1212	CLA	CHA-CBD-CGD-O2D
16	G	1213	CLA	C1A-C2A-CAA-CBA
16	G	1214	CLA	C3A-C2A-CAA-CBA
16	G	1214	CLA	C4B-C3B-CAB-CBB
16	G	1217	CLA	C1A-C2A-CAA-CBA
16	G	1217	CLA	C2B-C3B-CAB-CBB
16	G	1218	CLA	C1A-C2A-CAA-CBA
16	G	1218	CLA	O1A-CGA-O2A-C1
16	G	1220	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	G	1221	CLA	C1A-C2A-CAA-CBA
16	G	1221	CLA	C3A-C2A-CAA-CBA
16	G	1222	CLA	CHA-CBD-CGD-O1D
16	G	1222	CLA	CHA-CBD-CGD-O2D
16	G	1227	CLA	C4B-C3B-CAB-CBB
16	G	1230	CLA	C1A-C2A-CAA-CBA
16	G	1231	CLA	C1A-C2A-CAA-CBA
16	G	1231	CLA	C4B-C3B-CAB-CBB
16	G	1232	CLA	C4B-C3B-CAB-CBB
16	G	1232	CLA	CBD-CGD-O2D-CED
16	G	1235	CLA	CBD-CGD-O2D-CED
16	G	1235	CLA	O1D-CGD-O2D-CED
16	G	1236	CLA	C1A-C2A-CAA-CBA
16	G	1238	CLA	C4B-C3B-CAB-CBB
16	G	1239	CLA	C1A-C2A-CAA-CBA
16	G	1239	CLA	C3A-C2A-CAA-CBA
16	G	1239	CLA	C4B-C3B-CAB-CBB
16	G	1240	CLA	C4B-C3B-CAB-CBB
16	G	1240	CLA	CBD-CGD-O2D-CED
16	H	1013	CLA	CBD-CGD-O2D-CED
16	H	1022	CLA	C1A-C2A-CAA-CBA
16	H	1101	CLA	C1A-C2A-CAA-CBA
16	H	1104	CLA	CHA-CBD-CGD-O2D
16	H	1106	CLA	CHA-CBD-CGD-O1D
16	H	1106	CLA	CHA-CBD-CGD-O2D
16	H	1106	CLA	C11-C12-C13-C14
16	H	1107	CLA	C1A-C2A-CAA-CBA
16	H	1108	CLA	C1A-C2A-CAA-CBA
16	H	1110	CLA	C4B-C3B-CAB-CBB
16	H	1111	CLA	C1A-C2A-CAA-CBA
16	H	1111	CLA	C3A-C2A-CAA-CBA
16	H	1112	CLA	C1A-C2A-CAA-CBA
16	H	1114	CLA	C1A-C2A-CAA-CBA
16	H	1114	CLA	C3A-C2A-CAA-CBA
16	H	1114	CLA	C4B-C3B-CAB-CBB
16	H	1115	CLA	C1A-C2A-CAA-CBA
16	H	1116	CLA	C3A-C2A-CAA-CBA
16	H	1116	CLA	C2B-C3B-CAB-CBB
16	H	1118	CLA	C1A-C2A-CAA-CBA
16	H	1121	CLA	C1A-C2A-CAA-CBA
16	H	1121	CLA	C4B-C3B-CAB-CBB
16	H	1122	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	H	1128	CLA	C1A-C2A-CAA-CBA
16	H	1128	CLA	CHA-CBD-CGD-O1D
16	H	1128	CLA	CHA-CBD-CGD-O2D
16	H	1129	CLA	C4B-C3B-CAB-CBB
16	H	1130	CLA	C1A-C2A-CAA-CBA
16	H	1131	CLA	CBD-CGD-O2D-CED
16	H	1132	CLA	CHA-CBD-CGD-O1D
16	H	1132	CLA	CHA-CBD-CGD-O2D
16	H	1133	CLA	C2B-C3B-CAB-CBB
16	H	1133	CLA	C4B-C3B-CAB-CBB
16	H	1134	CLA	C4B-C3B-CAB-CBB
16	H	1135	CLA	C1A-C2A-CAA-CBA
16	H	1135	CLA	C3A-C2A-CAA-CBA
16	H	1136	CLA	C4B-C3B-CAB-CBB
16	H	1137	CLA	C1A-C2A-CAA-CBA
16	H	1137	CLA	C4B-C3B-CAB-CBB
16	H	1137	CLA	CBD-CGD-O2D-CED
16	H	1138	CLA	C4B-C3B-CAB-CBB
16	H	1139	CLA	C2B-C3B-CAB-CBB
16	H	1140	CLA	C1A-C2A-CAA-CBA
16	H	1140	CLA	C4B-C3B-CAB-CBB
16	H	1237	CLA	C4B-C3B-CAB-CBB
16	H	1237	CLA	C11-C10-C8-C9
16	H	1801	CLA	CBA-CGA-O2A-C1
16	H	1801	CLA	CAD-CBD-CGD-O1D
16	H	1801	CLA	CAD-CBD-CGD-O2D
16	J	1302	CLA	C4B-C3B-CAB-CBB
16	J	1303	CLA	C4B-C3B-CAB-CBB
16	K	4002	CLA	C4B-C3B-CAB-CBB
16	K	4003	CLA	C1A-C2A-CAA-CBA
16	K	4003	CLA	C3A-C2A-CAA-CBA
16	Q	1301	CLA	C2B-C3B-CAB-CBB
16	Q	1301	CLA	C4B-C3B-CAB-CBB
16	S	1302	CLA	C4B-C3B-CAB-CBB
16	S	1302	CLA	CBD-CGD-O2D-CED
16	S	1303	CLA	C4B-C3B-CAB-CBB
16	T	4002	CLA	C4B-C3B-CAB-CBB
16	T	4003	CLA	C1A-C2A-CAA-CBA
16	T	4003	CLA	C3A-C2A-CAA-CBA
16	W	501	CLA	C3A-C2A-CAA-CBA
16	W	501	CLA	CAD-CBD-CGD-O1D
16	W	501	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	W	502	CLA	C4B-C3B-CAB-CBB
16	W	502	CLA	CHA-CBD-CGD-O1D
16	W	502	CLA	CHA-CBD-CGD-O2D
16	W	503	CLA	C1A-C2A-CAA-CBA
16	W	503	CLA	C4B-C3B-CAB-CBB
16	W	504	CLA	C4B-C3B-CAB-CBB
16	W	505	CLA	C4B-C3B-CAB-CBB
16	W	505	CLA	CHA-CBD-CGD-O2D
16	W	506	CLA	CHA-CBD-CGD-O1D
16	W	506	CLA	CHA-CBD-CGD-O2D
16	W	508	CLA	C1A-C2A-CAA-CBA
16	W	508	CLA	C3A-C2A-CAA-CBA
16	W	508	CLA	C4B-C3B-CAB-CBB
16	W	508	CLA	CBD-CGD-O2D-CED
16	W	511	CLA	C1A-C2A-CAA-CBA
16	W	512	CLA	CBD-CGD-O2D-CED
16	W	513	CLA	CAD-CBD-CGD-O1D
16	W	513	CLA	CAD-CBD-CGD-O2D
16	W	513	CLA	CBD-CGD-O2D-CED
16	W	514	CLA	CBD-CGD-O2D-CED
16	W	516	CLA	C2B-C3B-CAB-CBB
16	X	501	CLA	C4B-C3B-CAB-CBB
16	X	502	CLA	C4B-C3B-CAB-CBB
16	X	502	CLA	CHA-CBD-CGD-O1D
16	X	502	CLA	CHA-CBD-CGD-O2D
16	X	503	CLA	C1A-C2A-CAA-CBA
16	X	504	CLA	C1A-C2A-CAA-CBA
16	X	504	CLA	C3A-C2A-CAA-CBA
16	X	504	CLA	CBD-CGD-O2D-CED
16	X	505	CLA	C4B-C3B-CAB-CBB
16	X	506	CLA	C1A-C2A-CAA-CBA
16	X	506	CLA	C3A-C2A-CAA-CBA
16	X	506	CLA	CBD-CGD-O2D-CED
16	X	506	CLA	O1D-CGD-O2D-CED
16	X	507	CLA	C4B-C3B-CAB-CBB
16	X	508	CLA	C4B-C3B-CAB-CBB
16	X	508	CLA	CBD-CGD-O2D-CED
16	X	513	CLA	C1A-C2A-CAA-CBA
16	X	513	CLA	C3A-C2A-CAA-CBA
16	X	513	CLA	C4B-C3B-CAB-CBB
16	X	513	CLA	CBD-CGD-O2D-CED
16	X	514	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	X	514	CLA	CBD-CGD-O2D-CED
16	X	514	CLA	O1D-CGD-O2D-CED
16	X	516	CLA	C1A-C2A-CAA-CBA
16	Y	501	CLA	CAD-CBD-CGD-O1D
16	Y	501	CLA	CAD-CBD-CGD-O2D
16	Y	502	CLA	C4B-C3B-CAB-CBB
16	Y	502	CLA	CHA-CBD-CGD-O1D
16	Y	502	CLA	CHA-CBD-CGD-O2D
16	Y	503	CLA	C1A-C2A-CAA-CBA
16	Y	503	CLA	C4B-C3B-CAB-CBB
16	Y	504	CLA	CHA-CBD-CGD-O1D
16	Y	504	CLA	CHA-CBD-CGD-O2D
16	Y	506	CLA	CBD-CGD-O2D-CED
16	Y	507	CLA	CBD-CGD-O2D-CED
16	Y	508	CLA	C1A-C2A-CAA-CBA
16	Y	508	CLA	C4B-C3B-CAB-CBB
16	Y	508	CLA	CHA-CBD-CGD-O1D
16	Y	508	CLA	CHA-CBD-CGD-O2D
16	Y	511	CLA	CBD-CGD-O2D-CED
16	Y	512	CLA	O1A-CGA-O2A-C1
16	Y	513	CLA	C1A-C2A-CAA-CBA
16	Y	513	CLA	C3A-C2A-CAA-CBA
16	Y	513	CLA	CBA-CGA-O2A-C1
16	Y	513	CLA	O1A-CGA-O2A-C1
16	Y	513	CLA	C4B-C3B-CAB-CBB
16	Y	514	CLA	CBD-CGD-O2D-CED
16	Y	515	CLA	O1A-CGA-O2A-C1
16	Y	515	CLA	CAD-CBD-CGD-O2D
16	Y	516	CLA	C1A-C2A-CAA-CBA
16	Y	516	CLA	C3A-C2A-CAA-CBA
16	Y	517	CLA	C3A-C2A-CAA-CBA
16	Y	517	CLA	C4B-C3B-CAB-CBB
16	Z	501	CLA	CAD-CBD-CGD-O1D
16	Z	501	CLA	CAD-CBD-CGD-O2D
16	Z	502	CLA	C4B-C3B-CAB-CBB
16	Z	503	CLA	C1A-C2A-CAA-CBA
16	Z	503	CLA	CBA-CGA-O2A-C1
16	Z	504	CLA	C3A-C2A-CAA-CBA
16	Z	504	CLA	C4B-C3B-CAB-CBB
16	Z	504	CLA	CBD-CGD-O2D-CED
16	Z	504	CLA	O1D-CGD-O2D-CED
16	Z	504	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	Z	507	CLA	CBA-CGA-O2A-C1
16	Z	507	CLA	CBD-CGD-O2D-CED
16	Z	508	CLA	C4B-C3B-CAB-CBB
16	Z	509	CLA	C1A-C2A-CAA-CBA
16	Z	509	CLA	C3A-C2A-CAA-CBA
16	Z	513	CLA	C4B-C3B-CAB-CBB
16	Z	513	CLA	CHA-CBD-CGD-O1D
16	Z	513	CLA	CHA-CBD-CGD-O2D
16	Z	516	CLA	C1A-C2A-CAA-CBA
16	Z	516	CLA	CAD-CBD-CGD-O1D
16	Z	516	CLA	CAD-CBD-CGD-O2D
16	Z	517	CLA	C2B-C3B-CAB-CBB
16	a	1101	CLA	C1A-C2A-CAA-CBA
16	a	1102	CLA	C3A-C2A-CAA-CBA
16	a	1104	CLA	CBD-CGD-O2D-CED
16	a	1106	CLA	CHA-CBD-CGD-O1D
16	a	1106	CLA	CHA-CBD-CGD-O2D
16	a	1107	CLA	C1A-C2A-CAA-CBA
16	a	1107	CLA	C4B-C3B-CAB-CBB
16	a	1108	CLA	C1A-C2A-CAA-CBA
16	a	1108	CLA	CBD-CGD-O2D-CED
16	a	1110	CLA	C4B-C3B-CAB-CBB
16	a	1111	CLA	C1A-C2A-CAA-CBA
16	a	1112	CLA	C1A-C2A-CAA-CBA
16	a	1114	CLA	C1A-C2A-CAA-CBA
16	a	1114	CLA	C4B-C3B-CAB-CBB
16	a	1114	CLA	CBD-CGD-O2D-CED
16	a	1115	CLA	C4-C3-C5-C6
16	a	1116	CLA	C3A-C2A-CAA-CBA
16	a	1118	CLA	C1A-C2A-CAA-CBA
16	a	1121	CLA	C1A-C2A-CAA-CBA
16	a	1121	CLA	C3A-C2A-CAA-CBA
16	a	1121	CLA	C4B-C3B-CAB-CBB
16	a	1122	CLA	C2B-C3B-CAB-CBB
16	a	1122	CLA	C4B-C3B-CAB-CBB
16	a	1128	CLA	CHA-CBD-CGD-O1D
16	a	1128	CLA	CHA-CBD-CGD-O2D
16	a	1130	CLA	C1A-C2A-CAA-CBA
16	a	1132	CLA	CHA-CBD-CGD-O1D
16	a	1132	CLA	CHA-CBD-CGD-O2D
16	a	1133	CLA	C2B-C3B-CAB-CBB
16	a	1133	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	a	1134	CLA	C4B-C3B-CAB-CBB
16	a	1135	CLA	C1A-C2A-CAA-CBA
16	a	1135	CLA	C3A-C2A-CAA-CBA
16	a	1136	CLA	C4B-C3B-CAB-CBB
16	a	1137	CLA	C1A-C2A-CAA-CBA
16	a	1137	CLA	C2B-C3B-CAB-CBB
16	a	1137	CLA	C4B-C3B-CAB-CBB
16	a	1137	CLA	CBD-CGD-O2D-CED
16	a	1138	CLA	C1A-C2A-CAA-CBA
16	a	1140	CLA	C1A-C2A-CAA-CBA
16	a	1140	CLA	C4B-C3B-CAB-CBB
16	a	1237	CLA	C1A-C2A-CAA-CBA
16	a	1237	CLA	C4B-C3B-CAB-CBB
16	b	1021	CLA	CBD-CGD-O2D-CED
16	b	1202	CLA	C1A-C2A-CAA-CBA
16	b	1202	CLA	C3A-C2A-CAA-CBA
16	b	1203	CLA	C4B-C3B-CAB-CBB
16	b	1203	CLA	CBD-CGD-O2D-CED
16	b	1204	CLA	C2B-C3B-CAB-CBB
16	b	1205	CLA	C4B-C3B-CAB-CBB
16	b	1205	CLA	CHA-CBD-CGD-O1D
16	b	1205	CLA	CHA-CBD-CGD-O2D
16	b	1206	CLA	C1A-C2A-CAA-CBA
16	b	1206	CLA	C3A-C2A-CAA-CBA
16	b	1206	CLA	CBD-CGD-O2D-CED
16	b	1207	CLA	C2B-C3B-CAB-CBB
16	b	1207	CLA	CHA-CBD-CGD-O2D
16	b	1207	CLA	CBD-CGD-O2D-CED
16	b	1208	CLA	C1A-C2A-CAA-CBA
16	b	1209	CLA	C1A-C2A-CAA-CBA
16	b	1209	CLA	C2B-C3B-CAB-CBB
16	b	1210	CLA	C1A-C2A-CAA-CBA
16	b	1210	CLA	C3A-C2A-CAA-CBA
16	b	1211	CLA	C1A-C2A-CAA-CBA
16	b	1213	CLA	C1A-C2A-CAA-CBA
16	b	1214	CLA	C1A-C2A-CAA-CBA
16	b	1214	CLA	C4B-C3B-CAB-CBB
16	b	1216	CLA	C4B-C3B-CAB-CBB
16	b	1217	CLA	C2B-C3B-CAB-CBB
16	b	1218	CLA	C2B-C3B-CAB-CBB
16	b	1219	CLA	CBD-CGD-O2D-CED
16	b	1222	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
16	b	1222	CLA	CHA-CBD-CGD-O2D
16	b	1227	CLA	C4B-C3B-CAB-CBB
16	b	1230	CLA	C1A-C2A-CAA-CBA
16	b	1230	CLA	C3A-C2A-CAA-CBA
16	b	1231	CLA	C1A-C2A-CAA-CBA
16	b	1231	CLA	C4B-C3B-CAB-CBB
16	b	1232	CLA	C4B-C3B-CAB-CBB
16	b	1232	CLA	CAD-CBD-CGD-O1D
16	b	1232	CLA	CAD-CBD-CGD-O2D
16	b	1235	CLA	C1A-C2A-CAA-CBA
16	b	1236	CLA	C1A-C2A-CAA-CBA
16	b	1238	CLA	C2B-C3B-CAB-CBB
16	b	1238	CLA	C4B-C3B-CAB-CBB
16	b	1239	CLA	C1A-C2A-CAA-CBA
16	b	1239	CLA	C4B-C3B-CAB-CBB
16	b	1239	CLA	CBD-CGD-O2D-CED
16	f	1301	CLA	C4B-C3B-CAB-CBB
16	f	1301	CLA	CBD-CGD-O2D-CED
16	g	501	CLA	C1A-C2A-CAA-CBA
16	g	501	CLA	CHA-CBD-CGD-O2D
16	g	502	CLA	C4B-C3B-CAB-CBB
16	g	503	CLA	C1A-C2A-CAA-CBA
16	g	504	CLA	C4B-C3B-CAB-CBB
16	g	504	CLA	CBD-CGD-O2D-CED
16	g	508	CLA	C1A-C2A-CAA-CBA
16	g	508	CLA	C3A-C2A-CAA-CBA
16	g	508	CLA	C4B-C3B-CAB-CBB
16	g	511	CLA	CBD-CGD-O2D-CED
16	g	512	CLA	C4B-C3B-CAB-CBB
16	g	512	CLA	C4-C3-C5-C6
16	g	513	CLA	C4B-C3B-CAB-CBB
16	g	513	CLA	CAD-CBD-CGD-O2D
16	g	513	CLA	CBD-CGD-O2D-CED
16	g	517	CLA	C1A-C2A-CAA-CBA
16	g	517	CLA	C4B-C3B-CAB-CBB
16	g	517	CLA	CBD-CGD-O2D-CED
16	h	501	CLA	C4B-C3B-CAB-CBB
16	h	501	CLA	CAD-CBD-CGD-O1D
16	h	501	CLA	CAD-CBD-CGD-O2D
16	h	502	CLA	C4B-C3B-CAB-CBB
16	h	503	CLA	CBA-CGA-O2A-C1
16	h	503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	h	503	CLA	CAD-CBD-CGD-O2D
16	h	504	CLA	C1A-C2A-CAA-CBA
16	h	504	CLA	CHA-CBD-CGD-O1D
16	h	504	CLA	CHA-CBD-CGD-O2D
16	h	505	CLA	CBD-CGD-O2D-CED
16	h	505	CLA	O1D-CGD-O2D-CED
16	h	506	CLA	C2B-C3B-CAB-CBB
16	h	506	CLA	C4B-C3B-CAB-CBB
16	h	507	CLA	C4B-C3B-CAB-CBB
16	h	507	CLA	CAD-CBD-CGD-O1D
16	h	507	CLA	CAD-CBD-CGD-O2D
16	h	507	CLA	C6-C7-C8-C9
16	h	508	CLA	C1A-C2A-CAA-CBA
16	h	508	CLA	C3A-C2A-CAA-CBA
16	h	508	CLA	C2B-C3B-CAB-CBB
16	h	509	CLA	C1A-C2A-CAA-CBA
16	h	509	CLA	C3A-C2A-CAA-CBA
16	h	509	CLA	CHA-CBD-CGD-O2D
16	h	510	CLA	CBD-CGD-O2D-CED
16	h	511	CLA	C2B-C3B-CAB-CBB
16	h	513	CLA	CBA-CGA-O2A-C1
16	h	513	CLA	O1A-CGA-O2A-C1
16	h	514	CLA	CBD-CGD-O2D-CED
16	h	515	CLA	CHA-CBD-CGD-O1D
16	h	515	CLA	CHA-CBD-CGD-O2D
16	h	515	CLA	C4-C3-C5-C6
16	h	516	CLA	C1A-C2A-CAA-CBA
16	h	516	CLA	CAD-CBD-CGD-O1D
16	h	516	CLA	CAD-CBD-CGD-O2D
16	j	1302	CLA	C4B-C3B-CAB-CBB
16	j	1302	CLA	CAD-CBD-CGD-O2D
16	j	1303	CLA	C4B-C3B-CAB-CBB
16	k	4002	CLA	C3A-C2A-CAA-CBA
16	k	4002	CLA	C4B-C3B-CAB-CBB
16	k	4003	CLA	C1A-C2A-CAA-CBA
16	k	4003	CLA	C3A-C2A-CAA-CBA
16	l	1503	CLA	C2-C1-O2A-CGA
16	n	501	CLA	C3A-C2A-CAA-CBA
16	n	501	CLA	C2B-C3B-CAB-CBB
16	n	501	CLA	C4B-C3B-CAB-CBB
16	n	502	CLA	C4B-C3B-CAB-CBB
16	n	503	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	n	503	CLA	CAD-CBD-CGD-O1D
16	n	503	CLA	CAD-CBD-CGD-O2D
16	n	505	CLA	C4B-C3B-CAB-CBB
16	n	505	CLA	CHA-CBD-CGD-O1D
16	n	505	CLA	CHA-CBD-CGD-O2D
16	n	506	CLA	CHA-CBD-CGD-O1D
16	n	506	CLA	CHA-CBD-CGD-O2D
16	n	507	CLA	C4B-C3B-CAB-CBB
16	n	507	CLA	CHA-CBD-CGD-O1D
16	n	507	CLA	CHA-CBD-CGD-O2D
16	n	508	CLA	C3A-C2A-CAA-CBA
16	n	508	CLA	C4B-C3B-CAB-CBB
16	n	508	CLA	CBD-CGD-O2D-CED
16	n	511	CLA	CBD-CGD-O2D-CED
16	n	512	CLA	CBD-CGD-O2D-CED
16	n	513	CLA	C1A-C2A-CAA-CBA
16	n	513	CLA	C3A-C2A-CAA-CBA
16	n	513	CLA	CBA-CGA-O2A-C1
16	n	513	CLA	O1A-CGA-O2A-C1
16	n	513	CLA	CAD-CBD-CGD-O1D
16	n	513	CLA	CAD-CBD-CGD-O2D
16	n	513	CLA	CBD-CGD-O2D-CED
16	n	514	CLA	CBD-CGD-O2D-CED
16	n	516	CLA	C1A-C2A-CAA-CBA
16	n	516	CLA	C2B-C3B-CAB-CBB
16	n	517	CLA	C4B-C3B-CAB-CBB
16	o	501	CLA	C1A-C2A-CAA-CBA
16	o	501	CLA	CBA-CGA-O2A-C1
16	o	501	CLA	O1A-CGA-O2A-C1
16	o	502	CLA	C4B-C3B-CAB-CBB
16	o	502	CLA	CHA-CBD-CGD-O1D
16	o	502	CLA	CHA-CBD-CGD-O2D
16	o	503	CLA	CBD-CGD-O2D-CED
16	o	504	CLA	C1A-C2A-CAA-CBA
16	o	504	CLA	CBD-CGD-O2D-CED
16	o	505	CLA	C4B-C3B-CAB-CBB
16	o	505	CLA	CBD-CGD-O2D-CED
16	o	506	CLA	CBD-CGD-O2D-CED
16	o	507	CLA	C2B-C3B-CAB-CBB
16	o	507	CLA	CBD-CGD-O2D-CED
16	o	508	CLA	C4B-C3B-CAB-CBB
16	o	508	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	o	511	CLA	C1A-C2A-CAA-CBA
16	o	513	CLA	C4B-C3B-CAB-CBB
16	o	514	CLA	CBD-CGD-O2D-CED
16	o	517	CLA	C1A-C2A-CAA-CBA
16	p	501	CLA	C2B-C3B-CAB-CBB
16	p	501	CLA	C4B-C3B-CAB-CBB
16	p	501	CLA	CAD-CBD-CGD-O1D
16	p	501	CLA	CAD-CBD-CGD-O2D
16	p	502	CLA	C4B-C3B-CAB-CBB
16	p	503	CLA	C4B-C3B-CAB-CBB
16	p	504	CLA	C3A-C2A-CAA-CBA
16	p	504	CLA	CHA-CBD-CGD-O1D
16	p	504	CLA	CHA-CBD-CGD-O2D
16	p	506	CLA	CHA-CBD-CGD-O2D
16	p	506	CLA	CBD-CGD-O2D-CED
16	p	507	CLA	CBD-CGD-O2D-CED
16	p	508	CLA	C1A-C2A-CAA-CBA
16	p	508	CLA	C4B-C3B-CAB-CBB
16	p	509	CLA	C2-C3-C5-C6
16	p	509	CLA	C4-C3-C5-C6
16	p	513	CLA	C1A-C2A-CAA-CBA
16	p	513	CLA	C3A-C2A-CAA-CBA
16	p	513	CLA	CBA-CGA-O2A-C1
16	p	513	CLA	O1A-CGA-O2A-C1
16	p	513	CLA	C4B-C3B-CAB-CBB
16	p	514	CLA	CBD-CGD-O2D-CED
16	p	515	CLA	CBA-CGA-O2A-C1
16	p	515	CLA	CAD-CBD-CGD-O1D
16	p	515	CLA	CAD-CBD-CGD-O2D
16	p	517	CLA	C3A-C2A-CAA-CBA
16	p	517	CLA	C4B-C3B-CAB-CBB
16	q	501	CLA	C1A-C2A-CAA-CBA
16	q	501	CLA	C3A-C2A-CAA-CBA
16	q	501	CLA	CAD-CBD-CGD-O1D
16	q	501	CLA	CAD-CBD-CGD-O2D
16	q	502	CLA	C4B-C3B-CAB-CBB
16	q	503	CLA	C1A-C2A-CAA-CBA
16	q	503	CLA	CBA-CGA-O2A-C1
16	q	503	CLA	O1A-CGA-O2A-C1
16	q	504	CLA	C1A-C2A-CAA-CBA
16	q	504	CLA	C4B-C3B-CAB-CBB
16	q	504	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	q	504	CLA	O1D-CGD-O2D-CED
16	q	508	CLA	C4B-C3B-CAB-CBB
16	q	510	CLA	C1A-C2A-CAA-CBA
16	q	510	CLA	C3A-C2A-CAA-CBA
16	q	510	CLA	C2B-C3B-CAB-CBB
16	q	513	CLA	C1A-C2A-CAA-CBA
16	q	513	CLA	C3A-C2A-CAA-CBA
16	q	513	CLA	C4B-C3B-CAB-CBB
16	q	513	CLA	CHA-CBD-CGD-O1D
16	q	513	CLA	CHA-CBD-CGD-O2D
16	q	514	CLA	C4B-C3B-CAB-CBB
16	q	516	CLA	C1A-C2A-CAA-CBA
16	q	516	CLA	C3A-C2A-CAA-CBA
16	q	516	CLA	CAD-CBD-CGD-O1D
16	q	516	CLA	CAD-CBD-CGD-O2D
16	q	517	CLA	C4B-C3B-CAB-CBB
16	q	517	CLA	CHA-CBD-CGD-O1D
16	q	517	CLA	CHA-CBD-CGD-O2D
16	r	501	CLA	C1A-C2A-CAA-CBA
16	r	501	CLA	C2B-C3B-CAB-CBB
16	r	501	CLA	C4B-C3B-CAB-CBB
16	r	502	CLA	C4B-C3B-CAB-CBB
16	r	503	CLA	C1A-C2A-CAA-CBA
16	r	504	CLA	CBD-CGD-O2D-CED
16	r	505	CLA	C4B-C3B-CAB-CBB
16	r	508	CLA	C4B-C3B-CAB-CBB
16	r	512	CLA	C2-C3-C5-C6
16	r	512	CLA	C4-C3-C5-C6
16	r	513	CLA	C1A-C2A-CAA-CBA
16	r	513	CLA	C3A-C2A-CAA-CBA
16	r	513	CLA	C4B-C3B-CAB-CBB
16	r	513	CLA	CAD-CBD-CGD-O1D
16	r	513	CLA	CAD-CBD-CGD-O2D
16	r	513	CLA	CBD-CGD-O2D-CED
16	r	515	CLA	O1A-CGA-O2A-C1
16	r	515	CLA	CHA-CBD-CGD-O1D
16	r	515	CLA	CHA-CBD-CGD-O2D
16	r	516	CLA	C4B-C3B-CAB-CBB
16	r	517	CLA	C1A-C2A-CAA-CBA
16	r	517	CLA	CHA-CBD-CGD-O1D
16	r	517	CLA	CHA-CBD-CGD-O2D
16	s	501	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	s	501	CLA	C4B-C3B-CAB-CBB
16	s	501	CLA	CAD-CBD-CGD-O1D
16	s	501	CLA	CAD-CBD-CGD-O2D
16	s	502	CLA	C4B-C3B-CAB-CBB
16	s	503	CLA	C1A-C2A-CAA-CBA
16	s	503	CLA	C4B-C3B-CAB-CBB
16	s	504	CLA	CHA-CBD-CGD-O1D
16	s	504	CLA	CHA-CBD-CGD-O2D
16	s	508	CLA	C1A-C2A-CAA-CBA
16	s	508	CLA	C4B-C3B-CAB-CBB
16	s	508	CLA	CHA-CBD-CGD-O1D
16	s	508	CLA	CHA-CBD-CGD-O2D
16	s	511	CLA	CBD-CGD-O2D-CED
16	s	513	CLA	C1A-C2A-CAA-CBA
16	s	513	CLA	CBA-CGA-O2A-C1
16	s	513	CLA	O1A-CGA-O2A-C1
16	s	513	CLA	C4B-C3B-CAB-CBB
16	s	513	CLA	CAD-CBD-CGD-O2D
16	s	514	CLA	CBD-CGD-O2D-CED
16	s	515	CLA	CAD-CBD-CGD-O1D
16	s	515	CLA	CAD-CBD-CGD-O2D
16	s	516	CLA	CAD-CBD-CGD-O1D
16	s	516	CLA	CAD-CBD-CGD-O2D
16	s	517	CLA	C4B-C3B-CAB-CBB
16	t	501	CLA	C1A-C2A-CAA-CBA
16	t	501	CLA	C3A-C2A-CAA-CBA
16	t	501	CLA	CAD-CBD-CGD-O1D
16	t	501	CLA	CAD-CBD-CGD-O2D
16	t	502	CLA	CHA-CBD-CGD-O1D
16	t	502	CLA	CHA-CBD-CGD-O2D
16	t	503	CLA	C4B-C3B-CAB-CBB
16	t	503	CLA	CAD-CBD-CGD-O1D
16	t	503	CLA	CAD-CBD-CGD-O2D
16	t	505	CLA	C4B-C3B-CAB-CBB
16	t	506	CLA	CHA-CBD-CGD-O1D
16	t	506	CLA	CHA-CBD-CGD-O2D
16	t	507	CLA	C4B-C3B-CAB-CBB
16	t	507	CLA	CBD-CGD-O2D-CED
16	t	508	CLA	C1A-C2A-CAA-CBA
16	t	508	CLA	C3A-C2A-CAA-CBA
16	t	508	CLA	C4B-C3B-CAB-CBB
16	t	508	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	t	508	CLA	O1D-CGD-O2D-CED
16	t	511	CLA	CBD-CGD-O2D-CED
16	t	512	CLA	CBD-CGD-O2D-CED
16	t	513	CLA	CAD-CBD-CGD-O1D
16	t	513	CLA	CAD-CBD-CGD-O2D
16	t	513	CLA	CBD-CGD-O2D-CED
16	t	514	CLA	CBD-CGD-O2D-CED
16	t	515	CLA	CHA-CBD-CGD-O1D
16	t	515	CLA	CHA-CBD-CGD-O2D
16	t	516	CLA	CAD-CBD-CGD-O2D
16	t	517	CLA	C4B-C3B-CAB-CBB
16	u	501	CLA	C1A-C2A-CAA-CBA
16	u	501	CLA	CBA-CGA-O2A-C1
16	u	501	CLA	O1A-CGA-O2A-C1
16	u	502	CLA	C4B-C3B-CAB-CBB
16	u	502	CLA	CHA-CBD-CGD-O1D
16	u	502	CLA	CHA-CBD-CGD-O2D
16	u	504	CLA	C1A-C2A-CAA-CBA
16	u	504	CLA	CBD-CGD-O2D-CED
16	u	504	CLA	C11-C10-C8-C9
16	u	505	CLA	C4B-C3B-CAB-CBB
16	u	505	CLA	CBD-CGD-O2D-CED
16	u	506	CLA	C1A-C2A-CAA-CBA
16	u	506	CLA	CBD-CGD-O2D-CED
16	u	507	CLA	C2B-C3B-CAB-CBB
16	u	508	CLA	C4B-C3B-CAB-CBB
16	u	508	CLA	CBD-CGD-O2D-CED
16	u	508	CLA	C2-C3-C5-C6
16	u	508	CLA	C4-C3-C5-C6
16	u	511	CLA	C1A-C2A-CAA-CBA
16	u	513	CLA	C1A-C2A-CAA-CBA
16	u	513	CLA	C4B-C3B-CAB-CBB
16	u	513	CLA	CBD-CGD-O2D-CED
16	u	514	CLA	C4B-C3B-CAB-CBB
16	u	514	CLA	CBD-CGD-O2D-CED
16	u	515	CLA	CBD-CGD-O2D-CED
16	u	516	CLA	CHA-CBD-CGD-O1D
16	u	516	CLA	CHA-CBD-CGD-O2D
16	u	516	CLA	CBD-CGD-O2D-CED
16	v	501	CLA	CAD-CBD-CGD-O1D
16	v	501	CLA	CAD-CBD-CGD-O2D
16	v	502	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	v	503	CLA	CAD-CBD-CGD-O1D
16	v	503	CLA	CAD-CBD-CGD-O2D
16	v	504	CLA	C1A-C2A-CAA-CBA
16	v	504	CLA	C3A-C2A-CAA-CBA
16	v	504	CLA	CHA-CBD-CGD-O1D
16	v	504	CLA	CHA-CBD-CGD-O2D
16	v	505	CLA	CBD-CGD-O2D-CED
16	v	505	CLA	O1D-CGD-O2D-CED
16	v	506	CLA	CBD-CGD-O2D-CED
16	v	507	CLA	C4B-C3B-CAB-CBB
16	v	508	CLA	C1A-C2A-CAA-CBA
16	v	508	CLA	C3A-C2A-CAA-CBA
16	v	508	CLA	C2B-C3B-CAB-CBB
16	v	508	CLA	C4B-C3B-CAB-CBB
16	v	509	CLA	C1A-C2A-CAA-CBA
16	v	509	CLA	C3A-C2A-CAA-CBA
16	v	509	CLA	CHA-CBD-CGD-O1D
16	v	509	CLA	CHA-CBD-CGD-O2D
16	v	511	CLA	CBD-CGD-O2D-CED
16	v	513	CLA	C1A-C2A-CAA-CBA
16	v	513	CLA	C3A-C2A-CAA-CBA
16	v	514	CLA	C1A-C2A-CAA-CBA
16	v	515	CLA	CHA-CBD-CGD-O1D
16	v	515	CLA	CHA-CBD-CGD-O2D
16	v	516	CLA	C1A-C2A-CAA-CBA
16	v	516	CLA	C4B-C3B-CAB-CBB
16	v	517	CLA	CBD-CGD-O2D-CED
16	w	501	CLA	C1A-C2A-CAA-CBA
16	w	501	CLA	CAD-CBD-CGD-O1D
16	w	501	CLA	CAD-CBD-CGD-O2D
16	w	502	CLA	C4B-C3B-CAB-CBB
16	w	503	CLA	C1A-C2A-CAA-CBA
16	w	503	CLA	CBA-CGA-O2A-C1
16	w	504	CLA	C1A-C2A-CAA-CBA
16	w	504	CLA	CBD-CGD-O2D-CED
16	w	504	CLA	O1D-CGD-O2D-CED
16	w	507	CLA	CBD-CGD-O2D-CED
16	w	508	CLA	C4B-C3B-CAB-CBB
16	w	509	CLA	C1A-C2A-CAA-CBA
16	w	509	CLA	C3A-C2A-CAA-CBA
16	w	510	CLA	C1A-C2A-CAA-CBA
16	w	510	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	w	511	CLA	CBD-CGD-O2D-CED
16	w	513	CLA	C1A-C2A-CAA-CBA
16	w	513	CLA	C4B-C3B-CAB-CBB
16	w	513	CLA	CHA-CBD-CGD-O1D
16	w	513	CLA	CHA-CBD-CGD-O2D
16	w	516	CLA	CBA-CGA-O2A-C1
16	w	516	CLA	CAD-CBD-CGD-O1D
16	w	516	CLA	CAD-CBD-CGD-O2D
16	w	517	CLA	C4B-C3B-CAB-CBB
16	x	501	CLA	C1A-C2A-CAA-CBA
16	x	501	CLA	CAD-CBD-CGD-O1D
16	x	501	CLA	CAD-CBD-CGD-O2D
16	x	503	CLA	C4B-C3B-CAB-CBB
16	x	504	CLA	C1A-C2A-CAA-CBA
16	x	504	CLA	CBD-CGD-O2D-CED
16	x	505	CLA	C4B-C3B-CAB-CBB
16	x	505	CLA	CBD-CGD-O2D-CED
16	x	506	CLA	C2B-C3B-CAB-CBB
16	x	508	CLA	C4B-C3B-CAB-CBB
16	x	508	CLA	CAD-CBD-CGD-O1D
16	x	508	CLA	CAD-CBD-CGD-O2D
16	x	509	CLA	C1A-C2A-CAA-CBA
16	x	509	CLA	C3A-C2A-CAA-CBA
16	x	513	CLA	CBA-CGA-O2A-C1
16	x	513	CLA	O1A-CGA-O2A-C1
16	x	513	CLA	C4B-C3B-CAB-CBB
16	x	513	CLA	CAD-CBD-CGD-O1D
16	x	513	CLA	CAD-CBD-CGD-O2D
16	x	515	CLA	CHA-CBD-CGD-O1D
16	x	515	CLA	CHA-CBD-CGD-O2D
16	x	516	CLA	CHA-CBD-CGD-O1D
16	x	516	CLA	CHA-CBD-CGD-O2D
16	x	517	CLA	C4B-C3B-CAB-CBB
16	x	517	CLA	CAD-CBD-CGD-O2D
16	y	501	CLA	C4B-C3B-CAB-CBB
16	y	501	CLA	CAD-CBD-CGD-O1D
16	y	501	CLA	CAD-CBD-CGD-O2D
16	y	502	CLA	C4B-C3B-CAB-CBB
16	y	502	CLA	CBD-CGD-O2D-CED
16	y	503	CLA	CBA-CGA-O2A-C1
16	y	503	CLA	O1A-CGA-O2A-C1
16	y	504	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
16	y	504	CLA	CHA-CBD-CGD-O2D
16	y	505	CLA	CBD-CGD-O2D-CED
16	y	506	CLA	CBD-CGD-O2D-CED
16	y	507	CLA	C4B-C3B-CAB-CBB
16	y	508	CLA	C1A-C2A-CAA-CBA
16	y	508	CLA	C3A-C2A-CAA-CBA
16	y	508	CLA	CAD-CBD-CGD-O1D
16	y	508	CLA	CAD-CBD-CGD-O2D
16	y	509	CLA	C1A-C2A-CAA-CBA
16	y	509	CLA	C3A-C2A-CAA-CBA
16	y	509	CLA	CHA-CBD-CGD-O1D
16	y	509	CLA	CHA-CBD-CGD-O2D
16	y	510	CLA	CBD-CGD-O2D-CED
16	y	511	CLA	CBD-CGD-O2D-CED
16	y	512	CLA	CBD-CGD-O2D-CED
16	y	513	CLA	CBA-CGA-O2A-C1
16	y	513	CLA	O1A-CGA-O2A-C1
16	y	514	CLA	C1A-C2A-CAA-CBA
16	y	514	CLA	C2B-C3B-CAB-CBB
16	y	514	CLA	C4B-C3B-CAB-CBB
16	y	515	CLA	CHA-CBD-CGD-O1D
16	y	515	CLA	CHA-CBD-CGD-O2D
16	y	516	CLA	C1A-C2A-CAA-CBA
16	y	516	CLA	CAD-CBD-CGD-O1D
16	y	516	CLA	CAD-CBD-CGD-O2D
16	y	517	CLA	C2-C1-O2A-CGA
16	y	517	CLA	CAD-CBD-CGD-O1D
16	y	517	CLA	CAD-CBD-CGD-O2D
19	A	4002	BCR	C7-C8-C9-C34
19	A	4002	BCR	C21-C22-C23-C24
19	A	4003	BCR	C6-C7-C8-C9
19	A	4003	BCR	C18-C19-C20-C21
19	A	4003	BCR	C20-C21-C22-C23
19	A	4003	BCR	C20-C21-C22-C37
19	A	4003	BCR	C22-C23-C24-C25
19	A	4007	BCR	C21-C22-C23-C24
19	A	4008	BCR	C7-C8-C9-C10
19	A	4008	BCR	C20-C21-C22-C37
19	A	4011	BCR	C11-C10-C9-C8
19	A	4011	BCR	C11-C10-C9-C34
19	A	4011	BCR	C18-C19-C20-C21
19	A	4011	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
19	A	4011	BCR	C21-C22-C23-C24
19	B	4004	BCR	C7-C8-C9-C10
19	B	4004	BCR	C18-C19-C20-C21
19	B	4004	BCR	C37-C22-C23-C24
19	B	4004	BCR	C22-C23-C24-C25
19	B	4005	BCR	C7-C8-C9-C34
19	B	4005	BCR	C21-C22-C23-C24
19	B	4005	BCR	C37-C22-C23-C24
19	B	4009	BCR	C18-C19-C20-C21
19	B	4009	BCR	C20-C21-C22-C23
19	B	4009	BCR	C20-C21-C22-C37
19	B	4010	BCR	C10-C11-C12-C13
19	B	4010	BCR	C17-C18-C19-C20
19	B	4010	BCR	C18-C19-C20-C21
19	B	4010	BCR	C20-C21-C22-C23
19	B	4010	BCR	C21-C22-C23-C24
19	B	4010	BCR	C22-C23-C24-C25
19	B	4014	BCR	C7-C8-C9-C10
19	B	4014	BCR	C7-C8-C9-C34
19	B	4014	BCR	C12-C13-C14-C15
19	B	4014	BCR	C35-C13-C14-C15
19	B	4014	BCR	C17-C18-C19-C20
19	B	4014	BCR	C18-C19-C20-C21
19	B	4014	BCR	C20-C21-C22-C37
19	B	4017	BCR	C11-C10-C9-C34
19	B	4017	BCR	C20-C21-C22-C23
19	B	4017	BCR	C20-C21-C22-C37
19	B	4017	BCR	C21-C22-C23-C24
19	G	4004	BCR	C18-C19-C20-C21
19	G	4005	BCR	C21-C22-C23-C24
19	G	4005	BCR	C37-C22-C23-C24
19	G	4010	BCR	C6-C7-C8-C9
19	G	4010	BCR	C15-C16-C17-C18
19	G	4010	BCR	C17-C18-C19-C20
19	G	4010	BCR	C18-C19-C20-C21
19	G	4010	BCR	C21-C22-C23-C24
19	G	4010	BCR	C22-C23-C24-C25
19	G	4014	BCR	C7-C8-C9-C10
19	G	4014	BCR	C7-C8-C9-C34
19	G	4014	BCR	C12-C13-C14-C15
19	G	4014	BCR	C35-C13-C14-C15
19	G	4014	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
19	G	4014	BCR	C37-C22-C23-C24
19	G	4017	BCR	C10-C11-C12-C13
19	G	4017	BCR	C20-C21-C22-C37
19	G	4017	BCR	C21-C22-C23-C24
19	H	4002	BCR	C6-C7-C8-C9
19	H	4002	BCR	C21-C22-C23-C24
19	H	4003	BCR	C7-C8-C9-C10
19	H	4003	BCR	C7-C8-C9-C34
19	H	4003	BCR	C21-C22-C23-C24
19	H	4007	BCR	C21-C22-C23-C24
19	H	4008	BCR	C7-C8-C9-C34
19	H	4008	BCR	C18-C19-C20-C21
19	H	4011	BCR	C11-C10-C9-C8
19	H	4011	BCR	C11-C10-C9-C34
19	H	4011	BCR	C10-C11-C12-C13
19	H	4011	BCR	C21-C22-C23-C24
19	I	4018	BCR	C20-C21-C22-C23
19	I	4018	BCR	C21-C22-C23-C24
19	I	4018	BCR	C37-C22-C23-C24
19	J	4012	BCR	C6-C7-C8-C9
19	J	4012	BCR	C7-C8-C9-C10
19	J	4012	BCR	C7-C8-C9-C34
19	J	4012	BCR	C21-C22-C23-C24
19	J	4012	BCR	C37-C22-C23-C24
19	J	4013	BCR	C18-C19-C20-C21
19	J	4013	BCR	C21-C22-C23-C24
19	J	4015	BCR	C7-C8-C9-C10
19	J	4015	BCR	C22-C23-C24-C25
19	K	4001	BCR	C21-C22-C23-C24
19	K	4005	BCR	C37-C22-C23-C24
19	L	4019	BCR	C7-C8-C9-C10
19	L	4022	BCR	C7-C8-C9-C10
19	L	4022	BCR	C20-C21-C22-C37
19	Q	4016	BCR	C11-C10-C9-C8
19	R	4018	BCR	C21-C22-C23-C24
19	S	4012	BCR	C6-C7-C8-C9
19	S	4012	BCR	C7-C8-C9-C10
19	S	4012	BCR	C7-C8-C9-C34
19	S	4012	BCR	C21-C22-C23-C24
19	S	4012	BCR	C37-C22-C23-C24
19	S	4013	BCR	C18-C19-C20-C21
19	S	4013	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	S	4015	BCR	C7-C8-C9-C10
19	S	4015	BCR	C7-C8-C9-C34
19	S	4015	BCR	C22-C23-C24-C25
19	T	4001	BCR	C21-C22-C23-C24
19	T	4001	BCR	C37-C22-C23-C24
19	T	4005	BCR	C6-C7-C8-C9
19	T	4005	BCR	C37-C22-C23-C24
19	U	4019	BCR	C7-C8-C9-C10
19	U	4019	BCR	C37-C22-C23-C24
19	U	4019	BCR	C23-C24-C25-C26
19	U	4019	BCR	C23-C24-C25-C30
19	U	4022	BCR	C6-C7-C8-C9
19	U	4022	BCR	C7-C8-C9-C10
19	W	601	BCR	C7-C8-C9-C10
19	W	601	BCR	C10-C11-C12-C13
19	W	601	BCR	C17-C18-C19-C20
19	W	601	BCR	C36-C18-C19-C20
19	W	601	BCR	C20-C21-C22-C23
19	W	601	BCR	C20-C21-C22-C37
19	W	601	BCR	C37-C22-C23-C24
19	W	601	BCR	C22-C23-C24-C25
19	W	603	BCR	C6-C7-C8-C9
19	W	603	BCR	C7-C8-C9-C10
19	W	603	BCR	C7-C8-C9-C34
19	W	603	BCR	C10-C11-C12-C13
19	W	604	BCR	C10-C11-C12-C13
19	W	604	BCR	C22-C23-C24-C25
19	X	601	BCR	C21-C22-C23-C24
19	X	602	BCR	C6-C7-C8-C9
19	X	602	BCR	C7-C8-C9-C10
19	X	602	BCR	C7-C8-C9-C34
19	X	602	BCR	C10-C11-C12-C13
19	X	602	BCR	C14-C15-C16-C17
19	X	602	BCR	C20-C21-C22-C23
19	X	602	BCR	C20-C21-C22-C37
19	X	603	BCR	C6-C7-C8-C9
19	X	603	BCR	C20-C21-C22-C37
19	X	603	BCR	C22-C23-C24-C25
19	X	604	BCR	C7-C8-C9-C10
19	X	604	BCR	C7-C8-C9-C34
19	X	604	BCR	C16-C17-C18-C19
19	X	604	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
19	X	604	BCR	C18-C19-C20-C21
19	X	604	BCR	C20-C21-C22-C23
19	X	604	BCR	C20-C21-C22-C37
19	Y	601	BCR	C7-C8-C9-C10
19	Y	601	BCR	C7-C8-C9-C34
19	Y	601	BCR	C20-C21-C22-C37
19	Y	602	BCR	C21-C22-C23-C24
19	Y	603	BCR	C20-C21-C22-C37
19	Y	603	BCR	C22-C23-C24-C25
19	Y	604	BCR	C6-C7-C8-C9
19	Y	604	BCR	C7-C8-C9-C34
19	Y	604	BCR	C11-C10-C9-C8
19	Y	604	BCR	C11-C12-C13-C14
19	Y	604	BCR	C11-C12-C13-C35
19	Y	604	BCR	C21-C22-C23-C24
19	Y	604	BCR	C37-C22-C23-C24
19	Z	602	BCR	C20-C21-C22-C37
19	Z	602	BCR	C21-C22-C23-C24
19	Z	603	BCR	C20-C21-C22-C37
19	Z	604	BCR	C7-C8-C9-C10
19	Z	604	BCR	C7-C8-C9-C34
19	Z	604	BCR	C11-C10-C9-C8
19	Z	604	BCR	C11-C10-C9-C34
19	Z	604	BCR	C10-C11-C12-C13
19	Z	604	BCR	C11-C12-C13-C14
19	Z	604	BCR	C11-C12-C13-C35
19	Z	604	BCR	C14-C15-C16-C17
19	a	4002	BCR	C11-C12-C13-C35
19	a	4002	BCR	C20-C21-C22-C37
19	a	4002	BCR	C21-C22-C23-C24
19	a	4003	BCR	C6-C7-C8-C9
19	a	4003	BCR	C21-C22-C23-C24
19	a	4008	BCR	C7-C8-C9-C10
19	a	4008	BCR	C7-C8-C9-C34
19	a	4008	BCR	C37-C22-C23-C24
19	a	4008	BCR	C22-C23-C24-C25
19	a	4008	BCR	C23-C24-C25-C26
19	a	4008	BCR	C23-C24-C25-C30
19	a	4011	BCR	C11-C10-C9-C8
19	a	4011	BCR	C11-C10-C9-C34
19	a	4011	BCR	C20-C21-C22-C37
19	a	4011	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	a	4011	BCR	C37-C22-C23-C24
19	b	4004	BCR	C37-C22-C23-C24
19	b	4005	BCR	C6-C7-C8-C9
19	b	4005	BCR	C7-C8-C9-C34
19	b	4005	BCR	C21-C22-C23-C24
19	b	4005	BCR	C37-C22-C23-C24
19	b	4009	BCR	C18-C19-C20-C21
19	b	4009	BCR	C20-C21-C22-C23
19	b	4009	BCR	C20-C21-C22-C37
19	b	4010	BCR	C10-C11-C12-C13
19	b	4010	BCR	C17-C18-C19-C20
19	b	4010	BCR	C18-C19-C20-C21
19	b	4010	BCR	C21-C22-C23-C24
19	b	4010	BCR	C22-C23-C24-C25
19	b	4014	BCR	C7-C8-C9-C10
19	b	4014	BCR	C35-C13-C14-C15
19	b	4017	BCR	C20-C21-C22-C23
19	b	4017	BCR	C20-C21-C22-C37
19	b	4017	BCR	C21-C22-C23-C24
19	f	4016	BCR	C37-C22-C23-C24
19	g	601	BCR	C7-C8-C9-C10
19	g	601	BCR	C7-C8-C9-C34
19	g	601	BCR	C16-C17-C18-C36
19	g	601	BCR	C37-C22-C23-C24
19	g	602	BCR	C10-C11-C12-C13
19	g	602	BCR	C20-C21-C22-C37
19	g	602	BCR	C37-C22-C23-C24
19	g	603	BCR	C6-C7-C8-C9
19	g	603	BCR	C9-C10-C11-C12
19	g	603	BCR	C10-C11-C12-C13
19	g	603	BCR	C18-C19-C20-C21
19	g	603	BCR	C20-C21-C22-C23
19	g	603	BCR	C20-C21-C22-C37
19	g	604	BCR	C6-C7-C8-C9
19	g	604	BCR	C7-C8-C9-C10
19	g	604	BCR	C18-C19-C20-C21
19	g	604	BCR	C21-C22-C23-C24
19	h	601	BCR	C20-C21-C22-C37
19	h	601	BCR	C37-C22-C23-C24
19	h	603	BCR	C6-C7-C8-C9
19	h	603	BCR	C7-C8-C9-C10
19	h	603	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
19	h	604	BCR	C7-C8-C9-C34
19	h	604	BCR	C21-C22-C23-C24
19	h	604	BCR	C22-C23-C24-C25
19	i	4018	BCR	C21-C22-C23-C24
19	i	4018	BCR	C37-C22-C23-C24
19	j	4012	BCR	C7-C8-C9-C10
19	j	4012	BCR	C7-C8-C9-C34
19	j	4012	BCR	C21-C22-C23-C24
19	j	4012	BCR	C37-C22-C23-C24
19	j	4013	BCR	C16-C17-C18-C36
19	j	4013	BCR	C18-C19-C20-C21
19	j	4013	BCR	C20-C21-C22-C23
19	j	4013	BCR	C21-C22-C23-C24
19	j	4015	BCR	C7-C8-C9-C34
19	j	4015	BCR	C16-C17-C18-C36
19	j	4015	BCR	C22-C23-C24-C25
19	k	4001	BCR	C21-C22-C23-C24
19	k	4005	BCR	C37-C22-C23-C24
19	l	4019	BCR	C37-C22-C23-C24
19	l	4022	BCR	C6-C7-C8-C9
19	l	4022	BCR	C7-C8-C9-C10
19	l	4022	BCR	C17-C18-C19-C20
19	l	4022	BCR	C19-C20-C21-C22
19	l	4022	BCR	C20-C21-C22-C37
19	n	601	BCR	C7-C8-C9-C10
19	n	601	BCR	C19-C20-C21-C22
19	n	601	BCR	C20-C21-C22-C37
19	n	601	BCR	C37-C22-C23-C24
19	n	603	BCR	C6-C7-C8-C9
19	n	603	BCR	C10-C11-C12-C13
19	n	604	BCR	C15-C16-C17-C18
19	n	604	BCR	C22-C23-C24-C25
19	o	601	BCR	C21-C22-C23-C24
19	o	601	BCR	C37-C22-C23-C24
19	o	602	BCR	C6-C7-C8-C9
19	o	602	BCR	C18-C19-C20-C21
19	o	602	BCR	C20-C21-C22-C23
19	o	602	BCR	C20-C21-C22-C37
19	o	603	BCR	C6-C7-C8-C9
19	o	603	BCR	C7-C8-C9-C10
19	o	603	BCR	C7-C8-C9-C34
19	o	604	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	p	601	BCR	C20-C21-C22-C37
19	p	601	BCR	C21-C22-C23-C24
19	p	602	BCR	C21-C22-C23-C24
19	p	603	BCR	C20-C21-C22-C37
19	p	604	BCR	C6-C7-C8-C9
19	p	604	BCR	C7-C8-C9-C34
19	p	604	BCR	C21-C22-C23-C24
19	p	604	BCR	C37-C22-C23-C24
19	q	602	BCR	C21-C22-C23-C24
19	q	604	BCR	C11-C12-C13-C14
19	q	604	BCR	C11-C12-C13-C35
19	q	604	BCR	C21-C22-C23-C24
19	r	601	BCR	C7-C8-C9-C10
19	r	601	BCR	C7-C8-C9-C34
19	r	601	BCR	C10-C11-C12-C13
19	r	601	BCR	C20-C21-C22-C37
19	r	601	BCR	C21-C22-C23-C24
19	r	601	BCR	C37-C22-C23-C24
19	r	602	BCR	C7-C8-C9-C34
19	r	602	BCR	C11-C10-C9-C8
19	r	602	BCR	C10-C11-C12-C13
19	r	602	BCR	C37-C22-C23-C24
19	r	603	BCR	C20-C21-C22-C23
19	r	603	BCR	C20-C21-C22-C37
19	r	604	BCR	C6-C7-C8-C9
19	r	604	BCR	C11-C10-C9-C34
19	r	604	BCR	C18-C19-C20-C21
19	r	604	BCR	C21-C22-C23-C24
19	s	601	BCR	C7-C8-C9-C10
19	s	601	BCR	C21-C22-C23-C24
19	s	601	BCR	C37-C22-C23-C24
19	s	604	BCR	C6-C7-C8-C9
19	s	604	BCR	C7-C8-C9-C34
19	s	604	BCR	C11-C12-C13-C14
19	s	604	BCR	C11-C12-C13-C35
19	s	604	BCR	C21-C22-C23-C24
19	t	601	BCR	C7-C8-C9-C10
19	t	601	BCR	C10-C11-C12-C13
19	t	601	BCR	C11-C12-C13-C14
19	t	601	BCR	C11-C12-C13-C35
19	t	601	BCR	C18-C19-C20-C21
19	t	601	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
19	t	603	BCR	C7-C8-C9-C10
19	t	603	BCR	C7-C8-C9-C34
19	t	603	BCR	C11-C10-C9-C8
19	t	603	BCR	C20-C21-C22-C37
19	t	604	BCR	C7-C8-C9-C10
19	t	604	BCR	C7-C8-C9-C34
19	t	604	BCR	C11-C10-C9-C8
19	t	604	BCR	C11-C10-C9-C34
19	t	604	BCR	C10-C11-C12-C13
19	t	604	BCR	C22-C23-C24-C25
19	u	601	BCR	C7-C8-C9-C10
19	u	601	BCR	C7-C8-C9-C34
19	u	601	BCR	C37-C22-C23-C24
19	u	602	BCR	C7-C8-C9-C34
19	u	603	BCR	C6-C7-C8-C9
19	u	603	BCR	C7-C8-C9-C10
19	u	603	BCR	C7-C8-C9-C34
19	u	604	BCR	C20-C21-C22-C23
19	u	604	BCR	C20-C21-C22-C37
19	u	604	BCR	C21-C22-C23-C24
19	u	604	BCR	C22-C23-C24-C25
19	v	601	BCR	C21-C22-C23-C24
19	v	601	BCR	C37-C22-C23-C24
19	v	601	BCR	C22-C23-C24-C25
19	v	603	BCR	C6-C7-C8-C9
19	v	603	BCR	C7-C8-C9-C10
19	v	603	BCR	C21-C22-C23-C24
19	v	603	BCR	C22-C23-C24-C25
19	v	604	BCR	C7-C8-C9-C34
19	v	604	BCR	C21-C22-C23-C24
19	v	604	BCR	C22-C23-C24-C25
19	v	604	BCR	C23-C24-C25-C26
19	w	603	BCR	C6-C7-C8-C9
19	w	603	BCR	C7-C8-C9-C10
19	w	603	BCR	C10-C11-C12-C13
19	w	603	BCR	C20-C21-C22-C37
19	w	604	BCR	C11-C10-C9-C34
19	w	604	BCR	C11-C12-C13-C14
19	w	604	BCR	C11-C12-C13-C35
19	w	604	BCR	C21-C22-C23-C24
19	x	601	BCR	C7-C8-C9-C10
19	x	601	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
19	x	602	BCR	C6-C7-C8-C9
19	x	602	BCR	C11-C10-C9-C8
19	x	602	BCR	C11-C10-C9-C34
19	x	602	BCR	C10-C11-C12-C13
19	x	602	BCR	C11-C12-C13-C35
19	x	602	BCR	C14-C15-C16-C17
19	x	602	BCR	C21-C22-C23-C24
19	x	602	BCR	C37-C22-C23-C24
19	x	603	BCR	C6-C7-C8-C9
19	x	603	BCR	C18-C19-C20-C21
19	x	604	BCR	C6-C7-C8-C9
19	x	604	BCR	C18-C19-C20-C21
19	x	604	BCR	C21-C22-C23-C24
19	y	601	BCR	C21-C22-C23-C24
19	y	601	BCR	C22-C23-C24-C25
19	y	603	BCR	C6-C7-C8-C9
19	y	603	BCR	C7-C8-C9-C10
19	y	603	BCR	C22-C23-C24-C25
19	y	604	BCR	C7-C8-C9-C34
19	y	604	BCR	C21-C22-C23-C24
19	y	604	BCR	C22-C23-C24-C25
21	B	4006	ECH	C7-C8-C9-C10
21	B	4006	ECH	C7-C8-C9-C34
21	B	4006	ECH	C21-C22-C23-C24
21	B	4006	ECH	C37-C22-C23-C24
21	G	4006	ECH	C7-C8-C9-C10
21	G	4006	ECH	C7-C8-C9-C34
21	G	4006	ECH	C21-C22-C23-C24
21	I	4020	ECH	C1-C6-C7-C8
21	I	4020	ECH	C7-C8-C9-C10
21	I	4020	ECH	C7-C8-C9-C34
21	I	4020	ECH	C9-C10-C11-C12
21	I	4020	ECH	C11-C12-C13-C14
21	I	4020	ECH	C11-C12-C13-C35
21	I	4020	ECH	C21-C22-C23-C24
21	I	4020	ECH	C37-C22-C23-C24
21	M	4021	ECH	C9-C10-C11-C12
21	M	4021	ECH	C21-C22-C23-C24
21	M	4021	ECH	C37-C22-C23-C24
21	M	4021	ECH	C23-C24-C25-C26
21	R	4020	ECH	C11-C12-C13-C14
21	R	4020	ECH	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
21	V	4021	ECH	C11-C12-C13-C35
21	V	4021	ECH	C21-C22-C23-C24
21	V	4021	ECH	C37-C22-C23-C24
21	V	4021	ECH	C23-C24-C25-C26
21	b	4006	ECH	C21-C22-C23-C24
21	i	4020	ECH	C11-C12-C13-C14
21	i	4020	ECH	C21-C22-C23-C24
21	i	4020	ECH	C37-C22-C23-C24
21	m	4021	ECH	C7-C8-C9-C10
21	m	4021	ECH	C7-C8-C9-C34
21	m	4021	ECH	C11-C12-C13-C35
21	m	4021	ECH	C23-C24-C25-C26
23	Y	606	LMU	C2'-C1'-O1'-C1
23	Y	606	LMU	O5'-C1'-O1'-C1
23	p	606	LMU	C2'-C1'-O1'-C1
23	p	606	LMU	O5'-C1'-O1'-C1
23	q	605	LMU	C2'-C1'-O1'-C1
23	s	606	LMU	C2'-C1'-O1'-C1
23	s	606	LMU	O5'-C1'-O1'-C1
23	x	606	LMU	C2'-C1'-O1'-C1
24	Z	601	LUT	C7-C8-C9-C10
24	Z	601	LUT	C7-C8-C9-C19
24	Z	601	LUT	C27-C28-C29-C30
24	Z	601	LUT	C27-C28-C29-C39
24	Z	601	LUT	C31-C32-C33-C34
24	q	601	LUT	C27-C28-C29-C30
24	q	601	LUT	C27-C28-C29-C39
24	q	601	LUT	C31-C32-C33-C34
24	q	601	LUT	C31-C32-C33-C40
24	w	601	LUT	C27-C28-C29-C30
24	w	601	LUT	C27-C28-C29-C39
24	w	601	LUT	C31-C32-C33-C34
24	w	601	LUT	C31-C32-C33-C40
16	A	1108	CLA	O1D-CGD-O2D-CED
16	B	1021	CLA	O1D-CGD-O2D-CED
16	B	1240	CLA	O1D-CGD-O2D-CED
16	H	1104	CLA	O1D-CGD-O2D-CED
16	H	1108	CLA	O1D-CGD-O2D-CED
16	W	508	CLA	O1D-CGD-O2D-CED
16	W	511	CLA	O1D-CGD-O2D-CED
16	W	514	CLA	O1D-CGD-O2D-CED
16	X	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	X	515	CLA	O1D-CGD-O2D-CED
16	Y	514	CLA	O1D-CGD-O2D-CED
16	a	1108	CLA	O1D-CGD-O2D-CED
16	b	1021	CLA	O1D-CGD-O2D-CED
16	b	1229	CLA	O1D-CGD-O2D-CED
16	h	512	CLA	O1D-CGD-O2D-CED
16	h	514	CLA	O1D-CGD-O2D-CED
16	n	512	CLA	O1D-CGD-O2D-CED
16	o	505	CLA	O1D-CGD-O2D-CED
16	o	506	CLA	O1D-CGD-O2D-CED
16	o	514	CLA	O1D-CGD-O2D-CED
16	p	511	CLA	O1D-CGD-O2D-CED
16	p	514	CLA	O1D-CGD-O2D-CED
16	q	503	CLA	O1D-CGD-O2D-CED
16	r	511	CLA	O1D-CGD-O2D-CED
16	s	511	CLA	O1D-CGD-O2D-CED
16	s	514	CLA	O1D-CGD-O2D-CED
16	t	511	CLA	O1D-CGD-O2D-CED
16	t	514	CLA	O1D-CGD-O2D-CED
16	u	506	CLA	O1D-CGD-O2D-CED
16	u	514	CLA	O1D-CGD-O2D-CED
16	u	515	CLA	O1D-CGD-O2D-CED
16	v	504	CLA	O1D-CGD-O2D-CED
16	w	503	CLA	O1D-CGD-O2D-CED
16	w	511	CLA	O1D-CGD-O2D-CED
16	y	504	CLA	O1D-CGD-O2D-CED
16	y	505	CLA	O1D-CGD-O2D-CED
16	y	512	CLA	O1D-CGD-O2D-CED
16	A	1112	CLA	O1D-CGD-O2D-CED
16	B	1229	CLA	O1D-CGD-O2D-CED
16	G	1021	CLA	O1D-CGD-O2D-CED
16	H	1131	CLA	O1D-CGD-O2D-CED
16	W	507	CLA	O1D-CGD-O2D-CED
16	Y	504	CLA	O1D-CGD-O2D-CED
16	Y	511	CLA	O1D-CGD-O2D-CED
16	Z	503	CLA	O1D-CGD-O2D-CED
16	Z	514	CLA	O1D-CGD-O2D-CED
16	b	1240	CLA	O1D-CGD-O2D-CED
16	f	1301	CLA	O1D-CGD-O2D-CED
16	h	506	CLA	O1D-CGD-O2D-CED
16	h	510	CLA	O1D-CGD-O2D-CED
16	n	508	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	u	505	CLA	O1D-CGD-O2D-CED
16	u	513	CLA	O1D-CGD-O2D-CED
16	A	1108	CLA	CBD-CGD-O2D-CED
16	A	1111	CLA	CBD-CGD-O2D-CED
16	A	1121	CLA	CBD-CGD-O2D-CED
16	A	1122	CLA	CBD-CGD-O2D-CED
16	A	1132	CLA	CBD-CGD-O2D-CED
16	A	1801	CLA	CBD-CGD-O2D-CED
16	B	1021	CLA	CBD-CGD-O2D-CED
16	B	1224	CLA	CBD-CGD-O2D-CED
16	B	1229	CLA	CBD-CGD-O2D-CED
16	B	1239	CLA	CBD-CGD-O2D-CED
16	B	1240	CLA	CBD-CGD-O2D-CED
16	G	1208	CLA	CBD-CGD-O2D-CED
16	G	1219	CLA	CBD-CGD-O2D-CED
16	G	1220	CLA	CBD-CGD-O2D-CED
16	G	1229	CLA	CBD-CGD-O2D-CED
16	G	1239	CLA	CBD-CGD-O2D-CED
16	H	1104	CLA	CBD-CGD-O2D-CED
16	H	1108	CLA	CBD-CGD-O2D-CED
16	H	1116	CLA	CBD-CGD-O2D-CED
16	H	1121	CLA	CBD-CGD-O2D-CED
16	K	4002	CLA	CBD-CGD-O2D-CED
16	W	502	CLA	CBD-CGD-O2D-CED
16	W	503	CLA	CBD-CGD-O2D-CED
16	W	507	CLA	CBD-CGD-O2D-CED
16	W	511	CLA	CBD-CGD-O2D-CED
16	X	503	CLA	CBD-CGD-O2D-CED
16	X	507	CLA	CBD-CGD-O2D-CED
16	X	511	CLA	CBD-CGD-O2D-CED
16	X	515	CLA	CBD-CGD-O2D-CED
16	Y	504	CLA	CBD-CGD-O2D-CED
16	Z	503	CLA	CBD-CGD-O2D-CED
16	Z	506	CLA	CBD-CGD-O2D-CED
16	Z	510	CLA	CBD-CGD-O2D-CED
16	Z	511	CLA	CBD-CGD-O2D-CED
16	Z	514	CLA	CBD-CGD-O2D-CED
16	a	1013	CLA	CBD-CGD-O2D-CED
16	a	1120	CLA	CBD-CGD-O2D-CED
16	a	1121	CLA	CBD-CGD-O2D-CED
16	a	1122	CLA	CBD-CGD-O2D-CED
16	a	1131	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	a	1801	CLA	CBD-CGD-O2D-CED
16	b	1023	CLA	CBD-CGD-O2D-CED
16	b	1215	CLA	CBD-CGD-O2D-CED
16	b	1220	CLA	CBD-CGD-O2D-CED
16	b	1224	CLA	CBD-CGD-O2D-CED
16	b	1229	CLA	CBD-CGD-O2D-CED
16	b	1230	CLA	CBD-CGD-O2D-CED
16	b	1232	CLA	CBD-CGD-O2D-CED
16	b	1240	CLA	CBD-CGD-O2D-CED
16	g	507	CLA	CBD-CGD-O2D-CED
16	g	514	CLA	CBD-CGD-O2D-CED
16	g	516	CLA	CBD-CGD-O2D-CED
16	h	504	CLA	CBD-CGD-O2D-CED
16	h	506	CLA	CBD-CGD-O2D-CED
16	h	512	CLA	CBD-CGD-O2D-CED
16	h	513	CLA	CBD-CGD-O2D-CED
16	k	4002	CLA	CBD-CGD-O2D-CED
16	n	502	CLA	CBD-CGD-O2D-CED
16	n	507	CLA	CBD-CGD-O2D-CED
16	o	511	CLA	CBD-CGD-O2D-CED
16	p	504	CLA	CBD-CGD-O2D-CED
16	p	511	CLA	CBD-CGD-O2D-CED
16	q	502	CLA	CBD-CGD-O2D-CED
16	q	503	CLA	CBD-CGD-O2D-CED
16	q	506	CLA	CBD-CGD-O2D-CED
16	q	511	CLA	CBD-CGD-O2D-CED
16	q	514	CLA	CBD-CGD-O2D-CED
16	r	505	CLA	CBD-CGD-O2D-CED
16	r	507	CLA	CBD-CGD-O2D-CED
16	r	510	CLA	CBD-CGD-O2D-CED
16	r	511	CLA	CBD-CGD-O2D-CED
16	s	504	CLA	CBD-CGD-O2D-CED
16	s	507	CLA	CBD-CGD-O2D-CED
16	u	503	CLA	CBD-CGD-O2D-CED
16	u	507	CLA	CBD-CGD-O2D-CED
16	v	504	CLA	CBD-CGD-O2D-CED
16	v	508	CLA	CBD-CGD-O2D-CED
16	v	510	CLA	CBD-CGD-O2D-CED
16	v	512	CLA	CBD-CGD-O2D-CED
16	w	503	CLA	CBD-CGD-O2D-CED
16	w	510	CLA	CBD-CGD-O2D-CED
16	w	514	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	x	507	CLA	CBD-CGD-O2D-CED
16	x	510	CLA	CBD-CGD-O2D-CED
16	x	511	CLA	CBD-CGD-O2D-CED
16	x	513	CLA	CBD-CGD-O2D-CED
16	x	517	CLA	CBD-CGD-O2D-CED
16	y	504	CLA	CBD-CGD-O2D-CED
16	y	507	CLA	CBD-CGD-O2D-CED
16	y	513	CLA	CBD-CGD-O2D-CED
16	A	1130	CLA	O1A-CGA-O2A-C1
16	B	1203	CLA	O1A-CGA-O2A-C1
16	B	1220	CLA	O1A-CGA-O2A-C1
16	G	1203	CLA	O1A-CGA-O2A-C1
16	G	1226	CLA	O1A-CGA-O2A-C1
16	H	1130	CLA	O1A-CGA-O2A-C1
16	L	1503	CLA	O1A-CGA-O2A-C1
16	W	502	CLA	O1A-CGA-O2A-C1
16	Y	509	CLA	O1A-CGA-O2A-C1
16	Y	517	CLA	O1A-CGA-O2A-C1
16	Z	501	CLA	O1A-CGA-O2A-C1
16	Z	507	CLA	O1A-CGA-O2A-C1
16	Z	513	CLA	O1A-CGA-O2A-C1
16	b	1203	CLA	O1A-CGA-O2A-C1
16	b	1226	CLA	O1A-CGA-O2A-C1
16	b	1227	CLA	O1A-CGA-O2A-C1
16	g	512	CLA	O1A-CGA-O2A-C1
16	h	515	CLA	O1A-CGA-O2A-C1
16	h	517	CLA	O1A-CGA-O2A-C1
16	l	1503	CLA	O1A-CGA-O2A-C1
16	o	505	CLA	O1A-CGA-O2A-C1
16	o	515	CLA	O1A-CGA-O2A-C1
16	p	509	CLA	O1A-CGA-O2A-C1
16	p	512	CLA	O1A-CGA-O2A-C1
16	p	515	CLA	O1A-CGA-O2A-C1
16	p	517	CLA	O1A-CGA-O2A-C1
16	q	507	CLA	O1A-CGA-O2A-C1
16	r	510	CLA	O1A-CGA-O2A-C1
16	s	509	CLA	O1A-CGA-O2A-C1
16	s	512	CLA	O1A-CGA-O2A-C1
16	s	517	CLA	O1A-CGA-O2A-C1
16	u	508	CLA	O1A-CGA-O2A-C1
16	v	515	CLA	O1A-CGA-O2A-C1
16	X	513	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	Z	503	CLA	O1A-CGA-O2A-C1
16	n	503	CLA	O1A-CGA-O2A-C1
16	w	503	CLA	O1A-CGA-O2A-C1
16	w	516	CLA	O1A-CGA-O2A-C1
16	g	511	CLA	O1D-CGD-O2D-CED
16	n	514	CLA	O1D-CGD-O2D-CED
16	s	504	CLA	O1D-CGD-O2D-CED
16	W	503	CLA	CBA-CGA-O2A-C1
16	X	503	CLA	CBA-CGA-O2A-C1
16	X	513	CLA	CBA-CGA-O2A-C1
16	h	516	CLA	CBA-CGA-O2A-C1
16	y	501	CLA	CBA-CGA-O2A-C1
16	G	1208	CLA	O1D-CGD-O2D-CED
16	G	1229	CLA	O1D-CGD-O2D-CED
16	a	1131	CLA	O1D-CGD-O2D-CED
16	g	507	CLA	O1D-CGD-O2D-CED
16	n	507	CLA	O1D-CGD-O2D-CED
16	o	511	CLA	O1D-CGD-O2D-CED
16	p	504	CLA	O1D-CGD-O2D-CED
16	q	511	CLA	O1D-CGD-O2D-CED
16	q	514	CLA	O1D-CGD-O2D-CED
16	r	507	CLA	O1D-CGD-O2D-CED
16	v	510	CLA	O1D-CGD-O2D-CED
16	v	512	CLA	O1D-CGD-O2D-CED
16	w	514	CLA	O1D-CGD-O2D-CED
16	x	507	CLA	O1D-CGD-O2D-CED
16	x	511	CLA	O1D-CGD-O2D-CED
14	a	852	LMG	C29-C28-O8-C9
16	B	1211	CLA	CBA-CGA-O2A-C1
16	G	1211	CLA	CBA-CGA-O2A-C1
16	Y	509	CLA	CBA-CGA-O2A-C1
16	Y	517	CLA	CBA-CGA-O2A-C1
16	a	1130	CLA	CBA-CGA-O2A-C1
16	g	512	CLA	CBA-CGA-O2A-C1
16	h	515	CLA	CBA-CGA-O2A-C1
16	h	517	CLA	CBA-CGA-O2A-C1
16	p	509	CLA	CBA-CGA-O2A-C1
16	p	512	CLA	CBA-CGA-O2A-C1
16	p	517	CLA	CBA-CGA-O2A-C1
16	q	507	CLA	CBA-CGA-O2A-C1
16	s	509	CLA	CBA-CGA-O2A-C1
16	s	512	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	t	501	CLA	CBA-CGA-O2A-C1
16	v	507	CLA	CBA-CGA-O2A-C1
16	v	515	CLA	CBA-CGA-O2A-C1
16	x	510	CLA	CBA-CGA-O2A-C1
16	B	1232	CLA	CBD-CGD-O2D-CED
16	G	1215	CLA	CBD-CGD-O2D-CED
16	J	1302	CLA	CBD-CGD-O2D-CED
16	L	1501	CLA	CBD-CGD-O2D-CED
16	a	1113	CLA	CBD-CGD-O2D-CED
16	b	1201	CLA	CBD-CGD-O2D-CED
16	h	508	CLA	CBD-CGD-O2D-CED
16	q	510	CLA	CBD-CGD-O2D-CED
14	A	852	LMG	O10-C28-O8-C9
14	H	4201	LMG	O10-C28-O8-C9
14	a	852	LMG	O10-C28-O8-C9
14	a	4201	LMG	O10-C28-O8-C9
16	A	1118	CLA	O1A-CGA-O2A-C1
16	A	1120	CLA	O1A-CGA-O2A-C1
16	A	1132	CLA	O1A-CGA-O2A-C1
16	A	1133	CLA	O1A-CGA-O2A-C1
16	A	1237	CLA	O1A-CGA-O2A-C1
16	B	1211	CLA	O1A-CGA-O2A-C1
16	B	1218	CLA	O1A-CGA-O2A-C1
16	B	1226	CLA	O1A-CGA-O2A-C1
16	B	1236	CLA	O1A-CGA-O2A-C1
16	G	1211	CLA	O1A-CGA-O2A-C1
16	G	1227	CLA	O1A-CGA-O2A-C1
16	G	1236	CLA	O1A-CGA-O2A-C1
16	H	1118	CLA	O1A-CGA-O2A-C1
16	H	1120	CLA	O1A-CGA-O2A-C1
16	H	1132	CLA	O1A-CGA-O2A-C1
16	H	1133	CLA	O1A-CGA-O2A-C1
16	H	1237	CLA	O1A-CGA-O2A-C1
16	W	505	CLA	O1A-CGA-O2A-C1
16	W	508	CLA	O1A-CGA-O2A-C1
16	W	515	CLA	O1A-CGA-O2A-C1
16	X	506	CLA	O1A-CGA-O2A-C1
16	Z	502	CLA	O1A-CGA-O2A-C1
16	a	1118	CLA	O1A-CGA-O2A-C1
16	a	1120	CLA	O1A-CGA-O2A-C1
16	a	1130	CLA	O1A-CGA-O2A-C1
16	a	1132	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	a	1237	CLA	O1A-CGA-O2A-C1
16	b	1211	CLA	O1A-CGA-O2A-C1
16	b	1218	CLA	O1A-CGA-O2A-C1
16	b	1236	CLA	O1A-CGA-O2A-C1
16	g	501	CLA	O1A-CGA-O2A-C1
16	g	505	CLA	O1A-CGA-O2A-C1
16	g	508	CLA	O1A-CGA-O2A-C1
16	g	515	CLA	O1A-CGA-O2A-C1
16	g	517	CLA	O1A-CGA-O2A-C1
16	h	502	CLA	O1A-CGA-O2A-C1
16	h	508	CLA	O1A-CGA-O2A-C1
16	h	510	CLA	O1A-CGA-O2A-C1
16	n	505	CLA	O1A-CGA-O2A-C1
16	n	508	CLA	O1A-CGA-O2A-C1
16	n	515	CLA	O1A-CGA-O2A-C1
16	o	508	CLA	O1A-CGA-O2A-C1
16	q	501	CLA	O1A-CGA-O2A-C1
16	r	505	CLA	O1A-CGA-O2A-C1
16	r	508	CLA	O1A-CGA-O2A-C1
16	r	512	CLA	O1A-CGA-O2A-C1
16	s	515	CLA	O1A-CGA-O2A-C1
16	t	501	CLA	O1A-CGA-O2A-C1
16	t	505	CLA	O1A-CGA-O2A-C1
16	t	508	CLA	O1A-CGA-O2A-C1
16	t	515	CLA	O1A-CGA-O2A-C1
16	v	502	CLA	O1A-CGA-O2A-C1
16	v	507	CLA	O1A-CGA-O2A-C1
16	v	510	CLA	O1A-CGA-O2A-C1
16	w	501	CLA	O1A-CGA-O2A-C1
16	w	507	CLA	O1A-CGA-O2A-C1
16	x	505	CLA	O1A-CGA-O2A-C1
16	x	508	CLA	O1A-CGA-O2A-C1
16	x	510	CLA	O1A-CGA-O2A-C1
16	x	512	CLA	O1A-CGA-O2A-C1
16	x	515	CLA	O1A-CGA-O2A-C1
16	y	508	CLA	O1A-CGA-O2A-C1
16	y	510	CLA	O1A-CGA-O2A-C1
16	y	515	CLA	O1A-CGA-O2A-C1
16	y	517	CLA	O1A-CGA-O2A-C1
16	H	1801	CLA	O1A-CGA-O2A-C1
16	y	501	CLA	O1A-CGA-O2A-C1
16	A	1104	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	A	1120	CLA	O1D-CGD-O2D-CED
16	A	1137	CLA	O1D-CGD-O2D-CED
16	G	1211	CLA	O1D-CGD-O2D-CED
16	G	1220	CLA	O1D-CGD-O2D-CED
16	G	1232	CLA	O1D-CGD-O2D-CED
16	G	1240	CLA	O1D-CGD-O2D-CED
16	S	1302	CLA	O1D-CGD-O2D-CED
16	Y	507	CLA	O1D-CGD-O2D-CED
16	a	1013	CLA	O1D-CGD-O2D-CED
16	b	1206	CLA	O1D-CGD-O2D-CED
16	b	1239	CLA	O1D-CGD-O2D-CED
16	g	504	CLA	O1D-CGD-O2D-CED
16	n	511	CLA	O1D-CGD-O2D-CED
16	o	503	CLA	O1D-CGD-O2D-CED
16	o	507	CLA	O1D-CGD-O2D-CED
16	p	506	CLA	O1D-CGD-O2D-CED
16	s	507	CLA	O1D-CGD-O2D-CED
16	u	507	CLA	O1D-CGD-O2D-CED
16	w	507	CLA	O1D-CGD-O2D-CED
16	x	505	CLA	O1D-CGD-O2D-CED
16	A	1113	CLA	O1D-CGD-O2D-CED
16	A	1116	CLA	O1D-CGD-O2D-CED
16	B	1203	CLA	O1D-CGD-O2D-CED
16	B	1207	CLA	O1D-CGD-O2D-CED
16	B	1211	CLA	O1D-CGD-O2D-CED
16	F	1302	CLA	O1D-CGD-O2D-CED
16	H	1013	CLA	O1D-CGD-O2D-CED
16	H	1137	CLA	O1D-CGD-O2D-CED
16	X	508	CLA	O1D-CGD-O2D-CED
16	Z	507	CLA	O1D-CGD-O2D-CED
16	a	1104	CLA	O1D-CGD-O2D-CED
16	a	1137	CLA	O1D-CGD-O2D-CED
16	b	1207	CLA	O1D-CGD-O2D-CED
16	g	517	CLA	O1D-CGD-O2D-CED
16	n	513	CLA	O1D-CGD-O2D-CED
16	o	504	CLA	O1D-CGD-O2D-CED
16	o	508	CLA	O1D-CGD-O2D-CED
16	p	507	CLA	O1D-CGD-O2D-CED
16	r	504	CLA	O1D-CGD-O2D-CED
16	r	513	CLA	O1D-CGD-O2D-CED
16	t	507	CLA	O1D-CGD-O2D-CED
16	t	512	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	u	504	CLA	O1D-CGD-O2D-CED
16	u	508	CLA	O1D-CGD-O2D-CED
16	u	516	CLA	O1D-CGD-O2D-CED
16	v	506	CLA	O1D-CGD-O2D-CED
16	v	511	CLA	O1D-CGD-O2D-CED
16	x	504	CLA	O1D-CGD-O2D-CED
16	y	502	CLA	O1D-CGD-O2D-CED
16	y	506	CLA	O1D-CGD-O2D-CED
16	y	510	CLA	O1D-CGD-O2D-CED
16	y	511	CLA	O1D-CGD-O2D-CED
16	H	1132	CLA	CBD-CGD-O2D-CED
16	r	517	CLA	CBD-CGD-O2D-CED
16	u	506	CLA	O1A-CGA-O2A-C1
16	v	508	CLA	O1A-CGA-O2A-C1
16	A	1131	CLA	O1D-CGD-O2D-CED
16	t	513	CLA	O1D-CGD-O2D-CED
16	X	501	CLA	CBA-CGA-O2A-C1
16	t	516	CLA	O1A-CGA-O2A-C1
16	A	1013	CLA	C3-C5-C6-C7
16	A	1109	CLA	C3-C5-C6-C7
16	A	1115	CLA	C3-C5-C6-C7
16	B	1204	CLA	C3-C5-C6-C7
16	B	1205	CLA	C3-C5-C6-C7
16	B	1218	CLA	C3-C5-C6-C7
16	B	1225	CLA	C3-C5-C6-C7
16	B	1226	CLA	C3-C5-C6-C7
16	G	1205	CLA	C3-C5-C6-C7
16	G	1225	CLA	C3-C5-C6-C7
16	H	1013	CLA	C3-C5-C6-C7
16	H	1104	CLA	C3-C5-C6-C7
16	H	1119	CLA	C3-C5-C6-C7
16	H	1124	CLA	C3-C5-C6-C7
16	H	1128	CLA	C3-C5-C6-C7
16	H	1131	CLA	C3-C5-C6-C7
16	H	1133	CLA	C3-C5-C6-C7
16	W	512	CLA	C3-C5-C6-C7
16	X	504	CLA	C3-C5-C6-C7
16	X	517	CLA	C3-C5-C6-C7
16	Y	509	CLA	C3-C5-C6-C7
16	Y	512	CLA	C3-C5-C6-C7
16	Y	515	CLA	C3-C5-C6-C7
16	Z	505	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	Z	510	CLA	C3-C5-C6-C7
16	a	1119	CLA	C3-C5-C6-C7
16	a	1124	CLA	C3-C5-C6-C7
16	b	1012	CLA	C3-C5-C6-C7
16	b	1205	CLA	C3-C5-C6-C7
16	b	1211	CLA	C3-C5-C6-C7
16	b	1223	CLA	C3-C5-C6-C7
16	b	1225	CLA	C3-C5-C6-C7
16	b	1226	CLA	C3-C5-C6-C7
16	b	1235	CLA	C3-C5-C6-C7
16	g	515	CLA	C3-C5-C6-C7
16	h	504	CLA	C3-C5-C6-C7
16	h	512	CLA	C3-C5-C6-C7
16	o	505	CLA	C3-C5-C6-C7
16	o	509	CLA	C3-C5-C6-C7
16	o	517	CLA	C3-C5-C6-C7
16	p	509	CLA	C3-C5-C6-C7
16	p	512	CLA	C3-C5-C6-C7
16	p	515	CLA	C3-C5-C6-C7
16	q	517	CLA	C3-C5-C6-C7
16	r	505	CLA	C3-C5-C6-C7
16	r	508	CLA	C3-C5-C6-C7
16	r	512	CLA	C3-C5-C6-C7
16	r	515	CLA	C3-C5-C6-C7
16	s	509	CLA	C3-C5-C6-C7
16	s	512	CLA	C3-C5-C6-C7
16	s	515	CLA	C3-C5-C6-C7
16	t	510	CLA	C3-C5-C6-C7
16	u	517	CLA	C3-C5-C6-C7
16	v	504	CLA	C3-C5-C6-C7
16	v	506	CLA	C3-C5-C6-C7
16	v	511	CLA	C3-C5-C6-C7
16	v	512	CLA	C3-C5-C6-C7
16	w	508	CLA	C3-C5-C6-C7
16	w	517	CLA	C3-C5-C6-C7
16	x	515	CLA	C3-C5-C6-C7
16	y	512	CLA	C3-C5-C6-C7
16	b	1219	CLA	O1D-CGD-O2D-CED
14	A	852	LMG	C29-C28-O8-C9
14	H	4201	LMG	C29-C28-O8-C9
16	A	1105	CLA	CBA-CGA-O2A-C1
16	A	1118	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	A	1120	CLA	CBA-CGA-O2A-C1
16	A	1130	CLA	CBA-CGA-O2A-C1
16	A	1132	CLA	CBA-CGA-O2A-C1
16	A	1237	CLA	CBA-CGA-O2A-C1
16	B	1203	CLA	CBA-CGA-O2A-C1
16	B	1218	CLA	CBA-CGA-O2A-C1
16	B	1220	CLA	CBA-CGA-O2A-C1
16	B	1236	CLA	CBA-CGA-O2A-C1
16	G	1203	CLA	CBA-CGA-O2A-C1
16	G	1218	CLA	CBA-CGA-O2A-C1
16	G	1226	CLA	CBA-CGA-O2A-C1
16	G	1227	CLA	CBA-CGA-O2A-C1
16	G	1236	CLA	CBA-CGA-O2A-C1
16	H	1118	CLA	CBA-CGA-O2A-C1
16	H	1120	CLA	CBA-CGA-O2A-C1
16	H	1130	CLA	CBA-CGA-O2A-C1
16	H	1132	CLA	CBA-CGA-O2A-C1
16	H	1237	CLA	CBA-CGA-O2A-C1
16	L	1503	CLA	CBA-CGA-O2A-C1
16	W	502	CLA	CBA-CGA-O2A-C1
16	W	505	CLA	CBA-CGA-O2A-C1
16	W	515	CLA	CBA-CGA-O2A-C1
16	X	506	CLA	CBA-CGA-O2A-C1
16	Y	512	CLA	CBA-CGA-O2A-C1
16	Y	515	CLA	CBA-CGA-O2A-C1
16	Z	501	CLA	CBA-CGA-O2A-C1
16	Z	502	CLA	CBA-CGA-O2A-C1
16	Z	513	CLA	CBA-CGA-O2A-C1
16	a	1105	CLA	CBA-CGA-O2A-C1
16	a	1118	CLA	CBA-CGA-O2A-C1
16	a	1120	CLA	CBA-CGA-O2A-C1
16	a	1132	CLA	CBA-CGA-O2A-C1
16	a	1237	CLA	CBA-CGA-O2A-C1
16	b	1021	CLA	CBA-CGA-O2A-C1
16	b	1203	CLA	CBA-CGA-O2A-C1
16	b	1211	CLA	CBA-CGA-O2A-C1
16	b	1218	CLA	CBA-CGA-O2A-C1
16	b	1226	CLA	CBA-CGA-O2A-C1
16	b	1227	CLA	CBA-CGA-O2A-C1
16	b	1236	CLA	CBA-CGA-O2A-C1
16	g	515	CLA	CBA-CGA-O2A-C1
16	h	502	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	h	508	CLA	CBA-CGA-O2A-C1
16	l	1503	CLA	CBA-CGA-O2A-C1
16	n	505	CLA	CBA-CGA-O2A-C1
16	n	508	CLA	CBA-CGA-O2A-C1
16	n	510	CLA	CBA-CGA-O2A-C1
16	n	515	CLA	CBA-CGA-O2A-C1
16	o	505	CLA	CBA-CGA-O2A-C1
16	o	515	CLA	CBA-CGA-O2A-C1
16	q	501	CLA	CBA-CGA-O2A-C1
16	q	513	CLA	CBA-CGA-O2A-C1
16	q	515	CLA	CBA-CGA-O2A-C1
16	r	501	CLA	CBA-CGA-O2A-C1
16	r	508	CLA	CBA-CGA-O2A-C1
16	r	510	CLA	CBA-CGA-O2A-C1
16	r	515	CLA	CBA-CGA-O2A-C1
16	s	501	CLA	CBA-CGA-O2A-C1
16	s	517	CLA	CBA-CGA-O2A-C1
16	t	505	CLA	CBA-CGA-O2A-C1
16	t	508	CLA	CBA-CGA-O2A-C1
16	t	515	CLA	CBA-CGA-O2A-C1
16	u	508	CLA	CBA-CGA-O2A-C1
16	w	501	CLA	CBA-CGA-O2A-C1
16	w	507	CLA	CBA-CGA-O2A-C1
16	x	505	CLA	CBA-CGA-O2A-C1
16	x	508	CLA	CBA-CGA-O2A-C1
16	x	515	CLA	CBA-CGA-O2A-C1
16	y	515	CLA	CBA-CGA-O2A-C1
16	y	517	CLA	CBA-CGA-O2A-C1
16	B	1201	CLA	CBD-CGD-O2D-CED
16	B	1206	CLA	CBD-CGD-O2D-CED
16	B	1216	CLA	CBD-CGD-O2D-CED
16	B	1231	CLA	CBD-CGD-O2D-CED
16	H	1117	CLA	CBD-CGD-O2D-CED
16	H	1126	CLA	CBD-CGD-O2D-CED
16	T	4002	CLA	CBD-CGD-O2D-CED
16	U	1501	CLA	CBD-CGD-O2D-CED
16	W	505	CLA	CBD-CGD-O2D-CED
16	Y	505	CLA	CBD-CGD-O2D-CED
16	Y	517	CLA	CBD-CGD-O2D-CED
16	Z	512	CLA	CBD-CGD-O2D-CED
16	a	1116	CLA	CBD-CGD-O2D-CED
16	a	1117	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	a	1126	CLA	CBD-CGD-O2D-CED
16	a	1132	CLA	CBD-CGD-O2D-CED
16	b	1208	CLA	CBD-CGD-O2D-CED
16	b	1228	CLA	CBD-CGD-O2D-CED
16	b	1231	CLA	CBD-CGD-O2D-CED
16	b	1235	CLA	CBD-CGD-O2D-CED
16	f	1302	CLA	CBD-CGD-O2D-CED
16	g	505	CLA	CBD-CGD-O2D-CED
16	g	510	CLA	CBD-CGD-O2D-CED
16	h	511	CLA	CBD-CGD-O2D-CED
16	l	1501	CLA	CBD-CGD-O2D-CED
16	n	517	CLA	CBD-CGD-O2D-CED
16	p	505	CLA	CBD-CGD-O2D-CED
16	p	516	CLA	CBD-CGD-O2D-CED
16	q	512	CLA	CBD-CGD-O2D-CED
16	r	509	CLA	CBD-CGD-O2D-CED
16	r	512	CLA	CBD-CGD-O2D-CED
16	s	502	CLA	CBD-CGD-O2D-CED
16	s	516	CLA	CBD-CGD-O2D-CED
16	t	516	CLA	CBD-CGD-O2D-CED
16	v	509	CLA	CBD-CGD-O2D-CED
16	w	512	CLA	CBD-CGD-O2D-CED
16	w	516	CLA	CBD-CGD-O2D-CED
16	y	509	CLA	CBD-CGD-O2D-CED
14	H	4101	LMG	C11-C10-O7-C8
14	a	4101	LMG	C11-C10-O7-C8
16	A	1117	CLA	O1D-CGD-O2D-CED
16	B	1215	CLA	O1D-CGD-O2D-CED
16	B	1219	CLA	O1D-CGD-O2D-CED
16	F	1301	CLA	O1D-CGD-O2D-CED
16	G	1219	CLA	O1D-CGD-O2D-CED
16	W	512	CLA	O1D-CGD-O2D-CED
16	W	513	CLA	O1D-CGD-O2D-CED
16	X	504	CLA	O1D-CGD-O2D-CED
16	Y	506	CLA	O1D-CGD-O2D-CED
16	Z	510	CLA	O1D-CGD-O2D-CED
16	b	1203	CLA	O1D-CGD-O2D-CED
16	b	1215	CLA	O1D-CGD-O2D-CED
16	g	513	CLA	O1D-CGD-O2D-CED
16	u	503	CLA	O1D-CGD-O2D-CED
16	v	517	CLA	O1D-CGD-O2D-CED
16	x	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	y	507	CLA	O1D-CGD-O2D-CED
16	B	1239	CLA	O1A-CGA-O2A-C1
16	t	502	CLA	O1A-CGA-O2A-C1
16	u	505	CLA	O1A-CGA-O2A-C1
16	A	1801	CLA	O1A-CGA-O2A-C1
16	W	516	CLA	O1A-CGA-O2A-C1
16	X	501	CLA	O1A-CGA-O2A-C1
16	X	503	CLA	O1A-CGA-O2A-C1
16	f	1302	CLA	O1A-CGA-O2A-C1
16	o	513	CLA	O1A-CGA-O2A-C1
16	u	513	CLA	O1A-CGA-O2A-C1
23	p	606	LMU	C4'-C5'-C6'-O6'
16	G	1207	CLA	O1D-CGD-O2D-CED
16	X	511	CLA	O1D-CGD-O2D-CED
16	a	1114	CLA	O1D-CGD-O2D-CED
16	B	1218	CLA	C4-C3-C5-C6
16	G	1203	CLA	C4-C3-C5-C6
16	h	504	CLA	C4-C3-C5-C6
16	p	504	CLA	C4-C3-C5-C6
16	s	504	CLA	C4-C3-C5-C6
16	a	1115	CLA	C2-C3-C5-C6
16	g	512	CLA	C2-C3-C5-C6
16	h	515	CLA	C2-C3-C5-C6
16	A	1801	CLA	CBA-CGA-O2A-C1
16	W	516	CLA	CBA-CGA-O2A-C1
16	f	1302	CLA	CBA-CGA-O2A-C1
16	o	513	CLA	CBA-CGA-O2A-C1
16	t	516	CLA	CBA-CGA-O2A-C1
16	u	513	CLA	CBA-CGA-O2A-C1
16	G	1216	CLA	CBD-CGD-O2D-CED
16	W	517	CLA	CBD-CGD-O2D-CED
16	a	1138	CLA	CBD-CGD-O2D-CED
16	A	1801	CLA	O1D-CGD-O2D-CED
16	G	1239	CLA	O1D-CGD-O2D-CED
16	W	503	CLA	O1D-CGD-O2D-CED
16	X	503	CLA	O1D-CGD-O2D-CED
16	Z	511	CLA	O1D-CGD-O2D-CED
16	g	516	CLA	O1D-CGD-O2D-CED
16	h	513	CLA	O1D-CGD-O2D-CED
16	q	506	CLA	O1D-CGD-O2D-CED
16	x	510	CLA	O1D-CGD-O2D-CED
16	B	1227	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	a	1127	CLA	C2A-CAA-CBA-CGA
16	r	508	CLA	C2A-CAA-CBA-CGA
16	t	510	CLA	O1A-CGA-O2A-C1
16	t	517	CLA	O1A-CGA-O2A-C1
16	w	515	CLA	O1A-CGA-O2A-C1
16	w	517	CLA	O1A-CGA-O2A-C1
16	A	1128	CLA	C3-C5-C6-C7
16	A	1133	CLA	C3-C5-C6-C7
16	B	1220	CLA	C3-C5-C6-C7
16	B	1223	CLA	C3-C5-C6-C7
16	G	1226	CLA	C3-C5-C6-C7
16	Z	517	CLA	C3-C5-C6-C7
16	a	1104	CLA	C3-C5-C6-C7
16	a	1115	CLA	C3-C5-C6-C7
16	a	1128	CLA	C3-C5-C6-C7
16	g	512	CLA	C3-C5-C6-C7
16	o	504	CLA	C3-C5-C6-C7
16	r	517	CLA	C3-C5-C6-C7
16	u	504	CLA	C3-C5-C6-C7
16	u	506	CLA	C3-C5-C6-C7
16	u	508	CLA	C3-C5-C6-C7
16	v	515	CLA	C3-C5-C6-C7
16	w	510	CLA	C3-C5-C6-C7
16	x	508	CLA	C3-C5-C6-C7
16	y	506	CLA	C3-C5-C6-C7
13	A	849	LHG	C24-C23-O8-C6
14	A	4101	LMG	C29-C28-O8-C9
14	a	4201	LMG	C29-C28-O8-C9
16	A	1124	CLA	CBA-CGA-O2A-C1
16	A	1131	CLA	CBA-CGA-O2A-C1
16	A	1133	CLA	CBA-CGA-O2A-C1
16	B	1021	CLA	CBA-CGA-O2A-C1
16	B	1226	CLA	CBA-CGA-O2A-C1
16	B	1227	CLA	CBA-CGA-O2A-C1
16	G	1021	CLA	CBA-CGA-O2A-C1
16	G	1223	CLA	CBA-CGA-O2A-C1
16	G	1229	CLA	CBA-CGA-O2A-C1
16	H	1128	CLA	CBA-CGA-O2A-C1
16	H	1133	CLA	CBA-CGA-O2A-C1
16	U	1502	CLA	CBA-CGA-O2A-C1
16	W	508	CLA	CBA-CGA-O2A-C1
16	X	504	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	Y	501	CLA	CBA-CGA-O2A-C1
16	Z	515	CLA	CBA-CGA-O2A-C1
16	Z	517	CLA	CBA-CGA-O2A-C1
16	b	1229	CLA	CBA-CGA-O2A-C1
16	g	501	CLA	CBA-CGA-O2A-C1
16	g	505	CLA	CBA-CGA-O2A-C1
16	g	508	CLA	CBA-CGA-O2A-C1
16	g	517	CLA	CBA-CGA-O2A-C1
16	h	510	CLA	CBA-CGA-O2A-C1
16	o	508	CLA	CBA-CGA-O2A-C1
16	o	509	CLA	CBA-CGA-O2A-C1
16	q	505	CLA	CBA-CGA-O2A-C1
16	r	505	CLA	CBA-CGA-O2A-C1
16	r	512	CLA	CBA-CGA-O2A-C1
16	s	515	CLA	CBA-CGA-O2A-C1
16	t	506	CLA	CBA-CGA-O2A-C1
16	t	510	CLA	CBA-CGA-O2A-C1
16	t	517	CLA	CBA-CGA-O2A-C1
16	u	504	CLA	CBA-CGA-O2A-C1
16	u	515	CLA	CBA-CGA-O2A-C1
16	v	502	CLA	CBA-CGA-O2A-C1
16	v	508	CLA	CBA-CGA-O2A-C1
16	v	510	CLA	CBA-CGA-O2A-C1
16	x	512	CLA	CBA-CGA-O2A-C1
16	x	517	CLA	CBA-CGA-O2A-C1
16	y	502	CLA	CBA-CGA-O2A-C1
16	y	504	CLA	CBA-CGA-O2A-C1
16	y	508	CLA	CBA-CGA-O2A-C1
16	y	510	CLA	CBA-CGA-O2A-C1
16	y	512	CLA	CBA-CGA-O2A-C1
16	W	503	CLA	O1A-CGA-O2A-C1
14	B	848	LMG	O6-C5-C6-O5
16	Z	509	CLA	CBD-CGD-O2D-CED
20	l	4101	LMT	O5B-C5B-C6B-O6B
19	Z	604	BCR	C9-C10-C11-C12
19	b	4014	BCR	C13-C14-C15-C16
19	g	602	BCR	C9-C10-C11-C12
19	g	602	BCR	C19-C20-C21-C22
19	o	604	BCR	C9-C10-C11-C12
19	r	604	BCR	C13-C14-C15-C16
19	t	604	BCR	C9-C10-C11-C12
19	x	601	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
21	R	4020	ECH	C9-C10-C11-C12
24	q	601	LUT	C29-C30-C31-C32
24	w	601	LUT	C29-C30-C31-C32
16	B	1227	CLA	O1A-CGA-O2A-C1
16	G	1021	CLA	O1A-CGA-O2A-C1
16	H	1105	CLA	O1A-CGA-O2A-C1
16	W	517	CLA	O1A-CGA-O2A-C1
16	X	505	CLA	O1A-CGA-O2A-C1
16	X	508	CLA	O1A-CGA-O2A-C1
16	X	515	CLA	O1A-CGA-O2A-C1
16	Z	515	CLA	O1A-CGA-O2A-C1
16	Z	517	CLA	O1A-CGA-O2A-C1
16	b	1021	CLA	O1A-CGA-O2A-C1
16	g	510	CLA	O1A-CGA-O2A-C1
16	n	510	CLA	O1A-CGA-O2A-C1
16	n	517	CLA	O1A-CGA-O2A-C1
16	q	513	CLA	O1A-CGA-O2A-C1
16	q	517	CLA	O1A-CGA-O2A-C1
16	r	501	CLA	O1A-CGA-O2A-C1
16	s	501	CLA	O1A-CGA-O2A-C1
16	u	510	CLA	O1A-CGA-O2A-C1
16	x	501	CLA	O1A-CGA-O2A-C1
16	x	517	CLA	O1A-CGA-O2A-C1
16	b	1023	CLA	O1D-CGD-O2D-CED
16	h	516	CLA	O1A-CGA-O2A-C1
20	H	4202	LMT	O5'-C5'-C6'-O6'
16	A	1121	CLA	O1D-CGD-O2D-CED
16	H	1116	CLA	O1D-CGD-O2D-CED
16	K	4002	CLA	O1D-CGD-O2D-CED
16	g	514	CLA	O1D-CGD-O2D-CED
16	k	4002	CLA	O1D-CGD-O2D-CED
16	r	505	CLA	O1D-CGD-O2D-CED
16	y	513	CLA	O1D-CGD-O2D-CED
16	A	1104	CLA	C3-C5-C6-C7
16	B	1012	CLA	C3-C5-C6-C7
16	G	1218	CLA	C3-C5-C6-C7
16	H	1106	CLA	C3-C5-C6-C7
16	H	1140	CLA	C3-C5-C6-C7
16	X	505	CLA	C3-C5-C6-C7
16	X	509	CLA	C3-C5-C6-C7
16	X	510	CLA	C3-C5-C6-C7
16	a	1109	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	b	1204	CLA	C3-C5-C6-C7
16	g	509	CLA	C3-C5-C6-C7
16	o	506	CLA	C3-C5-C6-C7
16	t	512	CLA	C3-C5-C6-C7
16	A	1107	CLA	CBD-CGD-O2D-CED
16	G	1203	CLA	CBD-CGD-O2D-CED
16	T	4004	CLA	CBD-CGD-O2D-CED
16	X	501	CLA	CBD-CGD-O2D-CED
16	q	517	CLA	CBD-CGD-O2D-CED
16	r	503	CLA	CBD-CGD-O2D-CED
16	x	503	CLA	CBD-CGD-O2D-CED
16	y	517	CLA	CBD-CGD-O2D-CED
23	p	606	LMU	C2B-C1B-O1B-C4'
13	g	605	LHG	O2-C2-C3-O3
13	r	605	LHG	O2-C2-C3-O3
16	H	1121	CLA	O1D-CGD-O2D-CED
16	W	502	CLA	O1D-CGD-O2D-CED
16	a	1121	CLA	O1D-CGD-O2D-CED
16	n	502	CLA	O1D-CGD-O2D-CED
16	v	508	CLA	O1D-CGD-O2D-CED
16	x	517	CLA	O1D-CGD-O2D-CED
16	A	1115	CLA	CBA-CGA-O2A-C1
16	A	1128	CLA	CBA-CGA-O2A-C1
16	B	1239	CLA	CBA-CGA-O2A-C1
16	H	1105	CLA	CBA-CGA-O2A-C1
16	H	1115	CLA	CBA-CGA-O2A-C1
16	H	1122	CLA	CBA-CGA-O2A-C1
16	H	1131	CLA	CBA-CGA-O2A-C1
16	L	1501	CLA	CBA-CGA-O2A-C1
16	L	1502	CLA	CBA-CGA-O2A-C1
16	U	1501	CLA	CBA-CGA-O2A-C1
16	W	510	CLA	CBA-CGA-O2A-C1
16	W	511	CLA	CBA-CGA-O2A-C1
16	W	517	CLA	CBA-CGA-O2A-C1
16	Y	502	CLA	CBA-CGA-O2A-C1
16	a	1122	CLA	CBA-CGA-O2A-C1
16	a	1128	CLA	CBA-CGA-O2A-C1
16	a	1131	CLA	CBA-CGA-O2A-C1
16	b	1239	CLA	CBA-CGA-O2A-C1
16	g	510	CLA	CBA-CGA-O2A-C1
16	l	1502	CLA	CBA-CGA-O2A-C1
16	n	517	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	o	504	CLA	CBA-CGA-O2A-C1
16	o	506	CLA	CBA-CGA-O2A-C1
16	r	517	CLA	CBA-CGA-O2A-C1
16	t	502	CLA	CBA-CGA-O2A-C1
16	u	505	CLA	CBA-CGA-O2A-C1
16	u	506	CLA	CBA-CGA-O2A-C1
16	u	510	CLA	CBA-CGA-O2A-C1
16	w	512	CLA	CBA-CGA-O2A-C1
16	w	517	CLA	CBA-CGA-O2A-C1
16	x	501	CLA	CBA-CGA-O2A-C1
16	x	506	CLA	CBA-CGA-O2A-C1
20	A	4202	LMT	O5'-C5'-C6'-O6'
20	a	4202	LMT	O5B-C5B-C6B-O6B
20	a	4202	LMT	O5'-C5'-C6'-O6'
23	q	605	LMU	O5'-C5'-C6'-O6'
16	A	1105	CLA	O1A-CGA-O2A-C1
16	B	1021	CLA	O1A-CGA-O2A-C1
16	G	1229	CLA	O1A-CGA-O2A-C1
16	H	1128	CLA	O1A-CGA-O2A-C1
16	a	1105	CLA	O1A-CGA-O2A-C1
16	b	1229	CLA	O1A-CGA-O2A-C1
16	q	515	CLA	O1A-CGA-O2A-C1
16	y	502	CLA	O1A-CGA-O2A-C1
16	B	1224	CLA	O1D-CGD-O2D-CED
16	B	1239	CLA	O1D-CGD-O2D-CED
16	X	507	CLA	O1D-CGD-O2D-CED
16	Z	506	CLA	O1D-CGD-O2D-CED
16	b	1220	CLA	O1D-CGD-O2D-CED
16	r	510	CLA	O1D-CGD-O2D-CED
23	Y	606	LMU	O5'-C5'-C6'-O6'
16	Y	513	CLA	CBD-CGD-O2D-CED
16	h	502	CLA	CBD-CGD-O2D-CED
16	s	505	CLA	CBD-CGD-O2D-CED
16	H	1114	CLA	CBA-CGA-O2A-C1
16	A	1132	CLA	O1D-CGD-O2D-CED
23	x	606	LMU	C2B-C1B-O1B-C4'
14	A	4101	LMG	O10-C28-O8-C9
16	L	1502	CLA	O1A-CGA-O2A-C1
16	a	1122	CLA	O1A-CGA-O2A-C1
16	l	1502	CLA	O1A-CGA-O2A-C1
16	u	504	CLA	O1A-CGA-O2A-C1
16	w	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	y	504	CLA	O1A-CGA-O2A-C1
16	y	512	CLA	O1A-CGA-O2A-C1
16	A	1111	CLA	O1D-CGD-O2D-CED
16	a	1120	CLA	O1D-CGD-O2D-CED
16	a	1122	CLA	O1D-CGD-O2D-CED
16	a	1140	CLA	C3-C5-C6-C7
16	u	509	CLA	C3-C5-C6-C7
16	A	1138	CLA	CBD-CGD-O2D-CED
16	H	1136	CLA	CBD-CGD-O2D-CED
16	j	1302	CLA	CBD-CGD-O2D-CED
16	o	501	CLA	CBD-CGD-O2D-CED
16	u	512	CLA	CBD-CGD-O2D-CED
16	x	509	CLA	CBD-CGD-O2D-CED
20	L	4101	LMT	O5B-C5B-C6B-O6B
16	q	502	CLA	O1D-CGD-O2D-CED
16	X	505	CLA	CBA-CGA-O2A-C1
16	X	508	CLA	CBA-CGA-O2A-C1
16	X	515	CLA	CBA-CGA-O2A-C1
16	q	517	CLA	CBA-CGA-O2A-C1
16	w	513	CLA	CBA-CGA-O2A-C1
16	w	515	CLA	CBA-CGA-O2A-C1
16	H	1133	CLA	C4-C3-C5-C6
16	Y	509	CLA	C4-C3-C5-C6
16	Z	507	CLA	C4-C3-C5-C6
16	a	1110	CLA	C4-C3-C5-C6
16	G	1203	CLA	C2-C3-C5-C6
16	h	504	CLA	C2-C3-C5-C6
16	s	504	CLA	C2-C3-C5-C6
16	A	1115	CLA	O1A-CGA-O2A-C1
16	A	1124	CLA	O1A-CGA-O2A-C1
16	A	1128	CLA	O1A-CGA-O2A-C1
16	A	1131	CLA	O1A-CGA-O2A-C1
16	H	1115	CLA	O1A-CGA-O2A-C1
16	H	1122	CLA	O1A-CGA-O2A-C1
16	L	1501	CLA	O1A-CGA-O2A-C1
16	U	1502	CLA	O1A-CGA-O2A-C1
16	Y	501	CLA	O1A-CGA-O2A-C1
16	b	1239	CLA	O1A-CGA-O2A-C1
16	o	504	CLA	O1A-CGA-O2A-C1
16	o	509	CLA	O1A-CGA-O2A-C1
16	q	505	CLA	O1A-CGA-O2A-C1
16	r	517	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	u	515	CLA	O1A-CGA-O2A-C1
16	A	1122	CLA	O1D-CGD-O2D-CED
16	w	510	CLA	O1D-CGD-O2D-CED
14	B	848	LMG	C4-C5-C6-O5
20	l	4101	LMT	C4B-C5B-C6B-O6B
16	A	1105	CLA	CBD-CGD-O2D-CED
16	A	1126	CLA	CBD-CGD-O2D-CED
16	A	1136	CLA	CBD-CGD-O2D-CED
16	B	1226	CLA	CBD-CGD-O2D-CED
16	G	1205	CLA	CBD-CGD-O2D-CED
16	G	1221	CLA	CBD-CGD-O2D-CED
16	G	1230	CLA	CBD-CGD-O2D-CED
16	H	1119	CLA	CBD-CGD-O2D-CED
16	b	1221	CLA	CBD-CGD-O2D-CED
16	w	508	CLA	CBD-CGD-O2D-CED
16	a	1801	CLA	O1D-CGD-O2D-CED
16	b	1232	CLA	O1D-CGD-O2D-CED
16	y	509	CLA	C5-C6-C7-C8
13	g	605	LHG	C5-C4-O6-P
23	s	606	LMU	O5'-C5'-C6'-O6'
20	L	4101	LMT	C4'-C5'-C6'-O6'
16	G	1218	CLA	C2A-CAA-CBA-CGA
16	H	1127	CLA	C2A-CAA-CBA-CGA
16	X	516	CLA	C2A-CAA-CBA-CGA
16	Y	509	CLA	C2A-CAA-CBA-CGA
16	o	515	CLA	C2A-CAA-CBA-CGA
16	p	509	CLA	C2A-CAA-CBA-CGA
23	Y	606	LMU	O5B-C1B-O1B-C4'
23	p	606	LMU	O5B-C1B-O1B-C4'
23	x	606	LMU	O5B-C1B-O1B-C4'
16	G	1215	CLA	O1D-CGD-O2D-CED
16	a	1113	CLA	O1D-CGD-O2D-CED
16	b	1224	CLA	O1D-CGD-O2D-CED
16	h	504	CLA	O1D-CGD-O2D-CED
16	G	1223	CLA	O1A-CGA-O2A-C1
16	H	1131	CLA	O1A-CGA-O2A-C1
16	W	511	CLA	O1A-CGA-O2A-C1
16	X	504	CLA	O1A-CGA-O2A-C1
16	a	1128	CLA	O1A-CGA-O2A-C1
16	a	1131	CLA	O1A-CGA-O2A-C1
16	o	506	CLA	O1A-CGA-O2A-C1
16	t	506	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	x	506	CLA	O1A-CGA-O2A-C1
16	B	1211	CLA	C3-C5-C6-C7
14	A	4201	LMG	O6-C1-O1-C7
14	H	4201	LMG	O6-C1-O1-C7
14	a	4201	LMG	O6-C1-O1-C7
23	p	606	LMU	O5'-C5'-C6'-O6'
23	Z	605	LMU	C4'-C5'-C6'-O6'
23	Y	606	LMU	C2B-C1B-O1B-C4'
16	h	508	CLA	O1D-CGD-O2D-CED
16	q	510	CLA	O1D-CGD-O2D-CED
16	B	1229	CLA	CBA-CGA-O2A-C1
16	G	1239	CLA	CBA-CGA-O2A-C1
16	U	1503	CLA	CBA-CGA-O2A-C1
16	W	512	CLA	CBA-CGA-O2A-C1
16	l	1501	CLA	CBA-CGA-O2A-C1
16	o	512	CLA	CBA-CGA-O2A-C1
16	p	501	CLA	CBA-CGA-O2A-C1
16	r	507	CLA	CBA-CGA-O2A-C1
16	u	509	CLA	CBA-CGA-O2A-C1
16	A	1139	CLA	CBD-CGD-O2D-CED
16	B	1210	CLA	CBD-CGD-O2D-CED
16	B	1220	CLA	CBD-CGD-O2D-CED
16	B	1227	CLA	CBD-CGD-O2D-CED
16	B	1230	CLA	CBD-CGD-O2D-CED
16	B	1238	CLA	CBD-CGD-O2D-CED
16	G	1214	CLA	CBD-CGD-O2D-CED
16	G	1218	CLA	CBD-CGD-O2D-CED
16	G	1224	CLA	CBD-CGD-O2D-CED
16	G	1228	CLA	CBD-CGD-O2D-CED
16	H	1107	CLA	CBD-CGD-O2D-CED
16	H	1111	CLA	CBD-CGD-O2D-CED
16	H	1122	CLA	CBD-CGD-O2D-CED
16	a	1107	CLA	CBD-CGD-O2D-CED
16	a	1128	CLA	CBD-CGD-O2D-CED
16	g	512	CLA	CBD-CGD-O2D-CED
16	n	503	CLA	CBD-CGD-O2D-CED
16	p	508	CLA	CBD-CGD-O2D-CED
16	u	502	CLA	CBD-CGD-O2D-CED
16	w	517	CLA	CBD-CGD-O2D-CED
16	x	502	CLA	CBD-CGD-O2D-CED
16	x	514	CLA	CBD-CGD-O2D-CED
16	y	514	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	U	4101	LMT	O5B-C5B-C6B-O6B
23	g	606	LMU	O5'-C5'-C6'-O6'
16	o	516	CLA	CBA-CGA-O2A-C1
16	v	503	CLA	CBA-CGA-O2A-C1
16	B	1229	CLA	O1A-CGA-O2A-C1
16	U	1501	CLA	O1A-CGA-O2A-C1
16	W	510	CLA	O1A-CGA-O2A-C1
16	Y	502	CLA	O1A-CGA-O2A-C1
16	l	1501	CLA	O1A-CGA-O2A-C1
16	w	513	CLA	O1A-CGA-O2A-C1
16	b	1230	CLA	O1D-CGD-O2D-CED
23	q	605	LMU	C4'-C5'-C6'-O6'
16	A	1022	CLA	CBD-CGD-O2D-CED
16	G	1226	CLA	CBD-CGD-O2D-CED
16	H	1115	CLA	CBD-CGD-O2D-CED
16	H	1139	CLA	CBD-CGD-O2D-CED
16	Y	509	CLA	CBD-CGD-O2D-CED
16	o	515	CLA	CBD-CGD-O2D-CED
16	q	516	CLA	CBD-CGD-O2D-CED
16	r	502	CLA	CBD-CGD-O2D-CED
16	x	512	CLA	CBD-CGD-O2D-CED
16	A	1106	CLA	C3-C5-C6-C7
16	n	506	CLA	C3-C5-C6-C7
16	b	1201	CLA	O1D-CGD-O2D-CED
20	U	4101	LMT	C4B-C5B-C6B-O6B
20	a	4202	LMT	C4'-C5'-C6'-O6'
23	p	606	LMU	C4B-C5B-C6B-O6B
19	Z	602	BCR	C19-C20-C21-C22
19	q	604	BCR	C9-C10-C11-C12
19	r	602	BCR	C9-C10-C11-C12
19	w	604	BCR	C9-C10-C11-C12
16	G	1239	CLA	O1A-CGA-O2A-C1
16	W	512	CLA	O1A-CGA-O2A-C1
16	p	501	CLA	O1A-CGA-O2A-C1
16	u	509	CLA	O1A-CGA-O2A-C1
13	R	103	LHG	O9-C7-O7-C5
13	B	4018	LHG	C1-C2-C3-O3
16	H	1132	CLA	O1D-CGD-O2D-CED
16	J	1302	CLA	O1D-CGD-O2D-CED
16	r	517	CLA	O1D-CGD-O2D-CED
14	A	4201	LMG	C29-C28-O8-C9
15	H	1011	CL0	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	A	1122	CLA	CBA-CGA-O2A-C1
16	B	1202	CLA	CBA-CGA-O2A-C1
16	B	1224	CLA	CBA-CGA-O2A-C1
16	B	1225	CLA	CBA-CGA-O2A-C1
16	G	1202	CLA	CBA-CGA-O2A-C1
16	G	1222	CLA	CBA-CGA-O2A-C1
16	G	1224	CLA	CBA-CGA-O2A-C1
16	H	1106	CLA	CBA-CGA-O2A-C1
16	X	507	CLA	CBA-CGA-O2A-C1
16	X	509	CLA	CBA-CGA-O2A-C1
16	Y	507	CLA	CBA-CGA-O2A-C1
16	Y	510	CLA	CBA-CGA-O2A-C1
16	Y	514	CLA	CBA-CGA-O2A-C1
16	Z	509	CLA	CBA-CGA-O2A-C1
16	Z	514	CLA	CBA-CGA-O2A-C1
16	a	1124	CLA	CBA-CGA-O2A-C1
16	b	1202	CLA	CBA-CGA-O2A-C1
16	b	1221	CLA	CBA-CGA-O2A-C1
16	b	1224	CLA	CBA-CGA-O2A-C1
16	b	1235	CLA	CBA-CGA-O2A-C1
16	b	1238	CLA	CBA-CGA-O2A-C1
16	g	504	CLA	CBA-CGA-O2A-C1
16	g	509	CLA	CBA-CGA-O2A-C1
16	h	507	CLA	CBA-CGA-O2A-C1
16	h	511	CLA	CBA-CGA-O2A-C1
16	n	506	CLA	CBA-CGA-O2A-C1
16	o	507	CLA	CBA-CGA-O2A-C1
16	p	510	CLA	CBA-CGA-O2A-C1
16	q	514	CLA	CBA-CGA-O2A-C1
16	s	510	CLA	CBA-CGA-O2A-C1
16	t	512	CLA	CBA-CGA-O2A-C1
16	v	505	CLA	CBA-CGA-O2A-C1
16	v	517	CLA	CBA-CGA-O2A-C1
16	w	509	CLA	CBA-CGA-O2A-C1
16	w	514	CLA	CBA-CGA-O2A-C1
16	x	509	CLA	CBA-CGA-O2A-C1
16	g	503	CLA	CBA-CGA-O2A-C1
16	Z	508	CLA	CBD-CGD-O2D-CED
16	p	515	CLA	CBD-CGD-O2D-CED
23	g	606	LMU	C4'-C5'-C6'-O6'
23	x	606	LMU	C4'-C5'-C6'-O6'
16	B	1232	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	L	1501	CLA	O1D-CGD-O2D-CED
16	a	1132	CLA	O1D-CGD-O2D-CED
20	l	4101	LMT	C4'-C5'-C6'-O6'
16	B	1203	CLA	C4-C3-C5-C6
16	b	1203	CLA	C4-C3-C5-C6
16	B	1203	CLA	C2-C3-C5-C6
16	B	1218	CLA	C2-C3-C5-C6
16	H	1133	CLA	C2-C3-C5-C6
16	Y	509	CLA	C2-C3-C5-C6
16	Z	507	CLA	C2-C3-C5-C6
16	b	1203	CLA	C2-C3-C5-C6
16	p	504	CLA	C2-C3-C5-C6
16	H	1103	CLA	C3-C5-C6-C7
16	b	1229	CLA	C3-C5-C6-C7
16	q	507	CLA	C3-C5-C6-C7
16	x	510	CLA	C3-C5-C6-C7
16	B	1228	CLA	CBD-CGD-O2D-CED
16	G	1201	CLA	CBD-CGD-O2D-CED
16	H	1128	CLA	CBD-CGD-O2D-CED
16	q	508	CLA	CBD-CGD-O2D-CED
16	A	1106	CLA	C11-C12-C13-C14
16	A	1237	CLA	C11-C10-C8-C9
16	G	1211	CLA	C11-C12-C13-C14
16	G	1221	CLA	C14-C13-C15-C16
16	H	1101	CLA	C14-C13-C15-C16
16	H	1140	CLA	C6-C7-C8-C9
16	X	504	CLA	C11-C10-C8-C9
16	Y	511	CLA	C14-C13-C15-C16
16	a	1106	CLA	C11-C12-C13-C14
16	a	1237	CLA	C11-C10-C8-C9
16	b	1023	CLA	C11-C12-C13-C14
16	g	504	CLA	C11-C10-C8-C9
16	g	506	CLA	C6-C7-C8-C9
16	h	512	CLA	C11-C12-C13-C14
16	h	515	CLA	C11-C10-C8-C9
16	p	511	CLA	C14-C13-C15-C16
16	r	504	CLA	C11-C10-C8-C9
16	r	506	CLA	C6-C7-C8-C9
16	s	511	CLA	C14-C13-C15-C16
16	v	515	CLA	C11-C10-C8-C9
16	v	515	CLA	C11-C12-C13-C14
16	x	504	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	x	506	CLA	C6-C7-C8-C9
16	y	510	CLA	C6-C7-C8-C9
20	A	4202	LMT	C4'-C5'-C6'-O6'
20	H	4202	LMT	C4'-C5'-C6'-O6'
16	g	510	CLA	O1D-CGD-O2D-CED
16	p	516	CLA	O1D-CGD-O2D-CED
16	q	512	CLA	O1D-CGD-O2D-CED
16	t	516	CLA	O1D-CGD-O2D-CED
14	A	4201	LMG	C2-C1-O1-C7
14	H	4201	LMG	C2-C1-O1-C7
14	a	4201	LMG	C2-C1-O1-C7
23	Z	605	LMU	C2'-C1'-O1'-C1
23	w	605	LMU	C2'-C1'-O1'-C1
16	p	503	CLA	CBA-CGA-O2A-C1
16	t	513	CLA	CBA-CGA-O2A-C1
13	X	605	LHG	O2-C2-C3-O3
13	u	605	LHG	O2-C2-C3-O3
16	B	1231	CLA	O1D-CGD-O2D-CED
16	Z	512	CLA	O1D-CGD-O2D-CED
16	a	1126	CLA	O1D-CGD-O2D-CED
16	g	505	CLA	O1D-CGD-O2D-CED
16	h	511	CLA	O1D-CGD-O2D-CED
16	n	517	CLA	O1D-CGD-O2D-CED
16	w	502	CLA	CBA-CGA-O2A-C1
16	G	1222	CLA	O1A-CGA-O2A-C1
16	Z	514	CLA	O1A-CGA-O2A-C1
16	o	507	CLA	O1A-CGA-O2A-C1
16	o	512	CLA	O1A-CGA-O2A-C1
16	q	514	CLA	O1A-CGA-O2A-C1
16	v	505	CLA	O1A-CGA-O2A-C1
16	A	1128	CLA	CBD-CGD-O2D-CED
16	H	1120	CLA	CBD-CGD-O2D-CED
16	b	1208	CLA	O1D-CGD-O2D-CED
16	b	1235	CLA	O1D-CGD-O2D-CED
16	v	509	CLA	O1D-CGD-O2D-CED
19	A	4002	BCR	C11-C12-C13-C35
19	A	4008	BCR	C7-C8-C9-C34
19	A	4008	BCR	C37-C22-C23-C24
19	A	4011	BCR	C7-C8-C9-C34
19	B	4004	BCR	C7-C8-C9-C34
19	B	4009	BCR	C36-C18-C19-C20
19	B	4010	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
19	B	4014	BCR	C36-C18-C19-C20
19	F	4016	BCR	C7-C8-C9-C34
19	F	4016	BCR	C37-C22-C23-C24
19	G	4004	BCR	C7-C8-C9-C34
19	G	4004	BCR	C37-C22-C23-C24
19	G	4005	BCR	C7-C8-C9-C34
19	G	4010	BCR	C37-C22-C23-C24
19	H	4002	BCR	C11-C12-C13-C35
19	H	4002	BCR	C37-C22-C23-C24
19	H	4003	BCR	C37-C22-C23-C24
19	H	4007	BCR	C37-C22-C23-C24
19	H	4008	BCR	C37-C22-C23-C24
19	H	4011	BCR	C7-C8-C9-C34
19	J	4013	BCR	C37-C22-C23-C24
19	J	4015	BCR	C7-C8-C9-C34
19	K	4001	BCR	C7-C8-C9-C34
19	L	4019	BCR	C7-C8-C9-C34
19	L	4019	BCR	C37-C22-C23-C24
19	L	4022	BCR	C7-C8-C9-C34
19	Q	4016	BCR	C7-C8-C9-C34
19	Q	4016	BCR	C37-C22-C23-C24
19	R	4018	BCR	C37-C22-C23-C24
19	U	4019	BCR	C7-C8-C9-C34
19	W	601	BCR	C7-C8-C9-C34
19	W	604	BCR	C7-C8-C9-C34
19	X	601	BCR	C7-C8-C9-C34
19	X	601	BCR	C37-C22-C23-C24
19	X	603	BCR	C7-C8-C9-C34
19	X	604	BCR	C37-C22-C23-C24
19	Y	601	BCR	C37-C22-C23-C24
19	Y	602	BCR	C7-C8-C9-C34
19	a	4002	BCR	C7-C8-C9-C34
19	a	4003	BCR	C37-C22-C23-C24
19	b	4004	BCR	C7-C8-C9-C34
19	b	4009	BCR	C36-C18-C19-C20
19	b	4010	BCR	C37-C22-C23-C24
19	b	4014	BCR	C7-C8-C9-C34
19	b	4014	BCR	C37-C22-C23-C24
19	g	602	BCR	C11-C12-C13-C35
19	g	603	BCR	C7-C8-C9-C34
19	g	603	BCR	C11-C12-C13-C35
19	g	604	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
19	h	603	BCR	C37-C22-C23-C24
19	k	4001	BCR	C37-C22-C23-C24
19	n	601	BCR	C7-C8-C9-C34
19	n	603	BCR	C7-C8-C9-C34
19	o	602	BCR	C7-C8-C9-C34
19	o	604	BCR	C7-C8-C9-C34
19	o	604	BCR	C37-C22-C23-C24
19	p	601	BCR	C7-C8-C9-C34
19	p	604	BCR	C11-C12-C13-C35
19	q	602	BCR	C7-C8-C9-C34
19	q	602	BCR	C37-C22-C23-C24
19	q	604	BCR	C7-C8-C9-C34
19	r	603	BCR	C11-C12-C13-C35
19	r	604	BCR	C11-C12-C13-C35
19	s	601	BCR	C7-C8-C9-C34
19	s	602	BCR	C37-C22-C23-C24
19	s	604	BCR	C37-C22-C23-C24
19	t	601	BCR	C7-C8-C9-C34
19	u	604	BCR	C7-C8-C9-C34
19	u	604	BCR	C37-C22-C23-C24
19	v	603	BCR	C37-C22-C23-C24
19	v	604	BCR	C37-C22-C23-C24
19	w	602	BCR	C7-C8-C9-C34
19	w	602	BCR	C37-C22-C23-C24
19	w	603	BCR	C7-C8-C9-C34
19	w	604	BCR	C7-C8-C9-C34
19	x	601	BCR	C7-C8-C9-C34
19	x	601	BCR	C37-C22-C23-C24
19	x	602	BCR	C7-C8-C9-C34
19	x	604	BCR	C7-C8-C9-C34
19	x	604	BCR	C11-C12-C13-C35
19	y	601	BCR	C37-C22-C23-C24
19	y	603	BCR	C37-C22-C23-C24
19	y	604	BCR	C37-C22-C23-C24
21	G	4006	ECH	C37-C22-C23-C24
21	M	4021	ECH	C7-C8-C9-C34
21	R	4020	ECH	C7-C8-C9-C34
21	b	4006	ECH	C37-C22-C23-C24
21	i	4020	ECH	C7-C8-C9-C34
21	i	4020	ECH	C11-C12-C13-C35
21	m	4021	ECH	C37-C22-C23-C24
24	Z	601	LUT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
20	L	4101	LMT	O5'-C5'-C6'-O6'
19	B	4009	BCR	C17-C18-C19-C20
19	G	4004	BCR	C7-C8-C9-C10
19	G	4004	BCR	C21-C22-C23-C24
19	H	4008	BCR	C7-C8-C9-C10
19	H	4008	BCR	C21-C22-C23-C24
19	K	4001	BCR	C7-C8-C9-C10
19	L	4019	BCR	C21-C22-C23-C24
19	S	4013	BCR	C21-C22-C23-C24
19	T	4001	BCR	C7-C8-C9-C10
19	X	601	BCR	C7-C8-C9-C10
19	Y	601	BCR	C21-C22-C23-C24
19	Y	604	BCR	C7-C8-C9-C10
19	Z	602	BCR	C7-C8-C9-C10
19	b	4004	BCR	C7-C8-C9-C10
19	b	4009	BCR	C17-C18-C19-C20
19	g	602	BCR	C11-C12-C13-C14
19	g	602	BCR	C21-C22-C23-C24
19	h	601	BCR	C21-C22-C23-C24
19	h	604	BCR	C7-C8-C9-C10
19	i	4018	BCR	C7-C8-C9-C10
19	j	4015	BCR	C7-C8-C9-C10
19	k	4001	BCR	C7-C8-C9-C10
19	l	4019	BCR	C7-C8-C9-C10
19	l	4019	BCR	C21-C22-C23-C24
19	n	603	BCR	C7-C8-C9-C10
19	n	604	BCR	C7-C8-C9-C10
19	o	601	BCR	C7-C8-C9-C10
19	o	604	BCR	C7-C8-C9-C10
19	p	602	BCR	C7-C8-C9-C10
19	q	602	BCR	C7-C8-C9-C10
19	r	602	BCR	C7-C8-C9-C10
19	s	602	BCR	C7-C8-C9-C10
19	s	603	BCR	C7-C8-C9-C10
19	u	601	BCR	C21-C22-C23-C24
19	v	604	BCR	C7-C8-C9-C10
19	w	602	BCR	C21-C22-C23-C24
19	x	601	BCR	C21-C22-C23-C24
19	y	604	BCR	C7-C8-C9-C10
21	M	4021	ECH	C7-C8-C9-C10
21	R	4020	ECH	C7-C8-C9-C10
21	V	4021	ECH	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	m	4021	ECH	C11-C12-C13-C14
16	A	1132	CLA	C2A-CAA-CBA-CGA
16	B	1217	CLA	C2A-CAA-CBA-CGA
16	B	1228	CLA	C2A-CAA-CBA-CGA
16	H	1106	CLA	C2A-CAA-CBA-CGA
16	H	1132	CLA	C2A-CAA-CBA-CGA
16	L	1501	CLA	C2A-CAA-CBA-CGA
16	a	1118	CLA	C2A-CAA-CBA-CGA
16	a	1129	CLA	C2A-CAA-CBA-CGA
16	b	1218	CLA	C2A-CAA-CBA-CGA
16	b	1228	CLA	C2A-CAA-CBA-CGA
16	g	505	CLA	C2A-CAA-CBA-CGA
16	h	503	CLA	C2A-CAA-CBA-CGA
16	q	517	CLA	C2A-CAA-CBA-CGA
16	x	508	CLA	C2A-CAA-CBA-CGA
13	R	103	LHG	C7-C8-C9-C10
16	T	4002	CLA	O1D-CGD-O2D-CED
16	A	1122	CLA	O1A-CGA-O2A-C1
16	X	507	CLA	O1A-CGA-O2A-C1
16	a	1124	CLA	O1A-CGA-O2A-C1
16	b	1235	CLA	O1A-CGA-O2A-C1
16	p	510	CLA	O1A-CGA-O2A-C1
16	w	514	CLA	O1A-CGA-O2A-C1
16	G	1225	CLA	C13-C15-C16-C17
16	A	1134	CLA	CBD-CGD-O2D-CED
14	F	4017	LMG	C11-C10-O7-C8
14	Q	4017	LMG	C11-C10-O7-C8
16	A	1129	CLA	CBA-CGA-O2A-C1
23	x	606	LMU	C4B-C5B-C6B-O6B
13	g	605	LHG	C24-C23-O8-C6
16	B	1228	CLA	CBA-CGA-O2A-C1
16	H	1124	CLA	CBA-CGA-O2A-C1
16	H	1140	CLA	CBA-CGA-O2A-C1
16	W	506	CLA	CBA-CGA-O2A-C1
16	a	1140	CLA	CBA-CGA-O2A-C1
16	r	509	CLA	CBA-CGA-O2A-C1
16	s	502	CLA	CBA-CGA-O2A-C1
16	x	502	CLA	CBA-CGA-O2A-C1
16	x	507	CLA	CBA-CGA-O2A-C1
16	G	1214	CLA	C5-C6-C7-C8
16	a	1237	CLA	C13-C15-C16-C17
13	I	103	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
16	B	1220	CLA	C2-C1-O2A-CGA
16	B	1228	CLA	C2-C1-O2A-CGA
16	G	1228	CLA	C2-C1-O2A-CGA
16	L	1503	CLA	C2-C1-O2A-CGA
16	t	501	CLA	C2-C1-O2A-CGA
16	h	511	CLA	O1A-CGA-O2A-C1
16	w	509	CLA	O1A-CGA-O2A-C1
16	B	1201	CLA	O1D-CGD-O2D-CED
16	B	1216	CLA	O1D-CGD-O2D-CED
16	H	1117	CLA	O1D-CGD-O2D-CED
16	H	1126	CLA	O1D-CGD-O2D-CED
16	Y	517	CLA	O1D-CGD-O2D-CED
16	a	1117	CLA	O1D-CGD-O2D-CED
16	s	516	CLA	O1D-CGD-O2D-CED
16	w	516	CLA	O1D-CGD-O2D-CED
20	U	4101	LMT	C4'-C5'-C6'-O6'
16	p	510	CLA	CBD-CGD-O2D-CED
16	A	1022	CLA	C8-C10-C11-C12
16	A	1125	CLA	C8-C10-C11-C12
16	B	1221	CLA	C8-C10-C11-C12
16	G	1202	CLA	C5-C6-C7-C8
16	Y	509	CLA	C10-C11-C12-C13
16	a	1101	CLA	C15-C16-C17-C18
16	a	1106	CLA	C5-C6-C7-C8
16	b	1202	CLA	C5-C6-C7-C8
13	G	4018	LHG	O1-C1-C2-O2
16	q	510	CLA	C3-C5-C6-C7
16	x	512	CLA	C3-C5-C6-C7
16	Y	505	CLA	O1D-CGD-O2D-CED
16	s	510	CLA	O1A-CGA-O2A-C1
16	x	509	CLA	O1A-CGA-O2A-C1
16	A	1101	CLA	C15-C16-C17-C18
16	s	509	CLA	C5-C6-C7-C8
17	B	2002	PQN	C18-C20-C21-C22
16	T	4003	CLA	CBD-CGD-O2D-CED
16	X	509	CLA	CBD-CGD-O2D-CED
16	b	1222	CLA	CBD-CGD-O2D-CED
16	g	502	CLA	CBD-CGD-O2D-CED
23	x	606	LMU	O5'-C5'-C6'-O6'
14	b	848	LMG	C4-C5-C6-O5
16	A	1104	CLA	C11-C10-C8-C7
16	A	1139	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	H	1136	CLA	C11-C10-C8-C7
16	H	1139	CLA	C11-C10-C8-C7
16	Z	507	CLA	C6-C7-C8-C10
16	a	1104	CLA	C11-C10-C8-C7
16	b	1210	CLA	C11-C10-C8-C7
16	v	505	CLA	C11-C12-C13-C15
16	B	1206	CLA	O1D-CGD-O2D-CED
16	A	1140	CLA	CBA-CGA-O2A-C1
16	H	1123	CLA	CBA-CGA-O2A-C1
16	h	512	CLA	CBA-CGA-O2A-C1
16	p	507	CLA	CBA-CGA-O2A-C1
16	q	509	CLA	CBA-CGA-O2A-C1
16	x	514	CLA	CBA-CGA-O2A-C1
16	r	504	CLA	C15-C16-C17-C18
16	t	517	CLA	C5-C6-C7-C8
16	f	1302	CLA	O1D-CGD-O2D-CED
16	l	1501	CLA	O1D-CGD-O2D-CED
13	R	103	LHG	C23-C24-C25-C26
14	G	848	LMG	C28-C29-C30-C31
19	G	4005	BCR	C19-C20-C21-C22
19	H	4011	BCR	C19-C20-C21-C22
19	W	603	BCR	C9-C10-C11-C12
19	X	604	BCR	C15-C16-C17-C18
19	g	604	BCR	C9-C10-C11-C12
19	n	603	BCR	C9-C10-C11-C12
19	r	604	BCR	C9-C10-C11-C12
19	u	604	BCR	C9-C10-C11-C12
19	u	604	BCR	C15-C16-C17-C18
19	v	603	BCR	C9-C10-C11-C12
19	x	603	BCR	C15-C16-C17-C18
19	x	604	BCR	C9-C10-C11-C12
16	G	1224	CLA	O1A-CGA-O2A-C1
16	a	1116	CLA	O1D-CGD-O2D-CED
16	r	512	CLA	O1D-CGD-O2D-CED
16	s	502	CLA	O1D-CGD-O2D-CED
16	B	1235	CLA	C3-C5-C6-C7
16	G	1235	CLA	C3-C5-C6-C7
16	Z	506	CLA	C3-C5-C6-C7
16	x	509	CLA	C3-C5-C6-C7
16	Y	512	CLA	C10-C11-C12-C13
16	h	508	CLA	C5-C6-C7-C8
16	q	509	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
16	v	504	CLA	C10-C11-C12-C13
17	G	2002	PQN	C18-C20-C21-C22
16	A	1114	CLA	CBA-CGA-O2A-C1
16	b	1231	CLA	O1D-CGD-O2D-CED
23	Z	605	LMU	O5'-C5'-C6'-O6'
13	B	4018	LHG	C7-C8-C9-C10
13	b	4018	LHG	C7-C8-C9-C10
13	x	605	LHG	C23-C24-C25-C26
13	A	849	LHG	O10-C23-O8-C6
16	U	1503	CLA	O1A-CGA-O2A-C1
16	X	509	CLA	O1A-CGA-O2A-C1
16	Y	507	CLA	O1A-CGA-O2A-C1
16	Y	510	CLA	O1A-CGA-O2A-C1
16	Y	514	CLA	O1A-CGA-O2A-C1
16	b	1224	CLA	O1A-CGA-O2A-C1
16	b	1238	CLA	O1A-CGA-O2A-C1
16	g	504	CLA	O1A-CGA-O2A-C1
16	t	512	CLA	O1A-CGA-O2A-C1
16	v	517	CLA	O1A-CGA-O2A-C1
16	U	1501	CLA	O1D-CGD-O2D-CED
16	b	1228	CLA	O1D-CGD-O2D-CED
16	r	509	CLA	O1D-CGD-O2D-CED
16	y	509	CLA	O1D-CGD-O2D-CED
16	A	1103	CLA	C15-C16-C17-C18
16	A	1104	CLA	C10-C11-C12-C13
16	A	1139	CLA	C10-C11-C12-C13
16	B	1023	CLA	C13-C15-C16-C17
16	B	1235	CLA	C8-C10-C11-C12
16	G	1229	CLA	C5-C6-C7-C8
16	H	1101	CLA	C13-C15-C16-C17
16	H	1103	CLA	C13-C15-C16-C17
16	H	1106	CLA	C5-C6-C7-C8
16	H	1128	CLA	C8-C10-C11-C12
16	L	1501	CLA	C10-C11-C12-C13
16	Y	509	CLA	C5-C6-C7-C8
16	Z	506	CLA	C5-C6-C7-C8
16	g	515	CLA	C8-C10-C11-C12
16	o	504	CLA	C5-C6-C7-C8
16	w	504	CLA	C13-C15-C16-C17
23	x	606	LMU	O5B-C5B-C6B-O6B
16	A	1105	CLA	C2A-CAA-CBA-CGA
16	A	1106	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	A	1118	CLA	C2A-CAA-CBA-CGA
16	A	1127	CLA	C2A-CAA-CBA-CGA
16	B	1229	CLA	C2A-CAA-CBA-CGA
16	G	1217	CLA	C2A-CAA-CBA-CGA
16	G	1238	CLA	C2A-CAA-CBA-CGA
16	H	1105	CLA	C2A-CAA-CBA-CGA
16	U	1501	CLA	C2A-CAA-CBA-CGA
16	W	501	CLA	C2A-CAA-CBA-CGA
16	W	504	CLA	C2A-CAA-CBA-CGA
16	W	505	CLA	C2A-CAA-CBA-CGA
16	W	517	CLA	C2A-CAA-CBA-CGA
16	X	515	CLA	C2A-CAA-CBA-CGA
16	Z	503	CLA	C2A-CAA-CBA-CGA
16	Z	517	CLA	C2A-CAA-CBA-CGA
16	a	1105	CLA	C2A-CAA-CBA-CGA
16	a	1106	CLA	C2A-CAA-CBA-CGA
16	a	1132	CLA	C2A-CAA-CBA-CGA
16	b	1211	CLA	C2A-CAA-CBA-CGA
16	b	1223	CLA	C2A-CAA-CBA-CGA
16	b	1238	CLA	C2A-CAA-CBA-CGA
16	n	505	CLA	C2A-CAA-CBA-CGA
16	n	515	CLA	C2A-CAA-CBA-CGA
16	n	517	CLA	C2A-CAA-CBA-CGA
16	o	505	CLA	C2A-CAA-CBA-CGA
16	o	506	CLA	C2A-CAA-CBA-CGA
16	q	503	CLA	C2A-CAA-CBA-CGA
16	r	504	CLA	C2A-CAA-CBA-CGA
16	r	505	CLA	C2A-CAA-CBA-CGA
16	r	517	CLA	C2A-CAA-CBA-CGA
16	s	501	CLA	C2A-CAA-CBA-CGA
16	s	509	CLA	C2A-CAA-CBA-CGA
16	t	504	CLA	C2A-CAA-CBA-CGA
16	t	505	CLA	C2A-CAA-CBA-CGA
16	t	506	CLA	C2A-CAA-CBA-CGA
16	t	515	CLA	C2A-CAA-CBA-CGA
16	t	517	CLA	C2A-CAA-CBA-CGA
16	u	515	CLA	C2A-CAA-CBA-CGA
16	v	504	CLA	C2A-CAA-CBA-CGA
16	w	515	CLA	C2A-CAA-CBA-CGA
16	x	504	CLA	C2A-CAA-CBA-CGA
16	x	517	CLA	C2A-CAA-CBA-CGA
16	y	503	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	4008	BCR	C18-C19-C20-C21
19	A	4011	BCR	C10-C11-C12-C13
19	G	4014	BCR	C18-C19-C20-C21
19	H	4011	BCR	C18-C19-C20-C21
19	K	4001	BCR	C10-C11-C12-C13
19	T	4001	BCR	C10-C11-C12-C13
19	X	602	BCR	C18-C19-C20-C21
19	a	4011	BCR	C10-C11-C12-C13
19	a	4011	BCR	C18-C19-C20-C21
19	b	4004	BCR	C18-C19-C20-C21
19	b	4005	BCR	C18-C19-C20-C21
19	k	4001	BCR	C10-C11-C12-C13
19	l	4022	BCR	C10-C11-C12-C13
19	o	604	BCR	C10-C11-C12-C13
19	r	603	BCR	C18-C19-C20-C21
19	t	603	BCR	C10-C11-C12-C13
19	u	603	BCR	C18-C19-C20-C21
16	A	1130	CLA	C8-C10-C11-C12
16	H	1101	CLA	C8-C10-C11-C12
16	H	1109	CLA	C13-C15-C16-C17
16	H	1126	CLA	C15-C16-C17-C18
16	L	1503	CLA	C15-C16-C17-C18
16	W	515	CLA	C10-C11-C12-C13
16	X	506	CLA	C8-C10-C11-C12
16	X	508	CLA	C5-C6-C7-C8
16	Z	504	CLA	C13-C15-C16-C17
16	a	1101	CLA	C13-C15-C16-C17
16	b	1021	CLA	C5-C6-C7-C8
16	b	1221	CLA	C10-C11-C12-C13
16	h	507	CLA	C15-C16-C17-C18
16	n	515	CLA	C10-C11-C12-C13
16	o	517	CLA	C5-C6-C7-C8
16	p	511	CLA	C8-C10-C11-C12
16	r	512	CLA	C5-C6-C7-C8
16	s	504	CLA	C15-C16-C17-C18
16	s	511	CLA	C8-C10-C11-C12
16	s	512	CLA	C10-C11-C12-C13
16	v	508	CLA	C5-C6-C7-C8
16	v	515	CLA	C5-C6-C7-C8
16	y	512	CLA	C5-C6-C7-C8
20	a	4202	LMT	C4B-C5B-C6B-O6B
23	x	606	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	A	849	LHG	C23-C24-C25-C26
13	g	605	LHG	C23-C24-C25-C26
13	i	103	LHG	C23-C24-C25-C26
13	r	605	LHG	C23-C24-C25-C26
13	s	605	LHG	C23-C24-C25-C26
14	B	848	LMG	C28-C29-C30-C31
16	W	505	CLA	O1D-CGD-O2D-CED
16	b	1240	CLA	CBA-CGA-O2A-C1
16	s	503	CLA	CBA-CGA-O2A-C1
16	B	1202	CLA	O1A-CGA-O2A-C1
16	B	1225	CLA	O1A-CGA-O2A-C1
16	G	1202	CLA	O1A-CGA-O2A-C1
16	Z	509	CLA	O1A-CGA-O2A-C1
16	g	509	CLA	O1A-CGA-O2A-C1
16	h	507	CLA	O1A-CGA-O2A-C1
16	n	506	CLA	O1A-CGA-O2A-C1
16	A	1139	CLA	C3-C5-C6-C7
14	G	848	LMG	O6-C1-O1-C7
14	b	848	LMG	O6-C1-O1-C7
19	A	4002	BCR	C6-C7-C8-C9
19	B	4005	BCR	C6-C7-C8-C9
19	h	604	BCR	C6-C7-C8-C9
19	j	4012	BCR	C6-C7-C8-C9
19	t	603	BCR	C6-C7-C8-C9
19	v	604	BCR	C6-C7-C8-C9
19	w	604	BCR	C22-C23-C24-C25
19	y	604	BCR	C6-C7-C8-C9
23	Z	605	LMU	O5'-C1'-O1'-C1
23	w	605	LMU	O5'-C1'-O1'-C1
23	x	606	LMU	O5'-C1'-O1'-C1
23	p	606	LMU	O5B-C5B-C6B-O6B
16	A	1101	CLA	C13-C15-C16-C17
16	A	1106	CLA	C5-C6-C7-C8
16	A	1131	CLA	C5-C6-C7-C8
16	B	1206	CLA	C10-C11-C12-C13
16	H	1013	CLA	C13-C15-C16-C17
16	H	1125	CLA	C5-C6-C7-C8
16	H	1128	CLA	C10-C11-C12-C13
16	H	1139	CLA	C10-C11-C12-C13
16	X	504	CLA	C8-C10-C11-C12
16	Y	504	CLA	C15-C16-C17-C18
16	Y	511	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	Z	504	CLA	C5-C6-C7-C8
16	Z	505	CLA	C8-C10-C11-C12
16	Z	509	CLA	C10-C11-C12-C13
16	a	1125	CLA	C5-C6-C7-C8
16	a	1125	CLA	C8-C10-C11-C12
16	a	1140	CLA	C5-C6-C7-C8
16	b	1229	CLA	C5-C6-C7-C8
16	b	1235	CLA	C8-C10-C11-C12
16	b	1238	CLA	C8-C10-C11-C12
16	h	506	CLA	C5-C6-C7-C8
16	h	512	CLA	C5-C6-C7-C8
16	o	506	CLA	C8-C10-C11-C12
16	o	508	CLA	C5-C6-C7-C8
16	p	509	CLA	C5-C6-C7-C8
16	q	506	CLA	C5-C6-C7-C8
16	t	515	CLA	C10-C11-C12-C13
16	u	508	CLA	C5-C6-C7-C8
16	y	511	CLA	C10-C11-C12-C13
13	B	4018	LHG	O2-C2-C3-O3
13	I	103	LHG	O2-C2-C3-O3
13	b	4018	LHG	O2-C2-C3-O3
13	x	605	LHG	O2-C2-C3-O3
13	H	849	LHG	C24-C23-O8-C6
16	G	1228	CLA	CBA-CGA-O2A-C1
16	B	1224	CLA	O1A-CGA-O2A-C1
16	H	1106	CLA	O1A-CGA-O2A-C1
16	b	1202	CLA	O1A-CGA-O2A-C1
16	b	1221	CLA	O1A-CGA-O2A-C1
16	r	507	CLA	O1A-CGA-O2A-C1
16	w	502	CLA	O1A-CGA-O2A-C1
16	H	1140	CLA	C5-C6-C7-C8
16	W	506	CLA	C8-C10-C11-C12
16	a	1103	CLA	C15-C16-C17-C18
16	b	1023	CLA	C13-C15-C16-C17
16	b	1205	CLA	C13-C15-C16-C17
16	n	512	CLA	C10-C11-C12-C13
16	n	517	CLA	C5-C6-C7-C8
16	p	504	CLA	C15-C16-C17-C18
16	q	504	CLA	C8-C10-C11-C12
16	q	504	CLA	C13-C15-C16-C17
16	r	505	CLA	C5-C6-C7-C8
23	g	606	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
16	G	1216	CLA	O1D-CGD-O2D-CED
16	T	4004	CLA	O1D-CGD-O2D-CED
16	p	516	CLA	CBA-CGA-O2A-C1
16	t	503	CLA	CBA-CGA-O2A-C1
16	H	1139	CLA	C3-C5-C6-C7
16	W	517	CLA	C3-C5-C6-C7
16	b	1207	CLA	C3-C5-C6-C7
16	A	1107	CLA	O1D-CGD-O2D-CED
16	W	517	CLA	O1D-CGD-O2D-CED
16	Z	509	CLA	O1D-CGD-O2D-CED
16	a	1138	CLA	O1D-CGD-O2D-CED
16	p	505	CLA	O1D-CGD-O2D-CED
16	A	1105	CLA	C5-C6-C7-C8
16	A	1127	CLA	C8-C10-C11-C12
16	A	1128	CLA	C10-C11-C12-C13
16	G	1023	CLA	C15-C16-C17-C18
16	H	1022	CLA	C15-C16-C17-C18
16	H	1103	CLA	C15-C16-C17-C18
16	H	1105	CLA	C5-C6-C7-C8
16	U	1501	CLA	C10-C11-C12-C13
16	Y	511	CLA	C8-C10-C11-C12
16	a	1105	CLA	C5-C6-C7-C8
16	a	1109	CLA	C15-C16-C17-C18
16	q	512	CLA	C10-C11-C12-C13
16	t	505	CLA	C15-C16-C17-C18
16	u	505	CLA	C5-C6-C7-C8
16	u	506	CLA	C8-C10-C11-C12
16	y	515	CLA	C5-C6-C7-C8
20	l	4101	LMT	O5'-C5'-C6'-O6'
15	H	1011	CL0	O1A-CGA-O2A-C1
16	W	506	CLA	O1A-CGA-O2A-C1
16	s	502	CLA	O1A-CGA-O2A-C1
16	a	1110	CLA	C2-C3-C5-C6
13	G	4018	LHG	C23-C24-C25-C26
13	a	851	LHG	C7-C8-C9-C10
16	G	1203	CLA	O1D-CGD-O2D-CED
16	X	501	CLA	O1D-CGD-O2D-CED
16	r	503	CLA	O1D-CGD-O2D-CED
16	w	512	CLA	O1D-CGD-O2D-CED
16	y	517	CLA	O1D-CGD-O2D-CED
16	H	1114	CLA	O1A-CGA-O2A-C1
16	A	1109	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	A	1140	CLA	C15-C16-C17-C18
16	B	1021	CLA	C5-C6-C7-C8
16	B	1202	CLA	C5-C6-C7-C8
16	G	1238	CLA	C13-C15-C16-C17
16	H	1127	CLA	C15-C16-C17-C18
16	Y	504	CLA	C8-C10-C11-C12
16	Y	510	CLA	C15-C16-C17-C18
16	Y	512	CLA	C15-C16-C17-C18
16	Z	505	CLA	C15-C16-C17-C18
16	h	507	CLA	C8-C10-C11-C12
16	p	510	CLA	C15-C16-C17-C18
16	q	517	CLA	C5-C6-C7-C8
16	w	509	CLA	C10-C11-C12-C13
16	w	515	CLA	C15-C16-C17-C18
16	y	509	CLA	C10-C11-C12-C13
16	G	1220	CLA	CBA-CGA-O2A-C1
16	b	1220	CLA	CBA-CGA-O2A-C1
16	g	502	CLA	CBA-CGA-O2A-C1
16	g	507	CLA	CBA-CGA-O2A-C1
16	h	504	CLA	CBA-CGA-O2A-C1
16	k	4004	CLA	CBA-CGA-O2A-C1
16	n	507	CLA	CBA-CGA-O2A-C1
16	p	506	CLA	CBA-CGA-O2A-C1
16	Y	508	CLA	CBD-CGD-O2D-CED
16	a	1136	CLA	CBD-CGD-O2D-CED
16	n	505	CLA	CBD-CGD-O2D-CED
16	o	509	CLA	CBD-CGD-O2D-CED
16	u	511	CLA	CBD-CGD-O2D-CED
16	w	502	CLA	CBD-CGD-O2D-CED
16	x	508	CLA	CBD-CGD-O2D-CED
16	H	1124	CLA	O1A-CGA-O2A-C1
16	a	1140	CLA	O1A-CGA-O2A-C1
16	p	507	CLA	O1A-CGA-O2A-C1
16	r	509	CLA	O1A-CGA-O2A-C1
16	q	517	CLA	O1D-CGD-O2D-CED
16	G	1240	CLA	CBA-CGA-O2A-C1
16	Z	516	CLA	CBA-CGA-O2A-C1
16	r	516	CLA	CBA-CGA-O2A-C1
16	u	503	CLA	CBA-CGA-O2A-C1
16	x	503	CLA	CBA-CGA-O2A-C1
23	r	606	LMU	C4'-C5'-C6'-O6'
16	A	1128	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	a	1022	CLA	C15-C16-C17-C18
16	x	512	CLA	C5-C6-C7-C8
16	B	1203	CLA	C3-C5-C6-C7
16	a	1106	CLA	C3-C5-C6-C7
16	a	1132	CLA	C3-C5-C6-C7
16	q	508	CLA	C3-C5-C6-C7
16	x	506	CLA	C3-C5-C6-C7
16	a	1111	CLA	CBD-CGD-O2D-CED
19	W	601	BCR	C19-C20-C21-C22
19	h	603	BCR	C9-C10-C11-C12
19	o	602	BCR	C19-C20-C21-C22
19	r	602	BCR	C19-C20-C21-C22
19	s	603	BCR	C9-C10-C11-C12
19	x	602	BCR	C13-C14-C15-C16
19	x	604	BCR	C13-C14-C15-C16
16	G	1021	CLA	C13-C15-C16-C17
16	H	1101	CLA	C15-C16-C17-C18
16	H	1125	CLA	C8-C10-C11-C12
16	H	1237	CLA	C8-C10-C11-C12
16	a	1128	CLA	C10-C11-C12-C13
16	B	1228	CLA	O1A-CGA-O2A-C1
16	h	512	CLA	O1A-CGA-O2A-C1
16	q	509	CLA	O1A-CGA-O2A-C1
14	b	848	LMG	O6-C5-C6-O5
14	A	4101	LMG	C28-C29-C30-C31
13	b	4018	LHG	C1-C2-C3-O3
13	x	605	LHG	C1-C2-C3-O3
16	B	1235	CLA	C2A-CAA-CBA-CGA
16	B	1238	CLA	C2A-CAA-CBA-CGA
16	G	1228	CLA	C2A-CAA-CBA-CGA
16	H	1118	CLA	C2A-CAA-CBA-CGA
16	L	1503	CLA	C2A-CAA-CBA-CGA
16	W	515	CLA	C2A-CAA-CBA-CGA
16	X	508	CLA	C2A-CAA-CBA-CGA
16	Z	515	CLA	C2A-CAA-CBA-CGA
16	l	1501	CLA	C2A-CAA-CBA-CGA
16	o	516	CLA	C2A-CAA-CBA-CGA
16	w	517	CLA	C2A-CAA-CBA-CGA
16	x	503	CLA	O1D-CGD-O2D-CED
13	r	605	LHG	C24-C23-O8-C6
15	a	1011	CL0	CBA-CGA-O2A-C1
16	Z	512	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	a	1123	CLA	CBA-CGA-O2A-C1
16	b	1222	CLA	CBA-CGA-O2A-C1
16	q	502	CLA	CBA-CGA-O2A-C1
16	r	514	CLA	CBA-CGA-O2A-C1
16	u	507	CLA	CBA-CGA-O2A-C1
16	A	1013	CLA	C8-C10-C11-C12
16	A	1126	CLA	C15-C16-C17-C18
16	B	1203	CLA	C10-C11-C12-C13
16	B	1205	CLA	C13-C15-C16-C17
16	G	1021	CLA	C5-C6-C7-C8
16	H	1013	CLA	C8-C10-C11-C12
16	H	1022	CLA	C8-C10-C11-C12
16	H	1118	CLA	C5-C6-C7-C8
16	H	1139	CLA	C5-C6-C7-C8
16	H	1237	CLA	C10-C11-C12-C13
16	W	510	CLA	C13-C15-C16-C17
16	X	517	CLA	C5-C6-C7-C8
16	b	1204	CLA	C13-C15-C16-C17
16	g	504	CLA	C13-C15-C16-C17
16	g	512	CLA	C5-C6-C7-C8
16	h	511	CLA	C5-C6-C7-C8
16	o	504	CLA	C8-C10-C11-C12
16	p	504	CLA	C5-C6-C7-C8
16	p	512	CLA	C10-C11-C12-C13
16	s	509	CLA	C10-C11-C12-C13
16	u	515	CLA	C15-C16-C17-C18
16	v	512	CLA	C5-C6-C7-C8
16	w	504	CLA	C5-C6-C7-C8
16	w	510	CLA	C5-C6-C7-C8
16	x	511	CLA	C5-C6-C7-C8
17	B	2002	PQN	C23-C25-C26-C27
17	G	2002	PQN	C23-C25-C26-C27
16	K	4003	CLA	CBD-CGD-O2D-CED
16	Z	516	CLA	CBD-CGD-O2D-CED
16	n	510	CLA	CBD-CGD-O2D-CED
16	u	510	CLA	CBD-CGD-O2D-CED
16	A	1109	CLA	C10-C11-C12-C13
16	G	1221	CLA	C13-C15-C16-C17
16	G	1225	CLA	C15-C16-C17-C18
16	a	1126	CLA	C15-C16-C17-C18
16	a	1237	CLA	C10-C11-C12-C13
16	b	1221	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	l	1501	CLA	C10-C11-C12-C13
16	n	510	CLA	C13-C15-C16-C17
16	o	505	CLA	C5-C6-C7-C8
16	p	511	CLA	C5-C6-C7-C8
16	p	515	CLA	C8-C10-C11-C12
16	u	504	CLA	C8-C10-C11-C12
23	w	605	LMU	C4'-C5'-C6'-O6'
23	r	606	LMU	O5'-C5'-C6'-O6'
16	A	1125	CLA	C5-C6-C7-C8
16	A	1128	CLA	C15-C16-C17-C18
16	B	1221	CLA	C13-C15-C16-C17
16	B	1229	CLA	C5-C6-C7-C8
16	W	517	CLA	C5-C6-C7-C8
16	a	1237	CLA	C8-C10-C11-C12
16	b	1021	CLA	C13-C15-C16-C17
16	b	1203	CLA	C10-C11-C12-C13
16	b	1211	CLA	C13-C15-C16-C17
16	b	1238	CLA	C5-C6-C7-C8
16	q	511	CLA	C5-C6-C7-C8
16	s	510	CLA	C5-C6-C7-C8
16	s	511	CLA	C5-C6-C7-C8
16	v	511	CLA	C5-C6-C7-C8
16	w	504	CLA	C8-C10-C11-C12
16	B	1235	CLA	CBA-CGA-O2A-C1
16	W	501	CLA	CBA-CGA-O2A-C1
16	a	1104	CLA	CBA-CGA-O2A-C1
16	n	511	CLA	CBA-CGA-O2A-C1
16	p	508	CLA	CBA-CGA-O2A-C1
16	r	506	CLA	CBA-CGA-O2A-C1
16	s	507	CLA	CBA-CGA-O2A-C1
16	L	1502	CLA	C4-C3-C5-C6
16	r	505	CLA	C4-C3-C5-C6
16	Y	513	CLA	O1D-CGD-O2D-CED
16	x	509	CLA	O1D-CGD-O2D-CED
16	A	1139	CLA	C5-C6-C7-C8
16	G	1203	CLA	C10-C11-C12-C13
16	G	1224	CLA	C5-C6-C7-C8
16	H	1131	CLA	C5-C6-C7-C8
16	a	1130	CLA	C8-C10-C11-C12
16	b	1238	CLA	C10-C11-C12-C13
16	g	504	CLA	C15-C16-C17-C18
16	h	515	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
16	u	517	CLA	C5-C6-C7-C8
16	x	504	CLA	C13-C15-C16-C17
16	X	508	CLA	C3-C5-C6-C7
16	Z	508	CLA	C3-C5-C6-C7
16	a	1133	CLA	C3-C5-C6-C7
16	b	1203	CLA	C3-C5-C6-C7
16	a	1106	CLA	CBD-CGD-O2D-CED
16	W	510	CLA	C11-C10-C8-C9
16	h	502	CLA	O1D-CGD-O2D-CED
16	x	507	CLA	O1A-CGA-O2A-C1
13	A	851	LHG	O9-C7-O7-C5
14	G	848	LMG	C2-C1-O1-C7
14	b	848	LMG	C2-C1-O1-C7
16	a	1104	CLA	C10-C11-C12-C13
16	a	1128	CLA	C13-C15-C16-C17
16	r	504	CLA	C13-C15-C16-C17
16	x	504	CLA	C15-C16-C17-C18
13	p	605	LHG	C23-C24-C25-C26
16	j	1302	CLA	O1D-CGD-O2D-CED
16	s	505	CLA	O1D-CGD-O2D-CED
13	R	103	LHG	O2-C2-C3-O3
16	K	4004	CLA	CBA-CGA-O2A-C1
16	G	1226	CLA	C11-C12-C13-C14
16	b	1012	CLA	C6-C7-C8-C9
16	W	515	CLA	C5-C6-C7-C8
16	s	515	CLA	C5-C6-C7-C8
16	H	1123	CLA	O1A-CGA-O2A-C1
16	H	1140	CLA	O1A-CGA-O2A-C1
16	x	502	CLA	O1A-CGA-O2A-C1
19	A	4002	BCR	C20-C21-C22-C37
19	A	4011	BCR	C20-C21-C22-C37
19	B	4010	BCR	C20-C21-C22-C37
19	B	4017	BCR	C35-C13-C14-C15
19	G	4005	BCR	C20-C21-C22-C37
19	H	4002	BCR	C20-C21-C22-C37
19	H	4003	BCR	C20-C21-C22-C37
19	H	4008	BCR	C20-C21-C22-C37
19	H	4011	BCR	C20-C21-C22-C37
19	I	4018	BCR	C35-C13-C14-C15
19	J	4013	BCR	C16-C17-C18-C36
19	J	4015	BCR	C16-C17-C18-C36
19	L	4022	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
19	R	4018	BCR	C35-C13-C14-C15
19	S	4015	BCR	C16-C17-C18-C36
19	T	4005	BCR	C16-C17-C18-C36
19	a	4003	BCR	C20-C21-C22-C37
19	b	4005	BCR	C20-C21-C22-C37
19	b	4010	BCR	C11-C10-C9-C34
19	b	4014	BCR	C20-C21-C22-C37
19	f	4016	BCR	C35-C13-C14-C15
19	g	602	BCR	C11-C10-C9-C34
19	g	604	BCR	C11-C10-C9-C34
19	g	604	BCR	C16-C17-C18-C36
19	h	604	BCR	C20-C21-C22-C37
19	l	4022	BCR	C16-C17-C18-C36
19	n	604	BCR	C16-C17-C18-C36
19	o	601	BCR	C20-C21-C22-C37
19	o	604	BCR	C20-C21-C22-C37
19	q	603	BCR	C20-C21-C22-C37
19	q	604	BCR	C11-C10-C9-C34
19	r	601	BCR	C16-C17-C18-C36
19	r	602	BCR	C11-C10-C9-C34
19	r	602	BCR	C16-C17-C18-C36
19	r	602	BCR	C20-C21-C22-C37
19	r	604	BCR	C16-C17-C18-C36
19	s	601	BCR	C16-C17-C18-C36
19	s	601	BCR	C20-C21-C22-C37
19	t	601	BCR	C20-C21-C22-C37
19	u	602	BCR	C20-C21-C22-C37
19	u	603	BCR	C20-C21-C22-C37
19	v	601	BCR	C20-C21-C22-C37
19	v	603	BCR	C20-C21-C22-C37
19	v	604	BCR	C20-C21-C22-C37
19	w	604	BCR	C35-C13-C14-C15
19	w	604	BCR	C16-C17-C18-C36
19	x	602	BCR	C20-C21-C22-C37
19	y	601	BCR	C20-C21-C22-C37
15	a	1011	CL0	C3-C5-C6-C7
20	U	4101	LMT	O5'-C5'-C6'-O6'
16	A	1013	CLA	C13-C15-C16-C17
16	A	1237	CLA	C13-C15-C16-C17
16	p	515	CLA	C15-C16-C17-C18
19	A	4007	BCR	C37-C22-C23-C24
19	A	4011	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	G	4017	BCR	C37-C22-C23-C24
19	H	4002	BCR	C7-C8-C9-C34
19	H	4011	BCR	C37-C22-C23-C24
19	I	4018	BCR	C7-C8-C9-C34
19	K	4001	BCR	C37-C22-C23-C24
19	R	4018	BCR	C7-C8-C9-C34
19	T	4001	BCR	C7-C8-C9-C34
19	U	4022	BCR	C7-C8-C9-C34
19	U	4022	BCR	C11-C12-C13-C35
19	W	601	BCR	C11-C12-C13-C35
19	Y	602	BCR	C37-C22-C23-C24
19	Z	602	BCR	C7-C8-C9-C34
19	f	4016	BCR	C7-C8-C9-C34
19	g	601	BCR	C11-C12-C13-C35
19	g	604	BCR	C7-C8-C9-C34
19	h	604	BCR	C37-C22-C23-C24
19	i	4018	BCR	C7-C8-C9-C34
19	k	4001	BCR	C7-C8-C9-C34
19	l	4019	BCR	C7-C8-C9-C34
19	l	4022	BCR	C7-C8-C9-C34
19	o	601	BCR	C7-C8-C9-C34
19	p	601	BCR	C37-C22-C23-C24
19	p	602	BCR	C7-C8-C9-C34
19	p	602	BCR	C37-C22-C23-C24
19	s	602	BCR	C7-C8-C9-C34
19	s	603	BCR	C7-C8-C9-C34
21	M	4021	ECH	C11-C12-C13-C35
21	R	4020	ECH	C37-C22-C23-C24
21	i	4020	ECH	C36-C18-C19-C20
19	A	4008	BCR	C21-C22-C23-C24
19	B	4004	BCR	C21-C22-C23-C24
19	G	4014	BCR	C17-C18-C19-C20
19	H	4008	BCR	C17-C18-C19-C20
19	I	4018	BCR	C7-C8-C9-C10
19	R	4018	BCR	C7-C8-C9-C10
19	U	4019	BCR	C21-C22-C23-C24
19	W	601	BCR	C21-C22-C23-C24
19	W	604	BCR	C7-C8-C9-C10
19	X	603	BCR	C7-C8-C9-C10
19	Y	602	BCR	C7-C8-C9-C10
19	Y	603	BCR	C21-C22-C23-C24
19	b	4004	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	g	601	BCR	C21-C22-C23-C24
19	g	603	BCR	C7-C8-C9-C10
19	h	603	BCR	C21-C22-C23-C24
19	k	4005	BCR	C21-C22-C23-C24
19	o	602	BCR	C21-C22-C23-C24
19	p	604	BCR	C7-C8-C9-C10
19	r	602	BCR	C21-C22-C23-C24
19	s	604	BCR	C7-C8-C9-C10
19	u	604	BCR	C7-C8-C9-C10
19	w	602	BCR	C7-C8-C9-C10
19	x	603	BCR	C7-C8-C9-C10
19	y	603	BCR	C21-C22-C23-C24
21	M	4021	ECH	C11-C12-C13-C14
21	i	4020	ECH	C7-C8-C9-C10
21	m	4021	ECH	C21-C22-C23-C24
16	A	1140	CLA	O1A-CGA-O2A-C1
16	a	1123	CLA	O1A-CGA-O2A-C1
16	k	4004	CLA	O1A-CGA-O2A-C1
16	x	514	CLA	O1A-CGA-O2A-C1
16	A	1116	CLA	C2A-CAA-CBA-CGA
16	B	1218	CLA	C2A-CAA-CBA-CGA
16	B	1220	CLA	C2A-CAA-CBA-CGA
16	G	1229	CLA	C2A-CAA-CBA-CGA
16	G	1235	CLA	C2A-CAA-CBA-CGA
16	H	1126	CLA	C2A-CAA-CBA-CGA
16	H	1138	CLA	C2A-CAA-CBA-CGA
16	Y	516	CLA	C2A-CAA-CBA-CGA
16	a	1110	CLA	C2A-CAA-CBA-CGA
16	b	1201	CLA	C2A-CAA-CBA-CGA
16	g	508	CLA	C2A-CAA-CBA-CGA
16	g	511	CLA	C2A-CAA-CBA-CGA
16	g	515	CLA	C2A-CAA-CBA-CGA
16	n	501	CLA	C2A-CAA-CBA-CGA
16	o	502	CLA	C2A-CAA-CBA-CGA
16	p	502	CLA	C2A-CAA-CBA-CGA
16	q	515	CLA	C2A-CAA-CBA-CGA
16	r	513	CLA	C2A-CAA-CBA-CGA
16	r	515	CLA	C2A-CAA-CBA-CGA
16	s	515	CLA	C2A-CAA-CBA-CGA
16	s	516	CLA	C2A-CAA-CBA-CGA
16	s	517	CLA	C2A-CAA-CBA-CGA
16	u	508	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	u	516	CLA	C2A-CAA-CBA-CGA
16	v	505	CLA	C2A-CAA-CBA-CGA
16	w	503	CLA	C2A-CAA-CBA-CGA
16	x	505	CLA	C2A-CAA-CBA-CGA
16	x	515	CLA	C2A-CAA-CBA-CGA
16	y	517	CLA	C2A-CAA-CBA-CGA
17	b	2002	PQN	C15-C16-C17-C18
13	I	103	LHG	O1-C1-C2-C3
13	X	605	LHG	O1-C1-C2-C3
16	G	1222	CLA	CBD-CGD-O2D-CED
16	H	1136	CLA	O1D-CGD-O2D-CED
23	Y	606	LMU	C4'-C5'-C6'-O6'
16	A	1140	CLA	C16-C17-C18-C20
16	G	1206	CLA	C16-C17-C18-C20
16	G	1215	CLA	C11-C12-C13-C14
16	H	1140	CLA	C16-C17-C18-C20
16	X	505	CLA	C16-C17-C18-C19
16	Z	510	CLA	C11-C12-C13-C15
16	b	1021	CLA	C16-C17-C18-C19
16	b	1206	CLA	C16-C17-C18-C19
16	h	510	CLA	C16-C17-C18-C19
16	h	510	CLA	C16-C17-C18-C20
16	k	4004	CLA	C6-C7-C8-C9
16	o	505	CLA	C16-C17-C18-C19
16	A	1138	CLA	O1D-CGD-O2D-CED
16	o	501	CLA	O1D-CGD-O2D-CED
16	u	512	CLA	O1D-CGD-O2D-CED
16	G	1220	CLA	O1A-CGA-O2A-C1
16	G	1228	CLA	O1A-CGA-O2A-C1
16	n	507	CLA	O1A-CGA-O2A-C1
16	p	506	CLA	O1A-CGA-O2A-C1
15	A	1011	CL0	C3-C5-C6-C7
16	B	1229	CLA	C3-C5-C6-C7
16	H	1115	CLA	C3-C5-C6-C7
16	s	505	CLA	C3-C5-C6-C7
16	G	1226	CLA	C10-C11-C12-C13
16	q	512	CLA	C13-C15-C16-C17
19	A	4008	BCR	C20-C21-C22-C23
19	B	4010	BCR	C16-C17-C18-C19
19	B	4014	BCR	C20-C21-C22-C23
19	F	4016	BCR	C11-C10-C9-C8
19	G	4009	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	G	4010	BCR	C11-C10-C9-C8
19	G	4010	BCR	C16-C17-C18-C19
19	G	4014	BCR	C20-C21-C22-C23
19	G	4017	BCR	C20-C21-C22-C23
19	K	4005	BCR	C16-C17-C18-C19
19	R	4018	BCR	C12-C13-C14-C15
19	R	4018	BCR	C20-C21-C22-C23
19	S	4013	BCR	C20-C21-C22-C23
19	T	4005	BCR	C16-C17-C18-C19
19	U	4022	BCR	C11-C10-C9-C8
19	W	603	BCR	C11-C10-C9-C8
19	X	603	BCR	C20-C21-C22-C23
19	X	604	BCR	C11-C10-C9-C8
19	Y	601	BCR	C20-C21-C22-C23
19	Y	603	BCR	C20-C21-C22-C23
19	Z	603	BCR	C20-C21-C22-C23
19	Z	604	BCR	C12-C13-C14-C15
19	a	4002	BCR	C20-C21-C22-C23
19	a	4003	BCR	C11-C10-C9-C8
19	a	4003	BCR	C16-C17-C18-C19
19	a	4008	BCR	C20-C21-C22-C23
19	a	4011	BCR	C20-C21-C22-C23
19	b	4010	BCR	C16-C17-C18-C19
19	b	4014	BCR	C11-C10-C9-C8
19	b	4014	BCR	C12-C13-C14-C15
19	b	4014	BCR	C16-C17-C18-C19
19	g	601	BCR	C16-C17-C18-C19
19	g	601	BCR	C20-C21-C22-C23
19	g	602	BCR	C11-C10-C9-C8
19	g	604	BCR	C11-C10-C9-C8
19	h	601	BCR	C20-C21-C22-C23
19	h	604	BCR	C11-C10-C9-C8
19	i	4018	BCR	C11-C10-C9-C8
19	i	4018	BCR	C16-C17-C18-C19
19	i	4018	BCR	C20-C21-C22-C23
19	j	4013	BCR	C16-C17-C18-C19
19	l	4022	BCR	C11-C10-C9-C8
19	n	601	BCR	C20-C21-C22-C23
19	n	603	BCR	C11-C10-C9-C8
19	n	604	BCR	C16-C17-C18-C19
19	o	604	BCR	C20-C21-C22-C23
19	p	601	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
19	p	603	BCR	C20-C21-C22-C23
19	p	604	BCR	C11-C10-C9-C8
19	q	604	BCR	C11-C10-C9-C8
19	r	601	BCR	C20-C21-C22-C23
19	r	604	BCR	C11-C10-C9-C8
19	r	604	BCR	C20-C21-C22-C23
19	s	604	BCR	C11-C10-C9-C8
19	s	604	BCR	C12-C13-C14-C15
19	u	602	BCR	C20-C21-C22-C23
19	v	601	BCR	C12-C13-C14-C15
19	v	604	BCR	C11-C10-C9-C8
19	w	603	BCR	C20-C21-C22-C23
19	w	604	BCR	C11-C10-C9-C8
19	x	603	BCR	C16-C17-C18-C19
19	x	603	BCR	C20-C21-C22-C23
20	A	4202	LMT	O5'-C1'-O1'-C1
20	H	4202	LMT	O5'-C1'-O1'-C1
20	a	4202	LMT	O5'-C1'-O1'-C1
23	q	605	LMU	O5'-C1'-O1'-C1
16	A	1136	CLA	O1D-CGD-O2D-CED
13	H	851	LHG	C8-C7-O7-C5
13	R	103	LHG	C8-C7-O7-C5
16	b	1239	CLA	C15-C16-C17-C18
16	s	504	CLA	C5-C6-C7-C8
16	A	1105	CLA	O1D-CGD-O2D-CED
16	B	1210	CLA	O1D-CGD-O2D-CED
16	G	1205	CLA	O1D-CGD-O2D-CED
16	B	1220	CLA	O1D-CGD-O2D-CED
16	B	1226	CLA	O1D-CGD-O2D-CED
16	G	1221	CLA	O1D-CGD-O2D-CED
16	b	1221	CLA	O1D-CGD-O2D-CED
16	w	508	CLA	O1D-CGD-O2D-CED
13	a	849	LHG	C24-C23-O8-C6
16	b	1213	CLA	CBA-CGA-O2A-C1
16	s	508	CLA	CBA-CGA-O2A-C1
16	u	512	CLA	CBA-CGA-O2A-C1
16	X	505	CLA	C5-C6-C7-C8
16	b	1238	CLA	CBD-CGD-O2D-CED
16	H	1119	CLA	O1D-CGD-O2D-CED
16	H	1123	CLA	C2-C1-O2A-CGA
16	Z	509	CLA	C2-C1-O2A-CGA
16	a	1123	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
16	b	1228	CLA	C2-C1-O2A-CGA
16	o	516	CLA	O1A-CGA-O2A-C1
16	p	517	CLA	C2-C1-O2A-CGA
16	q	509	CLA	C2-C1-O2A-CGA
16	w	509	CLA	C2-C1-O2A-CGA
16	B	1226	CLA	C11-C12-C13-C15
16	B	1228	CLA	C6-C7-C8-C9
16	G	1021	CLA	C16-C17-C18-C19
16	G	1206	CLA	C16-C17-C18-C19
16	H	1140	CLA	C16-C17-C18-C19
16	W	512	CLA	C11-C12-C13-C14
16	X	515	CLA	C16-C17-C18-C20
16	a	1124	CLA	C11-C12-C13-C14
16	a	1140	CLA	C16-C17-C18-C19
16	b	1204	CLA	C16-C17-C18-C20
16	o	515	CLA	C16-C17-C18-C20
17	b	2002	PQN	C26-C27-C28-C29
16	b	1220	CLA	O1A-CGA-O2A-C1
16	g	502	CLA	O1A-CGA-O2A-C1
16	g	507	CLA	O1A-CGA-O2A-C1
16	h	504	CLA	O1A-CGA-O2A-C1
16	A	1127	CLA	C15-C16-C17-C18
16	G	1211	CLA	C10-C11-C12-C13
16	H	1127	CLA	C5-C6-C7-C8
16	h	504	CLA	C8-C10-C11-C12
16	y	505	CLA	C15-C16-C17-C18
14	a	852	LMG	O6-C5-C6-O5
13	G	4018	LHG	C11-C12-C13-C14
16	g	516	CLA	CBA-CGA-O2A-C1
19	G	4009	BCR	C14-C15-C16-C17
19	b	4017	BCR	C14-C15-C16-C17
19	o	604	BCR	C14-C15-C16-C17
19	x	603	BCR	C14-C15-C16-C17
14	A	852	LMG	C30-C31-C32-C33
16	G	1230	CLA	O1D-CGD-O2D-CED
16	x	502	CLA	O1D-CGD-O2D-CED
23	w	605	LMU	O5'-C5'-C6'-O6'
16	A	1022	CLA	C15-C16-C17-C18
16	G	1206	CLA	C8-C10-C11-C12
16	X	506	CLA	C10-C11-C12-C13
16	p	517	CLA	C5-C6-C7-C8
13	R	103	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
16	n	503	CLA	O1D-CGD-O2D-CED
16	g	514	CLA	CBA-CGA-O2A-C1
13	I	103	LHG	O1-C1-C2-O2
13	X	605	LHG	O1-C1-C2-O2
13	b	4018	LHG	O1-C1-C2-O2
13	o	605	LHG	O1-C1-C2-O2
20	A	4202	LMT	C2-C1-O1'-C1'
20	H	4202	LMT	C2-C1-O1'-C1'
20	a	4202	LMT	C2-C1-O1'-C1'
23	x	606	LMU	C2-C1-O1'-C1'
16	u	505	CLA	C3-C5-C6-C7
16	G	1218	CLA	O1D-CGD-O2D-CED
16	G	1228	CLA	O1D-CGD-O2D-CED
16	a	1107	CLA	O1D-CGD-O2D-CED
16	p	508	CLA	O1D-CGD-O2D-CED
16	y	514	CLA	O1D-CGD-O2D-CED
16	A	1107	CLA	C4B-C3B-CAB-CBB
16	A	1116	CLA	C4B-C3B-CAB-CBB
16	A	1118	CLA	C4B-C3B-CAB-CBB
16	A	1129	CLA	C4B-C3B-CAB-CBB
16	B	1021	CLA	C4B-C3B-CAB-CBB
16	B	1204	CLA	C4B-C3B-CAB-CBB
16	B	1214	CLA	C4B-C3B-CAB-CBB
16	B	1215	CLA	C4B-C3B-CAB-CBB
16	B	1216	CLA	C4B-C3B-CAB-CBB
16	B	1222	CLA	C4B-C3B-CAB-CBB
16	B	1223	CLA	C4B-C3B-CAB-CBB
16	B	1227	CLA	C4B-C3B-CAB-CBB
16	G	1204	CLA	C4B-C3B-CAB-CBB
16	G	1208	CLA	C4B-C3B-CAB-CBB
16	G	1216	CLA	C4B-C3B-CAB-CBB
16	G	1217	CLA	C4B-C3B-CAB-CBB
16	G	1222	CLA	C4B-C3B-CAB-CBB
16	G	1235	CLA	C4B-C3B-CAB-CBB
16	H	1104	CLA	C4B-C3B-CAB-CBB
16	H	1109	CLA	C4B-C3B-CAB-CBB
16	H	1122	CLA	C4B-C3B-CAB-CBB
16	H	1139	CLA	C4B-C3B-CAB-CBB
16	L	1501	CLA	C4B-C3B-CAB-CBB
16	T	4004	CLA	C4B-C3B-CAB-CBB
16	W	513	CLA	C4B-C3B-CAB-CBB
16	W	514	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	W	517	CLA	C4B-C3B-CAB-CBB
16	X	503	CLA	C4B-C3B-CAB-CBB
16	X	509	CLA	C4B-C3B-CAB-CBB
16	Y	504	CLA	C4B-C3B-CAB-CBB
16	Y	505	CLA	C4B-C3B-CAB-CBB
16	Y	506	CLA	C4B-C3B-CAB-CBB
16	Y	514	CLA	C4B-C3B-CAB-CBB
16	Z	506	CLA	C4B-C3B-CAB-CBB
16	Z	512	CLA	C4B-C3B-CAB-CBB
16	Z	514	CLA	C4B-C3B-CAB-CBB
16	Z	516	CLA	C4B-C3B-CAB-CBB
16	a	1101	CLA	C4B-C3B-CAB-CBB
16	a	1129	CLA	C4B-C3B-CAB-CBB
16	b	1021	CLA	C4B-C3B-CAB-CBB
16	b	1204	CLA	C4B-C3B-CAB-CBB
16	b	1208	CLA	C4B-C3B-CAB-CBB
16	b	1219	CLA	C4B-C3B-CAB-CBB
16	f	1302	CLA	C4B-C3B-CAB-CBB
16	g	503	CLA	C4B-C3B-CAB-CBB
16	g	505	CLA	C4B-C3B-CAB-CBB
16	h	508	CLA	C4B-C3B-CAB-CBB
16	h	509	CLA	C4B-C3B-CAB-CBB
16	l	1501	CLA	C4B-C3B-CAB-CBB
16	n	503	CLA	C4B-C3B-CAB-CBB
16	n	504	CLA	C4B-C3B-CAB-CBB
16	n	513	CLA	C4B-C3B-CAB-CBB
16	n	516	CLA	C4B-C3B-CAB-CBB
16	o	503	CLA	C4B-C3B-CAB-CBB
16	o	504	CLA	C4B-C3B-CAB-CBB
16	o	514	CLA	C4B-C3B-CAB-CBB
16	p	504	CLA	C4B-C3B-CAB-CBB
16	p	506	CLA	C4B-C3B-CAB-CBB
16	p	514	CLA	C4B-C3B-CAB-CBB
16	r	503	CLA	C4B-C3B-CAB-CBB
16	r	504	CLA	C4B-C3B-CAB-CBB
16	r	512	CLA	C4B-C3B-CAB-CBB
16	r	514	CLA	C4B-C3B-CAB-CBB
16	s	514	CLA	C4B-C3B-CAB-CBB
16	t	506	CLA	C4B-C3B-CAB-CBB
16	t	513	CLA	C4B-C3B-CAB-CBB
16	u	504	CLA	C4B-C3B-CAB-CBB
16	v	509	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	w	504	CLA	C4B-C3B-CAB-CBB
16	w	514	CLA	C4B-C3B-CAB-CBB
16	x	502	CLA	C4B-C3B-CAB-CBB
16	x	504	CLA	C4B-C3B-CAB-CBB
16	x	507	CLA	C4B-C3B-CAB-CBB
16	x	516	CLA	C4B-C3B-CAB-CBB
16	y	505	CLA	C4B-C3B-CAB-CBB
16	W	513	CLA	CBA-CGA-O2A-C1
16	u	516	CLA	CBA-CGA-O2A-C1
16	B	1206	CLA	C16-C17-C18-C19
16	B	1206	CLA	C16-C17-C18-C20
16	G	1215	CLA	C11-C12-C13-C15
16	G	1228	CLA	C6-C7-C8-C9
16	G	1228	CLA	C6-C7-C8-C10
16	X	505	CLA	C16-C17-C18-C20
16	Z	510	CLA	C11-C12-C13-C14
16	a	1124	CLA	C11-C12-C13-C15
16	a	1140	CLA	C16-C17-C18-C20
16	b	1021	CLA	C16-C17-C18-C20
16	b	1206	CLA	C16-C17-C18-C20
16	b	1228	CLA	C6-C7-C8-C9
16	h	515	CLA	C16-C17-C18-C20
16	k	4004	CLA	C6-C7-C8-C10
16	v	517	CLA	C6-C7-C8-C9
16	w	509	CLA	C16-C17-C18-C19
16	x	509	CLA	C16-C17-C18-C19
16	x	509	CLA	C16-C17-C18-C20
16	A	1126	CLA	O1D-CGD-O2D-CED
16	G	1224	CLA	O1D-CGD-O2D-CED
16	x	514	CLA	O1D-CGD-O2D-CED
16	v	503	CLA	O1A-CGA-O2A-C1
16	b	1222	CLA	O1A-CGA-O2A-C1
16	A	1110	CLA	C2A-CAA-CBA-CGA
16	A	1126	CLA	C2A-CAA-CBA-CGA
16	B	1201	CLA	C2A-CAA-CBA-CGA
16	H	1110	CLA	C2A-CAA-CBA-CGA
16	a	1138	CLA	C2A-CAA-CBA-CGA
16	y	515	CLA	C2A-CAA-CBA-CGA
14	a	852	LMG	C34-C35-C36-C37
16	A	1133	CLA	C5-C6-C7-C8
16	H	1125	CLA	C15-C16-C17-C18
16	Y	512	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	a	1125	CLA	C15-C16-C17-C18
16	a	1128	CLA	C8-C10-C11-C12
16	b	1225	CLA	C15-C16-C17-C18
16	w	511	CLA	C5-C6-C7-C8
13	A	851	LHG	C8-C7-O7-C5
14	f	4017	LMG	C11-C10-O7-C8
16	A	1139	CLA	O1D-CGD-O2D-CED
16	w	517	CLA	O1D-CGD-O2D-CED
16	G	1210	CLA	C11-C10-C8-C7
16	H	1128	CLA	C11-C12-C13-C15
16	a	1125	CLA	C11-C10-C8-C7
16	v	512	CLA	C6-C7-C8-C10
17	B	2002	PQN	C21-C22-C23-C25
17	G	2002	PQN	C21-C22-C23-C25
13	B	4018	LHG	C11-C12-C13-C14
13	H	849	LHG	C28-C29-C30-C31
16	B	1207	CLA	C5-C6-C7-C8
16	B	1221	CLA	C10-C11-C12-C13
16	Z	515	CLA	C8-C10-C11-C12
16	a	1131	CLA	C5-C6-C7-C8
16	n	504	CLA	C5-C6-C7-C8
16	r	509	CLA	C13-C15-C16-C17
16	v	509	CLA	C13-C15-C16-C17
13	I	103	LHG	C28-C29-C30-C31
14	a	852	LMG	C30-C31-C32-C33
16	g	503	CLA	O1A-CGA-O2A-C1
15	a	1011	CL0	O1A-CGA-O2A-C1
16	Z	512	CLA	O1A-CGA-O2A-C1
16	q	502	CLA	O1A-CGA-O2A-C1
16	s	507	CLA	O1A-CGA-O2A-C1
16	u	507	CLA	O1A-CGA-O2A-C1
16	a	1103	CLA	C3-C5-C6-C7
16	A	1022	CLA	C3A-C2A-CAA-CBA
16	A	1115	CLA	C3A-C2A-CAA-CBA
16	A	1118	CLA	C3A-C2A-CAA-CBA
16	A	1121	CLA	C3A-C2A-CAA-CBA
16	A	1130	CLA	C3A-C2A-CAA-CBA
16	A	1137	CLA	C3A-C2A-CAA-CBA
16	B	1023	CLA	C3A-C2A-CAA-CBA
16	B	1210	CLA	C3A-C2A-CAA-CBA
16	B	1211	CLA	C3A-C2A-CAA-CBA
16	B	1213	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	B	1216	CLA	C3A-C2A-CAA-CBA
16	B	1217	CLA	C3A-C2A-CAA-CBA
16	B	1223	CLA	C3A-C2A-CAA-CBA
16	B	1234	CLA	C3A-C2A-CAA-CBA
16	B	1236	CLA	C3A-C2A-CAA-CBA
16	F	1302	CLA	C3A-C2A-CAA-CBA
16	G	1023	CLA	C3A-C2A-CAA-CBA
16	G	1203	CLA	C3A-C2A-CAA-CBA
16	G	1206	CLA	C3A-C2A-CAA-CBA
16	G	1209	CLA	C3A-C2A-CAA-CBA
16	G	1210	CLA	C3A-C2A-CAA-CBA
16	G	1211	CLA	C3A-C2A-CAA-CBA
16	G	1213	CLA	C3A-C2A-CAA-CBA
16	G	1218	CLA	C3A-C2A-CAA-CBA
16	G	1230	CLA	C3A-C2A-CAA-CBA
16	G	1231	CLA	C3A-C2A-CAA-CBA
16	G	1236	CLA	C3A-C2A-CAA-CBA
16	H	1022	CLA	C3A-C2A-CAA-CBA
16	H	1115	CLA	C3A-C2A-CAA-CBA
16	H	1118	CLA	C3A-C2A-CAA-CBA
16	H	1121	CLA	C3A-C2A-CAA-CBA
16	H	1123	CLA	C3A-C2A-CAA-CBA
16	H	1130	CLA	C3A-C2A-CAA-CBA
16	H	1140	CLA	C3A-C2A-CAA-CBA
16	Q	1302	CLA	C3A-C2A-CAA-CBA
16	T	4002	CLA	C3A-C2A-CAA-CBA
16	W	511	CLA	C3A-C2A-CAA-CBA
16	X	503	CLA	C3A-C2A-CAA-CBA
16	X	517	CLA	C3A-C2A-CAA-CBA
16	Y	504	CLA	C3A-C2A-CAA-CBA
16	Y	508	CLA	C3A-C2A-CAA-CBA
16	Y	509	CLA	C3A-C2A-CAA-CBA
16	Z	501	CLA	C3A-C2A-CAA-CBA
16	Z	510	CLA	C3A-C2A-CAA-CBA
16	a	1022	CLA	C3A-C2A-CAA-CBA
16	a	1111	CLA	C3A-C2A-CAA-CBA
16	a	1115	CLA	C3A-C2A-CAA-CBA
16	a	1118	CLA	C3A-C2A-CAA-CBA
16	a	1123	CLA	C3A-C2A-CAA-CBA
16	a	1130	CLA	C3A-C2A-CAA-CBA
16	a	1140	CLA	C3A-C2A-CAA-CBA
16	b	1012	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	b	1023	CLA	C3A-C2A-CAA-CBA
16	b	1203	CLA	C3A-C2A-CAA-CBA
16	b	1209	CLA	C3A-C2A-CAA-CBA
16	b	1211	CLA	C3A-C2A-CAA-CBA
16	b	1213	CLA	C3A-C2A-CAA-CBA
16	b	1221	CLA	C3A-C2A-CAA-CBA
16	b	1223	CLA	C3A-C2A-CAA-CBA
16	b	1231	CLA	C3A-C2A-CAA-CBA
16	b	1236	CLA	C3A-C2A-CAA-CBA
16	b	1239	CLA	C3A-C2A-CAA-CBA
16	f	1302	CLA	C3A-C2A-CAA-CBA
16	g	501	CLA	C3A-C2A-CAA-CBA
16	g	509	CLA	C3A-C2A-CAA-CBA
16	g	513	CLA	C3A-C2A-CAA-CBA
16	g	517	CLA	C3A-C2A-CAA-CBA
16	h	507	CLA	C3A-C2A-CAA-CBA
16	n	516	CLA	C3A-C2A-CAA-CBA
16	o	504	CLA	C3A-C2A-CAA-CBA
16	o	517	CLA	C3A-C2A-CAA-CBA
16	p	508	CLA	C3A-C2A-CAA-CBA
16	p	509	CLA	C3A-C2A-CAA-CBA
16	q	503	CLA	C3A-C2A-CAA-CBA
16	q	504	CLA	C3A-C2A-CAA-CBA
16	q	509	CLA	C3A-C2A-CAA-CBA
16	r	504	CLA	C3A-C2A-CAA-CBA
16	r	509	CLA	C3A-C2A-CAA-CBA
16	r	517	CLA	C3A-C2A-CAA-CBA
16	s	503	CLA	C3A-C2A-CAA-CBA
16	s	504	CLA	C3A-C2A-CAA-CBA
16	s	508	CLA	C3A-C2A-CAA-CBA
16	s	509	CLA	C3A-C2A-CAA-CBA
16	s	513	CLA	C3A-C2A-CAA-CBA
16	u	501	CLA	C3A-C2A-CAA-CBA
16	u	504	CLA	C3A-C2A-CAA-CBA
16	u	506	CLA	C3A-C2A-CAA-CBA
16	u	517	CLA	C3A-C2A-CAA-CBA
16	w	501	CLA	C3A-C2A-CAA-CBA
16	w	504	CLA	C3A-C2A-CAA-CBA
16	x	501	CLA	C3A-C2A-CAA-CBA
16	x	504	CLA	C3A-C2A-CAA-CBA
16	x	513	CLA	C3A-C2A-CAA-CBA
16	B	1227	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	B	1230	CLA	O1D-CGD-O2D-CED
16	g	512	CLA	O1D-CGD-O2D-CED
13	R	103	LHG	C31-C32-C33-C34
16	B	1214	CLA	C4C-C3C-CAC-CBC
16	A	1130	CLA	C10-C11-C12-C13
16	A	1237	CLA	C8-C10-C11-C12
16	B	1202	CLA	C13-C15-C16-C17
16	Y	511	CLA	C13-C15-C16-C17
16	a	1109	CLA	C10-C11-C12-C13
16	q	504	CLA	C5-C6-C7-C8
16	s	510	CLA	C15-C16-C17-C18
16	w	505	CLA	C15-C16-C17-C18
17	B	2002	PQN	C20-C21-C22-C23
17	G	2002	PQN	C25-C26-C27-C28
14	F	4017	LMG	C28-C29-C30-C31
14	Q	4017	LMG	C28-C29-C30-C31
16	H	1111	CLA	O1D-CGD-O2D-CED
13	A	851	LHG	C7-C8-C9-C10
13	G	4018	LHG	C7-C8-C9-C10
13	a	849	LHG	C23-C24-C25-C26
19	B	4014	BCR	C19-C20-C21-C22
19	L	4022	BCR	C19-C20-C21-C22
19	X	602	BCR	C9-C10-C11-C12
19	t	604	BCR	C13-C14-C15-C16
21	V	4021	ECH	C9-C10-C11-C12
16	A	1140	CLA	C16-C17-C18-C19
16	B	1228	CLA	C6-C7-C8-C10
16	G	1238	CLA	C16-C17-C18-C19
16	G	1238	CLA	C16-C17-C18-C20
16	b	1228	CLA	C6-C7-C8-C10
16	o	505	CLA	C16-C17-C18-C20
16	v	517	CLA	C6-C7-C8-C10
23	w	605	LMU	O5B-C5B-C6B-O6B
16	W	501	CLA	O1A-CGA-O2A-C1
16	p	508	CLA	O1A-CGA-O2A-C1
20	L	4101	LMT	O5B-C1B-O1B-C4'
16	H	1106	CLA	CBD-CGD-O2D-CED
16	W	506	CLA	CBD-CGD-O2D-CED
16	X	502	CLA	CBD-CGD-O2D-CED
16	s	509	CLA	CBD-CGD-O2D-CED
16	a	1128	CLA	O1D-CGD-O2D-CED
16	u	502	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	H	1104	CLA	CBA-CGA-O2A-C1
16	a	1110	CLA	CBA-CGA-O2A-C1
16	a	1115	CLA	CBA-CGA-O2A-C1
16	b	1228	CLA	CBA-CGA-O2A-C1
16	h	514	CLA	CBA-CGA-O2A-C1
16	n	501	CLA	CBA-CGA-O2A-C1
16	o	502	CLA	CBA-CGA-O2A-C1
13	x	605	LHG	C11-C10-C9-C8
16	A	1132	CLA	C3-C5-C6-C7
16	B	1238	CLA	C3-C5-C6-C7
16	G	1203	CLA	C3-C5-C6-C7
16	Y	505	CLA	C3-C5-C6-C7
16	a	1110	CLA	C3-C5-C6-C7
13	H	849	LHG	C23-C24-C25-C26
16	n	512	CLA	C8-C10-C11-C12
16	x	504	CLA	C8-C10-C11-C12
23	s	606	LMU	C2B-C1B-O1B-C4'
13	H	849	LHG	C30-C31-C32-C33
13	R	103	LHG	C25-C26-C27-C28
13	i	103	LHG	C27-C28-C29-C30
23	x	606	LMU	C2-C3-C4-C5
16	K	4004	CLA	O1A-CGA-O2A-C1
16	a	1104	CLA	O1A-CGA-O2A-C1
16	n	511	CLA	O1A-CGA-O2A-C1
16	r	514	CLA	O1A-CGA-O2A-C1
16	u	512	CLA	O1A-CGA-O2A-C1
20	L	4101	LMT	C4B-C5B-C6B-O6B
13	b	4018	LHG	C14-C15-C16-C17
13	b	4018	LHG	C16-C17-C18-C19
16	A	1022	CLA	O1D-CGD-O2D-CED
16	H	1107	CLA	O1D-CGD-O2D-CED
16	B	1012	CLA	C5-C6-C7-C8
16	K	4003	CLA	C4C-C3C-CAC-CBC
16	H	1122	CLA	O1D-CGD-O2D-CED
16	B	1226	CLA	C11-C12-C13-C14
16	G	1021	CLA	C16-C17-C18-C20
16	X	515	CLA	C16-C17-C18-C19
16	o	515	CLA	C16-C17-C18-C19
16	B	1235	CLA	O1A-CGA-O2A-C1
16	b	1213	CLA	O1A-CGA-O2A-C1
16	r	506	CLA	O1A-CGA-O2A-C1
16	A	1101	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	A	1109	CLA	C2B-C3B-CAB-CBB
16	A	1116	CLA	C2B-C3B-CAB-CBB
16	A	1133	CLA	C2B-C3B-CAB-CBB
16	B	1203	CLA	C2B-C3B-CAB-CBB
16	B	1211	CLA	C2B-C3B-CAB-CBB
16	B	1218	CLA	C2B-C3B-CAB-CBB
16	B	1221	CLA	C2B-C3B-CAB-CBB
16	B	1230	CLA	C2B-C3B-CAB-CBB
16	B	1236	CLA	C2B-C3B-CAB-CBB
16	B	1238	CLA	C2B-C3B-CAB-CBB
16	G	1209	CLA	C2B-C3B-CAB-CBB
16	G	1211	CLA	C2B-C3B-CAB-CBB
16	G	1218	CLA	C2B-C3B-CAB-CBB
16	G	1222	CLA	C2B-C3B-CAB-CBB
16	G	1230	CLA	C2B-C3B-CAB-CBB
16	G	1236	CLA	C2B-C3B-CAB-CBB
16	G	1238	CLA	C2B-C3B-CAB-CBB
16	H	1124	CLA	C2B-C3B-CAB-CBB
16	H	1136	CLA	C2B-C3B-CAB-CBB
16	H	1137	CLA	C2B-C3B-CAB-CBB
16	L	1502	CLA	C2B-C3B-CAB-CBB
16	W	504	CLA	C2B-C3B-CAB-CBB
16	W	507	CLA	C2B-C3B-CAB-CBB
16	W	515	CLA	C2B-C3B-CAB-CBB
16	X	507	CLA	C2B-C3B-CAB-CBB
16	X	516	CLA	C2B-C3B-CAB-CBB
16	Y	507	CLA	C2B-C3B-CAB-CBB
16	Y	516	CLA	C2B-C3B-CAB-CBB
16	a	1102	CLA	C2B-C3B-CAB-CBB
16	a	1109	CLA	C2B-C3B-CAB-CBB
16	a	1138	CLA	C2B-C3B-CAB-CBB
16	b	1211	CLA	C2B-C3B-CAB-CBB
16	b	1223	CLA	C2B-C3B-CAB-CBB
16	b	1229	CLA	C2B-C3B-CAB-CBB
16	b	1230	CLA	C2B-C3B-CAB-CBB
16	g	501	CLA	C2B-C3B-CAB-CBB
16	g	516	CLA	C2B-C3B-CAB-CBB
16	h	516	CLA	C2B-C3B-CAB-CBB
16	j	1303	CLA	C2B-C3B-CAB-CBB
16	n	517	CLA	C2B-C3B-CAB-CBB
16	o	503	CLA	C2B-C3B-CAB-CBB
16	o	505	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	p	507	CLA	C2B-C3B-CAB-CBB
16	p	512	CLA	C2B-C3B-CAB-CBB
16	q	517	CLA	C2B-C3B-CAB-CBB
16	r	506	CLA	C2B-C3B-CAB-CBB
16	r	517	CLA	C2B-C3B-CAB-CBB
16	s	504	CLA	C2B-C3B-CAB-CBB
16	s	506	CLA	C2B-C3B-CAB-CBB
16	s	507	CLA	C2B-C3B-CAB-CBB
16	t	506	CLA	C2B-C3B-CAB-CBB
16	t	516	CLA	C2B-C3B-CAB-CBB
16	t	517	CLA	C2B-C3B-CAB-CBB
16	u	516	CLA	C2B-C3B-CAB-CBB
16	v	505	CLA	C2B-C3B-CAB-CBB
16	v	513	CLA	C2B-C3B-CAB-CBB
16	w	516	CLA	C2B-C3B-CAB-CBB
16	x	510	CLA	C2B-C3B-CAB-CBB
16	y	517	CLA	C2B-C3B-CAB-CBB
19	A	4003	BCR	C1-C6-C7-C8
19	A	4003	BCR	C5-C6-C7-C8
19	A	4008	BCR	C1-C6-C7-C8
19	A	4008	BCR	C23-C24-C25-C30
19	A	4011	BCR	C1-C6-C7-C8
19	A	4011	BCR	C23-C24-C25-C26
19	A	4011	BCR	C23-C24-C25-C30
19	B	4009	BCR	C23-C24-C25-C30
19	G	4004	BCR	C23-C24-C25-C30
19	G	4010	BCR	C1-C6-C7-C8
19	G	4010	BCR	C5-C6-C7-C8
19	H	4002	BCR	C1-C6-C7-C8
19	H	4011	BCR	C1-C6-C7-C8
19	H	4011	BCR	C23-C24-C25-C26
19	H	4011	BCR	C23-C24-C25-C30
19	J	4012	BCR	C1-C6-C7-C8
19	J	4012	BCR	C5-C6-C7-C8
19	L	4022	BCR	C23-C24-C25-C26
19	L	4022	BCR	C23-C24-C25-C30
19	R	4018	BCR	C1-C6-C7-C8
19	R	4018	BCR	C5-C6-C7-C8
19	S	4012	BCR	C5-C6-C7-C8
19	S	4013	BCR	C23-C24-C25-C26
19	S	4013	BCR	C23-C24-C25-C30
19	T	4001	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	W	601	BCR	C1-C6-C7-C8
19	W	601	BCR	C23-C24-C25-C26
19	W	601	BCR	C23-C24-C25-C30
19	W	603	BCR	C1-C6-C7-C8
19	X	601	BCR	C1-C6-C7-C8
19	Y	601	BCR	C23-C24-C25-C26
19	Y	601	BCR	C23-C24-C25-C30
19	Y	604	BCR	C1-C6-C7-C8
19	Y	604	BCR	C5-C6-C7-C8
19	Y	604	BCR	C23-C24-C25-C26
19	Y	604	BCR	C23-C24-C25-C30
19	Z	602	BCR	C23-C24-C25-C26
19	Z	602	BCR	C23-C24-C25-C30
19	a	4002	BCR	C1-C6-C7-C8
19	a	4003	BCR	C1-C6-C7-C8
19	a	4003	BCR	C5-C6-C7-C8
19	a	4011	BCR	C23-C24-C25-C26
19	a	4011	BCR	C23-C24-C25-C30
19	g	603	BCR	C1-C6-C7-C8
19	g	603	BCR	C5-C6-C7-C8
19	g	604	BCR	C23-C24-C25-C30
19	h	601	BCR	C1-C6-C7-C8
19	h	601	BCR	C5-C6-C7-C8
19	h	601	BCR	C23-C24-C25-C26
19	h	601	BCR	C23-C24-C25-C30
19	h	603	BCR	C23-C24-C25-C30
19	h	604	BCR	C23-C24-C25-C26
19	h	604	BCR	C23-C24-C25-C30
19	j	4012	BCR	C1-C6-C7-C8
19	j	4012	BCR	C5-C6-C7-C8
19	p	601	BCR	C1-C6-C7-C8
19	p	601	BCR	C23-C24-C25-C26
19	p	601	BCR	C23-C24-C25-C30
19	p	604	BCR	C1-C6-C7-C8
19	p	604	BCR	C5-C6-C7-C8
19	p	604	BCR	C23-C24-C25-C26
19	p	604	BCR	C23-C24-C25-C30
19	q	604	BCR	C1-C6-C7-C8
19	q	604	BCR	C5-C6-C7-C8
19	r	603	BCR	C1-C6-C7-C8
19	r	603	BCR	C5-C6-C7-C8
19	s	604	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	s	604	BCR	C5-C6-C7-C8
19	s	604	BCR	C23-C24-C25-C26
19	s	604	BCR	C23-C24-C25-C30
19	t	603	BCR	C1-C6-C7-C8
19	t	603	BCR	C5-C6-C7-C8
19	v	601	BCR	C23-C24-C25-C26
19	v	601	BCR	C23-C24-C25-C30
19	v	604	BCR	C23-C24-C25-C30
19	w	604	BCR	C1-C6-C7-C8
19	w	604	BCR	C5-C6-C7-C8
19	x	603	BCR	C1-C6-C7-C8
19	x	603	BCR	C5-C6-C7-C8
19	x	604	BCR	C1-C6-C7-C8
19	y	601	BCR	C1-C6-C7-C8
19	y	601	BCR	C5-C6-C7-C8
19	y	601	BCR	C23-C24-C25-C26
19	y	601	BCR	C23-C24-C25-C30
19	y	604	BCR	C23-C24-C25-C26
19	y	604	BCR	C23-C24-C25-C30
21	I	4020	ECH	C5-C6-C7-C8
21	M	4021	ECH	C5-C6-C7-C8
21	i	4020	ECH	C1-C6-C7-C8
21	i	4020	ECH	C5-C6-C7-C8
21	m	4021	ECH	C5-C6-C7-C8
24	q	601	LUT	C1-C6-C7-C8
24	q	601	LUT	C5-C6-C7-C8
16	B	1214	CLA	CBD-CGD-O2D-CED
16	t	513	CLA	O1A-CGA-O2A-C1
16	k	4003	CLA	C4C-C3C-CAC-CBC
16	G	1214	CLA	O1D-CGD-O2D-CED
16	G	1235	CLA	CBA-CGA-O2A-C1
16	w	505	CLA	CBA-CGA-O2A-C1
16	A	1237	CLA	C10-C11-C12-C13
16	B	1211	CLA	C13-C15-C16-C17
16	X	512	CLA	C3-C5-C6-C7
16	r	509	CLA	C3-C5-C6-C7
16	v	501	CLA	CBA-CGA-O2A-C1
14	G	848	LMG	C34-C35-C36-C37
16	A	1138	CLA	C2A-CAA-CBA-CGA
16	G	1201	CLA	C2A-CAA-CBA-CGA
16	W	508	CLA	C2A-CAA-CBA-CGA
16	X	505	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	Y	501	CLA	C2A-CAA-CBA-CGA
16	a	1116	CLA	C2A-CAA-CBA-CGA
16	a	1126	CLA	C2A-CAA-CBA-CGA
16	b	1229	CLA	C2A-CAA-CBA-CGA
16	g	504	CLA	C2A-CAA-CBA-CGA
16	g	513	CLA	C2A-CAA-CBA-CGA
16	k	4002	CLA	C2A-CAA-CBA-CGA
16	o	508	CLA	C2A-CAA-CBA-CGA
16	p	501	CLA	C2A-CAA-CBA-CGA
16	q	505	CLA	C2A-CAA-CBA-CGA
16	u	505	CLA	C2A-CAA-CBA-CGA
16	x	503	CLA	C2A-CAA-CBA-CGA
16	y	504	CLA	C2A-CAA-CBA-CGA
16	y	505	CLA	C2A-CAA-CBA-CGA
16	h	515	CLA	C8-C10-C11-C12
16	n	509	CLA	C10-C11-C12-C13
13	Y	605	LHG	C24-C25-C26-C27
14	A	4201	LMG	O10-C28-O8-C9
16	a	1115	CLA	O1A-CGA-O2A-C1
16	g	514	CLA	O1A-CGA-O2A-C1
16	n	501	CLA	O1A-CGA-O2A-C1
16	s	508	CLA	O1A-CGA-O2A-C1
16	p	503	CLA	O1A-CGA-O2A-C1
13	I	103	LHG	C27-C28-C29-C30
13	H	851	LHG	O9-C7-O7-C5
13	a	849	LHG	O9-C7-O7-C5
16	A	1022	CLA	C4C-C3C-CAC-CBC
16	Y	504	CLA	C4-C3-C5-C6
16	a	1136	CLA	C4-C3-C5-C6
16	b	1228	CLA	C4-C3-C5-C6
16	B	1238	CLA	O1D-CGD-O2D-CED
16	r	502	CLA	O1D-CGD-O2D-CED
19	A	4003	BCR	C10-C11-C12-C13
19	G	4005	BCR	C18-C19-C20-C21
19	J	4012	BCR	C10-C11-C12-C13
19	K	4001	BCR	C18-C19-C20-C21
19	L	4019	BCR	C10-C11-C12-C13
19	T	4001	BCR	C18-C19-C20-C21
19	Y	604	BCR	C10-C11-C12-C13
19	a	4008	BCR	C10-C11-C12-C13
19	b	4014	BCR	C10-C11-C12-C13
19	f	4016	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
19	g	601	BCR	C18-C19-C20-C21
19	g	604	BCR	C10-C11-C12-C13
19	j	4015	BCR	C18-C19-C20-C21
19	l	4019	BCR	C10-C11-C12-C13
19	o	604	BCR	C18-C19-C20-C21
19	q	604	BCR	C10-C11-C12-C13
19	u	602	BCR	C18-C19-C20-C21
19	u	604	BCR	C10-C11-C12-C13
19	v	603	BCR	C18-C19-C20-C21
19	w	604	BCR	C10-C11-C12-C13
19	y	601	BCR	C10-C11-C12-C13
16	G	1221	CLA	C10-C11-C12-C13
16	X	512	CLA	C15-C16-C17-C18
16	L	1502	CLA	C2-C3-C5-C6
16	r	505	CLA	C2-C3-C5-C6
16	b	1204	CLA	C16-C17-C18-C19
20	H	4202	LMT	O1'-C1-C2-C3
14	H	4101	LMG	C28-C29-C30-C31
13	x	605	LHG	C24-C23-O8-C6
16	G	1213	CLA	CBA-CGA-O2A-C1
16	g	506	CLA	CBA-CGA-O2A-C1
16	p	502	CLA	CBA-CGA-O2A-C1
16	t	514	CLA	CBA-CGA-O2A-C1
16	g	505	CLA	C3-C5-C6-C7
16	a	1106	CLA	C11-C10-C8-C9
16	v	515	CLA	C6-C7-C8-C9
14	a	4101	LMG	C30-C31-C32-C33
16	b	1207	CLA	C5-C6-C7-C8
16	A	1122	CLA	C4C-C3C-CAC-CBC
16	Y	509	CLA	O1D-CGD-O2D-CED
19	A	4008	BCR	C6-C7-C8-C9
19	B	4010	BCR	C6-C7-C8-C9
19	B	4017	BCR	C22-C23-C24-C25
19	a	4002	BCR	C6-C7-C8-C9
19	g	601	BCR	C6-C7-C8-C9
19	v	601	BCR	C6-C7-C8-C9
14	B	848	LMG	C13-C14-C15-C16
16	a	1112	CLA	CBD-CGD-O2D-CED
16	X	511	CLA	C8-C10-C11-C12
16	a	1101	CLA	C5-C6-C7-C8
16	g	509	CLA	C13-C15-C16-C17
16	q	515	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	v	505	CLA	C10-C11-C12-C13
14	A	4101	LMG	C30-C31-C32-C33
14	b	848	LMG	C34-C35-C36-C37
20	l	4101	LMT	C4-C5-C6-C7
16	A	1114	CLA	O1A-CGA-O2A-C1
14	H	4101	LMG	C30-C31-C32-C33
20	a	4202	LMT	O1'-C1-C2-C3
16	H	1109	CLA	C10-C11-C12-C13
16	v	517	CLA	C3-C5-C6-C7
16	G	1210	CLA	CBA-CGA-O2A-C1
16	v	511	CLA	CBA-CGA-O2A-C1
19	G	4010	BCR	C13-C14-C15-C16
19	G	4014	BCR	C13-C14-C15-C16
19	U	4019	BCR	C9-C10-C11-C12
19	X	602	BCR	C19-C20-C21-C22
19	Z	604	BCR	C13-C14-C15-C16
19	p	604	BCR	C13-C14-C15-C16
19	u	604	BCR	C19-C20-C21-C22
15	A	1011	CL0	C16-C17-C18-C19
16	W	512	CLA	C11-C12-C13-C15
16	p	509	CLA	C11-C12-C13-C15
16	u	515	CLA	C16-C17-C18-C20
13	A	849	LHG	C8-C7-O7-C5
13	H	849	LHG	C8-C7-O7-C5
13	a	849	LHG	C8-C7-O7-C5
14	a	4201	LMG	C11-C10-O7-C8
16	H	1104	CLA	O1A-CGA-O2A-C1
14	b	848	LMG	C35-C36-C37-C38
16	B	1021	CLA	C13-C15-C16-C17
16	Z	512	CLA	C8-C10-C11-C12
16	a	1127	CLA	C15-C16-C17-C18
16	n	515	CLA	C13-C15-C16-C17
14	Q	4017	LMG	O9-C10-O7-C8
16	A	1129	CLA	O1A-CGA-O2A-C1
14	B	848	LMG	C34-C35-C36-C37
16	a	1133	CLA	C5-C6-C7-C8
16	q	503	CLA	C2C-C3C-CAC-CBC
16	a	1110	CLA	O1A-CGA-O2A-C1
16	G	1223	CLA	C13-C15-C16-C17
19	A	4002	BCR	C37-C22-C23-C24
19	a	4007	BCR	C37-C22-C23-C24
19	h	603	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
19	n	604	BCR	C7-C8-C9-C34
19	r	603	BCR	C7-C8-C9-C34
19	r	604	BCR	C7-C8-C9-C34
19	u	602	BCR	C37-C22-C23-C24
19	v	603	BCR	C7-C8-C9-C34
19	y	603	BCR	C7-C8-C9-C34
24	w	601	LUT	C7-C8-C9-C19
16	H	1129	CLA	CBA-CGA-O2A-C1
14	b	848	LMG	C28-C29-C30-C31
15	H	1011	CL0	C3-C5-C6-C7
16	H	1102	CLA	C3-C5-C6-C7
16	W	515	CLA	C3-C5-C6-C7
19	B	4014	BCR	C21-C22-C23-C24
19	K	4005	BCR	C21-C22-C23-C24
19	L	4022	BCR	C21-C22-C23-C24
19	l	4022	BCR	C21-C22-C23-C24
19	u	602	BCR	C21-C22-C23-C24
19	x	602	BCR	C11-C12-C13-C14
13	a	849	LHG	C30-C31-C32-C33
16	l	1503	CLA	C2A-CAA-CBA-CGA
16	o	501	CLA	C2A-CAA-CBA-CGA
16	A	1117	CLA	C16-C17-C18-C20
16	b	1012	CLA	C6-C7-C8-C10
16	b	1215	CLA	C11-C12-C13-C15
16	p	509	CLA	C11-C12-C13-C14
17	b	2002	PQN	C26-C27-C28-C30
16	Y	510	CLA	CBD-CGD-O2D-CED
16	a	1119	CLA	CBD-CGD-O2D-CED
16	G	1205	CLA	C4-C3-C5-C6
16	G	1213	CLA	C4-C3-C5-C6
16	W	512	CLA	C4-C3-C5-C6
16	X	508	CLA	C4-C3-C5-C6
16	a	1136	CLA	C2-C3-C5-C6
13	Y	605	LHG	C23-C24-C25-C26
16	G	1023	CLA	C10-C11-C12-C13
16	H	1130	CLA	C8-C10-C11-C12
16	Y	505	CLA	C8-C10-C11-C12
16	a	1022	CLA	C13-C15-C16-C17
16	g	505	CLA	C8-C10-C11-C12
16	o	506	CLA	C10-C11-C12-C13
13	A	849	LHG	C30-C31-C32-C33
16	w	503	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
16	G	1226	CLA	O1D-CGD-O2D-CED
16	H	1139	CLA	O1D-CGD-O2D-CED
16	b	1228	CLA	O1A-CGA-O2A-C1
16	h	514	CLA	O1A-CGA-O2A-C1
16	o	502	CLA	O1A-CGA-O2A-C1
16	b	1218	CLA	C3-C5-C6-C7
16	H	1109	CLA	C15-C16-C17-C18
16	w	506	CLA	C5-C6-C7-C8
15	A	1011	CL0	CBA-CGA-O2A-C1
16	v	512	CLA	CBA-CGA-O2A-C1
13	i	103	LHG	C7-C8-C9-C10
13	I	103	LHG	C30-C31-C32-C33
14	F	4017	LMG	O9-C10-O7-C8
14	A	852	LMG	O6-C5-C6-O5
16	B	1225	CLA	C15-C16-C17-C18
16	X	504	CLA	C5-C6-C7-C8
16	Y	504	CLA	C5-C6-C7-C8
16	q	505	CLA	C15-C16-C17-C18
16	u	515	CLA	C10-C11-C12-C13
20	A	4202	LMT	O1'-C1-C2-C3
16	G	1226	CLA	C11-C12-C13-C15
16	W	505	CLA	C16-C17-C18-C20
13	H	851	LHG	C7-C8-C9-C10
13	b	4018	LHG	C23-C24-C25-C26
16	A	1125	CLA	C15-C16-C17-C18
16	A	1126	CLA	C8-C10-C11-C12
16	H	1127	CLA	C8-C10-C11-C12
16	Y	510	CLA	C5-C6-C7-C8
16	b	1207	CLA	C13-C15-C16-C17
16	q	512	CLA	C8-C10-C11-C12
16	w	509	CLA	C15-C16-C17-C18
16	x	515	CLA	C8-C10-C11-C12
16	y	505	CLA	C8-C10-C11-C12
16	H	1115	CLA	O1D-CGD-O2D-CED
16	o	515	CLA	O1D-CGD-O2D-CED
16	x	512	CLA	O1D-CGD-O2D-CED
14	A	4101	LMG	O6-C5-C6-O5
14	H	4101	LMG	O6-C5-C6-O5
16	b	1240	CLA	O1A-CGA-O2A-C1
16	s	517	CLA	C3-C5-C6-C7
13	o	605	LHG	O7-C5-C6-O8
13	u	605	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
14	B	848	LMG	O7-C8-C9-O8
14	G	848	LMG	O7-C8-C9-O8
14	a	4201	LMG	O7-C8-C9-O8
16	q	516	CLA	O1D-CGD-O2D-CED
16	a	1101	CLA	CBA-CGA-O2A-C1
16	n	514	CLA	CBA-CGA-O2A-C1
16	u	505	CLA	C15-C16-C17-C18
16	v	505	CLA	C5-C6-C7-C8
16	y	508	CLA	C5-C6-C7-C8
23	Z	605	LMU	O5B-C5B-C6B-O6B
23	s	606	LMU	C4'-C5'-C6'-O6'
16	G	1220	CLA	C2-C1-O2A-CGA
16	B	1012	CLA	C6-C7-C8-C9
16	W	505	CLA	C16-C17-C18-C19
16	H	1140	CLA	C15-C16-C17-C18
16	p	504	CLA	C8-C10-C11-C12
17	G	2002	PQN	C20-C21-C22-C23
16	H	1132	CLA	C4-C3-C5-C6
16	a	1013	CLA	C4-C3-C5-C6
16	b	1205	CLA	C4-C3-C5-C6
16	h	507	CLA	C4-C3-C5-C6
16	n	512	CLA	C4-C3-C5-C6
16	q	512	CLA	C4-C3-C5-C6
16	G	1229	CLA	C3-C5-C6-C7
16	H	1132	CLA	C3-C5-C6-C7
16	h	506	CLA	C3-C5-C6-C7
16	W	512	CLA	C2-C3-C5-C6
16	t	509	CLA	C10-C11-C12-C13
16	A	1122	CLA	C2A-CAA-CBA-CGA
16	A	1237	CLA	C2A-CAA-CBA-CGA
16	B	1219	CLA	C2A-CAA-CBA-CGA
16	B	1223	CLA	C2A-CAA-CBA-CGA
16	B	1224	CLA	C2A-CAA-CBA-CGA
16	G	1219	CLA	C2A-CAA-CBA-CGA
16	H	1116	CLA	C2A-CAA-CBA-CGA
16	H	1122	CLA	C2A-CAA-CBA-CGA
16	H	1237	CLA	C2A-CAA-CBA-CGA
16	Y	515	CLA	C2A-CAA-CBA-CGA
16	a	1022	CLA	C2A-CAA-CBA-CGA
16	a	1237	CLA	C2A-CAA-CBA-CGA
16	b	1224	CLA	C2A-CAA-CBA-CGA
16	h	501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	h	505	CLA	C2A-CAA-CBA-CGA
16	h	515	CLA	C2A-CAA-CBA-CGA
16	n	509	CLA	C2A-CAA-CBA-CGA
16	o	513	CLA	C2A-CAA-CBA-CGA
16	p	508	CLA	C2A-CAA-CBA-CGA
16	p	515	CLA	C2A-CAA-CBA-CGA
16	q	507	CLA	C2A-CAA-CBA-CGA
16	t	508	CLA	C2A-CAA-CBA-CGA
16	w	505	CLA	C2A-CAA-CBA-CGA
16	w	513	CLA	C2A-CAA-CBA-CGA
16	h	517	CLA	CBD-CGD-O2D-CED
16	B	1228	CLA	O1D-CGD-O2D-CED
16	A	1101	CLA	CBA-CGA-O2A-C1
16	W	507	CLA	CBA-CGA-O2A-C1
16	t	511	CLA	CBA-CGA-O2A-C1
16	p	516	CLA	O1A-CGA-O2A-C1
16	t	503	CLA	O1A-CGA-O2A-C1
16	x	503	CLA	O1A-CGA-O2A-C1
16	H	1128	CLA	O1D-CGD-O2D-CED
16	Z	508	CLA	O1D-CGD-O2D-CED
16	a	1140	CLA	C15-C16-C17-C18
16	q	505	CLA	C10-C11-C12-C13
16	t	515	CLA	C13-C15-C16-C17
14	H	4201	LMG	C10-C11-C12-C13
16	u	515	CLA	C16-C17-C18-C19
13	a	849	LHG	O1-C1-C2-O2
16	G	1213	CLA	O1A-CGA-O2A-C1
16	t	514	CLA	O1A-CGA-O2A-C1
16	w	505	CLA	O1A-CGA-O2A-C1
16	G	1211	CLA	C3-C5-C6-C7
16	Y	517	CLA	C3-C5-C6-C7
13	a	849	LHG	C24-C25-C26-C27
16	A	1109	CLA	C1A-C2A-CAA-CBA
16	A	1116	CLA	C1A-C2A-CAA-CBA
16	A	1119	CLA	C1A-C2A-CAA-CBA
16	A	1122	CLA	C1A-C2A-CAA-CBA
16	A	1126	CLA	C1A-C2A-CAA-CBA
16	A	1128	CLA	C1A-C2A-CAA-CBA
16	A	1133	CLA	C1A-C2A-CAA-CBA
16	A	1237	CLA	C1A-C2A-CAA-CBA
16	B	1208	CLA	C1A-C2A-CAA-CBA
16	B	1212	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	B	1213	CLA	C1A-C2A-CAA-CBA
16	B	1216	CLA	C1A-C2A-CAA-CBA
16	B	1218	CLA	C1A-C2A-CAA-CBA
16	B	1223	CLA	C1A-C2A-CAA-CBA
16	B	1224	CLA	C1A-C2A-CAA-CBA
16	B	1225	CLA	C1A-C2A-CAA-CBA
16	B	1226	CLA	C1A-C2A-CAA-CBA
16	F	1302	CLA	C1A-C2A-CAA-CBA
16	G	1203	CLA	C1A-C2A-CAA-CBA
16	G	1206	CLA	C1A-C2A-CAA-CBA
16	G	1208	CLA	C1A-C2A-CAA-CBA
16	G	1212	CLA	C1A-C2A-CAA-CBA
16	G	1214	CLA	C1A-C2A-CAA-CBA
16	G	1216	CLA	C1A-C2A-CAA-CBA
16	G	1224	CLA	C1A-C2A-CAA-CBA
16	G	1225	CLA	C1A-C2A-CAA-CBA
16	G	1226	CLA	C1A-C2A-CAA-CBA
16	G	1228	CLA	C1A-C2A-CAA-CBA
16	H	1109	CLA	C1A-C2A-CAA-CBA
16	H	1116	CLA	C1A-C2A-CAA-CBA
16	H	1119	CLA	C1A-C2A-CAA-CBA
16	H	1126	CLA	C1A-C2A-CAA-CBA
16	H	1129	CLA	C1A-C2A-CAA-CBA
16	H	1138	CLA	C1A-C2A-CAA-CBA
16	H	1237	CLA	C1A-C2A-CAA-CBA
16	Q	1302	CLA	C1A-C2A-CAA-CBA
16	T	4002	CLA	C1A-C2A-CAA-CBA
16	W	501	CLA	C1A-C2A-CAA-CBA
16	W	512	CLA	C1A-C2A-CAA-CBA
16	W	515	CLA	C1A-C2A-CAA-CBA
16	X	501	CLA	C1A-C2A-CAA-CBA
16	X	511	CLA	C1A-C2A-CAA-CBA
16	X	517	CLA	C1A-C2A-CAA-CBA
16	Y	501	CLA	C1A-C2A-CAA-CBA
16	Y	504	CLA	C1A-C2A-CAA-CBA
16	Y	506	CLA	C1A-C2A-CAA-CBA
16	Y	509	CLA	C1A-C2A-CAA-CBA
16	Y	511	CLA	C1A-C2A-CAA-CBA
16	Y	514	CLA	C1A-C2A-CAA-CBA
16	Y	515	CLA	C1A-C2A-CAA-CBA
16	Y	517	CLA	C1A-C2A-CAA-CBA
16	Z	501	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	Z	504	CLA	C1A-C2A-CAA-CBA
16	Z	505	CLA	C1A-C2A-CAA-CBA
16	Z	506	CLA	C1A-C2A-CAA-CBA
16	Z	510	CLA	C1A-C2A-CAA-CBA
16	a	1022	CLA	C1A-C2A-CAA-CBA
16	a	1102	CLA	C1A-C2A-CAA-CBA
16	a	1109	CLA	C1A-C2A-CAA-CBA
16	a	1115	CLA	C1A-C2A-CAA-CBA
16	a	1116	CLA	C1A-C2A-CAA-CBA
16	a	1119	CLA	C1A-C2A-CAA-CBA
16	a	1126	CLA	C1A-C2A-CAA-CBA
16	a	1128	CLA	C1A-C2A-CAA-CBA
16	a	1129	CLA	C1A-C2A-CAA-CBA
16	a	1134	CLA	C1A-C2A-CAA-CBA
16	b	1012	CLA	C1A-C2A-CAA-CBA
16	b	1023	CLA	C1A-C2A-CAA-CBA
16	b	1203	CLA	C1A-C2A-CAA-CBA
16	b	1212	CLA	C1A-C2A-CAA-CBA
16	b	1217	CLA	C1A-C2A-CAA-CBA
16	b	1218	CLA	C1A-C2A-CAA-CBA
16	b	1219	CLA	C1A-C2A-CAA-CBA
16	b	1221	CLA	C1A-C2A-CAA-CBA
16	b	1223	CLA	C1A-C2A-CAA-CBA
16	b	1224	CLA	C1A-C2A-CAA-CBA
16	b	1225	CLA	C1A-C2A-CAA-CBA
16	b	1228	CLA	C1A-C2A-CAA-CBA
16	f	1302	CLA	C1A-C2A-CAA-CBA
16	g	509	CLA	C1A-C2A-CAA-CBA
16	g	513	CLA	C1A-C2A-CAA-CBA
16	g	514	CLA	C1A-C2A-CAA-CBA
16	h	512	CLA	C1A-C2A-CAA-CBA
16	h	514	CLA	C1A-C2A-CAA-CBA
16	h	517	CLA	C1A-C2A-CAA-CBA
16	k	4002	CLA	C1A-C2A-CAA-CBA
16	n	501	CLA	C1A-C2A-CAA-CBA
16	n	503	CLA	C1A-C2A-CAA-CBA
16	n	504	CLA	C1A-C2A-CAA-CBA
16	n	508	CLA	C1A-C2A-CAA-CBA
16	n	511	CLA	C1A-C2A-CAA-CBA
16	n	512	CLA	C1A-C2A-CAA-CBA
16	n	514	CLA	C1A-C2A-CAA-CBA
16	n	515	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	o	514	CLA	C1A-C2A-CAA-CBA
16	o	515	CLA	C1A-C2A-CAA-CBA
16	o	516	CLA	C1A-C2A-CAA-CBA
16	p	504	CLA	C1A-C2A-CAA-CBA
16	p	505	CLA	C1A-C2A-CAA-CBA
16	p	506	CLA	C1A-C2A-CAA-CBA
16	p	509	CLA	C1A-C2A-CAA-CBA
16	p	511	CLA	C1A-C2A-CAA-CBA
16	p	514	CLA	C1A-C2A-CAA-CBA
16	p	515	CLA	C1A-C2A-CAA-CBA
16	p	516	CLA	C1A-C2A-CAA-CBA
16	p	517	CLA	C1A-C2A-CAA-CBA
16	q	506	CLA	C1A-C2A-CAA-CBA
16	q	509	CLA	C1A-C2A-CAA-CBA
16	q	512	CLA	C1A-C2A-CAA-CBA
16	q	514	CLA	C1A-C2A-CAA-CBA
16	r	504	CLA	C1A-C2A-CAA-CBA
16	r	509	CLA	C1A-C2A-CAA-CBA
16	s	504	CLA	C1A-C2A-CAA-CBA
16	s	506	CLA	C1A-C2A-CAA-CBA
16	s	509	CLA	C1A-C2A-CAA-CBA
16	s	511	CLA	C1A-C2A-CAA-CBA
16	s	514	CLA	C1A-C2A-CAA-CBA
16	t	503	CLA	C1A-C2A-CAA-CBA
16	t	512	CLA	C1A-C2A-CAA-CBA
16	t	514	CLA	C1A-C2A-CAA-CBA
16	u	517	CLA	C1A-C2A-CAA-CBA
16	v	501	CLA	C1A-C2A-CAA-CBA
16	v	503	CLA	C1A-C2A-CAA-CBA
16	v	511	CLA	C1A-C2A-CAA-CBA
16	v	517	CLA	C1A-C2A-CAA-CBA
16	w	506	CLA	C1A-C2A-CAA-CBA
16	w	512	CLA	C1A-C2A-CAA-CBA
16	w	516	CLA	C1A-C2A-CAA-CBA
16	x	506	CLA	C1A-C2A-CAA-CBA
16	x	513	CLA	C1A-C2A-CAA-CBA
16	x	514	CLA	C1A-C2A-CAA-CBA
16	x	515	CLA	C1A-C2A-CAA-CBA
16	y	501	CLA	C1A-C2A-CAA-CBA
16	y	504	CLA	C1A-C2A-CAA-CBA
16	y	506	CLA	C1A-C2A-CAA-CBA
16	y	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	A	1134	CLA	O1D-CGD-O2D-CED
13	Y	605	LHG	C24-C23-O8-C6
16	a	1105	CLA	CBD-CGD-O2D-CED
16	b	1012	CLA	C5-C6-C7-C8
13	B	4018	LHG	C12-C13-C14-C15
16	G	1201	CLA	O1D-CGD-O2D-CED
16	G	1235	CLA	O1A-CGA-O2A-C1
14	a	852	LMG	C32-C33-C34-C35
16	G	1218	CLA	C5-C6-C7-C8
13	X	605	LHG	O6-C4-C5-C6
13	H	849	LHG	O9-C7-O7-C5
13	i	103	LHG	O9-C7-O7-C5
13	H	849	LHG	C24-C25-C26-C27
16	A	1013	CLA	C11-C12-C13-C15
16	A	1022	CLA	C12-C13-C15-C16
16	A	1101	CLA	C11-C10-C8-C7
16	A	1119	CLA	C6-C7-C8-C10
16	A	1125	CLA	C11-C10-C8-C7
16	B	1202	CLA	C6-C7-C8-C10
16	B	1204	CLA	C6-C7-C8-C10
16	B	1206	CLA	C11-C10-C8-C7
16	B	1207	CLA	C12-C13-C15-C16
16	B	1210	CLA	C11-C10-C8-C7
16	B	1211	CLA	C6-C7-C8-C10
16	B	1221	CLA	C12-C13-C15-C16
16	B	1225	CLA	C6-C7-C8-C10
16	B	1225	CLA	C12-C13-C15-C16
16	B	1235	CLA	C6-C7-C8-C10
16	G	1023	CLA	C12-C13-C15-C16
16	G	1202	CLA	C6-C7-C8-C10
16	G	1211	CLA	C6-C7-C8-C10
16	G	1211	CLA	C11-C12-C13-C15
16	G	1225	CLA	C6-C7-C8-C10
16	G	1235	CLA	C6-C7-C8-C10
16	H	1022	CLA	C12-C13-C15-C16
16	H	1101	CLA	C6-C7-C8-C10
16	H	1117	CLA	C11-C12-C13-C15
16	W	510	CLA	C6-C7-C8-C10
16	W	512	CLA	C6-C7-C8-C10
16	W	515	CLA	C12-C13-C15-C16
16	X	506	CLA	C6-C7-C8-C10
16	X	511	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
16	Y	505	CLA	C11-C10-C8-C7
16	Y	506	CLA	C11-C10-C8-C7
16	Y	511	CLA	C6-C7-C8-C10
16	Z	505	CLA	C11-C12-C13-C15
16	Z	507	CLA	C11-C10-C8-C7
16	Z	512	CLA	C11-C12-C13-C15
16	a	1013	CLA	C11-C10-C8-C7
16	a	1022	CLA	C12-C13-C15-C16
16	a	1119	CLA	C12-C13-C15-C16
16	a	1123	CLA	C11-C12-C13-C15
16	a	1131	CLA	C6-C7-C8-C10
16	b	1202	CLA	C6-C7-C8-C10
16	b	1204	CLA	C6-C7-C8-C10
16	b	1206	CLA	C12-C13-C15-C16
16	b	1207	CLA	C12-C13-C15-C16
16	b	1210	CLA	C6-C7-C8-C10
16	b	1221	CLA	C11-C10-C8-C7
16	b	1225	CLA	C6-C7-C8-C10
16	b	1225	CLA	C12-C13-C15-C16
16	g	506	CLA	C11-C10-C8-C7
16	g	510	CLA	C6-C7-C8-C10
16	h	506	CLA	C11-C10-C8-C7
16	h	511	CLA	C12-C13-C15-C16
16	h	512	CLA	C11-C12-C13-C15
16	h	515	CLA	C6-C7-C8-C10
16	n	510	CLA	C6-C7-C8-C10
16	n	512	CLA	C6-C7-C8-C10
16	n	512	CLA	C11-C12-C13-C15
16	n	515	CLA	C6-C7-C8-C10
16	o	511	CLA	C11-C12-C13-C15
16	q	512	CLA	C12-C13-C15-C16
16	r	515	CLA	C11-C12-C13-C15
16	s	511	CLA	C11-C12-C13-C15
16	t	506	CLA	C11-C10-C8-C7
16	t	512	CLA	C11-C12-C13-C15
16	u	511	CLA	C11-C12-C13-C15
16	u	512	CLA	C6-C7-C8-C10
16	v	507	CLA	C11-C10-C8-C7
16	y	507	CLA	C11-C10-C8-C7
16	y	511	CLA	C12-C13-C15-C16
16	y	515	CLA	C11-C10-C8-C7
16	G	1207	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	t	505	CLA	C8-C10-C11-C12
16	r	516	CLA	O1A-CGA-O2A-C1
16	G	1210	CLA	O1A-CGA-O2A-C1
16	p	502	CLA	O1A-CGA-O2A-C1
14	f	4017	LMG	O6-C5-C6-O5
16	p	515	CLA	O1D-CGD-O2D-CED
16	y	514	CLA	CBA-CGA-O2A-C1
14	G	848	LMG	C4-C5-C6-O5
16	n	515	CLA	CBD-CGD-O2D-CED
16	H	1120	CLA	O1D-CGD-O2D-CED
16	a	1103	CLA	C13-C15-C16-C17
23	s	606	LMU	O5B-C1B-O1B-C4'
16	A	1132	CLA	C4-C3-C5-C6
16	B	1204	CLA	C4-C3-C5-C6
16	b	1204	CLA	C4-C3-C5-C6
16	A	1132	CLA	C2-C3-C5-C6
16	G	1205	CLA	C2-C3-C5-C6
16	a	1132	CLA	C2-C3-C5-C6
16	b	1204	CLA	C2-C3-C5-C6
16	o	509	CLA	C2-C3-C5-C6
16	h	509	CLA	C4C-C3C-CAC-CBC
16	v	511	CLA	O1A-CGA-O2A-C1
13	r	605	LHG	C11-C10-C9-C8
16	H	1122	CLA	C4C-C3C-CAC-CBC
16	p	506	CLA	C4C-C3C-CAC-CBC
16	B	1210	CLA	C10-C11-C12-C13
16	H	1125	CLA	C13-C15-C16-C17
16	h	509	CLA	C15-C16-C17-C18
14	f	4017	LMG	C28-C29-C30-C31
16	A	1022	CLA	C2A-CAA-CBA-CGA
16	B	1012	CLA	C2A-CAA-CBA-CGA
16	H	1022	CLA	C2A-CAA-CBA-CGA
16	H	1129	CLA	C2A-CAA-CBA-CGA
16	X	513	CLA	C2A-CAA-CBA-CGA
16	s	505	CLA	C2A-CAA-CBA-CGA
16	s	508	CLA	C2A-CAA-CBA-CGA
16	u	501	CLA	C2A-CAA-CBA-CGA
16	v	515	CLA	C2A-CAA-CBA-CGA
16	y	501	CLA	C2A-CAA-CBA-CGA
16	A	1125	CLA	C11-C10-C8-C9
16	A	1128	CLA	C11-C12-C13-C14
16	A	1131	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	B	1202	CLA	C6-C7-C8-C9
16	B	1203	CLA	C14-C13-C15-C16
16	B	1204	CLA	C6-C7-C8-C9
16	B	1211	CLA	C6-C7-C8-C9
16	B	1221	CLA	C11-C10-C8-C9
16	G	1221	CLA	C6-C7-C8-C9
16	G	1221	CLA	C11-C10-C8-C9
16	G	1224	CLA	C11-C10-C8-C9
16	G	1225	CLA	C6-C7-C8-C9
16	H	1022	CLA	C14-C13-C15-C16
16	H	1131	CLA	C11-C10-C8-C9
16	W	505	CLA	C11-C12-C13-C14
16	W	512	CLA	C6-C7-C8-C9
16	W	515	CLA	C6-C7-C8-C9
16	X	515	CLA	C6-C7-C8-C9
16	Y	506	CLA	C11-C10-C8-C9
16	Z	512	CLA	C11-C12-C13-C14
16	a	1104	CLA	C11-C10-C8-C9
16	a	1128	CLA	C11-C12-C13-C14
16	b	1210	CLA	C6-C7-C8-C9
16	b	1211	CLA	C6-C7-C8-C9
16	b	1225	CLA	C14-C13-C15-C16
16	b	1226	CLA	C6-C7-C8-C9
16	g	511	CLA	C11-C10-C8-C9
16	h	506	CLA	C11-C10-C8-C9
16	n	506	CLA	C11-C10-C8-C9
16	n	510	CLA	C6-C7-C8-C9
16	n	512	CLA	C11-C10-C8-C9
16	o	515	CLA	C6-C7-C8-C9
16	p	505	CLA	C11-C10-C8-C9
16	q	506	CLA	C6-C7-C8-C9
16	q	506	CLA	C11-C10-C8-C9
16	r	511	CLA	C11-C10-C8-C9
16	r	515	CLA	C11-C12-C13-C14
16	u	504	CLA	C6-C7-C8-C9
16	u	506	CLA	C6-C7-C8-C9
16	x	506	CLA	C11-C10-C8-C9
16	x	511	CLA	C14-C13-C15-C16
16	y	507	CLA	C11-C10-C8-C9
16	y	511	CLA	C6-C7-C8-C9
16	y	511	CLA	C14-C13-C15-C16
17	b	2002	PQN	C24-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
20	U	4101	LMT	C4-C5-C6-C7
14	a	4101	LMG	C28-C29-C30-C31
19	y	603	BCR	C9-C10-C11-C12
16	A	1128	CLA	O1D-CGD-O2D-CED
13	R	103	LHG	C24-C23-O8-C6
14	H	852	LMG	C29-C28-O8-C9
16	A	1123	CLA	CBA-CGA-O2A-C1
16	W	514	CLA	CBA-CGA-O2A-C1
16	X	512	CLA	CBA-CGA-O2A-C1
16	h	509	CLA	CBA-CGA-O2A-C1
16	x	504	CLA	CBA-CGA-O2A-C1
16	a	1130	CLA	C10-C11-C12-C13
16	Z	516	CLA	O1A-CGA-O2A-C1
14	A	4101	LMG	C17-C18-C19-C20
14	F	4017	LMG	O6-C5-C6-O5
16	B	1222	CLA	CBD-CGD-O2D-CED
16	H	1138	CLA	CBD-CGD-O2D-CED
16	Y	516	CLA	CBD-CGD-O2D-CED
13	A	849	LHG	C29-C30-C31-C32
16	X	505	CLA	C10-C11-C12-C13
16	a	1101	CLA	C8-C10-C11-C12
16	a	1138	CLA	C10-C11-C12-C13
14	A	4201	LMG	C28-C29-C30-C31
16	q	508	CLA	O1D-CGD-O2D-CED
13	X	605	LHG	C4-C5-C6-O8
13	p	605	LHG	C4-C5-C6-O8
13	u	605	LHG	C4-C5-C6-O8
14	A	852	LMG	C7-C8-C9-O8
14	H	4201	LMG	C7-C8-C9-O8
14	a	852	LMG	C7-C8-C9-O8
14	a	4201	LMG	C7-C8-C9-O8
23	q	605	LMU	O5B-C5B-C6B-O6B
13	b	4018	LHG	C17-C18-C19-C20
16	G	1207	CLA	C5-C6-C7-C8
16	Y	505	CLA	C13-C15-C16-C17
16	g	502	CLA	O1D-CGD-O2D-CED
16	H	1127	CLA	CBA-CGA-O2A-C1
16	Y	508	CLA	CBA-CGA-O2A-C1
16	a	1136	CLA	CBA-CGA-O2A-C1
16	b	1210	CLA	CBA-CGA-O2A-C1
16	p	514	CLA	CBA-CGA-O2A-C1
16	s	506	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	s	511	CLA	CBA-CGA-O2A-C1
14	H	852	LMG	O6-C5-C6-O5
14	Q	4017	LMG	O6-C5-C6-O5
16	B	1012	CLA	C6-C7-C8-C10
16	G	1202	CLA	C16-C17-C18-C20
16	Z	509	CLA	C16-C17-C18-C19
16	b	1215	CLA	C11-C12-C13-C14
16	n	505	CLA	C16-C17-C18-C20
14	A	852	LMG	C34-C35-C36-C37
20	a	4202	LMT	C1-C2-C3-C4
15	A	1011	CL0	O1A-CGA-O2A-C1
16	g	506	CLA	O1A-CGA-O2A-C1
16	T	4003	CLA	O1D-CGD-O2D-CED
19	I	4018	BCR	C20-C21-C22-C37
19	X	602	BCR	C11-C10-C9-C34
19	a	4007	BCR	C16-C17-C18-C36
19	b	4017	BCR	C16-C17-C18-C36
19	j	4015	BCR	C11-C10-C9-C34
19	l	4019	BCR	C20-C21-C22-C37
19	o	603	BCR	C20-C21-C22-C37
19	s	602	BCR	C16-C17-C18-C36
19	y	604	BCR	C20-C21-C22-C37
16	A	1127	CLA	C5-C6-C7-C8
16	a	1127	CLA	C8-C10-C11-C12
16	p	505	CLA	C13-C15-C16-C17
16	W	507	CLA	O1A-CGA-O2A-C1
16	n	514	CLA	O1A-CGA-O2A-C1
16	v	512	CLA	O1A-CGA-O2A-C1
14	A	4101	LMG	C14-C15-C16-C17
16	o	509	CLA	C4-C3-C5-C6
16	v	504	CLA	C4-C3-C5-C6
16	A	1101	CLA	C2-C3-C5-C6
16	A	1123	CLA	C2-C3-C5-C6
16	B	1204	CLA	C2-C3-C5-C6
16	H	1132	CLA	C2-C3-C5-C6
16	Y	504	CLA	C2-C3-C5-C6
16	b	1205	CLA	C2-C3-C5-C6
16	n	512	CLA	C2-C3-C5-C6
16	q	512	CLA	C2-C3-C5-C6
16	G	1240	CLA	O1A-CGA-O2A-C1
16	B	1205	CLA	C10-C11-C12-C13
16	H	1131	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	a	1101	CLA	C10-C11-C12-C13
16	a	1131	CLA	C13-C15-C16-C17
16	q	509	CLA	C8-C10-C11-C12
16	u	504	CLA	C5-C6-C7-C8
19	B	4014	BCR	C37-C22-C23-C24
19	L	4022	BCR	C37-C22-C23-C24
19	S	4013	BCR	C7-C8-C9-C34
19	U	4022	BCR	C37-C22-C23-C24
19	X	602	BCR	C37-C22-C23-C24
19	l	4022	BCR	C37-C22-C23-C24
19	r	601	BCR	C11-C12-C13-C35
19	x	603	BCR	C7-C8-C9-C34
19	y	601	BCR	C7-C8-C9-C34
20	l	4101	LMT	O5B-C1B-O1B-C4'
16	A	1117	CLA	C16-C17-C18-C19
16	n	505	CLA	C16-C17-C18-C19
13	i	103	LHG	C29-C30-C31-C32
14	a	4101	LMG	O6-C5-C6-O5
19	G	4014	BCR	C21-C22-C23-C24
19	U	4022	BCR	C21-C22-C23-C24
19	X	602	BCR	C21-C22-C23-C24
19	h	601	BCR	C7-C8-C9-C10
19	n	601	BCR	C21-C22-C23-C24
19	q	604	BCR	C7-C8-C9-C10
16	t	511	CLA	O1A-CGA-O2A-C1
16	Z	510	CLA	C5-C6-C7-C8
16	p	511	CLA	C13-C15-C16-C17
13	I	103	LHG	C29-C30-C31-C32
16	Y	508	CLA	C2A-CAA-CBA-CGA
16	t	516	CLA	C2A-CAA-CBA-CGA
16	v	507	CLA	C2A-CAA-CBA-CGA
16	x	511	CLA	C2A-CAA-CBA-CGA
16	r	503	CLA	CBA-CGA-O2A-C1
16	y	516	CLA	CBA-CGA-O2A-C1
16	g	504	CLA	C8-C10-C11-C12
16	a	1101	CLA	O1A-CGA-O2A-C1
16	b	1222	CLA	O1D-CGD-O2D-CED
16	A	1110	CLA	CBA-CGA-O2A-C1
16	B	1222	CLA	CBA-CGA-O2A-C1
13	a	849	LHG	C10-C11-C12-C13
14	G	848	LMG	C13-C14-C15-C16
16	u	503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	S	4012	BCR	C10-C11-C12-C13
19	a	4003	BCR	C10-C11-C12-C13
19	k	4001	BCR	C18-C19-C20-C21
16	A	1125	CLA	C13-C15-C16-C17
16	G	1224	CLA	C8-C10-C11-C12
19	S	4015	BCR	C9-C10-C11-C12
19	b	4005	BCR	C19-C20-C21-C22
19	w	604	BCR	C15-C16-C17-C18
15	A	1011	CL0	C16-C17-C18-C20
16	H	1101	CLA	C16-C17-C18-C20
13	B	4018	LHG	C16-C17-C18-C19
16	q	516	CLA	CBA-CGA-O2A-C1
13	g	605	LHG	O10-C23-O8-C6
16	y	514	CLA	O1A-CGA-O2A-C1
14	a	4101	LMG	C31-C32-C33-C34
16	s	503	CLA	O1A-CGA-O2A-C1
19	A	4003	BCR	C16-C17-C18-C19
19	G	4004	BCR	C20-C21-C22-C23
19	R	4018	BCR	C16-C17-C18-C19
19	X	601	BCR	C16-C17-C18-C19
19	g	603	BCR	C11-C10-C9-C8
19	i	4018	BCR	C12-C13-C14-C15
19	n	604	BCR	C20-C21-C22-C23
19	t	603	BCR	C20-C21-C22-C23
14	a	4101	LMG	C14-C15-C16-C17
13	p	605	LHG	O6-C4-C5-O7
19	K	4001	BCR	C6-C7-C8-C9
19	Z	604	BCR	C22-C23-C24-C25
19	b	4017	BCR	C22-C23-C24-C25
19	o	603	BCR	C22-C23-C24-C25
16	B	1225	CLA	C13-C15-C16-C17
16	X	509	CLA	O1D-CGD-O2D-CED
13	I	103	LHG	C24-C23-O8-C6
16	A	1116	CLA	CBA-CGA-O2A-C1
16	p	511	CLA	CBA-CGA-O2A-C1
16	r	502	CLA	CBA-CGA-O2A-C1
16	s	514	CLA	CBA-CGA-O2A-C1
16	g	503	CLA	CBD-CGD-O2D-CED
16	X	512	CLA	O1A-CGA-O2A-C1
16	Y	508	CLA	O1A-CGA-O2A-C1
13	H	849	LHG	C27-C28-C29-C30
16	A	1101	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	A	1110	CLA	C4-C3-C5-C6
16	B	1228	CLA	C4-C3-C5-C6
16	G	1220	CLA	C4-C3-C5-C6
16	G	1228	CLA	C4-C3-C5-C6
16	U	1502	CLA	C4-C3-C5-C6
16	a	1132	CLA	C4-C3-C5-C6
16	B	1205	CLA	C2-C3-C5-C6
16	b	1228	CLA	C2-C3-C5-C6
16	l	1501	CLA	C2-C3-C5-C6
16	A	1110	CLA	C3-C5-C6-C7
16	o	506	CLA	C11-C12-C13-C15
13	H	849	LHG	C25-C26-C27-C28
14	H	852	LMG	C30-C31-C32-C33
13	p	605	LHG	C27-C28-C29-C30
14	H	4201	LMG	C14-C15-C16-C17
16	x	506	CLA	C5-C6-C7-C8
13	R	103	LHG	O7-C5-C6-O8
13	Y	605	LHG	O7-C5-C6-O8
13	x	605	LHG	O7-C5-C6-O8
14	b	848	LMG	O7-C8-C9-O8
14	H	4101	LMG	C13-C14-C15-C16
16	p	510	CLA	O1D-CGD-O2D-CED
15	A	1011	CL0	CAA-CBA-CGA-O2A
16	X	509	CLA	CAA-CBA-CGA-O2A
16	T	4003	CLA	C4C-C3C-CAC-CBC
16	s	503	CLA	C4C-C3C-CAC-CBC
16	G	1211	CLA	C2A-CAA-CBA-CGA
16	G	1224	CLA	C2A-CAA-CBA-CGA
16	H	1120	CLA	C2A-CAA-CBA-CGA
16	A	1140	CLA	C3-C5-C6-C7
16	B	1224	CLA	C3-C5-C6-C7
16	G	1238	CLA	C3-C5-C6-C7
16	b	1224	CLA	C3-C5-C6-C7
16	n	517	CLA	C3-C5-C6-C7
13	X	605	LHG	C11-C10-C9-C8
16	G	1221	CLA	C8-C10-C11-C12
16	Y	517	CLA	C2-C1-O2A-CGA
16	A	1101	CLA	O1A-CGA-O2A-C1
14	H	4101	LMG	C31-C32-C33-C34
14	b	848	LMG	C29-C28-O8-C9
16	Y	511	CLA	CBA-CGA-O2A-C1
16	a	1106	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
16	n	504	CLA	CBA-CGA-O2A-C1
16	g	515	CLA	CBD-CGD-O2D-CED
16	t	502	CLA	CBD-CGD-O2D-CED
16	a	1122	CLA	C4C-C3C-CAC-CBC
16	A	1013	CLA	C10-C11-C12-C13
16	b	1023	CLA	C10-C11-C12-C13
16	w	515	CLA	C13-C15-C16-C17
16	A	1123	CLA	O1A-CGA-O2A-C1
16	s	506	CLA	O1A-CGA-O2A-C1
16	y	517	CLA	C3-C5-C6-C7
14	a	852	LMG	C33-C34-C35-C36
16	Y	508	CLA	O1D-CGD-O2D-CED
16	a	1136	CLA	O1D-CGD-O2D-CED
16	u	511	CLA	O1D-CGD-O2D-CED
16	w	502	CLA	O1D-CGD-O2D-CED
16	b	1220	CLA	C6-C7-C8-C9
16	A	1132	CLA	C13-C15-C16-C17
16	Y	506	CLA	C8-C10-C11-C12
16	r	504	CLA	C8-C10-C11-C12
16	s	504	CLA	C8-C10-C11-C12
16	u	506	CLA	C5-C6-C7-C8
16	u	509	CLA	C10-C11-C12-C13
20	A	4202	LMT	C1-C2-C3-C4
16	H	1102	CLA	C11-C10-C8-C9
16	a	1117	CLA	C16-C17-C18-C20
16	A	1123	CLA	C4-C3-C5-C6
16	B	1223	CLA	C4-C3-C5-C6
16	G	1214	CLA	C4-C3-C5-C6
16	L	1501	CLA	C4-C3-C5-C6
16	b	1223	CLA	C4-C3-C5-C6
16	h	509	CLA	C4-C3-C5-C6
16	l	1501	CLA	C4-C3-C5-C6
16	l	1502	CLA	C4-C3-C5-C6
16	v	512	CLA	C4-C3-C5-C6
16	X	509	CLA	C2-C3-C5-C6
13	R	103	LHG	C27-C28-C29-C30
16	H	1133	CLA	C5-C6-C7-C8
16	H	1110	CLA	CBA-CGA-O2A-C1
16	Z	505	CLA	CBA-CGA-O2A-C1
16	u	517	CLA	CBA-CGA-O2A-C1
16	A	1109	CLA	C5-C6-C7-C8
16	B	1203	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	G	1205	CLA	C13-C15-C16-C17
16	H	1136	CLA	C8-C10-C11-C12
16	b	1205	CLA	C10-C11-C12-C13
16	h	515	CLA	C5-C6-C7-C8
16	a	1133	CLA	C6-C7-C8-C9
13	A	849	LHG	C10-C11-C12-C13
13	r	605	LHG	O1-C1-C2-O2
16	A	1013	CLA	C11-C12-C13-C14
16	A	1022	CLA	C14-C13-C15-C16
16	A	1101	CLA	C11-C10-C8-C9
16	A	1117	CLA	C11-C12-C13-C14
16	A	1119	CLA	C6-C7-C8-C9
16	A	1131	CLA	C6-C7-C8-C9
16	B	1206	CLA	C11-C10-C8-C9
16	B	1206	CLA	C11-C12-C13-C14
16	B	1207	CLA	C14-C13-C15-C16
16	B	1223	CLA	C14-C13-C15-C16
16	B	1225	CLA	C6-C7-C8-C9
16	B	1225	CLA	C14-C13-C15-C16
16	B	1226	CLA	C6-C7-C8-C9
16	G	1207	CLA	C14-C13-C15-C16
16	G	1211	CLA	C6-C7-C8-C9
16	G	1211	CLA	C14-C13-C15-C16
16	H	1013	CLA	C11-C12-C13-C14
16	H	1117	CLA	C11-C12-C13-C14
16	H	1119	CLA	C14-C13-C15-C16
16	H	1125	CLA	C11-C10-C8-C9
16	H	1125	CLA	C14-C13-C15-C16
16	H	1128	CLA	C11-C12-C13-C14
16	L	1502	CLA	C11-C10-C8-C9
16	W	510	CLA	C6-C7-C8-C9
16	X	504	CLA	C6-C7-C8-C9
16	X	506	CLA	C6-C7-C8-C9
16	X	511	CLA	C11-C12-C13-C14
16	Y	505	CLA	C11-C10-C8-C9
16	Y	511	CLA	C6-C7-C8-C9
16	Z	505	CLA	C11-C12-C13-C14
16	Z	507	CLA	C11-C10-C8-C9
16	a	1022	CLA	C14-C13-C15-C16
16	a	1117	CLA	C11-C12-C13-C14
16	a	1119	CLA	C14-C13-C15-C16
16	a	1123	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	a	1125	CLA	C11-C10-C8-C9
16	a	1131	CLA	C6-C7-C8-C9
16	b	1202	CLA	C6-C7-C8-C9
16	b	1204	CLA	C6-C7-C8-C9
16	b	1206	CLA	C6-C7-C8-C9
16	b	1207	CLA	C14-C13-C15-C16
16	b	1210	CLA	C11-C10-C8-C9
16	b	1221	CLA	C6-C7-C8-C9
16	b	1221	CLA	C11-C10-C8-C9
16	b	1221	CLA	C11-C12-C13-C14
16	b	1225	CLA	C6-C7-C8-C9
16	g	506	CLA	C11-C10-C8-C9
16	g	510	CLA	C6-C7-C8-C9
16	h	511	CLA	C14-C13-C15-C16
16	h	515	CLA	C6-C7-C8-C9
16	n	510	CLA	C11-C10-C8-C9
16	n	512	CLA	C6-C7-C8-C9
16	n	512	CLA	C11-C12-C13-C14
16	n	515	CLA	C6-C7-C8-C9
16	o	506	CLA	C6-C7-C8-C9
16	o	511	CLA	C11-C12-C13-C14
16	p	506	CLA	C11-C10-C8-C9
16	q	504	CLA	C11-C12-C13-C14
16	q	512	CLA	C14-C13-C15-C16
16	s	505	CLA	C11-C10-C8-C9
16	s	506	CLA	C11-C10-C8-C9
16	s	511	CLA	C11-C12-C13-C14
16	t	506	CLA	C11-C10-C8-C9
16	t	512	CLA	C11-C12-C13-C14
16	t	515	CLA	C6-C7-C8-C9
16	u	511	CLA	C11-C12-C13-C14
16	u	515	CLA	C14-C13-C15-C16
16	v	507	CLA	C11-C10-C8-C9
16	w	506	CLA	C6-C7-C8-C9
16	y	515	CLA	C11-C10-C8-C9
16	x	508	CLA	O1D-CGD-O2D-CED
16	H	1237	CLA	C13-C15-C16-C17
16	l	1503	CLA	C13-C15-C16-C17
16	t	512	CLA	C5-C6-C7-C8
16	y	507	CLA	C5-C6-C7-C8
16	A	1108	CLA	C4B-C3B-CAB-CBB
16	A	1109	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	A	1111	CLA	C4B-C3B-CAB-CBB
16	B	1207	CLA	C4B-C3B-CAB-CBB
16	B	1209	CLA	C4B-C3B-CAB-CBB
16	B	1221	CLA	C4B-C3B-CAB-CBB
16	B	1231	CLA	C4B-C3B-CAB-CBB
16	B	1235	CLA	C4B-C3B-CAB-CBB
16	F	1302	CLA	C4B-C3B-CAB-CBB
16	G	1207	CLA	C4B-C3B-CAB-CBB
16	G	1215	CLA	C4B-C3B-CAB-CBB
16	G	1225	CLA	C4B-C3B-CAB-CBB
16	H	1105	CLA	C4B-C3B-CAB-CBB
16	H	1108	CLA	C4B-C3B-CAB-CBB
16	H	1116	CLA	C4B-C3B-CAB-CBB
16	H	1118	CLA	C4B-C3B-CAB-CBB
16	Q	1302	CLA	C4B-C3B-CAB-CBB
16	U	1501	CLA	C4B-C3B-CAB-CBB
16	W	507	CLA	C4B-C3B-CAB-CBB
16	W	516	CLA	C4B-C3B-CAB-CBB
16	Y	507	CLA	C4B-C3B-CAB-CBB
16	Z	503	CLA	C4B-C3B-CAB-CBB
16	Z	509	CLA	C4B-C3B-CAB-CBB
16	Z	517	CLA	C4B-C3B-CAB-CBB
16	a	1108	CLA	C4B-C3B-CAB-CBB
16	a	1109	CLA	C4B-C3B-CAB-CBB
16	a	1118	CLA	C4B-C3B-CAB-CBB
16	a	1130	CLA	C4B-C3B-CAB-CBB
16	a	1138	CLA	C4B-C3B-CAB-CBB
16	b	1207	CLA	C4B-C3B-CAB-CBB
16	b	1209	CLA	C4B-C3B-CAB-CBB
16	b	1217	CLA	C4B-C3B-CAB-CBB
16	b	1218	CLA	C4B-C3B-CAB-CBB
16	b	1220	CLA	C4B-C3B-CAB-CBB
16	b	1223	CLA	C4B-C3B-CAB-CBB
16	b	1235	CLA	C4B-C3B-CAB-CBB
16	g	501	CLA	C4B-C3B-CAB-CBB
16	g	514	CLA	C4B-C3B-CAB-CBB
16	g	515	CLA	C4B-C3B-CAB-CBB
16	h	516	CLA	C4B-C3B-CAB-CBB
16	h	517	CLA	C4B-C3B-CAB-CBB
16	n	509	CLA	C4B-C3B-CAB-CBB
16	o	507	CLA	C4B-C3B-CAB-CBB
16	p	505	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	p	507	CLA	C4B-C3B-CAB-CBB
16	q	503	CLA	C4B-C3B-CAB-CBB
16	q	505	CLA	C4B-C3B-CAB-CBB
16	q	506	CLA	C4B-C3B-CAB-CBB
16	q	509	CLA	C4B-C3B-CAB-CBB
16	q	510	CLA	C4B-C3B-CAB-CBB
16	s	505	CLA	C4B-C3B-CAB-CBB
16	s	507	CLA	C4B-C3B-CAB-CBB
16	t	502	CLA	C4B-C3B-CAB-CBB
16	t	514	CLA	C4B-C3B-CAB-CBB
16	t	516	CLA	C4B-C3B-CAB-CBB
16	u	501	CLA	C4B-C3B-CAB-CBB
16	u	503	CLA	C4B-C3B-CAB-CBB
16	v	503	CLA	C4B-C3B-CAB-CBB
16	v	512	CLA	C4B-C3B-CAB-CBB
16	v	514	CLA	C4B-C3B-CAB-CBB
16	v	517	CLA	C4B-C3B-CAB-CBB
16	w	505	CLA	C4B-C3B-CAB-CBB
16	w	506	CLA	C4B-C3B-CAB-CBB
16	w	515	CLA	C4B-C3B-CAB-CBB
16	w	516	CLA	C4B-C3B-CAB-CBB
16	x	510	CLA	C4B-C3B-CAB-CBB
16	x	512	CLA	C4B-C3B-CAB-CBB
16	x	514	CLA	C4B-C3B-CAB-CBB
16	x	515	CLA	C4B-C3B-CAB-CBB
16	y	517	CLA	C4B-C3B-CAB-CBB
20	U	4101	LMT	O5B-C1B-O1B-C4'
16	a	1111	CLA	O1D-CGD-O2D-CED
16	A	1138	CLA	C10-C11-C12-C13
16	G	1210	CLA	C10-C11-C12-C13
16	p	510	CLA	C5-C6-C7-C8
16	H	1127	CLA	O1A-CGA-O2A-C1
16	B	1209	CLA	C2A-CAA-CBA-CGA
16	H	1130	CLA	C2A-CAA-CBA-CGA
16	n	508	CLA	C2A-CAA-CBA-CGA
16	o	509	CLA	O1D-CGD-O2D-CED
14	a	4101	LMG	C2-C1-O1-C7
16	A	1106	CLA	C10-C11-C12-C13
16	H	1132	CLA	C13-C15-C16-C17
16	y	509	CLA	C8-C10-C11-C12
13	R	103	LHG	C29-C30-C31-C32
13	b	4018	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
16	X	506	CLA	C3-C5-C6-C7
16	a	1125	CLA	C3-C5-C6-C7
16	q	505	CLA	C3-C5-C6-C7
17	G	2002	PQN	C13-C15-C16-C17
13	R	103	LHG	C32-C33-C34-C35
13	o	605	LHG	C11-C10-C9-C8
13	G	4018	LHG	O6-C4-C5-C6
13	b	4018	LHG	O6-C4-C5-C6
13	o	605	LHG	O6-C4-C5-C6
13	p	605	LHG	O6-C4-C5-C6
13	x	605	LHG	O6-C4-C5-C6
13	A	849	LHG	C28-C29-C30-C31
14	H	4101	LMG	C34-C35-C36-C37
16	a	1111	CLA	C4C-C3C-CAC-CBC
13	H	849	LHG	C32-C33-C34-C35
14	A	4201	LMG	C14-C15-C16-C17
16	h	509	CLA	CAA-CBA-CGA-O2A
16	A	1117	CLA	C11-C12-C13-C15
16	A	1119	CLA	C12-C13-C15-C16
16	A	1128	CLA	C11-C12-C13-C15
16	A	1131	CLA	C6-C7-C8-C10
16	A	1131	CLA	C11-C10-C8-C7
16	B	1202	CLA	C11-C12-C13-C15
16	B	1203	CLA	C12-C13-C15-C16
16	B	1221	CLA	C11-C10-C8-C7
16	B	1226	CLA	C6-C7-C8-C10
16	G	1204	CLA	C12-C13-C15-C16
16	G	1207	CLA	C12-C13-C15-C16
16	G	1211	CLA	C12-C13-C15-C16
16	G	1221	CLA	C6-C7-C8-C10
16	G	1221	CLA	C11-C10-C8-C7
16	G	1224	CLA	C11-C10-C8-C7
16	H	1013	CLA	C11-C12-C13-C15
16	H	1106	CLA	C6-C7-C8-C10
16	H	1109	CLA	C6-C7-C8-C10
16	H	1109	CLA	C11-C12-C13-C15
16	H	1119	CLA	C12-C13-C15-C16
16	H	1125	CLA	C11-C10-C8-C7
16	H	1125	CLA	C12-C13-C15-C16
16	H	1130	CLA	C11-C10-C8-C7
16	H	1131	CLA	C11-C10-C8-C7
16	L	1501	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	W	505	CLA	C11-C12-C13-C15
16	W	515	CLA	C6-C7-C8-C10
16	X	515	CLA	C6-C7-C8-C10
16	Y	510	CLA	C11-C12-C13-C15
16	Y	511	CLA	C12-C13-C15-C16
16	Z	510	CLA	C6-C7-C8-C10
16	a	1117	CLA	C11-C12-C13-C15
16	a	1128	CLA	C11-C12-C13-C15
16	a	1130	CLA	C11-C10-C8-C7
16	a	1131	CLA	C11-C10-C8-C7
16	b	1203	CLA	C12-C13-C15-C16
16	b	1211	CLA	C6-C7-C8-C10
16	b	1221	CLA	C6-C7-C8-C10
16	b	1226	CLA	C6-C7-C8-C10
16	g	504	CLA	C12-C13-C15-C16
16	g	510	CLA	C11-C12-C13-C15
16	g	511	CLA	C11-C10-C8-C7
16	l	1503	CLA	C11-C10-C8-C7
16	n	505	CLA	C11-C12-C13-C15
16	n	506	CLA	C11-C10-C8-C7
16	n	512	CLA	C11-C10-C8-C7
16	n	512	CLA	C12-C13-C15-C16
16	o	505	CLA	C6-C7-C8-C10
16	o	506	CLA	C6-C7-C8-C10
16	o	515	CLA	C6-C7-C8-C10
16	p	505	CLA	C11-C10-C8-C7
16	p	506	CLA	C11-C10-C8-C7
16	q	504	CLA	C11-C12-C13-C15
16	q	510	CLA	C6-C7-C8-C10
16	r	511	CLA	C11-C10-C8-C7
16	s	505	CLA	C11-C10-C8-C7
16	s	506	CLA	C11-C10-C8-C7
16	s	509	CLA	C6-C7-C8-C10
16	s	510	CLA	C11-C12-C13-C15
16	t	515	CLA	C6-C7-C8-C10
16	u	504	CLA	C11-C10-C8-C7
16	u	506	CLA	C6-C7-C8-C10
16	u	507	CLA	C11-C10-C8-C7
16	u	515	CLA	C12-C13-C15-C16
16	v	509	CLA	C6-C7-C8-C10
16	w	506	CLA	C6-C7-C8-C10
16	x	504	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
16	x	511	CLA	C12-C13-C15-C16
16	y	504	CLA	C11-C10-C8-C7
16	y	509	CLA	C6-C7-C8-C10
16	y	511	CLA	C6-C7-C8-C10
17	b	2002	PQN	C22-C23-C25-C26
16	H	1013	CLA	C10-C11-C12-C13
16	s	505	CLA	C13-C15-C16-C17
16	u	515	CLA	C8-C10-C11-C12
16	h	509	CLA	O1A-CGA-O2A-C1
16	x	504	CLA	O1A-CGA-O2A-C1
13	i	103	LHG	O2-C2-C3-O3
13	u	605	LHG	C11-C10-C9-C8
16	K	4003	CLA	O1D-CGD-O2D-CED
16	p	514	CLA	O1A-CGA-O2A-C1
16	s	511	CLA	O1A-CGA-O2A-C1
16	A	1138	CLA	C3A-C2A-CAA-CBA
16	A	1139	CLA	C3A-C2A-CAA-CBA
16	B	1205	CLA	C4-C3-C5-C6
16	B	1210	CLA	C4-C3-C5-C6
16	B	1220	CLA	C3A-C2A-CAA-CBA
16	B	1226	CLA	C3A-C2A-CAA-CBA
16	G	1204	CLA	C4-C3-C5-C6
16	G	1226	CLA	C3A-C2A-CAA-CBA
16	H	1107	CLA	C3A-C2A-CAA-CBA
16	H	1118	CLA	C4-C3-C5-C6
16	H	1138	CLA	C3A-C2A-CAA-CBA
16	H	1139	CLA	C3A-C2A-CAA-CBA
16	X	516	CLA	C3A-C2A-CAA-CBA
16	Z	516	CLA	C3A-C2A-CAA-CBA
16	a	1101	CLA	C4-C3-C5-C6
16	a	1137	CLA	C3A-C2A-CAA-CBA
16	a	1138	CLA	C3A-C2A-CAA-CBA
16	b	1210	CLA	C4-C3-C5-C6
16	b	1214	CLA	C3A-C2A-CAA-CBA
16	g	503	CLA	C3A-C2A-CAA-CBA
16	o	516	CLA	C3A-C2A-CAA-CBA
16	p	516	CLA	C3A-C2A-CAA-CBA
16	r	501	CLA	C3A-C2A-CAA-CBA
16	s	516	CLA	C3A-C2A-CAA-CBA
16	u	513	CLA	C3A-C2A-CAA-CBA
16	v	516	CLA	C3A-C2A-CAA-CBA
16	w	513	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	x	504	CLA	C4-C3-C5-C6
16	y	512	CLA	C4-C3-C5-C6
16	y	514	CLA	C3A-C2A-CAA-CBA
16	y	517	CLA	C4-C3-C5-C6
16	o	512	CLA	C5-C6-C7-C8
16	G	1222	CLA	O1D-CGD-O2D-CED
16	p	514	CLA	CAA-CBA-CGA-O2A
16	H	1118	CLA	C2-C3-C5-C6
16	h	509	CLA	C2-C3-C5-C6
16	u	510	CLA	O1D-CGD-O2D-CED
16	A	1110	CLA	O1A-CGA-O2A-C1
16	W	514	CLA	O1A-CGA-O2A-C1
16	b	1210	CLA	O1A-CGA-O2A-C1
16	u	512	CLA	C13-C15-C16-C17
16	v	509	CLA	CBA-CGA-O2A-C1
19	B	4005	BCR	C19-C20-C21-C22
19	B	4010	BCR	C15-C16-C17-C18
19	G	4014	BCR	C19-C20-C21-C22
19	H	4011	BCR	C9-C10-C11-C12
19	S	4013	BCR	C19-C20-C21-C22
19	T	4001	BCR	C9-C10-C11-C12
19	U	4022	BCR	C19-C20-C21-C22
19	a	4011	BCR	C9-C10-C11-C12
19	n	604	BCR	C13-C14-C15-C16
19	o	604	BCR	C15-C16-C17-C18
19	o	604	BCR	C19-C20-C21-C22
19	p	604	BCR	C9-C10-C11-C12
19	s	604	BCR	C9-C10-C11-C12
19	s	604	BCR	C13-C14-C15-C16
19	u	602	BCR	C19-C20-C21-C22
19	w	602	BCR	C19-C20-C21-C22
19	y	601	BCR	C9-C10-C11-C12
21	m	4021	ECH	C9-C10-C11-C12
16	o	506	CLA	C11-C12-C13-C14
16	o	505	CLA	C15-C16-C17-C18
19	h	601	BCR	C7-C8-C9-C34
16	a	1136	CLA	O1A-CGA-O2A-C1
16	n	505	CLA	O1D-CGD-O2D-CED
16	n	510	CLA	O1D-CGD-O2D-CED
14	a	4101	LMG	C33-C34-C35-C36
16	a	1126	CLA	C13-C15-C16-C17
16	o	511	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	Z	603	BCR	C21-C22-C23-C24
19	f	4016	BCR	C21-C22-C23-C24
19	s	602	BCR	C21-C22-C23-C24
13	A	851	LHG	C4-C5-C6-O8
13	H	851	LHG	C4-C5-C6-O8
13	R	103	LHG	C4-C5-C6-O8
13	o	605	LHG	C4-C5-C6-O8
14	A	4101	LMG	O1-C7-C8-C9
14	B	848	LMG	C7-C8-C9-O8
14	H	4101	LMG	O1-C7-C8-C9
14	H	4101	LMG	C7-C8-C9-O8
14	a	4101	LMG	C7-C8-C9-O8
13	A	849	LHG	C24-C25-C26-C27
16	t	506	CLA	CBD-CGD-O2D-CED
16	w	509	CLA	C16-C17-C18-C20
16	A	1103	CLA	C13-C15-C16-C17
16	G	1211	CLA	C8-C10-C11-C12
16	a	1106	CLA	C10-C11-C12-C13
16	x	509	CLA	C13-C15-C16-C17
14	a	4201	LMG	C14-C15-C16-C17
16	g	505	CLA	C5-C6-C7-C8
16	H	1123	CLA	C4-C3-C5-C6
16	X	509	CLA	C4-C3-C5-C6
16	a	1103	CLA	C4-C3-C5-C6
16	h	512	CLA	C4-C3-C5-C6
16	u	512	CLA	C4-C3-C5-C6
16	v	509	CLA	C4-C3-C5-C6
16	w	512	CLA	C4-C3-C5-C6
16	t	514	CLA	CAA-CBA-CGA-O2A
16	B	1210	CLA	C2-C3-C5-C6
16	L	1501	CLA	C2-C3-C5-C6
16	b	1210	CLA	C2-C3-C5-C6
16	h	512	CLA	C2-C3-C5-C6
16	v	512	CLA	C2-C3-C5-C6
16	y	512	CLA	C2-C3-C5-C6
20	H	4202	LMT	C1-C2-C3-C4
16	A	1126	CLA	C3-C5-C6-C7
16	o	510	CLA	C3-C5-C6-C7
16	t	506	CLA	C3-C5-C6-C7
17	B	2002	PQN	C13-C15-C16-C17
16	a	1106	CLA	O1D-CGD-O2D-CED
16	W	510	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	H	1114	CLA	C4C-C3C-CAC-CBC
16	Z	516	CLA	O1D-CGD-O2D-CED
16	B	1238	CLA	C16-C17-C18-C19
16	L	1503	CLA	C16-C17-C18-C19
13	I	103	LHG	O9-C7-O7-C5
13	G	4018	LHG	O6-C4-C5-O7
13	a	849	LHG	O6-C4-C5-O7
13	b	4018	LHG	O6-C4-C5-O7
13	g	605	LHG	O6-C4-C5-O7
13	u	605	LHG	O6-C4-C5-O7
16	r	502	CLA	O1A-CGA-O2A-C1
16	Z	503	CLA	C2C-C3C-CAC-CBC
13	a	849	LHG	C32-C33-C34-C35
16	H	1109	CLA	C2B-C3B-CAB-CBB
16	Y	503	CLA	C2B-C3B-CAB-CBB
16	q	508	CLA	C2B-C3B-CAB-CBB
16	s	503	CLA	C2B-C3B-CAB-CBB
16	t	512	CLA	C2B-C3B-CAB-CBB
16	u	503	CLA	C2B-C3B-CAB-CBB
16	w	502	CLA	C2B-C3B-CAB-CBB
19	A	4002	BCR	C1-C6-C7-C8
19	A	4002	BCR	C23-C24-C25-C30
19	A	4007	BCR	C1-C6-C7-C8
19	A	4007	BCR	C23-C24-C25-C30
19	B	4004	BCR	C1-C6-C7-C8
19	B	4004	BCR	C23-C24-C25-C30
19	B	4005	BCR	C1-C6-C7-C8
19	B	4010	BCR	C1-C6-C7-C8
19	B	4014	BCR	C23-C24-C25-C30
19	B	4017	BCR	C1-C6-C7-C8
19	B	4017	BCR	C23-C24-C25-C30
19	F	4016	BCR	C1-C6-C7-C8
19	G	4004	BCR	C1-C6-C7-C8
19	G	4005	BCR	C1-C6-C7-C8
19	G	4009	BCR	C23-C24-C25-C30
19	G	4014	BCR	C1-C6-C7-C8
19	G	4014	BCR	C23-C24-C25-C30
19	G	4017	BCR	C1-C6-C7-C8
19	G	4017	BCR	C23-C24-C25-C30
19	H	4002	BCR	C23-C24-C25-C30
19	H	4003	BCR	C1-C6-C7-C8
19	H	4007	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	H	4007	BCR	C23-C24-C25-C30
19	H	4008	BCR	C1-C6-C7-C8
19	H	4008	BCR	C23-C24-C25-C30
19	I	4018	BCR	C1-C6-C7-C8
19	J	4015	BCR	C23-C24-C25-C30
19	K	4001	BCR	C1-C6-C7-C8
19	K	4005	BCR	C23-C24-C25-C30
19	L	4019	BCR	C1-C6-C7-C8
19	L	4022	BCR	C1-C6-C7-C8
19	Q	4016	BCR	C1-C6-C7-C8
19	Q	4016	BCR	C23-C24-C25-C30
19	S	4012	BCR	C1-C6-C7-C8
19	S	4012	BCR	C23-C24-C25-C30
19	S	4015	BCR	C1-C6-C7-C8
19	S	4015	BCR	C23-C24-C25-C30
19	T	4001	BCR	C23-C24-C25-C30
19	T	4005	BCR	C1-C6-C7-C8
19	T	4005	BCR	C23-C24-C25-C30
19	U	4019	BCR	C1-C6-C7-C8
19	U	4022	BCR	C23-C24-C25-C30
19	W	603	BCR	C23-C24-C25-C30
19	W	604	BCR	C1-C6-C7-C8
19	X	602	BCR	C1-C6-C7-C8
19	X	603	BCR	C1-C6-C7-C8
19	X	603	BCR	C5-C6-C7-C8
19	X	603	BCR	C23-C24-C25-C30
19	X	604	BCR	C1-C6-C7-C8
19	X	604	BCR	C23-C24-C25-C30
19	Y	601	BCR	C1-C6-C7-C8
19	Y	602	BCR	C23-C24-C25-C30
19	Y	603	BCR	C1-C6-C7-C8
19	Z	602	BCR	C1-C6-C7-C8
19	Z	603	BCR	C1-C6-C7-C8
19	Z	603	BCR	C23-C24-C25-C30
19	Z	604	BCR	C1-C6-C7-C8
19	Z	604	BCR	C23-C24-C25-C30
19	a	4007	BCR	C1-C6-C7-C8
19	a	4007	BCR	C23-C24-C25-C30
19	a	4008	BCR	C1-C6-C7-C8
19	b	4004	BCR	C1-C6-C7-C8
19	b	4004	BCR	C23-C24-C25-C30
19	b	4005	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	b	4009	BCR	C23-C24-C25-C30
19	b	4010	BCR	C1-C6-C7-C8
19	b	4017	BCR	C1-C6-C7-C8
19	f	4016	BCR	C1-C6-C7-C8
19	g	601	BCR	C23-C24-C25-C30
19	g	602	BCR	C1-C6-C7-C8
19	g	603	BCR	C23-C24-C25-C30
19	g	604	BCR	C1-C6-C7-C8
19	g	604	BCR	C23-C24-C25-C26
19	h	603	BCR	C1-C6-C7-C8
19	h	604	BCR	C1-C6-C7-C8
19	j	4013	BCR	C23-C24-C25-C30
19	j	4015	BCR	C1-C6-C7-C8
19	j	4015	BCR	C23-C24-C25-C30
19	k	4001	BCR	C1-C6-C7-C8
19	k	4001	BCR	C23-C24-C25-C30
19	k	4005	BCR	C23-C24-C25-C30
19	l	4019	BCR	C1-C6-C7-C8
19	l	4019	BCR	C23-C24-C25-C26
19	l	4019	BCR	C23-C24-C25-C30
19	l	4022	BCR	C23-C24-C25-C30
19	n	601	BCR	C1-C6-C7-C8
19	n	601	BCR	C23-C24-C25-C30
19	n	603	BCR	C1-C6-C7-C8
19	n	603	BCR	C23-C24-C25-C30
19	n	604	BCR	C1-C6-C7-C8
19	o	601	BCR	C1-C6-C7-C8
19	o	602	BCR	C1-C6-C7-C8
19	o	602	BCR	C23-C24-C25-C30
19	o	603	BCR	C1-C6-C7-C8
19	o	603	BCR	C23-C24-C25-C30
19	p	602	BCR	C23-C24-C25-C30
19	p	603	BCR	C1-C6-C7-C8
19	p	603	BCR	C23-C24-C25-C30
19	q	602	BCR	C1-C6-C7-C8
19	q	603	BCR	C1-C6-C7-C8
19	q	603	BCR	C23-C24-C25-C30
19	q	604	BCR	C23-C24-C25-C30
19	r	601	BCR	C1-C6-C7-C8
19	r	602	BCR	C1-C6-C7-C8
19	r	603	BCR	C23-C24-C25-C30
19	r	604	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	r	604	BCR	C23-C24-C25-C30
19	s	601	BCR	C1-C6-C7-C8
19	s	601	BCR	C5-C6-C7-C8
19	s	602	BCR	C1-C6-C7-C8
19	s	602	BCR	C23-C24-C25-C30
19	s	603	BCR	C1-C6-C7-C8
19	s	603	BCR	C23-C24-C25-C30
19	t	601	BCR	C1-C6-C7-C8
19	t	601	BCR	C23-C24-C25-C30
19	t	603	BCR	C23-C24-C25-C30
19	t	604	BCR	C1-C6-C7-C8
19	u	601	BCR	C1-C6-C7-C8
19	u	602	BCR	C1-C6-C7-C8
19	u	602	BCR	C23-C24-C25-C30
19	u	603	BCR	C1-C6-C7-C8
19	u	603	BCR	C23-C24-C25-C30
19	v	601	BCR	C1-C6-C7-C8
19	v	603	BCR	C1-C6-C7-C8
19	v	604	BCR	C1-C6-C7-C8
19	w	602	BCR	C1-C6-C7-C8
19	w	603	BCR	C23-C24-C25-C30
19	w	604	BCR	C23-C24-C25-C30
19	x	601	BCR	C1-C6-C7-C8
19	x	601	BCR	C23-C24-C25-C30
19	x	602	BCR	C1-C6-C7-C8
19	x	603	BCR	C23-C24-C25-C30
19	x	604	BCR	C23-C24-C25-C30
19	y	603	BCR	C23-C24-C25-C30
19	y	604	BCR	C1-C6-C7-C8
21	B	4006	ECH	C23-C24-C25-C30
21	M	4021	ECH	C1-C6-C7-C8
21	b	4006	ECH	C23-C24-C25-C30
21	m	4021	ECH	C1-C6-C7-C8
23	g	606	LMU	C6-C7-C8-C9
16	H	1106	CLA	O1D-CGD-O2D-CED
13	p	605	LHG	C5-C4-O6-P
14	H	4101	LMG	C33-C34-C35-C36
16	Y	516	CLA	CBA-CGA-O2A-C1
16	B	1222	CLA	O1A-CGA-O2A-C1
16	k	4004	CLA	C5-C6-C7-C8
16	u	512	CLA	C8-C10-C11-C12
16	v	510	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	b	1238	CLA	O1D-CGD-O2D-CED
23	g	606	LMU	C4-C5-C6-C7
16	g	516	CLA	O1A-CGA-O2A-C1
16	W	509	CLA	C2A-CAA-CBA-CGA
16	b	1219	CLA	C2A-CAA-CBA-CGA
16	p	516	CLA	C2A-CAA-CBA-CGA
16	A	1132	CLA	C15-C16-C17-C18
16	H	1104	CLA	C10-C11-C12-C13
16	H	1106	CLA	C10-C11-C12-C13
16	Z	512	CLA	C10-C11-C12-C13
16	a	1103	CLA	C10-C11-C12-C13
16	a	1136	CLA	C8-C10-C11-C12
16	s	506	CLA	C8-C10-C11-C12
17	A	2001	PQN	C25-C26-C27-C28
13	A	851	LHG	O7-C5-C6-O8
13	X	605	LHG	O7-C5-C6-O8
13	g	605	LHG	O7-C5-C6-O8
13	s	605	LHG	C27-C28-C29-C30
16	o	515	CLA	C3-C5-C6-C7
16	W	506	CLA	O1D-CGD-O2D-CED
19	G	4004	BCR	C10-C11-C12-C13
19	G	4010	BCR	C10-C11-C12-C13
19	L	4022	BCR	C10-C11-C12-C13
19	Z	603	BCR	C18-C19-C20-C21
19	p	602	BCR	C10-C11-C12-C13
16	a	1132	CLA	C13-C15-C16-C17
16	b	1206	CLA	C15-C16-C17-C18
16	G	1214	CLA	C2-C3-C5-C6
16	a	1101	CLA	C2-C3-C5-C6
16	b	1223	CLA	C2-C3-C5-C6
16	u	512	CLA	C2-C3-C5-C6
16	w	512	CLA	C2-C3-C5-C6
14	A	4101	LMG	C18-C19-C20-C21
16	W	517	CLA	C6-C7-C8-C9
16	X	508	CLA	C6-C7-C8-C9
16	a	1117	CLA	C16-C17-C18-C19
16	h	515	CLA	C16-C17-C18-C19
13	B	4018	LHG	C9-C10-C11-C12
14	a	4101	LMG	C34-C35-C36-C37
16	W	512	CLA	C10-C11-C12-C13
16	A	1119	CLA	C14-C13-C15-C16
16	B	1210	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	G	1202	CLA	C6-C7-C8-C9
16	G	1204	CLA	C14-C13-C15-C16
16	H	1101	CLA	C6-C7-C8-C9
16	H	1106	CLA	C6-C7-C8-C9
16	H	1109	CLA	C11-C12-C13-C14
16	H	1126	CLA	C6-C7-C8-C9
16	H	1130	CLA	C11-C10-C8-C9
16	Y	510	CLA	C11-C12-C13-C14
16	Z	504	CLA	C11-C10-C8-C9
16	a	1130	CLA	C11-C10-C8-C9
16	b	1203	CLA	C14-C13-C15-C16
16	g	504	CLA	C11-C12-C13-C14
16	l	1503	CLA	C11-C10-C8-C9
16	q	510	CLA	C6-C7-C8-C9
16	s	510	CLA	C11-C12-C13-C14
16	v	505	CLA	C11-C12-C13-C14
16	v	506	CLA	C11-C10-C8-C9
16	v	509	CLA	C6-C7-C8-C9
14	B	848	LMG	O6-C1-O1-C7
19	G	4017	BCR	C22-C23-C24-C25
19	H	4008	BCR	C6-C7-C8-C9
19	L	4019	BCR	C6-C7-C8-C9
19	L	4022	BCR	C6-C7-C8-C9
19	T	4001	BCR	C6-C7-C8-C9
19	b	4004	BCR	C22-C23-C24-C25
19	h	601	BCR	C6-C7-C8-C9
19	n	604	BCR	C6-C7-C8-C9
19	t	604	BCR	C6-C7-C8-C9
19	u	602	BCR	C6-C7-C8-C9
19	x	602	BCR	C22-C23-C24-C25
16	G	1227	CLA	CBD-CGD-O2D-CED
16	s	514	CLA	O1A-CGA-O2A-C1
16	G	1210	CLA	C4C-C3C-CAC-CBC
16	B	1214	CLA	O1D-CGD-O2D-CED
16	q	512	CLA	C15-C16-C17-C18
19	j	4015	BCR	C14-C15-C16-C17
19	r	602	BCR	C14-C15-C16-C17
19	u	604	BCR	C14-C15-C16-C17
16	L	1503	CLA	C16-C17-C18-C20
16	b	1226	CLA	C11-C12-C13-C15
16	B	1239	CLA	C3-C5-C6-C7
16	n	515	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	q	515	CLA	C3-C5-C6-C7
16	u	515	CLA	C3-C5-C6-C7
16	A	1104	CLA	CBA-CGA-O2A-C1
13	p	605	LHG	C11-C10-C9-C8
14	A	4101	LMG	C2-C1-O1-C7
14	H	4101	LMG	C2-C1-O1-C7
16	G	1227	CLA	O2A-C1-C2-C3
16	b	1227	CLA	O2A-C1-C2-C3
16	a	1123	CLA	CBD-CGD-O2D-CED
13	a	851	LHG	C11-C10-C9-C8
16	a	1022	CLA	C4C-C3C-CAC-CBC
16	h	511	CLA	C2C-C3C-CAC-CBC
16	q	510	CLA	C5-C6-C7-C8
16	s	509	CLA	O1D-CGD-O2D-CED
16	p	511	CLA	O1A-CGA-O2A-C1
16	x	507	CLA	C5-C6-C7-C8
13	x	605	LHG	O1-C1-C2-O2
14	B	848	LMG	C29-C28-O8-C9
16	H	1103	CLA	CBA-CGA-O2A-C1
19	X	604	BCR	C13-C14-C15-C16
19	a	4007	BCR	C19-C20-C21-C22
19	h	601	BCR	C9-C10-C11-C12
15	a	1011	CL0	CAA-CBA-CGA-O2A
16	r	503	CLA	CAA-CBA-CGA-O2A
13	Y	605	LHG	C27-C28-C29-C30
16	B	1223	CLA	C2-C3-C5-C6
16	G	1204	CLA	C2-C3-C5-C6
16	H	1123	CLA	C2-C3-C5-C6
16	a	1103	CLA	C2-C3-C5-C6
16	v	509	CLA	C2-C3-C5-C6
16	y	517	CLA	C2-C3-C5-C6
14	G	848	LMG	O6-C5-C6-O5
16	H	1138	CLA	C8-C10-C11-C12
16	Z	511	CLA	C4C-C3C-CAC-CBC
16	G	1220	CLA	C2C-C3C-CAC-CBC
16	X	502	CLA	O1D-CGD-O2D-CED
16	H	1138	CLA	C10-C11-C12-C13
16	u	516	CLA	O1A-CGA-O2A-C1
13	I	103	LHG	C1-C2-C3-O3
19	G	4009	BCR	C16-C17-C18-C36
19	H	4007	BCR	C16-C17-C18-C36
19	J	4012	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
19	K	4005	BCR	C16-C17-C18-C36
19	L	4019	BCR	C20-C21-C22-C37
19	Q	4016	BCR	C11-C10-C9-C34
19	U	4022	BCR	C16-C17-C18-C36
19	a	4011	BCR	C16-C17-C18-C36
19	g	601	BCR	C11-C10-C9-C34
19	j	4013	BCR	C35-C13-C14-C15
19	j	4013	BCR	C20-C21-C22-C37
19	q	604	BCR	C16-C17-C18-C36
19	s	604	BCR	C16-C17-C18-C36
19	t	601	BCR	C16-C17-C18-C36
19	y	601	BCR	C35-C13-C14-C15
16	H	1109	CLA	C3-C5-C6-C7
16	y	515	CLA	C3-C5-C6-C7
16	a	1140	CLA	C8-C10-C11-C12
16	b	1211	CLA	C8-C10-C11-C12
14	a	4101	LMG	C13-C14-C15-C16
13	g	605	LHG	O6-C4-C5-C6
13	u	605	LHG	O6-C4-C5-C6
16	v	504	CLA	C8-C10-C11-C12
19	G	4017	BCR	C7-C8-C9-C34
19	S	4015	BCR	C11-C12-C13-C35
19	n	601	BCR	C11-C12-C13-C35
19	o	602	BCR	C37-C22-C23-C24
13	Y	605	LHG	C11-C10-C9-C8
16	a	1114	CLA	CBA-CGA-O2A-C1
16	A	1106	CLA	C6-C7-C8-C10
16	A	1125	CLA	C12-C13-C15-C16
16	A	1128	CLA	C12-C13-C15-C16
16	A	1130	CLA	C11-C10-C8-C7
16	A	1131	CLA	C12-C13-C15-C16
16	B	1021	CLA	C11-C12-C13-C15
16	B	1021	CLA	C12-C13-C15-C16
16	B	1210	CLA	C6-C7-C8-C10
16	B	1211	CLA	C12-C13-C15-C16
16	G	1021	CLA	C11-C12-C13-C15
16	G	1021	CLA	C12-C13-C15-C16
16	G	1203	CLA	C12-C13-C15-C16
16	G	1206	CLA	C11-C10-C8-C7
16	G	1210	CLA	C6-C7-C8-C10
16	H	1103	CLA	C11-C10-C8-C7
16	H	1104	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
16	H	1126	CLA	C6-C7-C8-C10
16	H	1128	CLA	C12-C13-C15-C16
16	H	1140	CLA	C6-C7-C8-C10
16	U	1501	CLA	C11-C10-C8-C7
16	U	1502	CLA	C6-C7-C8-C10
16	U	1503	CLA	C12-C13-C15-C16
16	Y	507	CLA	C11-C10-C8-C7
16	Y	512	CLA	C11-C12-C13-C15
16	a	1101	CLA	C11-C10-C8-C7
16	a	1106	CLA	C6-C7-C8-C10
16	a	1109	CLA	C11-C12-C13-C15
16	b	1021	CLA	C11-C12-C13-C15
16	b	1021	CLA	C12-C13-C15-C16
16	b	1206	CLA	C6-C7-C8-C10
16	g	504	CLA	C11-C12-C13-C15
16	h	505	CLA	C11-C12-C13-C15
16	h	507	CLA	C6-C7-C8-C10
16	l	1502	CLA	C6-C7-C8-C10
16	o	510	CLA	C11-C10-C8-C7
16	p	509	CLA	C11-C10-C8-C7
16	p	510	CLA	C11-C12-C13-C15
16	q	515	CLA	C11-C12-C13-C15
16	r	504	CLA	C11-C12-C13-C15
16	w	504	CLA	C11-C10-C8-C7
16	w	510	CLA	C6-C7-C8-C10
16	w	511	CLA	C6-C7-C8-C10
14	a	4101	LMG	C17-C18-C19-C20
16	w	501	CLA	CBD-CGD-O2D-CED
16	X	515	CLA	C13-C15-C16-C17
16	b	1223	CLA	C8-C10-C11-C12
16	s	511	CLA	C13-C15-C16-C17
19	T	4005	BCR	C21-C22-C23-C24
19	W	603	BCR	C11-C12-C13-C14
19	g	603	BCR	C11-C12-C13-C14
19	o	602	BCR	C17-C18-C19-C20
19	p	604	BCR	C11-C12-C13-C14
19	r	603	BCR	C7-C8-C9-C10
19	r	603	BCR	C11-C12-C13-C14
19	u	602	BCR	C7-C8-C9-C10
19	w	603	BCR	C11-C12-C13-C14
19	w	604	BCR	C7-C8-C9-C10
19	y	601	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	R	4020	ECH	C21-C22-C23-C24
21	i	4020	ECH	C17-C18-C19-C20
16	G	1221	CLA	CBA-CGA-O2A-C1
16	n	502	CLA	CBA-CGA-O2A-C1
16	t	507	CLA	CBA-CGA-O2A-C1
16	W	513	CLA	O1A-CGA-O2A-C1
16	Z	505	CLA	O1A-CGA-O2A-C1
16	u	517	CLA	O1A-CGA-O2A-C1
16	W	506	CLA	C4C-C3C-CAC-CBC
16	r	505	CLA	C8-C10-C11-C12
17	B	2002	PQN	C25-C26-C27-C28
16	A	1120	CLA	C2A-CAA-CBA-CGA
16	W	516	CLA	C2A-CAA-CBA-CGA
16	Y	505	CLA	C2A-CAA-CBA-CGA
16	Z	513	CLA	C2A-CAA-CBA-CGA
16	a	1122	CLA	C2A-CAA-CBA-CGA
16	A	1124	CLA	C11-C12-C13-C14
16	X	508	CLA	C6-C7-C8-C10
16	x	504	CLA	C16-C17-C18-C20
16	a	1112	CLA	O1D-CGD-O2D-CED
14	f	4017	LMG	O9-C10-O7-C8
13	s	605	LHG	C11-C10-C9-C8
16	A	1115	CLA	C4-C3-C5-C6
16	G	1210	CLA	C4-C3-C5-C6
16	H	1101	CLA	C4-C3-C5-C6
16	U	1501	CLA	C4-C3-C5-C6
16	X	515	CLA	C4-C3-C5-C6
16	a	1104	CLA	C4-C3-C5-C6
16	A	1104	CLA	O1A-CGA-O2A-C1
16	A	1116	CLA	O1A-CGA-O2A-C1
16	a	1106	CLA	O1A-CGA-O2A-C1
16	n	504	CLA	O1A-CGA-O2A-C1
16	x	504	CLA	C2-C3-C5-C6
16	X	509	CLA	C10-C11-C12-C13
16	n	505	CLA	C8-C10-C11-C12
14	H	4201	LMG	C28-C29-C30-C31
16	p	505	CLA	C3-C5-C6-C7
13	i	103	LHG	C10-C11-C12-C13
16	G	1217	CLA	CBD-CGD-O2D-CED
13	r	605	LHG	O10-C23-O8-C6
16	H	1110	CLA	O1A-CGA-O2A-C1
13	a	849	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
16	w	507	CLA	C5-C6-C7-C8
19	h	604	BCR	C19-C20-C21-C22
19	j	4015	BCR	C9-C10-C11-C12
19	w	602	BCR	C15-C16-C17-C18
19	a	4003	BCR	C14-C15-C16-C17
19	w	602	BCR	C14-C15-C16-C17
13	I	103	LHG	C10-C11-C12-C13
14	A	4101	LMG	C34-C35-C36-C37
16	H	1101	CLA	C16-C17-C18-C19
16	W	517	CLA	C6-C7-C8-C10
16	H	1013	CLA	O1A-CGA-O2A-C1
16	Y	511	CLA	O1A-CGA-O2A-C1
16	v	509	CLA	O1A-CGA-O2A-C1
16	B	1207	CLA	C13-C15-C16-C17
16	G	1239	CLA	C8-C10-C11-C12
16	a	1102	CLA	C5-C6-C7-C8
16	p	512	CLA	C8-C10-C11-C12
16	t	505	CLA	C10-C11-C12-C13
13	i	103	LHG	C25-C26-C27-C28
19	X	601	BCR	C20-C21-C22-C23
19	l	4022	BCR	C20-C21-C22-C23
19	s	601	BCR	C16-C17-C18-C19
16	a	1117	CLA	C8-C10-C11-C12
16	q	505	CLA	C5-C6-C7-C8
13	A	849	LHG	O6-C4-C5-O7
16	B	1227	CLA	O2A-C1-C2-C3
13	s	605	LHG	C4-C5-C6-O8
14	a	4101	LMG	O1-C7-C8-C9
14	b	848	LMG	O1-C7-C8-C9
16	H	1103	CLA	C10-C11-C12-C13
16	r	507	CLA	C5-C6-C7-C8
16	G	1202	CLA	C16-C17-C18-C19
16	a	1139	CLA	C6-C7-C8-C10
16	H	1125	CLA	C3-C5-C6-C7
16	w	515	CLA	C3-C5-C6-C7
16	A	1013	CLA	O1A-CGA-O2A-C1
16	A	1102	CLA	C5-C6-C7-C8
16	H	1110	CLA	C4-C3-C5-C6
16	o	512	CLA	C4-C3-C5-C6
16	A	1129	CLA	C2A-CAA-CBA-CGA
16	B	1213	CLA	C2A-CAA-CBA-CGA
16	F	1302	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	S	1302	CLA	C2A-CAA-CBA-CGA
16	X	509	CLA	C2A-CAA-CBA-CGA
16	a	1107	CLA	C2A-CAA-CBA-CGA
16	p	505	CLA	C2A-CAA-CBA-CGA
16	X	508	CLA	C2-C3-C5-C6
16	h	507	CLA	C2-C3-C5-C6
13	G	4018	LHG	C16-C17-C18-C19
13	H	849	LHG	C10-C11-C12-C13
16	B	1222	CLA	O1D-CGD-O2D-CED
16	G	1206	CLA	C5-C6-C7-C8
16	W	505	CLA	C8-C10-C11-C12
16	W	509	CLA	C10-C11-C12-C13
16	a	1132	CLA	C15-C16-C17-C18
16	p	505	CLA	C8-C10-C11-C12
16	v	512	CLA	C8-C10-C11-C12
13	i	103	LHG	O7-C5-C6-O8
13	r	605	LHG	O7-C5-C6-O8
14	H	4101	LMG	O7-C8-C9-O8
14	a	4101	LMG	O7-C8-C9-O8
14	b	848	LMG	O1-C7-C8-O7
16	B	1226	CLA	C8-C10-C11-C12
16	H	1132	CLA	C8-C10-C11-C12
16	A	1125	CLA	C14-C13-C15-C16
16	G	1021	CLA	C11-C12-C13-C14
16	G	1021	CLA	C14-C13-C15-C16
16	G	1206	CLA	C11-C10-C8-C9
16	G	1210	CLA	C6-C7-C8-C9
16	Z	507	CLA	C6-C7-C8-C9
16	a	1013	CLA	C11-C10-C8-C9
16	a	1109	CLA	C11-C12-C13-C14
16	n	505	CLA	C14-C13-C15-C16
16	o	510	CLA	C11-C10-C8-C9
16	p	509	CLA	C11-C10-C8-C9
16	p	510	CLA	C11-C12-C13-C14
16	r	504	CLA	C11-C12-C13-C14
16	w	510	CLA	C6-C7-C8-C9
16	w	511	CLA	C6-C7-C8-C9
16	y	506	CLA	C11-C10-C8-C9
16	y	509	CLA	C6-C7-C8-C9
16	Z	509	CLA	C16-C17-C18-C20
16	Z	512	CLA	C16-C17-C18-C19
16	W	514	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	q	508	CLA	CAA-CBA-CGA-O2A
16	t	507	CLA	O1A-CGA-O2A-C1
16	H	1117	CLA	C15-C16-C17-C18
16	b	1221	CLA	C8-C10-C11-C12
16	v	516	CLA	CBD-CGD-O2D-CED
14	A	4101	LMG	C33-C34-C35-C36
16	G	1211	CLA	C13-C15-C16-C17
16	a	1126	CLA	C8-C10-C11-C12
16	b	1226	CLA	C8-C10-C11-C12
16	u	511	CLA	C8-C10-C11-C12
16	b	1238	CLA	C3-C5-C6-C7
14	b	848	LMG	C31-C32-C33-C34
16	a	1119	CLA	O1D-CGD-O2D-CED
16	b	1220	CLA	C2-C1-O2A-CGA
19	Y	602	BCR	C13-C14-C15-C16
19	p	602	BCR	C13-C14-C15-C16
23	r	606	LMU	C2'-C1'-O1'-C1
16	H	1116	CLA	CBA-CGA-O2A-C1
15	H	1011	CL0	C16-C17-C18-C19
16	a	1237	CLA	C16-C17-C18-C20
16	b	1221	CLA	C16-C17-C18-C20
16	A	1136	CLA	C8-C10-C11-C12
16	q	509	CLA	C13-C15-C16-C17
16	t	511	CLA	C10-C11-C12-C13
16	a	1105	CLA	O1D-CGD-O2D-CED
16	y	509	CLA	C4C-C3C-CAC-CBC
16	A	1118	CLA	C4-C3-C5-C6
16	G	1224	CLA	C4-C3-C5-C6
16	v	508	CLA	C4-C3-C5-C6
16	y	508	CLA	C4-C3-C5-C6
16	B	1229	CLA	C2C-C3C-CAC-CBC
16	t	515	CLA	C3-C5-C6-C7
16	G	1210	CLA	C2-C3-C5-C6
16	G	1213	CLA	C2-C3-C5-C6
13	R	103	LHG	C1-C2-C3-O3
16	H	1130	CLA	C10-C11-C12-C13
16	Z	509	CLA	C15-C16-C17-C18
16	q	509	CLA	C15-C16-C17-C18
16	x	505	CLA	C8-C10-C11-C12
13	i	103	LHG	C31-C32-C33-C34
16	Q	1302	CLA	C2A-CAA-CBA-CGA
16	y	513	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	Y	510	CLA	O1D-CGD-O2D-CED
13	H	849	LHG	O10-C23-O8-C6
16	G	1221	CLA	O1A-CGA-O2A-C1
16	H	1103	CLA	O1A-CGA-O2A-C1
16	n	502	CLA	O1A-CGA-O2A-C1
13	b	4018	LHG	C11-C12-C13-C14
16	A	1123	CLA	C5-C6-C7-C8
16	b	1225	CLA	C13-C15-C16-C17
16	B	1214	CLA	C3-C5-C6-C7
16	W	506	CLA	C3-C5-C6-C7
16	w	512	CLA	C8-C10-C11-C12
13	A	849	LHG	C32-C33-C34-C35
16	h	517	CLA	O1D-CGD-O2D-CED
16	B	1224	CLA	C11-C12-C13-C15
16	G	1221	CLA	C16-C17-C18-C20
16	g	504	CLA	C16-C17-C18-C20
16	t	517	CLA	C6-C7-C8-C9
14	A	4201	LMG	C4-C5-C6-O5
19	Z	602	BCR	C36-C18-C19-C20
16	A	1139	CLA	C1A-C2A-CAA-CBA
16	A	1801	CLA	C1A-C2A-CAA-CBA
16	B	1023	CLA	C1A-C2A-CAA-CBA
16	B	1227	CLA	C1A-C2A-CAA-CBA
16	G	1021	CLA	C4B-C3B-CAB-CBB
16	G	1023	CLA	C1A-C2A-CAA-CBA
16	G	1234	CLA	C1A-C2A-CAA-CBA
16	H	1123	CLA	C1A-C2A-CAA-CBA
16	H	1129	CLA	O1A-CGA-O2A-C1
16	H	1131	CLA	C4B-C3B-CAB-CBB
16	H	1139	CLA	C1A-C2A-CAA-CBA
16	K	4004	CLA	C1A-C2A-CAA-CBA
16	W	505	CLA	C1A-C2A-CAA-CBA
16	W	514	CLA	C1A-C2A-CAA-CBA
16	Y	505	CLA	C1A-C2A-CAA-CBA
16	Z	514	CLA	C1A-C2A-CAA-CBA
16	a	1116	CLA	C4B-C3B-CAB-CBB
16	a	1120	CLA	C1A-C2A-CAA-CBA
16	a	1122	CLA	C1A-C2A-CAA-CBA
16	a	1123	CLA	C1A-C2A-CAA-CBA
16	a	1131	CLA	C4B-C3B-CAB-CBB
16	b	1234	CLA	C1A-C2A-CAA-CBA
16	g	506	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	g	515	CLA	C1A-C2A-CAA-CBA
16	h	507	CLA	C1A-C2A-CAA-CBA
16	p	503	CLA	C1A-C2A-CAA-CBA
16	r	516	CLA	C1A-C2A-CAA-CBA
16	s	505	CLA	C1A-C2A-CAA-CBA
16	t	511	CLA	C1A-C2A-CAA-CBA
16	v	501	CLA	O1A-CGA-O2A-C1
16	y	503	CLA	C1A-C2A-CAA-CBA
16	y	507	CLA	C1A-C2A-CAA-CBA
16	Y	516	CLA	O1D-CGD-O2D-CED
16	g	503	CLA	O1D-CGD-O2D-CED
16	n	515	CLA	O1D-CGD-O2D-CED
16	t	502	CLA	O1D-CGD-O2D-CED
13	B	4018	LHG	C18-C19-C20-C21
13	A	851	LHG	C9-C10-C11-C12
19	K	4005	BCR	C6-C7-C8-C9
19	k	4001	BCR	C6-C7-C8-C9
19	l	4019	BCR	C6-C7-C8-C9
16	n	514	CLA	CAA-CBA-CGA-O2A
16	U	1501	CLA	C2-C3-C5-C6
16	a	1013	CLA	C2-C3-C5-C6
16	o	512	CLA	C2-C3-C5-C6
19	U	4019	BCR	C11-C12-C13-C14
19	x	604	BCR	C7-C8-C9-C10
16	B	1238	CLA	C16-C17-C18-C20
16	l	1501	CLA	C11-C12-C13-C14
16	H	1118	CLA	C3-C5-C6-C7
16	h	512	CLA	C15-C16-C17-C18
16	b	1213	CLA	C2A-CAA-CBA-CGA
16	g	503	CLA	C2A-CAA-CBA-CGA
16	v	503	CLA	C2A-CAA-CBA-CGA
16	u	504	CLA	C10-C11-C12-C13
13	H	849	LHG	O6-C4-C5-C6
13	a	849	LHG	O6-C4-C5-C6
16	G	1210	CLA	CBD-CGD-O2D-CED
16	x	516	CLA	CBA-CGA-O2A-C1
13	i	103	LHG	C32-C33-C34-C35
16	B	1207	CLA	C3-C5-C6-C7
16	A	1103	CLA	C11-C10-C8-C7
16	A	1109	CLA	C11-C12-C13-C15
16	A	1126	CLA	C6-C7-C8-C10
16	B	1206	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
16	B	1239	CLA	C12-C13-C15-C16
16	G	1239	CLA	C6-C7-C8-C10
16	H	1104	CLA	C11-C12-C13-C15
16	L	1502	CLA	C6-C7-C8-C10
16	W	504	CLA	C6-C7-C8-C10
16	W	507	CLA	C11-C10-C8-C7
16	X	507	CLA	C11-C10-C8-C7
16	X	510	CLA	C11-C10-C8-C7
16	Z	515	CLA	C11-C12-C13-C15
16	a	1103	CLA	C11-C10-C8-C7
16	a	1126	CLA	C6-C7-C8-C10
16	a	1128	CLA	C12-C13-C15-C16
16	a	1131	CLA	C12-C13-C15-C16
16	a	1138	CLA	C11-C10-C8-C7
16	a	1237	CLA	C11-C10-C8-C7
16	b	1204	CLA	C12-C13-C15-C16
16	b	1211	CLA	C12-C13-C15-C16
16	b	1239	CLA	C6-C7-C8-C10
16	g	507	CLA	C11-C10-C8-C7
16	h	504	CLA	C11-C10-C8-C7
16	h	511	CLA	C6-C7-C8-C10
16	l	1501	CLA	C11-C10-C8-C7
16	l	1503	CLA	C12-C13-C15-C16
16	n	507	CLA	C11-C10-C8-C7
16	n	510	CLA	C12-C13-C15-C16
16	o	505	CLA	C11-C10-C8-C7
16	o	507	CLA	C11-C10-C8-C7
16	p	507	CLA	C11-C10-C8-C7
16	p	511	CLA	C12-C13-C15-C16
16	p	512	CLA	C11-C12-C13-C15
16	q	504	CLA	C6-C7-C8-C10
16	q	507	CLA	C11-C10-C8-C7
16	q	512	CLA	C6-C7-C8-C10
16	r	504	CLA	C12-C13-C15-C16
16	r	507	CLA	C11-C10-C8-C7
16	r	510	CLA	C11-C12-C13-C15
16	s	507	CLA	C11-C10-C8-C7
16	s	512	CLA	C11-C12-C13-C15
16	s	515	CLA	C6-C7-C8-C10
16	t	504	CLA	C6-C7-C8-C10
16	t	507	CLA	C11-C10-C8-C7
16	t	511	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
16	v	506	CLA	C11-C10-C8-C7
16	w	504	CLA	C6-C7-C8-C10
16	w	507	CLA	C11-C10-C8-C7
16	w	515	CLA	C11-C12-C13-C15
16	x	504	CLA	C12-C13-C15-C16
16	x	506	CLA	C11-C10-C8-C7
16	x	510	CLA	C6-C7-C8-C10
16	y	509	CLA	C11-C12-C13-C15
17	a	2001	PQN	C16-C17-C18-C20
17	a	2001	PQN	C21-C22-C23-C25
16	b	1221	CLA	C16-C17-C18-C19
16	b	1226	CLA	C11-C12-C13-C14
16	q	507	CLA	C5-C6-C7-C8
16	A	1103	CLA	CBA-CGA-O2A-C1
16	A	1106	CLA	CBA-CGA-O2A-C1
16	H	1013	CLA	CBA-CGA-O2A-C1
16	X	511	CLA	CBA-CGA-O2A-C1
16	a	1103	CLA	CBA-CGA-O2A-C1
13	R	103	LHG	C10-C11-C12-C13
16	b	1205	CLA	CBD-CGD-O2D-CED
13	Y	605	LHG	C5-C4-O6-P
13	r	605	LHG	C2-C3-O3-P
16	G	1220	CLA	C3A-C2A-CAA-CBA
16	a	1118	CLA	C4-C3-C5-C6
16	p	503	CLA	C3A-C2A-CAA-CBA
16	w	503	CLA	C3A-C2A-CAA-CBA
16	y	504	CLA	C3A-C2A-CAA-CBA
16	H	1117	CLA	C16-C17-C18-C20
16	Z	512	CLA	C16-C17-C18-C20
16	o	508	CLA	C6-C7-C8-C9
16	r	506	CLA	C11-C12-C13-C14
16	H	1138	CLA	O1D-CGD-O2D-CED
13	I	103	LHG	C11-C10-C9-C8
13	H	849	LHG	O6-C4-C5-O7
13	X	605	LHG	O6-C4-C5-O7
13	o	605	LHG	O6-C4-C5-O7
13	x	605	LHG	O6-C4-C5-O7
13	i	103	LHG	C8-C7-O7-C5
16	b	1235	CLA	C2A-CAA-CBA-CGA
16	q	508	CLA	C2A-CAA-CBA-CGA
16	A	1104	CLA	C11-C10-C8-C9
16	A	1130	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	A	1131	CLA	C14-C13-C15-C16
16	B	1021	CLA	C11-C12-C13-C14
16	B	1021	CLA	C14-C13-C15-C16
16	B	1202	CLA	C11-C12-C13-C14
16	B	1211	CLA	C14-C13-C15-C16
16	B	1223	CLA	C11-C10-C8-C9
16	G	1023	CLA	C14-C13-C15-C16
16	G	1203	CLA	C14-C13-C15-C16
16	H	1103	CLA	C11-C10-C8-C9
16	H	1109	CLA	C6-C7-C8-C9
16	U	1501	CLA	C11-C10-C8-C9
16	U	1503	CLA	C11-C10-C8-C9
16	U	1503	CLA	C14-C13-C15-C16
16	a	1101	CLA	C11-C10-C8-C9
16	a	1131	CLA	C11-C10-C8-C9
16	b	1021	CLA	C11-C12-C13-C14
16	b	1021	CLA	C14-C13-C15-C16
16	g	504	CLA	C14-C13-C15-C16
16	g	510	CLA	C11-C12-C13-C14
16	h	505	CLA	C11-C12-C13-C14
16	l	1502	CLA	C6-C7-C8-C9
16	l	1503	CLA	C6-C7-C8-C9
16	n	512	CLA	C14-C13-C15-C16
16	q	515	CLA	C11-C12-C13-C14
16	r	506	CLA	C11-C10-C8-C9
16	s	515	CLA	C6-C7-C8-C9
16	w	504	CLA	C6-C7-C8-C9
19	A	4011	BCR	C9-C10-C11-C12
19	U	4022	BCR	C13-C14-C15-C16
19	W	604	BCR	C15-C16-C17-C18
19	g	601	BCR	C13-C14-C15-C16
19	h	601	BCR	C19-C20-C21-C22
19	q	602	BCR	C19-C20-C21-C22
19	r	601	BCR	C9-C10-C11-C12
19	s	602	BCR	C13-C14-C15-C16
19	t	601	BCR	C15-C16-C17-C18
21	M	4021	ECH	C13-C14-C15-C16
16	r	513	CLA	CBA-CGA-O2A-C1
16	t	506	CLA	O1D-CGD-O2D-CED
16	g	506	CLA	C5-C6-C7-C8
16	s	512	CLA	C15-C16-C17-C18
16	A	1120	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
16	B	1227	CLA	C1-C2-C3-C4
16	G	1227	CLA	C1-C2-C3-C4
16	H	1120	CLA	C1-C2-C3-C4
16	a	1120	CLA	C1-C2-C3-C4
16	b	1227	CLA	C1-C2-C3-C4
16	A	1138	CLA	C8-C10-C11-C12
13	H	851	LHG	O7-C5-C6-O8
14	G	848	LMG	O1-C7-C8-O7
16	G	1227	CLA	O1D-CGD-O2D-CED
14	b	848	LMG	C16-C17-C18-C19
16	a	1801	CLA	CBA-CGA-O2A-C1
16	h	501	CLA	CBA-CGA-O2A-C1
15	A	1011	CL0	C2C-C3C-CAC-CBC
14	H	4101	LMG	C18-C19-C20-C21
13	Y	605	LHG	C4-C5-C6-O8
13	i	103	LHG	C4-C5-C6-O8
14	G	848	LMG	C7-C8-C9-O8
16	n	515	CLA	C5-C6-C7-C8
16	v	509	CLA	CAA-CBA-CGA-O2A
16	G	1224	CLA	C2-C3-C5-C6
16	v	504	CLA	C2-C3-C5-C6
14	A	4201	LMG	O6-C5-C6-O5
16	G	1212	CLA	CBD-CGD-O2D-CED
16	A	1801	CLA	CAD-CBD-CGD-O2D
16	B	1012	CLA	CAD-CBD-CGD-O2D
16	B	1202	CLA	CAD-CBD-CGD-O2D
16	B	1210	CLA	CAD-CBD-CGD-O2D
16	B	1234	CLA	CAD-CBD-CGD-O2D
16	G	1012	CLA	CAD-CBD-CGD-O2D
16	H	1103	CLA	CAD-CBD-CGD-O2D
16	H	1111	CLA	CAD-CBD-CGD-O2D
16	W	503	CLA	CAD-CBD-CGD-O2D
16	W	510	CLA	CAD-CBD-CGD-O2D
16	W	516	CLA	CAD-CBD-CGD-O2D
16	X	503	CLA	CAD-CBD-CGD-O2D
16	X	510	CLA	CAD-CBD-CGD-O2D
16	Y	513	CLA	CAD-CBD-CGD-O2D
16	Y	516	CLA	CAD-CBD-CGD-O2D
16	Z	514	CLA	CAD-CBD-CGD-O2D
16	a	1103	CLA	CAD-CBD-CGD-O2D
16	a	1111	CLA	CAD-CBD-CGD-O2D
16	b	1012	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	b	1202	CLA	CAD-CBD-CGD-O2D
16	h	506	CLA	CAD-CBD-CGD-O2D
16	h	517	CLA	CAD-CBD-CGD-O2D
16	n	501	CLA	CAD-CBD-CGD-O2D
16	n	510	CLA	CAD-CBD-CGD-O2D
16	n	516	CLA	CAD-CBD-CGD-O2D
16	n	517	CLA	CAD-CBD-CGD-O2D
16	o	507	CLA	CAD-CBD-CGD-O2D
16	p	513	CLA	CAD-CBD-CGD-O2D
16	q	514	CLA	CAD-CBD-CGD-O2D
16	r	514	CLA	CAD-CBD-CGD-O2D
16	s	503	CLA	CAD-CBD-CGD-O2D
16	t	510	CLA	CAD-CBD-CGD-O2D
16	u	503	CLA	CAD-CBD-CGD-O2D
16	v	508	CLA	CAD-CBD-CGD-O2D
16	v	517	CLA	CAD-CBD-CGD-O2D
16	y	506	CLA	CAD-CBD-CGD-O2D
16	y	507	CLA	CAD-CBD-CGD-O2D
13	x	605	LHG	O10-C23-O8-C6
16	A	1103	CLA	O1A-CGA-O2A-C1
16	W	510	CLA	O1D-CGD-O2D-CED
14	G	848	LMG	C29-C28-O8-C9
16	H	1136	CLA	CBA-CGA-O2A-C1
16	t	504	CLA	CBA-CGA-O2A-C1
16	b	1238	CLA	C16-C17-C18-C19
16	B	1211	CLA	C2A-CAA-CBA-CGA
16	B	1231	CLA	C2A-CAA-CBA-CGA
16	h	512	CLA	C2A-CAA-CBA-CGA
16	h	513	CLA	C2A-CAA-CBA-CGA
16	t	509	CLA	C2A-CAA-CBA-CGA
16	w	508	CLA	C2A-CAA-CBA-CGA
16	G	1226	CLA	C5-C6-C7-C8
16	X	515	CLA	C15-C16-C17-C18
16	A	1106	CLA	O1A-CGA-O2A-C1
16	H	1116	CLA	O1A-CGA-O2A-C1
13	B	4018	LHG	C3-O3-P-O6
13	B	4018	LHG	C4-O6-P-O5
13	H	849	LHG	C3-O3-P-O5
13	R	103	LHG	C3-O3-P-O5
13	R	103	LHG	C4-O6-P-O3
13	Y	605	LHG	C3-O3-P-O5
13	Y	605	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
13	a	849	LHG	C3-O3-P-O5
13	g	605	LHG	C3-O3-P-O5
13	g	605	LHG	C4-O6-P-O4
13	i	103	LHG	C3-O3-P-O5
13	o	605	LHG	C3-O3-P-O5
13	o	605	LHG	C4-O6-P-O3
13	o	605	LHG	C4-O6-P-O5
13	p	605	LHG	C4-O6-P-O5
13	r	605	LHG	C3-O3-P-O6
13	s	605	LHG	C4-O6-P-O5
13	x	605	LHG	C3-O3-P-O4
13	x	605	LHG	C3-O3-P-O6
16	A	1104	CLA	CHA-CBD-CGD-O1D
16	A	1104	CLA	CHA-CBD-CGD-O2D
16	A	1801	CLA	CAD-CBD-CGD-O1D
16	B	1012	CLA	CAD-CBD-CGD-O1D
16	B	1202	CLA	CAD-CBD-CGD-O1D
16	B	1210	CLA	CAD-CBD-CGD-O1D
16	B	1212	CLA	CHA-CBD-CGD-O1D
16	B	1212	CLA	CHA-CBD-CGD-O2D
16	B	1227	CLA	CHA-CBD-CGD-O1D
16	B	1234	CLA	CAD-CBD-CGD-O1D
16	G	1012	CLA	CAD-CBD-CGD-O1D
16	G	1207	CLA	CHA-CBD-CGD-O1D
16	G	1207	CLA	CHA-CBD-CGD-O2D
16	G	1210	CLA	CAD-CBD-CGD-O1D
16	G	1218	CLA	CHA-CBD-CGD-O1D
16	G	1218	CLA	CHA-CBD-CGD-O2D
16	G	1227	CLA	CHA-CBD-CGD-O1D
16	G	1227	CLA	CHA-CBD-CGD-O2D
16	G	1234	CLA	CAD-CBD-CGD-O1D
16	H	1103	CLA	CAD-CBD-CGD-O1D
16	H	1104	CLA	CHA-CBD-CGD-O1D
16	H	1111	CLA	CAD-CBD-CGD-O1D
16	H	1135	CLA	CAD-CBD-CGD-O1D
16	T	4003	CLA	CHA-CBD-CGD-O1D
16	T	4003	CLA	CHA-CBD-CGD-O2D
16	W	503	CLA	CAD-CBD-CGD-O1D
16	W	505	CLA	CHA-CBD-CGD-O1D
16	W	507	CLA	CHA-CBD-CGD-O1D
16	W	507	CLA	CHA-CBD-CGD-O2D
16	W	510	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
16	W	515	CLA	CHA-CBD-CGD-O1D
16	W	515	CLA	CHA-CBD-CGD-O2D
16	W	516	CLA	CAD-CBD-CGD-O1D
16	X	503	CLA	CAD-CBD-CGD-O1D
16	X	510	CLA	CAD-CBD-CGD-O1D
16	Y	506	CLA	CHA-CBD-CGD-O1D
16	Y	506	CLA	CHA-CBD-CGD-O2D
16	Y	513	CLA	CAD-CBD-CGD-O1D
16	Y	515	CLA	CAD-CBD-CGD-O1D
16	Y	516	CLA	CAD-CBD-CGD-O1D
16	Z	514	CLA	CAD-CBD-CGD-O1D
16	a	1103	CLA	CAD-CBD-CGD-O1D
16	a	1104	CLA	CHA-CBD-CGD-O1D
16	a	1104	CLA	CHA-CBD-CGD-O2D
16	a	1111	CLA	CAD-CBD-CGD-O1D
16	a	1114	CLA	CHA-CBD-CGD-O1D
16	a	1114	CLA	CHA-CBD-CGD-O2D
16	b	1012	CLA	CAD-CBD-CGD-O1D
16	b	1202	CLA	CAD-CBD-CGD-O1D
16	b	1207	CLA	CHA-CBD-CGD-O1D
16	b	1226	CLA	CAD-CBD-CGD-O1D
16	f	1302	CLA	CAD-CBD-CGD-O1D
16	g	501	CLA	CHA-CBD-CGD-O1D
16	g	513	CLA	CAD-CBD-CGD-O1D
16	h	503	CLA	CAD-CBD-CGD-O1D
16	h	506	CLA	CAD-CBD-CGD-O1D
16	h	509	CLA	CHA-CBD-CGD-O1D
16	h	517	CLA	CAD-CBD-CGD-O1D
16	j	1302	CLA	CAD-CBD-CGD-O1D
16	n	501	CLA	CAD-CBD-CGD-O1D
16	n	510	CLA	CAD-CBD-CGD-O1D
16	n	516	CLA	CAD-CBD-CGD-O1D
16	n	517	CLA	CAD-CBD-CGD-O1D
16	o	507	CLA	CAD-CBD-CGD-O1D
16	o	516	CLA	CHA-CBD-CGD-O1D
16	o	516	CLA	CHA-CBD-CGD-O2D
16	p	506	CLA	CHA-CBD-CGD-O1D
16	p	513	CLA	CAD-CBD-CGD-O1D
16	q	512	CLA	CHA-CBD-CGD-O1D
16	q	514	CLA	CAD-CBD-CGD-O1D
16	r	508	CLA	CHA-CBD-CGD-O1D
16	r	508	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	r	514	CLA	CAD-CBD-CGD-O1D
16	s	503	CLA	CAD-CBD-CGD-O1D
16	s	513	CLA	CAD-CBD-CGD-O1D
16	t	510	CLA	CAD-CBD-CGD-O1D
16	t	516	CLA	CAD-CBD-CGD-O1D
16	u	503	CLA	CAD-CBD-CGD-O1D
16	v	508	CLA	CAD-CBD-CGD-O1D
16	v	514	CLA	CAD-CBD-CGD-O1D
16	v	517	CLA	CAD-CBD-CGD-O1D
16	w	515	CLA	CHA-CBD-CGD-O1D
16	w	515	CLA	CHA-CBD-CGD-O2D
16	x	517	CLA	CAD-CBD-CGD-O1D
16	y	506	CLA	CAD-CBD-CGD-O1D
16	y	507	CLA	CAD-CBD-CGD-O1D
16	y	511	CLA	CAD-CBD-CGD-O1D
19	L	4019	BCR	C9-C10-C11-C12
19	Q	4016	BCR	C35-C13-C14-C15
19	X	604	BCR	C19-C20-C21-C22
19	b	4017	BCR	C13-C14-C15-C16
21	R	4020	ECH	C13-C14-C15-C16
21	V	4021	ECH	C13-C14-C15-C16
16	G	1202	CLA	C4-C3-C5-C6
16	h	508	CLA	C4-C3-C5-C6
16	A	1113	CLA	C2B-C3B-CAB-CBB
16	A	1114	CLA	C2B-C3B-CAB-CBB
16	A	1124	CLA	C2B-C3B-CAB-CBB
16	A	1130	CLA	C2B-C3B-CAB-CBB
16	A	1131	CLA	C2B-C3B-CAB-CBB
16	A	1801	CLA	C2B-C3B-CAB-CBB
16	B	1214	CLA	C2B-C3B-CAB-CBB
16	B	1223	CLA	C2B-C3B-CAB-CBB
16	G	1202	CLA	C2B-C3B-CAB-CBB
16	G	1206	CLA	C2B-C3B-CAB-CBB
16	G	1212	CLA	C2B-C3B-CAB-CBB
16	G	1213	CLA	C2B-C3B-CAB-CBB
16	G	1223	CLA	C2B-C3B-CAB-CBB
16	G	1235	CLA	C2B-C3B-CAB-CBB
16	H	1101	CLA	C2B-C3B-CAB-CBB
16	H	1114	CLA	C2B-C3B-CAB-CBB
16	H	1120	CLA	C2B-C3B-CAB-CBB
16	H	1125	CLA	C2B-C3B-CAB-CBB
16	H	1801	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	S	1302	CLA	C2B-C3B-CAB-CBB
16	S	1303	CLA	C2B-C3B-CAB-CBB
16	U	1502	CLA	C2B-C3B-CAB-CBB
16	W	503	CLA	C2B-C3B-CAB-CBB
16	W	505	CLA	C2B-C3B-CAB-CBB
16	W	506	CLA	C2B-C3B-CAB-CBB
16	W	508	CLA	C2B-C3B-CAB-CBB
16	W	509	CLA	C2B-C3B-CAB-CBB
16	X	517	CLA	C2B-C3B-CAB-CBB
16	Z	505	CLA	C2B-C3B-CAB-CBB
16	Z	507	CLA	C2B-C3B-CAB-CBB
16	Z	508	CLA	C2B-C3B-CAB-CBB
16	Z	515	CLA	C2B-C3B-CAB-CBB
16	a	1104	CLA	C2B-C3B-CAB-CBB
16	a	1120	CLA	C2B-C3B-CAB-CBB
16	a	1128	CLA	C2B-C3B-CAB-CBB
16	a	1135	CLA	C2B-C3B-CAB-CBB
16	a	1139	CLA	C2B-C3B-CAB-CBB
16	b	1205	CLA	C2B-C3B-CAB-CBB
16	b	1212	CLA	C2B-C3B-CAB-CBB
16	b	1213	CLA	C2B-C3B-CAB-CBB
16	b	1214	CLA	C2B-C3B-CAB-CBB
16	b	1215	CLA	C2B-C3B-CAB-CBB
16	b	1220	CLA	C2B-C3B-CAB-CBB
16	g	506	CLA	C2B-C3B-CAB-CBB
16	g	507	CLA	C2B-C3B-CAB-CBB
16	g	510	CLA	C2B-C3B-CAB-CBB
16	g	513	CLA	C2B-C3B-CAB-CBB
16	l	1502	CLA	C2B-C3B-CAB-CBB
16	n	507	CLA	C2B-C3B-CAB-CBB
16	n	508	CLA	C2B-C3B-CAB-CBB
16	n	515	CLA	C2B-C3B-CAB-CBB
16	o	501	CLA	C2B-C3B-CAB-CBB
16	o	506	CLA	C2B-C3B-CAB-CBB
16	o	512	CLA	C2B-C3B-CAB-CBB
16	o	516	CLA	C2B-C3B-CAB-CBB
16	o	517	CLA	C2B-C3B-CAB-CBB
16	p	509	CLA	C2B-C3B-CAB-CBB
16	p	516	CLA	C2B-C3B-CAB-CBB
16	q	506	CLA	C2B-C3B-CAB-CBB
16	q	507	CLA	C2B-C3B-CAB-CBB
16	q	515	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	q	516	CLA	C2B-C3B-CAB-CBB
16	r	509	CLA	C2B-C3B-CAB-CBB
16	s	509	CLA	C2B-C3B-CAB-CBB
16	s	512	CLA	C2B-C3B-CAB-CBB
16	s	516	CLA	C2B-C3B-CAB-CBB
16	t	503	CLA	C2B-C3B-CAB-CBB
16	t	515	CLA	C2B-C3B-CAB-CBB
16	u	517	CLA	C2B-C3B-CAB-CBB
16	v	515	CLA	C2B-C3B-CAB-CBB
16	v	516	CLA	C2B-C3B-CAB-CBB
16	w	506	CLA	C2B-C3B-CAB-CBB
16	w	507	CLA	C2B-C3B-CAB-CBB
16	w	508	CLA	C2B-C3B-CAB-CBB
16	w	509	CLA	C2B-C3B-CAB-CBB
16	w	510	CLA	C2B-C3B-CAB-CBB
16	w	511	CLA	C2B-C3B-CAB-CBB
16	w	517	CLA	C2B-C3B-CAB-CBB
16	x	505	CLA	C2B-C3B-CAB-CBB
16	x	507	CLA	C2B-C3B-CAB-CBB
16	x	509	CLA	C2B-C3B-CAB-CBB
16	y	501	CLA	C2B-C3B-CAB-CBB
16	y	513	CLA	C2B-C3B-CAB-CBB
16	y	516	CLA	C2B-C3B-CAB-CBB
19	A	4008	BCR	C23-C24-C25-C26
19	G	4004	BCR	C23-C24-C25-C26
19	H	4003	BCR	C23-C24-C25-C30
19	Y	601	BCR	C5-C6-C7-C8
19	Y	602	BCR	C1-C6-C7-C8
19	Y	603	BCR	C23-C24-C25-C30
19	Z	604	BCR	C5-C6-C7-C8
19	j	4012	BCR	C23-C24-C25-C30
19	k	4005	BCR	C1-C6-C7-C8
19	p	602	BCR	C1-C6-C7-C8
19	t	604	BCR	C23-C24-C25-C30
19	w	603	BCR	C1-C6-C7-C8
19	y	604	BCR	C5-C6-C7-C8
16	Z	514	CLA	CAA-CBA-CGA-O2A
16	A	1110	CLA	C2-C3-C5-C6
16	A	1118	CLA	C2-C3-C5-C6
16	G	1220	CLA	C2-C3-C5-C6
16	H	1101	CLA	C2-C3-C5-C6
16	U	1502	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	a	1104	CLA	C2-C3-C5-C6
16	y	508	CLA	C2-C3-C5-C6
16	K	4004	CLA	C5-C6-C7-C8
13	Y	605	LHG	C2-C3-O3-P
13	g	605	LHG	C2-C3-O3-P
13	s	605	LHG	C2-C3-O3-P
13	x	605	LHG	C2-C3-O3-P
16	F	1302	CLA	CBA-CGA-O2A-C1
16	B	1211	CLA	C10-C11-C12-C13
16	a	1140	CLA	C10-C11-C12-C13
13	b	4018	LHG	C15-C16-C17-C18
16	A	1124	CLA	C11-C12-C13-C15
16	B	1202	CLA	C16-C17-C18-C19
16	G	1221	CLA	C16-C17-C18-C19
16	x	504	CLA	C16-C17-C18-C19
16	B	1235	CLA	CAA-CBA-CGA-O2A
24	w	601	LUT	C7-C8-C9-C10
16	X	511	CLA	O1A-CGA-O2A-C1
16	t	504	CLA	O1A-CGA-O2A-C1
16	g	515	CLA	O1D-CGD-O2D-CED
16	H	1128	CLA	C13-C15-C16-C17
16	q	514	CLA	CAA-CBA-CGA-O2A
16	w	512	CLA	C16-C17-C18-C19
17	G	2002	PQN	C26-C27-C28-C29
16	H	1132	CLA	C5-C6-C7-C8
16	a	1132	CLA	C5-C6-C7-C8
16	q	511	CLA	C13-C15-C16-C17
16	r	506	CLA	C5-C6-C7-C8
16	v	507	CLA	C5-C6-C7-C8
16	A	1102	CLA	C11-C10-C8-C7
13	x	605	LHG	C24-C25-C26-C27
16	r	503	CLA	O1A-CGA-O2A-C1
16	y	516	CLA	O1A-CGA-O2A-C1
19	Z	602	BCR	C10-C11-C12-C13
19	l	4022	BCR	C18-C19-C20-C21
16	w	508	CLA	CAA-CBA-CGA-O2A
23	p	606	LMU	C1-C2-C3-C4
16	G	1228	CLA	C2-C3-C5-C6
19	h	601	BCR	C15-C16-C17-C18
16	g	504	CLA	C16-C17-C18-C19
16	A	1126	CLA	C13-C15-C16-C17
16	B	1023	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
16	s	507	CLA	C8-C10-C11-C12
17	b	2002	PQN	C20-C21-C22-C23
13	A	849	LHG	O6-C4-C5-C6
14	B	848	LMG	C29-C30-C31-C32
14	G	848	LMG	C29-C30-C31-C32
16	a	1116	CLA	CBA-CGA-O2A-C1
16	X	516	CLA	CBA-CGA-O2A-C1
16	a	1103	CLA	O1A-CGA-O2A-C1
16	x	505	CLA	C3-C5-C6-C7
16	Z	515	CLA	C10-C11-C12-C13
16	Y	503	CLA	CAA-CBA-CGA-O2A
16	Y	508	CLA	CAA-CBA-CGA-O2A
16	A	1106	CLA	C6-C7-C8-C9
16	B	1206	CLA	C6-C7-C8-C9
16	B	1221	CLA	C6-C7-C8-C9
16	G	1211	CLA	C11-C10-C8-C9
16	G	1223	CLA	C14-C13-C15-C16
16	G	1239	CLA	C6-C7-C8-C9
16	H	1104	CLA	C11-C12-C13-C14
16	H	1128	CLA	C14-C13-C15-C16
16	L	1501	CLA	C11-C10-C8-C9
16	U	1502	CLA	C6-C7-C8-C9
16	W	505	CLA	C14-C13-C15-C16
16	X	510	CLA	C11-C10-C8-C9
16	Z	505	CLA	C6-C7-C8-C9
16	Z	510	CLA	C6-C7-C8-C9
16	a	1101	CLA	C6-C7-C8-C9
16	a	1103	CLA	C11-C10-C8-C9
16	a	1106	CLA	C6-C7-C8-C9
16	b	1021	CLA	C11-C10-C8-C9
16	b	1202	CLA	C14-C13-C15-C16
16	b	1239	CLA	C6-C7-C8-C9
16	h	504	CLA	C11-C10-C8-C9
16	n	515	CLA	C11-C12-C13-C14
16	o	505	CLA	C6-C7-C8-C9
16	o	505	CLA	C11-C10-C8-C9
16	o	507	CLA	C11-C10-C8-C9
16	q	504	CLA	C6-C7-C8-C9
16	q	507	CLA	C11-C10-C8-C9
16	s	509	CLA	C6-C7-C8-C9
16	s	512	CLA	C11-C12-C13-C14
16	t	505	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
16	t	515	CLA	C11-C12-C13-C14
16	u	507	CLA	C11-C10-C8-C9
16	w	507	CLA	C11-C10-C8-C9
16	x	504	CLA	C11-C12-C13-C14
16	y	504	CLA	C11-C10-C8-C9
16	y	509	CLA	C11-C10-C8-C9
16	A	1136	CLA	C11-C10-C8-C7
16	B	1221	CLA	C6-C7-C8-C10
16	X	504	CLA	C11-C10-C8-C7
16	X	512	CLA	C6-C7-C8-C10
16	a	1101	CLA	C6-C7-C8-C10
16	a	1128	CLA	C11-C10-C8-C7
16	q	506	CLA	C6-C7-C8-C10
16	t	505	CLA	C11-C10-C8-C7
16	u	510	CLA	C6-C7-C8-C10
16	y	506	CLA	C11-C10-C8-C7
19	A	4011	BCR	C16-C17-C18-C19
19	B	4010	BCR	C11-C10-C9-C8
19	G	4005	BCR	C11-C10-C9-C8
19	G	4017	BCR	C11-C10-C9-C8
19	L	4022	BCR	C11-C10-C9-C8
19	U	4022	BCR	C20-C21-C22-C23
19	b	4010	BCR	C20-C21-C22-C23
19	p	603	BCR	C11-C10-C9-C8
19	v	601	BCR	C20-C21-C22-C23
19	y	601	BCR	C12-C13-C14-C15
19	y	601	BCR	C20-C21-C22-C23
14	H	4101	LMG	C10-C11-C12-C13
19	A	4011	BCR	C22-C23-C24-C25
15	H	1011	CL0	C16-C17-C18-C20
16	b	1202	CLA	C16-C17-C18-C20
16	o	508	CLA	C6-C7-C8-C10
14	H	4101	LMG	C14-C15-C16-C17
15	H	1011	CL0	CAA-CBA-CGA-O2A
16	Y	504	CLA	CAA-CBA-CGA-O2A
16	w	514	CLA	CAA-CBA-CGA-O2A
16	b	1201	CLA	C6-C7-C8-C9
16	o	510	CLA	CBD-CGD-O2D-CED
16	H	1126	CLA	C13-C15-C16-C17
16	n	505	CLA	C10-C11-C12-C13
16	s	505	CLA	C8-C10-C11-C12
14	A	4201	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	w	504	CLA	CAA-CBA-CGA-O2A
16	B	1228	CLA	C2-C3-C5-C6
16	l	1502	CLA	C2-C3-C5-C6
16	u	512	CLA	C3-C5-C6-C7
16	G	1210	CLA	O1D-CGD-O2D-CED
16	o	511	CLA	CBA-CGA-O2A-C1
16	a	1237	CLA	C16-C17-C18-C19
16	q	506	CLA	C11-C12-C13-C14
16	q	506	CLA	C11-C12-C13-C15
16	t	517	CLA	C6-C7-C8-C10
14	H	4101	LMG	C29-C30-C31-C32
16	H	1136	CLA	O1A-CGA-O2A-C1
16	G	1235	CLA	CAA-CBA-CGA-O2A
16	a	1801	CLA	CAA-CBA-CGA-O2A
13	o	605	LHG	C24-C25-C26-C27
16	v	516	CLA	O1D-CGD-O2D-CED
16	w	501	CLA	O1D-CGD-O2D-CED
16	n	512	CLA	C13-C15-C16-C17
16	G	1207	CLA	C3-C5-C6-C7
16	A	1013	CLA	CBA-CGA-O2A-C1
19	b	4004	BCR	C13-C14-C15-C16
19	i	4018	BCR	C9-C10-C11-C12
13	p	605	LHG	C26-C27-C28-C29
14	b	848	LMG	C11-C10-O7-C8
16	s	516	CLA	CBA-CGA-O2A-C1
16	Z	508	CLA	CAA-CBA-CGA-O2A
16	s	508	CLA	CAA-CBA-CGA-O2A
16	G	1203	CLA	C2A-CAA-CBA-CGA
16	b	1209	CLA	C2A-CAA-CBA-CGA
16	n	509	CLA	C3-C5-C6-C7
16	a	1013	CLA	O1A-CGA-O2A-C1
16	o	511	CLA	O1A-CGA-O2A-C1
16	G	1239	CLA	C15-C16-C17-C18
16	w	501	CLA	C2-C1-O2A-CGA
16	v	507	CLA	C16-C17-C18-C19
16	x	506	CLA	C11-C12-C13-C14
14	a	4201	LMG	O7-C10-C11-C12
16	g	513	CLA	CAA-CBA-CGA-O2A
16	g	514	CLA	CAA-CBA-CGA-O2A
16	p	508	CLA	CAA-CBA-CGA-O2A
14	A	4101	LMG	C11-C12-C13-C14
16	b	1205	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	G	848	LMG	O1-C7-C8-C9
16	a	1119	CLA	C5-C6-C7-C8
16	B	1012	CLA	C2C-C3C-CAC-CBC
19	W	603	BCR	C11-C12-C13-C35
19	a	4002	BCR	C37-C22-C23-C24
16	q	516	CLA	O1A-CGA-O2A-C1
16	b	1202	CLA	C16-C17-C18-C19
16	B	1206	CLA	C3-C5-C6-C7
16	b	1012	CLA	C2C-C3C-CAC-CBC
16	G	1229	CLA	C2C-C3C-CAC-CBC
14	F	4017	LMG	C8-C7-O1-C1
16	G	1217	CLA	O1D-CGD-O2D-CED
16	a	1116	CLA	O1A-CGA-O2A-C1
16	Z	512	CLA	C5-C6-C7-C8
16	B	1203	CLA	C2A-CAA-CBA-CGA
16	G	1012	CLA	C2A-CAA-CBA-CGA
16	Z	516	CLA	C2A-CAA-CBA-CGA
16	a	1130	CLA	C2A-CAA-CBA-CGA
16	a	1136	CLA	C2A-CAA-CBA-CGA
16	b	1227	CLA	C2A-CAA-CBA-CGA
16	b	1231	CLA	C2A-CAA-CBA-CGA
16	u	514	CLA	C2A-CAA-CBA-CGA
16	v	502	CLA	C2A-CAA-CBA-CGA
16	G	1212	CLA	O1D-CGD-O2D-CED
19	g	604	BCR	C13-C14-C15-C16
19	l	4019	BCR	C9-C10-C11-C12
16	A	1102	CLA	C11-C10-C8-C9
16	h	511	CLA	C16-C17-C18-C19
16	l	1501	CLA	C11-C12-C13-C15
16	L	1502	CLA	C3-C5-C6-C7
23	x	606	LMU	C11-C10-C9-C8
16	b	1220	CLA	C4-C3-C5-C6
17	b	2002	PQN	C14-C13-C15-C16
16	G	1202	CLA	C15-C16-C17-C18
16	s	504	CLA	CAA-CBA-CGA-O2A
16	h	508	CLA	C2-C3-C5-C6
16	v	508	CLA	C2-C3-C5-C6
16	n	512	CLA	CBA-CGA-O2A-C1
16	q	515	CLA	C13-C15-C16-C17
16	a	1123	CLA	O1D-CGD-O2D-CED
16	G	1218	CLA	C4C-C3C-CAC-CBC
16	G	1239	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
16	y	517	CLA	C6-C7-C8-C10
16	b	1214	CLA	C4C-C3C-CAC-CBC
14	a	852	LMG	C28-C29-C30-C31
16	A	1126	CLA	C6-C7-C8-C9
16	A	1128	CLA	C14-C13-C15-C16
16	X	507	CLA	C11-C10-C8-C9
16	X	511	CLA	C11-C10-C8-C9
16	Z	504	CLA	C6-C7-C8-C9
16	a	1128	CLA	C11-C10-C8-C9
16	a	1131	CLA	C14-C13-C15-C16
16	h	511	CLA	C6-C7-C8-C9
16	n	505	CLA	C11-C12-C13-C14
16	n	507	CLA	C11-C10-C8-C9
16	q	512	CLA	C6-C7-C8-C9
16	t	504	CLA	C6-C7-C8-C9
16	u	510	CLA	C6-C7-C8-C9
16	w	515	CLA	C11-C12-C13-C14
16	x	510	CLA	C6-C7-C8-C9
16	y	505	CLA	C11-C10-C8-C9
17	B	2002	PQN	C21-C22-C23-C24
17	G	2002	PQN	C21-C22-C23-C24
17	a	2001	PQN	C16-C17-C18-C19
16	B	1236	CLA	O1D-CGD-O2D-CED
16	b	1206	CLA	C13-C15-C16-C17
16	B	1218	CLA	C4B-C3B-CAB-CBB
16	G	1209	CLA	C4B-C3B-CAB-CBB
16	G	1210	CLA	C4B-C3B-CAB-CBB
16	G	1220	CLA	C4B-C3B-CAB-CBB
16	W	506	CLA	C4B-C3B-CAB-CBB
16	X	512	CLA	C4B-C3B-CAB-CBB
16	Y	512	CLA	C4B-C3B-CAB-CBB
16	Z	510	CLA	C4B-C3B-CAB-CBB
16	a	1139	CLA	C4B-C3B-CAB-CBB
16	a	1801	CLA	C4B-C3B-CAB-CBB
16	b	1230	CLA	C4B-C3B-CAB-CBB
16	b	1240	CLA	C4B-C3B-CAB-CBB
16	g	506	CLA	C4B-C3B-CAB-CBB
16	g	507	CLA	C4B-C3B-CAB-CBB
16	o	501	CLA	C4B-C3B-CAB-CBB
16	r	510	CLA	C4B-C3B-CAB-CBB
16	u	510	CLA	C4B-C3B-CAB-CBB
16	x	506	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	x	509	CLA	C4B-C3B-CAB-CBB
16	A	1133	CLA	C6-C7-C8-C9
16	A	1132	CLA	C5-C6-C7-C8
16	w	512	CLA	C16-C17-C18-C20
13	i	103	LHG	C28-C29-C30-C31
13	X	605	LHG	C24-C23-O8-C6
16	A	1124	CLA	C5-C6-C7-C8
16	b	1238	CLA	C13-C15-C16-C17
16	n	505	CLA	C15-C16-C17-C18
16	n	512	CLA	O1A-CGA-O2A-C1
13	r	605	LHG	C11-C12-C13-C14
16	Z	508	CLA	C2A-CAA-CBA-CGA
16	n	502	CLA	C2A-CAA-CBA-CGA
14	A	852	LMG	C29-C30-C31-C32
14	H	4201	LMG	O7-C10-C11-C12
16	X	515	CLA	C2-C3-C5-C6
16	t	506	CLA	C8-C10-C11-C12
13	s	605	LHG	C24-C25-C26-C27
13	G	4018	LHG	C12-C13-C14-C15
19	J	4013	BCR	C19-C20-C21-C22
19	q	602	BCR	C15-C16-C17-C18
16	B	1207	CLA	C15-C16-C17-C18
15	a	1011	CL0	C16-C17-C18-C19
16	B	1224	CLA	C11-C12-C13-C14
16	q	509	CLA	C16-C17-C18-C19
14	a	4101	LMG	C29-C30-C31-C32
20	L	4101	LMT	C2B-C1B-O1B-C4'
14	b	848	LMG	C17-C18-C19-C20
16	G	1221	CLA	C12-C13-C15-C16
16	H	1106	CLA	C11-C12-C13-C15
16	U	1503	CLA	C11-C10-C8-C7
16	a	1106	CLA	C11-C12-C13-C15
16	a	1138	CLA	C11-C12-C13-C15
16	g	505	CLA	C6-C7-C8-C10
16	h	515	CLA	C11-C10-C8-C7
16	n	505	CLA	C11-C10-C8-C7
16	p	511	CLA	C6-C7-C8-C10
16	r	506	CLA	C11-C10-C8-C7
16	v	515	CLA	C11-C12-C13-C15
16	b	1225	CLA	C5-C6-C7-C8
16	A	1111	CLA	CBA-CGA-O2A-C1
16	H	1117	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	b	1238	CLA	C16-C17-C18-C20
16	r	506	CLA	C11-C12-C13-C15
16	v	507	CLA	C16-C17-C18-C20
14	b	848	LMG	C33-C34-C35-C36
16	Z	509	CLA	C13-C15-C16-C17
16	A	1111	CLA	O1A-CGA-O2A-C1
16	b	1206	CLA	C3-C5-C6-C7
13	a	851	LHG	O7-C5-C6-O8
16	A	1105	CLA	C3A-C2A-CAA-CBA
16	A	1107	CLA	C3A-C2A-CAA-CBA
16	A	1112	CLA	C3A-C2A-CAA-CBA
16	B	1209	CLA	C3A-C2A-CAA-CBA
16	G	1217	CLA	C3A-C2A-CAA-CBA
16	G	1232	CLA	C3A-C2A-CAA-CBA
16	G	1234	CLA	C3A-C2A-CAA-CBA
16	H	1105	CLA	C3A-C2A-CAA-CBA
16	H	1128	CLA	C3A-C2A-CAA-CBA
16	H	1137	CLA	C3A-C2A-CAA-CBA
16	W	513	CLA	C3A-C2A-CAA-CBA
16	Y	503	CLA	C3A-C2A-CAA-CBA
16	Z	503	CLA	C3A-C2A-CAA-CBA
16	Z	513	CLA	C3A-C2A-CAA-CBA
16	a	1105	CLA	C3A-C2A-CAA-CBA
16	a	1107	CLA	C3A-C2A-CAA-CBA
16	a	1108	CLA	C3A-C2A-CAA-CBA
16	a	1114	CLA	C3A-C2A-CAA-CBA
16	h	516	CLA	C3A-C2A-CAA-CBA
16	o	503	CLA	C3A-C2A-CAA-CBA
16	o	506	CLA	C3A-C2A-CAA-CBA
16	o	511	CLA	C3A-C2A-CAA-CBA
16	r	503	CLA	C3A-C2A-CAA-CBA
16	s	517	CLA	C3A-C2A-CAA-CBA
16	u	503	CLA	C3A-C2A-CAA-CBA
16	y	507	CLA	C3A-C2A-CAA-CBA
16	y	516	CLA	C3A-C2A-CAA-CBA
16	W	501	CLA	CAA-CBA-CGA-O2A
16	a	1116	CLA	CAA-CBA-CGA-O2A
17	b	2002	PQN	C12-C13-C15-C16
16	u	502	CLA	C2A-CAA-CBA-CGA
16	H	1125	CLA	C10-C11-C12-C13
16	W	511	CLA	C10-C11-C12-C13
16	B	1240	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	4011	BCR	C16-C17-C18-C36
19	F	4016	BCR	C35-C13-C14-C15
19	G	4009	BCR	C20-C21-C22-C37
19	H	4007	BCR	C20-C21-C22-C37
19	H	4011	BCR	C16-C17-C18-C36
19	U	4022	BCR	C20-C21-C22-C37
19	X	604	BCR	C35-C13-C14-C15
19	Z	604	BCR	C35-C13-C14-C15
19	a	4002	BCR	C11-C10-C9-C34
19	b	4014	BCR	C16-C17-C18-C36
19	b	4017	BCR	C35-C13-C14-C15
19	n	603	BCR	C11-C10-C9-C34
19	w	603	BCR	C35-C13-C14-C15
21	B	4006	ECH	C11-C10-C9-C34
21	B	4006	ECH	C20-C21-C22-C37
21	G	4006	ECH	C11-C10-C9-C34
21	G	4006	ECH	C20-C21-C22-C37
21	I	4020	ECH	C11-C10-C9-C34
21	M	4021	ECH	C11-C10-C9-C34
21	R	4020	ECH	C11-C10-C9-C34
21	V	4021	ECH	C11-C10-C9-C34
21	b	4006	ECH	C11-C10-C9-C34
21	b	4006	ECH	C20-C21-C22-C37
21	i	4020	ECH	C11-C10-C9-C34
21	m	4021	ECH	C11-C10-C9-C34
16	W	505	CLA	C15-C16-C17-C18
16	o	509	CLA	C10-C11-C12-C13
14	A	4101	LMG	C29-C30-C31-C32
16	G	1214	CLA	C4C-C3C-CAC-CBC
16	b	1203	CLA	C15-C16-C17-C18
14	H	4101	LMG	C17-C18-C19-C20
14	b	848	LMG	C13-C14-C15-C16
16	B	1236	CLA	CBD-CGD-O2D-CED
16	G	1012	CLA	C2C-C3C-CAC-CBC
15	A	1011	CL0	CAA-CBA-CGA-O1A
16	A	1123	CLA	C2-C1-O2A-CGA
16	W	507	CLA	C2-C1-O2A-CGA
16	X	512	CLA	C2-C1-O2A-CGA
19	H	4008	BCR	C19-C20-C21-C22
19	b	4010	BCR	C15-C16-C17-C18
19	k	4005	BCR	C13-C14-C15-C16
19	l	4022	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
21	M	4021	ECH	C15-C16-C17-C18
23	r	606	LMU	C1-C2-C3-C4
16	B	1023	CLA	C15-C16-C17-C18
16	b	1206	CLA	C8-C10-C11-C12
19	G	4010	BCR	C7-C8-C9-C34
19	J	4012	BCR	C11-C12-C13-C35
19	J	4013	BCR	C11-C12-C13-C35
16	G	1235	CLA	C5-C6-C7-C8
16	t	515	CLA	C5-C6-C7-C8
16	X	504	CLA	C10-C11-C12-C13
16	h	510	CLA	C13-C15-C16-C17
19	B	4005	BCR	C7-C8-C9-C10
19	b	4005	BCR	C7-C8-C9-C10
13	i	103	LHG	C11-C10-C9-C8
14	B	848	LMG	C17-C18-C19-C20
16	H	1124	CLA	C4-C3-C5-C6
16	H	1123	CLA	C4C-C3C-CAC-CBC
13	H	849	LHG	C7-C8-C9-C10
16	a	1118	CLA	C2-C3-C5-C6
17	G	2002	PQN	C26-C27-C28-C30
16	G	1023	CLA	C13-C15-C16-C17
16	H	1101	CLA	C10-C11-C12-C13
16	H	1123	CLA	C8-C10-C11-C12
16	A	1136	CLA	C2A-CAA-CBA-CGA
16	G	1220	CLA	C2A-CAA-CBA-CGA
16	q	514	CLA	C2A-CAA-CBA-CGA
16	q	516	CLA	C2A-CAA-CBA-CGA
16	A	1113	CLA	CAA-CBA-CGA-O1A
16	A	1134	CLA	CAA-CBA-CGA-O1A
19	A	4007	BCR	C14-C15-C16-C17
19	q	602	BCR	C14-C15-C16-C17
16	X	515	CLA	C3-C5-C6-C7
16	y	509	CLA	C3-C5-C6-C7
16	t	510	CLA	C5-C6-C7-C8
16	A	1106	CLA	C11-C10-C8-C9
16	A	1139	CLA	C6-C7-C8-C9
16	B	1202	CLA	C14-C13-C15-C16
16	G	1226	CLA	C6-C7-C8-C9
16	H	1106	CLA	C11-C10-C8-C9
16	H	1132	CLA	C6-C7-C8-C9
16	H	1139	CLA	C6-C7-C8-C9
16	L	1503	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	U	1502	CLA	C11-C10-C8-C9
16	U	1503	CLA	C6-C7-C8-C9
16	W	504	CLA	C6-C7-C8-C9
16	W	507	CLA	C11-C10-C8-C9
16	b	1221	CLA	C14-C13-C15-C16
16	b	1223	CLA	C14-C13-C15-C16
16	b	1238	CLA	C6-C7-C8-C9
16	l	1501	CLA	C11-C10-C8-C9
16	l	1502	CLA	C11-C10-C8-C9
16	n	505	CLA	C11-C10-C8-C9
16	p	507	CLA	C11-C10-C8-C9
16	p	511	CLA	C6-C7-C8-C9
16	p	511	CLA	C11-C12-C13-C14
16	t	507	CLA	C11-C10-C8-C9
16	t	511	CLA	C6-C7-C8-C9
16	v	511	CLA	C6-C7-C8-C9
16	x	504	CLA	C14-C13-C15-C16
16	b	1220	CLA	C2C-C3C-CAC-CBC
16	B	1228	CLA	C5-C6-C7-C8
16	G	1203	CLA	C15-C16-C17-C18
16	H	1132	CLA	C15-C16-C17-C18
16	b	1206	CLA	C10-C11-C12-C13
16	r	515	CLA	C8-C10-C11-C12
14	H	852	LMG	C37-C38-C39-C40
16	A	1116	CLA	CAA-CBA-CGA-O2A
14	A	4101	LMG	C9-C8-O7-C10
14	a	4101	LMG	C7-C8-O7-C10
16	n	516	CLA	CBD-CGD-O2D-CED
19	W	604	BCR	C13-C14-C15-C16
19	Y	604	BCR	C13-C14-C15-C16
24	Z	601	LUT	C29-C30-C31-C32
16	H	1104	CLA	C4-C3-C5-C6
16	H	1115	CLA	C4-C3-C5-C6
16	q	509	CLA	C16-C17-C18-C20
16	H	1123	CLA	C2C-C3C-CAC-CBC
16	B	1213	CLA	CBD-CGD-O2D-CED
16	p	509	CLA	CBD-CGD-O2D-CED
16	G	1202	CLA	CAA-CBA-CGA-O2A
16	u	509	CLA	CAA-CBA-CGA-O2A
16	H	1124	CLA	C2-C3-C5-C6
16	v	517	CLA	C4C-C3C-CAC-CBC
16	A	1013	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
16	A	1130	CLA	C2A-CAA-CBA-CGA
16	G	1215	CLA	C2A-CAA-CBA-CGA
16	G	1231	CLA	C2A-CAA-CBA-CGA
16	Z	505	CLA	C2A-CAA-CBA-CGA
16	a	1120	CLA	C2A-CAA-CBA-CGA
16	u	509	CLA	C2A-CAA-CBA-CGA
16	B	1213	CLA	O1D-CGD-O2D-CED
16	X	509	CLA	CAA-CBA-CGA-O1A
16	X	506	CLA	C5-C6-C7-C8
16	A	1129	CLA	C1A-C2A-CAA-CBA
16	G	1207	CLA	C1A-C2A-CAA-CBA
16	G	1215	CLA	C1A-C2A-CAA-CBA
16	G	1232	CLA	C1A-C2A-CAA-CBA
16	H	1103	CLA	C1A-C2A-CAA-CBA
16	H	1120	CLA	C1A-C2A-CAA-CBA
16	W	504	CLA	C1A-C2A-CAA-CBA
16	Z	513	CLA	C1A-C2A-CAA-CBA
16	a	1139	CLA	C1A-C2A-CAA-CBA
16	b	1220	CLA	C1A-C2A-CAA-CBA
16	p	512	CLA	C1A-C2A-CAA-CBA
16	q	508	CLA	C1A-C2A-CAA-CBA
16	r	512	CLA	C1A-C2A-CAA-CBA
16	s	515	CLA	C1A-C2A-CAA-CBA
16	s	516	CLA	C1A-C2A-CAA-CBA
16	t	515	CLA	C1A-C2A-CAA-CBA
16	w	508	CLA	C1A-C2A-CAA-CBA
16	w	511	CLA	C1A-C2A-CAA-CBA
16	w	514	CLA	C1A-C2A-CAA-CBA
19	F	4016	BCR	C12-C13-C14-C15
19	H	4003	BCR	C16-C17-C18-C19
19	H	4011	BCR	C16-C17-C18-C19
19	Q	4016	BCR	C12-C13-C14-C15
19	X	604	BCR	C12-C13-C14-C15
19	Y	601	BCR	C12-C13-C14-C15
19	a	4011	BCR	C16-C17-C18-C19
19	f	4016	BCR	C12-C13-C14-C15
19	j	4015	BCR	C16-C17-C18-C19
21	B	4006	ECH	C11-C10-C9-C8
21	B	4006	ECH	C20-C21-C22-C23
21	G	4006	ECH	C11-C10-C9-C8
21	G	4006	ECH	C20-C21-C22-C23
21	I	4020	ECH	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	M	4021	ECH	C11-C10-C9-C8
21	R	4020	ECH	C11-C10-C9-C8
21	V	4021	ECH	C11-C10-C9-C8
21	b	4006	ECH	C11-C10-C9-C8
21	b	4006	ECH	C20-C21-C22-C23
21	i	4020	ECH	C11-C10-C9-C8
21	m	4021	ECH	C11-C10-C9-C8
16	b	1229	CLA	C2C-C3C-CAC-CBC
16	X	504	CLA	C11-C12-C13-C14
16	S	1302	CLA	CAA-CBA-CGA-O1A
13	I	103	LHG	C7-C8-C9-C10
16	Z	507	CLA	C3-C5-C6-C7
16	A	1013	CLA	C2B-C3B-CAB-CBB
16	A	1110	CLA	C2B-C3B-CAB-CBB
16	A	1117	CLA	C2B-C3B-CAB-CBB
16	A	1121	CLA	C2B-C3B-CAB-CBB
16	A	1125	CLA	C2B-C3B-CAB-CBB
16	A	1127	CLA	C2B-C3B-CAB-CBB
16	A	1134	CLA	C2B-C3B-CAB-CBB
16	A	1135	CLA	C2B-C3B-CAB-CBB
16	A	1136	CLA	C2B-C3B-CAB-CBB
16	A	1138	CLA	C2B-C3B-CAB-CBB
16	B	1023	CLA	C2B-C3B-CAB-CBB
16	B	1204	CLA	C2B-C3B-CAB-CBB
16	B	1205	CLA	C2B-C3B-CAB-CBB
16	B	1208	CLA	C2B-C3B-CAB-CBB
16	B	1212	CLA	C2B-C3B-CAB-CBB
16	B	1220	CLA	C2B-C3B-CAB-CBB
16	B	1229	CLA	C2B-C3B-CAB-CBB
16	B	1232	CLA	C2B-C3B-CAB-CBB
16	G	1203	CLA	C2B-C3B-CAB-CBB
16	G	1205	CLA	C2B-C3B-CAB-CBB
16	G	1208	CLA	C2B-C3B-CAB-CBB
16	G	1214	CLA	C2B-C3B-CAB-CBB
16	G	1215	CLA	C2B-C3B-CAB-CBB
16	G	1220	CLA	C2B-C3B-CAB-CBB
16	G	1228	CLA	C2B-C3B-CAB-CBB
16	G	1229	CLA	C2B-C3B-CAB-CBB
16	G	1231	CLA	C2B-C3B-CAB-CBB
16	H	1104	CLA	C2B-C3B-CAB-CBB
16	H	1106	CLA	C2B-C3B-CAB-CBB
16	H	1110	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	H	1113	CLA	C2B-C3B-CAB-CBB
16	H	1118	CLA	C2B-C3B-CAB-CBB
16	H	1119	CLA	C2B-C3B-CAB-CBB
16	H	1129	CLA	C2B-C3B-CAB-CBB
16	H	1130	CLA	C2B-C3B-CAB-CBB
16	H	1134	CLA	C2B-C3B-CAB-CBB
16	H	1138	CLA	C2B-C3B-CAB-CBB
16	H	1140	CLA	C2B-C3B-CAB-CBB
16	J	1302	CLA	C2B-C3B-CAB-CBB
16	J	1303	CLA	C2B-C3B-CAB-CBB
16	K	4002	CLA	C2B-C3B-CAB-CBB
16	T	4002	CLA	C2B-C3B-CAB-CBB
16	W	512	CLA	C2B-C3B-CAB-CBB
16	X	505	CLA	C2B-C3B-CAB-CBB
16	X	508	CLA	C2B-C3B-CAB-CBB
16	X	513	CLA	C2B-C3B-CAB-CBB
16	Y	502	CLA	C2B-C3B-CAB-CBB
16	Y	505	CLA	C2B-C3B-CAB-CBB
16	Y	508	CLA	C2B-C3B-CAB-CBB
16	Y	513	CLA	C2B-C3B-CAB-CBB
16	Z	504	CLA	C2B-C3B-CAB-CBB
16	a	1107	CLA	C2B-C3B-CAB-CBB
16	a	1110	CLA	C2B-C3B-CAB-CBB
16	a	1113	CLA	C2B-C3B-CAB-CBB
16	a	1114	CLA	C2B-C3B-CAB-CBB
16	a	1118	CLA	C2B-C3B-CAB-CBB
16	a	1127	CLA	C2B-C3B-CAB-CBB
16	a	1134	CLA	C2B-C3B-CAB-CBB
16	a	1136	CLA	C2B-C3B-CAB-CBB
16	a	1140	CLA	C2B-C3B-CAB-CBB
16	b	1203	CLA	C2B-C3B-CAB-CBB
16	b	1208	CLA	C2B-C3B-CAB-CBB
16	b	1216	CLA	C2B-C3B-CAB-CBB
16	b	1222	CLA	C2B-C3B-CAB-CBB
16	b	1231	CLA	C2B-C3B-CAB-CBB
16	b	1232	CLA	C2B-C3B-CAB-CBB
16	b	1235	CLA	C2B-C3B-CAB-CBB
16	f	1301	CLA	C2B-C3B-CAB-CBB
16	g	504	CLA	C2B-C3B-CAB-CBB
16	g	505	CLA	C2B-C3B-CAB-CBB
16	g	508	CLA	C2B-C3B-CAB-CBB
16	h	501	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	h	502	CLA	C2B-C3B-CAB-CBB
16	h	507	CLA	C2B-C3B-CAB-CBB
16	h	509	CLA	C2B-C3B-CAB-CBB
16	h	510	CLA	C2B-C3B-CAB-CBB
16	k	4002	CLA	C2B-C3B-CAB-CBB
16	n	502	CLA	C2B-C3B-CAB-CBB
16	n	511	CLA	C2B-C3B-CAB-CBB
16	o	508	CLA	C2B-C3B-CAB-CBB
16	o	515	CLA	C2B-C3B-CAB-CBB
16	p	502	CLA	C2B-C3B-CAB-CBB
16	p	506	CLA	C2B-C3B-CAB-CBB
16	p	508	CLA	C2B-C3B-CAB-CBB
16	p	511	CLA	C2B-C3B-CAB-CBB
16	p	513	CLA	C2B-C3B-CAB-CBB
16	p	517	CLA	C2B-C3B-CAB-CBB
16	q	512	CLA	C2B-C3B-CAB-CBB
16	r	505	CLA	C2B-C3B-CAB-CBB
16	r	508	CLA	C2B-C3B-CAB-CBB
16	r	512	CLA	C2B-C3B-CAB-CBB
16	r	513	CLA	C2B-C3B-CAB-CBB
16	s	505	CLA	C2B-C3B-CAB-CBB
16	s	508	CLA	C2B-C3B-CAB-CBB
16	s	511	CLA	C2B-C3B-CAB-CBB
16	s	513	CLA	C2B-C3B-CAB-CBB
16	t	507	CLA	C2B-C3B-CAB-CBB
16	t	508	CLA	C2B-C3B-CAB-CBB
16	t	509	CLA	C2B-C3B-CAB-CBB
16	u	505	CLA	C2B-C3B-CAB-CBB
16	u	508	CLA	C2B-C3B-CAB-CBB
16	u	509	CLA	C2B-C3B-CAB-CBB
16	u	515	CLA	C2B-C3B-CAB-CBB
16	v	511	CLA	C2B-C3B-CAB-CBB
16	x	508	CLA	C2B-C3B-CAB-CBB
16	x	512	CLA	C2B-C3B-CAB-CBB
16	x	513	CLA	C2B-C3B-CAB-CBB
16	x	517	CLA	C2B-C3B-CAB-CBB
16	y	507	CLA	C2B-C3B-CAB-CBB
16	y	508	CLA	C2B-C3B-CAB-CBB
19	A	4002	BCR	C5-C6-C7-C8
19	A	4002	BCR	C23-C24-C25-C26
19	A	4007	BCR	C5-C6-C7-C8
19	A	4007	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
19	A	4008	BCR	C5-C6-C7-C8
19	A	4011	BCR	C5-C6-C7-C8
19	B	4004	BCR	C5-C6-C7-C8
19	B	4004	BCR	C23-C24-C25-C26
19	B	4005	BCR	C5-C6-C7-C8
19	B	4009	BCR	C23-C24-C25-C26
19	B	4010	BCR	C5-C6-C7-C8
19	B	4010	BCR	C23-C24-C25-C26
19	B	4010	BCR	C23-C24-C25-C30
19	B	4014	BCR	C1-C6-C7-C8
19	B	4014	BCR	C5-C6-C7-C8
19	B	4014	BCR	C23-C24-C25-C26
19	B	4017	BCR	C5-C6-C7-C8
19	B	4017	BCR	C23-C24-C25-C26
19	F	4016	BCR	C5-C6-C7-C8
19	F	4016	BCR	C23-C24-C25-C30
19	G	4004	BCR	C5-C6-C7-C8
19	G	4005	BCR	C5-C6-C7-C8
19	G	4009	BCR	C23-C24-C25-C26
19	G	4010	BCR	C23-C24-C25-C30
19	G	4014	BCR	C5-C6-C7-C8
19	G	4014	BCR	C23-C24-C25-C26
19	G	4017	BCR	C5-C6-C7-C8
19	G	4017	BCR	C23-C24-C25-C26
19	H	4002	BCR	C5-C6-C7-C8
19	H	4002	BCR	C23-C24-C25-C26
19	H	4003	BCR	C5-C6-C7-C8
19	H	4003	BCR	C23-C24-C25-C26
19	H	4007	BCR	C5-C6-C7-C8
19	H	4007	BCR	C23-C24-C25-C26
19	H	4008	BCR	C5-C6-C7-C8
19	H	4008	BCR	C23-C24-C25-C26
19	H	4011	BCR	C5-C6-C7-C8
19	I	4018	BCR	C5-C6-C7-C8
19	J	4012	BCR	C23-C24-C25-C30
19	J	4013	BCR	C1-C6-C7-C8
19	J	4013	BCR	C23-C24-C25-C30
19	J	4015	BCR	C23-C24-C25-C26
19	K	4001	BCR	C5-C6-C7-C8
19	K	4005	BCR	C1-C6-C7-C8
19	K	4005	BCR	C5-C6-C7-C8
19	K	4005	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
19	L	4019	BCR	C5-C6-C7-C8
19	L	4019	BCR	C23-C24-C25-C26
19	L	4019	BCR	C23-C24-C25-C30
19	L	4022	BCR	C5-C6-C7-C8
19	Q	4016	BCR	C5-C6-C7-C8
19	Q	4016	BCR	C23-C24-C25-C26
19	S	4012	BCR	C23-C24-C25-C26
19	S	4013	BCR	C1-C6-C7-C8
19	S	4015	BCR	C5-C6-C7-C8
19	S	4015	BCR	C23-C24-C25-C26
19	T	4001	BCR	C5-C6-C7-C8
19	T	4001	BCR	C23-C24-C25-C26
19	T	4005	BCR	C5-C6-C7-C8
19	T	4005	BCR	C23-C24-C25-C26
19	U	4019	BCR	C5-C6-C7-C8
19	U	4022	BCR	C23-C24-C25-C26
19	W	601	BCR	C5-C6-C7-C8
19	W	603	BCR	C5-C6-C7-C8
19	W	603	BCR	C23-C24-C25-C26
19	W	604	BCR	C5-C6-C7-C8
19	W	604	BCR	C23-C24-C25-C30
19	X	601	BCR	C5-C6-C7-C8
19	X	601	BCR	C23-C24-C25-C26
19	X	601	BCR	C23-C24-C25-C30
19	X	602	BCR	C5-C6-C7-C8
19	X	602	BCR	C23-C24-C25-C26
19	X	602	BCR	C23-C24-C25-C30
19	X	603	BCR	C23-C24-C25-C26
19	X	604	BCR	C5-C6-C7-C8
19	X	604	BCR	C23-C24-C25-C26
19	Y	602	BCR	C5-C6-C7-C8
19	Y	602	BCR	C23-C24-C25-C26
19	Y	603	BCR	C5-C6-C7-C8
19	Z	602	BCR	C5-C6-C7-C8
19	Z	603	BCR	C5-C6-C7-C8
19	Z	603	BCR	C23-C24-C25-C26
19	Z	604	BCR	C23-C24-C25-C26
19	a	4002	BCR	C5-C6-C7-C8
19	a	4002	BCR	C23-C24-C25-C30
19	a	4003	BCR	C23-C24-C25-C30
19	a	4007	BCR	C5-C6-C7-C8
19	a	4007	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
19	a	4008	BCR	C5-C6-C7-C8
19	b	4004	BCR	C5-C6-C7-C8
19	b	4004	BCR	C23-C24-C25-C26
19	b	4005	BCR	C5-C6-C7-C8
19	b	4005	BCR	C23-C24-C25-C30
19	b	4009	BCR	C23-C24-C25-C26
19	b	4010	BCR	C5-C6-C7-C8
19	b	4010	BCR	C23-C24-C25-C30
19	b	4014	BCR	C1-C6-C7-C8
19	b	4014	BCR	C5-C6-C7-C8
19	b	4017	BCR	C5-C6-C7-C8
19	b	4017	BCR	C23-C24-C25-C30
19	f	4016	BCR	C5-C6-C7-C8
19	f	4016	BCR	C23-C24-C25-C26
19	f	4016	BCR	C23-C24-C25-C30
19	g	601	BCR	C1-C6-C7-C8
19	g	601	BCR	C5-C6-C7-C8
19	g	601	BCR	C23-C24-C25-C26
19	g	602	BCR	C5-C6-C7-C8
19	g	602	BCR	C23-C24-C25-C26
19	g	602	BCR	C23-C24-C25-C30
19	g	603	BCR	C23-C24-C25-C26
19	g	604	BCR	C5-C6-C7-C8
19	h	603	BCR	C5-C6-C7-C8
19	h	603	BCR	C23-C24-C25-C26
19	h	604	BCR	C5-C6-C7-C8
19	i	4018	BCR	C1-C6-C7-C8
19	j	4012	BCR	C23-C24-C25-C26
19	j	4013	BCR	C23-C24-C25-C26
19	j	4015	BCR	C5-C6-C7-C8
19	j	4015	BCR	C23-C24-C25-C26
19	k	4001	BCR	C5-C6-C7-C8
19	k	4001	BCR	C23-C24-C25-C26
19	k	4005	BCR	C5-C6-C7-C8
19	k	4005	BCR	C23-C24-C25-C26
19	l	4019	BCR	C5-C6-C7-C8
19	l	4022	BCR	C23-C24-C25-C26
19	n	601	BCR	C5-C6-C7-C8
19	n	601	BCR	C23-C24-C25-C26
19	n	603	BCR	C5-C6-C7-C8
19	n	603	BCR	C23-C24-C25-C26
19	n	604	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	n	604	BCR	C23-C24-C25-C30
19	o	601	BCR	C5-C6-C7-C8
19	o	601	BCR	C23-C24-C25-C30
19	o	602	BCR	C5-C6-C7-C8
19	o	602	BCR	C23-C24-C25-C26
19	o	603	BCR	C5-C6-C7-C8
19	o	603	BCR	C23-C24-C25-C26
19	p	601	BCR	C5-C6-C7-C8
19	p	602	BCR	C5-C6-C7-C8
19	p	602	BCR	C23-C24-C25-C26
19	p	603	BCR	C5-C6-C7-C8
19	p	603	BCR	C23-C24-C25-C26
19	q	602	BCR	C5-C6-C7-C8
19	q	602	BCR	C23-C24-C25-C30
19	q	603	BCR	C5-C6-C7-C8
19	q	603	BCR	C23-C24-C25-C26
19	q	604	BCR	C23-C24-C25-C26
19	r	601	BCR	C5-C6-C7-C8
19	r	601	BCR	C23-C24-C25-C30
19	r	602	BCR	C5-C6-C7-C8
19	r	602	BCR	C23-C24-C25-C30
19	r	603	BCR	C23-C24-C25-C26
19	r	604	BCR	C5-C6-C7-C8
19	r	604	BCR	C23-C24-C25-C26
19	s	602	BCR	C5-C6-C7-C8
19	s	602	BCR	C23-C24-C25-C26
19	s	603	BCR	C5-C6-C7-C8
19	s	603	BCR	C23-C24-C25-C26
19	t	601	BCR	C5-C6-C7-C8
19	t	601	BCR	C23-C24-C25-C26
19	t	603	BCR	C23-C24-C25-C26
19	t	604	BCR	C5-C6-C7-C8
19	t	604	BCR	C23-C24-C25-C26
19	u	601	BCR	C5-C6-C7-C8
19	u	601	BCR	C23-C24-C25-C30
19	u	602	BCR	C5-C6-C7-C8
19	u	602	BCR	C23-C24-C25-C26
19	u	603	BCR	C5-C6-C7-C8
19	u	603	BCR	C23-C24-C25-C26
19	u	604	BCR	C1-C6-C7-C8
19	v	601	BCR	C5-C6-C7-C8
19	v	603	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	v	603	BCR	C23-C24-C25-C30
19	v	604	BCR	C5-C6-C7-C8
19	w	602	BCR	C5-C6-C7-C8
19	w	602	BCR	C23-C24-C25-C30
19	w	603	BCR	C5-C6-C7-C8
19	w	603	BCR	C23-C24-C25-C26
19	w	604	BCR	C23-C24-C25-C26
19	x	601	BCR	C5-C6-C7-C8
19	x	601	BCR	C23-C24-C25-C26
19	x	602	BCR	C5-C6-C7-C8
19	x	602	BCR	C23-C24-C25-C30
19	x	603	BCR	C23-C24-C25-C26
19	x	604	BCR	C5-C6-C7-C8
19	x	604	BCR	C23-C24-C25-C26
19	y	603	BCR	C1-C6-C7-C8
19	y	603	BCR	C5-C6-C7-C8
19	y	603	BCR	C23-C24-C25-C26
21	G	4006	ECH	C23-C24-C25-C30
21	V	4021	ECH	C5-C6-C7-C8
21	V	4021	ECH	C23-C24-C25-C30
21	b	4006	ECH	C1-C6-C7-C8
21	m	4021	ECH	C23-C24-C25-C30
16	p	503	CLA	C4C-C3C-CAC-CBC
16	j	1302	CLA	CAA-CBA-CGA-O2A
16	w	509	CLA	C13-C15-C16-C17
13	G	4018	LHG	C2-C3-O3-P
13	u	605	LHG	C2-C3-O3-P
16	h	511	CLA	C16-C17-C18-C20
16	G	1228	CLA	C5-C6-C7-C8
16	A	1134	CLA	CAA-CBA-CGA-O2A
16	U	1503	CLA	C4-C3-C5-C6
16	a	1124	CLA	C4-C3-C5-C6
16	a	1138	CLA	C4-C3-C5-C6
16	b	1238	CLA	C4-C3-C5-C6
16	g	517	CLA	C4-C3-C5-C6
16	o	508	CLA	C4-C3-C5-C6
16	r	514	CLA	O1D-CGD-O2D-CED
14	A	4101	LMG	C31-C32-C33-C34
16	S	1302	CLA	CAA-CBA-CGA-O2A
16	j	1302	CLA	CAA-CBA-CGA-O1A
16	Y	516	CLA	O1A-CGA-O2A-C1
19	k	4001	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	A	1104	CLA	C12-C13-C15-C16
16	A	1138	CLA	C11-C10-C8-C7
16	A	1237	CLA	C11-C10-C8-C7
16	B	1023	CLA	C11-C10-C8-C7
16	G	1202	CLA	C11-C12-C13-C15
16	G	1225	CLA	C12-C13-C15-C16
16	G	1226	CLA	C6-C7-C8-C10
16	X	511	CLA	C11-C10-C8-C7
16	Y	509	CLA	C6-C7-C8-C10
16	Z	504	CLA	C6-C7-C8-C10
16	Z	506	CLA	C6-C7-C8-C10
16	b	1235	CLA	C12-C13-C15-C16
16	b	1238	CLA	C6-C7-C8-C10
16	g	504	CLA	C11-C10-C8-C7
16	g	506	CLA	C6-C7-C8-C10
16	g	511	CLA	C12-C13-C15-C16
16	h	509	CLA	C6-C7-C8-C10
16	r	506	CLA	C6-C7-C8-C10
16	s	504	CLA	C12-C13-C15-C16
16	w	511	CLA	C12-C13-C15-C16
16	x	506	CLA	C6-C7-C8-C10
16	x	507	CLA	C11-C10-C8-C7
16	y	505	CLA	C11-C10-C8-C7
16	H	1136	CLA	C2A-CAA-CBA-CGA
16	b	1203	CLA	C2A-CAA-CBA-CGA
16	b	1221	CLA	C2A-CAA-CBA-CGA
16	r	510	CLA	C2A-CAA-CBA-CGA
16	x	510	CLA	C2A-CAA-CBA-CGA
16	p	509	CLA	O1D-CGD-O2D-CED
13	B	4018	LHG	C23-C24-C25-C26
16	G	1205	CLA	C15-C16-C17-C18
16	L	1503	CLA	C10-C11-C12-C13
13	H	849	LHG	O7-C5-C6-O8
13	I	103	LHG	O7-C5-C6-O8
13	a	849	LHG	O7-C5-C6-O8
16	A	1113	CLA	CAA-CBA-CGA-O2A
16	o	513	CLA	C4C-C3C-CAC-CBC
16	A	1115	CLA	C5-C6-C7-C8
16	n	501	CLA	CAA-CBA-CGA-O2A
16	a	1114	CLA	O1A-CGA-O2A-C1
16	b	1239	CLA	C5-C6-C7-C8
16	x	506	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
16	y	517	CLA	C6-C7-C8-C9
16	H	1102	CLA	C11-C10-C8-C7
16	H	1101	CLA	C5-C6-C7-C8
19	j	4015	BCR	C11-C12-C13-C35
16	a	1133	CLA	O1A-CGA-O2A-C1
16	b	1218	CLA	C4-C3-C5-C6
16	u	505	CLA	C4-C3-C5-C6
16	v	517	CLA	C4-C3-C5-C6
16	A	1101	CLA	CBD-CGD-O2D-CED
16	n	509	CLA	CBA-CGA-O2A-C1
16	H	1116	CLA	CAA-CBA-CGA-O2A
16	y	509	CLA	CAA-CBA-CGA-O2A
16	B	1211	CLA	C15-C16-C17-C18
16	A	1115	CLA	C2-C3-C5-C6
16	H	1104	CLA	C2-C3-C5-C6
16	H	1110	CLA	C2-C3-C5-C6
16	a	1124	CLA	C2-C3-C5-C6
16	a	1138	CLA	C2-C3-C5-C6
16	n	516	CLA	O1D-CGD-O2D-CED
16	o	510	CLA	O1D-CGD-O2D-CED
16	Y	507	CLA	C2-C1-O2A-CGA
16	X	512	CLA	CBD-CGD-O2D-CED
16	r	514	CLA	CBD-CGD-O2D-CED
16	a	1139	CLA	C6-C7-C8-C9
16	b	1223	CLA	C10-C11-C12-C13
16	a	1133	CLA	CBA-CGA-O2A-C1
13	i	103	LHG	C9-C10-C11-C12
16	g	510	CLA	C2A-CAA-CBA-CGA
16	r	502	CLA	C2A-CAA-CBA-CGA
16	J	1302	CLA	CAA-CBA-CGA-O2A
16	A	1013	CLA	C11-C10-C8-C9
16	B	1023	CLA	C11-C10-C8-C9
16	G	1226	CLA	C11-C10-C8-C9
16	a	1104	CLA	C11-C12-C13-C14
16	h	512	CLA	C6-C7-C8-C9
16	q	507	CLA	C14-C13-C15-C16
16	H	1117	CLA	C8-C10-C11-C12
16	A	1123	CLA	C4C-C3C-CAC-CBC
19	Q	4016	BCR	C9-C10-C11-C12
19	o	604	BCR	C13-C14-C15-C16
19	q	604	BCR	C15-C16-C17-C18
21	m	4021	ECH	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
16	A	1139	CLA	C8-C10-C11-C12
16	Z	509	CLA	C8-C10-C11-C12
16	Z	515	CLA	C15-C16-C17-C18
14	G	848	LMG	C17-C18-C19-C20
16	A	1104	CLA	C4-C3-C5-C6
16	B	1206	CLA	C4-C3-C5-C6
16	B	1224	CLA	C4-C3-C5-C6
16	Y	505	CLA	C4-C3-C5-C6
16	b	1225	CLA	C4-C3-C5-C6
16	b	1235	CLA	C4-C3-C5-C6
16	g	504	CLA	C4-C3-C5-C6
16	s	509	CLA	C4-C3-C5-C6
17	H	2001	PQN	C14-C13-C15-C16
16	A	1128	CLA	C13-C15-C16-C17
16	G	1225	CLA	C5-C6-C7-C8
16	H	1104	CLA	C15-C16-C17-C18
16	b	1232	CLA	CAA-CBA-CGA-O2A
16	A	1104	CLA	C2-C3-C5-C6
16	G	1202	CLA	C2-C3-C5-C6
16	v	517	CLA	C2-C3-C5-C6
16	H	1022	CLA	O1D-CGD-O2D-CED
16	n	509	CLA	O1A-CGA-O2A-C1
16	A	1103	CLA	C3-C5-C6-C7
16	b	1214	CLA	O1D-CGD-O2D-CED
16	G	1205	CLA	C10-C11-C12-C13
16	a	1136	CLA	C5-C6-C7-C8
13	R	103	LHG	C9-C10-C11-C12
16	q	504	CLA	CAA-CBA-CGA-O2A
13	a	851	LHG	C4-C5-C6-O8
16	B	1208	CLA	CAA-CBA-CGA-O2A
16	a	1108	CLA	CAA-CBA-CGA-O2A
16	B	1220	CLA	C2C-C3C-CAC-CBC
14	H	852	LMG	O10-C28-O8-C9
16	H	1013	CLA	C2A-CAA-CBA-CGA
16	X	502	CLA	C2A-CAA-CBA-CGA
16	Y	517	CLA	C2A-CAA-CBA-CGA
16	a	1115	CLA	C2A-CAA-CBA-CGA
16	r	511	CLA	C2A-CAA-CBA-CGA
16	s	504	CLA	C2A-CAA-CBA-CGA
16	H	1119	CLA	C16-C17-C18-C20
16	Z	508	CLA	C6-C7-C8-C10
16	A	1801	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	B	1202	CLA	CAA-CBA-CGA-O2A
16	b	1210	CLA	CBD-CGD-O2D-CED
13	a	849	LHG	O10-C23-O8-C6
16	A	1133	CLA	C4-C3-C5-C6
16	A	1138	CLA	C4-C3-C5-C6
16	g	506	CLA	C4-C3-C5-C6
16	o	515	CLA	C4-C3-C5-C6
16	x	506	CLA	C4-C3-C5-C6
16	h	509	CLA	CAA-CBA-CGA-O1A
16	H	1138	CLA	CAA-CBA-CGA-O2A
16	Z	504	CLA	CAA-CBA-CGA-O2A
16	b	1202	CLA	CAA-CBA-CGA-O2A
16	g	503	CLA	CAA-CBA-CGA-O2A
16	A	1104	CLA	C15-C16-C17-C18
16	A	1104	CLA	C4B-C3B-CAB-CBB
16	B	1210	CLA	C4B-C3B-CAB-CBB
16	G	1211	CLA	C4B-C3B-CAB-CBB
16	G	1218	CLA	C4B-C3B-CAB-CBB
16	G	1223	CLA	C4B-C3B-CAB-CBB
16	G	1236	CLA	C4B-C3B-CAB-CBB
16	H	1120	CLA	C4B-C3B-CAB-CBB
16	H	1132	CLA	C4B-C3B-CAB-CBB
16	K	4004	CLA	C4B-C3B-CAB-CBB
16	X	516	CLA	C4B-C3B-CAB-CBB
16	X	517	CLA	C4B-C3B-CAB-CBB
16	Y	516	CLA	C4B-C3B-CAB-CBB
16	Z	505	CLA	C4B-C3B-CAB-CBB
16	a	1104	CLA	C4B-C3B-CAB-CBB
16	a	1125	CLA	C4B-C3B-CAB-CBB
16	b	1224	CLA	C4B-C3B-CAB-CBB
16	g	510	CLA	C4B-C3B-CAB-CBB
16	h	505	CLA	C4B-C3B-CAB-CBB
16	h	510	CLA	C4B-C3B-CAB-CBB
16	o	516	CLA	C4B-C3B-CAB-CBB
16	o	517	CLA	C4B-C3B-CAB-CBB
16	p	516	CLA	C4B-C3B-CAB-CBB
16	q	515	CLA	C4B-C3B-CAB-CBB
16	q	516	CLA	C4B-C3B-CAB-CBB
16	s	504	CLA	C4B-C3B-CAB-CBB
16	s	510	CLA	C4B-C3B-CAB-CBB
16	u	507	CLA	C4B-C3B-CAB-CBB
16	u	509	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	u	516	CLA	C4B-C3B-CAB-CBB
16	u	517	CLA	C4B-C3B-CAB-CBB
16	v	511	CLA	C4B-C3B-CAB-CBB
16	y	513	CLA	C4B-C3B-CAB-CBB
16	B	1235	CLA	C5-C6-C7-C8
16	A	1125	CLA	O1A-CGA-O2A-C1
16	A	1139	CLA	O1A-CGA-O2A-C1
16	r	504	CLA	O1A-CGA-O2A-C1
16	p	504	CLA	CAA-CBA-CGA-O2A
16	s	514	CLA	CAA-CBA-CGA-O2A
16	r	509	CLA	C4C-C3C-CAC-CBC
16	B	1213	CLA	O1A-CGA-O2A-C1
16	B	1215	CLA	C11-C12-C13-C14
16	h	509	CLA	C16-C17-C18-C19
16	y	515	CLA	C16-C17-C18-C19
14	A	4201	LMG	O9-C10-O7-C8
16	r	513	CLA	O1A-CGA-O2A-C1
16	x	516	CLA	O1A-CGA-O2A-C1
13	X	605	LHG	C1-C2-C3-O3
15	A	1011	CL0	CHA-CBD-CGD-O1D
15	A	1011	CL0	CHA-CBD-CGD-O2D
15	H	1011	CL0	CHA-CBD-CGD-O2D
15	a	1011	CL0	CHA-CBD-CGD-O1D
15	a	1011	CL0	CHA-CBD-CGD-O2D
19	H	4002	BCR	C11-C10-C9-C34
19	Z	604	BCR	C16-C17-C18-C36
19	x	603	BCR	C20-C21-C22-C37
16	B	1206	CLA	C8-C10-C11-C12
16	B	1223	CLA	C10-C11-C12-C13
16	x	510	CLA	C13-C15-C16-C17
20	L	4101	LMT	O1'-C1-C2-C3
16	B	1231	CLA	CAA-CBA-CGA-O2A
16	H	1134	CLA	CAA-CBA-CGA-O1A
13	B	4018	LHG	O6-C4-C5-C6
13	Y	605	LHG	O6-C4-C5-C6
16	A	1128	CLA	C16-C17-C18-C19
16	q	505	CLA	C16-C17-C18-C19
16	H	1139	CLA	C4-C3-C5-C6
16	b	1224	CLA	C4-C3-C5-C6
13	g	605	LHG	C11-C10-C9-C8
16	w	515	CLA	C10-C11-C12-C13
16	H	1134	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	k	4003	CLA	CAA-CBA-CGA-O2A
14	B	848	LMG	C11-C10-O7-C8
13	o	605	LHG	C2-C3-O3-P
16	A	1013	CLA	C11-C10-C8-C7
16	A	1106	CLA	C11-C12-C13-C15
16	G	1226	CLA	C11-C10-C8-C7
16	H	1237	CLA	C11-C10-C8-C7
16	W	511	CLA	C6-C7-C8-C10
16	h	512	CLA	C6-C7-C8-C10
16	r	510	CLA	C6-C7-C8-C10
16	v	511	CLA	C6-C7-C8-C10
16	a	1134	CLA	O1D-CGD-O2D-CED
16	b	1210	CLA	O1D-CGD-O2D-CED
16	a	1112	CLA	CAA-CBA-CGA-O2A
16	a	1801	CLA	O1A-CGA-O2A-C1
19	t	604	BCR	C15-C16-C17-C18
19	x	603	BCR	C9-C10-C11-C12
21	V	4021	ECH	C15-C16-C17-C18
16	U	1503	CLA	C13-C15-C16-C17
16	B	1210	CLA	C4C-C3C-CAC-CBC
14	A	4201	LMG	C10-C11-C12-C13
16	J	1302	CLA	CAA-CBA-CGA-O1A
16	p	514	CLA	CAA-CBA-CGA-O1A
16	A	1104	CLA	C11-C12-C13-C14
16	B	1021	CLA	C11-C10-C8-C9
16	B	1204	CLA	C14-C13-C15-C16
16	B	1207	CLA	C11-C12-C13-C14
16	G	1221	CLA	C11-C12-C13-C14
16	L	1503	CLA	C11-C10-C8-C9
16	Y	504	CLA	C6-C7-C8-C9
16	Y	511	CLA	C11-C12-C13-C14
16	Z	515	CLA	C11-C12-C13-C14
16	b	1204	CLA	C14-C13-C15-C16
16	g	507	CLA	C11-C10-C8-C9
16	p	512	CLA	C11-C12-C13-C14
16	r	507	CLA	C11-C10-C8-C9
16	r	507	CLA	C14-C13-C15-C16
16	r	510	CLA	C6-C7-C8-C9
16	s	507	CLA	C11-C10-C8-C9
16	s	511	CLA	C6-C7-C8-C9
16	u	507	CLA	C6-C7-C8-C9
16	u	512	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	v	505	CLA	C11-C10-C8-C9
16	y	505	CLA	C11-C12-C13-C14
16	y	515	CLA	C11-C12-C13-C14
17	B	2002	PQN	C24-C23-C25-C26
14	H	852	LMG	C33-C34-C35-C36
14	G	848	LMG	O10-C28-O8-C9
14	Q	4017	LMG	C8-C7-O1-C1
14	f	4017	LMG	C8-C7-O1-C1
16	a	1134	CLA	CBD-CGD-O2D-CED
16	x	514	CLA	CAA-CBA-CGA-O2A
16	t	514	CLA	CAA-CBA-CGA-O1A
16	G	1217	CLA	CAA-CBA-CGA-O2A
16	a	1108	CLA	CAA-CBA-CGA-O1A
16	A	1124	CLA	C2A-CAA-CBA-CGA
16	a	1013	CLA	C2A-CAA-CBA-CGA
16	o	514	CLA	C2A-CAA-CBA-CGA
16	v	517	CLA	C2A-CAA-CBA-CGA
16	B	1012	CLA	C2-C1-O2A-CGA
16	B	1206	CLA	C2-C1-O2A-CGA
16	G	1214	CLA	C2-C1-O2A-CGA
16	W	505	CLA	C2-C1-O2A-CGA
16	Y	506	CLA	C2-C1-O2A-CGA
16	a	1104	CLA	C2-C1-O2A-CGA
16	b	1239	CLA	C2-C1-O2A-CGA
16	p	515	CLA	C2-C1-O2A-CGA
16	r	514	CLA	C2-C1-O2A-CGA
16	s	506	CLA	C2-C1-O2A-CGA
16	s	507	CLA	C2-C1-O2A-CGA
16	s	517	CLA	C2-C1-O2A-CGA
16	u	515	CLA	C2-C1-O2A-CGA
16	v	502	CLA	C2-C1-O2A-CGA
16	h	509	CLA	C16-C17-C18-C20
16	y	515	CLA	C16-C17-C18-C20
16	G	1207	CLA	C15-C16-C17-C18
16	H	1140	CLA	C10-C11-C12-C13
16	Z	507	CLA	C5-C6-C7-C8
16	A	1125	CLA	CBA-CGA-O2A-C1
16	A	1113	CLA	C3A-C2A-CAA-CBA
16	A	1114	CLA	C3A-C2A-CAA-CBA
16	A	1140	CLA	C3A-C2A-CAA-CBA
16	B	1228	CLA	C3A-C2A-CAA-CBA
16	H	1103	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	W	503	CLA	C3A-C2A-CAA-CBA
16	a	1139	CLA	C3A-C2A-CAA-CBA
16	a	1237	CLA	C3A-C2A-CAA-CBA
16	b	1208	CLA	C3A-C2A-CAA-CBA
16	b	1234	CLA	C3A-C2A-CAA-CBA
16	g	504	CLA	C3A-C2A-CAA-CBA
16	h	504	CLA	C3A-C2A-CAA-CBA
16	o	501	CLA	C3A-C2A-CAA-CBA
16	p	512	CLA	C3A-C2A-CAA-CBA
16	u	511	CLA	C3A-C2A-CAA-CBA
16	B	1208	CLA	CAA-CBA-CGA-O1A
16	B	1209	CLA	CAA-CBA-CGA-O2A
16	Y	503	CLA	C4C-C3C-CAC-CBC
16	h	511	CLA	C3-C5-C6-C7
16	B	1217	CLA	CAA-CBA-CGA-O2A
16	T	4003	CLA	CAA-CBA-CGA-O2A
16	b	1234	CLA	CBD-CGD-O2D-CED
16	p	517	CLA	CBD-CGD-O2D-CED
16	B	1213	CLA	CBA-CGA-O2A-C1
16	B	1021	CLA	CAA-CBA-CGA-O2A
16	a	1133	CLA	CAA-CBA-CGA-O2A
16	a	1138	CLA	CAA-CBA-CGA-O2A
16	r	514	CLA	CAA-CBA-CGA-O2A
14	A	4101	LMG	C7-C8-O7-C10
14	H	4101	LMG	C9-C8-O7-C10
14	a	4101	LMG	C9-C8-O7-C10
16	Y	506	CLA	O1A-CGA-O2A-C1
19	A	4002	BCR	C10-C11-C12-C13
19	R	4018	BCR	C10-C11-C12-C13
19	W	603	BCR	C18-C19-C20-C21
19	i	4018	BCR	C10-C11-C12-C13
19	r	601	BCR	C18-C19-C20-C21
16	B	1230	CLA	CAA-CBA-CGA-O2A
16	B	1225	CLA	C5-C6-C7-C8
16	A	1138	CLA	CAA-CBA-CGA-O2A
16	K	4003	CLA	CAA-CBA-CGA-O2A
16	b	1232	CLA	CAA-CBA-CGA-O1A
16	b	1220	CLA	C5-C6-C7-C8
16	u	504	CLA	C4C-C3C-CAC-CBC
14	A	852	LMG	C36-C37-C38-C39
16	B	1231	CLA	CAA-CBA-CGA-O1A
20	L	4101	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
16	A	1139	CLA	CBA-CGA-O2A-C1
16	r	504	CLA	CBA-CGA-O2A-C1
13	A	849	LHG	C26-C27-C28-C29
16	y	511	CLA	C8-C10-C11-C12
13	Y	605	LHG	O10-C23-O8-C6
15	a	1011	CL0	C16-C17-C18-C20
16	H	1126	CLA	C16-C17-C18-C20
16	q	505	CLA	C16-C17-C18-C20
19	X	603	BCR	C11-C10-C9-C8
16	B	1217	CLA	CAA-CBA-CGA-O1A
16	X	509	CLA	C4C-C3C-CAC-CBC
16	H	1140	CLA	C8-C10-C11-C12
17	H	2001	PQN	C20-C21-C22-C23
13	X	605	LHG	C2-C3-O3-P
13	u	605	LHG	C1-C2-C3-O3
16	a	1102	CLA	CBD-CGD-O2D-CED
16	A	1140	CLA	O1D-CGD-O2D-CED
19	A	4002	BCR	C22-C23-C24-C25
19	X	604	BCR	C22-C23-C24-C25
19	q	603	BCR	C22-C23-C24-C25
16	Z	504	CLA	C10-C11-C12-C13
16	b	1205	CLA	C15-C16-C17-C18
16	n	515	CLA	C15-C16-C17-C18
16	p	509	CLA	C8-C10-C11-C12
16	y	511	CLA	C5-C6-C7-C8
16	K	4003	CLA	CAA-CBA-CGA-O1A
13	I	103	LHG	C4-C5-C6-O8
13	g	605	LHG	C4-C5-C6-O8
13	x	605	LHG	C4-C5-C6-O8
14	A	4101	LMG	C7-C8-C9-O8
14	A	4201	LMG	C7-C8-C9-O8
14	B	848	LMG	O1-C7-C8-C9
16	o	517	CLA	O1A-CGA-O2A-C1
16	w	509	CLA	C8-C10-C11-C12
16	o	509	CLA	CAA-CBA-CGA-O2A
16	h	501	CLA	O1A-CGA-O2A-C1
16	G	1217	CLA	CAA-CBA-CGA-O1A
16	w	501	CLA	C4C-C3C-CAC-CBC
16	G	1225	CLA	C4-C3-C5-C6
16	p	505	CLA	C4-C3-C5-C6
16	x	515	CLA	C4-C3-C5-C6
19	w	603	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	a	1126	CLA	C3-C5-C6-C7
16	B	1240	CLA	C4C-C3C-CAC-CBC
16	W	515	CLA	O1D-CGD-O2D-CED
16	B	1221	CLA	C16-C17-C18-C19
16	a	1117	CLA	C13-C15-C16-C17
16	B	1209	CLA	CAA-CBA-CGA-O1A
16	a	1112	CLA	CAA-CBA-CGA-O1A
16	B	1206	CLA	CAA-CBA-CGA-O2A
14	B	848	LMG	C35-C36-C37-C38
16	U	1502	CLA	C3-C5-C6-C7
16	w	506	CLA	C3-C5-C6-C7
16	A	1116	CLA	C5-C6-C7-C8
14	A	852	LMG	O1-C7-C8-O7
14	A	4101	LMG	O7-C8-C9-O8
16	B	1230	CLA	CAA-CBA-CGA-O1A
16	T	4003	CLA	CAA-CBA-CGA-O1A
16	q	504	CLA	C10-C11-C12-C13
19	G	4010	BCR	C14-C15-C16-C17
16	A	1103	CLA	C11-C10-C8-C9
16	A	1109	CLA	C11-C12-C13-C14
16	A	1132	CLA	C6-C7-C8-C9
16	L	1502	CLA	C6-C7-C8-C9
16	W	515	CLA	C14-C13-C15-C16
16	Y	507	CLA	C11-C10-C8-C9
16	a	1126	CLA	C6-C7-C8-C9
16	a	1128	CLA	C14-C13-C15-C16
16	a	1132	CLA	C6-C7-C8-C9
16	a	1138	CLA	C11-C10-C8-C9
16	r	504	CLA	C14-C13-C15-C16
16	v	512	CLA	C6-C7-C8-C9
17	G	2002	PQN	C24-C23-C25-C26
17	a	2001	PQN	C21-C22-C23-C24
16	H	1110	CLA	CAA-CBA-CGA-O2A
16	n	509	CLA	CAA-CBA-CGA-O2A
16	y	507	CLA	CAA-CBA-CGA-O2A
16	r	503	CLA	CAA-CBA-CGA-O1A
16	B	1212	CLA	CAA-CBA-CGA-O2A
16	b	1208	CLA	CAA-CBA-CGA-O2A
16	k	4003	CLA	CAA-CBA-CGA-O1A
19	n	603	BCR	C11-C12-C13-C14
19	o	602	BCR	C7-C8-C9-C10
16	l	1503	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	u	515	CLA	C13-C15-C16-C17
16	A	1139	CLA	C4-C3-C5-C6
16	l	1503	CLA	C4-C3-C5-C6
16	b	1226	CLA	CAA-CBA-CGA-O2A
16	u	514	CLA	CAA-CBA-CGA-O2A
16	b	1225	CLA	CBA-CGA-O2A-C1
16	A	1121	CLA	C2A-CAA-CBA-CGA
16	Y	503	CLA	C2A-CAA-CBA-CGA
16	q	513	CLA	C2A-CAA-CBA-CGA
16	A	1013	CLA	C6-C7-C8-C10
16	A	1104	CLA	C11-C12-C13-C15
16	B	1239	CLA	C11-C10-C8-C7
16	H	1101	CLA	C12-C13-C15-C16
16	L	1503	CLA	C11-C10-C8-C7
16	W	510	CLA	C11-C10-C8-C7
16	X	504	CLA	C6-C7-C8-C10
16	X	505	CLA	C12-C13-C15-C16
16	Y	504	CLA	C6-C7-C8-C10
16	Z	512	CLA	C6-C7-C8-C10
16	a	1013	CLA	C12-C13-C15-C16
16	a	1104	CLA	C11-C12-C13-C15
16	b	1221	CLA	C11-C12-C13-C15
16	o	512	CLA	C6-C7-C8-C10
16	p	504	CLA	C12-C13-C15-C16
16	p	511	CLA	C11-C12-C13-C15
16	q	507	CLA	C12-C13-C15-C16
16	r	504	CLA	C11-C10-C8-C7
16	r	507	CLA	C12-C13-C15-C16
16	s	511	CLA	C6-C7-C8-C10
16	u	504	CLA	C6-C7-C8-C10
16	v	505	CLA	C11-C10-C8-C7
16	x	504	CLA	C11-C10-C8-C7
16	x	509	CLA	C11-C10-C8-C7
16	y	510	CLA	C6-C7-C8-C10
16	y	515	CLA	C11-C12-C13-C15
17	A	2001	PQN	C16-C17-C18-C20
17	H	2001	PQN	C16-C17-C18-C20
16	Z	515	CLA	C3-C5-C6-C7
15	a	1011	CL0	CAA-CBA-CGA-O1A
16	A	1103	CLA	C2B-C3B-CAB-CBB
16	A	1106	CLA	C2B-C3B-CAB-CBB
16	A	1107	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	A	1120	CLA	C2B-C3B-CAB-CBB
16	A	1128	CLA	C2B-C3B-CAB-CBB
16	A	1139	CLA	C2B-C3B-CAB-CBB
16	B	1213	CLA	C2B-C3B-CAB-CBB
16	B	1228	CLA	C2B-C3B-CAB-CBB
16	G	1204	CLA	C2B-C3B-CAB-CBB
16	H	1107	CLA	C2B-C3B-CAB-CBB
16	H	1115	CLA	C2B-C3B-CAB-CBB
16	H	1117	CLA	C2B-C3B-CAB-CBB
16	H	1126	CLA	C2B-C3B-CAB-CBB
16	H	1127	CLA	C2B-C3B-CAB-CBB
16	H	1128	CLA	C2B-C3B-CAB-CBB
16	Q	1302	CLA	C2B-C3B-CAB-CBB
16	W	511	CLA	C2B-C3B-CAB-CBB
16	W	513	CLA	C2B-C3B-CAB-CBB
16	X	501	CLA	C2B-C3B-CAB-CBB
16	X	514	CLA	C2B-C3B-CAB-CBB
16	X	515	CLA	C2B-C3B-CAB-CBB
16	Y	506	CLA	C2B-C3B-CAB-CBB
16	Y	511	CLA	C2B-C3B-CAB-CBB
16	Z	511	CLA	C2B-C3B-CAB-CBB
16	Z	516	CLA	C2B-C3B-CAB-CBB
16	a	1106	CLA	C2B-C3B-CAB-CBB
16	a	1112	CLA	C2B-C3B-CAB-CBB
16	a	1117	CLA	C2B-C3B-CAB-CBB
16	a	1119	CLA	C2B-C3B-CAB-CBB
16	b	1023	CLA	C2B-C3B-CAB-CBB
16	b	1228	CLA	C2B-C3B-CAB-CBB
16	b	1234	CLA	C2B-C3B-CAB-CBB
16	g	502	CLA	C2B-C3B-CAB-CBB
16	g	511	CLA	C2B-C3B-CAB-CBB
16	g	512	CLA	C2B-C3B-CAB-CBB
16	n	505	CLA	C2B-C3B-CAB-CBB
16	n	506	CLA	C2B-C3B-CAB-CBB
16	n	512	CLA	C2B-C3B-CAB-CBB
16	o	509	CLA	C2B-C3B-CAB-CBB
16	o	511	CLA	C2B-C3B-CAB-CBB
16	p	505	CLA	C2B-C3B-CAB-CBB
16	p	515	CLA	C2B-C3B-CAB-CBB
16	q	511	CLA	C2B-C3B-CAB-CBB
16	r	516	CLA	C2B-C3B-CAB-CBB
16	s	515	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	t	511	CLA	C2B-C3B-CAB-CBB
16	t	513	CLA	C2B-C3B-CAB-CBB
16	u	511	CLA	C2B-C3B-CAB-CBB
16	u	514	CLA	C2B-C3B-CAB-CBB
16	v	509	CLA	C2B-C3B-CAB-CBB
16	x	511	CLA	C2B-C3B-CAB-CBB
19	F	4016	BCR	C23-C24-C25-C26
19	G	4005	BCR	C23-C24-C25-C26
19	G	4005	BCR	C23-C24-C25-C30
19	G	4010	BCR	C23-C24-C25-C26
19	I	4018	BCR	C23-C24-C25-C26
19	I	4018	BCR	C23-C24-C25-C30
19	J	4012	BCR	C23-C24-C25-C26
19	J	4013	BCR	C23-C24-C25-C26
19	J	4015	BCR	C5-C6-C7-C8
19	K	4001	BCR	C23-C24-C25-C26
19	K	4001	BCR	C23-C24-C25-C30
19	R	4018	BCR	C23-C24-C25-C26
19	R	4018	BCR	C23-C24-C25-C30
19	S	4013	BCR	C5-C6-C7-C8
19	U	4022	BCR	C1-C6-C7-C8
19	U	4022	BCR	C5-C6-C7-C8
19	W	604	BCR	C23-C24-C25-C26
19	Y	603	BCR	C23-C24-C25-C26
19	a	4002	BCR	C23-C24-C25-C26
19	a	4003	BCR	C23-C24-C25-C26
19	a	4011	BCR	C1-C6-C7-C8
19	a	4011	BCR	C5-C6-C7-C8
19	b	4005	BCR	C23-C24-C25-C26
19	b	4010	BCR	C23-C24-C25-C26
19	b	4014	BCR	C23-C24-C25-C26
19	b	4014	BCR	C23-C24-C25-C30
19	b	4017	BCR	C23-C24-C25-C26
19	i	4018	BCR	C5-C6-C7-C8
19	i	4018	BCR	C23-C24-C25-C30
19	j	4013	BCR	C1-C6-C7-C8
19	j	4013	BCR	C5-C6-C7-C8
19	l	4022	BCR	C1-C6-C7-C8
19	l	4022	BCR	C5-C6-C7-C8
19	n	604	BCR	C23-C24-C25-C26
19	o	604	BCR	C1-C6-C7-C8
19	o	604	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	o	604	BCR	C23-C24-C25-C26
19	o	604	BCR	C23-C24-C25-C30
19	q	602	BCR	C23-C24-C25-C26
19	r	601	BCR	C23-C24-C25-C26
19	r	602	BCR	C23-C24-C25-C26
19	s	601	BCR	C23-C24-C25-C26
19	s	601	BCR	C23-C24-C25-C30
19	u	601	BCR	C23-C24-C25-C26
19	u	604	BCR	C5-C6-C7-C8
19	u	604	BCR	C23-C24-C25-C26
19	u	604	BCR	C23-C24-C25-C30
19	w	602	BCR	C23-C24-C25-C26
19	x	602	BCR	C23-C24-C25-C26
21	B	4006	ECH	C23-C24-C25-C26
21	G	4006	ECH	C23-C24-C25-C26
21	M	4021	ECH	C23-C24-C25-C30
21	R	4020	ECH	C1-C6-C7-C8
21	V	4021	ECH	C1-C6-C7-C8
21	b	4006	ECH	C5-C6-C7-C8
16	Y	514	CLA	CAA-CBA-CGA-O2A
16	v	501	CLA	CAA-CBA-CGA-O2A
16	x	503	CLA	CAA-CBA-CGA-O2A
13	A	849	LHG	O9-C7-O7-C5
16	A	1104	CLA	C2-C1-O2A-CGA
16	G	1239	CLA	C2-C1-O2A-CGA
16	W	502	CLA	C2-C1-O2A-CGA
16	X	507	CLA	C2-C1-O2A-CGA
16	Z	515	CLA	C2-C1-O2A-CGA
16	g	507	CLA	C2-C1-O2A-CGA
16	h	508	CLA	C2-C1-O2A-CGA
16	p	506	CLA	C2-C1-O2A-CGA
16	p	507	CLA	C2-C1-O2A-CGA
16	q	515	CLA	C2-C1-O2A-CGA
16	r	511	CLA	C2-C1-O2A-CGA
16	x	507	CLA	C2-C1-O2A-CGA
16	X	510	CLA	C11-C12-C13-C15
16	a	1013	CLA	C8-C10-C11-C12
16	h	515	CLA	C13-C15-C16-C17
13	u	605	LHG	C24-C25-C26-C27
16	G	1023	CLA	C8-C10-C11-C12
20	L	4101	LMT	C4-C5-C6-C7
16	A	1110	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	G	1220	CLA	CAA-CBA-CGA-O2A
16	Q	1302	CLA	CAA-CBA-CGA-O2A
20	l	4101	LMT	C2B-C1B-O1B-C4'
13	B	4018	LHG	C15-C16-C17-C18
16	Y	506	CLA	CBA-CGA-O2A-C1
16	a	1013	CLA	CBA-CGA-O2A-C1
16	a	1125	CLA	O1A-CGA-O2A-C1
16	B	1221	CLA	C16-C17-C18-C20
16	v	515	CLA	C16-C17-C18-C20
16	G	1211	CLA	C4-C3-C5-C6
16	H	1119	CLA	C4-C3-C5-C6
13	I	103	LHG	O8-C23-C24-C25
13	R	103	LHG	O8-C23-C24-C25
14	a	4101	LMG	O8-C28-C29-C30
16	A	1101	CLA	CAA-CBA-CGA-O2A
16	A	1133	CLA	CAA-CBA-CGA-O2A
16	L	1501	CLA	CAA-CBA-CGA-O2A
16	n	505	CLA	CAA-CBA-CGA-O2A
16	o	517	CLA	CAA-CBA-CGA-O2A
16	q	507	CLA	CAA-CBA-CGA-O2A
16	A	1139	CLA	C2-C3-C5-C6
16	G	1211	CLA	C2-C3-C5-C6
16	H	1119	CLA	C2-C3-C5-C6
16	H	1139	CLA	C2-C3-C5-C6
16	a	1123	CLA	C2-C3-C5-C6
16	b	1225	CLA	O1A-CGA-O2A-C1
16	F	1302	CLA	O1A-CGA-O2A-C1
16	A	1114	CLA	C4C-C3C-CAC-CBC
16	A	1101	CLA	C2A-CAA-CBA-CGA
16	B	1215	CLA	C2A-CAA-CBA-CGA
16	a	1117	CLA	C2A-CAA-CBA-CGA
16	w	514	CLA	C2A-CAA-CBA-CGA
16	B	1238	CLA	C13-C15-C16-C17
16	W	505	CLA	CAA-CBA-CGA-O2A
16	a	1118	CLA	CAA-CBA-CGA-O2A
16	b	1236	CLA	CAA-CBA-CGA-O2A
16	o	514	CLA	CAA-CBA-CGA-O2A
16	r	513	CLA	CAA-CBA-CGA-O2A
16	v	514	CLA	CAA-CBA-CGA-O2A
16	y	512	CLA	CAA-CBA-CGA-O2A
16	p	517	CLA	O1D-CGD-O2D-CED
16	X	516	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	G	4018	LHG	C15-C16-C17-C18
16	A	1128	CLA	C16-C17-C18-C20
16	A	1123	CLA	C8-C10-C11-C12
13	R	103	LHG	C30-C31-C32-C33
16	b	1226	CLA	O1D-CGD-O2D-CED
16	b	1207	CLA	C15-C16-C17-C18
16	n	509	CLA	C5-C6-C7-C8
16	p	515	CLA	C10-C11-C12-C13
13	A	849	LHG	C25-C26-C27-C28
16	H	1102	CLA	CAA-CBA-CGA-O2A
16	p	505	CLA	CAA-CBA-CGA-O2A
16	s	517	CLA	CAA-CBA-CGA-O2A
16	u	505	CLA	CAA-CBA-CGA-O2A
14	a	4201	LMG	O9-C10-C11-C12
19	B	4004	BCR	C15-C16-C17-C18
20	H	4202	LMT	C4B-C5B-C6B-O6B
16	Z	508	CLA	C6-C7-C8-C9
16	t	509	CLA	C4C-C3C-CAC-CBC
16	H	1022	CLA	C4-C3-C5-C6
19	Y	602	BCR	C10-C11-C12-C13
13	a	851	LHG	O7-C7-C8-C9
16	X	508	CLA	CAA-CBA-CGA-O2A
16	o	502	CLA	CAA-CBA-CGA-O2A
16	t	502	CLA	CAA-CBA-CGA-O2A
16	u	507	CLA	CAA-CBA-CGA-O2A
16	H	1115	CLA	C2-C3-C5-C6
16	b	1220	CLA	C2-C3-C5-C6
16	g	517	CLA	C2-C3-C5-C6
16	Z	502	CLA	O1D-CGD-O2D-CED
16	H	1114	CLA	CBD-CGD-O2D-CED
16	G	1230	CLA	CAA-CBA-CGA-O2A
16	H	1111	CLA	C4C-C3C-CAC-CBC
16	T	4002	CLA	C2A-CAA-CBA-CGA
20	U	4101	LMT	C2B-C1B-O1B-C4'
16	Z	502	CLA	CAA-CBA-CGA-O2A
16	p	510	CLA	CAA-CBA-CGA-O2A
16	x	508	CLA	CAA-CBA-CGA-O2A
13	p	605	LHG	C24-C23-O8-C6
16	o	517	CLA	CBA-CGA-O2A-C1
16	a	1102	CLA	O1A-CGA-O2A-C1
16	G	1202	CLA	C11-C12-C13-C14
16	Y	509	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
16	Y	512	CLA	C11-C12-C13-C14
16	h	509	CLA	C6-C7-C8-C9
16	l	1503	CLA	C14-C13-C15-C16
16	r	510	CLA	C11-C12-C13-C14
16	v	504	CLA	C11-C10-C8-C9
16	a	1104	CLA	C15-C16-C17-C18
16	H	1105	CLA	CAA-CBA-CGA-O2A
16	H	1133	CLA	CAA-CBA-CGA-O2A
16	U	1501	CLA	CAA-CBA-CGA-O2A
16	Y	505	CLA	CAA-CBA-CGA-O2A
16	o	508	CLA	CAA-CBA-CGA-O2A
16	s	510	CLA	CAA-CBA-CGA-O2A
16	t	505	CLA	CAA-CBA-CGA-O2A
14	b	848	LMG	C7-C8-C9-O8
16	y	504	CLA	C8-C10-C11-C12
16	A	1102	CLA	C1A-C2A-CAA-CBA
16	A	1113	CLA	C1A-C2A-CAA-CBA
16	B	1207	CLA	C1A-C2A-CAA-CBA
16	B	1208	CLA	C4B-C3B-CAB-CBB
16	B	1211	CLA	C4B-C3B-CAB-CBB
16	B	1215	CLA	C1A-C2A-CAA-CBA
16	B	1236	CLA	C4B-C3B-CAB-CBB
16	G	1202	CLA	C4B-C3B-CAB-CBB
16	G	1204	CLA	C1A-C2A-CAA-CBA
16	G	1228	CLA	C4B-C3B-CAB-CBB
16	G	1230	CLA	C4B-C3B-CAB-CBB
16	H	1122	CLA	C1A-C2A-CAA-CBA
16	H	1135	CLA	C4B-C3B-CAB-CBB
16	T	4004	CLA	C1A-C2A-CAA-CBA
16	W	512	CLA	C4B-C3B-CAB-CBB
16	X	504	CLA	C4B-C3B-CAB-CBB
16	X	506	CLA	C4B-C3B-CAB-CBB
16	Y	510	CLA	C4B-C3B-CAB-CBB
16	a	1801	CLA	C1A-C2A-CAA-CBA
16	b	1023	CLA	C4B-C3B-CAB-CBB
16	b	1207	CLA	C1A-C2A-CAA-CBA
16	g	504	CLA	C1A-C2A-CAA-CBA
16	h	511	CLA	C4B-C3B-CAB-CBB
16	n	514	CLA	C4B-C3B-CAB-CBB
16	o	509	CLA	C4B-C3B-CAB-CBB
16	p	510	CLA	C4B-C3B-CAB-CBB
16	r	506	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
16	r	514	CLA	C1A-C2A-CAA-CBA
16	r	515	CLA	C1A-C2A-CAA-CBA
16	r	515	CLA	C4B-C3B-CAB-CBB
16	r	517	CLA	C4B-C3B-CAB-CBB
16	s	501	CLA	C1A-C2A-CAA-CBA
16	s	506	CLA	C4B-C3B-CAB-CBB
16	t	504	CLA	C4B-C3B-CAB-CBB
16	t	512	CLA	C4B-C3B-CAB-CBB
16	t	515	CLA	C4B-C3B-CAB-CBB
16	v	505	CLA	C4B-C3B-CAB-CBB
16	v	513	CLA	C4B-C3B-CAB-CBB
16	w	505	CLA	C1A-C2A-CAA-CBA
16	A	1140	CLA	CBD-CGD-O2D-CED
16	W	515	CLA	CBD-CGD-O2D-CED
16	a	1106	CLA	C4-C3-C5-C6
16	a	1123	CLA	C4-C3-C5-C6
16	x	512	CLA	C4-C3-C5-C6
19	p	604	BCR	C22-C23-C24-C25
23	r	606	LMU	O5'-C1'-O1'-C1
13	r	605	LHG	O8-C23-C24-C25
16	A	1118	CLA	CAA-CBA-CGA-O2A
16	W	502	CLA	CAA-CBA-CGA-O2A
16	Y	510	CLA	CAA-CBA-CGA-O2A
16	a	1101	CLA	CAA-CBA-CGA-O2A
16	q	502	CLA	CAA-CBA-CGA-O2A
16	s	505	CLA	CAA-CBA-CGA-O2A
16	w	502	CLA	CAA-CBA-CGA-O2A
16	w	505	CLA	CAA-CBA-CGA-O2A
16	x	510	CLA	CAA-CBA-CGA-O2A
16	b	1238	CLA	C2-C3-C5-C6
13	A	849	LHG	O7-C5-C6-O8
14	A	4201	LMG	O7-C8-C9-O8
19	X	603	BCR	C21-C22-C23-C24
19	g	601	BCR	C11-C12-C13-C14
21	V	4021	ECH	C7-C8-C9-C10
19	B	4017	BCR	C13-C14-C15-C16
19	G	4017	BCR	C9-C10-C11-C12
19	f	4016	BCR	C19-C20-C21-C22
16	W	510	CLA	C15-C16-C17-C18
16	b	1214	CLA	CBD-CGD-O2D-CED
23	x	606	LMU	C6-C7-C8-C9
13	a	851	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
16	a	1125	CLA	CBA-CGA-O2A-C1
13	p	605	LHG	C24-C25-C26-C27
16	G	1208	CLA	CAA-CBA-CGA-O2A
16	G	1219	CLA	CAA-CBA-CGA-O2A
14	A	4101	LMG	O8-C28-C29-C30
16	A	1013	CLA	CAA-CBA-CGA-O2A
16	A	1102	CLA	CAA-CBA-CGA-O2A
16	B	1214	CLA	CAA-CBA-CGA-O2A
16	B	1226	CLA	CAA-CBA-CGA-O2A
16	B	1236	CLA	CAA-CBA-CGA-O2A
16	G	1226	CLA	CAA-CBA-CGA-O2A
16	H	1013	CLA	CAA-CBA-CGA-O2A
16	W	509	CLA	CAA-CBA-CGA-O2A
16	Z	505	CLA	CAA-CBA-CGA-O2A
16	Z	507	CLA	CAA-CBA-CGA-O2A
16	Z	509	CLA	CAA-CBA-CGA-O2A
16	a	1013	CLA	CAA-CBA-CGA-O2A
16	h	501	CLA	CAA-CBA-CGA-O2A
16	l	1501	CLA	CAA-CBA-CGA-O2A
16	o	516	CLA	CAA-CBA-CGA-O2A
16	q	505	CLA	CAA-CBA-CGA-O2A
16	a	1125	CLA	C4C-C3C-CAC-CBC
16	B	1204	CLA	C2A-CAA-CBA-CGA
16	G	1204	CLA	C2A-CAA-CBA-CGA
16	G	1209	CLA	C2A-CAA-CBA-CGA
16	b	1215	CLA	C2A-CAA-CBA-CGA
16	b	1236	CLA	C2A-CAA-CBA-CGA
14	G	848	LMG	C14-C15-C16-C17
16	a	1121	CLA	C4C-C3C-CAC-CBC
16	v	515	CLA	C4C-C3C-CAC-CBC
16	H	1119	CLA	C5-C6-C7-C8
16	b	1021	CLA	C8-C10-C11-C12
16	p	506	CLA	C8-C10-C11-C12
16	q	506	CLA	C8-C10-C11-C12
16	x	505	CLA	C10-C11-C12-C13
16	G	1212	CLA	CAA-CBA-CGA-O2A
16	G	1238	CLA	O1A-CGA-O2A-C1
14	B	848	LMG	C14-C15-C16-C17
16	H	1118	CLA	CAA-CBA-CGA-O2A
16	t	509	CLA	CAA-CBA-CGA-O2A
17	a	2001	PQN	C25-C26-C27-C28
14	b	848	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	B	1212	CLA	CAA-CBA-CGA-O1A
16	A	1121	CLA	C2-C3-C5-C6
16	H	1121	CLA	C2-C3-C5-C6
16	G	1238	CLA	O1D-CGD-O2D-CED
16	q	505	CLA	C4-C3-C5-C6
16	B	1202	CLA	C2-C1-O2A-CGA
16	G	1012	CLA	C2-C1-O2A-CGA
16	G	1206	CLA	C2-C1-O2A-CGA
16	H	1101	CLA	C2-C1-O2A-CGA
16	H	1119	CLA	C2-C1-O2A-CGA
16	a	1107	CLA	C2-C1-O2A-CGA
16	b	1202	CLA	C2-C1-O2A-CGA
16	b	1206	CLA	C2-C1-O2A-CGA
16	g	511	CLA	C2-C1-O2A-CGA
16	h	502	CLA	C2-C1-O2A-CGA
16	h	517	CLA	C2-C1-O2A-CGA
16	n	505	CLA	C2-C1-O2A-CGA
16	o	506	CLA	C2-C1-O2A-CGA
16	o	514	CLA	C2-C1-O2A-CGA
16	r	507	CLA	C2-C1-O2A-CGA
16	w	515	CLA	C2-C1-O2A-CGA
16	B	1207	CLA	CAA-CBA-CGA-O2A
16	B	1207	CLA	C11-C12-C13-C15
16	H	1104	CLA	C12-C13-C15-C16
16	H	1126	CLA	C11-C12-C13-C15
16	H	1138	CLA	C11-C10-C8-C7
16	X	512	CLA	C11-C10-C8-C7
16	Y	504	CLA	C12-C13-C15-C16
16	a	1109	CLA	C6-C7-C8-C10
16	b	1023	CLA	C11-C12-C13-C15
16	b	1202	CLA	C11-C12-C13-C15
16	h	507	CLA	C11-C10-C8-C7
16	o	506	CLA	C11-C10-C8-C7
16	o	515	CLA	C11-C10-C8-C7
16	p	504	CLA	C6-C7-C8-C10
16	p	509	CLA	C6-C7-C8-C10
16	u	507	CLA	C6-C7-C8-C10
16	v	510	CLA	C12-C13-C15-C16
17	B	2002	PQN	C22-C23-C25-C26
16	B	1239	CLA	C8-C10-C11-C12
16	a	1138	CLA	C8-C10-C11-C12
23	x	606	LMU	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
16	u	504	CLA	C11-C12-C13-C14
16	a	1102	CLA	O1D-CGD-O2D-CED
14	H	4101	LMG	C7-C8-O7-C10
16	A	1126	CLA	C5-C6-C7-C8
13	b	4018	LHG	C10-C11-C12-C13
20	H	4202	LMT	C11-C10-C9-C8
16	b	1212	CLA	CAA-CBA-CGA-O2A
16	Y	515	CLA	C8-C10-C11-C12
16	u	515	CLA	C5-C6-C7-C8
16	X	501	CLA	C2A-CAA-CBA-CGA
16	a	1101	CLA	C2A-CAA-CBA-CGA
16	b	1012	CLA	C2A-CAA-CBA-CGA
16	b	1204	CLA	C2A-CAA-CBA-CGA
16	g	517	CLA	C2A-CAA-CBA-CGA
16	o	507	CLA	C5-C6-C7-C8
16	B	1215	CLA	C11-C12-C13-C15
14	B	848	LMG	C33-C34-C35-C36
14	G	848	LMG	C33-C34-C35-C36
13	H	851	LHG	O8-C23-C24-C25
16	G	1239	CLA	C5-C6-C7-C8
16	w	512	CLA	C10-C11-C12-C13
16	y	506	CLA	C5-C6-C7-C8
13	x	605	LHG	O7-C7-C8-C9
16	X	503	CLA	CAA-CBA-CGA-O2A
16	g	509	CLA	CAA-CBA-CGA-O2A
16	r	505	CLA	CAA-CBA-CGA-O2A
16	B	1234	CLA	O1A-CGA-O2A-C1
16	n	511	CLA	C10-C11-C12-C13
16	B	1232	CLA	CAA-CBA-CGA-O1A
16	b	1208	CLA	CAA-CBA-CGA-O1A
16	A	1106	CLA	C4-C3-C5-C6
16	A	1128	CLA	C3A-C2A-CAA-CBA
16	A	1237	CLA	C3A-C2A-CAA-CBA
16	B	1208	CLA	C3A-C2A-CAA-CBA
16	B	1219	CLA	C3A-C2A-CAA-CBA
16	G	1208	CLA	C3A-C2A-CAA-CBA
16	G	1219	CLA	C3A-C2A-CAA-CBA
16	G	1228	CLA	C3A-C2A-CAA-CBA
16	G	1229	CLA	C4-C3-C5-C6
16	H	1101	CLA	C3A-C2A-CAA-CBA
16	H	1108	CLA	C3A-C2A-CAA-CBA
16	H	1112	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
16	W	512	CLA	C3A-C2A-CAA-CBA
16	X	501	CLA	C3A-C2A-CAA-CBA
16	Y	506	CLA	C3A-C2A-CAA-CBA
16	a	1101	CLA	C3A-C2A-CAA-CBA
16	b	1021	CLA	C3A-C2A-CAA-CBA
16	b	1202	CLA	C4-C3-C5-C6
16	b	1226	CLA	C3A-C2A-CAA-CBA
16	b	1235	CLA	C3A-C2A-CAA-CBA
16	p	506	CLA	C3A-C2A-CAA-CBA
16	s	506	CLA	C3A-C2A-CAA-CBA
16	v	514	CLA	C3A-C2A-CAA-CBA
16	y	512	CLA	C3A-C2A-CAA-CBA
16	o	517	CLA	CAA-CBA-CGA-O1A
16	X	515	CLA	C5-C6-C7-C8
16	h	512	CLA	C13-C15-C16-C17
16	q	515	CLA	C8-C10-C11-C12
20	U	4101	LMT	C3-C4-C5-C6
16	b	1021	CLA	CAA-CBA-CGA-O2A
16	b	1218	CLA	C2-C3-C5-C6
16	u	505	CLA	C2-C3-C5-C6
19	b	4010	BCR	C11-C10-C9-C8
19	q	602	BCR	C16-C17-C18-C19
19	s	601	BCR	C20-C21-C22-C23
16	G	1220	CLA	CAA-CBA-CGA-O1A
16	q	508	CLA	CAA-CBA-CGA-O1A
16	r	513	CLA	CAA-CBA-CGA-O1A
16	v	514	CLA	CAA-CBA-CGA-O1A
16	y	509	CLA	O1A-CGA-O2A-C1
13	B	4018	LHG	O6-C4-C5-O7
16	B	1205	CLA	C15-C16-C17-C18
16	A	1104	CLA	CAA-CBA-CGA-O2A
16	u	508	CLA	CAA-CBA-CGA-O2A
16	s	501	CLA	C4C-C3C-CAC-CBC
16	A	1133	CLA	CAA-CBA-CGA-O1A
16	L	1501	CLA	CAA-CBA-CGA-O1A
16	b	1226	CLA	CAA-CBA-CGA-O1A
16	p	505	CLA	CAA-CBA-CGA-O1A
16	u	505	CLA	CAA-CBA-CGA-O1A
16	b	1226	CLA	CBD-CGD-O2D-CED
16	A	1131	CLA	C2A-CAA-CBA-CGA
16	h	517	CLA	C2A-CAA-CBA-CGA
16	b	1231	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	B	1239	CLA	C11-C10-C8-C9
16	B	1239	CLA	C14-C13-C15-C16
16	G	1204	CLA	C6-C7-C8-C9
16	H	1136	CLA	C11-C10-C8-C9
16	W	512	CLA	C11-C10-C8-C9
16	X	512	CLA	C6-C7-C8-C9
16	Z	506	CLA	C6-C7-C8-C9
16	b	1211	CLA	C14-C13-C15-C16
16	b	1235	CLA	C14-C13-C15-C16
16	g	511	CLA	C14-C13-C15-C16
16	n	510	CLA	C14-C13-C15-C16
16	o	515	CLA	C11-C10-C8-C9
16	p	504	CLA	C6-C7-C8-C9
16	p	509	CLA	C6-C7-C8-C9
16	s	507	CLA	C14-C13-C15-C16
16	s	515	CLA	C11-C10-C8-C9
16	w	507	CLA	C14-C13-C15-C16
16	w	511	CLA	C14-C13-C15-C16
16	x	507	CLA	C11-C10-C8-C9
16	x	509	CLA	C11-C10-C8-C9
16	y	509	CLA	C11-C12-C13-C14
17	A	2001	PQN	C16-C17-C18-C19
16	B	1220	CLA	CAA-CBA-CGA-O2A
16	G	1021	CLA	CAA-CBA-CGA-O2A
16	A	1118	CLA	CAA-CBA-CGA-O1A
16	B	1236	CLA	CAA-CBA-CGA-O1A
16	W	514	CLA	CAA-CBA-CGA-O1A
16	X	508	CLA	CAA-CBA-CGA-O1A
16	a	1101	CLA	CAA-CBA-CGA-O1A
16	a	1118	CLA	CAA-CBA-CGA-O1A
16	n	509	CLA	CAA-CBA-CGA-O1A
13	a	849	LHG	C13-C14-C15-C16
16	y	515	CLA	C13-C15-C16-C17
16	H	1114	CLA	O1D-CGD-O2D-CED
20	A	4202	LMT	C11-C10-C9-C8
16	a	1123	CLA	C4C-C3C-CAC-CBC
16	A	1140	CLA	C5-C6-C7-C8
16	G	1225	CLA	C10-C11-C12-C13
16	g	510	CLA	C13-C15-C16-C17
16	t	507	CLA	C5-C6-C7-C8
16	g	513	CLA	C4C-C3C-CAC-CBC
19	q	604	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	X	510	CLA	C4-C3-C5-C6
16	q	508	CLA	C4-C3-C5-C6
16	w	510	CLA	C4-C3-C5-C6
16	A	1101	CLA	CAA-CBA-CGA-O1A
16	H	1105	CLA	CAA-CBA-CGA-O1A
16	b	1236	CLA	CAA-CBA-CGA-O1A
16	s	517	CLA	CAA-CBA-CGA-O1A
16	w	505	CLA	CAA-CBA-CGA-O1A
16	y	512	CLA	CAA-CBA-CGA-O1A
16	s	516	CLA	O1A-CGA-O2A-C1
16	s	506	CLA	O1D-CGD-O2D-CED
16	h	514	CLA	CAA-CBA-CGA-O2A
16	o	508	CLA	C2-C3-C5-C6
16	s	509	CLA	C2-C3-C5-C6
14	B	848	LMG	O10-C28-O8-C9
16	A	1116	CLA	C6-C7-C8-C9
16	B	1240	CLA	O1A-CGA-O2A-C1
16	H	1118	CLA	CAA-CBA-CGA-O1A
16	W	505	CLA	CAA-CBA-CGA-O1A
16	o	508	CLA	CAA-CBA-CGA-O1A
16	G	1206	CLA	C15-C16-C17-C18
16	b	1226	CLA	C5-C6-C7-C8
16	o	515	CLA	C5-C6-C7-C8
16	a	1122	CLA	C11-C12-C13-C14
16	Y	509	CLA	CAA-CBA-CGA-O2A
16	o	507	CLA	CAA-CBA-CGA-O2A
16	G	1219	CLA	CAA-CBA-CGA-O1A
16	b	1230	CLA	CAA-CBA-CGA-O2A
16	Y	507	CLA	C8-C10-C11-C12
16	G	1238	CLA	CBD-CGD-O2D-CED
19	G	4009	BCR	C17-C18-C19-C20
19	L	4019	BCR	C11-C12-C13-C14
19	Z	604	BCR	C21-C22-C23-C24
19	a	4011	BCR	C17-C18-C19-C20
19	u	604	BCR	C11-C12-C13-C14
16	G	1238	CLA	CBA-CGA-O2A-C1
16	Z	501	CLA	C4C-C3C-CAC-CBC
16	b	1239	CLA	C4C-C3C-CAC-CBC
16	A	1110	CLA	CAA-CBA-CGA-O1A
16	H	1110	CLA	CAA-CBA-CGA-O1A
16	U	1501	CLA	CAA-CBA-CGA-O1A
16	W	502	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
16	Y	505	CLA	CAA-CBA-CGA-O1A
16	Z	502	CLA	CAA-CBA-CGA-O1A
16	p	510	CLA	CAA-CBA-CGA-O1A
16	t	505	CLA	CAA-CBA-CGA-O1A
16	w	502	CLA	CAA-CBA-CGA-O1A
16	x	503	CLA	CAA-CBA-CGA-O1A
16	x	508	CLA	CAA-CBA-CGA-O1A
16	y	507	CLA	CAA-CBA-CGA-O1A
16	B	1239	CLA	C4C-C3C-CAC-CBC
14	a	4201	LMG	C28-C29-C30-C31
16	t	510	CLA	C8-C10-C11-C12
16	G	1212	CLA	CAA-CBA-CGA-O1A
16	G	1232	CLA	CAA-CBA-CGA-O2A
14	B	848	LMG	C2-C1-O1-C7
16	H	1102	CLA	CAA-CBA-CGA-O1A
16	Y	510	CLA	CAA-CBA-CGA-O1A
16	Z	507	CLA	CAA-CBA-CGA-O1A
16	Z	509	CLA	CAA-CBA-CGA-O1A
16	o	502	CLA	CAA-CBA-CGA-O1A
16	o	514	CLA	CAA-CBA-CGA-O1A
16	o	516	CLA	CAA-CBA-CGA-O1A
16	q	505	CLA	CAA-CBA-CGA-O1A
16	s	510	CLA	CAA-CBA-CGA-O1A
16	u	507	CLA	CAA-CBA-CGA-O1A
16	G	1214	CLA	CAA-CBA-CGA-O2A
16	W	510	CLA	CAA-CBA-CGA-O2A
16	a	1110	CLA	CAA-CBA-CGA-O2A
16	b	1023	CLA	CAA-CBA-CGA-O2A
16	n	510	CLA	CAA-CBA-CGA-O2A
16	r	510	CLA	CAA-CBA-CGA-O2A
16	u	510	CLA	CAA-CBA-CGA-O2A
16	B	1207	CLA	C2A-CAA-CBA-CGA
16	B	1236	CLA	C2A-CAA-CBA-CGA
16	H	1111	CLA	C2A-CAA-CBA-CGA
16	H	1121	CLA	C2A-CAA-CBA-CGA
16	u	504	CLA	C2A-CAA-CBA-CGA
16	v	515	CLA	C16-C17-C18-C19
16	G	1208	CLA	CAA-CBA-CGA-O1A
16	G	1230	CLA	CAA-CBA-CGA-O1A
16	W	513	CLA	C4C-C3C-CAC-CBC
16	q	501	CLA	C4C-C3C-CAC-CBC
16	G	1213	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	X	510	CLA	O1D-CGD-O2D-CED
16	B	1214	CLA	CAA-CBA-CGA-O1A
16	H	1133	CLA	CAA-CBA-CGA-O1A
16	W	509	CLA	CAA-CBA-CGA-O1A
16	Z	505	CLA	CAA-CBA-CGA-O1A
16	q	507	CLA	CAA-CBA-CGA-O1A
16	G	1239	CLA	C4-C3-C5-C6
16	r	506	CLA	C4-C3-C5-C6
16	W	507	CLA	C5-C6-C7-C8
16	G	1236	CLA	CAA-CBA-CGA-O2A
16	X	516	CLA	CAA-CBA-CGA-O2A
16	b	1207	CLA	CAA-CBA-CGA-O2A
16	g	504	CLA	CAA-CBA-CGA-O2A
16	t	510	CLA	CAA-CBA-CGA-O2A
16	w	516	CLA	CAA-CBA-CGA-O2A
16	Y	505	CLA	C2-C3-C5-C6
16	l	1502	CLA	C3-C5-C6-C7
16	X	512	CLA	O1D-CGD-O2D-CED
16	b	1212	CLA	CAA-CBA-CGA-O1A
19	p	602	BCR	C9-C10-C11-C12
19	s	602	BCR	C15-C16-C17-C18
13	i	103	LHG	O10-C23-C24-C25
16	n	505	CLA	CAA-CBA-CGA-O1A
16	h	506	CLA	O1A-CGA-O2A-C1
16	Y	508	CLA	C6-C7-C8-C10
16	A	1101	CLA	CAD-CBD-CGD-O2D
16	A	1105	CLA	CAD-CBD-CGD-O2D
16	A	1129	CLA	CAD-CBD-CGD-O2D
16	G	1210	CLA	CAD-CBD-CGD-O2D
16	H	1105	CLA	CAD-CBD-CGD-O2D
16	H	1121	CLA	CAD-CBD-CGD-O2D
16	K	4003	CLA	CAD-CBD-CGD-O2D
16	X	507	CLA	CAD-CBD-CGD-O2D
16	a	1123	CLA	CAD-CBD-CGD-O2D
16	b	1219	CLA	CAD-CBD-CGD-O2D
16	b	1226	CLA	CAD-CBD-CGD-O2D
16	h	513	CLA	CAD-CBD-CGD-O2D
16	o	517	CLA	CAD-CBD-CGD-O2D
16	r	507	CLA	CAD-CBD-CGD-O2D
16	s	502	CLA	CAD-CBD-CGD-O2D
16	u	510	CLA	CAD-CBD-CGD-O2D
16	v	514	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
16	w	507	CLA	CAD-CBD-CGD-O2D
16	y	511	CLA	CAD-CBD-CGD-O2D
16	A	1105	CLA	CAA-CBA-CGA-O2A
16	B	1201	CLA	CAA-CBA-CGA-O2A
16	G	1206	CLA	CAA-CBA-CGA-O2A
16	p	509	CLA	CAA-CBA-CGA-O2A
16	r	515	CLA	CAA-CBA-CGA-O2A
16	A	1102	CLA	CAA-CBA-CGA-O1A
16	h	501	CLA	CAA-CBA-CGA-O1A
16	l	1501	CLA	CAA-CBA-CGA-O1A
16	a	1111	CLA	O1A-CGA-O2A-C1
16	y	509	CLA	CBA-CGA-O2A-C1
19	Y	601	BCR	C6-C7-C8-C9
19	o	604	BCR	C22-C23-C24-C25
19	x	601	BCR	C6-C7-C8-C9
16	v	515	CLA	C8-C10-C11-C12
16	G	1202	CLA	C2-C1-O2A-CGA
16	Z	512	CLA	C2-C1-O2A-CGA
16	a	1126	CLA	C2-C1-O2A-CGA
16	b	1222	CLA	C2-C1-O2A-CGA
16	k	4004	CLA	C2-C1-O2A-CGA
16	n	507	CLA	C2-C1-O2A-CGA
16	t	502	CLA	C2-C1-O2A-CGA
16	t	507	CLA	C2-C1-O2A-CGA
16	B	1207	CLA	CAA-CBA-CGA-O1A
16	b	1023	CLA	CAA-CBA-CGA-O1A
16	t	502	CLA	CAA-CBA-CGA-O1A
14	G	848	LMG	O7-C10-C11-C12
16	X	517	CLA	CAA-CBA-CGA-O2A
16	r	508	CLA	CAA-CBA-CGA-O2A
16	t	507	CLA	CAA-CBA-CGA-O2A
16	v	515	CLA	CAA-CBA-CGA-O2A
16	H	1022	CLA	CBD-CGD-O2D-CED
16	G	1214	CLA	C6-C7-C8-C10
16	A	1132	CLA	C8-C10-C11-C12
16	G	1207	CLA	C2A-CAA-CBA-CGA
16	B	1232	CLA	CAA-CBA-CGA-O2A
16	g	509	CLA	CAA-CBA-CGA-O1A
16	n	510	CLA	CAA-CBA-CGA-O1A
16	t	509	CLA	CAA-CBA-CGA-O1A
16	w	505	CLA	C13-C15-C16-C17
13	i	103	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
14	H	4101	LMG	O8-C28-C29-C30
16	A	1137	CLA	CAA-CBA-CGA-O2A
16	G	1201	CLA	CAA-CBA-CGA-O2A
16	H	1237	CLA	CAA-CBA-CGA-O2A
16	X	505	CLA	CAA-CBA-CGA-O2A
16	o	512	CLA	CAA-CBA-CGA-O2A
16	s	503	CLA	CAA-CBA-CGA-O2A
16	y	515	CLA	CAA-CBA-CGA-O2A
16	v	502	CLA	O1D-CGD-O2D-CED
16	a	1134	CLA	CAA-CBA-CGA-O2A
16	H	1126	CLA	C16-C17-C18-C19
16	H	1013	CLA	CAA-CBA-CGA-O1A
16	r	510	CLA	CAA-CBA-CGA-O1A
13	i	103	LHG	C30-C31-C32-C33
16	Z	502	CLA	CBD-CGD-O2D-CED
16	B	1023	CLA	CAA-CBA-CGA-O2A
16	W	512	CLA	CAA-CBA-CGA-O2A
16	b	1239	CLA	CAA-CBA-CGA-O2A
16	s	513	CLA	CAA-CBA-CGA-O2A
16	u	502	CLA	CAA-CBA-CGA-O2A
16	G	1226	CLA	CAA-CBA-CGA-O1A
16	W	510	CLA	CAA-CBA-CGA-O1A
16	X	503	CLA	CAA-CBA-CGA-O1A
16	o	507	CLA	CAA-CBA-CGA-O1A
16	q	502	CLA	CAA-CBA-CGA-O1A
16	s	505	CLA	CAA-CBA-CGA-O1A
16	t	510	CLA	CAA-CBA-CGA-O1A
16	x	510	CLA	CAA-CBA-CGA-O1A
23	r	606	LMU	C7-C8-C9-C10

There are no ring outliers.

673 monomers are involved in 1441 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	1122	CLA	5	0
13	B	4018	LHG	1	0
16	a	1133	CLA	2	0
14	A	4201	LMG	1	0
16	B	1021	CLA	4	0
16	h	506	CLA	1	0
16	q	505	CLA	4	0
16	p	509	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1240	CLA	4	0
16	B	1205	CLA	4	0
16	G	1202	CLA	6	0
16	W	506	CLA	3	0
16	b	1238	CLA	2	0
19	x	603	BCR	2	0
19	x	601	BCR	5	0
16	G	1206	CLA	3	0
16	q	511	CLA	3	0
16	p	512	CLA	2	0
16	A	1108	CLA	1	0
16	b	1215	CLA	3	0
16	h	509	CLA	4	0
16	X	514	CLA	1	0
16	p	502	CLA	1	0
16	s	508	CLA	2	0
16	X	509	CLA	6	0
16	b	1228	CLA	1	0
16	B	1234	CLA	1	0
16	y	505	CLA	3	0
16	a	1126	CLA	4	0
16	p	513	CLA	1	0
16	g	509	CLA	3	0
16	n	510	CLA	6	0
16	H	1101	CLA	5	0
19	T	4001	BCR	3	0
14	H	852	LMG	2	0
17	b	2002	PQN	2	0
16	o	510	CLA	4	0
16	T	4003	CLA	2	0
19	H	4007	BCR	1	0
19	y	604	BCR	5	0
16	a	1119	CLA	6	0
16	t	504	CLA	2	0
19	I	4018	BCR	3	0
16	n	516	CLA	2	0
16	q	504	CLA	3	0
16	G	1228	CLA	2	0
16	a	1125	CLA	1	0
16	H	1122	CLA	3	0
16	o	501	CLA	1	0
19	x	604	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	H	1120	CLA	2	0
16	r	510	CLA	6	0
16	v	505	CLA	5	0
16	X	517	CLA	1	0
16	y	516	CLA	1	0
17	G	2002	PQN	5	0
16	B	1206	CLA	7	0
19	k	4001	BCR	4	0
16	n	503	CLA	1	0
16	y	502	CLA	2	0
19	y	601	BCR	1	0
16	G	1012	CLA	2	0
16	v	511	CLA	5	0
16	A	1127	CLA	4	0
16	b	1202	CLA	2	0
16	A	1121	CLA	1	0
21	I	4020	ECH	2	0
16	o	505	CLA	7	0
16	b	1205	CLA	3	0
19	v	604	BCR	3	0
16	L	1502	CLA	3	0
13	s	605	LHG	1	0
19	L	4019	BCR	3	0
19	w	602	BCR	3	0
16	n	509	CLA	5	0
19	q	602	BCR	4	0
16	G	1211	CLA	3	0
19	b	4014	BCR	7	0
16	G	1201	CLA	2	0
16	o	512	CLA	3	0
19	A	4007	BCR	1	0
19	A	4003	BCR	2	0
16	A	1122	CLA	3	0
16	A	1123	CLA	4	0
14	A	4101	LMG	5	0
16	a	1103	CLA	5	0
16	H	1118	CLA	2	0
16	w	505	CLA	3	0
16	a	1138	CLA	1	0
16	A	1102	CLA	2	0
16	H	1106	CLA	2	0
16	B	1202	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	1012	CLA	3	0
16	b	1021	CLA	2	0
16	b	1207	CLA	6	0
16	o	504	CLA	2	0
16	B	1224	CLA	2	0
16	G	1239	CLA	5	0
16	A	1103	CLA	3	0
16	A	1136	CLA	3	0
16	q	509	CLA	4	0
16	b	1211	CLA	2	0
16	b	1208	CLA	2	0
16	a	1114	CLA	1	0
16	B	1201	CLA	3	0
16	q	506	CLA	4	0
17	H	2001	PQN	4	0
19	g	604	BCR	4	0
16	W	501	CLA	2	0
16	a	1110	CLA	3	0
16	t	515	CLA	4	0
16	u	515	CLA	2	0
16	w	516	CLA	1	0
16	H	1237	CLA	3	0
16	X	510	CLA	6	0
16	A	1109	CLA	1	0
19	f	4016	BCR	4	0
20	L	4101	LMT	3	0
16	Y	509	CLA	5	0
16	B	1229	CLA	2	0
16	H	1121	CLA	1	0
16	Y	506	CLA	5	0
19	S	4012	BCR	4	0
16	x	508	CLA	1	0
16	q	517	CLA	3	0
16	n	507	CLA	6	0
19	K	4005	BCR	2	0
19	o	602	BCR	1	0
24	q	601	LUT	1	0
16	s	512	CLA	3	0
16	q	515	CLA	4	0
16	B	1239	CLA	3	0
16	W	505	CLA	2	0
16	A	1106	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	4002	CLA	1	0
16	B	1012	CLA	4	0
13	R	103	LHG	2	0
16	G	1213	CLA	2	0
16	s	504	CLA	6	0
16	H	1135	CLA	1	0
16	Y	517	CLA	2	0
16	b	1225	CLA	5	0
19	H	4003	BCR	2	0
16	J	1303	CLA	1	0
16	H	1123	CLA	2	0
16	t	510	CLA	3	0
20	H	4202	LMT	1	0
16	A	1113	CLA	1	0
16	b	1224	CLA	2	0
16	Y	515	CLA	3	0
16	w	511	CLA	1	0
16	B	1238	CLA	3	0
16	a	1135	CLA	3	0
19	a	4002	BCR	4	0
16	B	1219	CLA	1	0
13	G	4018	LHG	1	0
16	G	1224	CLA	2	0
16	a	1123	CLA	6	0
16	B	1215	CLA	3	0
16	a	1105	CLA	4	0
16	a	1118	CLA	1	0
23	r	606	LMU	3	0
16	A	1119	CLA	5	0
16	B	1225	CLA	8	0
16	p	511	CLA	1	0
16	p	515	CLA	6	0
16	q	507	CLA	6	0
19	U	4019	BCR	1	0
15	a	1011	CL0	4	0
16	a	1022	CLA	3	0
16	p	504	CLA	7	0
19	s	601	BCR	2	0
16	b	1218	CLA	1	0
16	Z	512	CLA	2	0
16	h	515	CLA	4	0
16	Z	502	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	1226	CLA	4	0
16	l	1502	CLA	2	0
23	Y	606	LMU	1	0
13	X	605	LHG	1	0
16	Y	507	CLA	5	0
16	g	515	CLA	3	0
16	x	514	CLA	1	0
16	x	506	CLA	2	0
16	h	504	CLA	2	0
16	X	504	CLA	4	0
16	A	1135	CLA	2	0
16	o	517	CLA	3	0
16	H	1140	CLA	4	0
16	b	1230	CLA	1	0
16	b	1240	CLA	2	0
19	B	4005	BCR	3	0
16	o	514	CLA	1	0
14	H	4201	LMG	1	0
16	q	503	CLA	2	0
16	L	1503	CLA	5	0
16	b	1221	CLA	6	0
16	A	1126	CLA	8	0
16	b	1220	CLA	3	0
19	L	4022	BCR	6	0
16	k	4002	CLA	1	0
16	x	511	CLA	6	0
16	H	1133	CLA	1	0
19	i	4018	BCR	5	0
16	y	512	CLA	4	0
16	A	1128	CLA	5	0
19	b	4004	BCR	1	0
16	H	1105	CLA	3	0
16	G	1231	CLA	1	0
16	r	516	CLA	3	0
19	J	4013	BCR	1	0
21	G	4006	ECH	2	0
19	B	4009	BCR	2	0
16	G	1210	CLA	6	0
16	s	509	CLA	4	0
16	B	1221	CLA	2	0
16	w	504	CLA	3	0
19	g	601	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1230	CLA	3	0
14	Q	4017	LMG	1	0
16	X	506	CLA	2	0
16	a	1101	CLA	5	0
16	p	517	CLA	2	0
16	a	1115	CLA	1	0
16	q	513	CLA	2	0
16	g	504	CLA	2	0
16	a	1120	CLA	2	0
16	B	1231	CLA	2	0
16	G	1227	CLA	2	0
16	a	1112	CLA	1	0
16	A	1105	CLA	1	0
16	A	1118	CLA	1	0
16	b	1210	CLA	5	0
16	s	515	CLA	2	0
19	H	4011	BCR	3	0
16	p	510	CLA	7	0
19	y	603	BCR	5	0
16	o	503	CLA	1	0
13	r	605	LHG	2	0
19	v	601	BCR	1	0
16	Y	505	CLA	4	0
16	A	1022	CLA	4	0
19	p	604	BCR	1	0
19	p	602	BCR	3	0
16	h	512	CLA	3	0
16	r	515	CLA	4	0
16	W	507	CLA	5	0
16	A	1129	CLA	1	0
16	B	1023	CLA	5	0
16	B	1226	CLA	2	0
16	b	1229	CLA	4	0
16	g	512	CLA	2	0
16	t	507	CLA	1	0
16	v	512	CLA	4	0
16	F	1301	CLA	1	0
13	I	103	LHG	2	0
16	w	507	CLA	6	0
16	A	1131	CLA	2	0
16	p	516	CLA	1	0
16	r	504	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	v	502	CLA	3	0
16	W	502	CLA	4	0
16	o	509	CLA	5	0
16	f	1301	CLA	2	0
16	x	504	CLA	2	0
19	W	601	BCR	5	0
19	v	603	BCR	3	0
16	g	513	CLA	1	0
16	B	1227	CLA	1	0
16	b	1239	CLA	5	0
16	y	510	CLA	5	0
16	x	510	CLA	8	0
19	l	4022	BCR	6	0
16	h	516	CLA	2	0
16	u	517	CLA	1	0
16	W	504	CLA	5	0
16	X	515	CLA	3	0
16	Z	508	CLA	1	0
16	Y	504	CLA	4	0
14	f	4017	LMG	1	0
16	g	516	CLA	2	0
16	B	1210	CLA	7	0
16	o	513	CLA	1	0
19	U	4022	BCR	12	0
19	n	603	BCR	1	0
16	q	510	CLA	7	0
16	b	1216	CLA	2	0
19	S	4013	BCR	3	0
16	v	514	CLA	2	0
21	B	4006	ECH	3	0
16	H	1013	CLA	3	0
16	H	1130	CLA	1	0
16	H	1103	CLA	8	0
16	s	510	CLA	5	0
16	W	517	CLA	1	0
16	G	1021	CLA	2	0
16	o	508	CLA	4	0
19	j	4012	BCR	3	0
16	L	1501	CLA	3	0
16	H	1108	CLA	1	0
19	n	604	BCR	4	0
19	t	603	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	w	603	BCR	3	0
19	Y	602	BCR	2	0
20	l	4101	LMT	3	0
16	a	1136	CLA	2	0
16	t	505	CLA	3	0
16	u	505	CLA	3	0
16	x	509	CLA	3	0
16	y	508	CLA	5	0
19	p	603	BCR	4	0
16	b	1234	CLA	1	0
19	X	602	BCR	3	0
16	H	1801	CLA	3	0
19	F	4016	BCR	4	0
16	G	1234	CLA	2	0
16	x	512	CLA	3	0
16	b	1219	CLA	1	0
19	H	4002	BCR	3	0
19	a	4007	BCR	1	0
15	A	1011	CL0	3	0
16	s	513	CLA	1	0
19	o	601	BCR	1	0
16	r	506	CLA	2	0
16	A	1110	CLA	1	0
16	H	1126	CLA	5	0
16	X	505	CLA	4	0
16	u	511	CLA	3	0
19	S	4015	BCR	2	0
16	Z	510	CLA	6	0
19	q	604	BCR	5	0
16	u	501	CLA	1	0
16	G	1238	CLA	2	0
16	x	515	CLA	4	0
16	r	513	CLA	1	0
16	G	1219	CLA	1	0
16	w	517	CLA	1	0
16	G	1215	CLA	2	0
16	G	1225	CLA	4	0
16	W	512	CLA	2	0
23	q	605	LMU	2	0
21	R	4020	ECH	2	0
16	p	507	CLA	2	0
16	A	1101	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	q	516	CLA	2	0
16	w	512	CLA	1	0
16	q	512	CLA	3	0
16	w	502	CLA	1	0
19	r	603	BCR	3	0
16	g	517	CLA	1	0
16	p	505	CLA	7	0
16	q	502	CLA	4	0
16	A	1112	CLA	1	0
19	B	4014	BCR	6	0
16	H	1109	CLA	2	0
16	Z	503	CLA	2	0
16	Y	512	CLA	3	0
16	X	513	CLA	2	0
16	A	1132	CLA	3	0
16	K	4004	CLA	1	0
16	H	1129	CLA	3	0
16	g	503	CLA	1	0
19	g	603	BCR	3	0
16	h	505	CLA	2	0
16	A	1134	CLA	1	0
16	Y	516	CLA	1	0
21	V	4021	ECH	4	0
16	A	1139	CLA	5	0
16	a	1127	CLA	1	0
19	a	4011	BCR	4	0
16	g	505	CLA	6	0
19	h	604	BCR	3	0
16	H	1128	CLA	5	0
16	w	508	CLA	2	0
16	A	1013	CLA	1	0
16	b	1206	CLA	4	0
16	n	505	CLA	3	0
16	Z	509	CLA	5	0
16	x	507	CLA	6	0
19	u	601	BCR	4	0
16	o	502	CLA	3	0
16	g	511	CLA	1	0
19	G	4010	BCR	3	0
16	y	504	CLA	2	0
16	G	1203	CLA	4	0
16	A	1107	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	l	1503	CLA	6	0
19	o	604	BCR	1	0
16	x	503	CLA	2	0
16	X	501	CLA	2	0
16	G	1218	CLA	2	0
19	Q	4016	BCR	2	0
16	A	1124	CLA	6	0
19	G	4004	BCR	2	0
16	U	1503	CLA	4	0
16	b	1227	CLA	1	0
16	a	1107	CLA	2	0
16	a	1108	CLA	1	0
16	b	1231	CLA	1	0
16	w	503	CLA	3	0
16	Y	511	CLA	3	0
16	t	502	CLA	1	0
19	A	4008	BCR	3	0
16	s	507	CLA	5	0
16	y	511	CLA	6	0
21	m	4021	ECH	2	0
16	n	514	CLA	1	0
19	B	4010	BCR	2	0
16	H	1110	CLA	2	0
16	B	1203	CLA	7	0
16	G	1230	CLA	2	0
19	Y	603	BCR	2	0
16	G	1220	CLA	3	0
16	g	510	CLA	4	0
16	a	1106	CLA	2	0
16	k	4003	CLA	1	0
16	h	511	CLA	6	0
19	X	603	BCR	2	0
16	H	1134	CLA	3	0
16	h	501	CLA	1	0
21	b	4006	ECH	2	0
19	a	4003	BCR	4	0
16	H	1104	CLA	5	0
16	H	1139	CLA	7	0
16	W	511	CLA	2	0
16	s	505	CLA	6	0
16	Z	507	CLA	6	0
16	A	1138	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	1221	CLA	8	0
16	s	506	CLA	4	0
19	h	601	BCR	1	0
16	H	1111	CLA	3	0
16	H	1119	CLA	9	0
16	g	507	CLA	4	0
19	G	4005	BCR	2	0
16	b	1222	CLA	2	0
16	X	512	CLA	3	0
16	r	505	CLA	7	0
16	v	504	CLA	4	0
19	A	4011	BCR	4	0
16	n	511	CLA	5	0
16	B	1220	CLA	3	0
16	s	516	CLA	1	0
16	r	511	CLA	3	0
16	G	1222	CLA	3	0
19	W	604	BCR	1	0
16	G	1232	CLA	1	0
13	A	851	LHG	2	0
16	s	517	CLA	2	0
16	A	1137	CLA	3	0
16	g	502	CLA	2	0
16	v	509	CLA	7	0
16	h	510	CLA	6	0
16	y	507	CLA	2	0
16	p	506	CLA	2	0
16	a	1013	CLA	2	0
16	a	1140	CLA	3	0
16	H	1022	CLA	2	0
16	w	506	CLA	3	0
16	B	1218	CLA	1	0
16	b	1235	CLA	3	0
19	J	4012	BCR	5	0
19	X	604	BCR	4	0
16	u	514	CLA	1	0
16	H	1117	CLA	4	0
16	b	1201	CLA	2	0
16	H	1137	CLA	5	0
16	h	507	CLA	4	0
16	n	504	CLA	5	0
19	u	603	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	t	601	BCR	3	0
16	Z	515	CLA	3	0
16	g	506	CLA	2	0
16	X	511	CLA	1	0
16	A	1125	CLA	1	0
16	B	1222	CLA	3	0
16	B	1223	CLA	2	0
16	a	1116	CLA	4	0
16	n	506	CLA	4	0
16	n	512	CLA	1	0
16	Z	517	CLA	1	0
16	v	516	CLA	3	0
16	y	509	CLA	8	0
16	n	501	CLA	3	0
19	s	602	BCR	1	0
16	B	1214	CLA	4	0
16	b	1236	CLA	1	0
13	i	103	LHG	2	0
19	b	4017	BCR	1	0
17	a	2001	PQN	4	0
19	j	4013	BCR	2	0
14	G	848	LMG	2	0
15	H	1011	CL0	4	0
16	G	1236	CLA	5	0
16	b	1209	CLA	1	0
19	G	4017	BCR	3	0
16	B	1207	CLA	6	0
16	n	502	CLA	3	0
19	r	602	BCR	2	0
16	u	510	CLA	3	0
20	A	4202	LMT	1	0
16	a	1237	CLA	2	0
16	B	1235	CLA	3	0
16	A	1116	CLA	4	0
16	y	517	CLA	3	0
13	o	605	LHG	1	0
16	w	510	CLA	5	0
16	A	1117	CLA	7	0
16	A	1104	CLA	4	0
21	i	4020	ECH	1	0
16	y	515	CLA	5	0
19	J	4015	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Z	511	CLA	2	0
16	A	1237	CLA	3	0
16	Y	508	CLA	1	0
16	G	1216	CLA	2	0
14	H	4101	LMG	6	0
14	a	4101	LMG	1	0
19	p	601	BCR	2	0
16	H	1136	CLA	2	0
16	Z	504	CLA	2	0
16	u	503	CLA	2	0
16	x	505	CLA	3	0
16	v	507	CLA	5	0
23	g	606	LMU	1	0
16	l	1501	CLA	7	0
14	B	848	LMG	2	0
16	b	1023	CLA	3	0
14	a	852	LMG	2	0
19	q	603	BCR	4	0
19	h	603	BCR	5	0
16	U	1501	CLA	4	0
16	X	503	CLA	2	0
16	b	1204	CLA	4	0
16	v	515	CLA	1	0
16	H	1138	CLA	4	0
16	G	1023	CLA	3	0
16	U	1502	CLA	3	0
16	G	1208	CLA	1	0
16	n	517	CLA	1	0
16	b	1203	CLA	7	0
16	H	1124	CLA	4	0
16	a	1131	CLA	3	0
19	w	604	BCR	2	0
16	H	1125	CLA	2	0
16	a	1801	CLA	1	0
19	A	4002	BCR	3	0
16	x	516	CLA	2	0
16	w	509	CLA	6	0
19	o	603	BCR	2	0
16	a	1109	CLA	2	0
16	n	515	CLA	2	0
16	x	501	CLA	1	0
16	o	515	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Z	506	CLA	3	0
19	G	4014	BCR	5	0
16	a	1129	CLA	2	0
23	p	606	LMU	1	0
13	u	605	LHG	1	0
19	b	4005	BCR	4	0
16	H	1116	CLA	3	0
16	W	515	CLA	1	0
16	a	1104	CLA	4	0
16	a	1130	CLA	2	0
16	H	1107	CLA	3	0
19	b	4010	BCR	2	0
16	B	1228	CLA	1	0
16	B	1236	CLA	3	0
16	Z	516	CLA	4	0
19	B	4017	BCR	2	0
16	H	1131	CLA	5	0
19	Y	601	BCR	2	0
16	B	1211	CLA	3	0
19	K	4001	BCR	3	0
19	n	601	BCR	4	0
16	a	1117	CLA	4	0
16	t	508	CLA	2	0
16	u	508	CLA	2	0
17	B	2002	PQN	5	0
16	K	4003	CLA	2	0
16	r	507	CLA	6	0
16	A	1140	CLA	2	0
16	Q	1301	CLA	2	0
21	M	4021	ECH	2	0
16	b	1213	CLA	1	0
19	r	601	BCR	2	0
16	a	1132	CLA	2	0
19	u	602	BCR	2	0
23	x	606	LMU	2	0
19	j	4015	BCR	2	0
19	Z	604	BCR	1	0
16	y	513	CLA	1	0
16	q	508	CLA	3	0
16	W	510	CLA	4	0
19	Z	602	BCR	2	0
16	X	508	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	1128	CLA	5	0
13	p	605	LHG	1	0
16	x	517	CLA	1	0
19	H	4008	BCR	4	0
20	a	4202	LMT	1	0
16	a	1111	CLA	4	0
16	v	506	CLA	3	0
16	a	1113	CLA	1	0
16	u	507	CLA	1	0
17	A	2001	PQN	4	0
16	b	1223	CLA	1	0
19	l	4019	BCR	4	0
16	G	1240	CLA	2	0
16	G	1205	CLA	5	0
19	G	4009	BCR	1	0
16	H	1112	CLA	1	0
16	w	515	CLA	4	0
16	o	511	CLA	1	0
16	p	508	CLA	2	0
16	b	1226	CLA	5	0
16	G	1223	CLA	2	0
16	o	506	CLA	3	0
13	H	851	LHG	2	0
16	H	1132	CLA	1	0
16	u	504	CLA	3	0
16	v	510	CLA	5	0
16	G	1204	CLA	5	0
16	t	506	CLA	3	0
16	B	1213	CLA	3	0
13	b	4018	LHG	3	0
16	s	502	CLA	2	0
16	u	506	CLA	5	0
19	s	603	BCR	5	0
16	r	509	CLA	6	0
16	A	1111	CLA	3	0
16	h	508	CLA	2	0
16	y	506	CLA	2	0
16	W	509	CLA	2	0
16	g	508	CLA	3	0
16	r	512	CLA	3	0
16	G	1207	CLA	5	0
16	r	502	CLA	1	0

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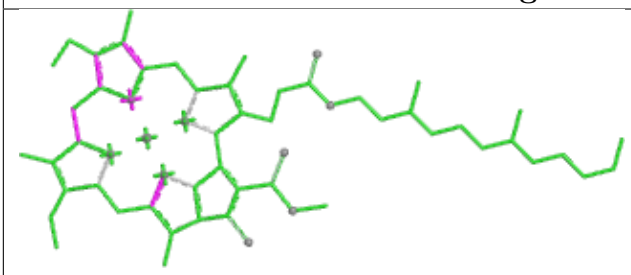
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	t	509	CLA	3	0
16	u	509	CLA	7	0
16	n	508	CLA	4	0
14	A	852	LMG	1	0
16	a	1102	CLA	5	0
16	Y	510	CLA	5	0
19	a	4008	BCR	3	0
16	G	1235	CLA	2	0
16	b	1214	CLA	2	0
16	B	1208	CLA	2	0
16	X	507	CLA	1	0
19	g	602	BCR	4	0
16	t	512	CLA	3	0
16	u	512	CLA	2	0
19	s	604	BCR	3	0
16	H	1127	CLA	1	0
16	u	502	CLA	2	0
16	A	1120	CLA	2	0
16	B	1204	CLA	5	0
16	w	513	CLA	1	0
19	X	601	BCR	3	0
19	Z	603	BCR	1	0
16	A	1801	CLA	2	0
16	X	502	CLA	3	0
16	r	508	CLA	2	0
20	U	4101	LMT	2	0
16	Z	505	CLA	7	0
16	G	1214	CLA	2	0
16	a	1124	CLA	7	0
16	a	1137	CLA	4	0
16	p	503	CLA	1	0
16	Q	1302	CLA	1	0
16	A	1130	CLA	4	0
16	t	511	CLA	2	0
19	x	602	BCR	1	0

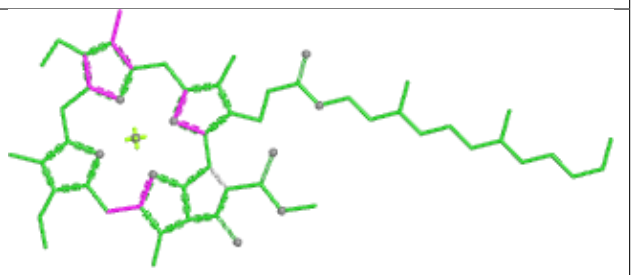
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

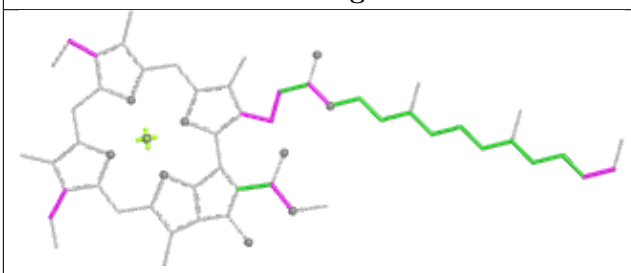
Ligand CLA a 1122



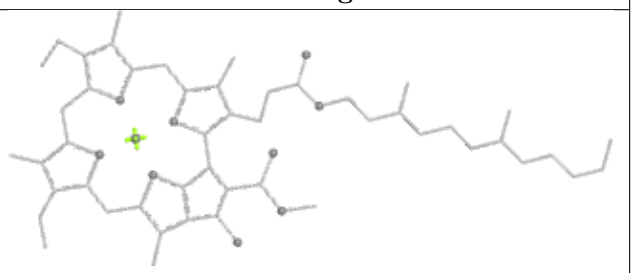
Bond lengths



Bond angles

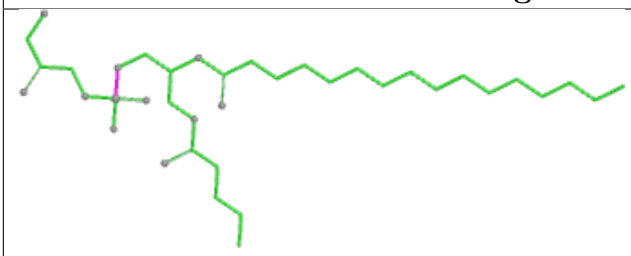


Torsions

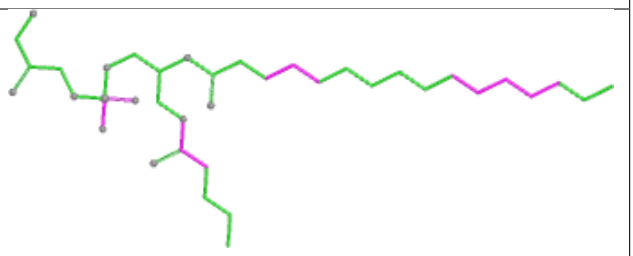


Rings

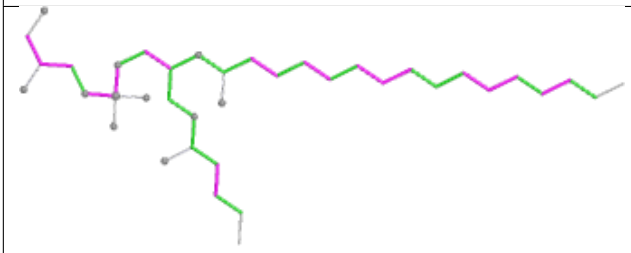
Ligand LHG B 4018



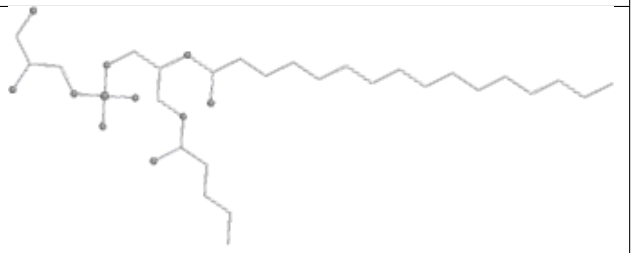
Bond lengths



Bond angles

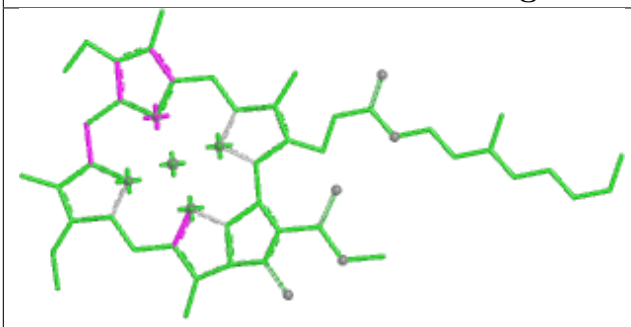


Torsions

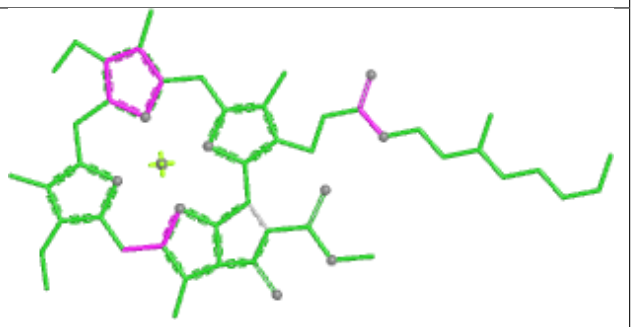


Rings

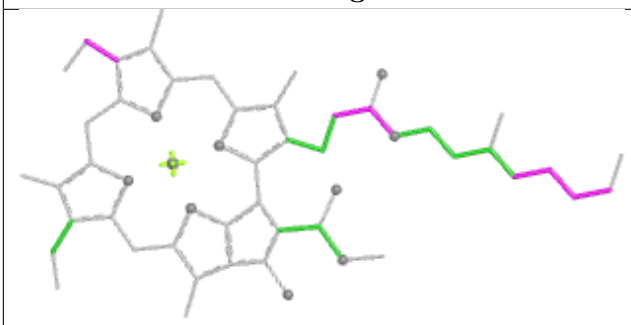
Ligand CLA a 1133



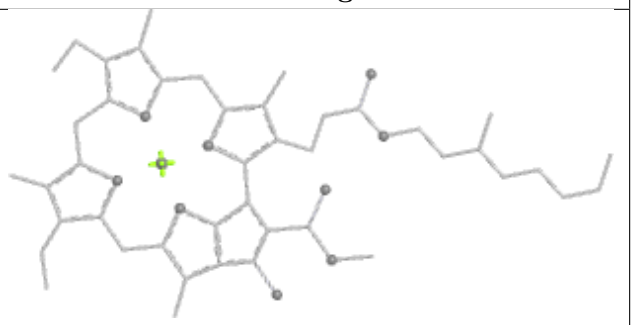
Bond lengths



Bond angles

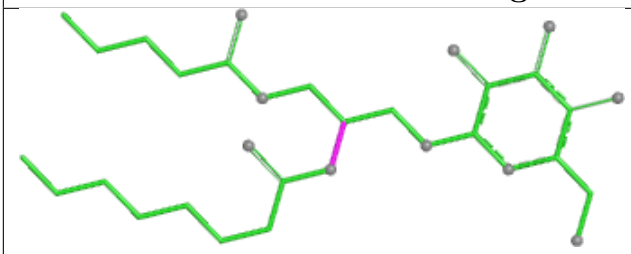


Torsions

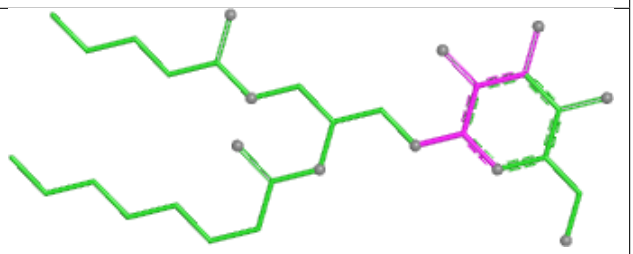


Rings

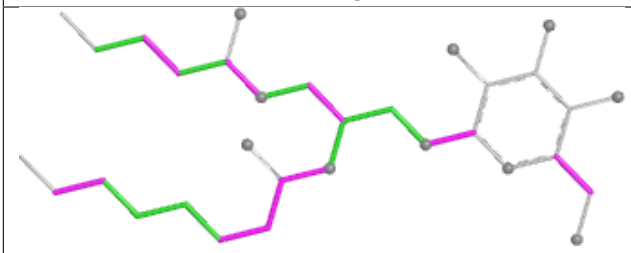
Ligand LMG A 4201



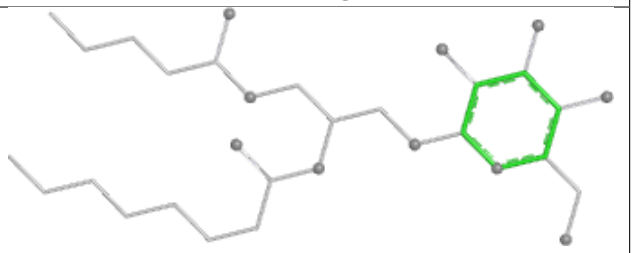
Bond lengths



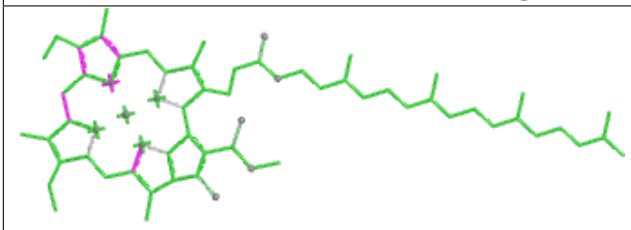
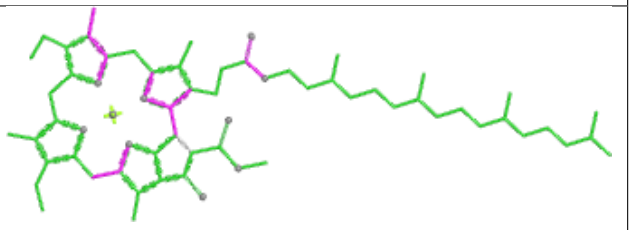
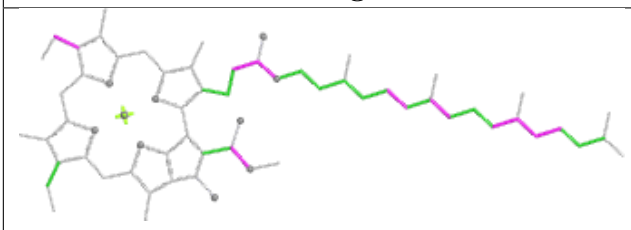
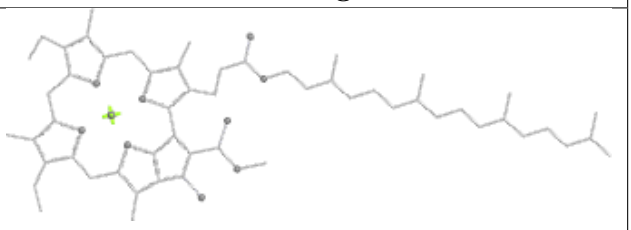
Bond angles

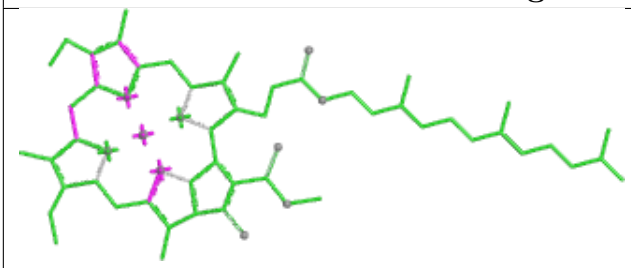
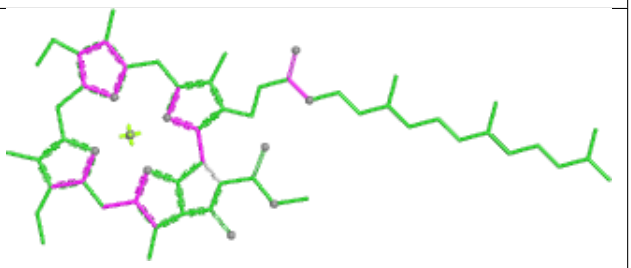
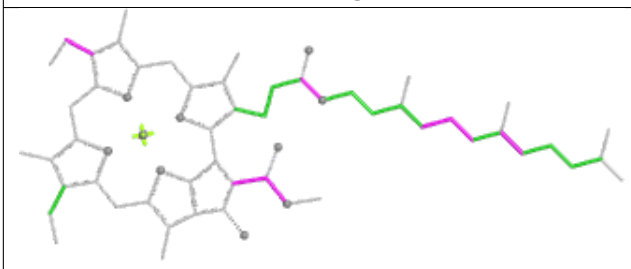
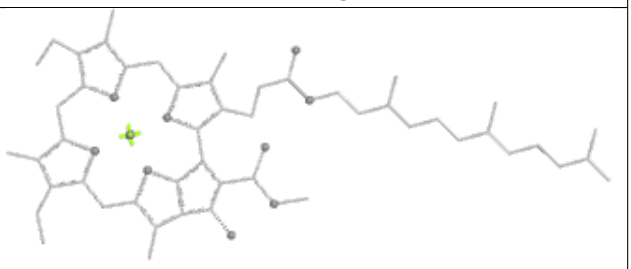


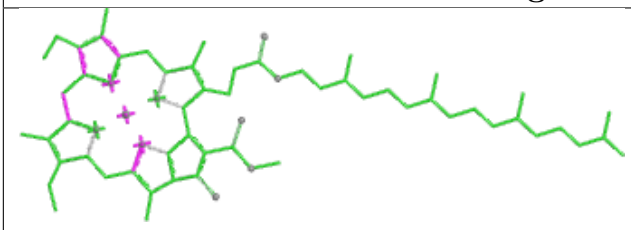
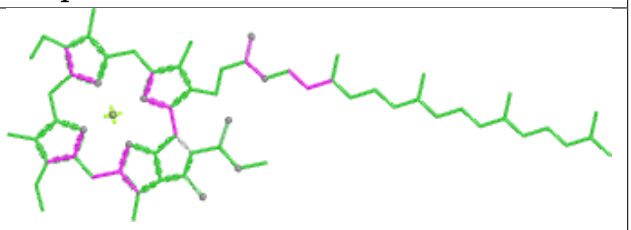
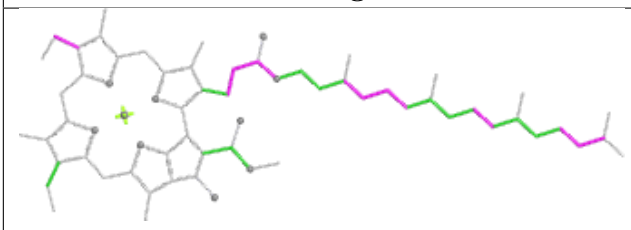
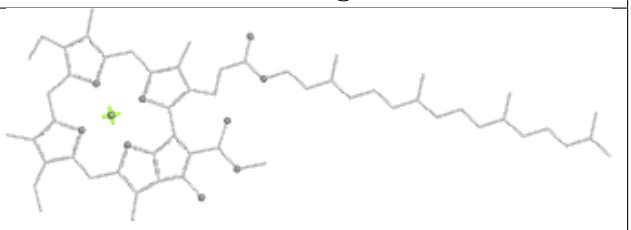
Torsions

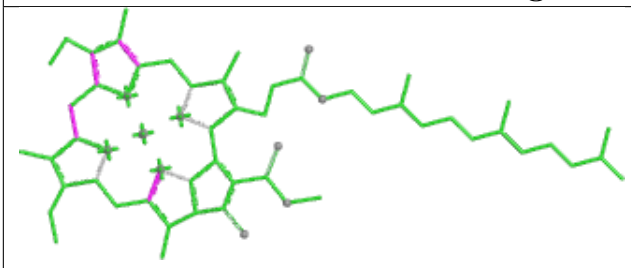
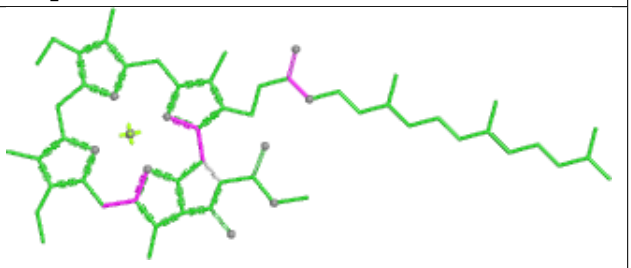
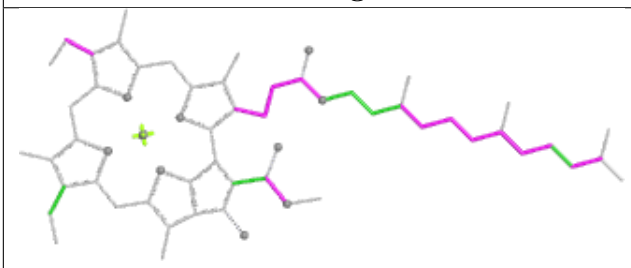
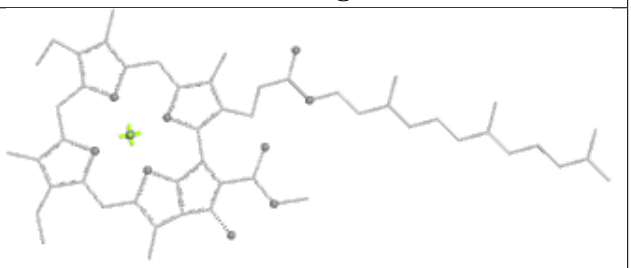


Rings

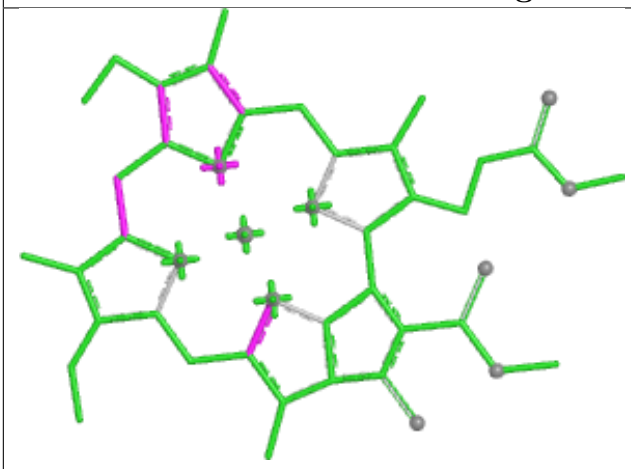
Ligand CLA B 1021	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA h 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1240



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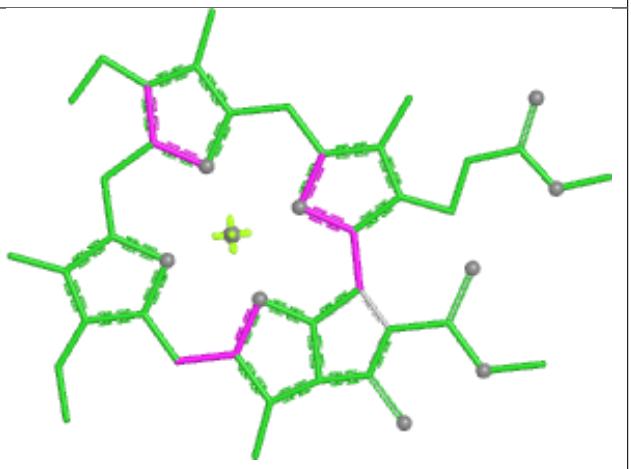
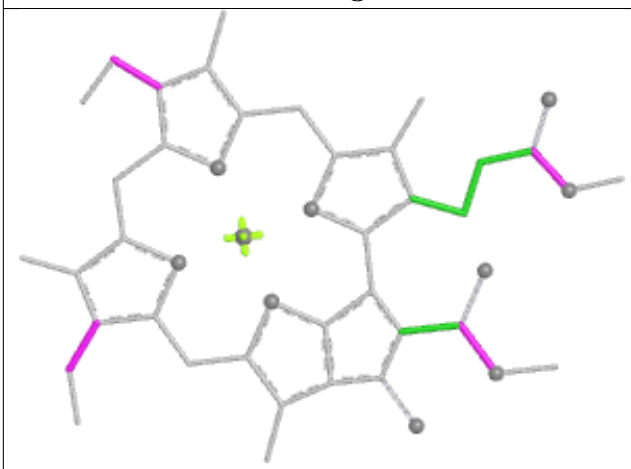
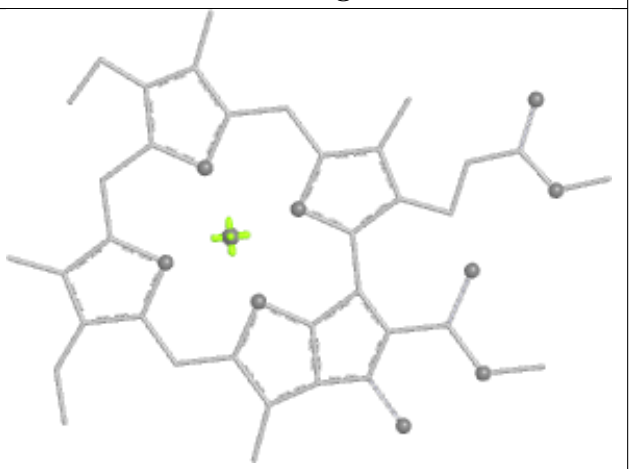


Bond angles

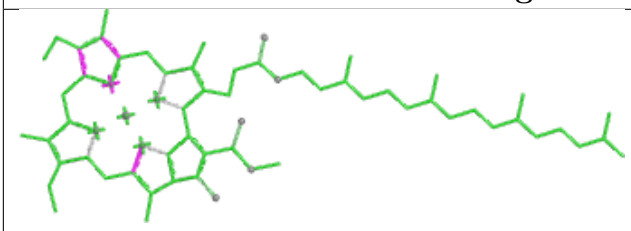


Torsions

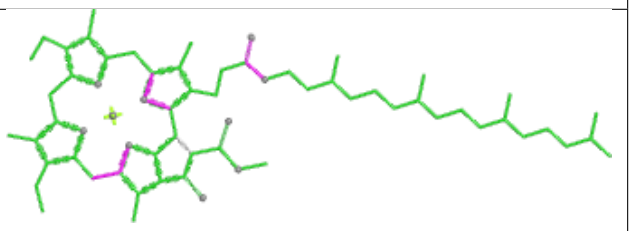


Rings

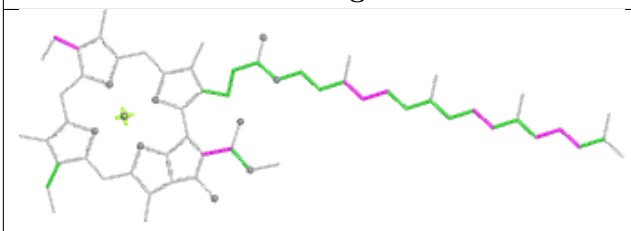
Ligand CLA B 1205



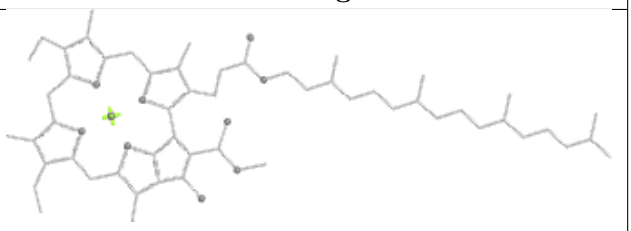
Bond lengths



Bond angles

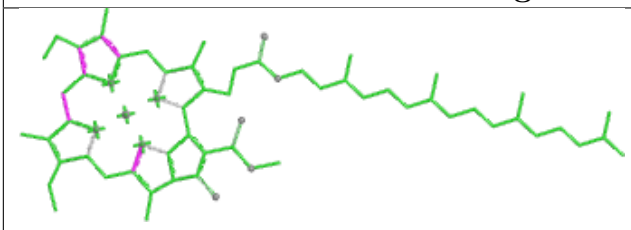


Torsions



Rings

Ligand CLA G 1202



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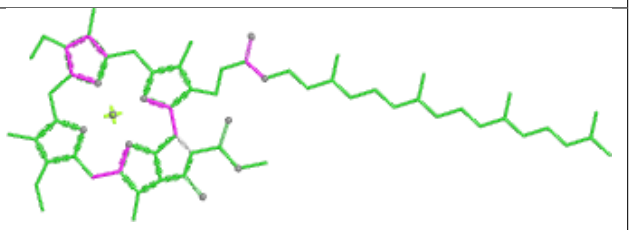
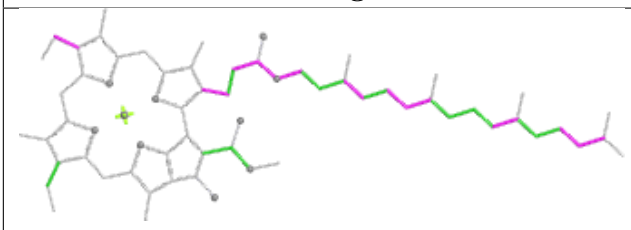
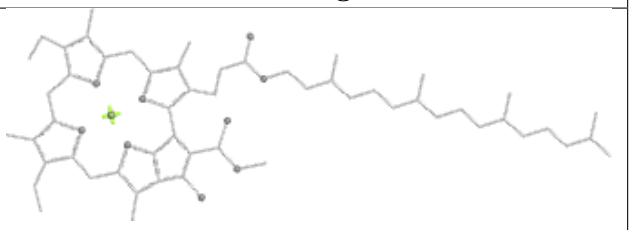


Bond angles

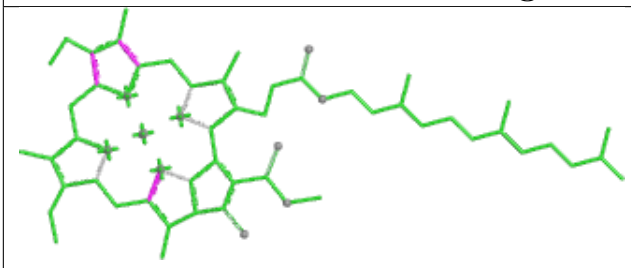


Torsions

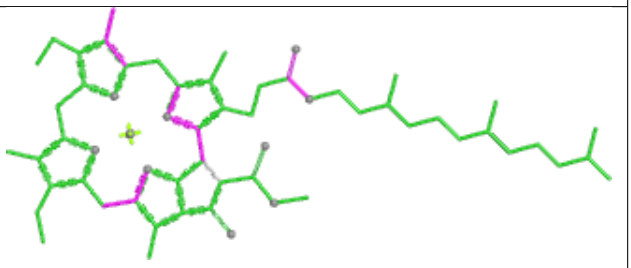


Rings

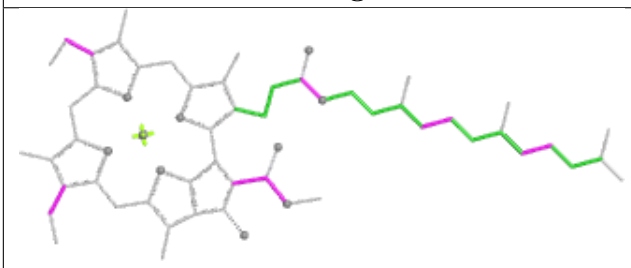
Ligand CLA W 506



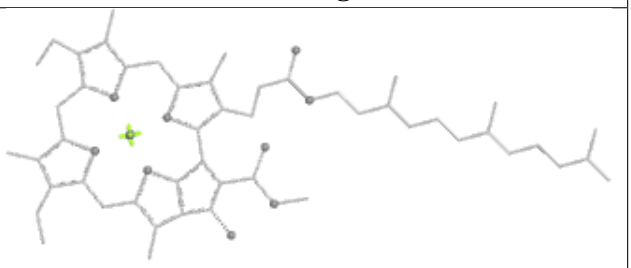
Bond lengths



Bond angles

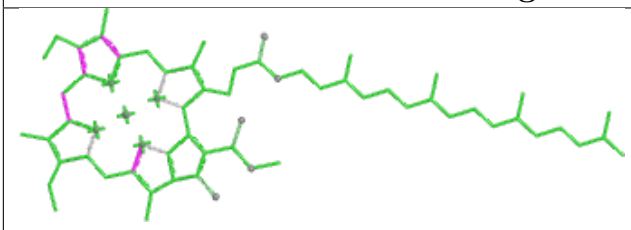


Torsions



Rings

Ligand CLA b 1238



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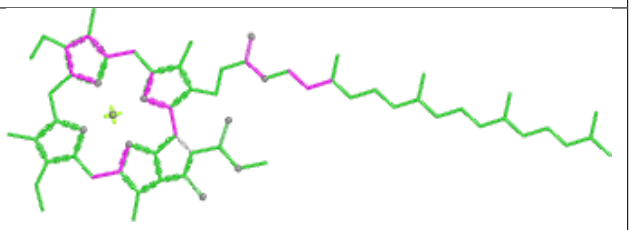
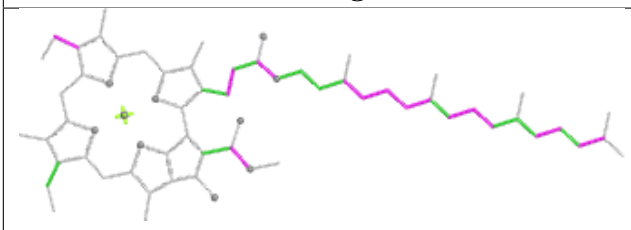
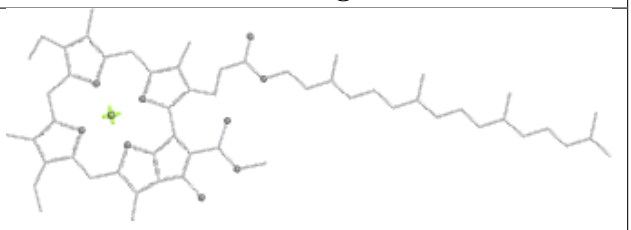


Bond angles

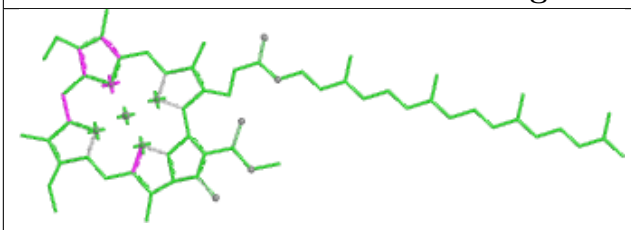


Torsions



Rings

Ligand CLA s 511



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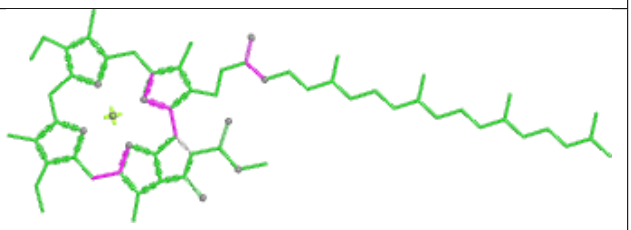
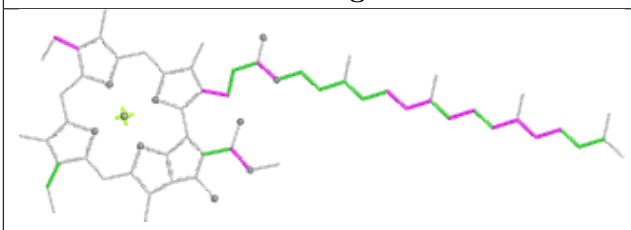


Bond angles



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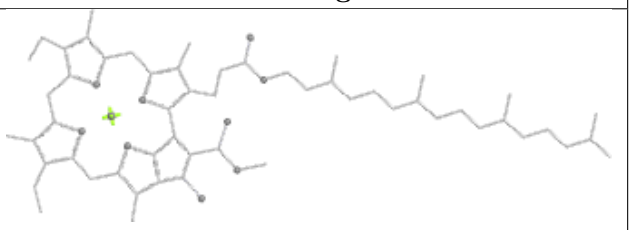
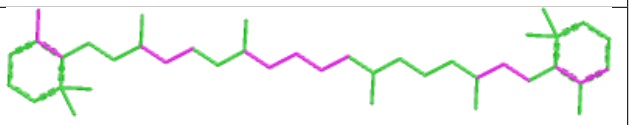


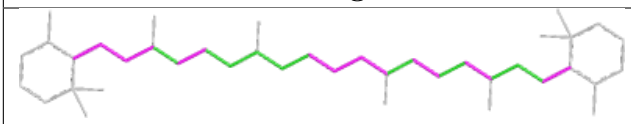
Rings

Ligand BCR x 603

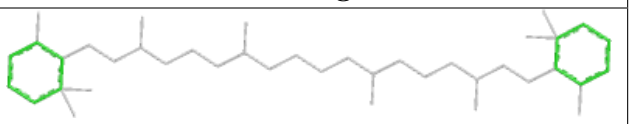
Bond lengths



Bond angles

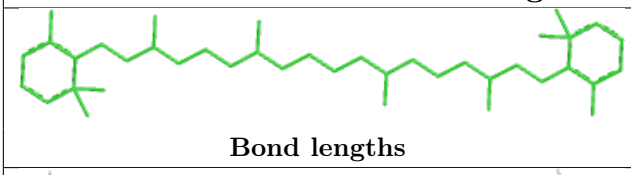


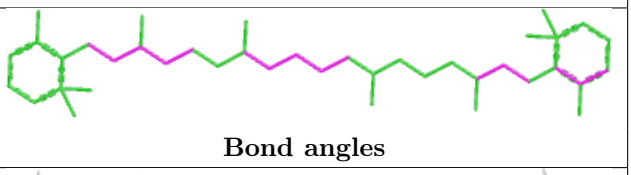
Torsions

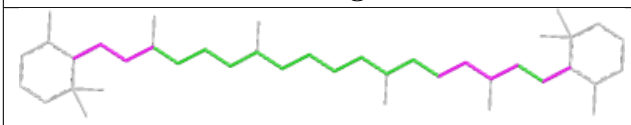


Rings

Ligand BCR x 601


Bond lengths


Bond angles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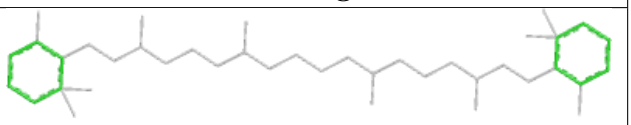
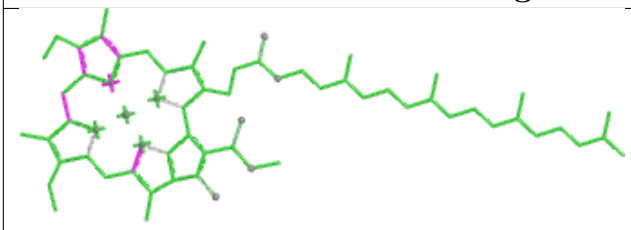

Rings

Ligand CLA G 1206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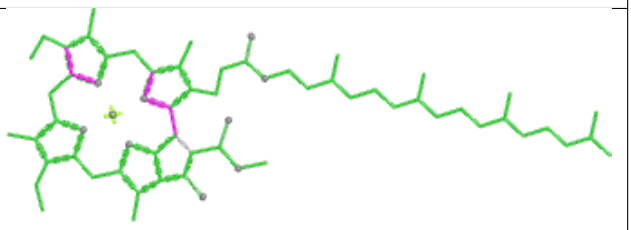
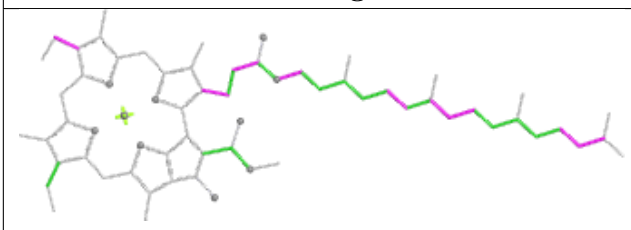
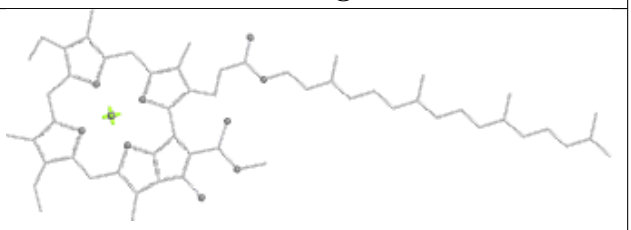
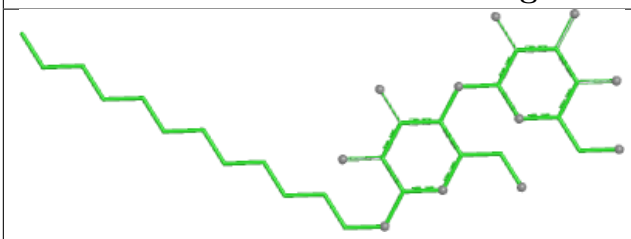

Bond angles


Torsions


Rings

Ligand LMU w 605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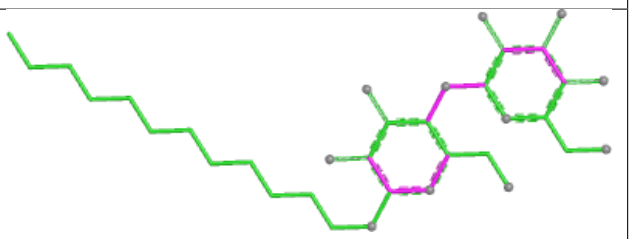
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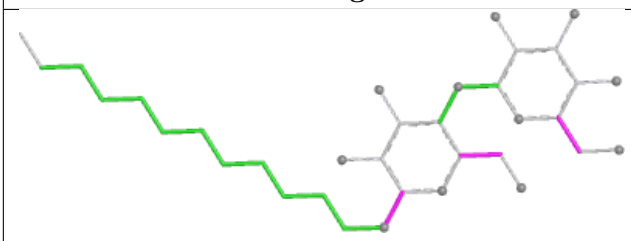
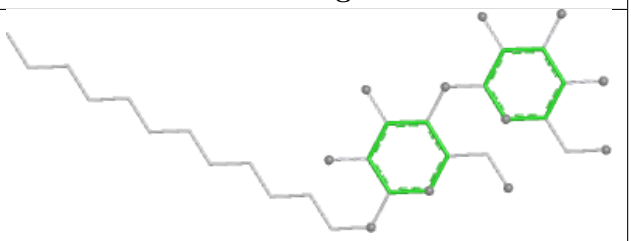
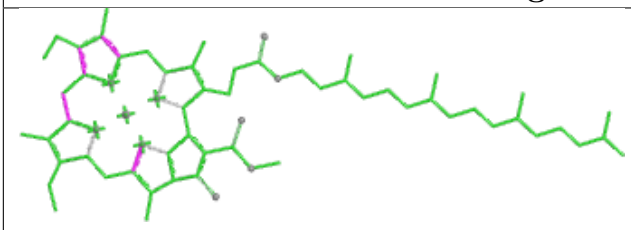
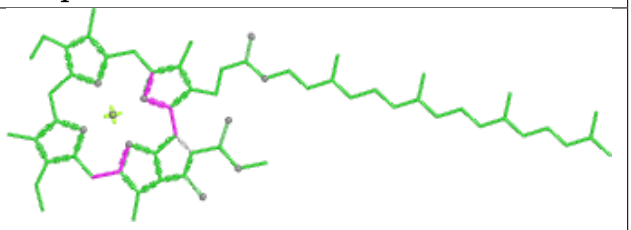
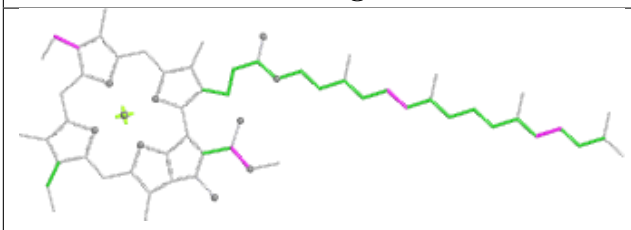
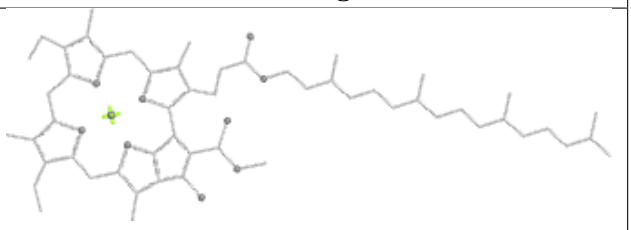
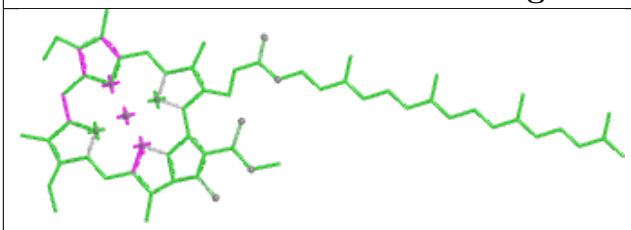
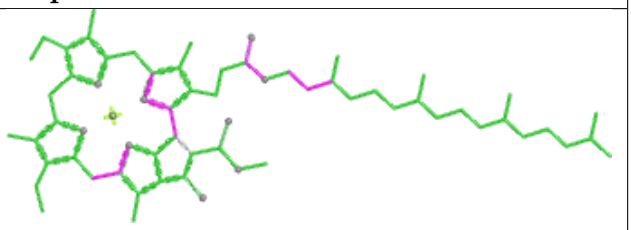
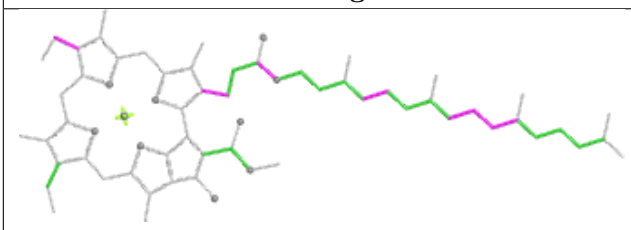
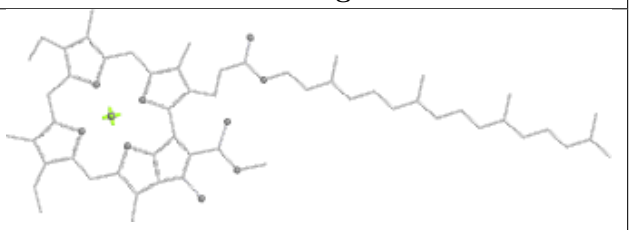
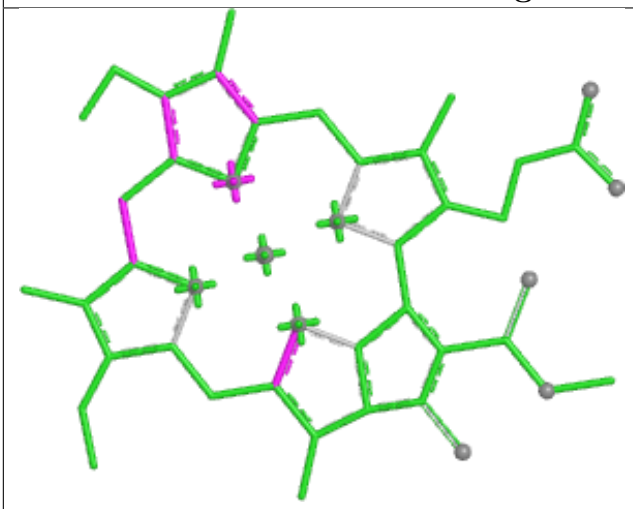

Torsions


Rings

Ligand CLA q 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1108



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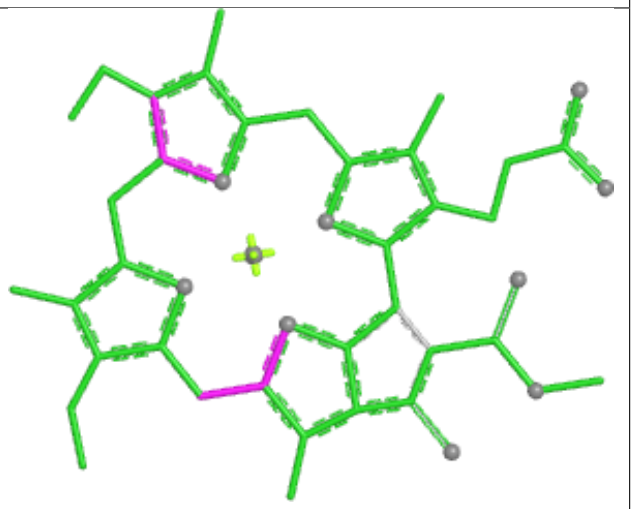
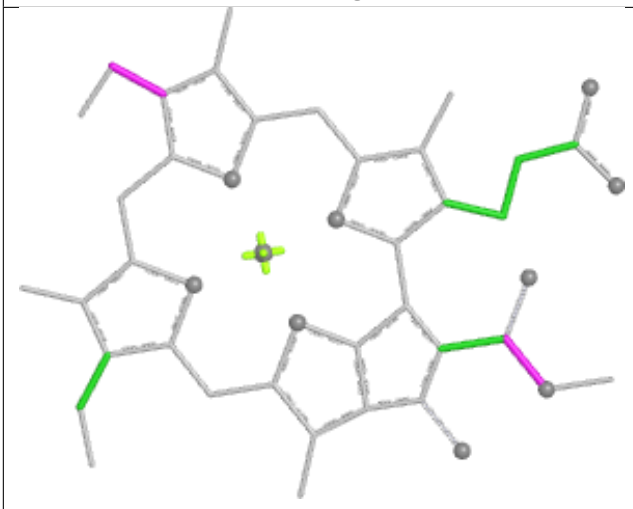


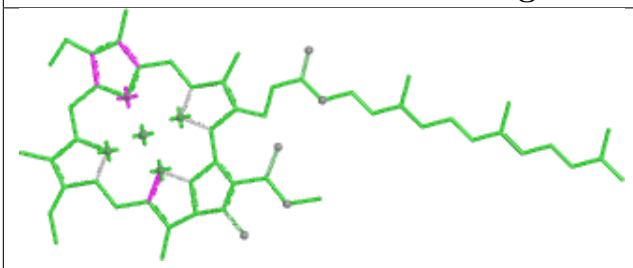
Bond angles



Torsions

Rings

Ligand CLA b 1215



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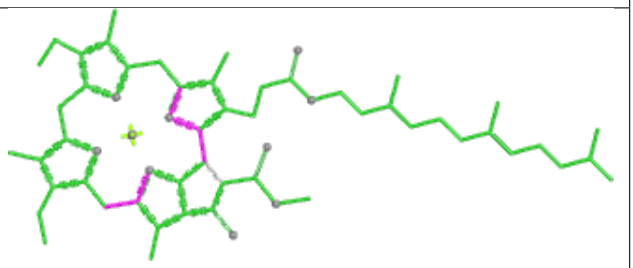
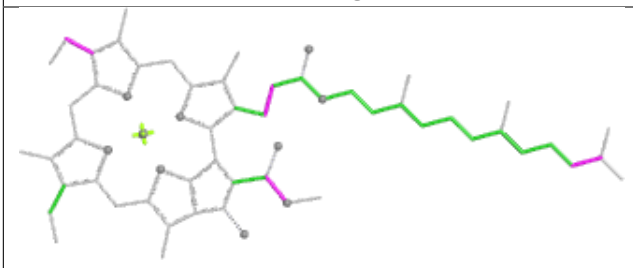
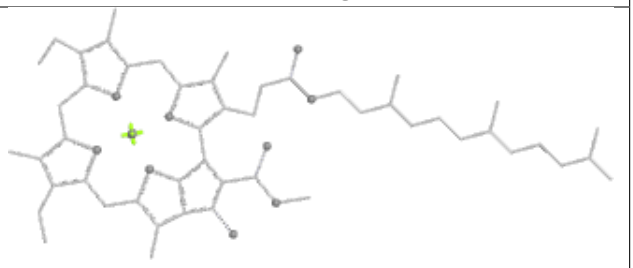


Bond angles

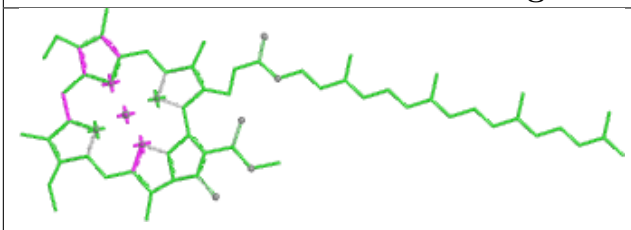


Torsions



Rings

Ligand CLA h 509



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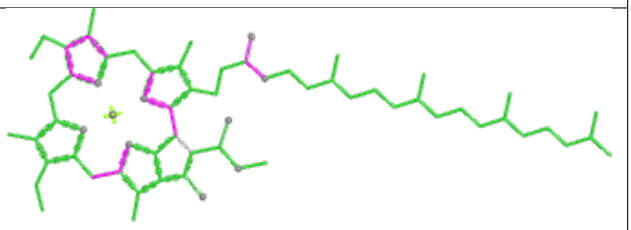
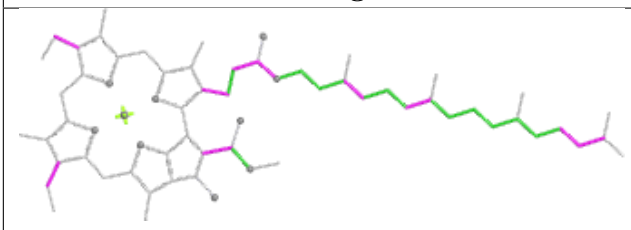
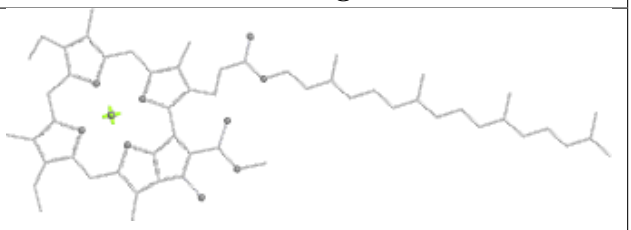


Bond angles

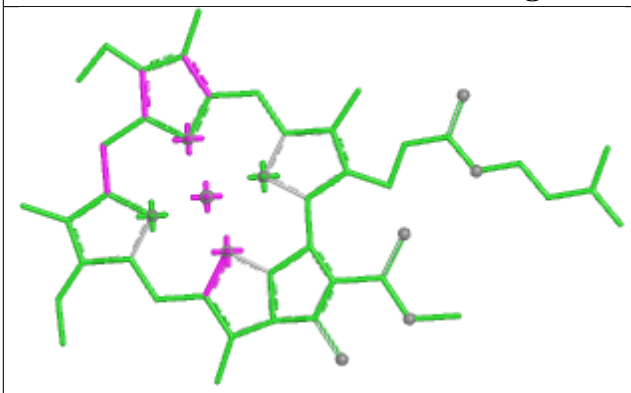


Torsions

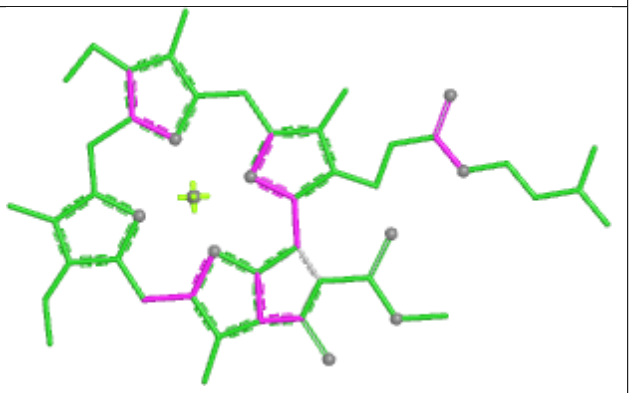


Rings

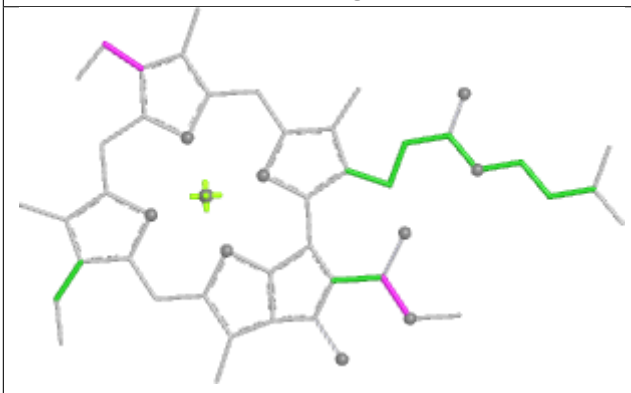
Ligand CLA X 514



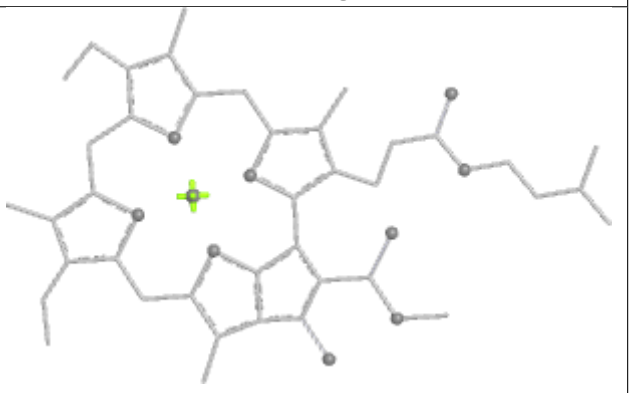
Bond lengths



Bond angles

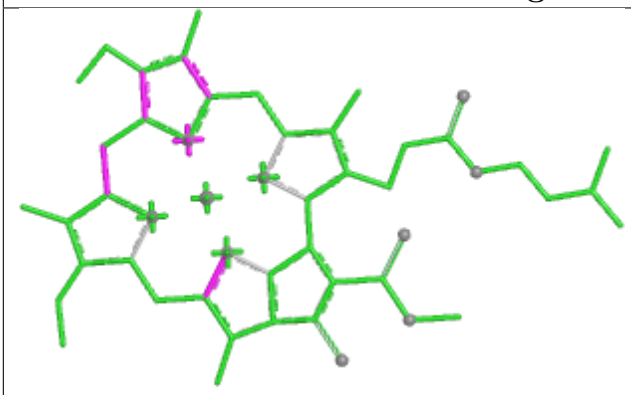


Torsions

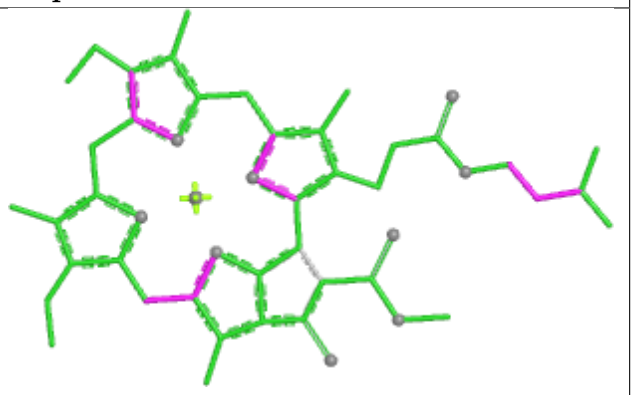


Rings

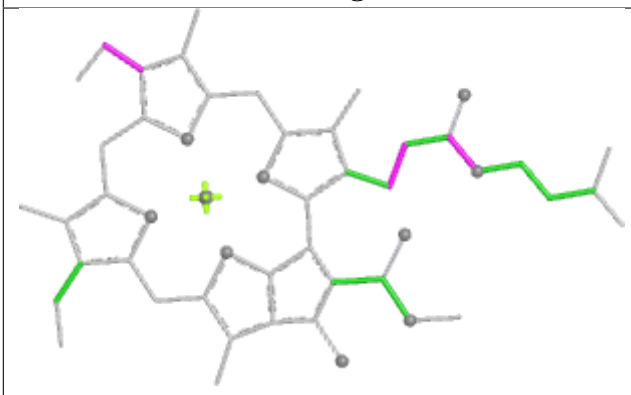
Ligand CLA p 502



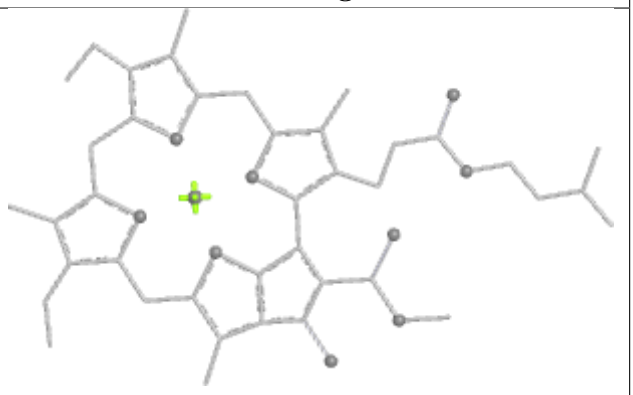
Bond lengths



Bond angles

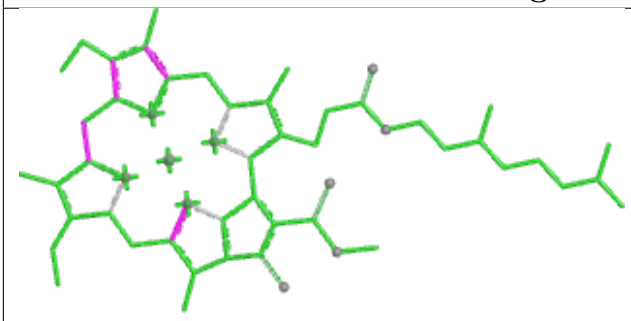


Torsions

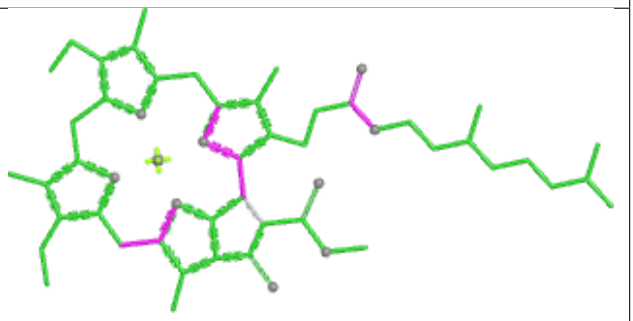


Rings

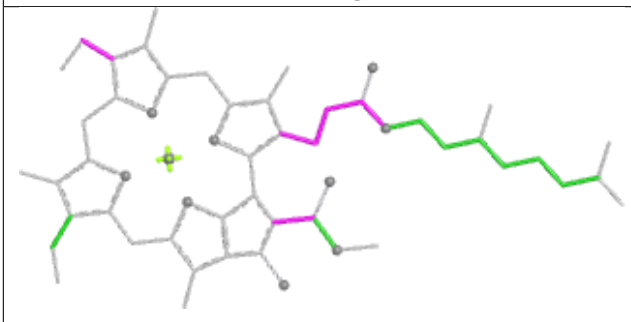
Ligand CLA s 508



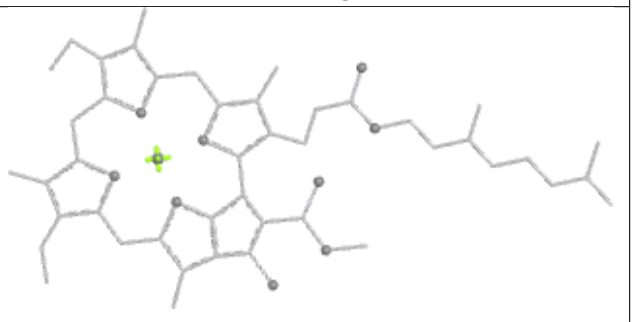
Bond lengths



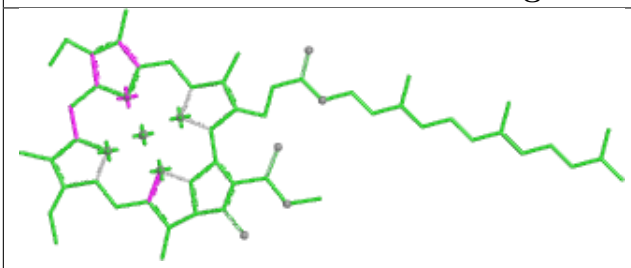
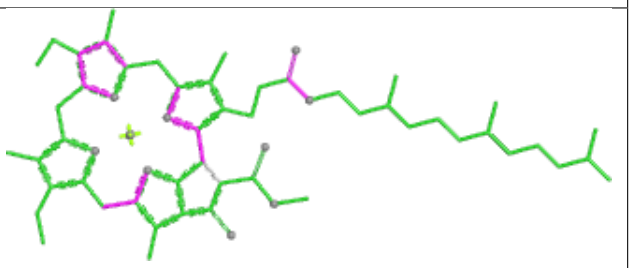
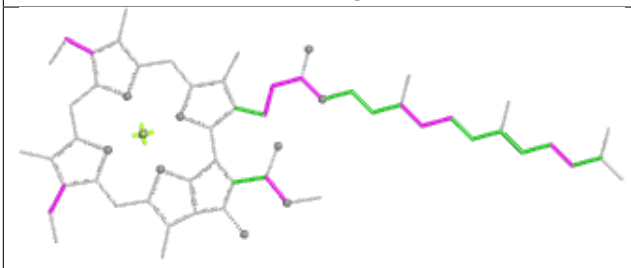
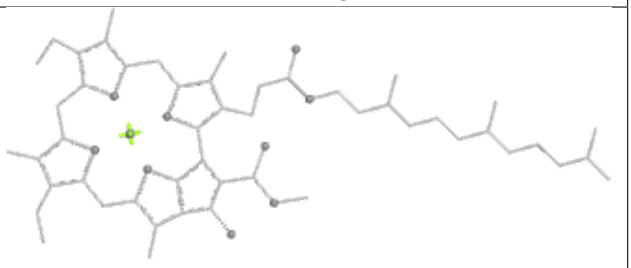
Bond angles

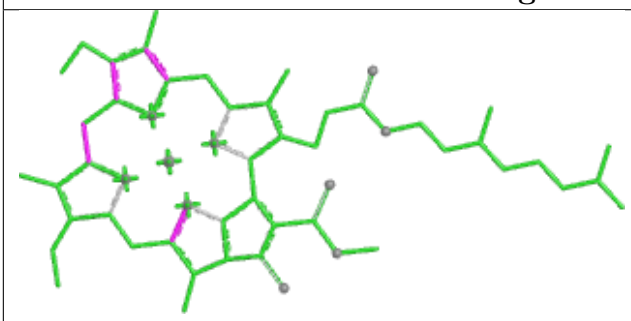
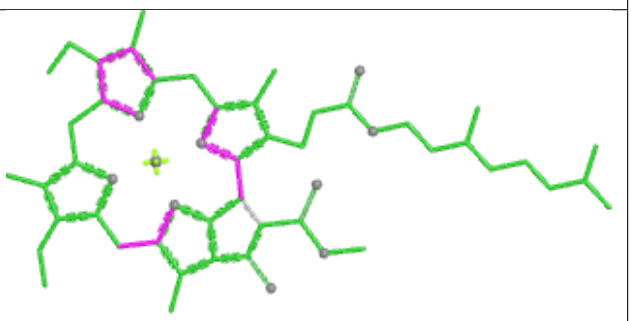
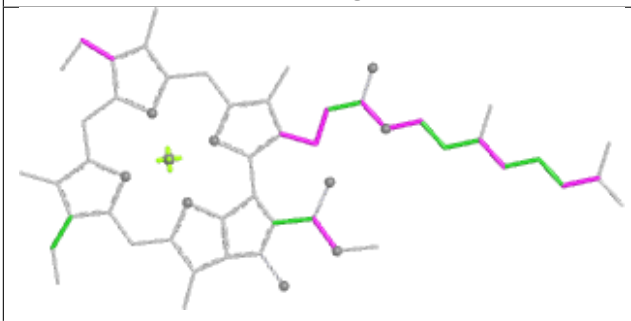
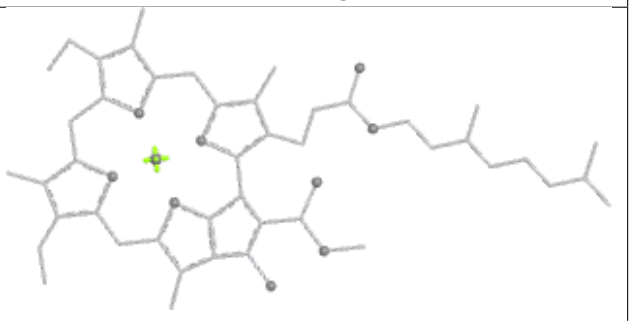


Torsions

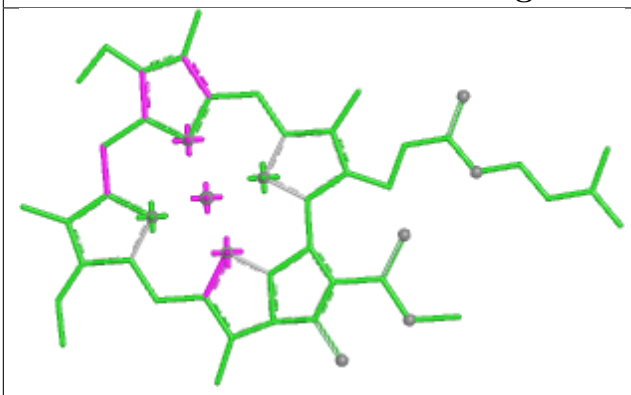


Rings

Ligand CLA X 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1228	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1234



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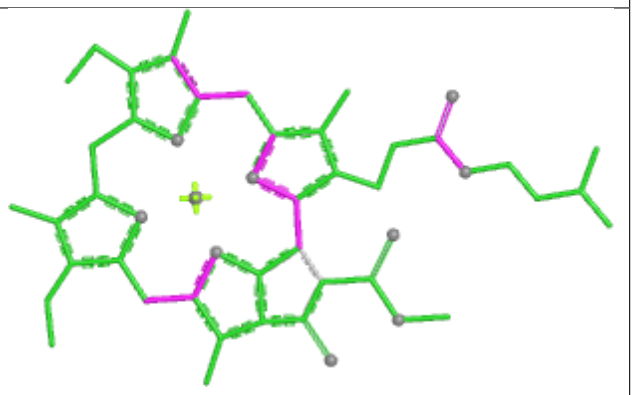
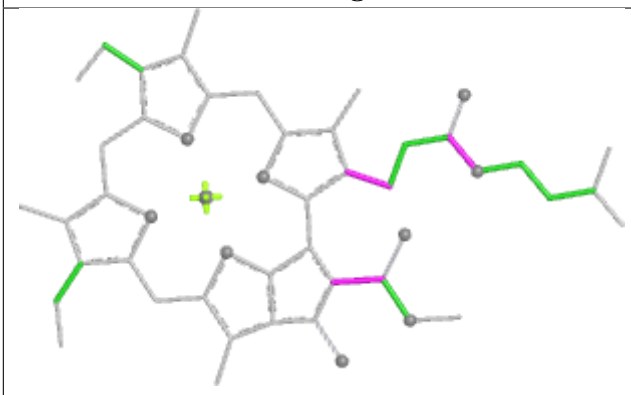
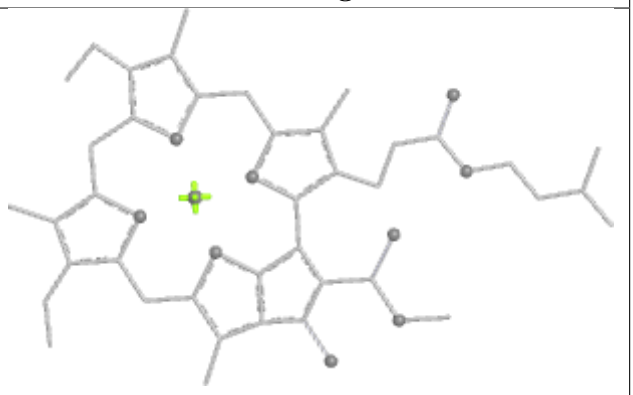


Bond angles

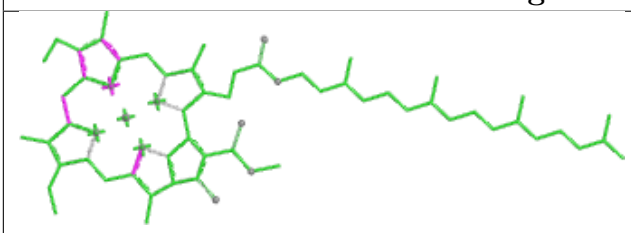


Torsions



Rings

Ligand CLA y 505



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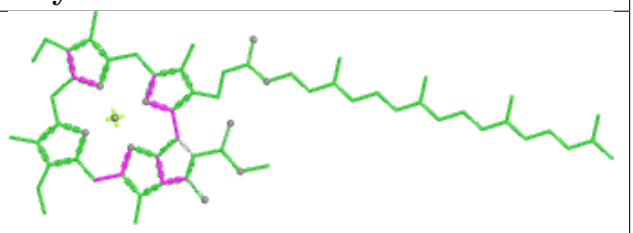
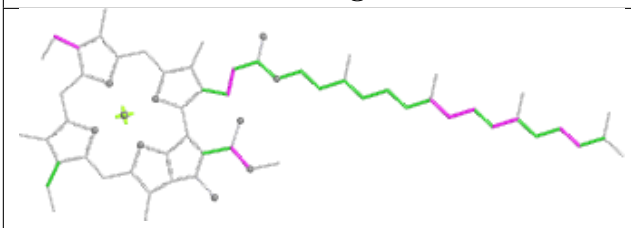


Bond angles



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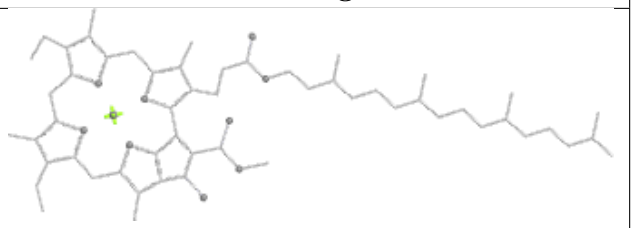
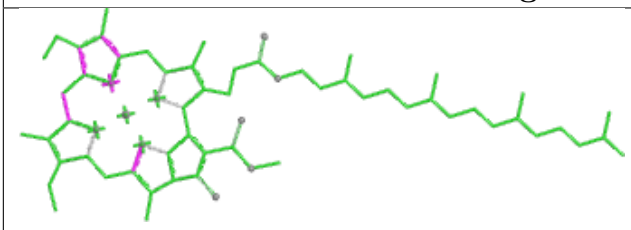


Rings

Ligand CLA a 1126



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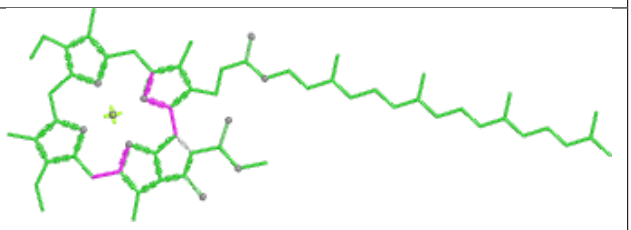
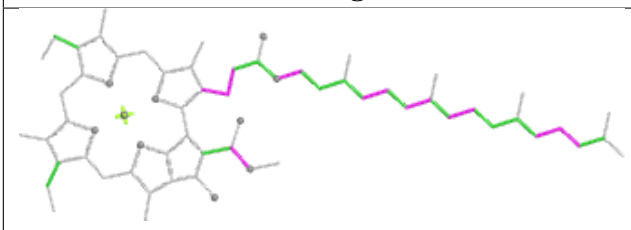


Bond angles



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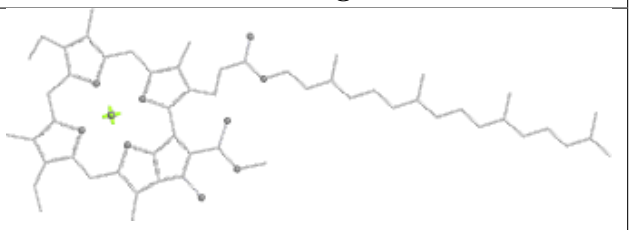
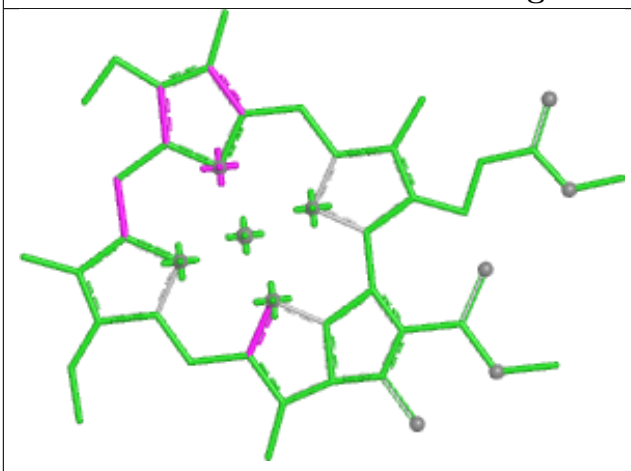


Rings

Ligand CLA p 513



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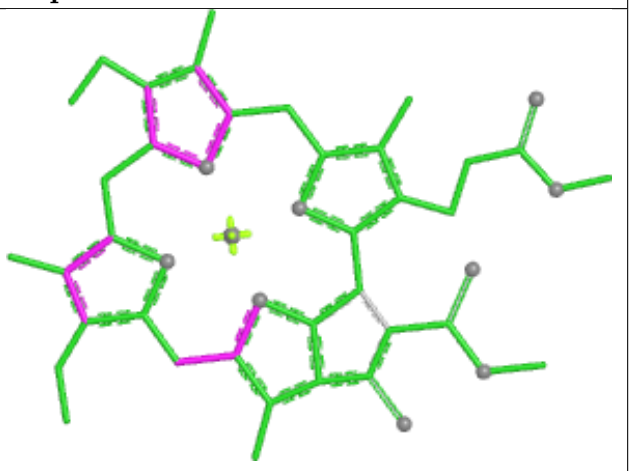
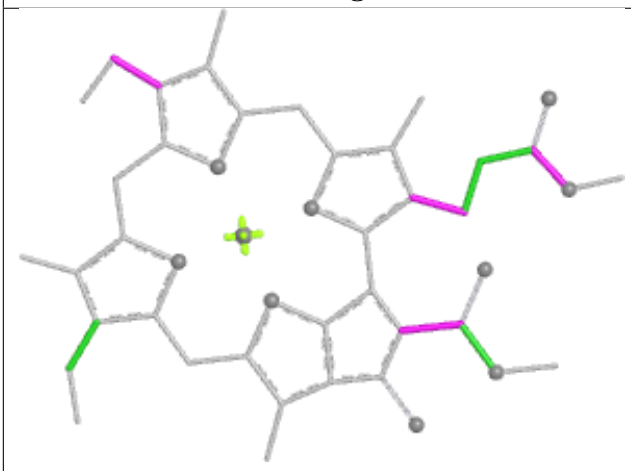


Bond angles



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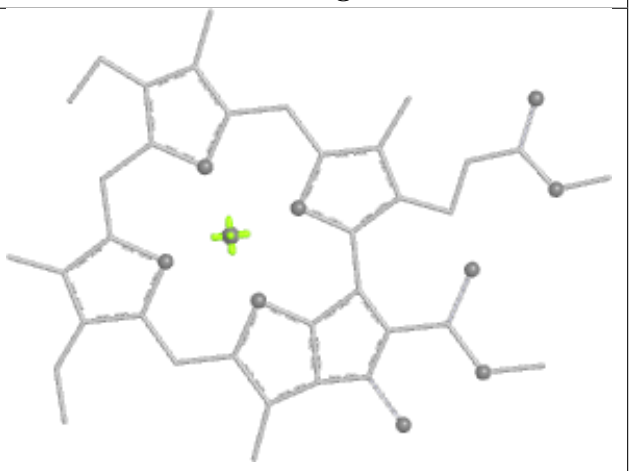
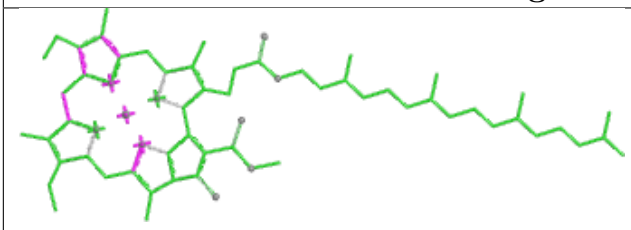


Rings

Ligand CLA g 509



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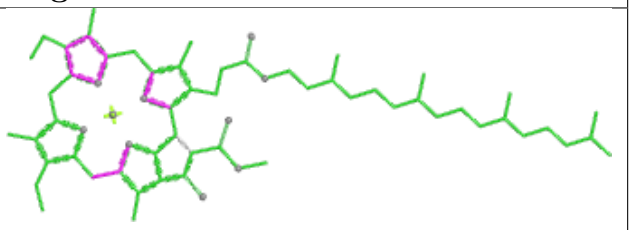

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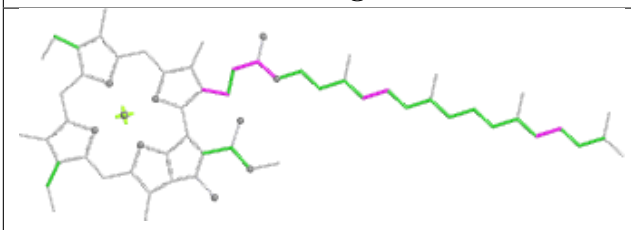

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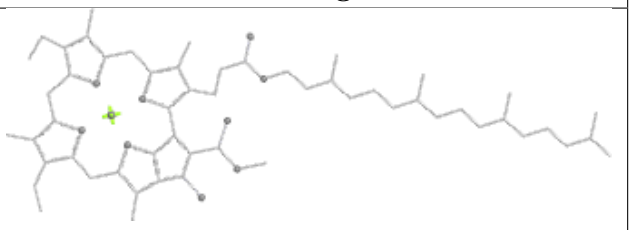
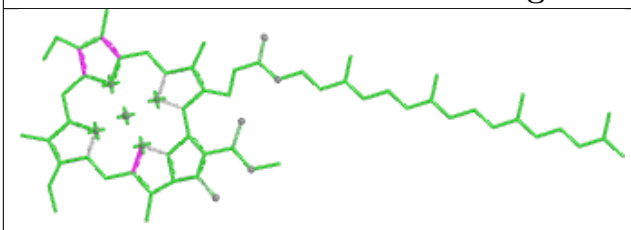


Rings

Ligand CLA n 510



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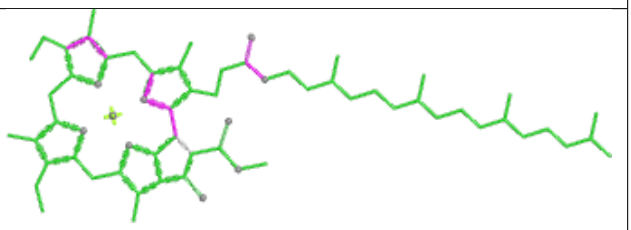
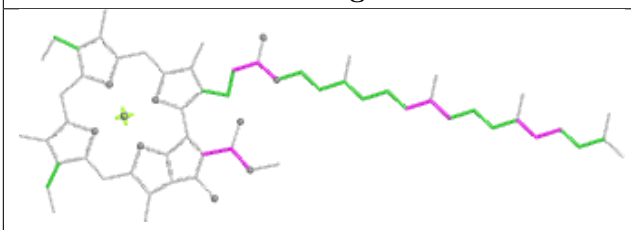


Bond angles



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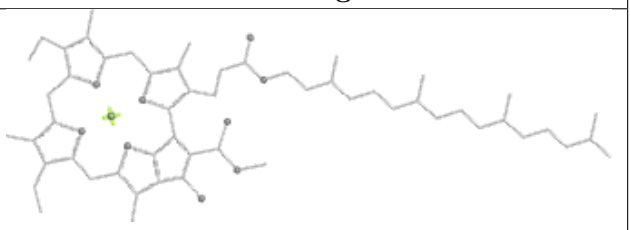
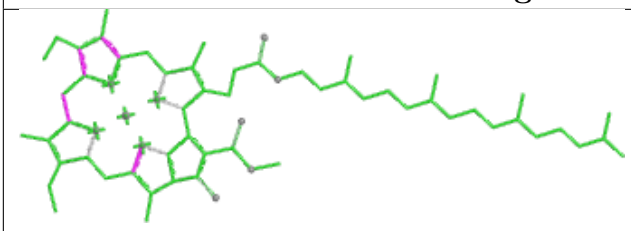


Rings

Ligand CLA H 1101



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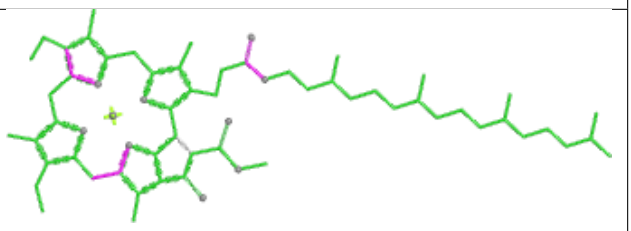
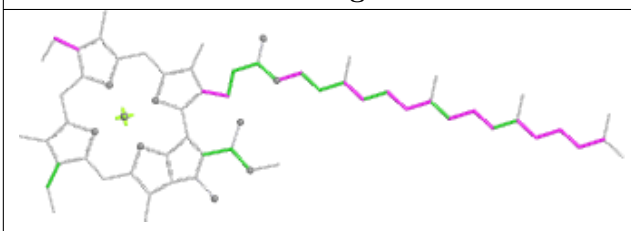


Bond angles



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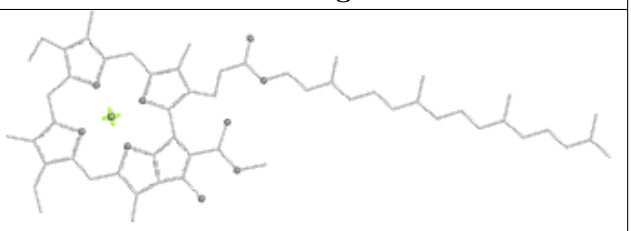
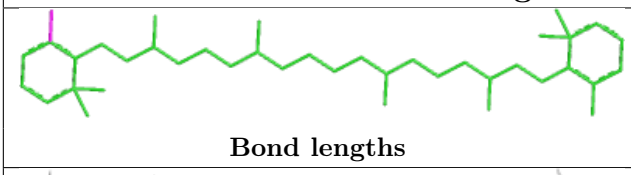


Rings

Ligand BCR T 4001



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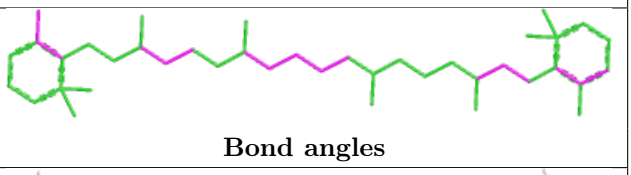
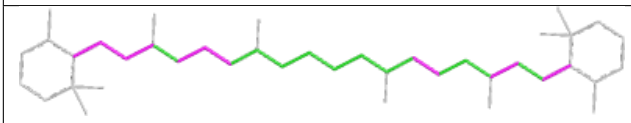


Bond angles



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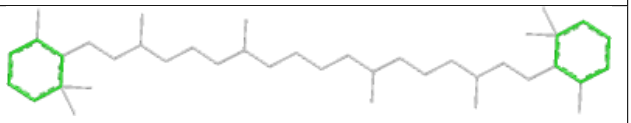
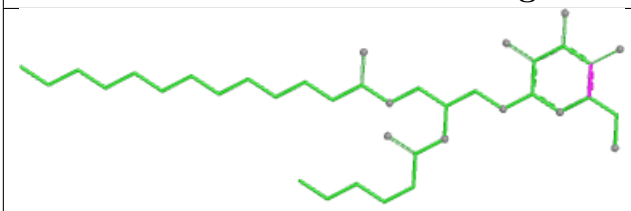


Rings

Ligand LMG H 852



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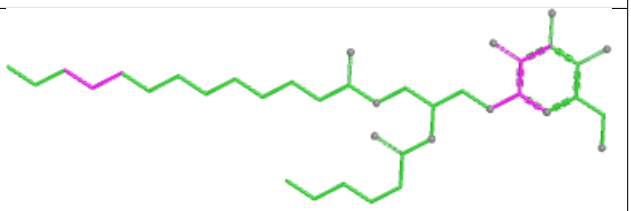
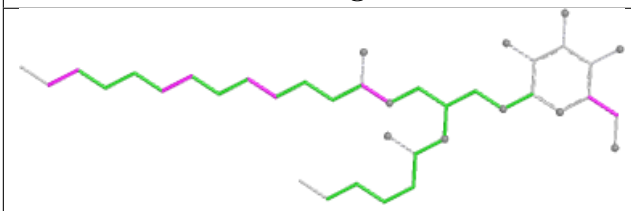


Bond angles



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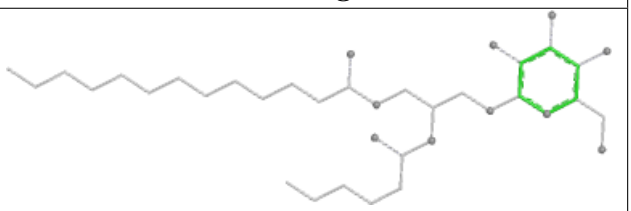
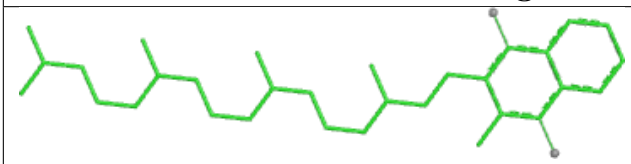
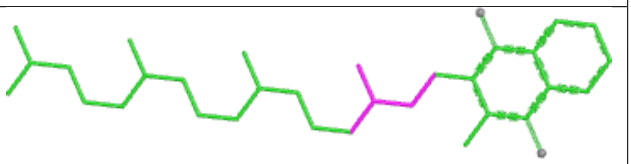


Rings

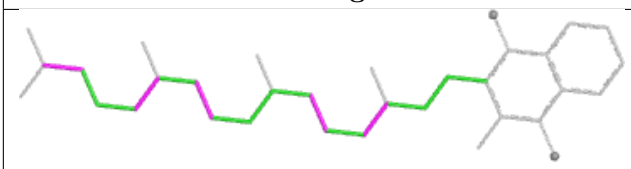
Ligand PQN b 2002



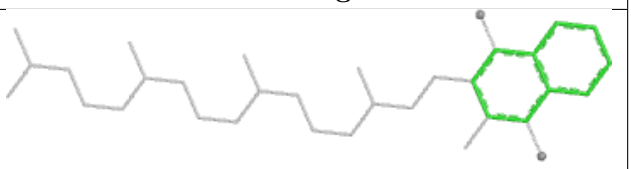
Bond lengths



Bond angles

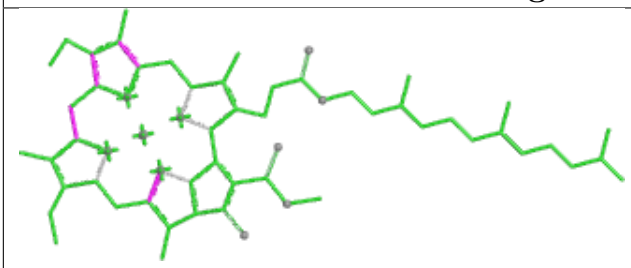


Torsions



Rings

Ligand CLA o 510



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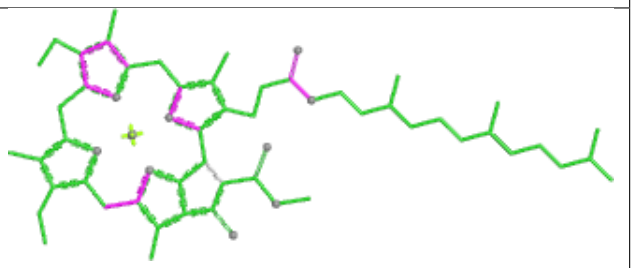
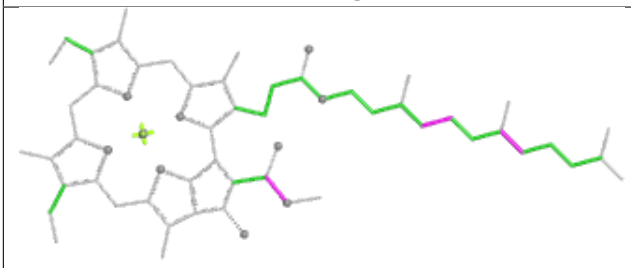


Bond angles



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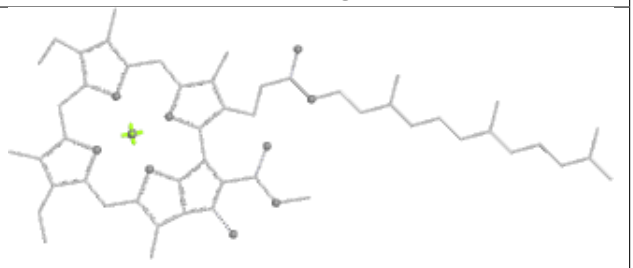
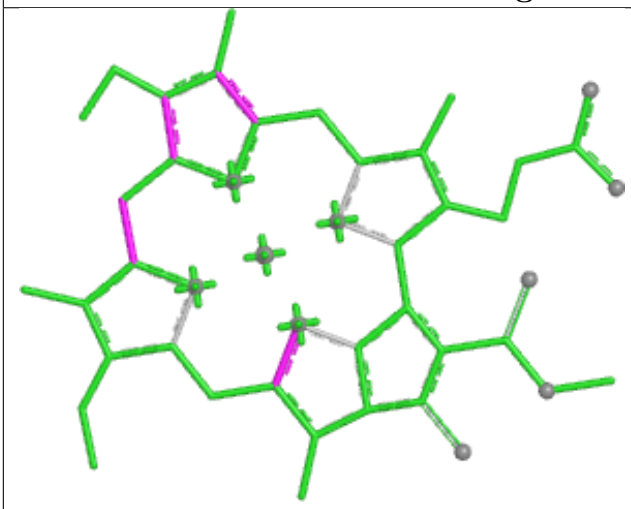
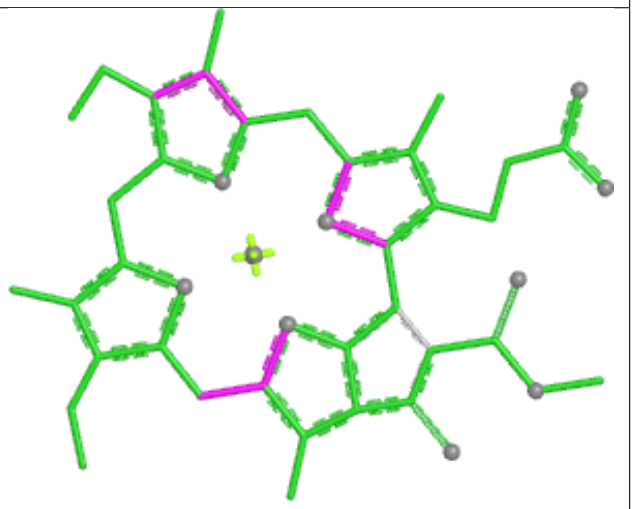


Rings

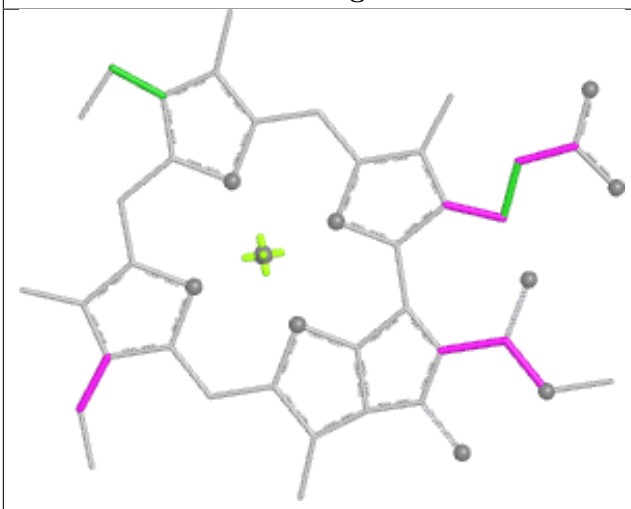
Ligand CLA T 4003



Bond lengths

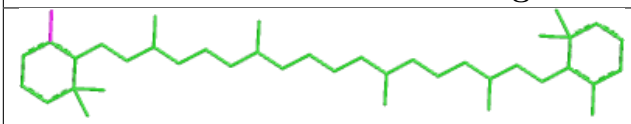
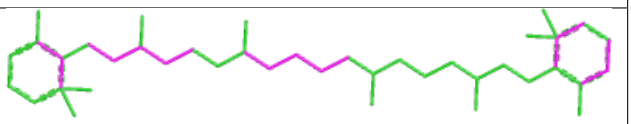
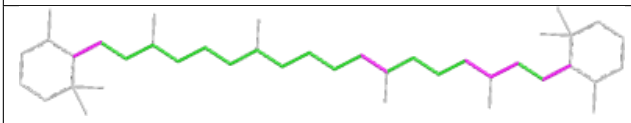
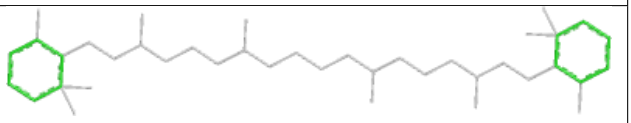


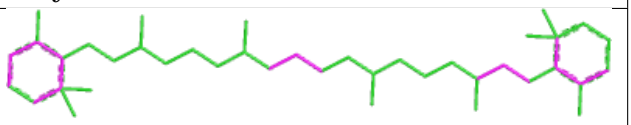
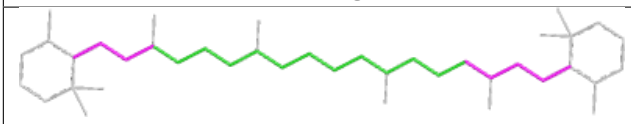
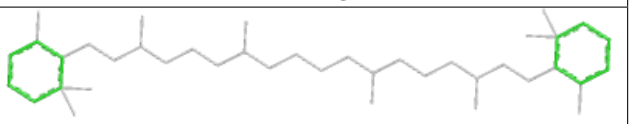
Bond angles

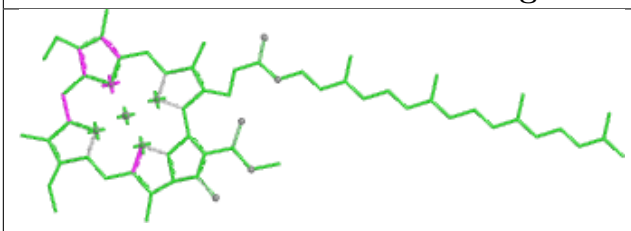
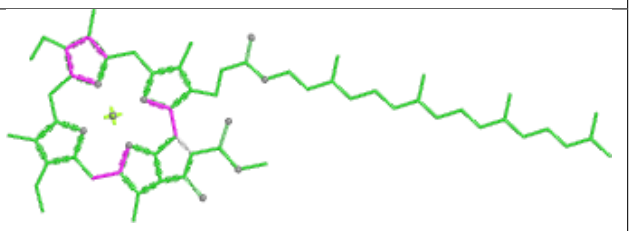
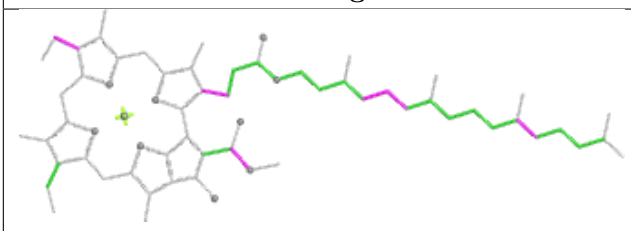
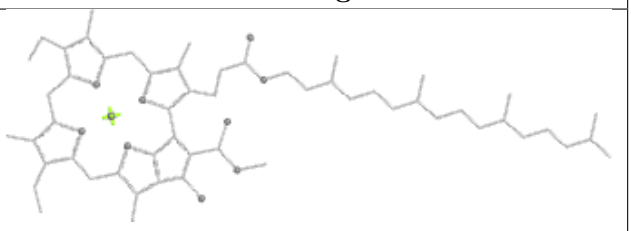


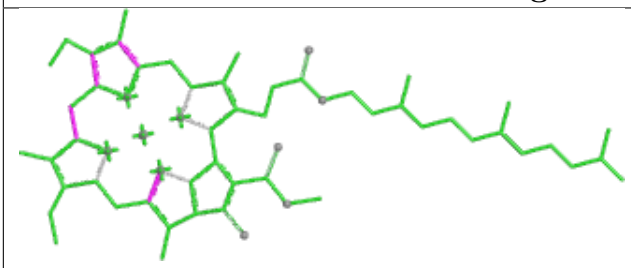
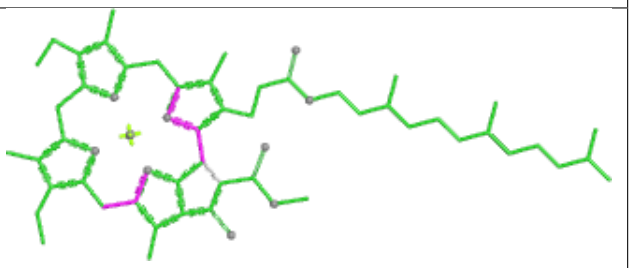
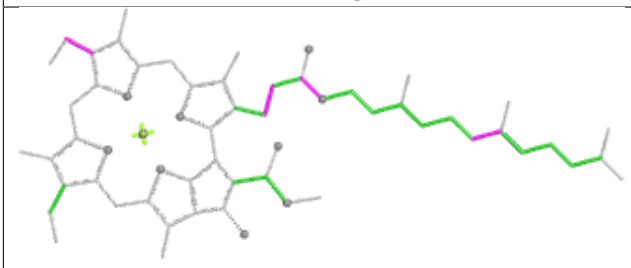
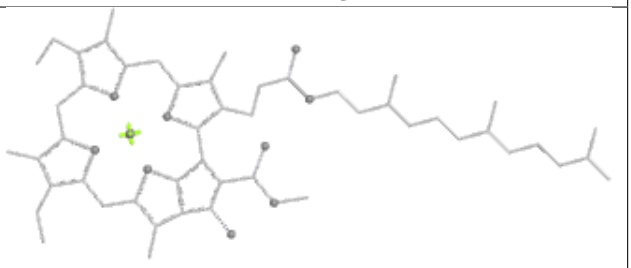
Torsions

Rings

Ligand BCR H 4007	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR y 604	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 1119	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA t 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

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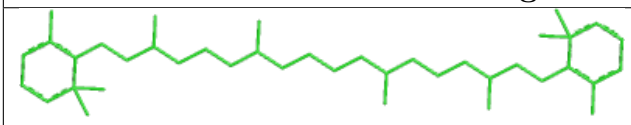
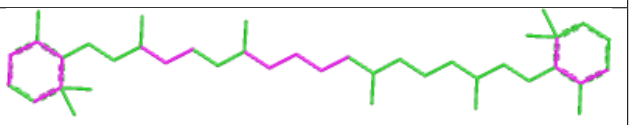
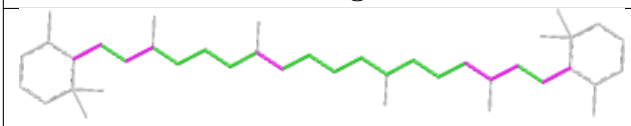
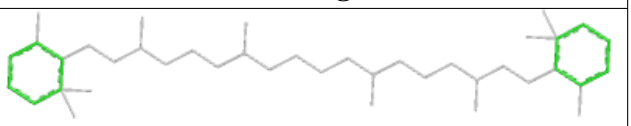
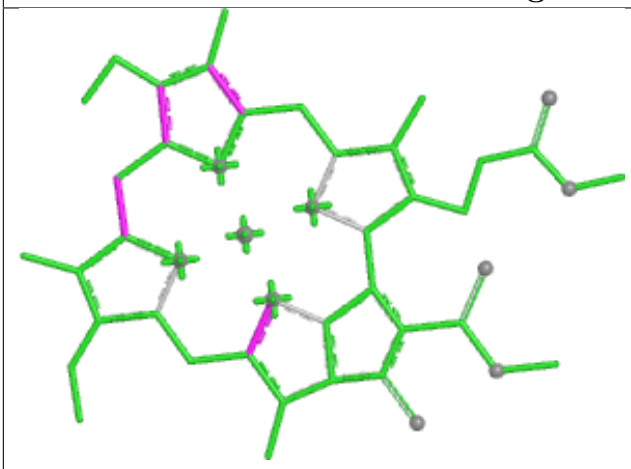
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 516



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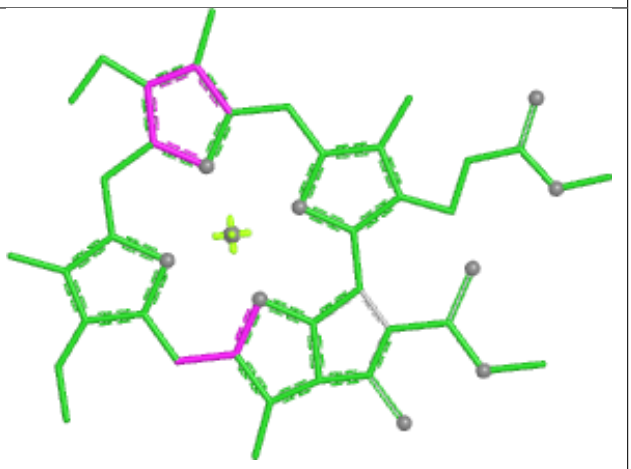

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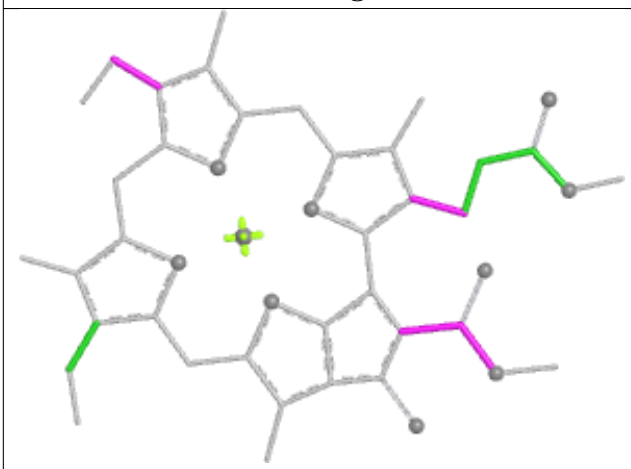
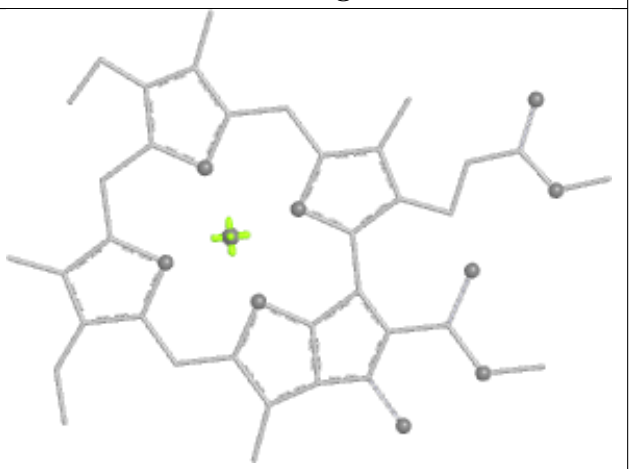
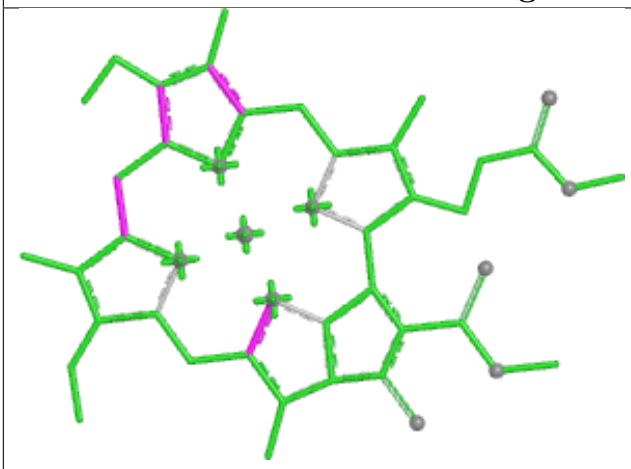


Torsions



Rings

Ligand CLA W 516



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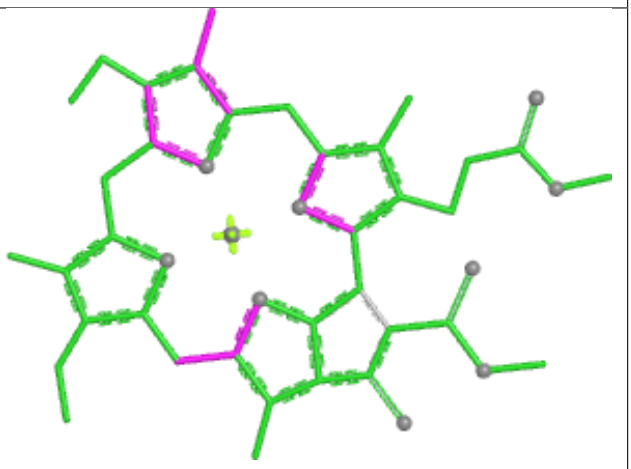

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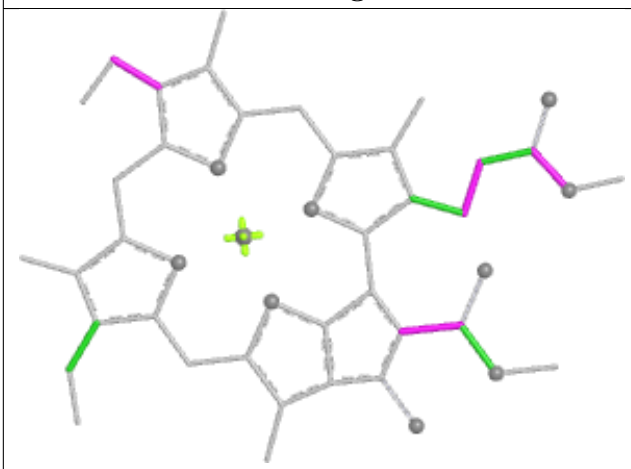

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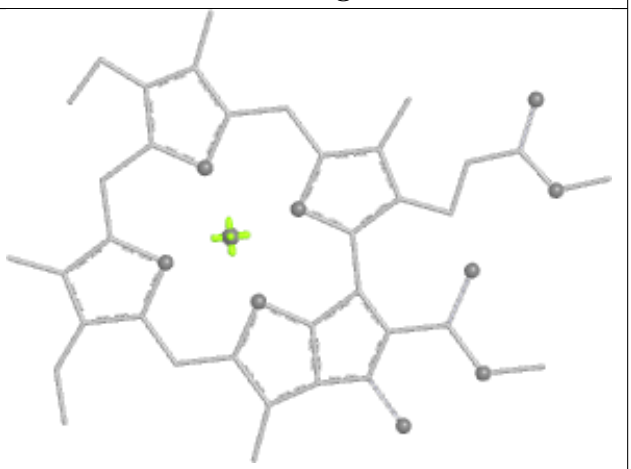
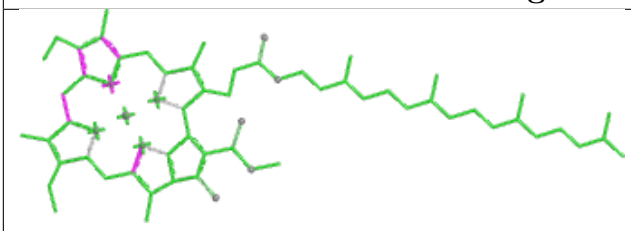


Rings

Ligand CLA q 504



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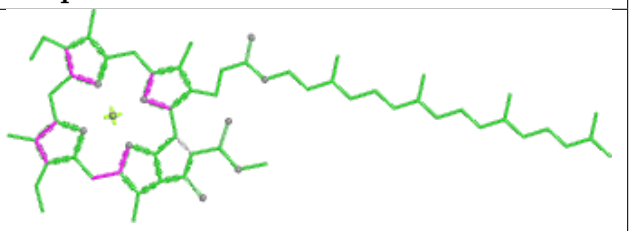

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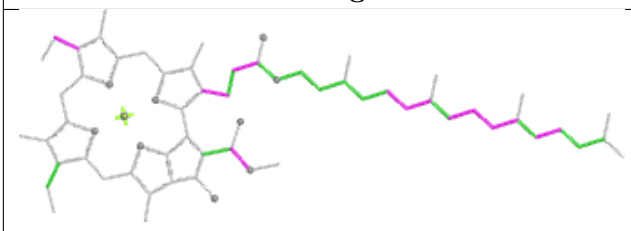

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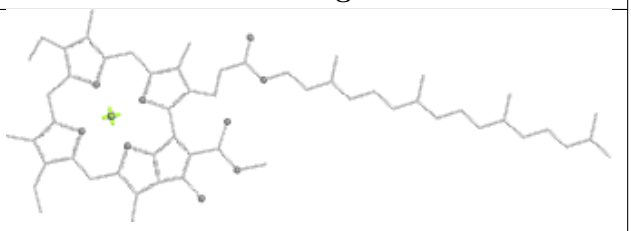
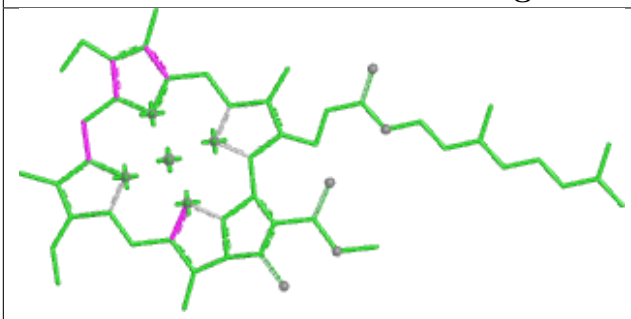
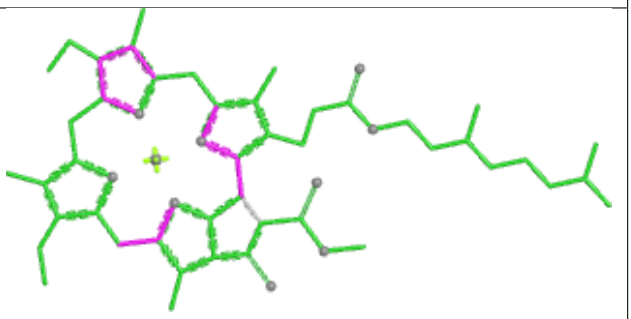
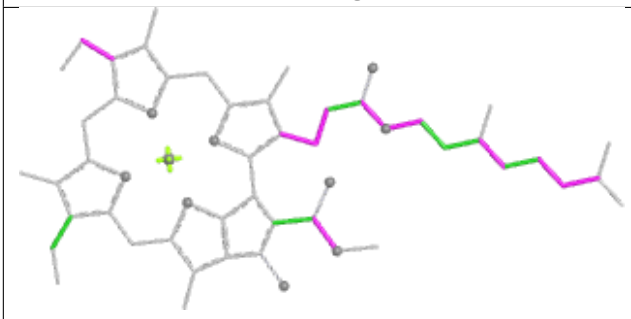
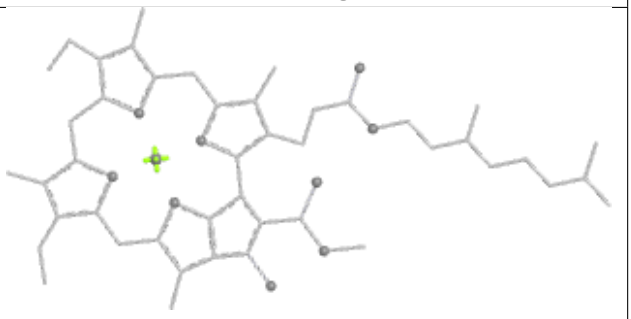


Rings

Ligand CLA G 1228	
 Bond lengths	 Bond angles
 Torsions	 Rings

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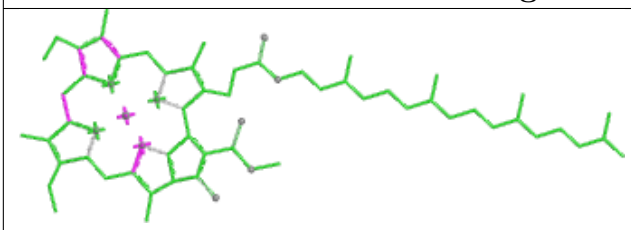
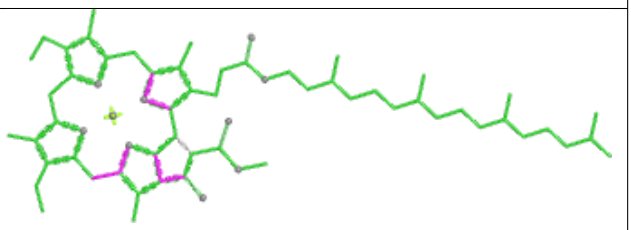
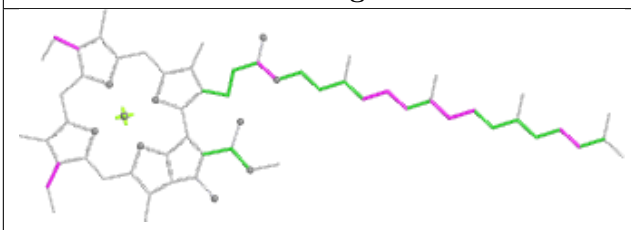
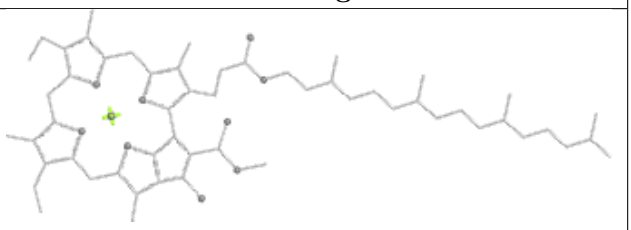
 Bond lengths	 Bond angles
 Torsions	 Rings

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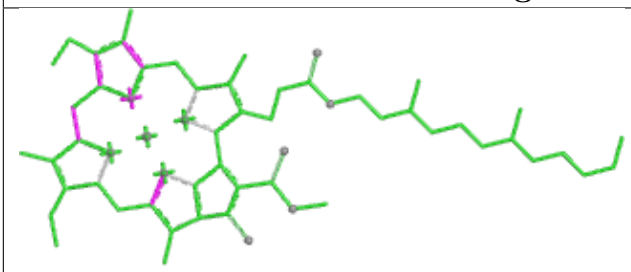
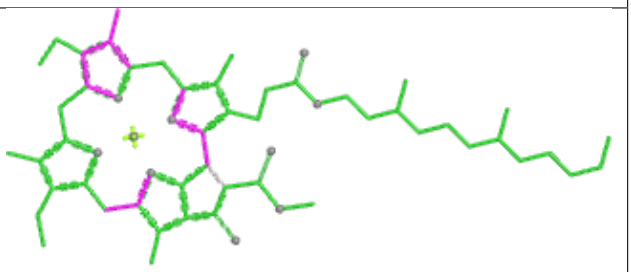
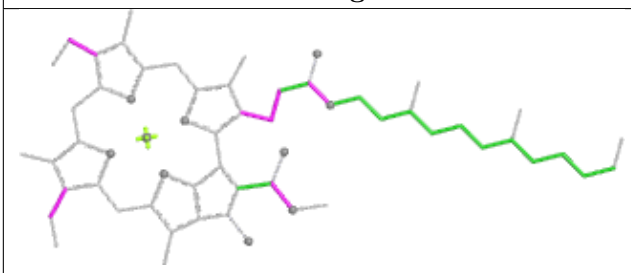
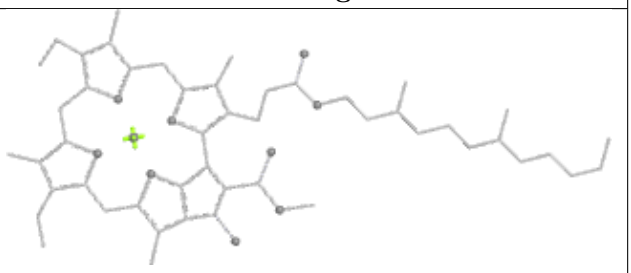
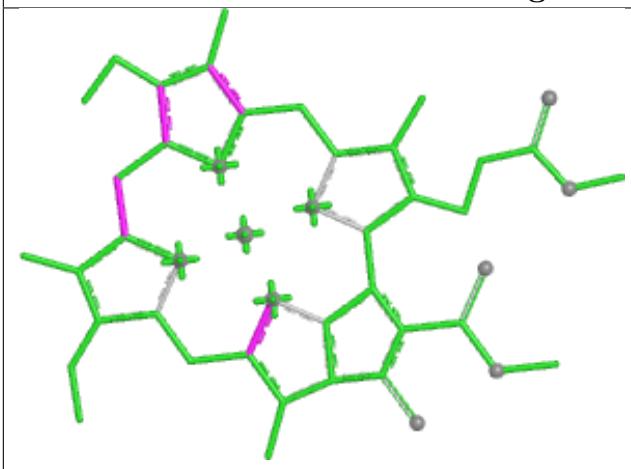
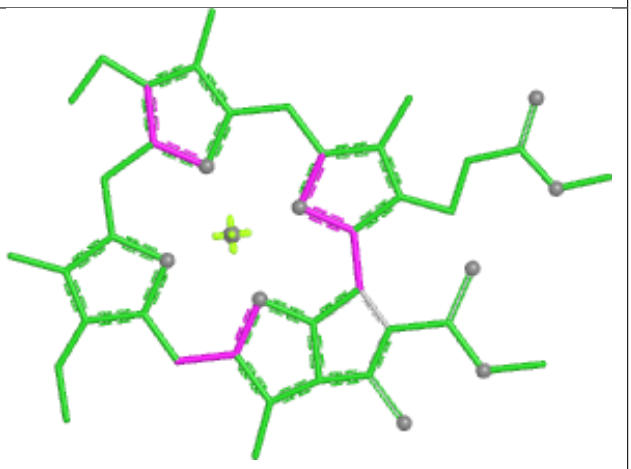
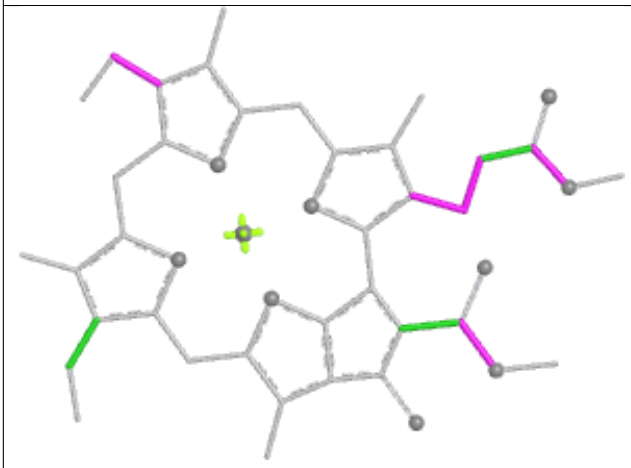
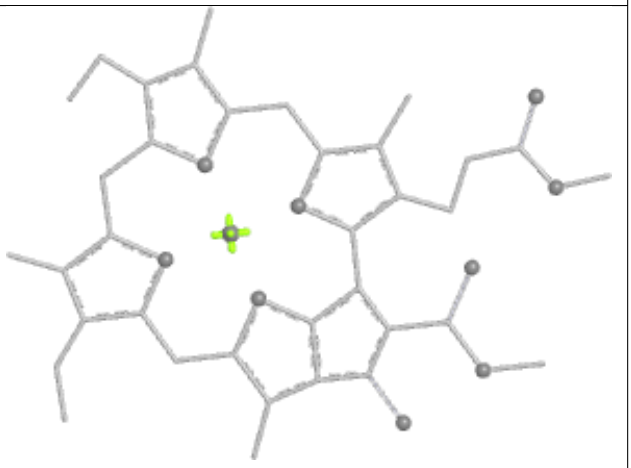
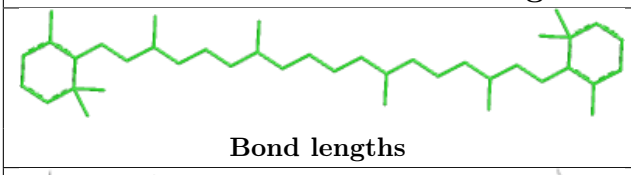
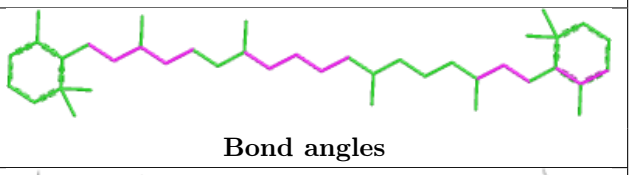
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA o 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

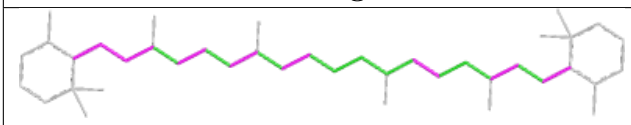
Ligand BCR x 604



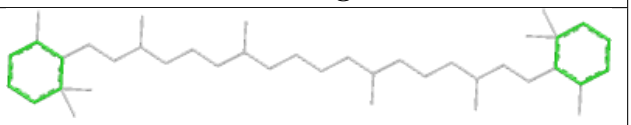
Bond lengths



Bond angles

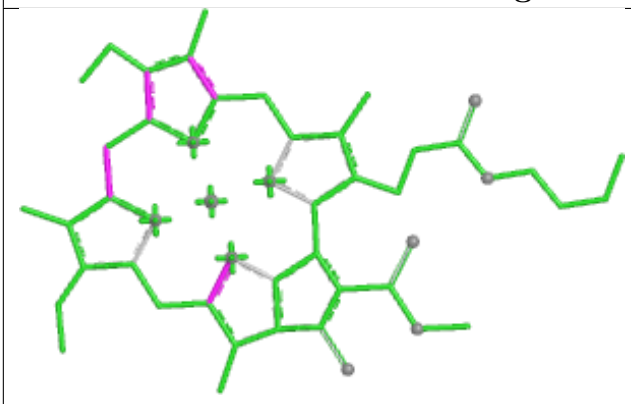


Torsions

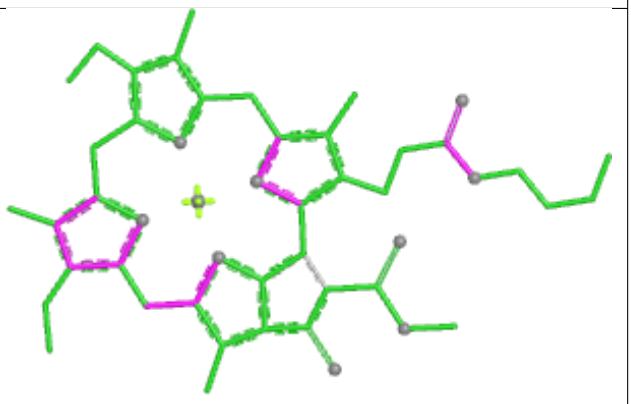


Rings

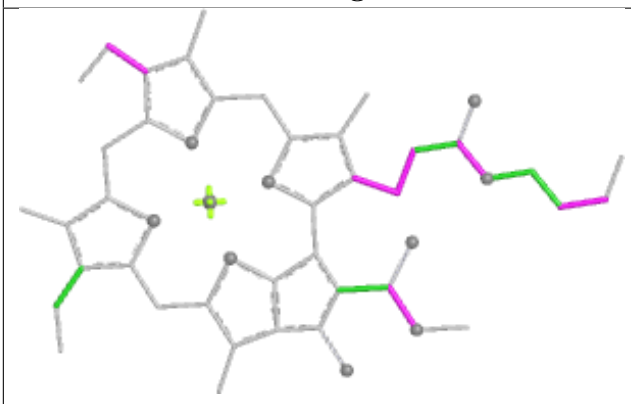
Ligand CLA H 1120



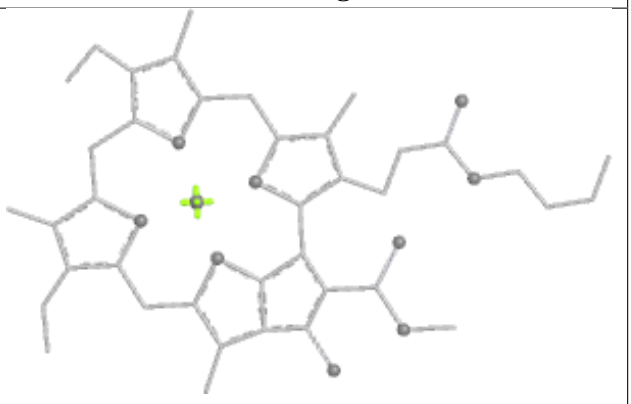
Bond lengths



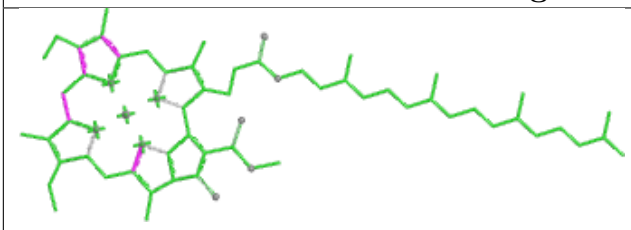
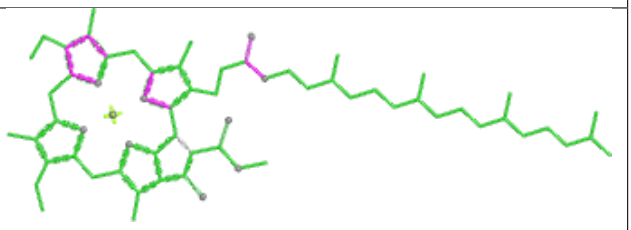
Bond angles



Torsions



Rings

Ligand CLA r 510	
	
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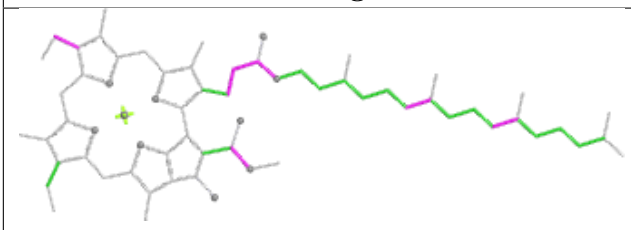
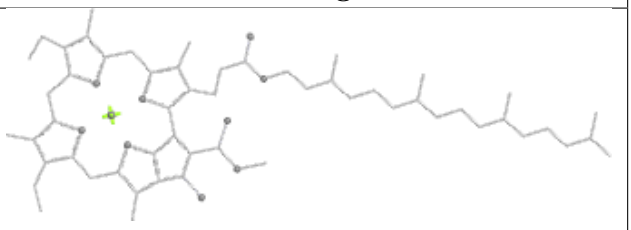
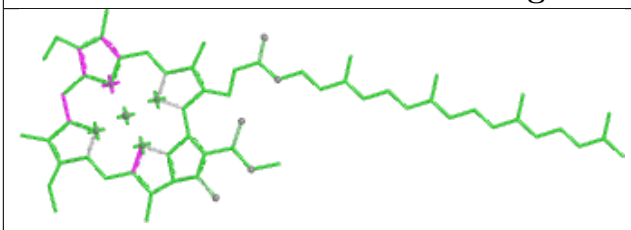
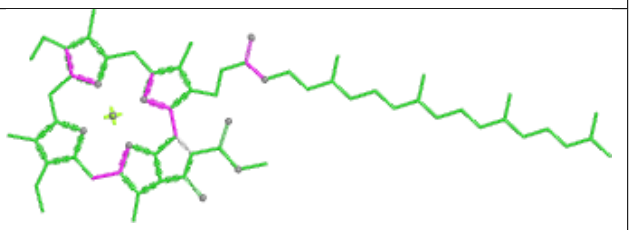
	
Torsions	**Rings**

Ligand CLA v 505	
	
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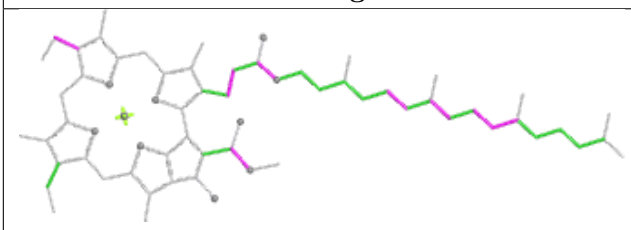
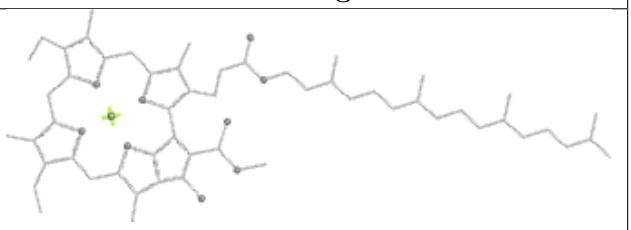
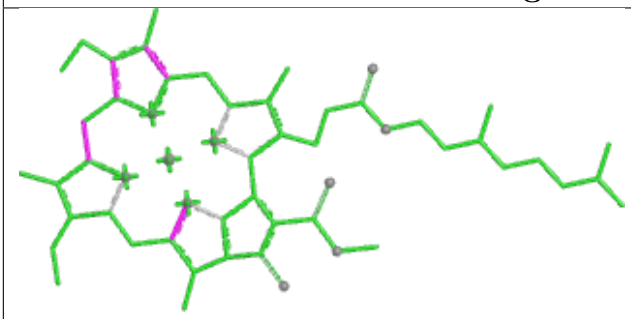
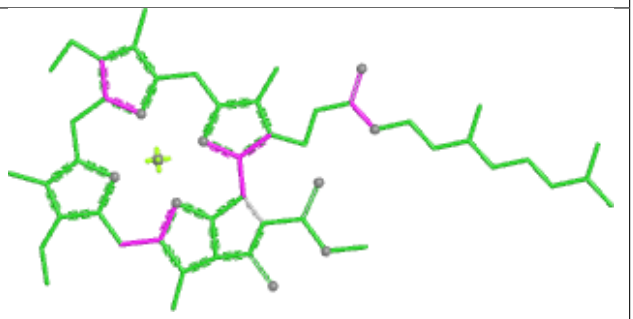
	
Torsions	**Rings**

Ligand CLA X 517



Bond lengths



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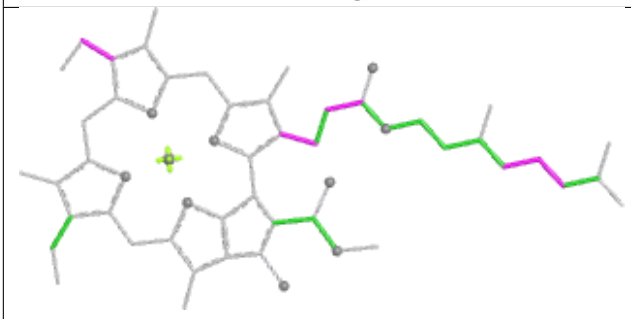
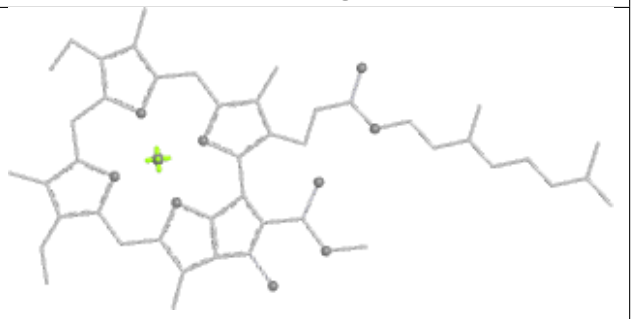
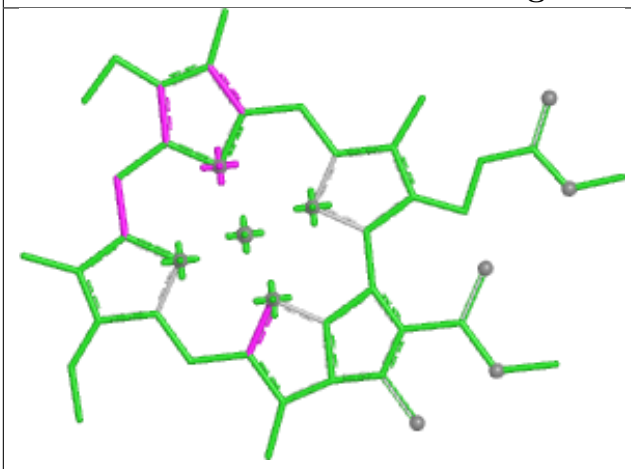


Torsions



Rings

Ligand CLA y 516



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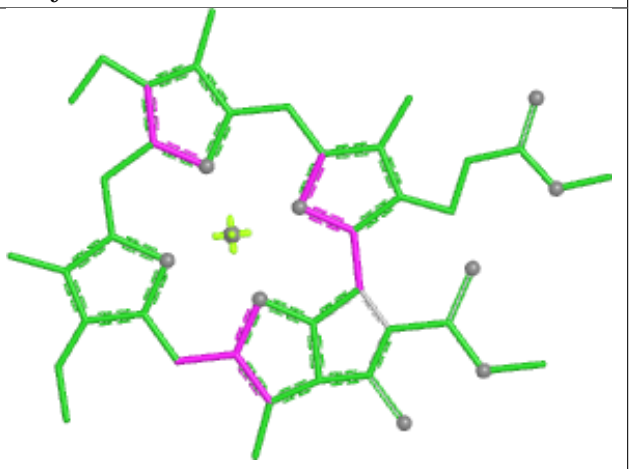
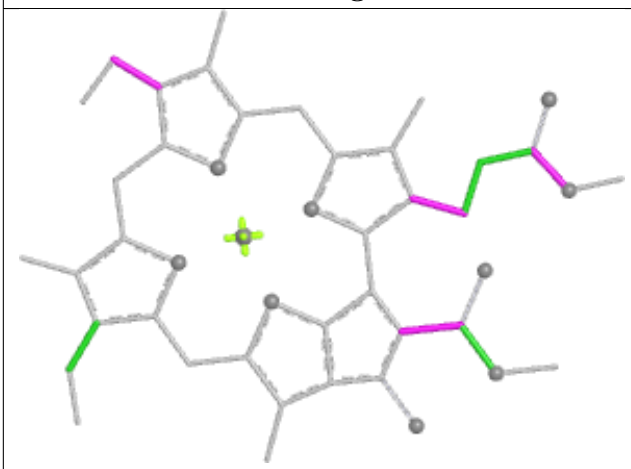
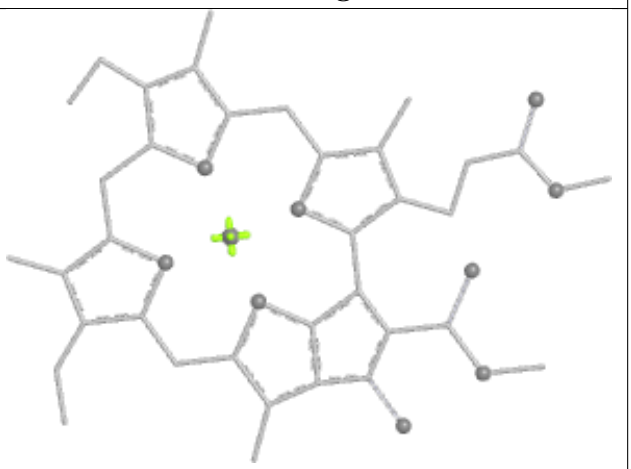


Bond angles

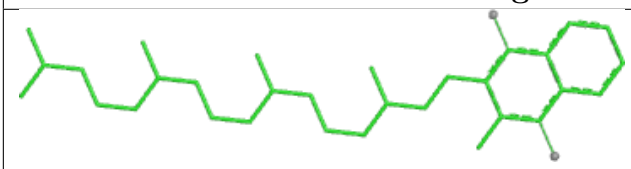


Torsions



Rings

Ligand PQN G 2002



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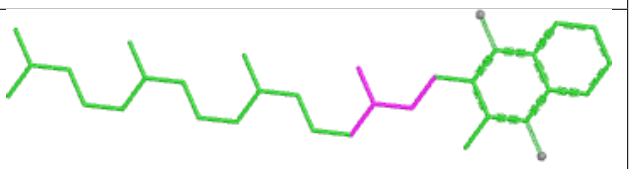
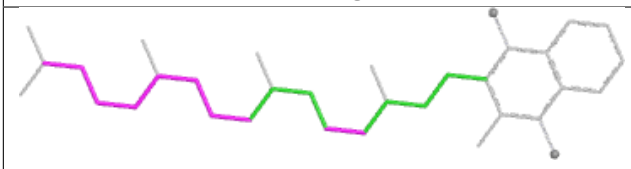


Bond angles



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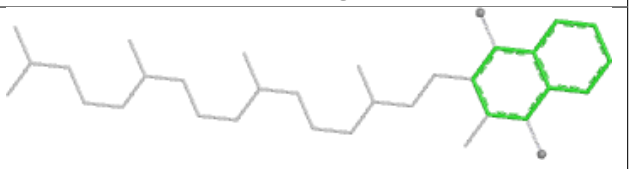
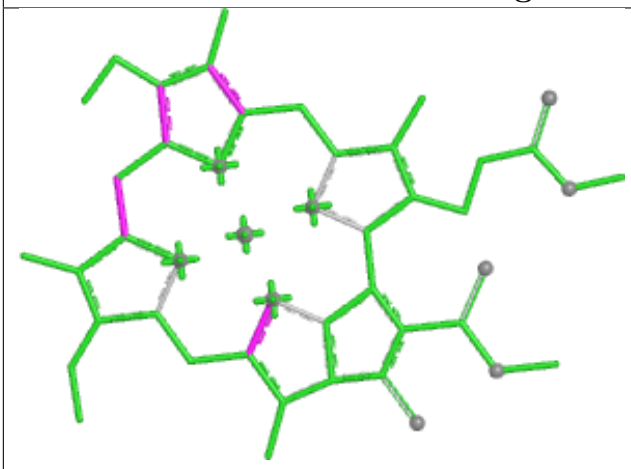
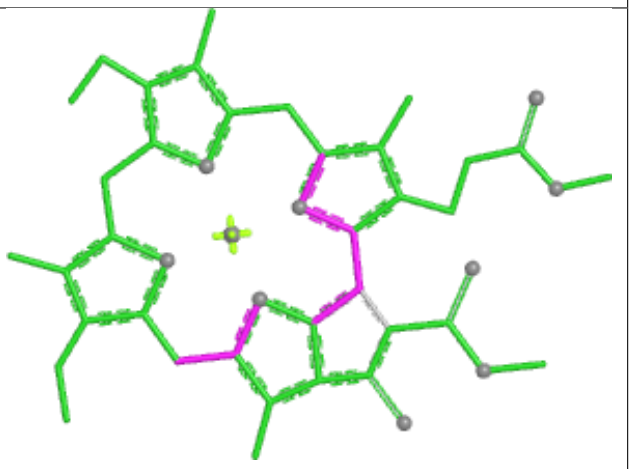


Rings

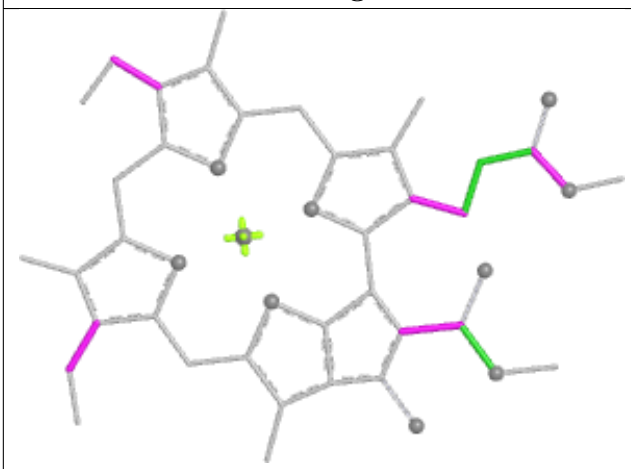
Ligand CLA A 1114



Bond lengths



Bond angles



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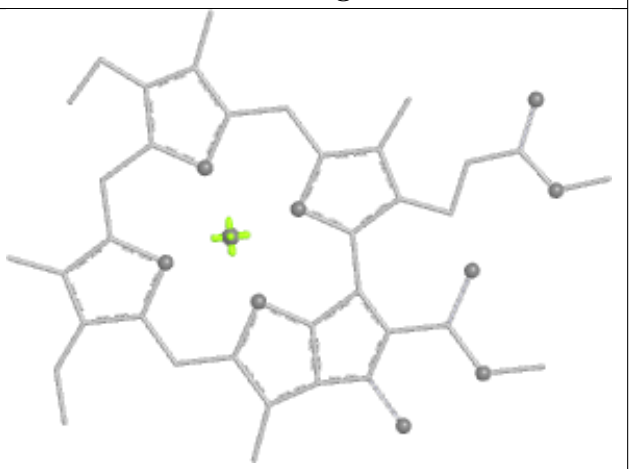
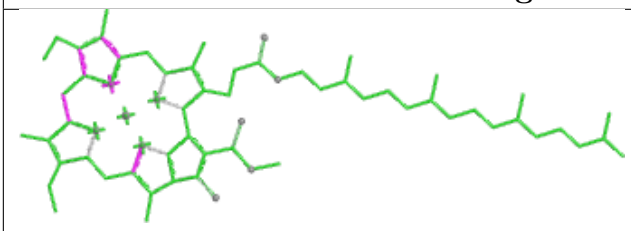


Rings

Ligand CLA B 1206



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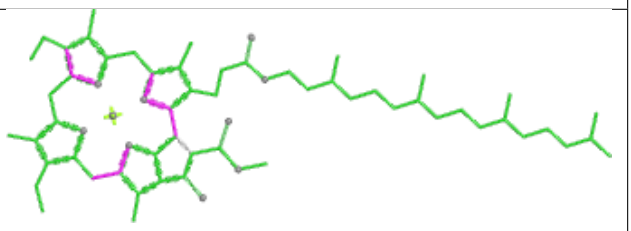
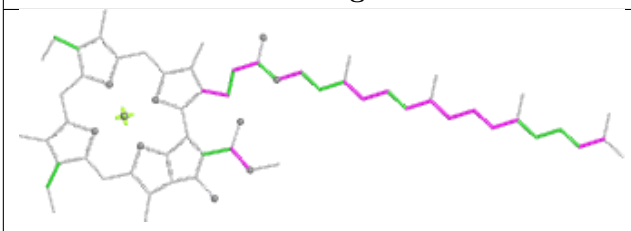


Bond angles



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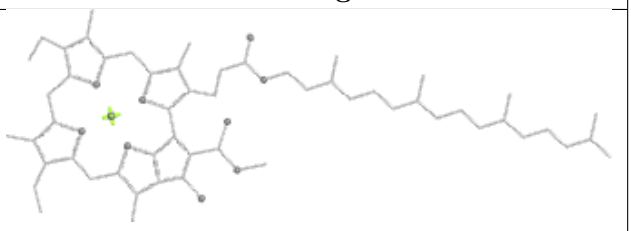
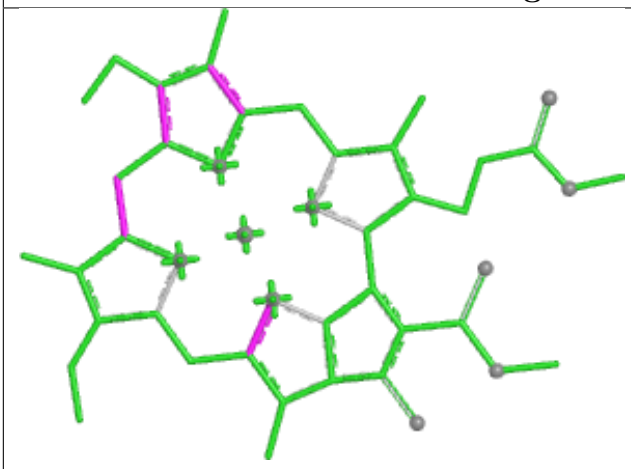
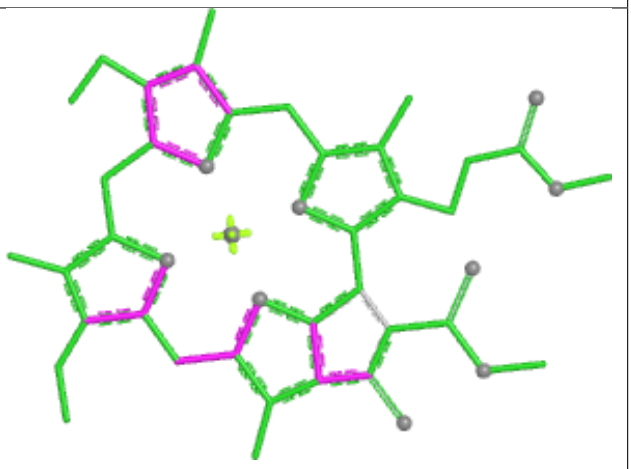


Rings

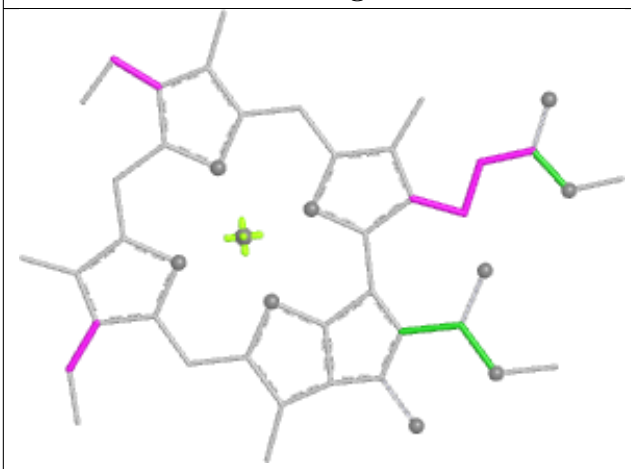
Ligand CLA Y 503



Bond lengths



Bond angles



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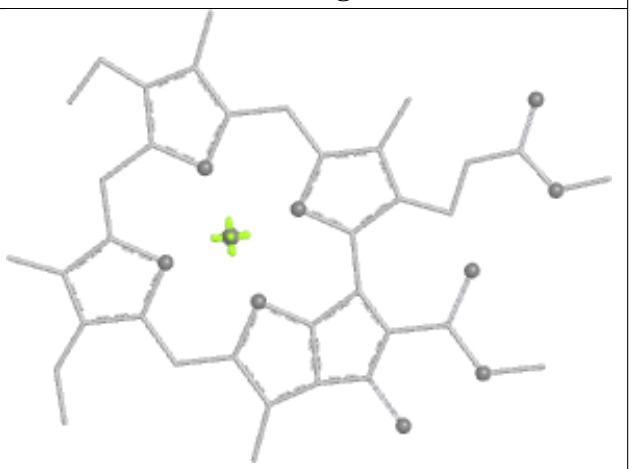
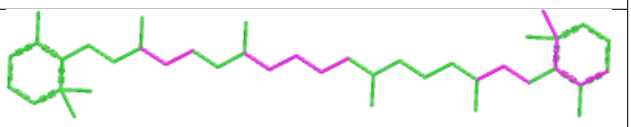


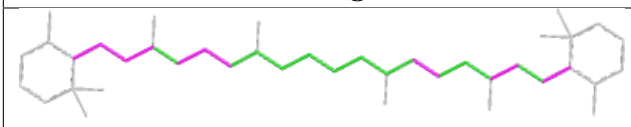
Rings

Ligand BCR k 4001

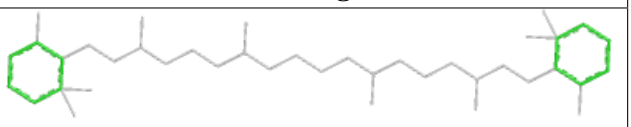
Bond lengths



Bond angles

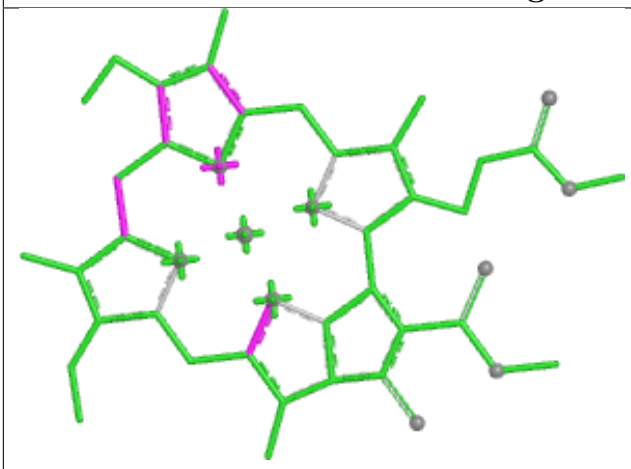


Torsions



Rings

Ligand CLA n 503



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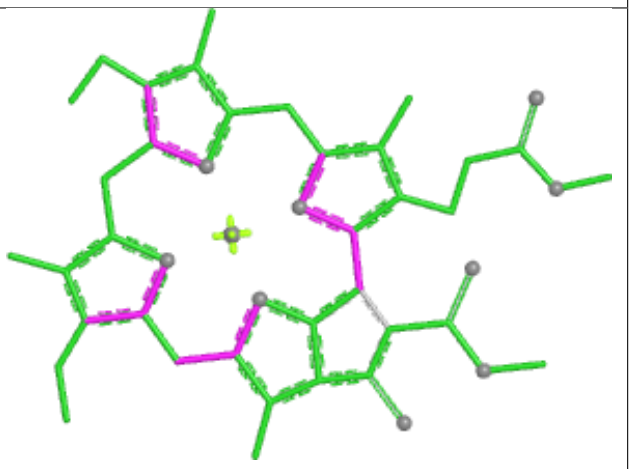

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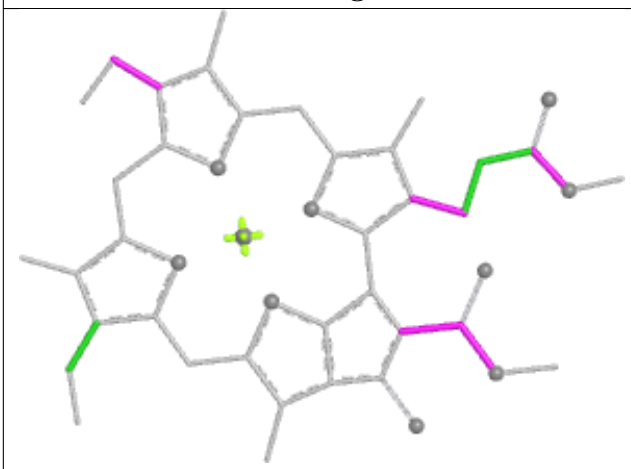

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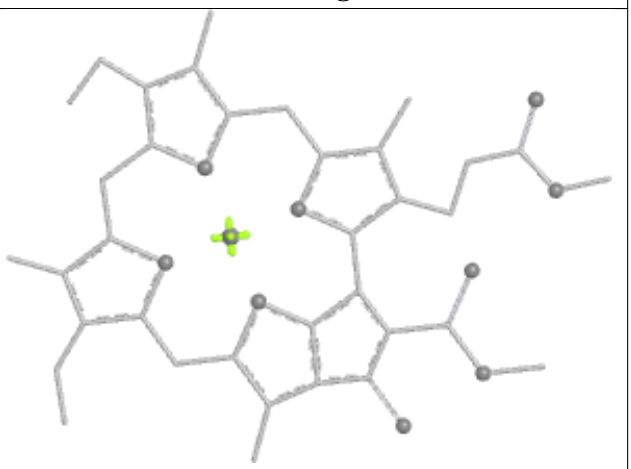
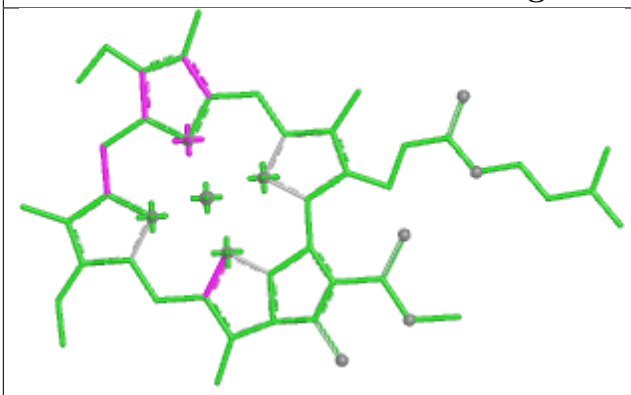


Rings

Ligand CLA y 502



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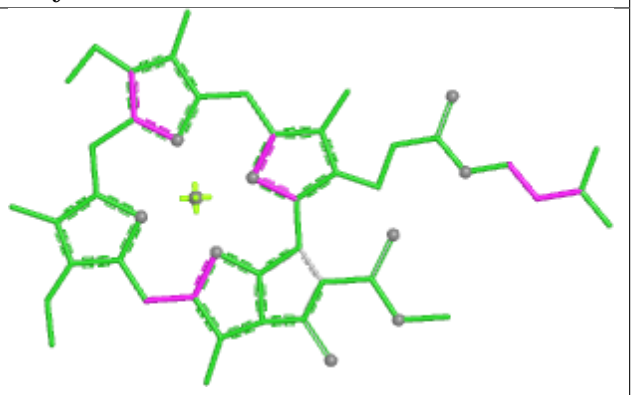
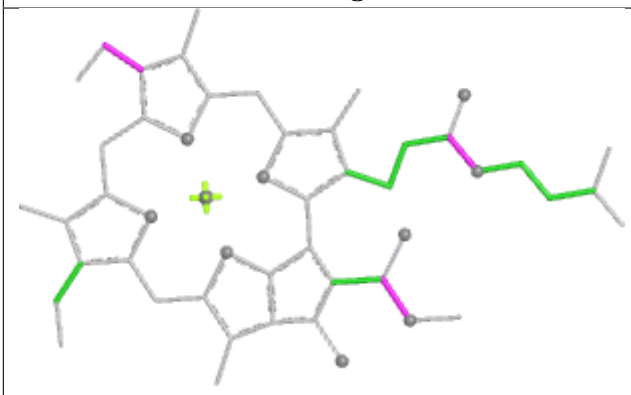


Bond angles



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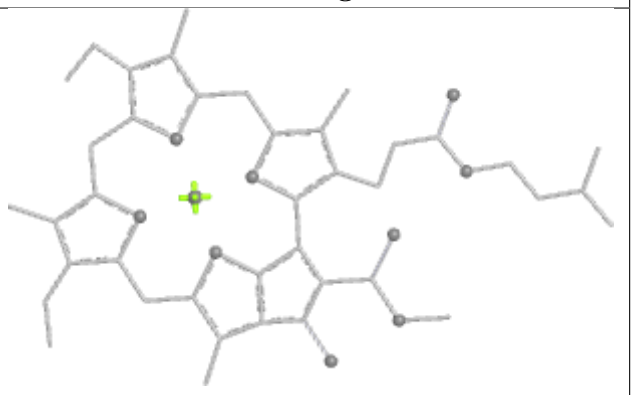
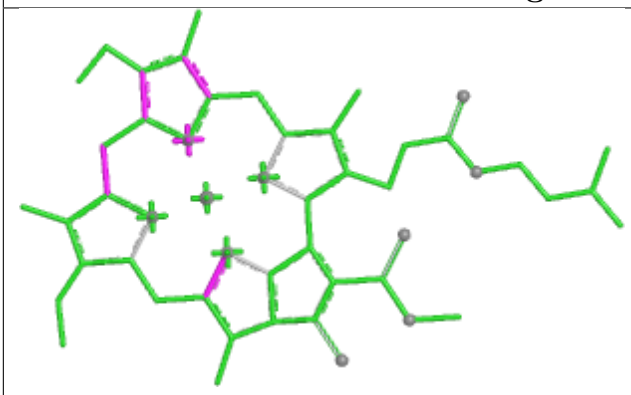


Rings

Ligand CLA Z 501



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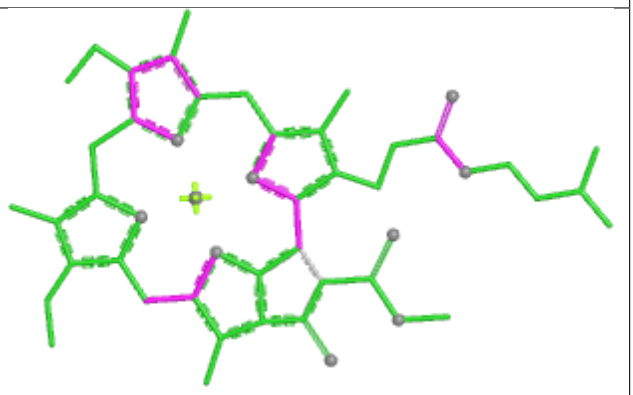
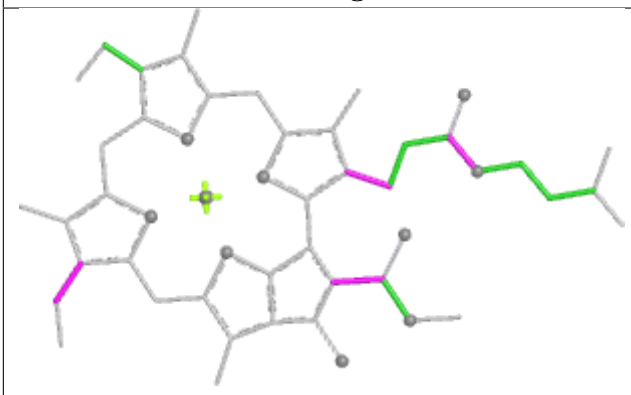


Bond angles



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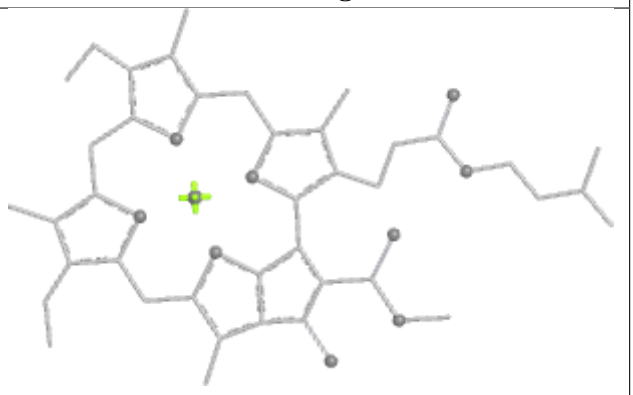
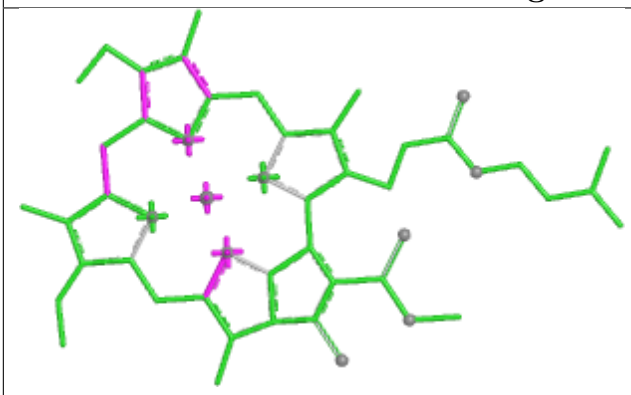


Rings

Ligand CLA x 502



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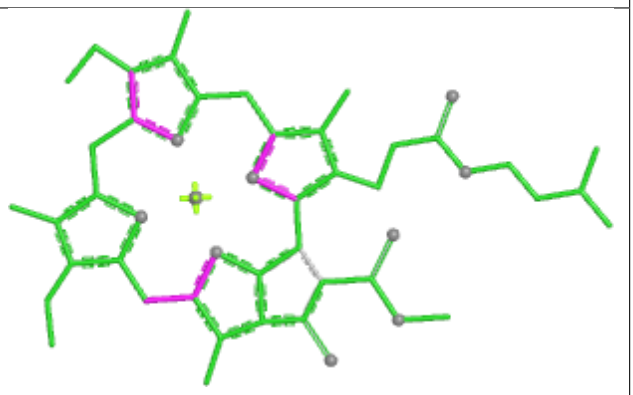
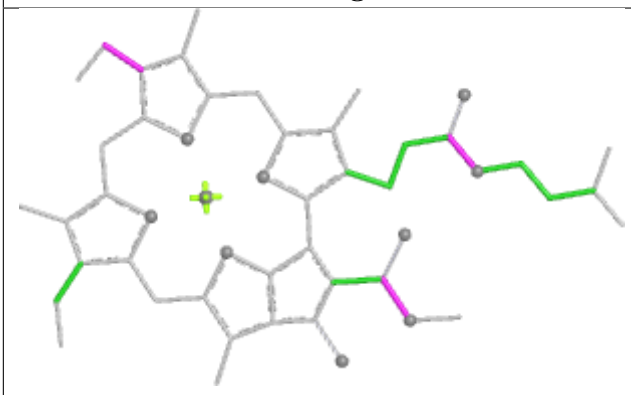


Bond angles



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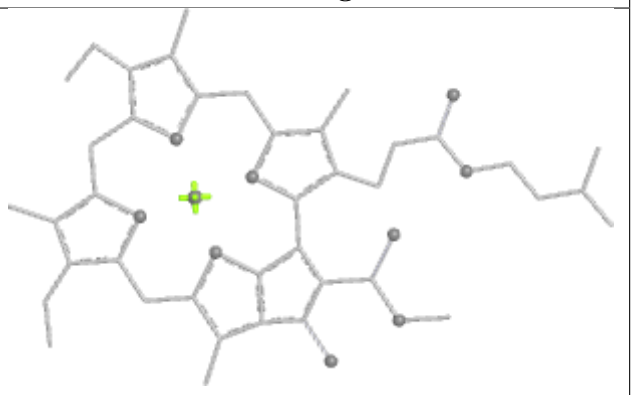
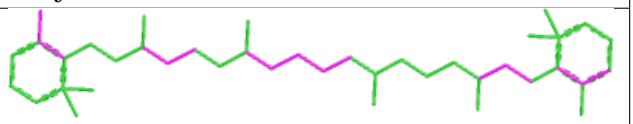


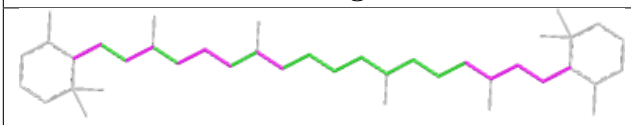
Rings

Ligand BCR y 601

Bond lengths



Bond angles



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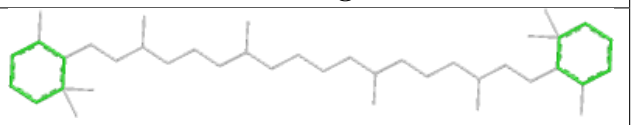
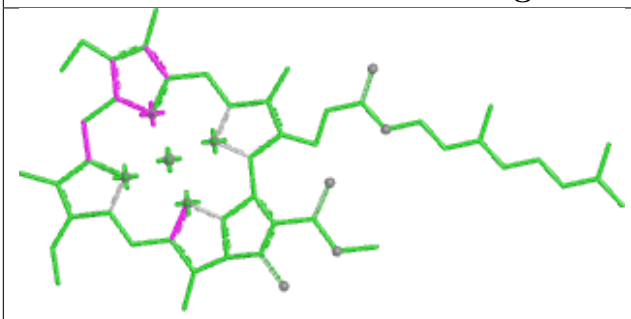
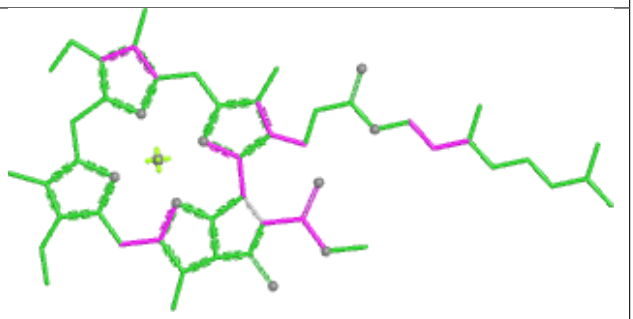


Rings

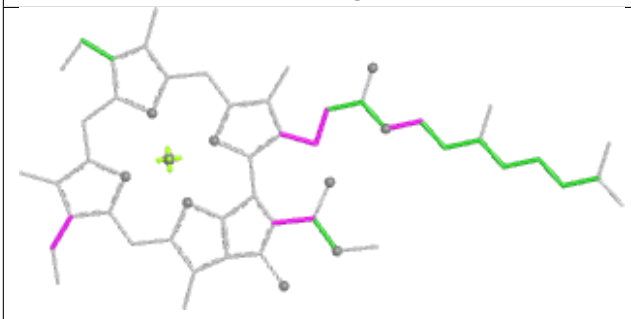
Ligand CLA G 1012



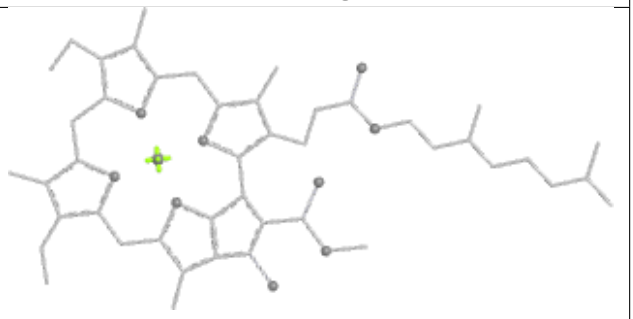
Bond lengths



Bond angles

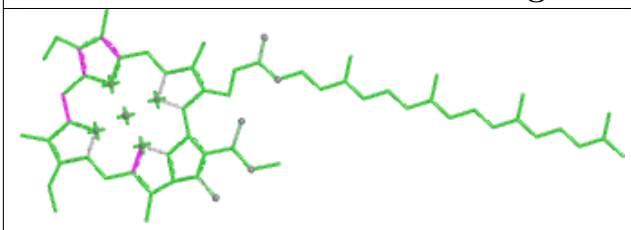


Torsions



Rings

Ligand CLA v 511



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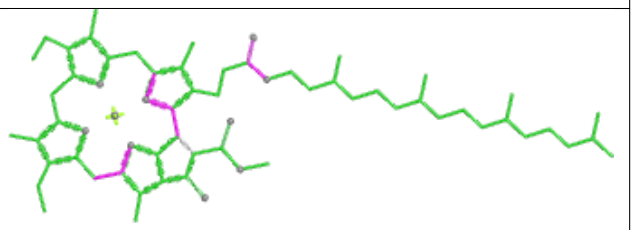

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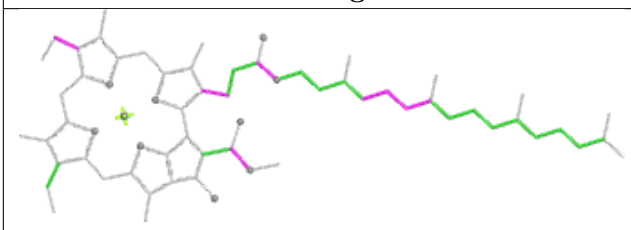

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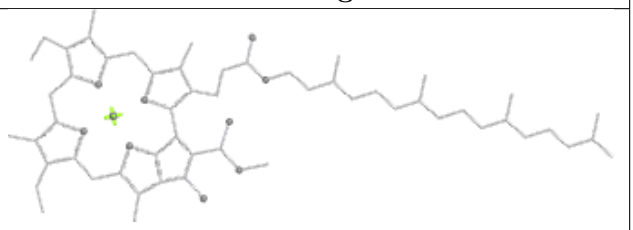
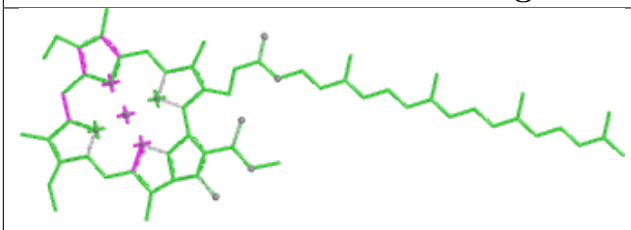


Rings

Ligand CLA A 1127



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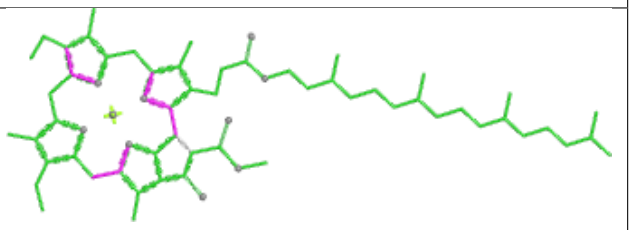
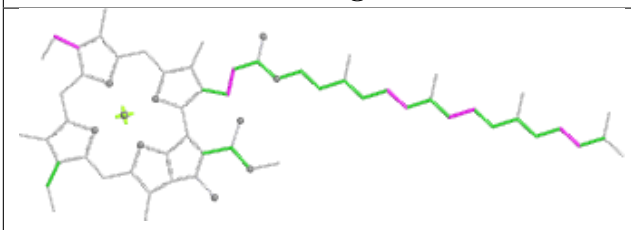


Bond angles



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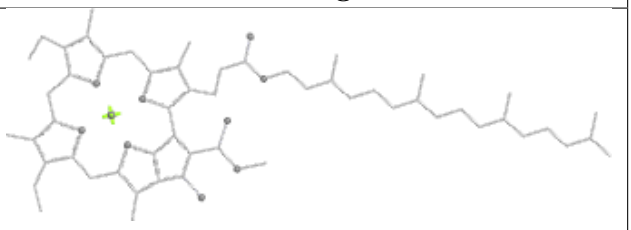
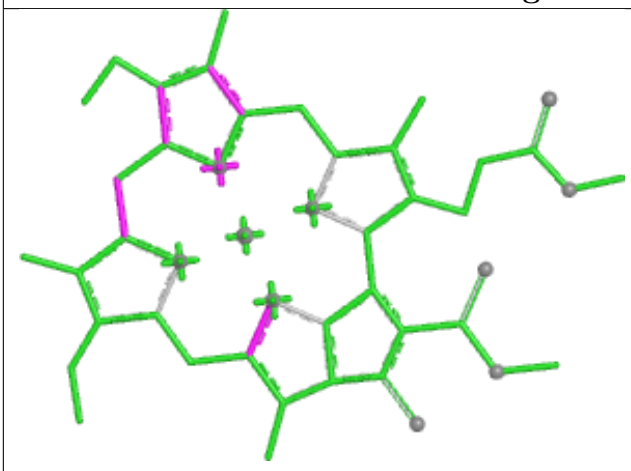


Rings

Ligand CLA f 1302



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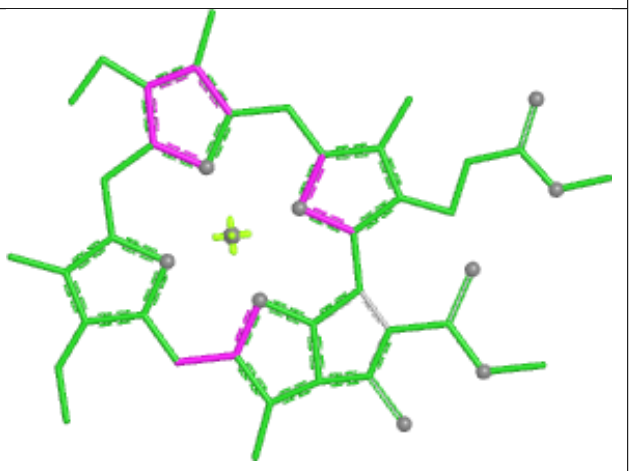
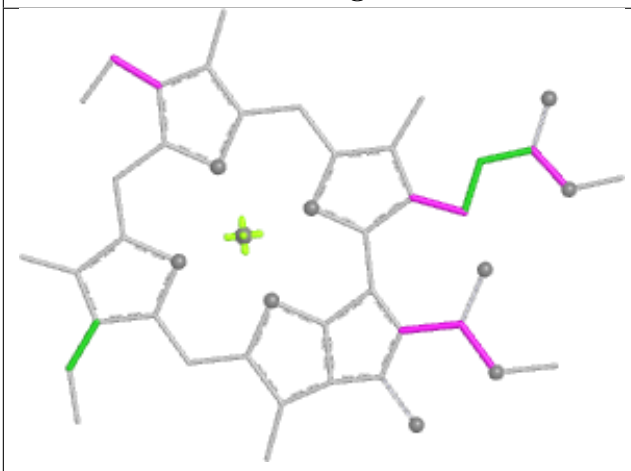


Bond angles



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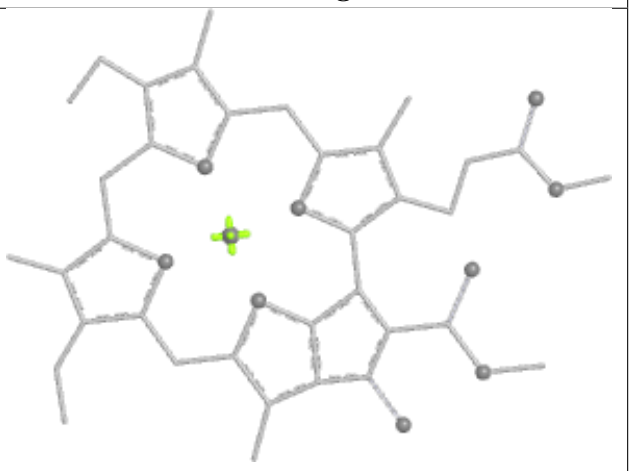
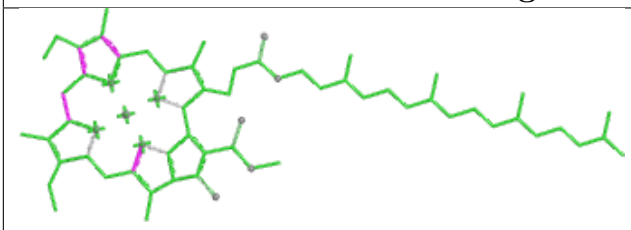


Rings

Ligand CLA b 1202



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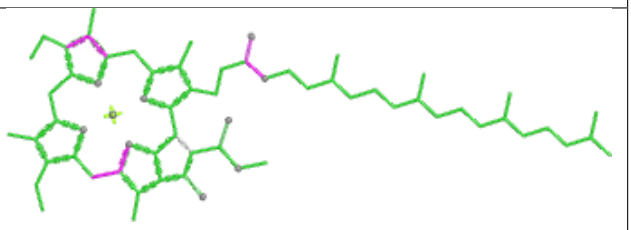
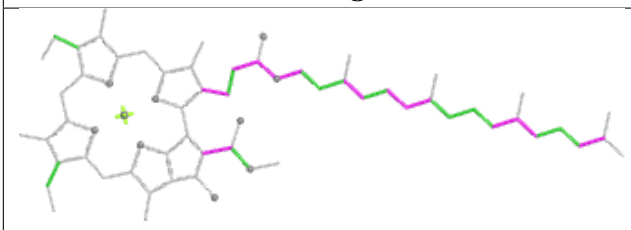


Bond angles



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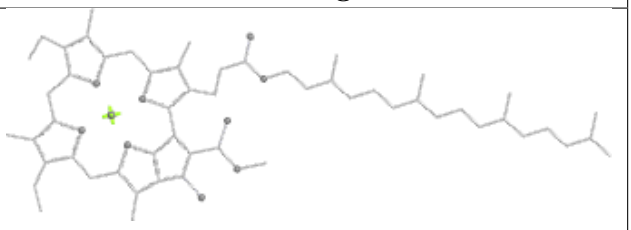
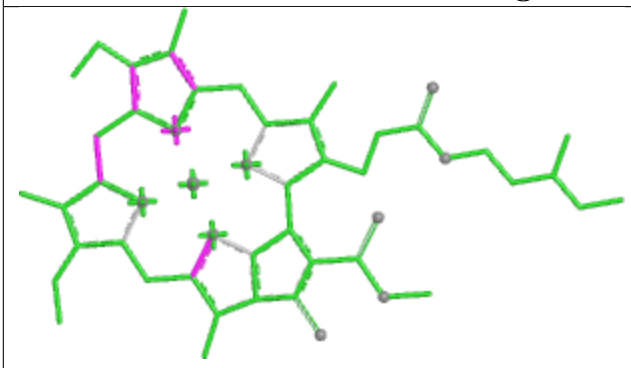


Rings

Ligand CLA A 1121



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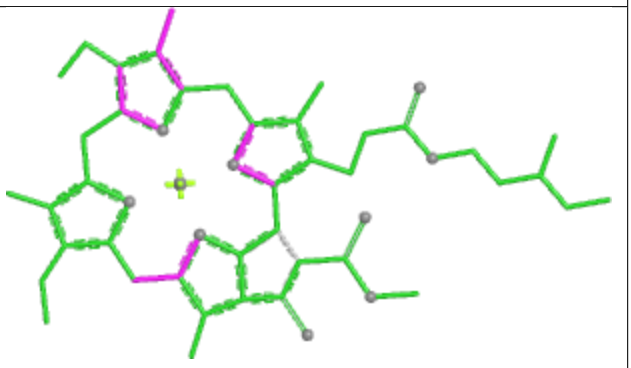
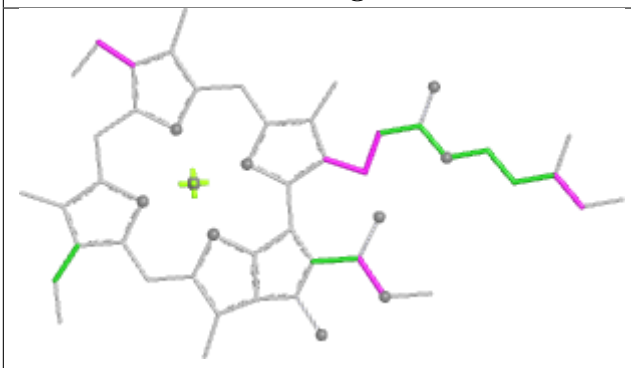


Bond angles



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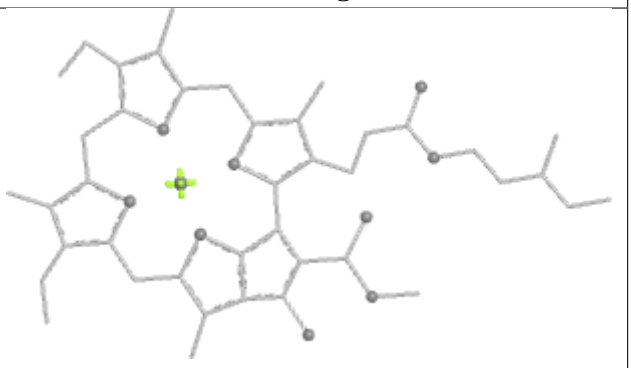
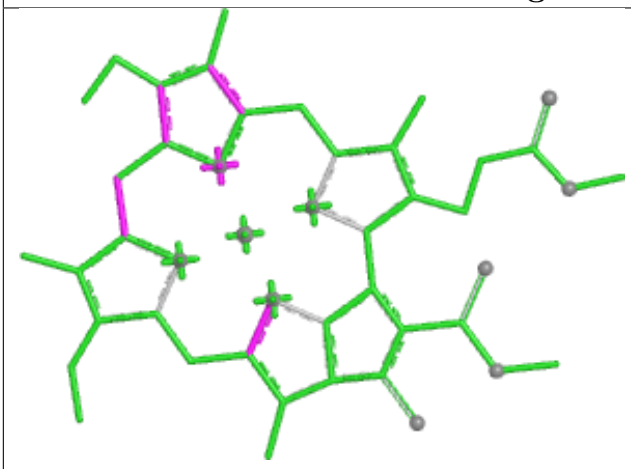


Rings

Ligand CLA v 501



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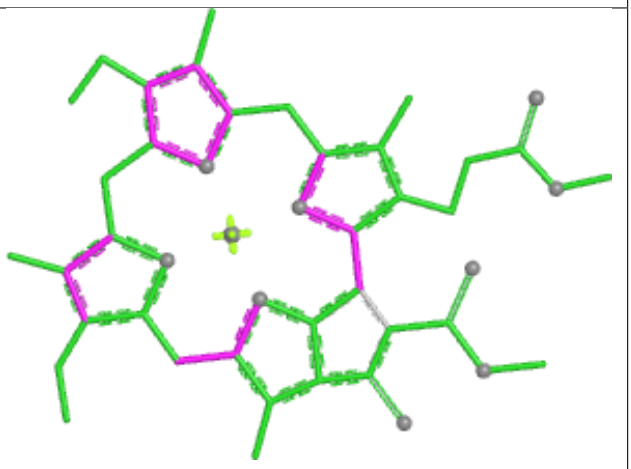

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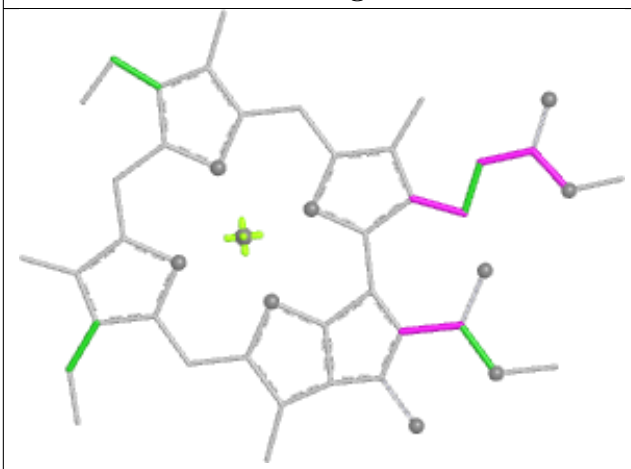

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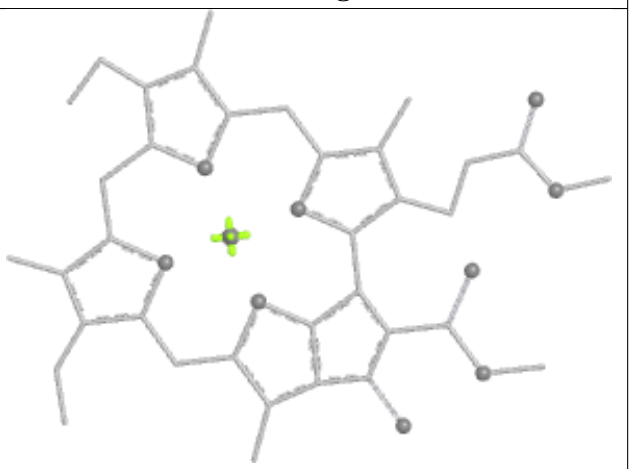

Rings

Ligand ECH I 4020

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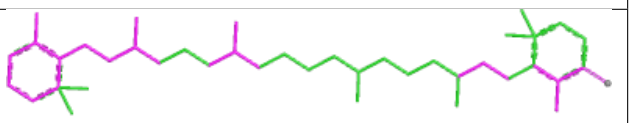
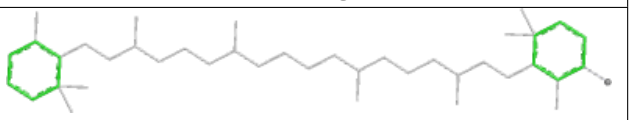


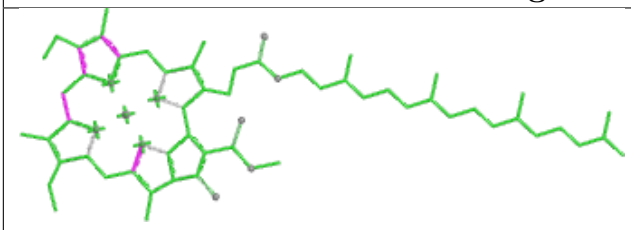
Bond angles

Torsions



Rings

Ligand CLA o 505



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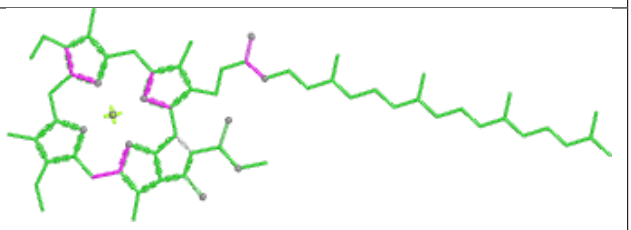
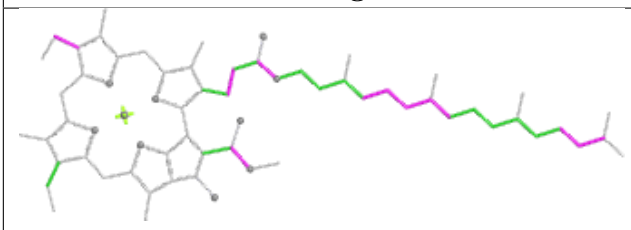


Bond angles



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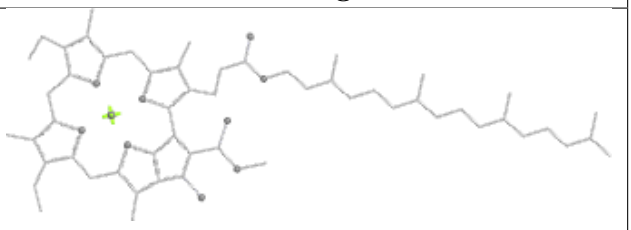
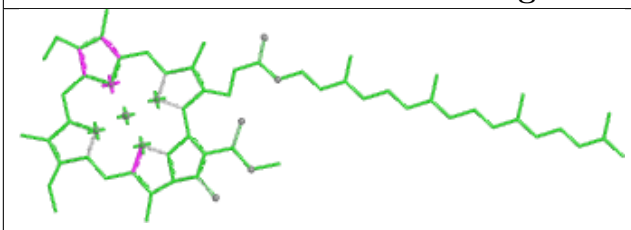


Rings

Ligand CLA b 1205



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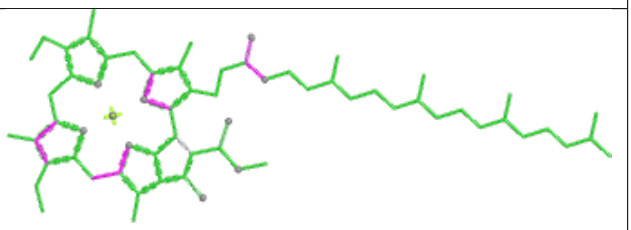

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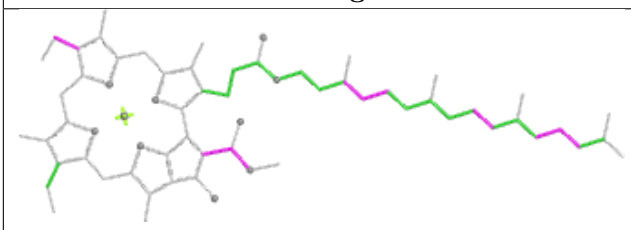

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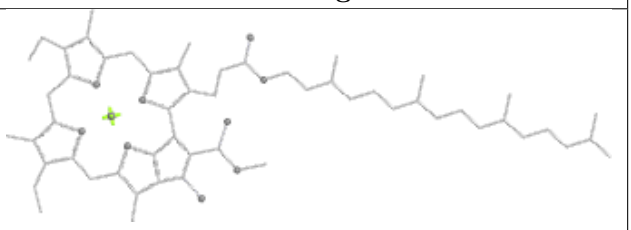
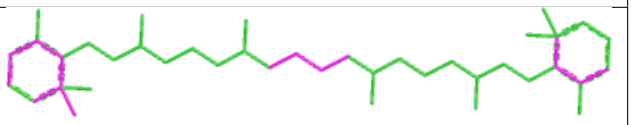


Rings

Ligand BCR v 604

Bond lengths



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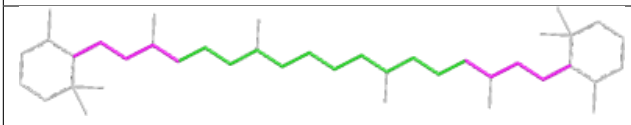

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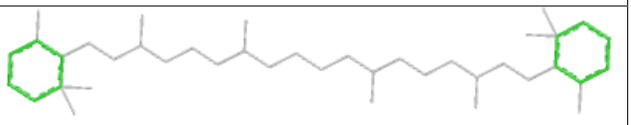
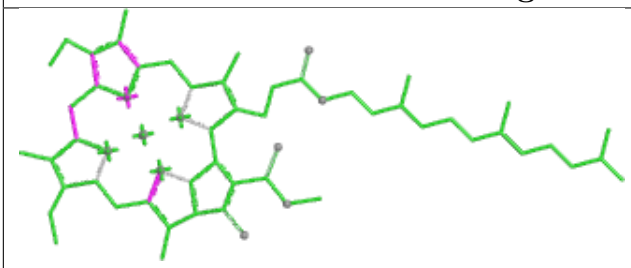


Rings

Ligand CLA L 1502



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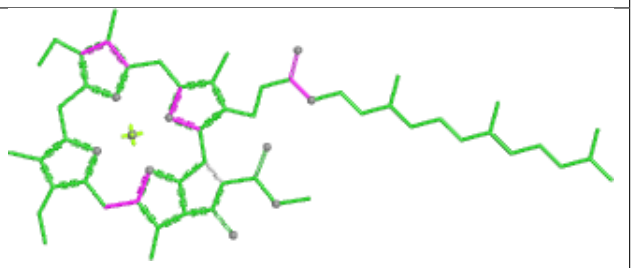
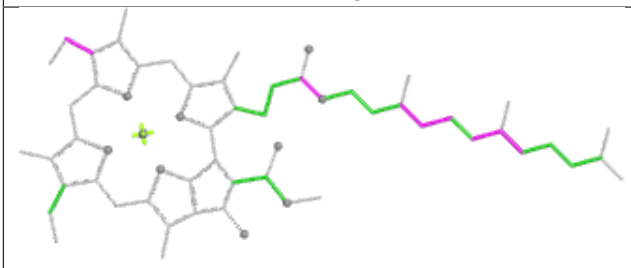


Bond angles



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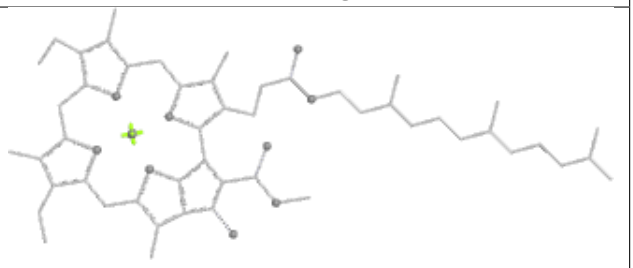
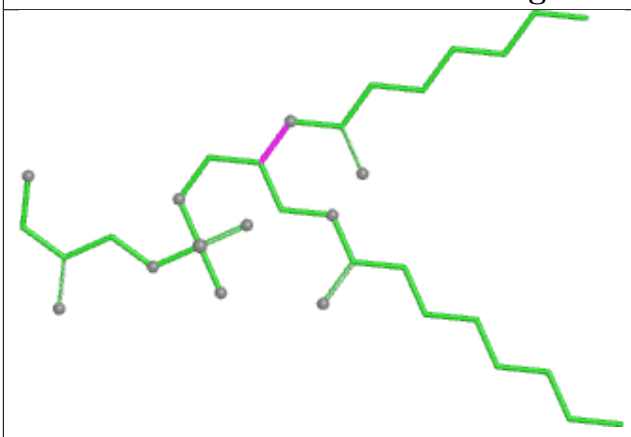


Rings

Ligand LHG s 605



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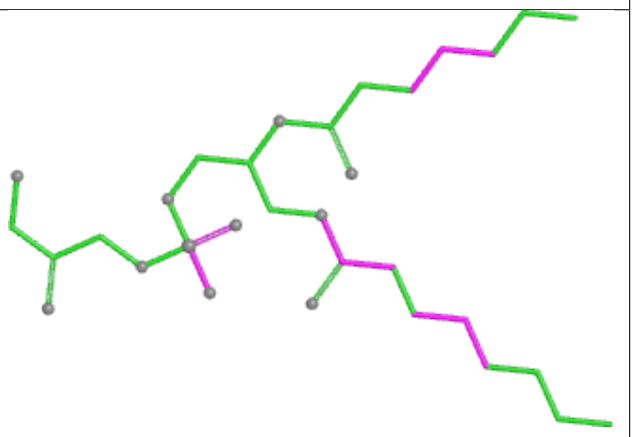
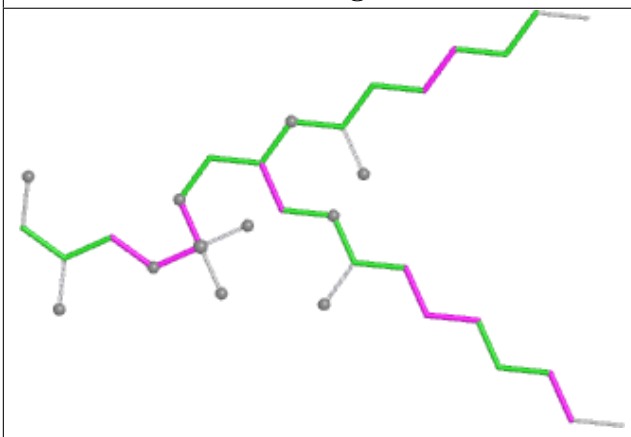
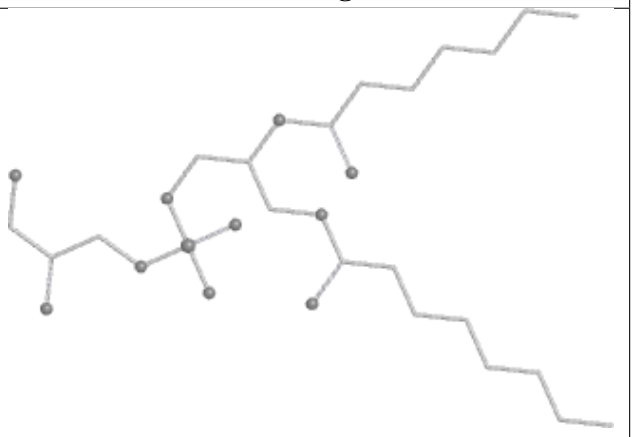


Bond angles

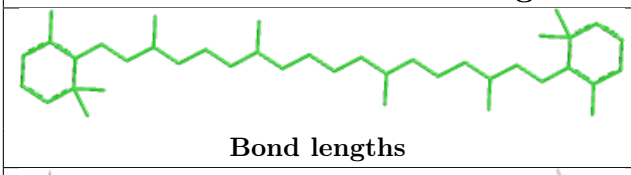


Torsions



Rings

Ligand BCR L 4019



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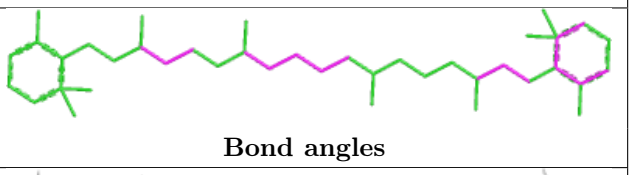
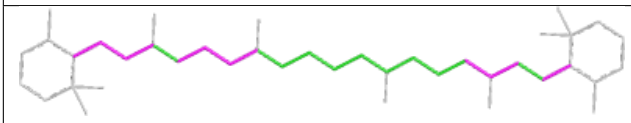


Bond angles



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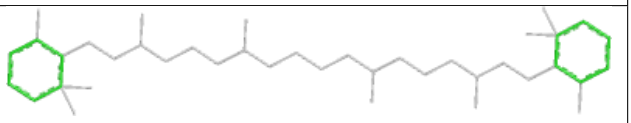
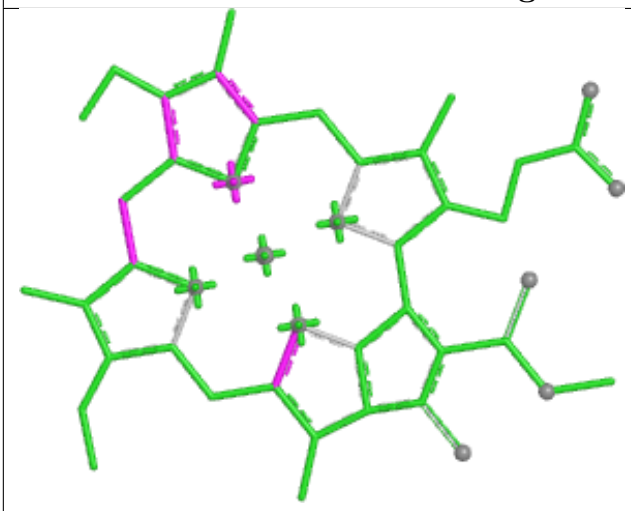


Rings

Ligand CLA b 1212



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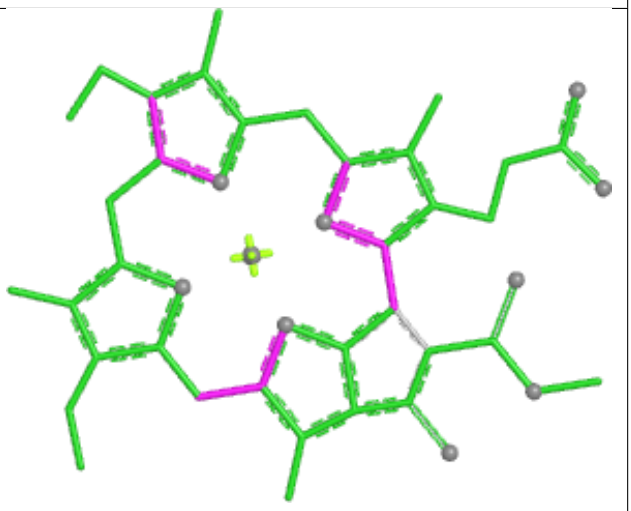
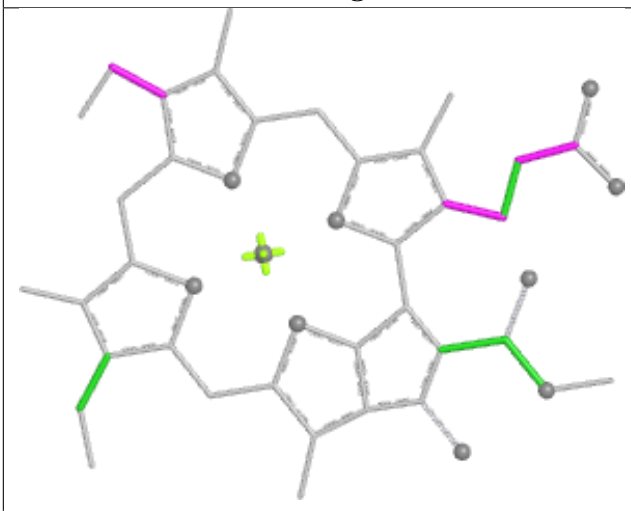


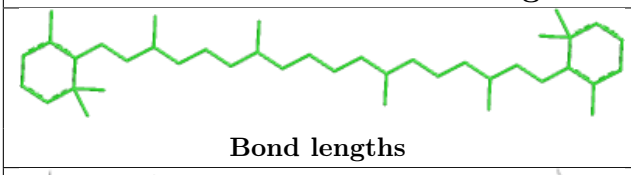
Bond angles



Torsions

Rings

Ligand BCR w 602



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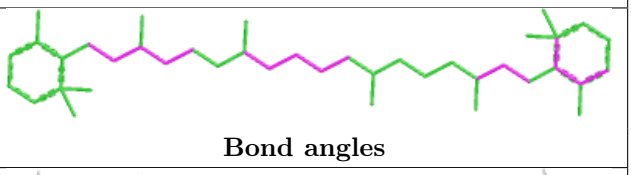
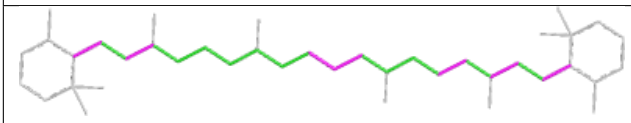
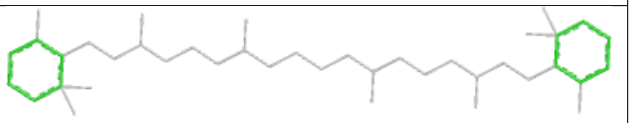


Bond angles

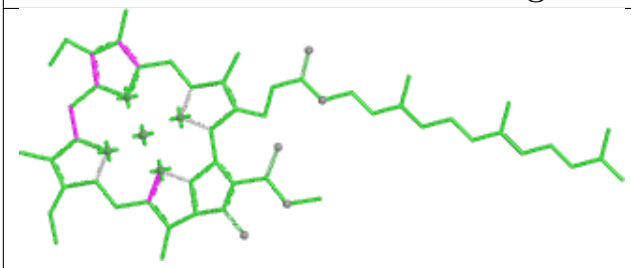


Torsions



Rings

Ligand CLA n 509



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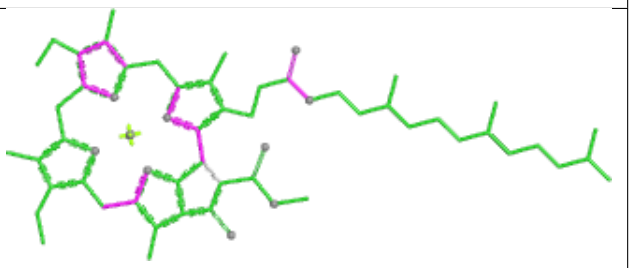

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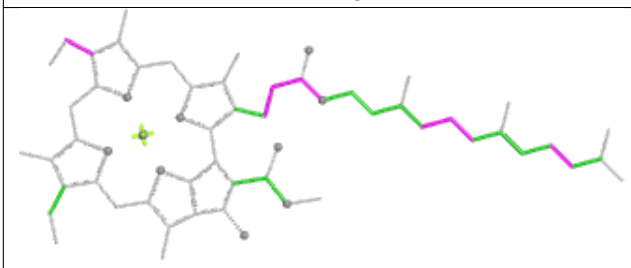

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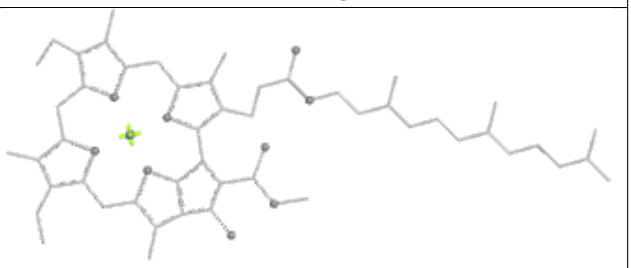

Rings

Ligand BCR q 602

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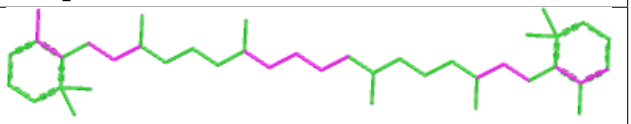

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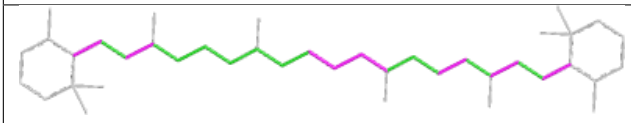

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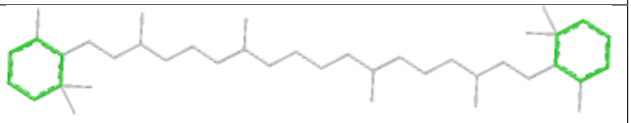
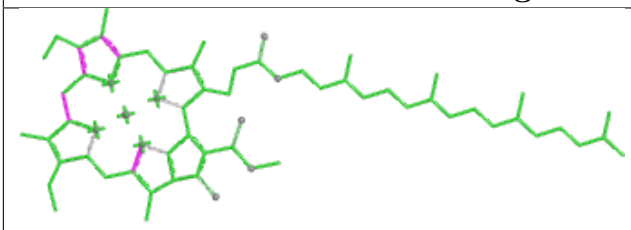


Rings

Ligand CLA G 1211



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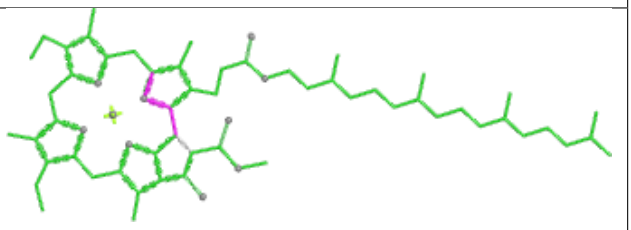

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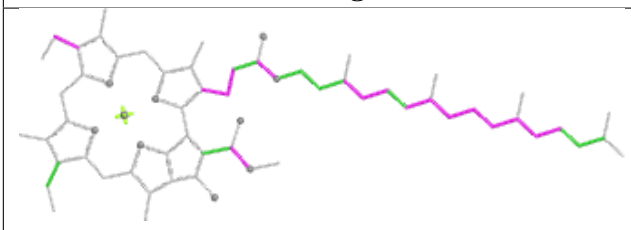

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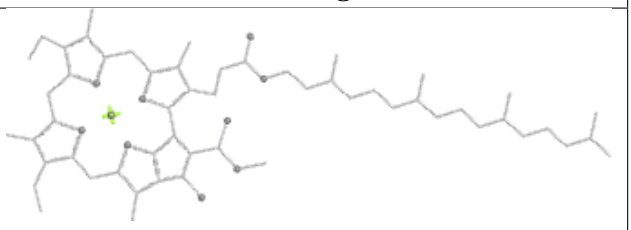
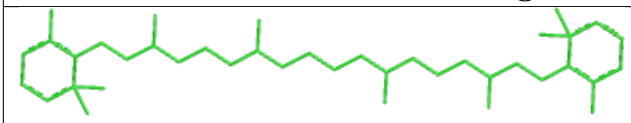


Rings

Ligand BCR b 4014



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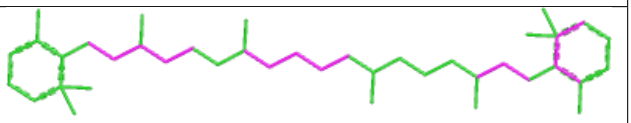

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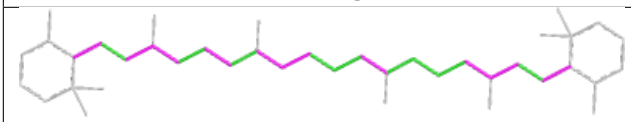

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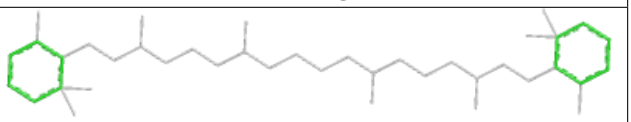
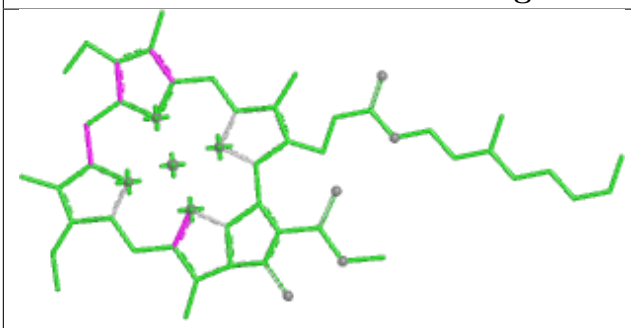


Rings

Ligand CLA G 1201



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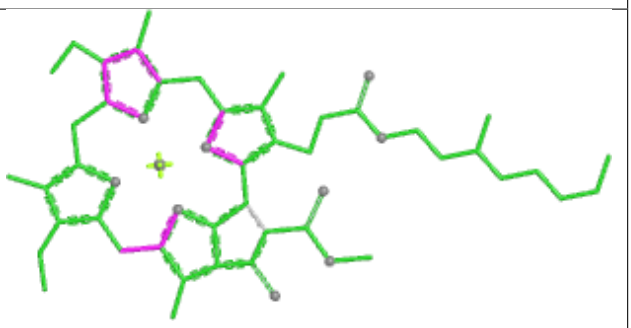

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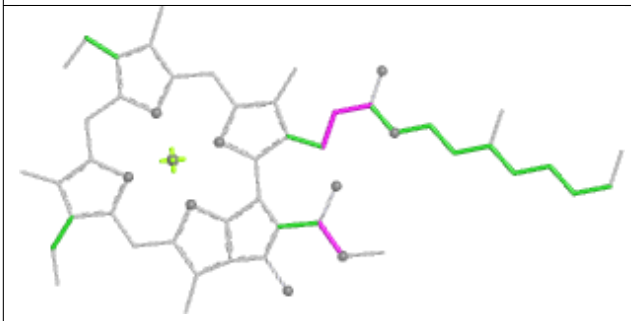

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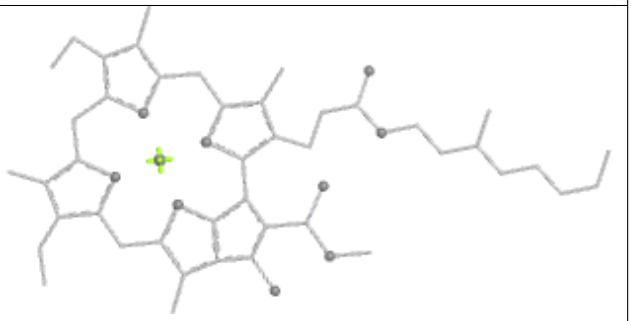
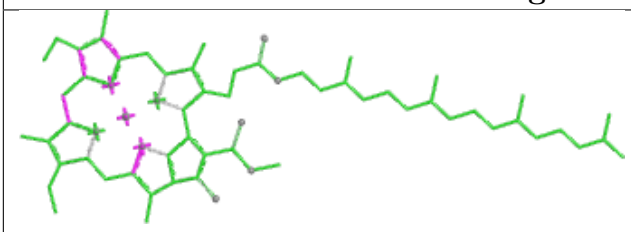


Rings

Ligand CLA o 512



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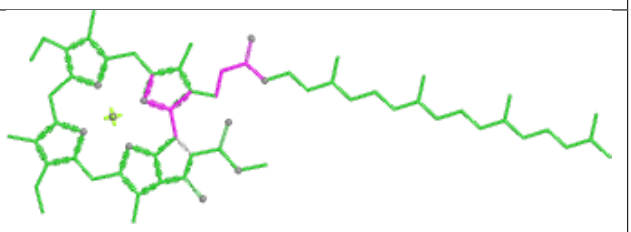

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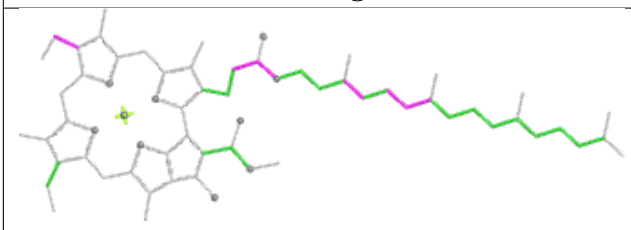

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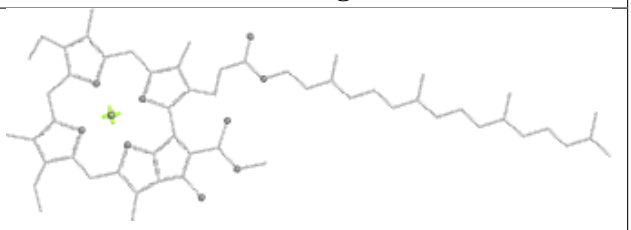
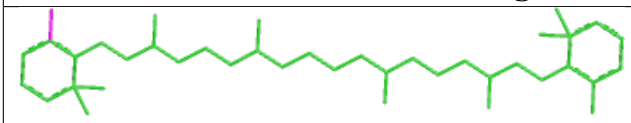


Rings

Ligand BCR A 4007



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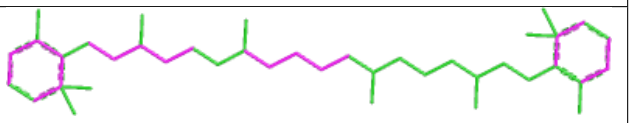

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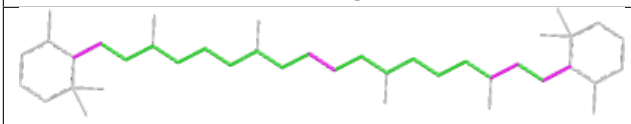

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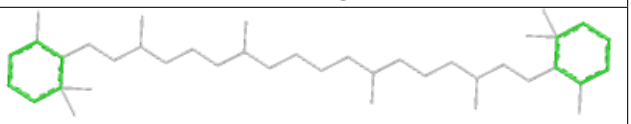
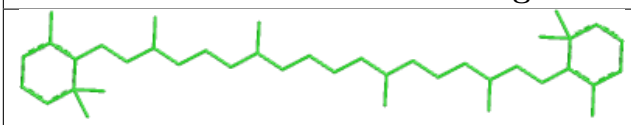


Rings

Ligand BCR A 4003



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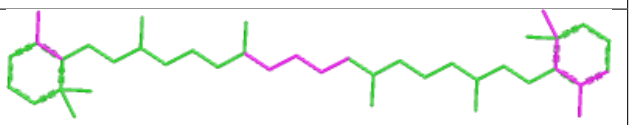
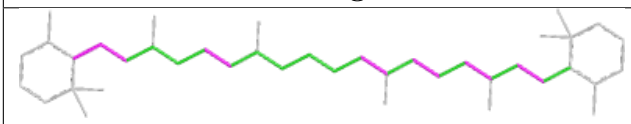
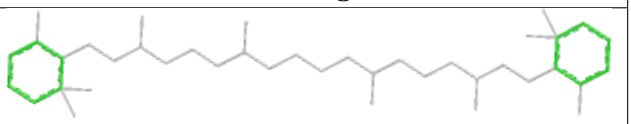


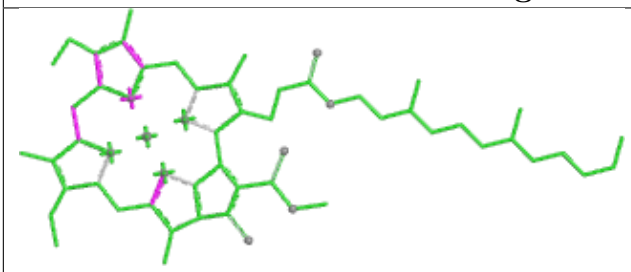
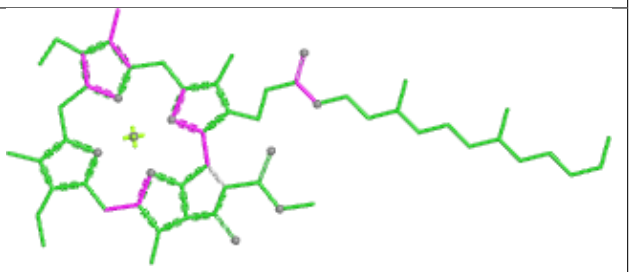
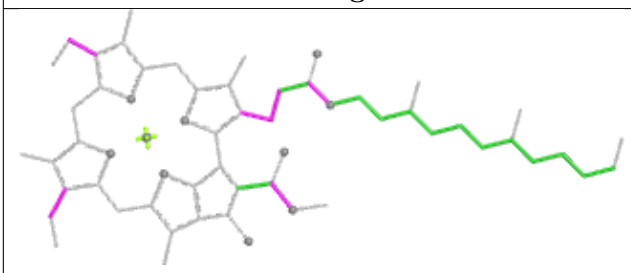
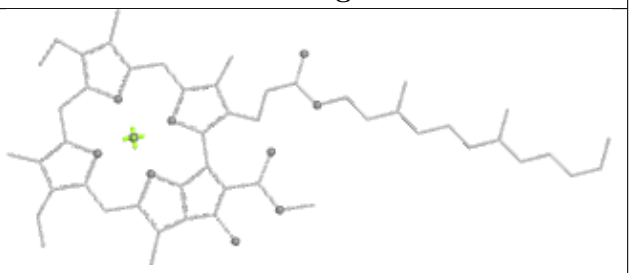
Bond angles

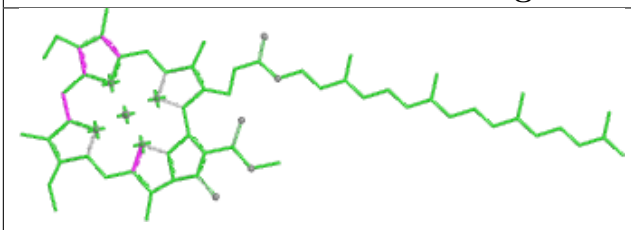
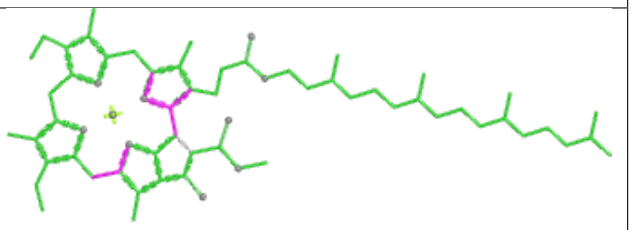
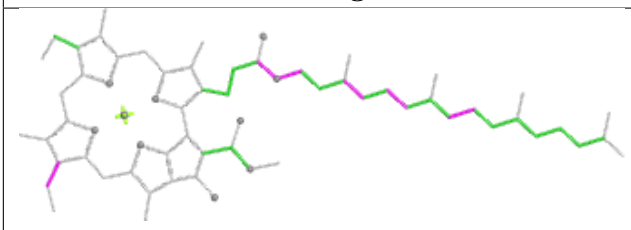
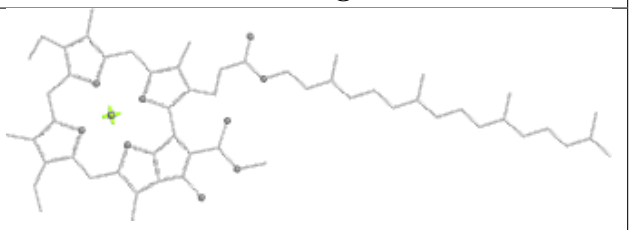


Torsions

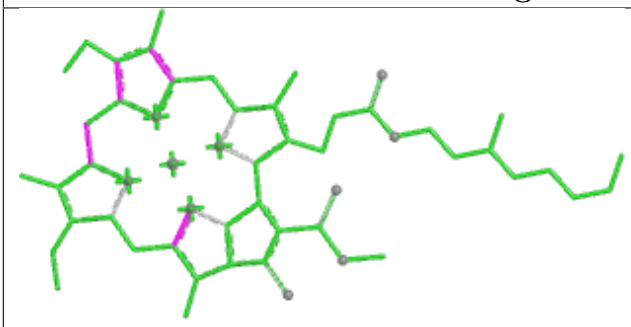


Rings

Ligand CLA A 1122	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1123	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1115



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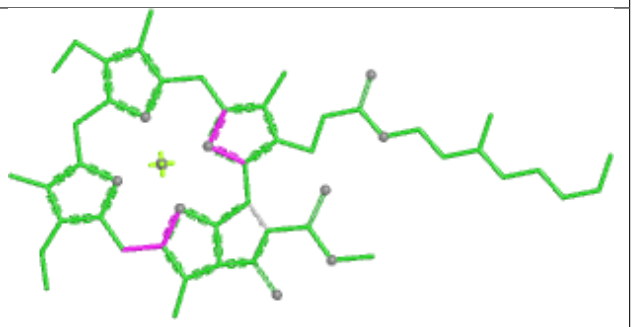
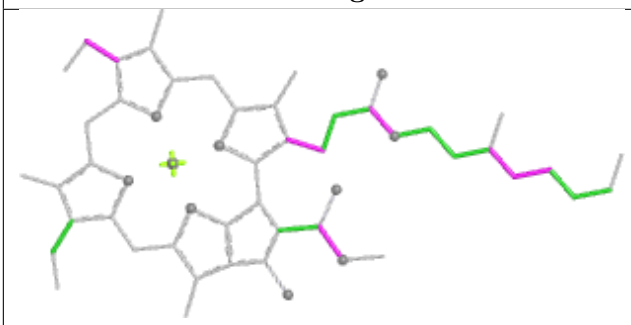
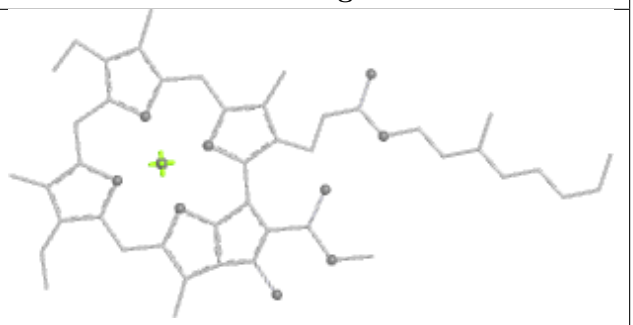


Bond angles

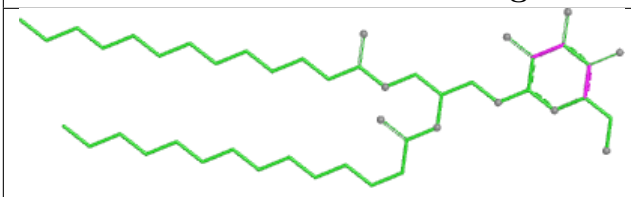


Torsions



Rings

Ligand LMG A 4101



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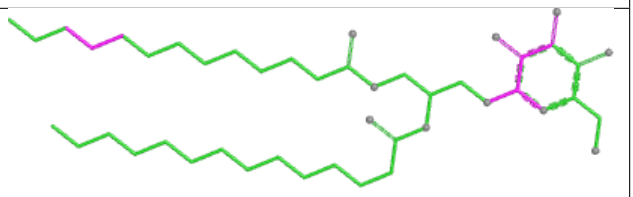
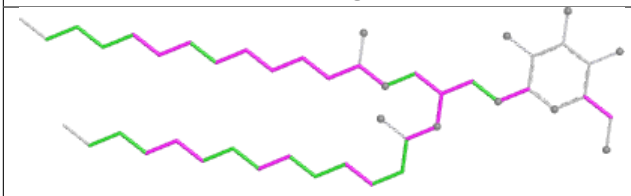
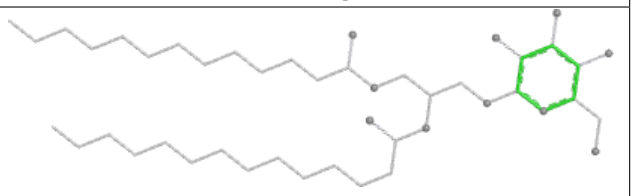


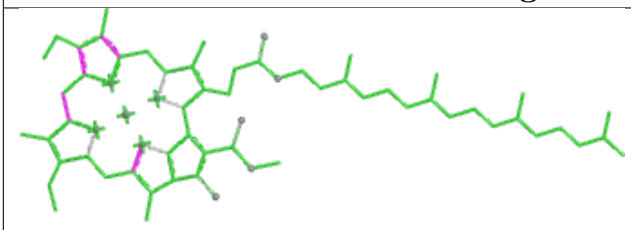
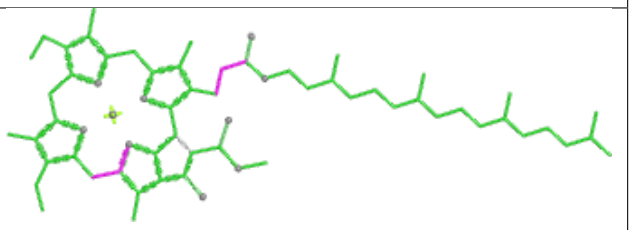
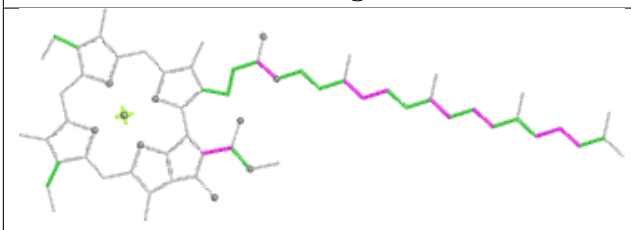
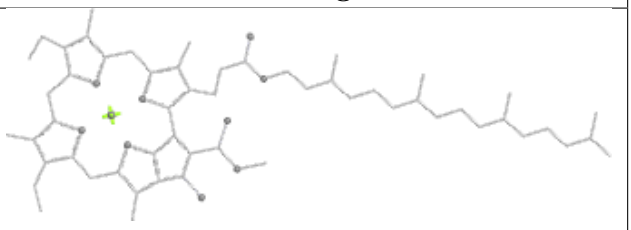
Bond angles

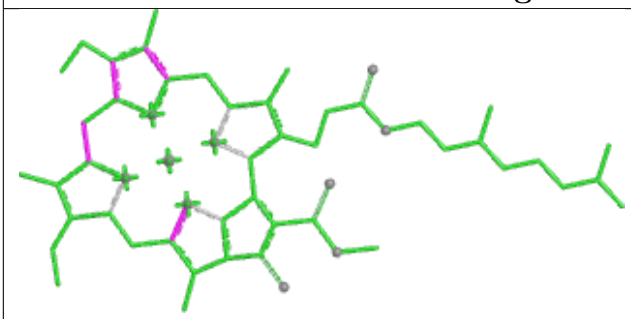
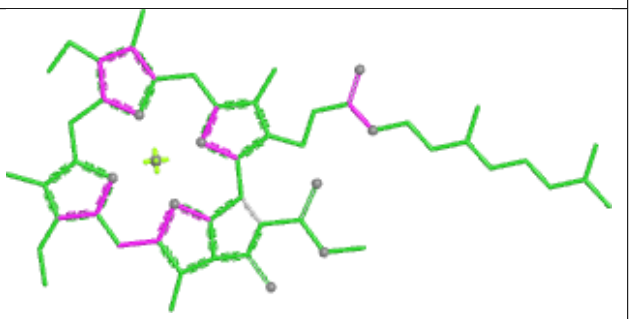
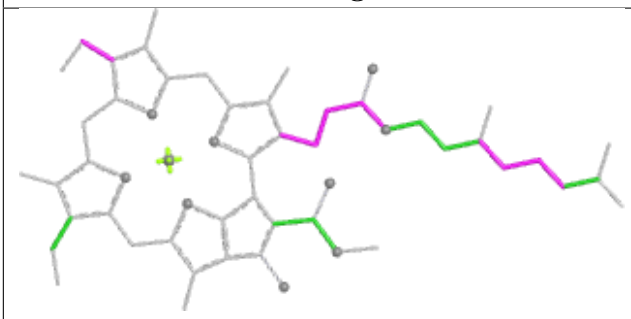
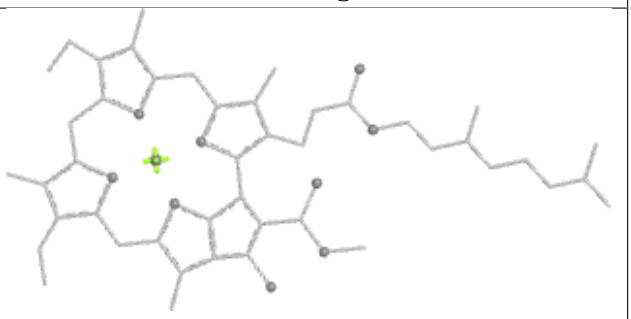


Torsions



Rings

Ligand CLA a 1103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 1118	
 Bond lengths	 Bond angles
 Torsions	 Rings

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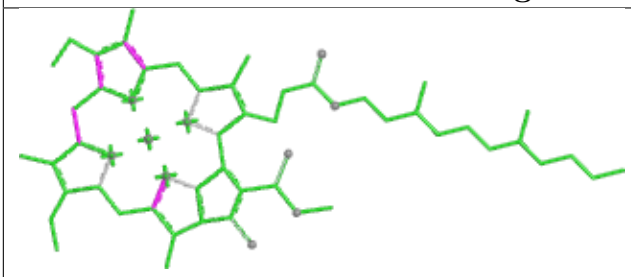

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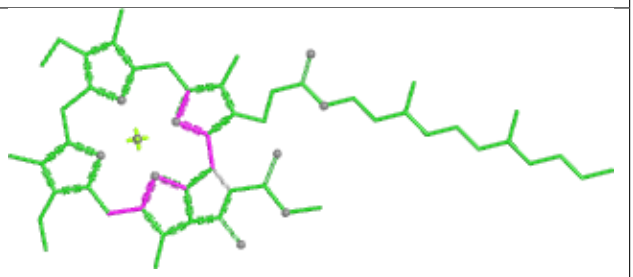

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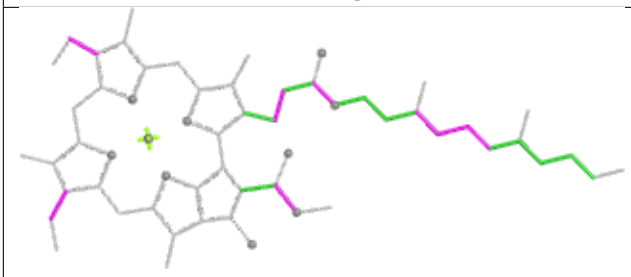

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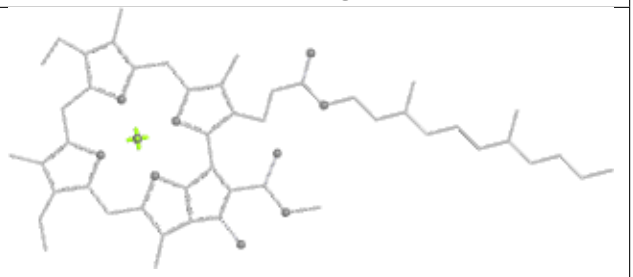
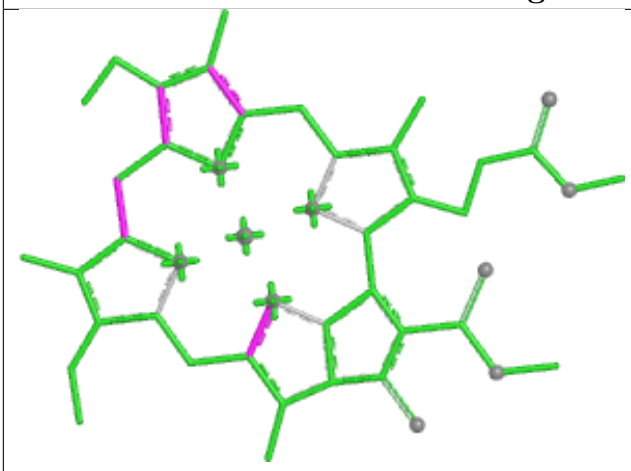


Rings

Ligand CLA y 501



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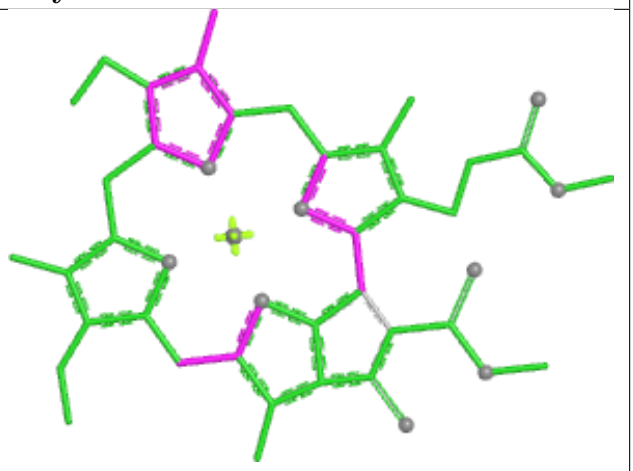

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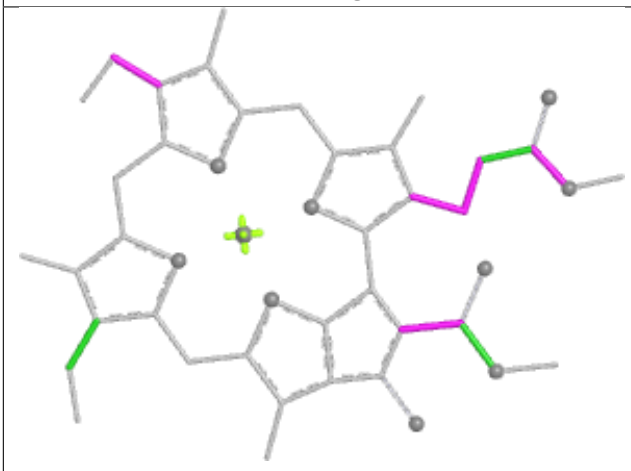

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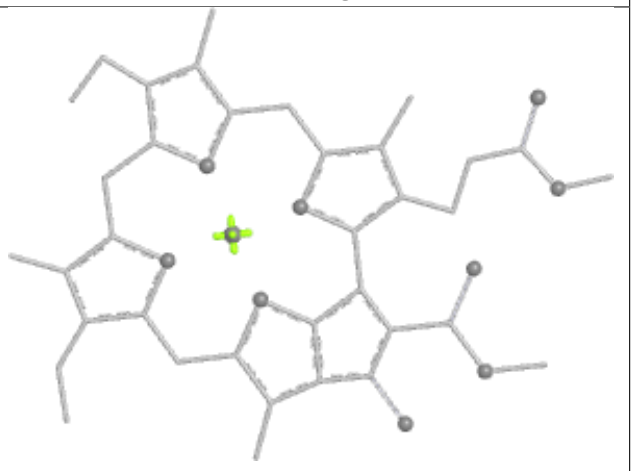

Rings

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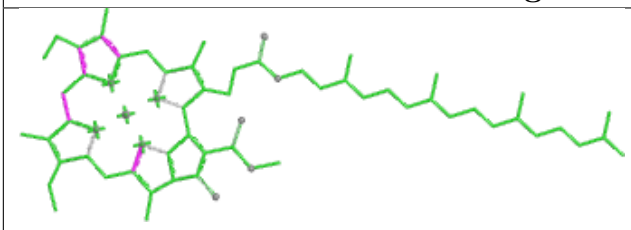
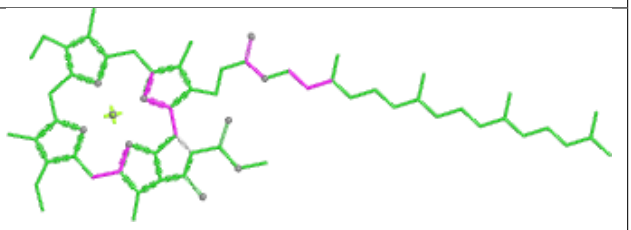
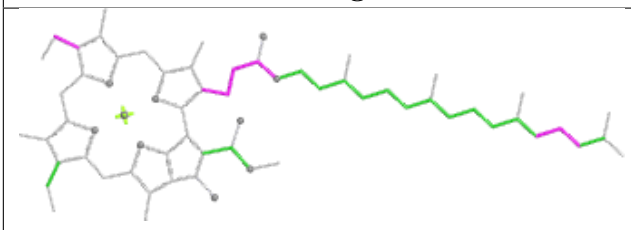
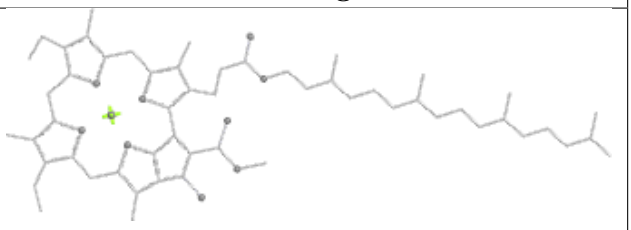
	
Bond lengths	Bond angles
	
Torsions	Rings

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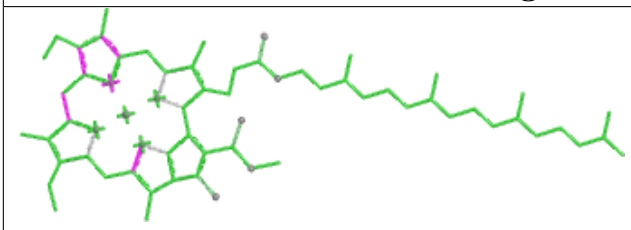	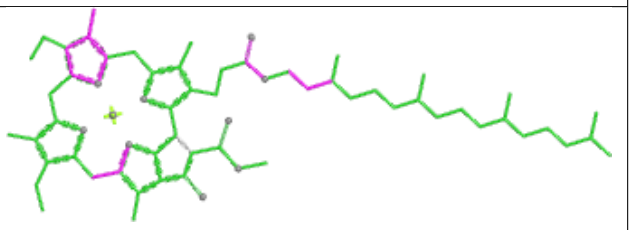
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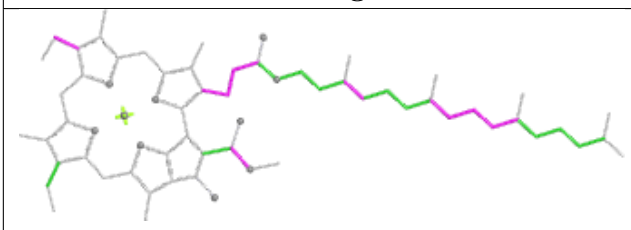	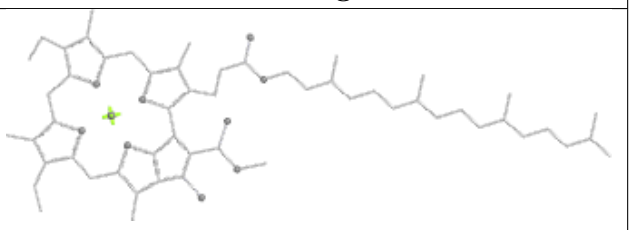
Torsions	Rings

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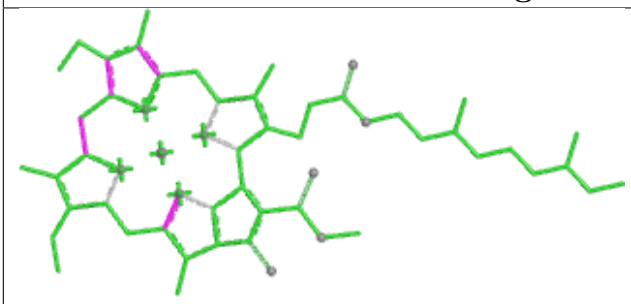	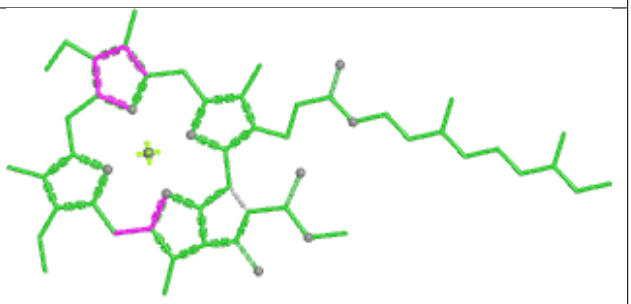
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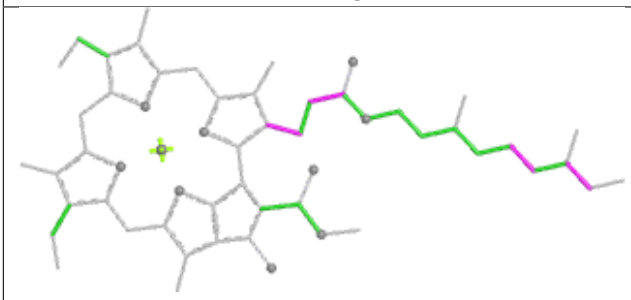	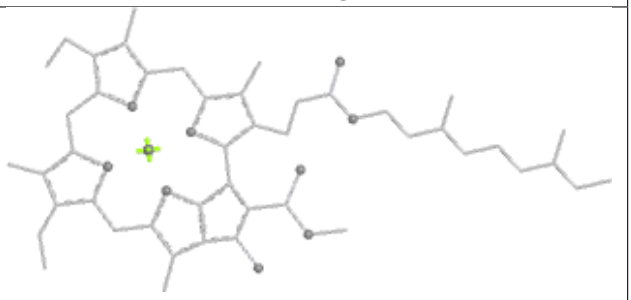
Torsions	Rings

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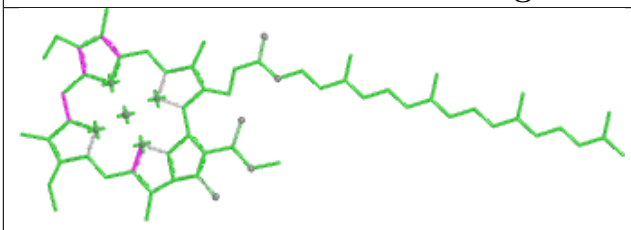	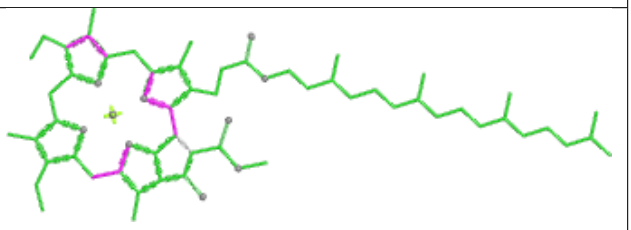
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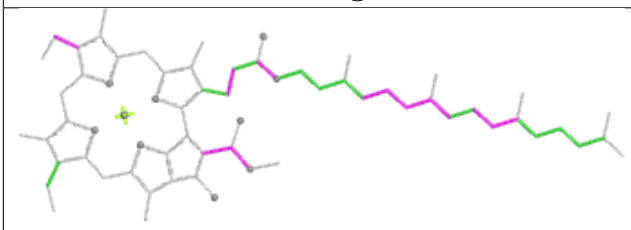	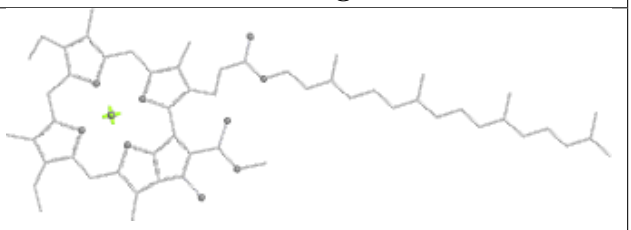
Torsions	Rings

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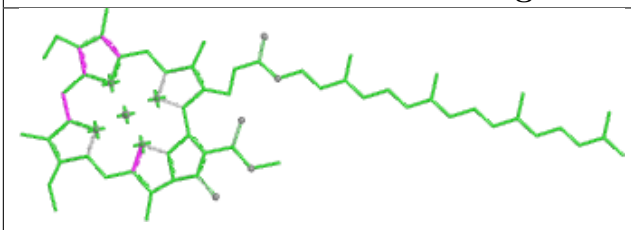

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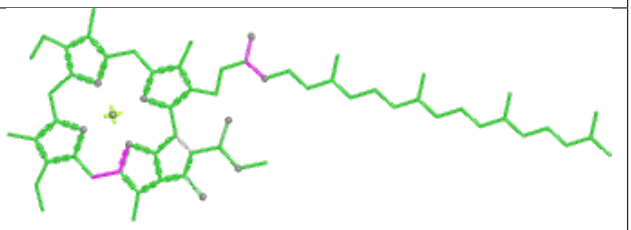

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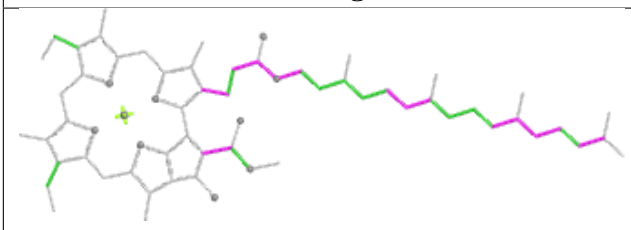

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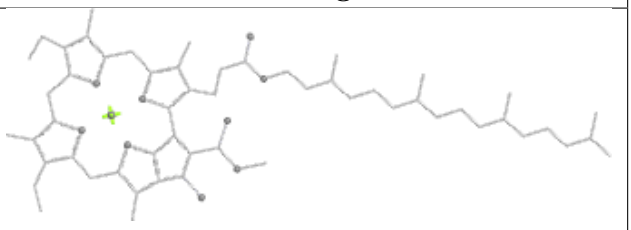
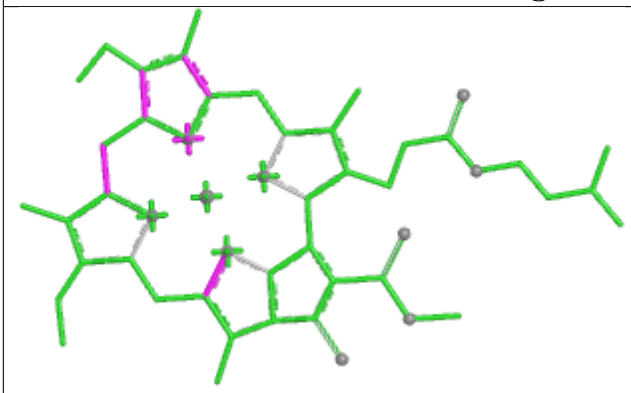


Rings

Ligand CLA r 514



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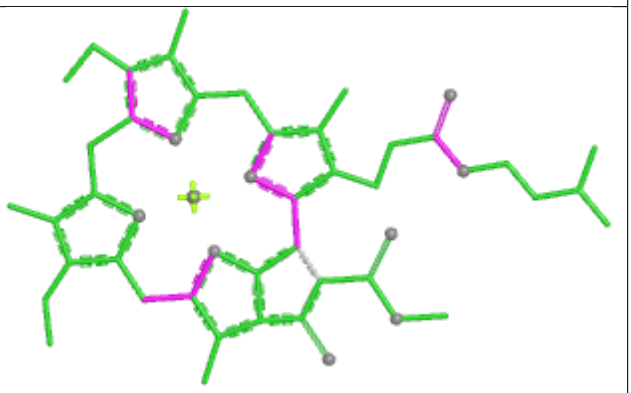

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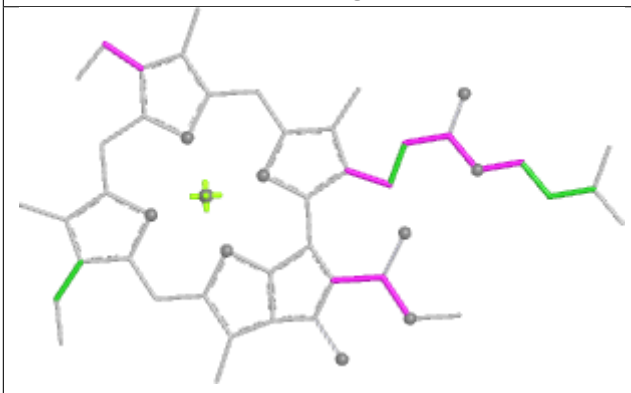

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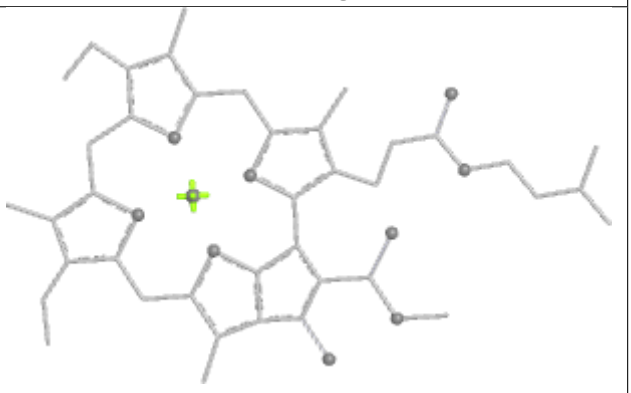

Rings

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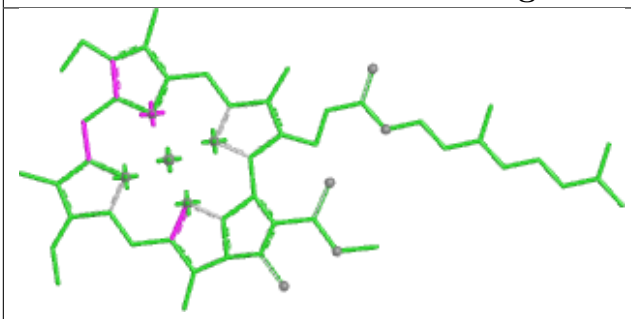
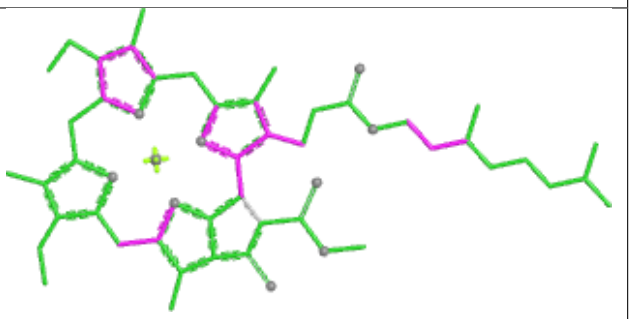
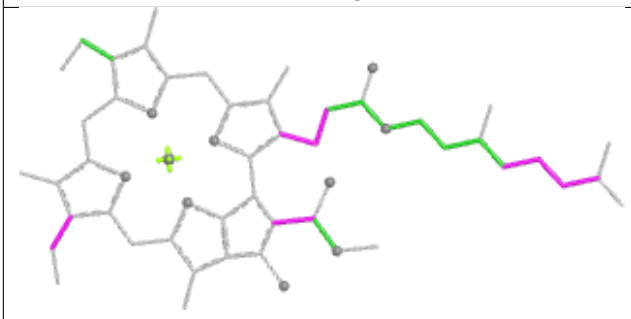
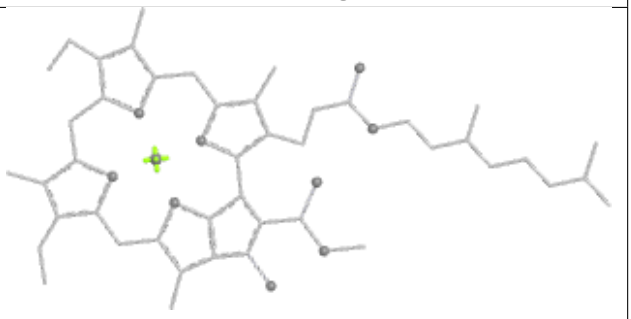
	
Bond lengths	Bond angles
	
Torsions	Rings

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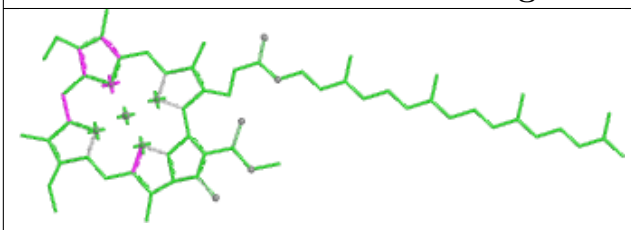
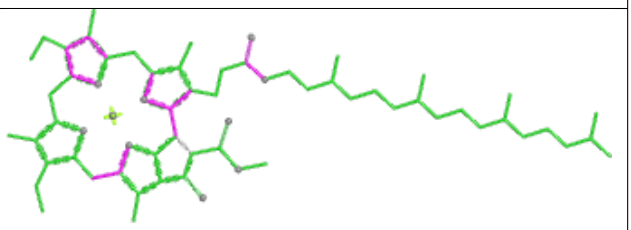
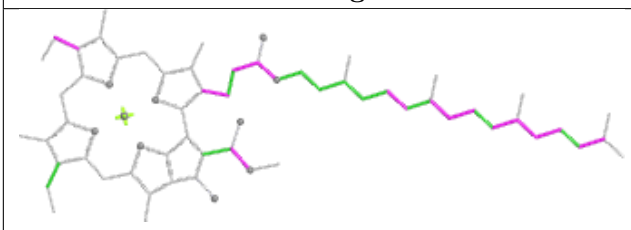
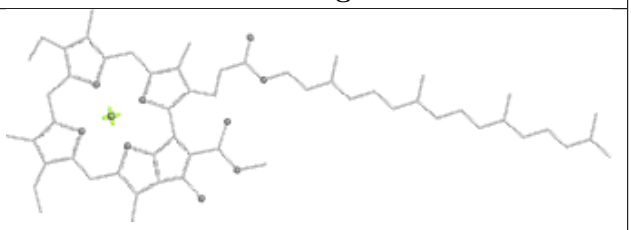
	
Bond lengths	Bond angles
	
Torsions	Rings

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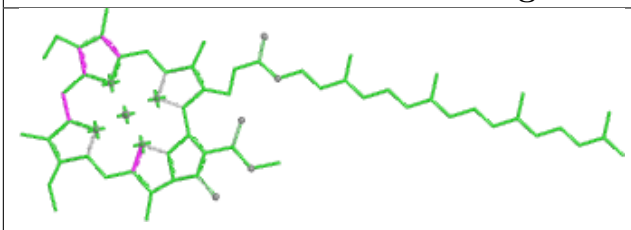	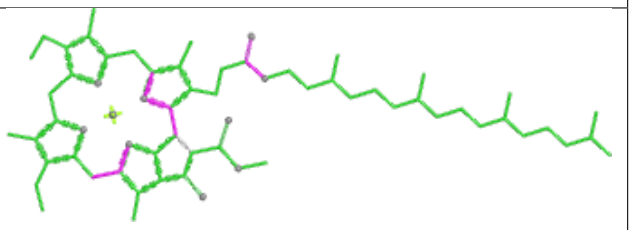
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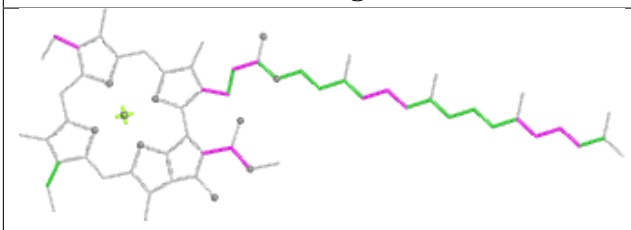	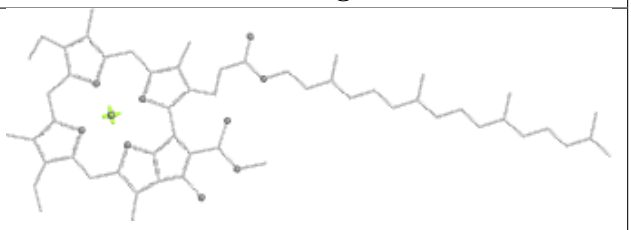
Torsions	Rings

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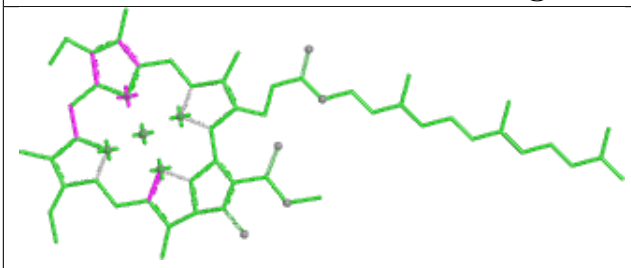
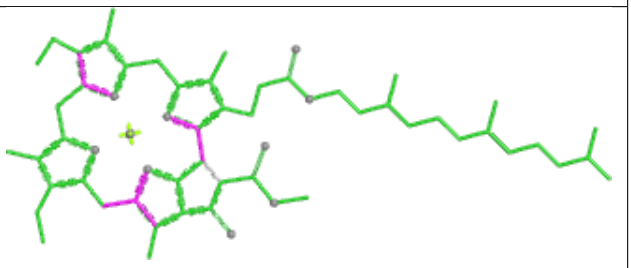
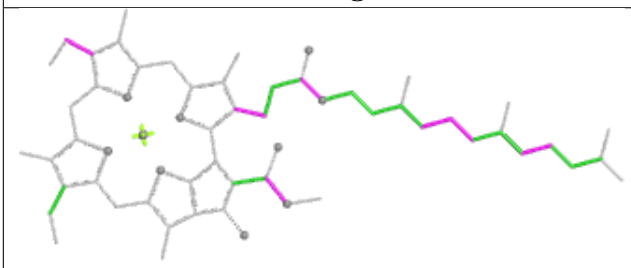
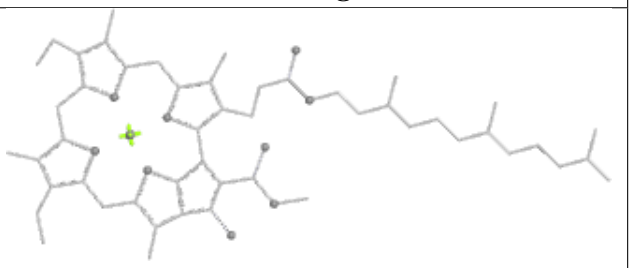
	
Bond lengths	Bond angles
	
Torsions	Rings

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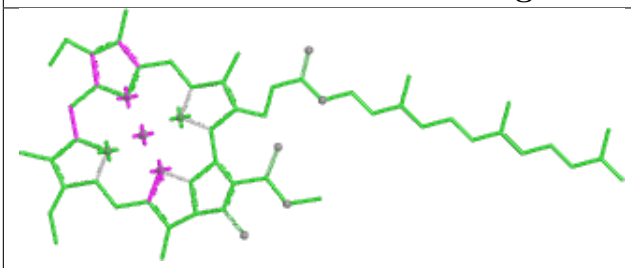
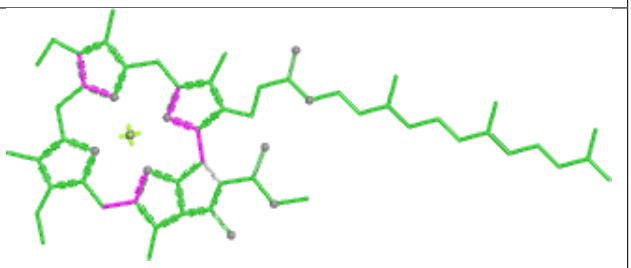
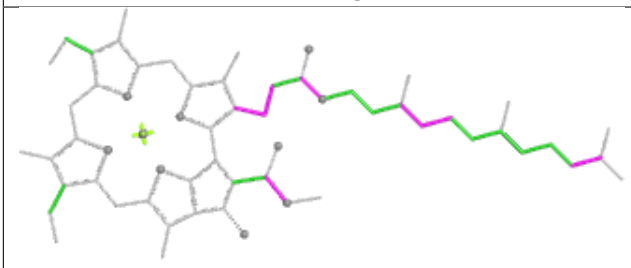
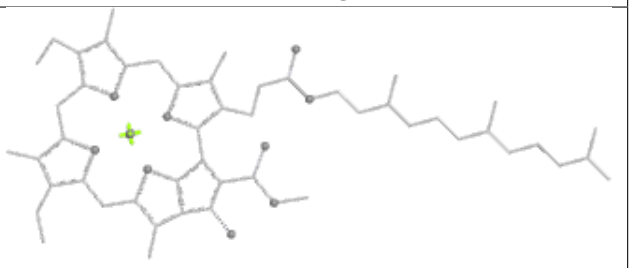
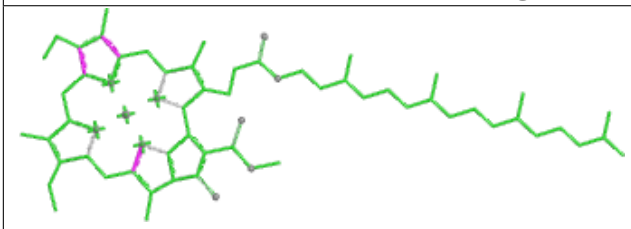
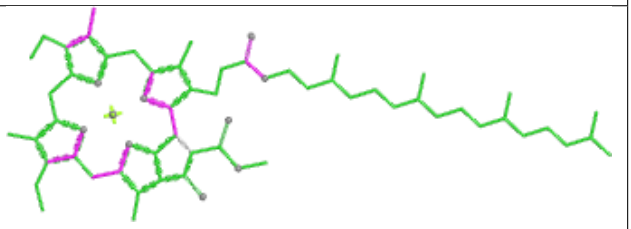
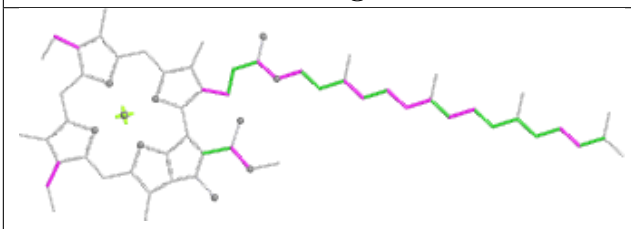
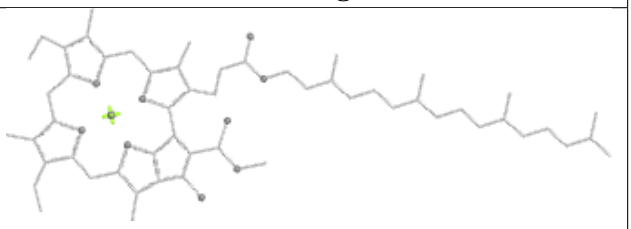
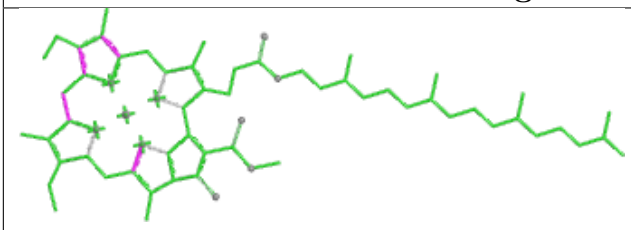
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1239	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1103



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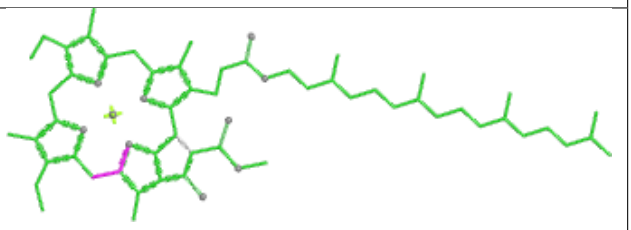
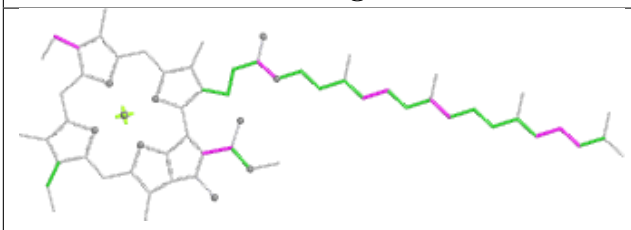
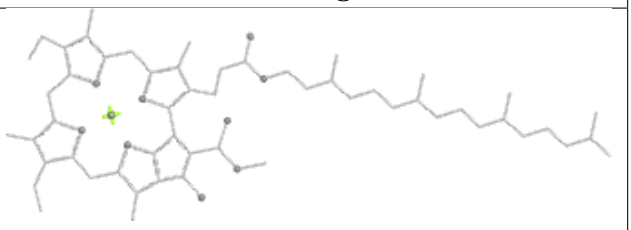


Bond angles

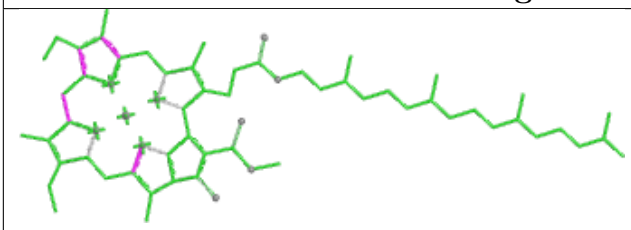


Torsions



Rings

Ligand CLA A 1136



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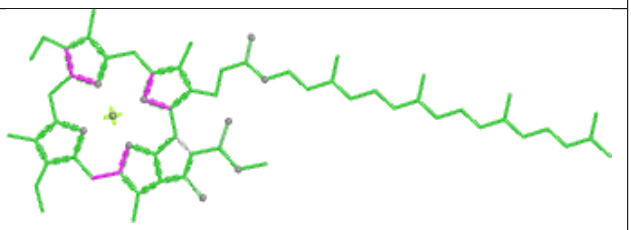

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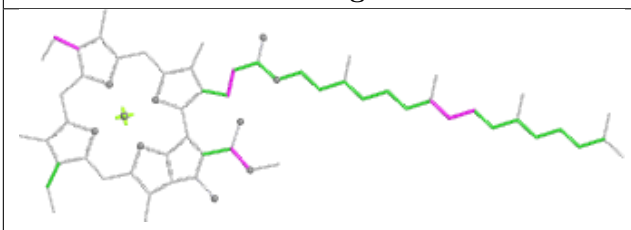
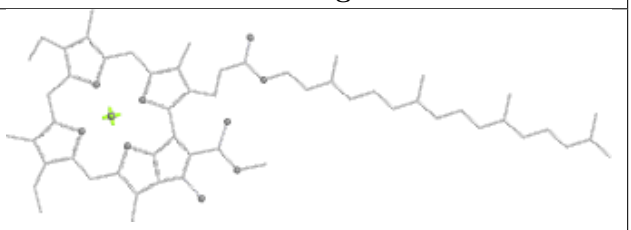
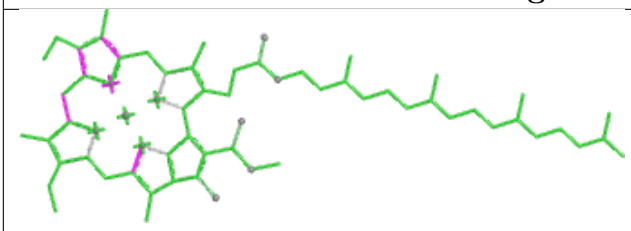


Torsions



Rings

Ligand CLA q 509



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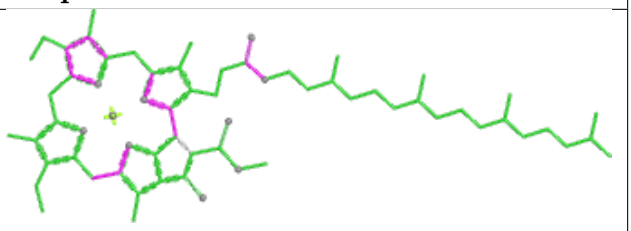
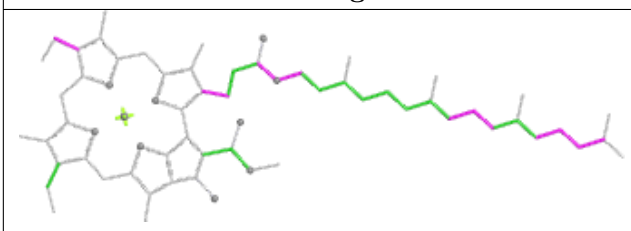


Bond angles



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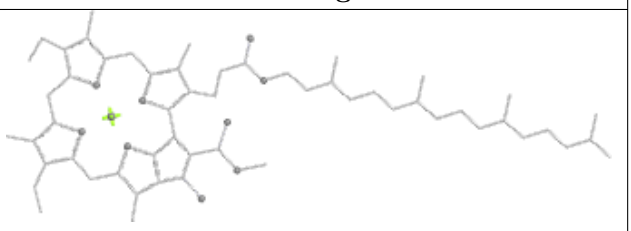
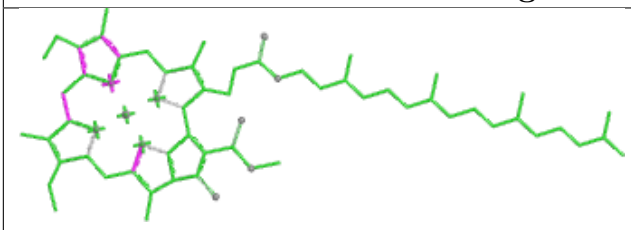


Rings

Ligand CLA b 1211



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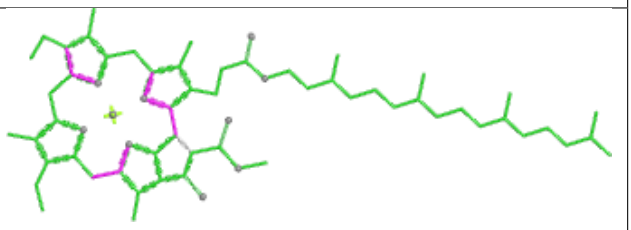
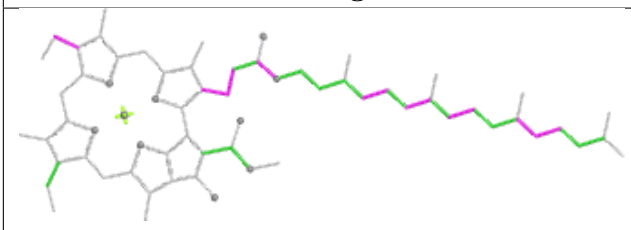


Bond angles



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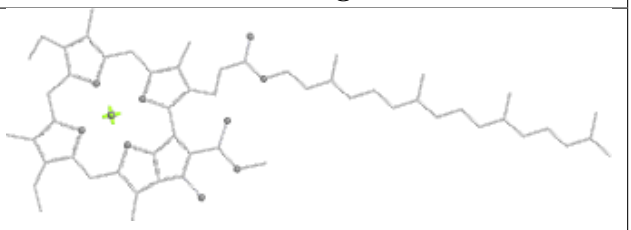
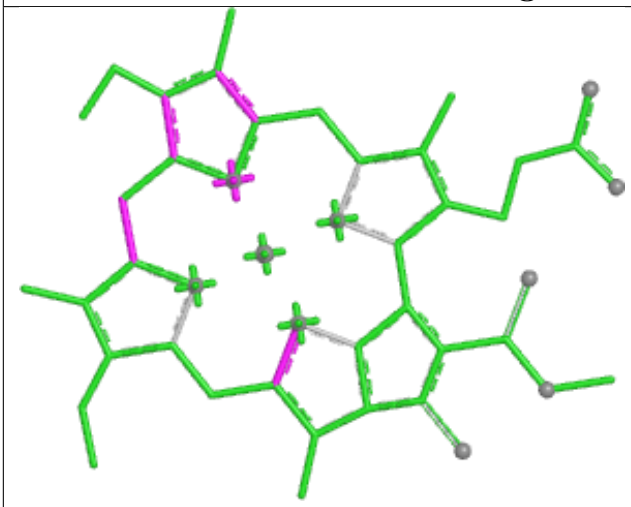


Rings

Ligand CLA b 1208



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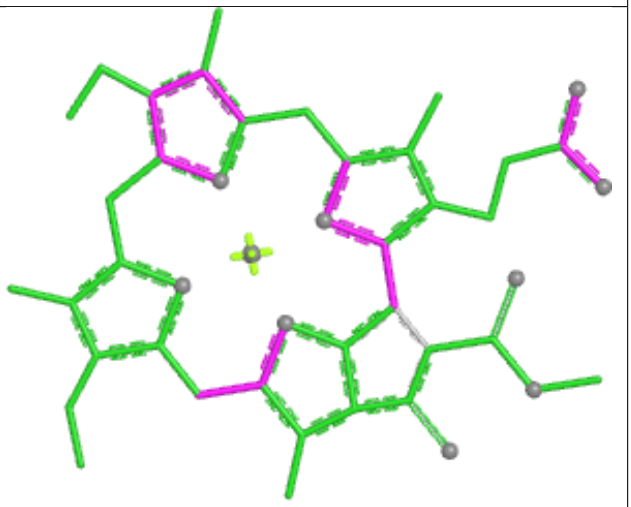

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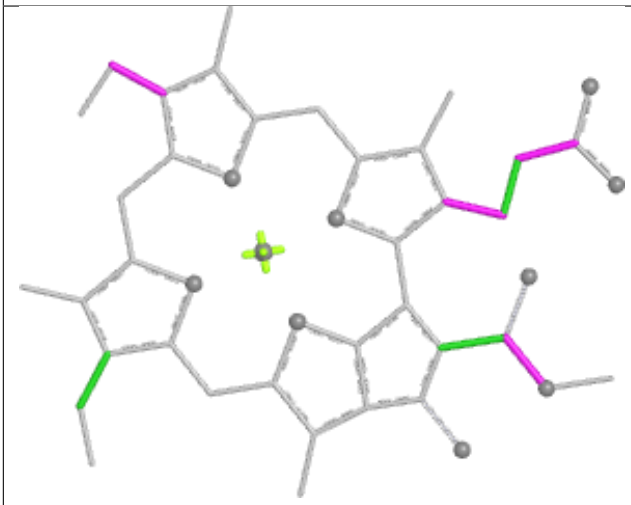
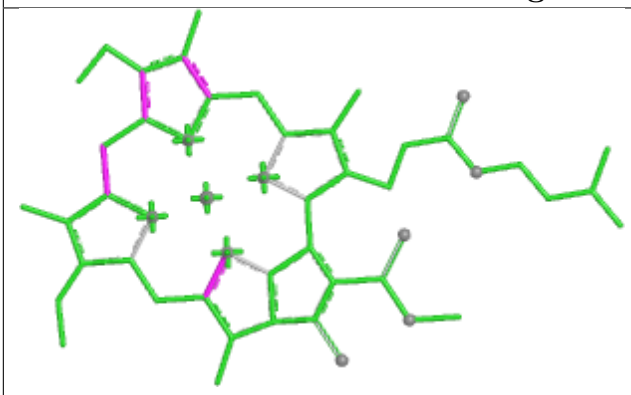


Torsions

Rings

Ligand CLA h 514



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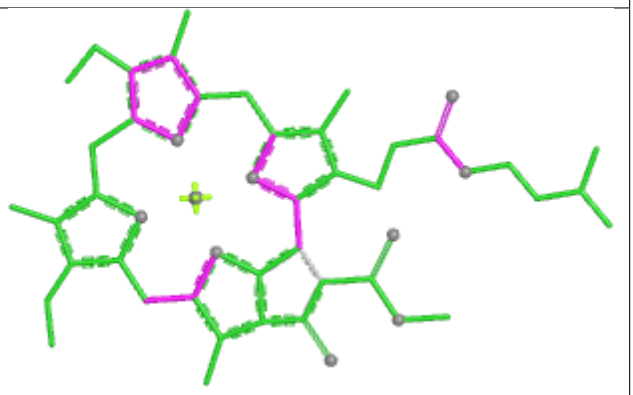

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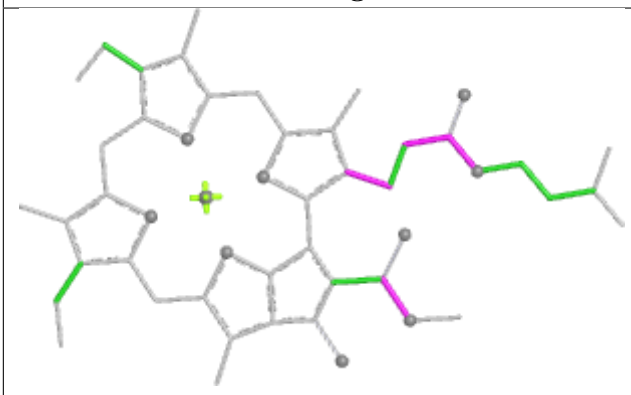

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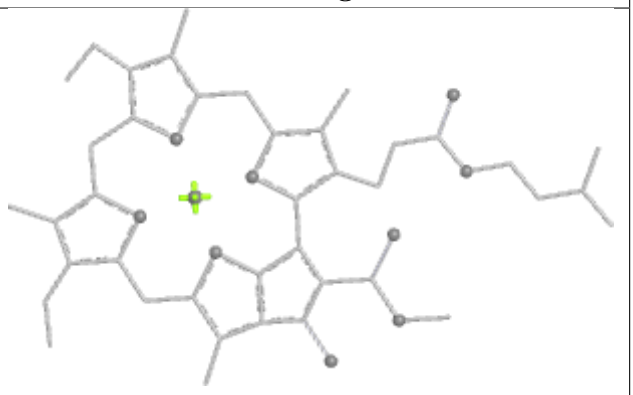
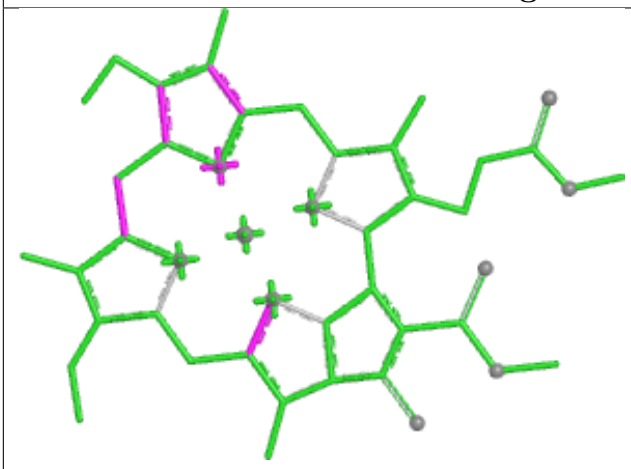


Rings

Ligand CLA a 1114



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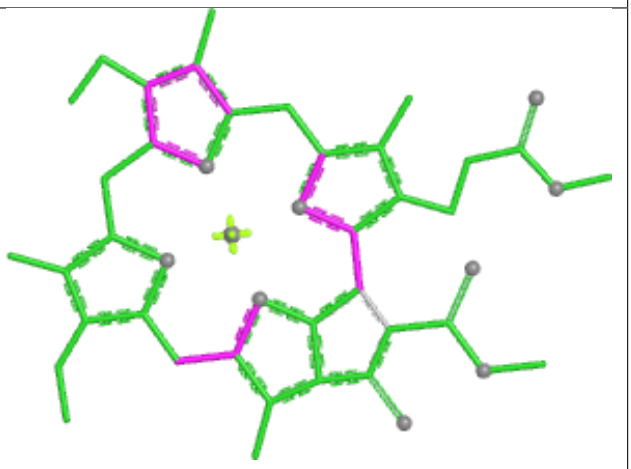
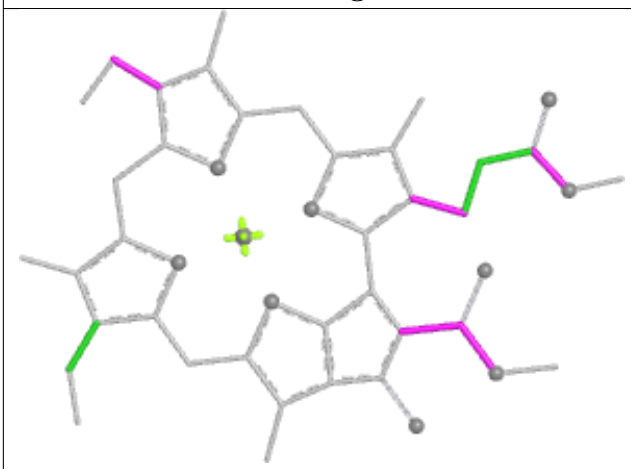


Bond angles



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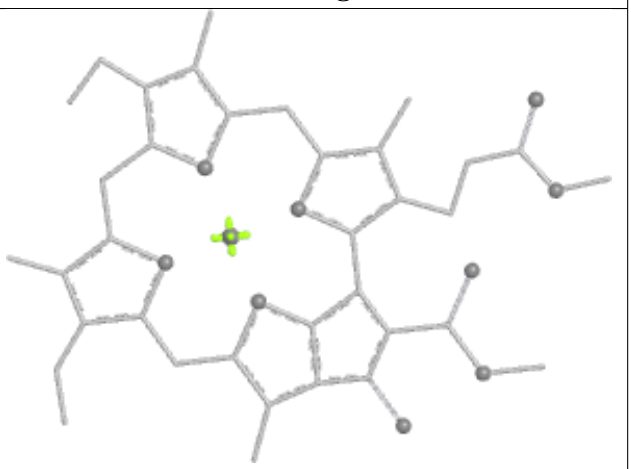
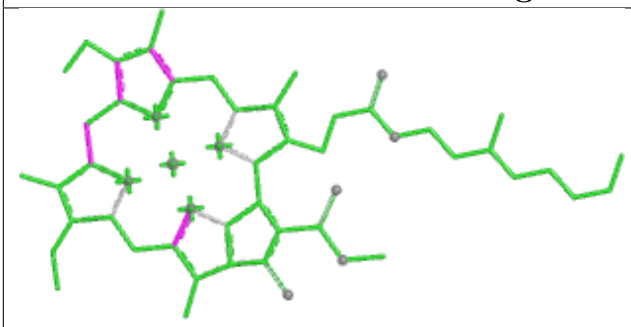


Rings

Ligand CLA B 1201



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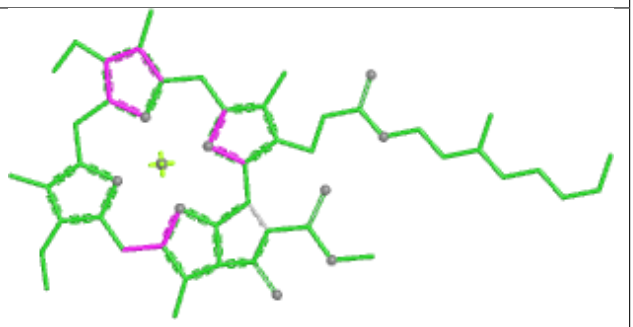
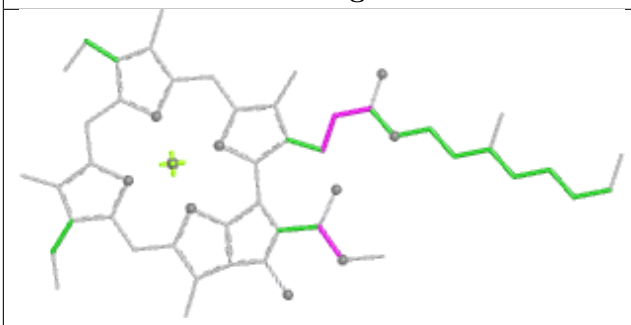


Bond angles



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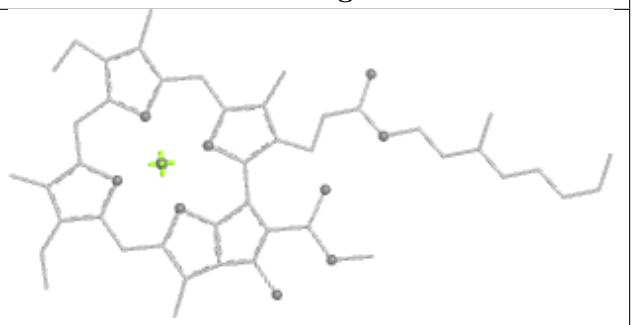
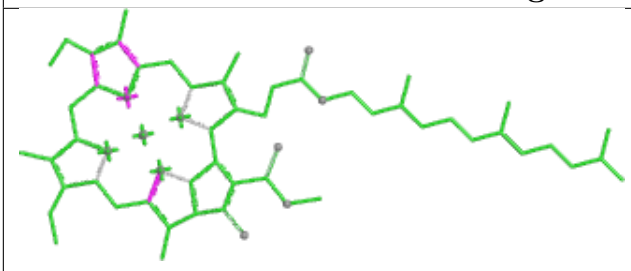


Rings

Ligand CLA q 506



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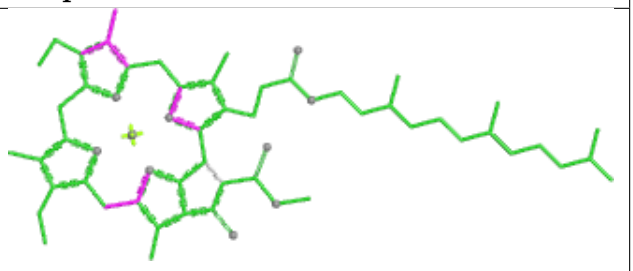

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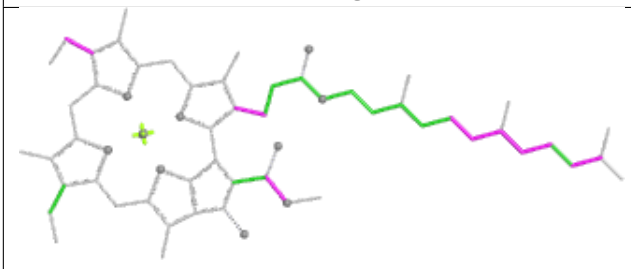

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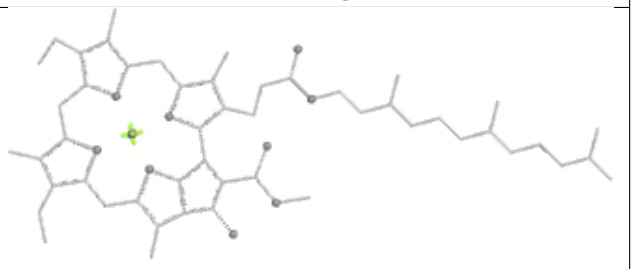
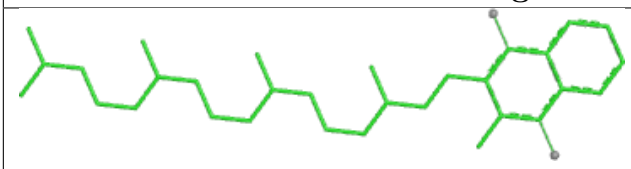


Rings

Ligand PQN H 2001



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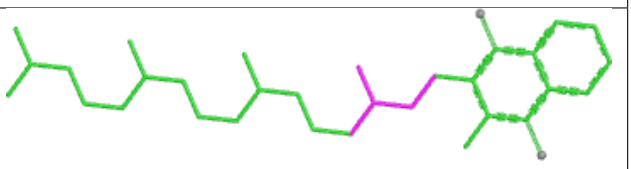
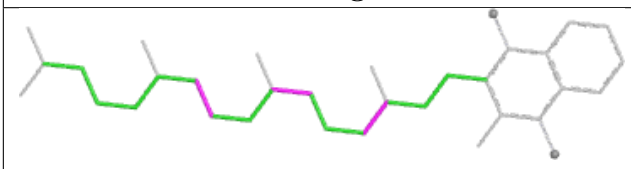


Bond angles



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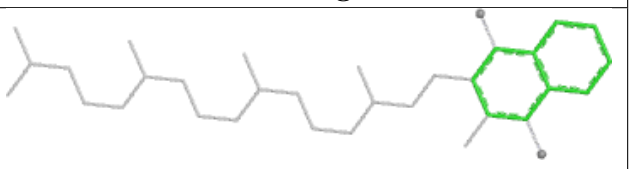
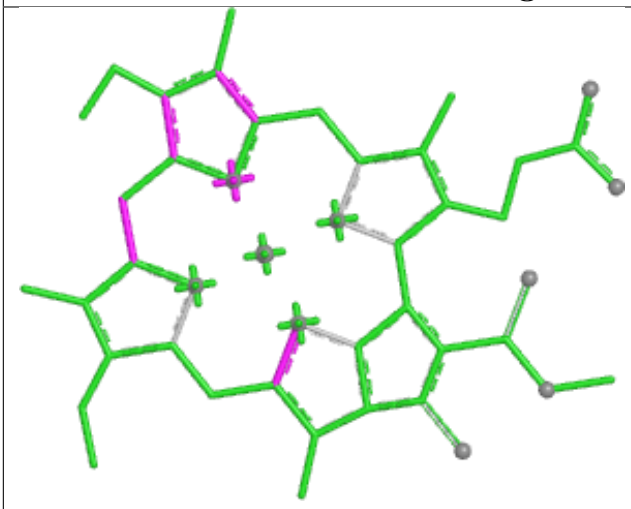


Rings

Ligand CLA S 1302



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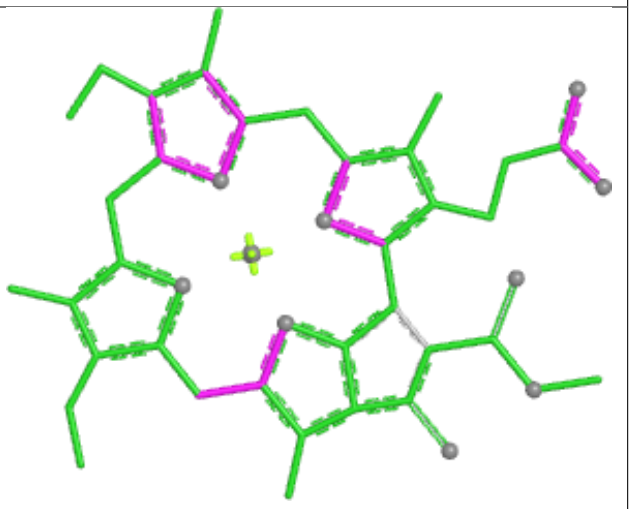
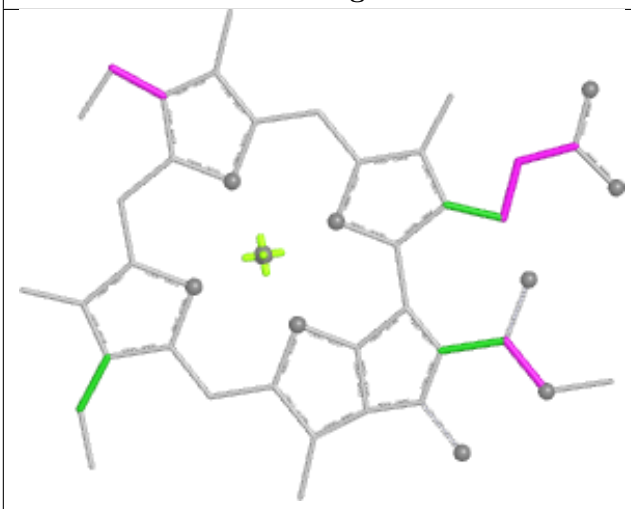


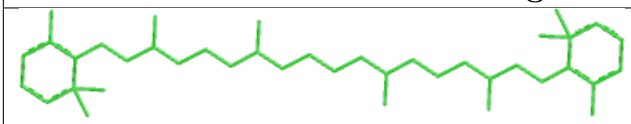
Bond angles



Torsions

Rings

Ligand BCR g 604



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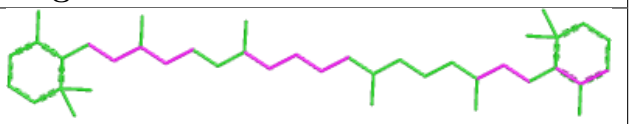
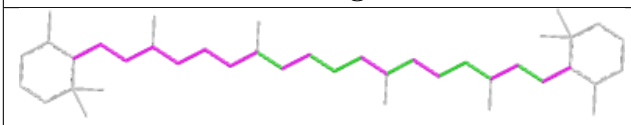


Bond angles



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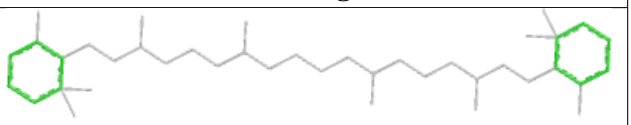
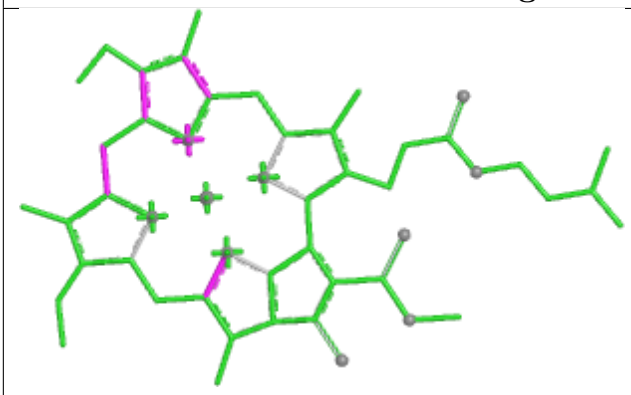
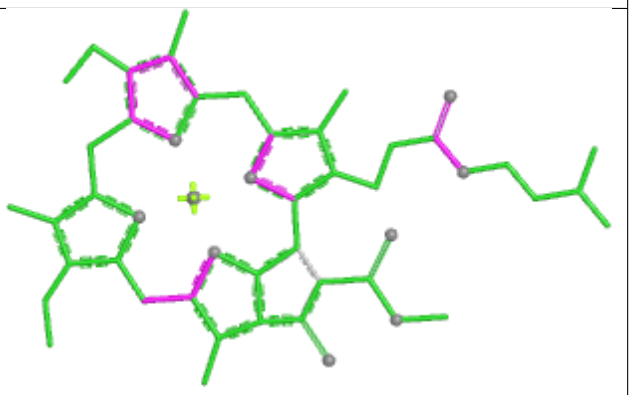


Rings

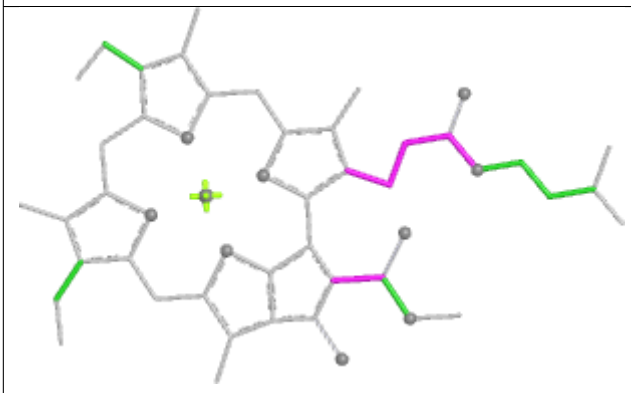
Ligand CLA W 501



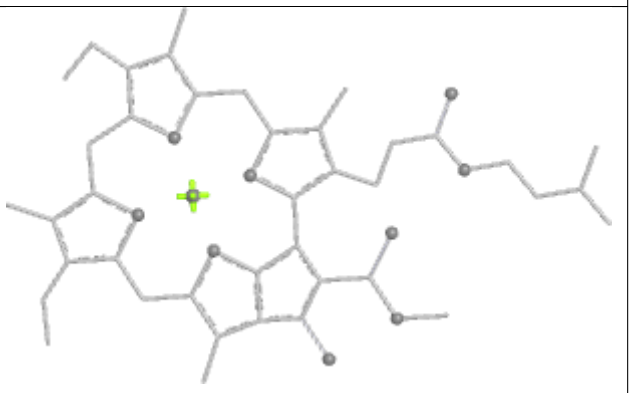
Bond lengths



Bond angles

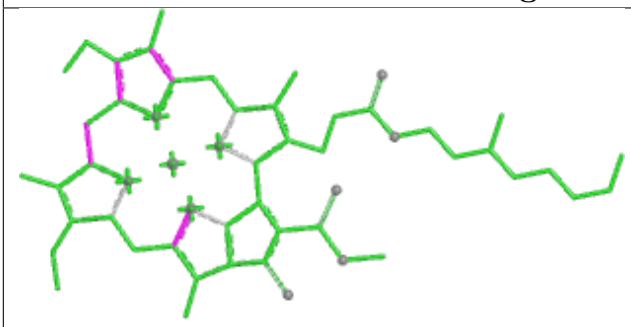


Torsions



Rings

Ligand CLA a 1110



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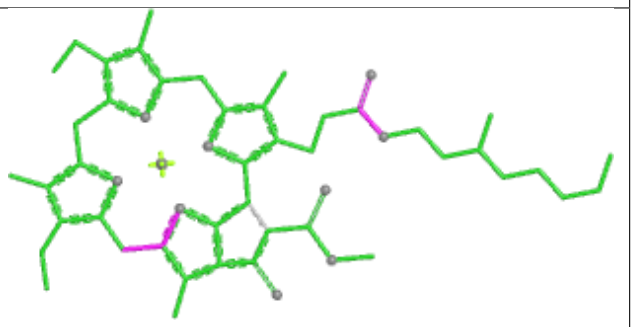
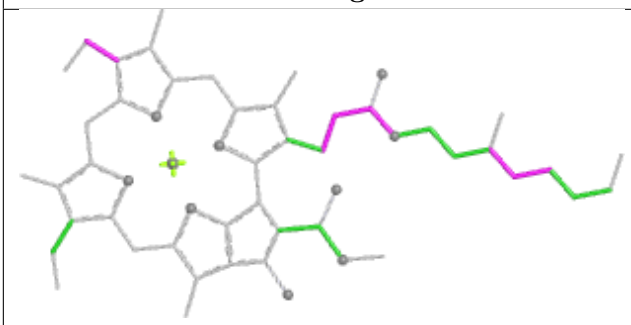
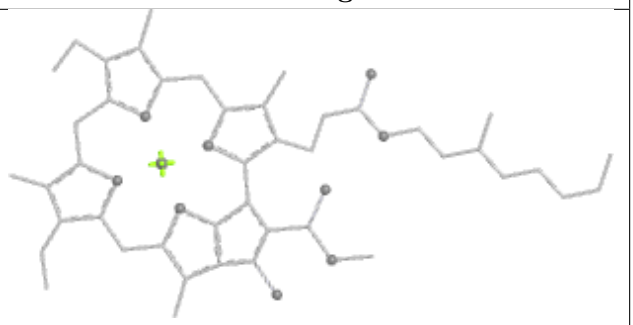


Bond angles

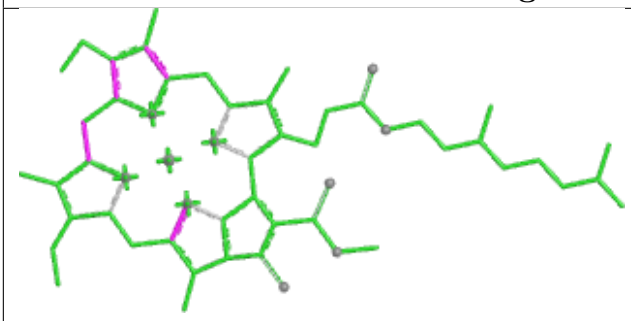


Torsions



Rings

Ligand CLA k 4004



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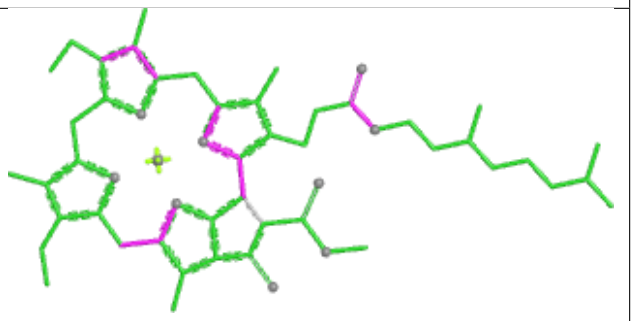

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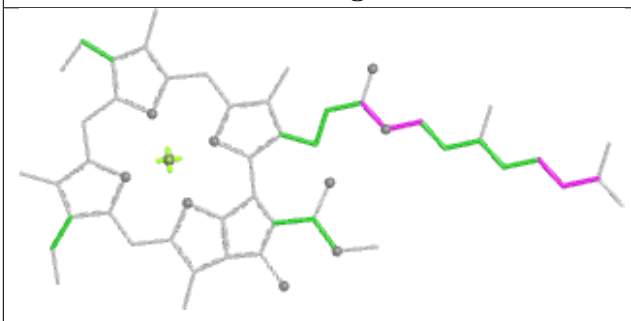
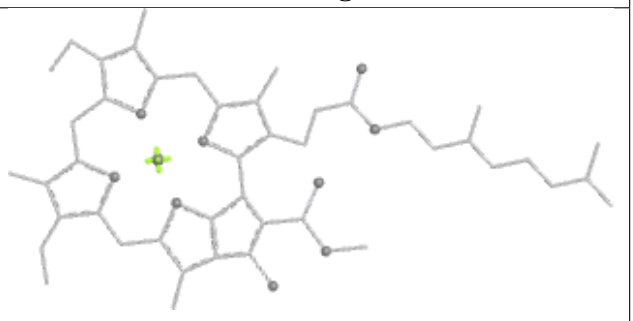
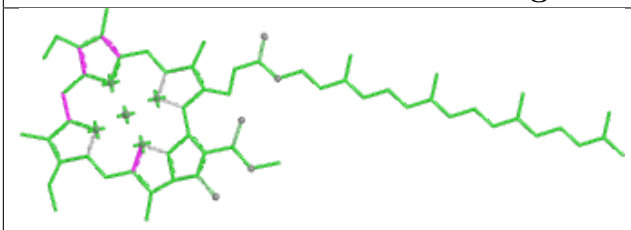
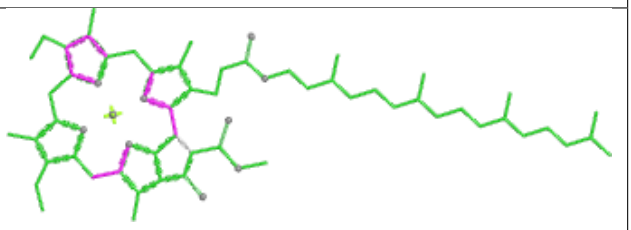
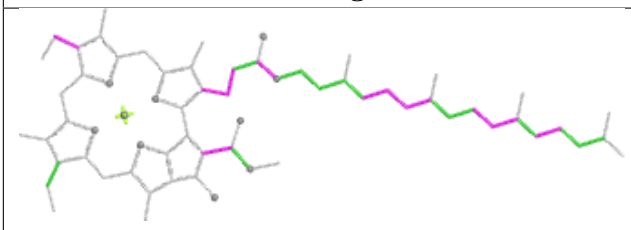
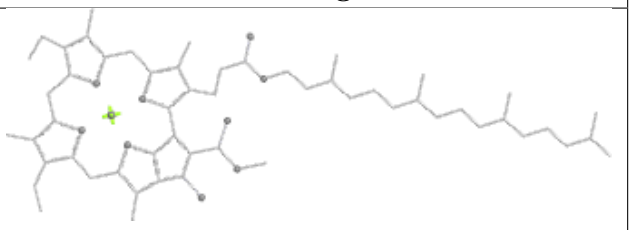
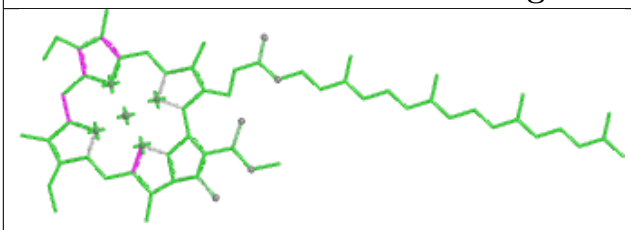
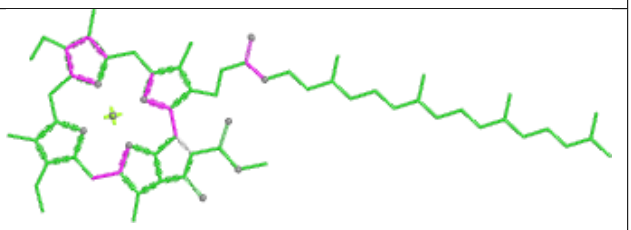
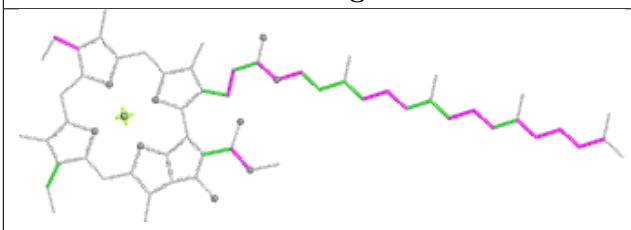
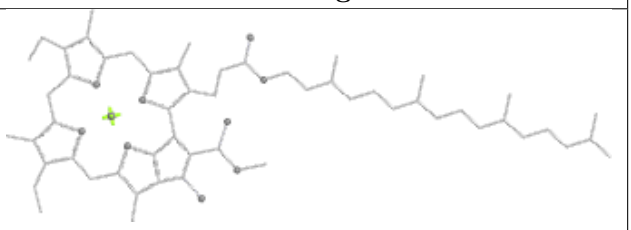


Torsions

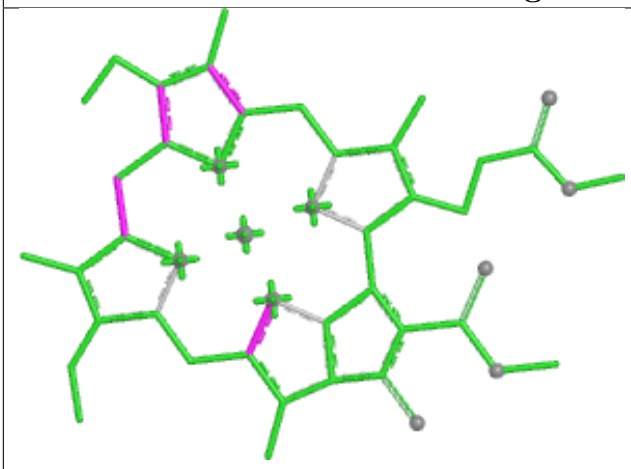


Rings

Ligand CLA t 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA w 516



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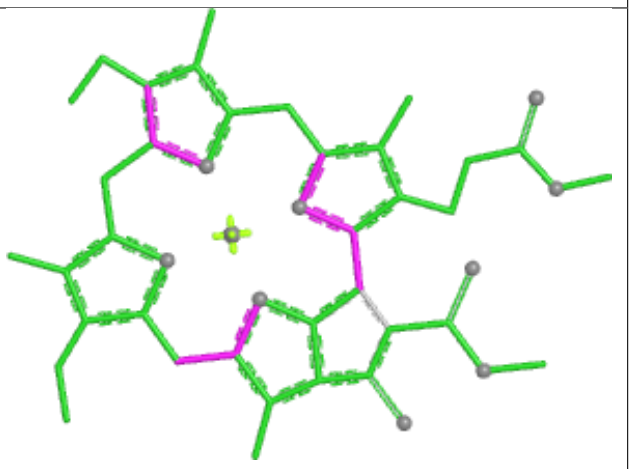
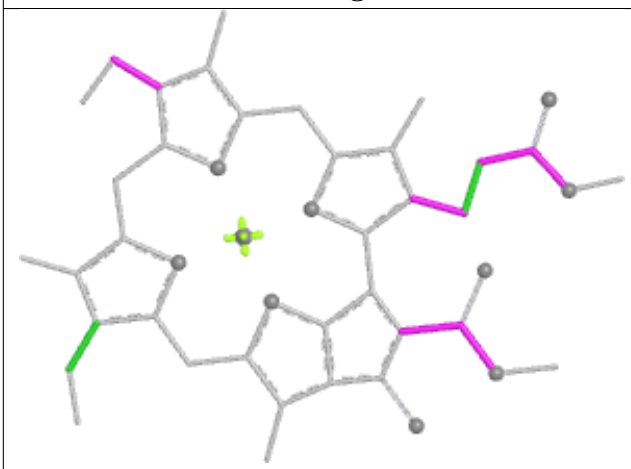
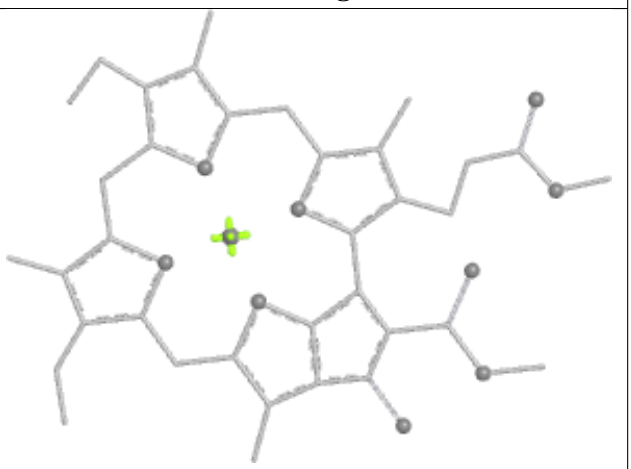


Bond angles

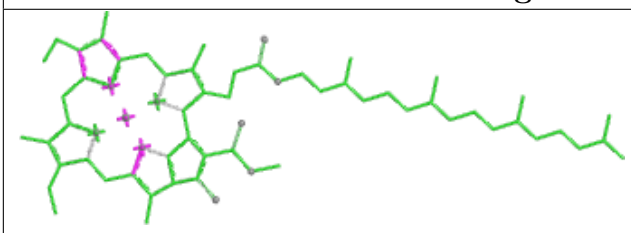


Torsions



Rings

Ligand CLA H 1237



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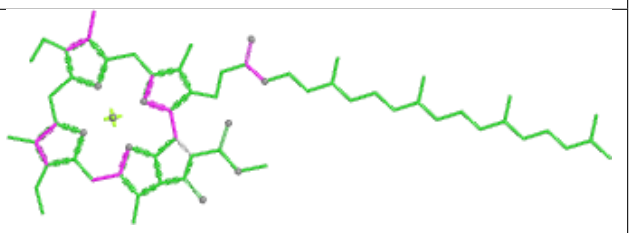
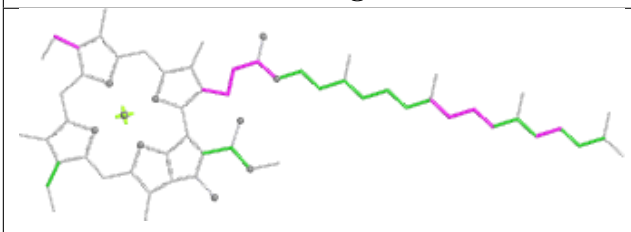


Bond angles



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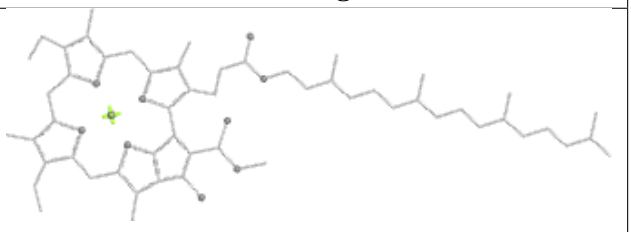
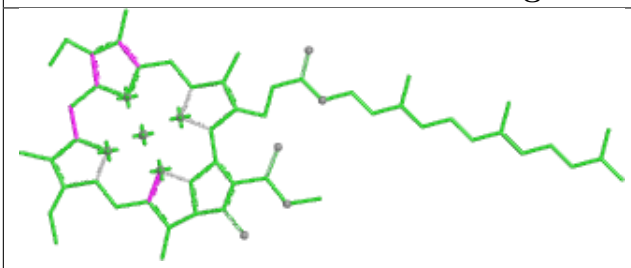


Rings

Ligand CLA X 510



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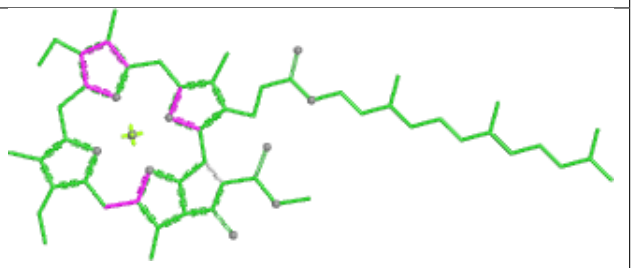
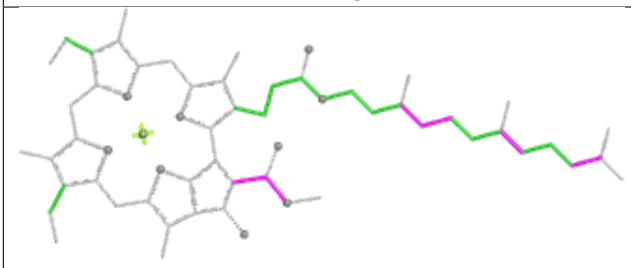


Bond angles



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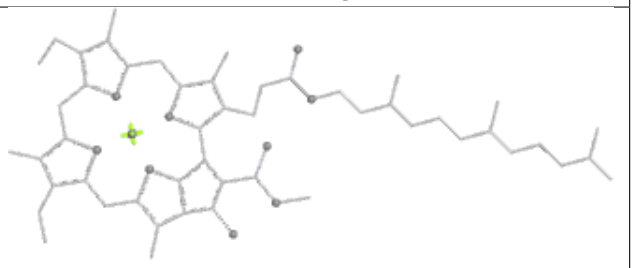
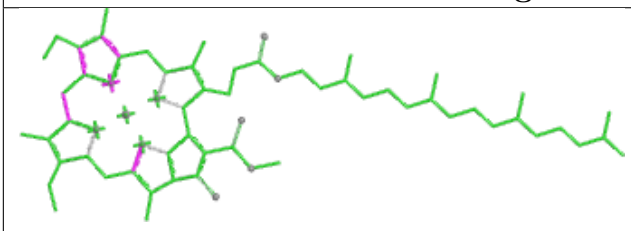
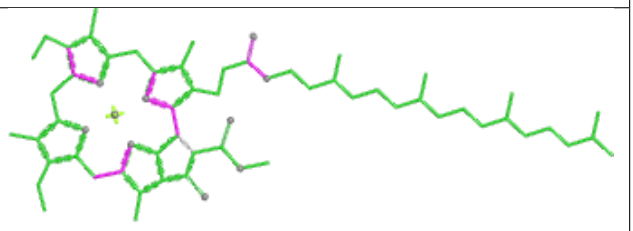


Rings

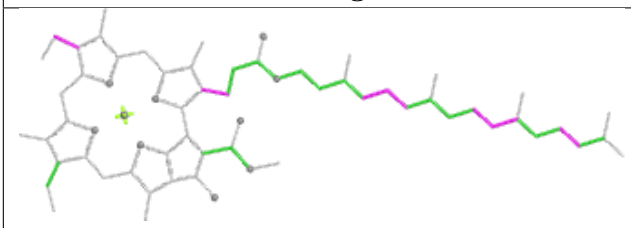
Ligand CLA A 1109



Bond lengths



Bond angles



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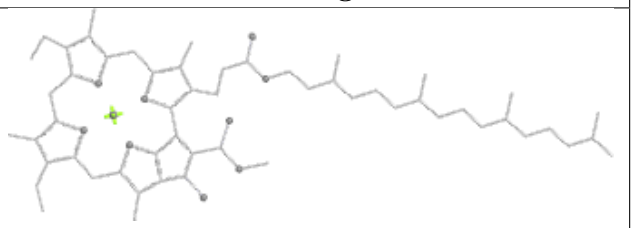
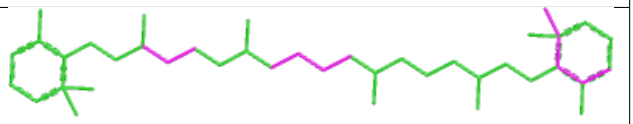


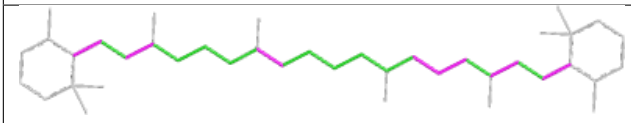
Rings

Ligand BCR f 4016

Bond lengths



Bond angles



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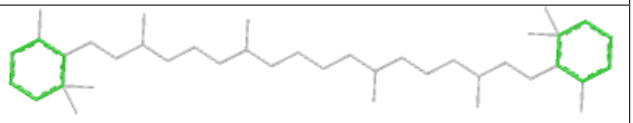
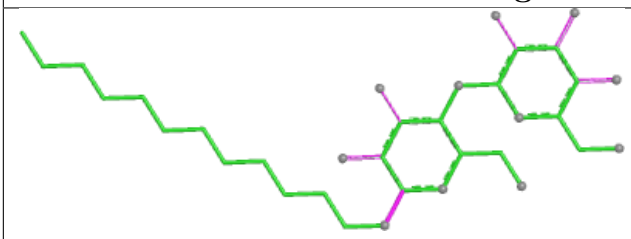


Rings

Ligand LMT L 4101



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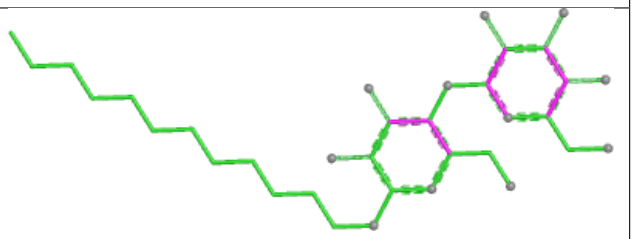
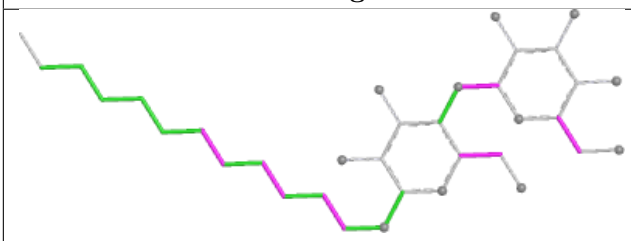


Bond angles



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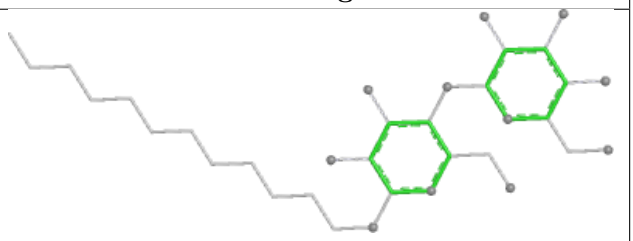
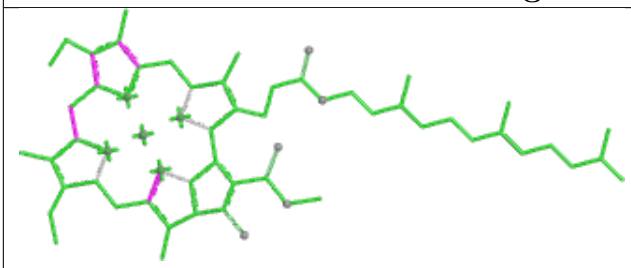


Rings

Ligand CLA Y 509



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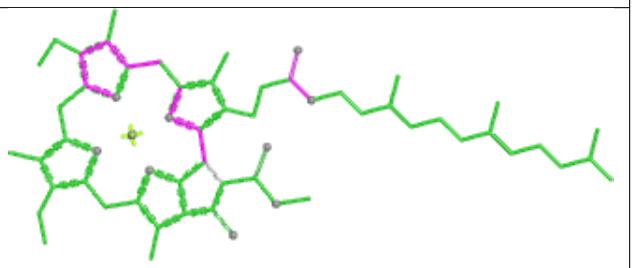
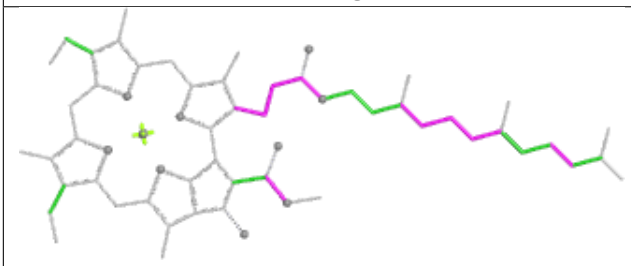


Bond angles



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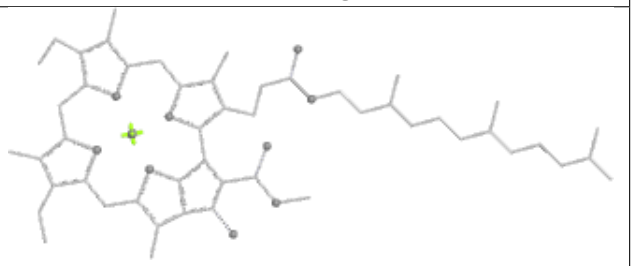
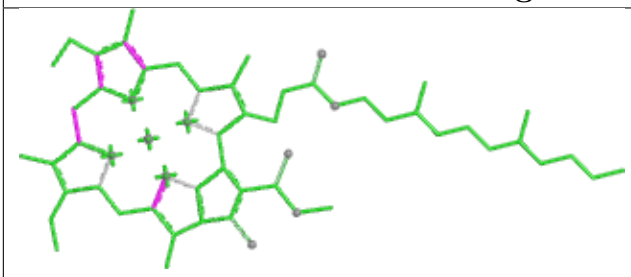


Rings

Ligand CLA B 1229



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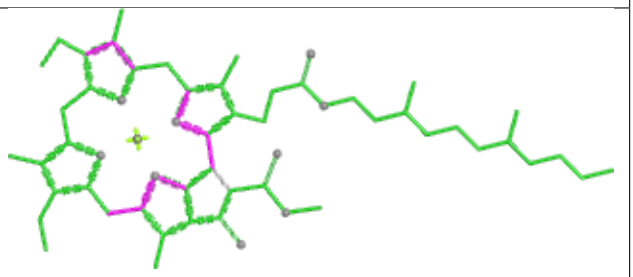
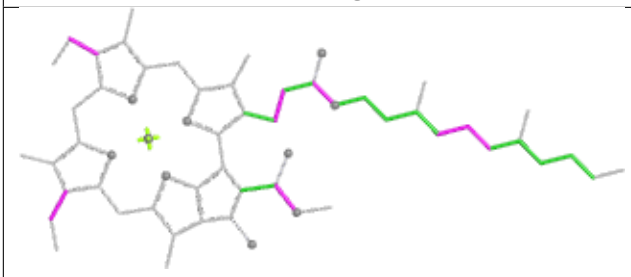


Bond angles



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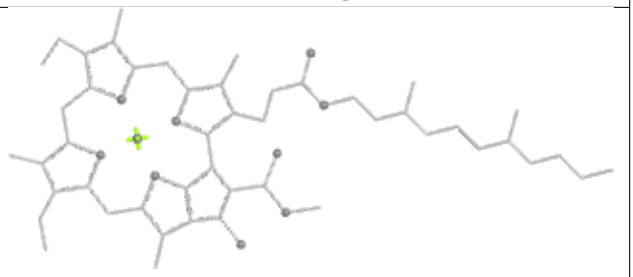
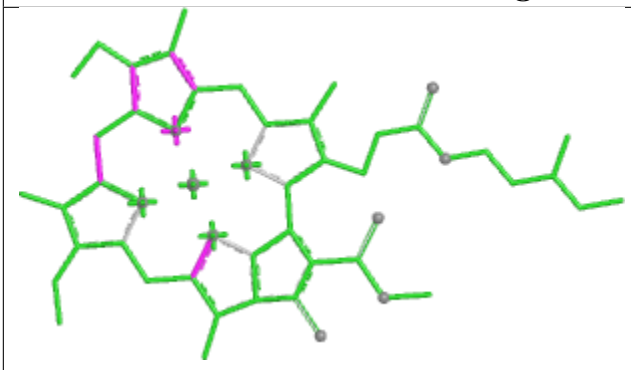


Rings

Ligand CLA H 1121



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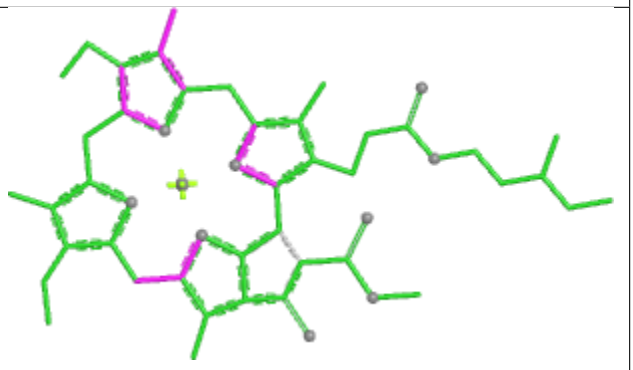
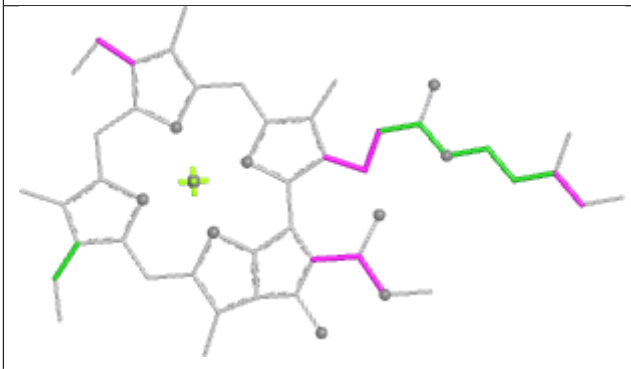


Bond angles



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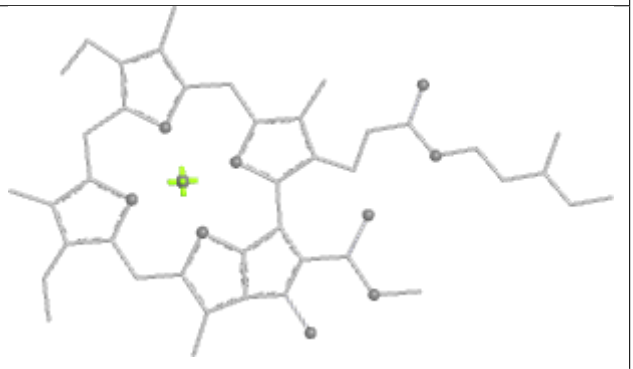
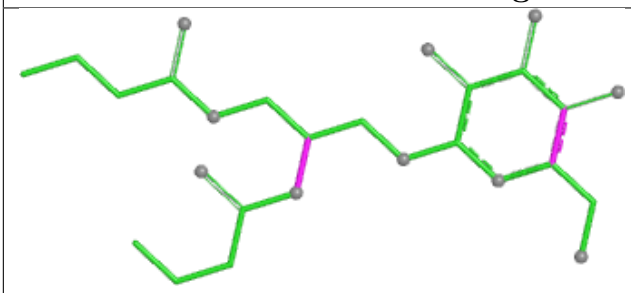


Rings

Ligand LMG F 4017



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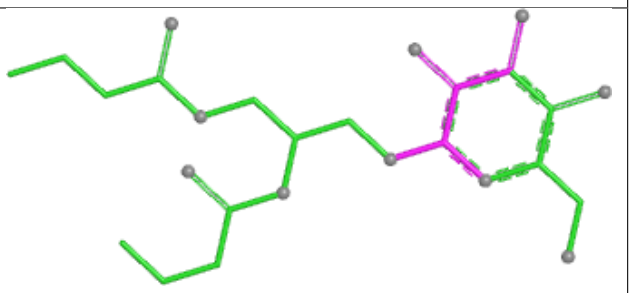
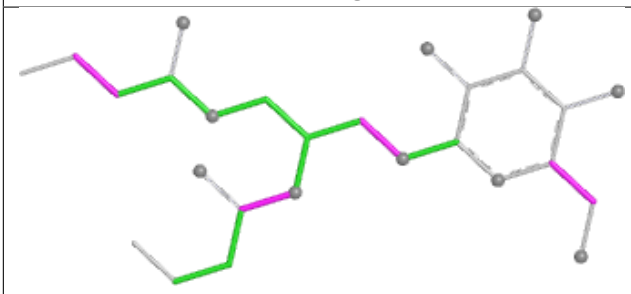


Bond angles



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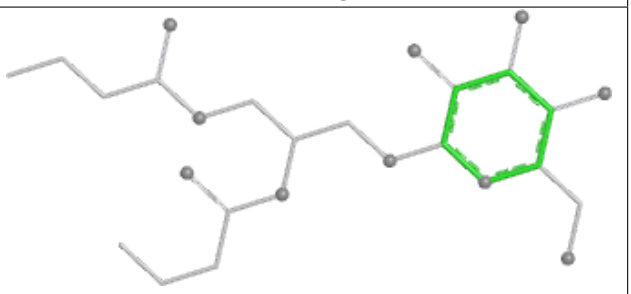
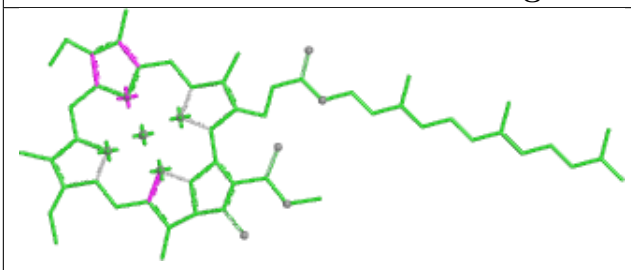
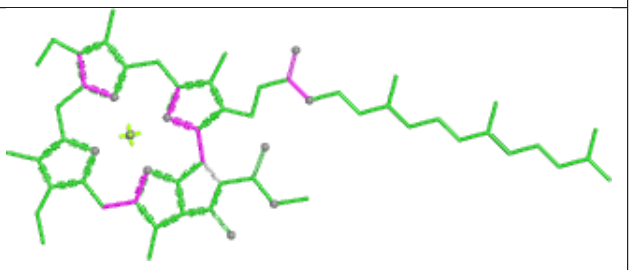


Rings

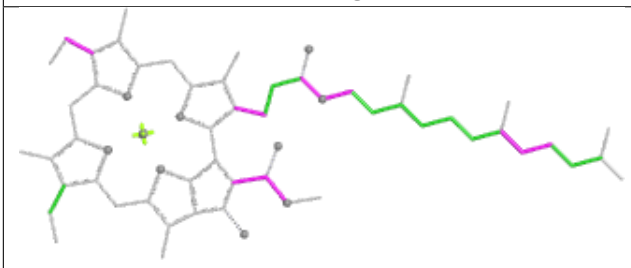
Ligand CLA Y 506



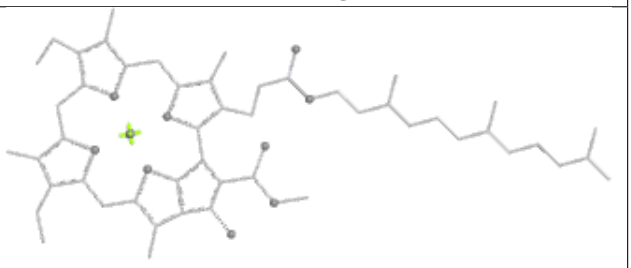
Bond lengths



Bond angles



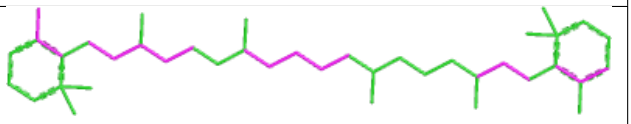
Torsions



Rings

Ligand BCR S 4012

Bond lengths



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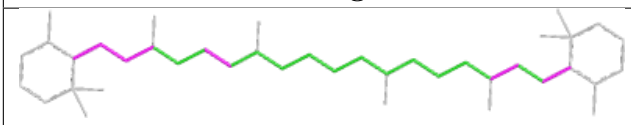
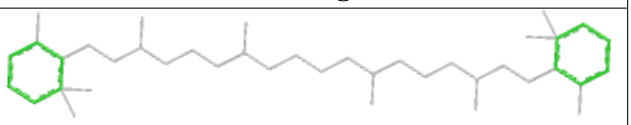
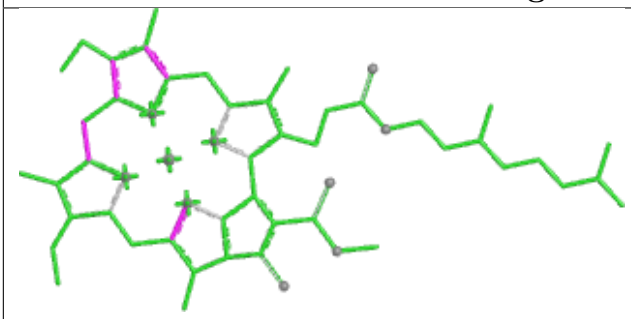
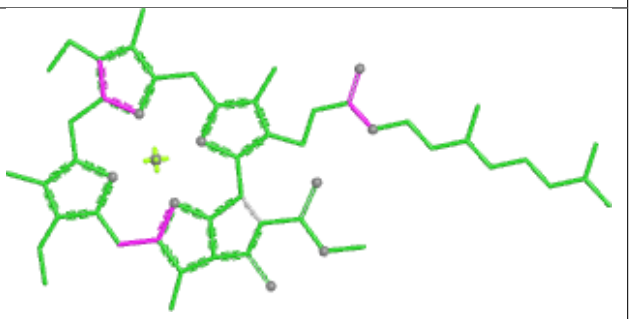
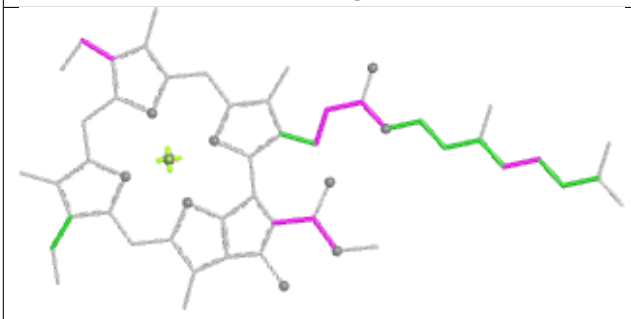
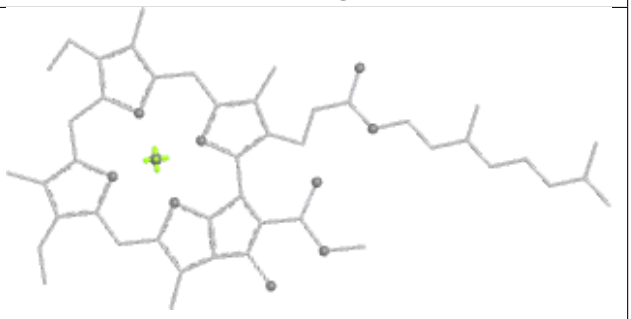
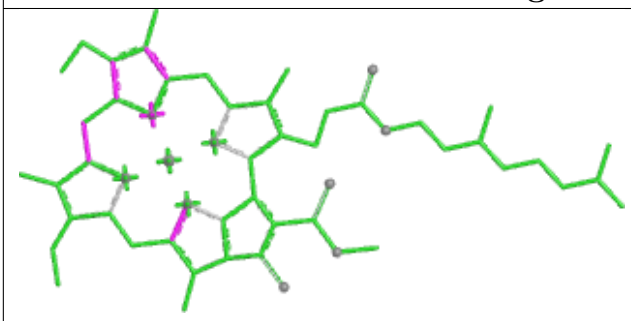
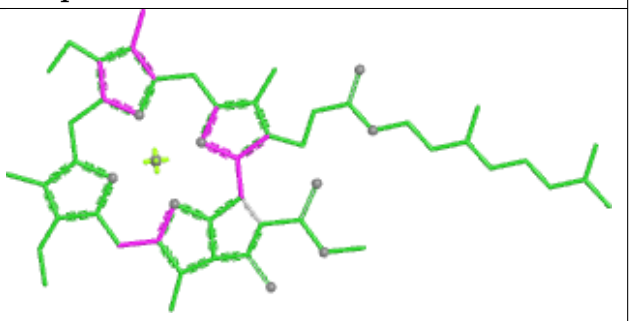
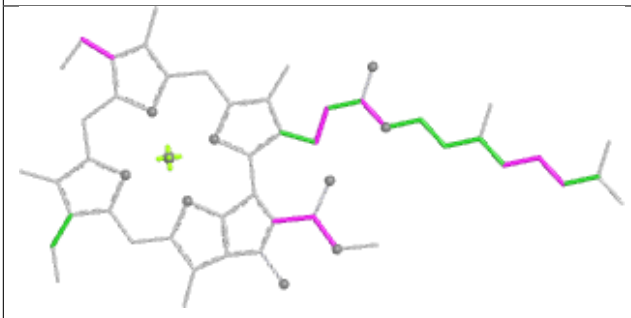
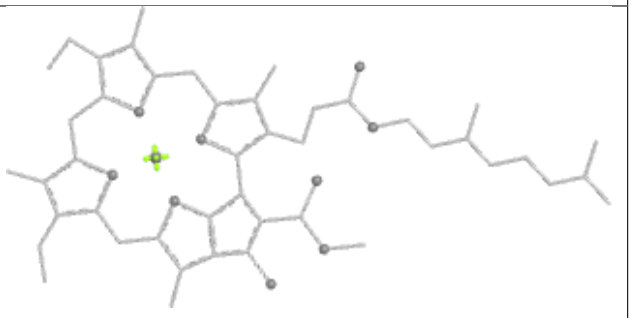


Torsions

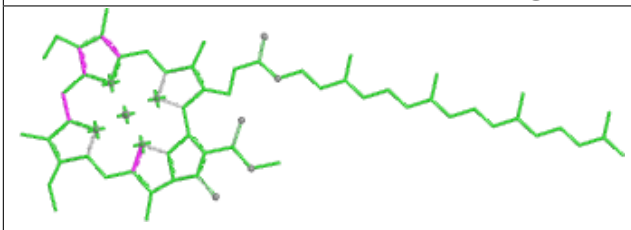


Rings

Ligand CLA x 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA n 507



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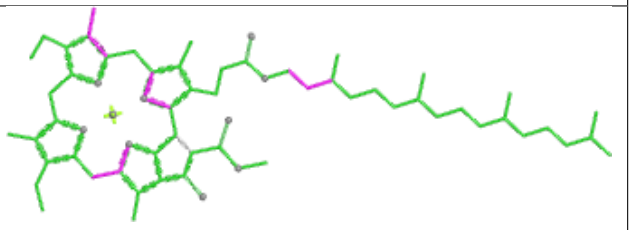
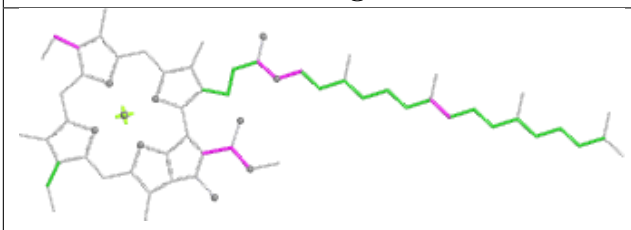


Bond angles



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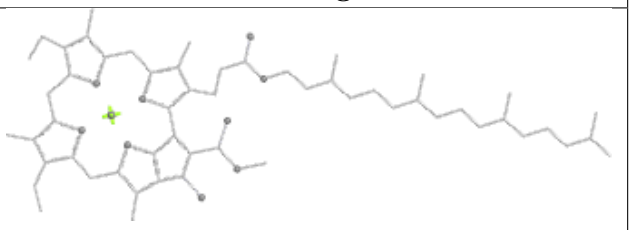
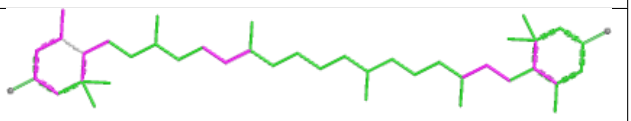


Rings

Ligand LUT Z 601

Bond lengths



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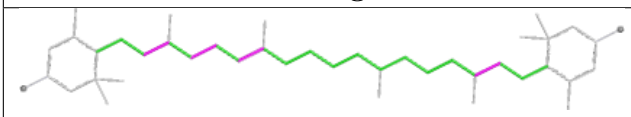

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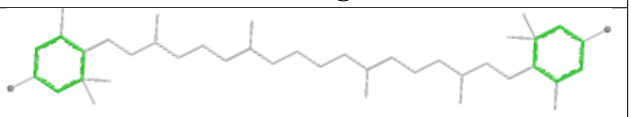
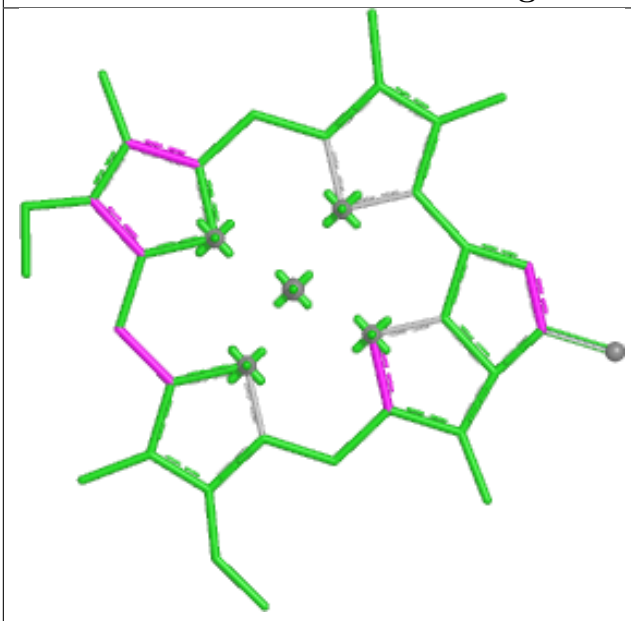
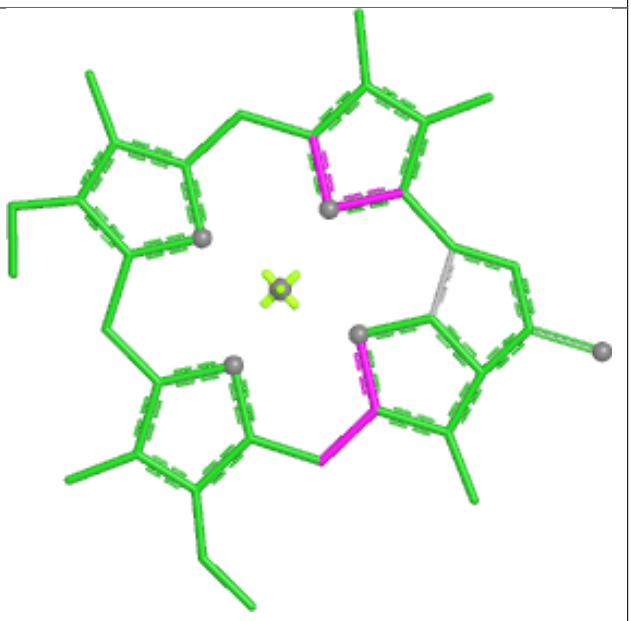


Rings

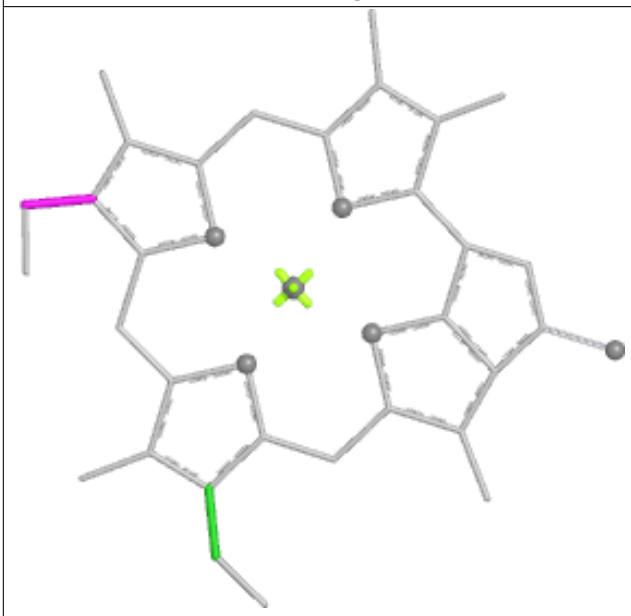
Ligand CLA S 1303



Bond lengths



Bond angles



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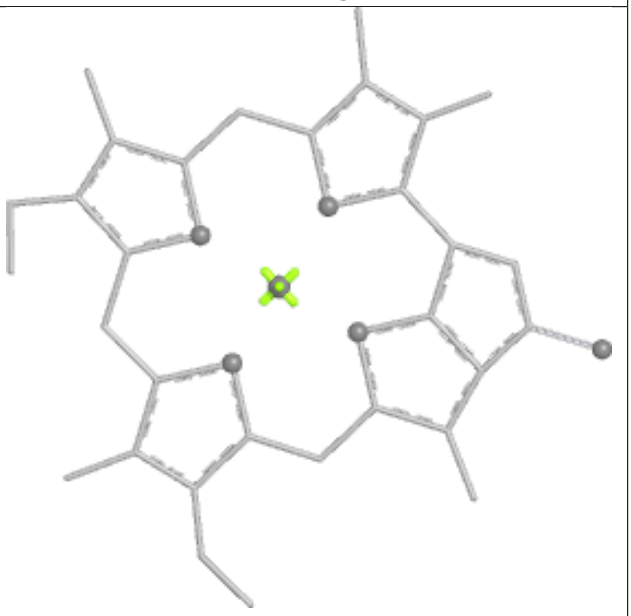
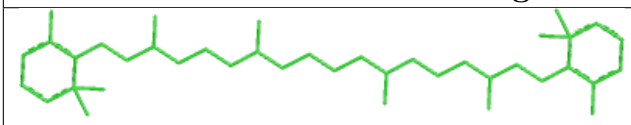


Rings

Ligand BCR K 4005



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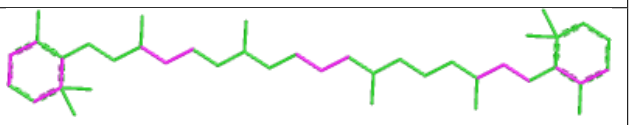
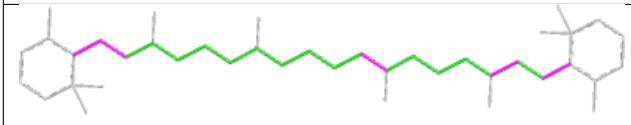


Bond angles



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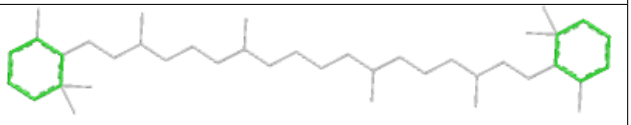
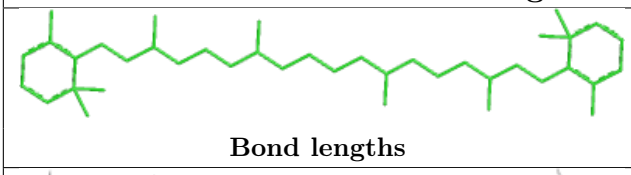


Rings

Ligand BCR o 602



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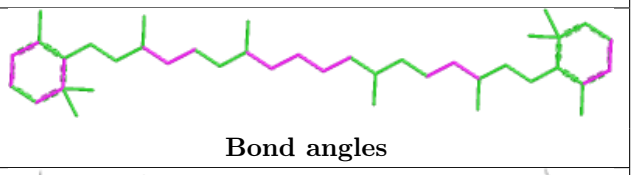
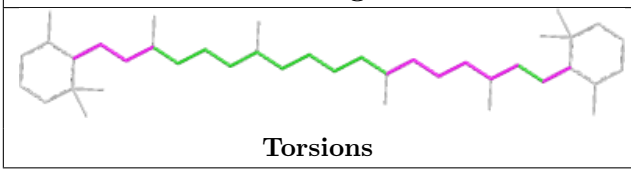
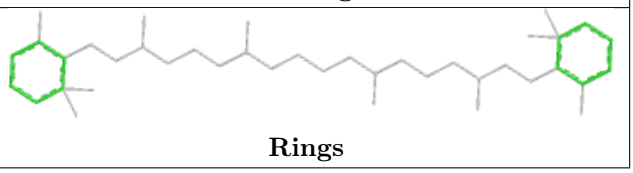


Bond angles

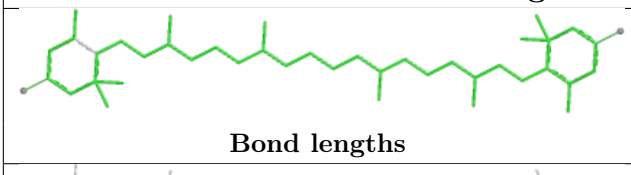


Torsions



Rings

Ligand LUT q 601



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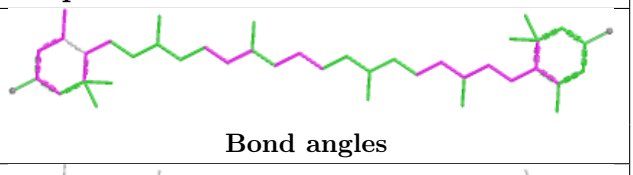
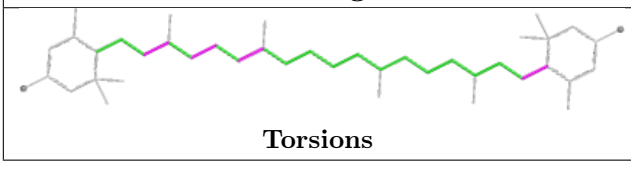


Bond angles



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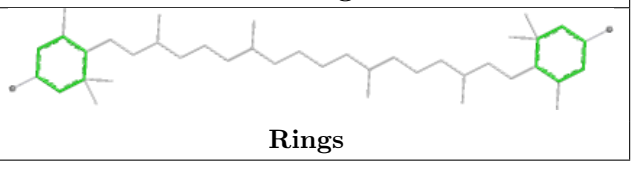
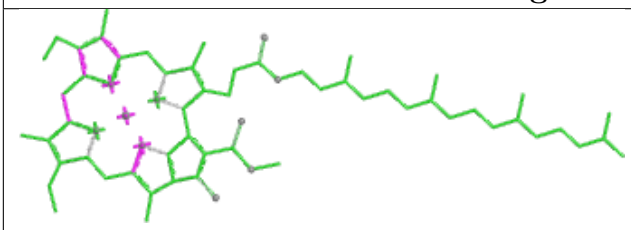


Rings

Ligand CLA s 512



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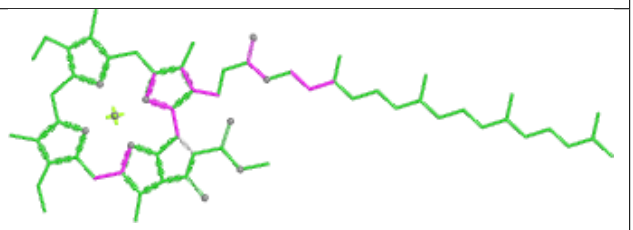

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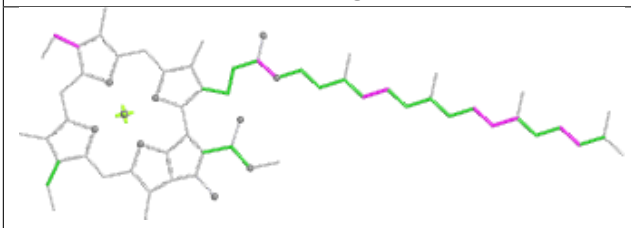

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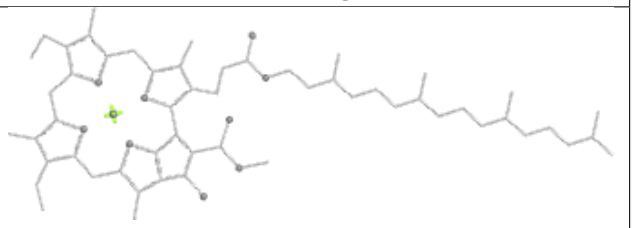
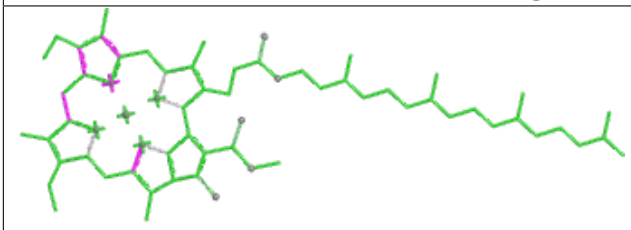


Rings

Ligand CLA q 515



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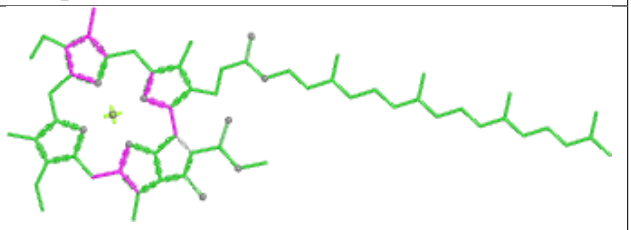
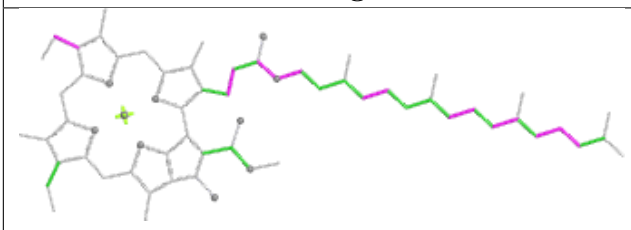


Bond angles



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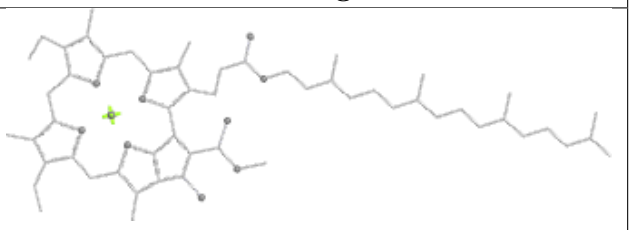
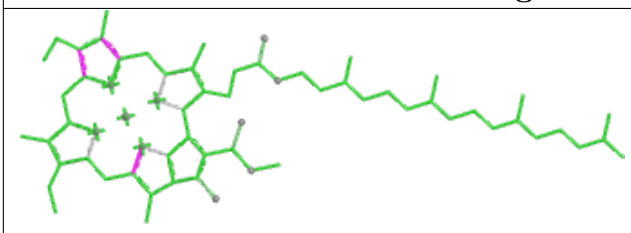


Rings

Ligand CLA B 1239



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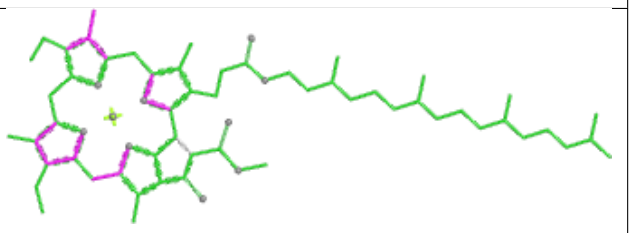
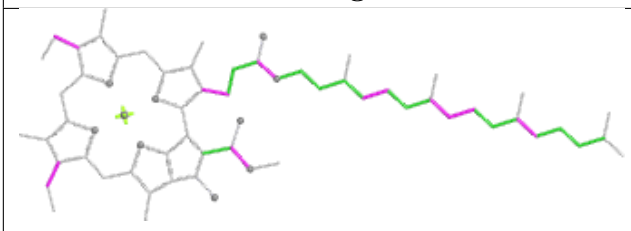
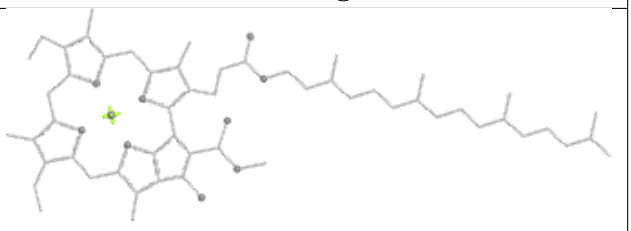


Bond angles

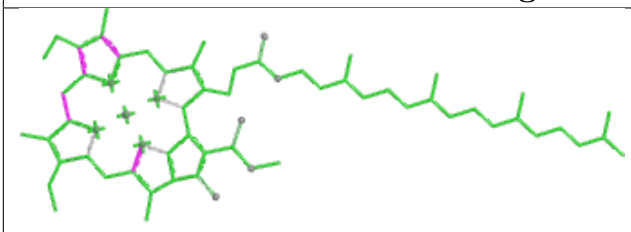


Torsions



Rings

Ligand CLA W 505



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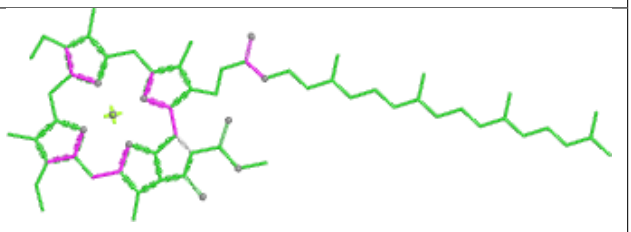
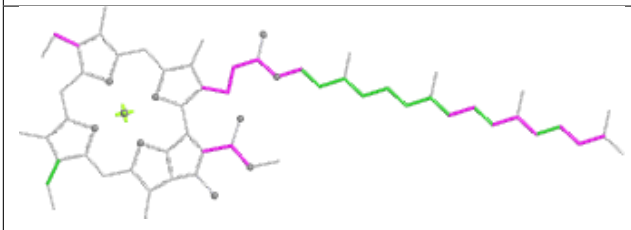
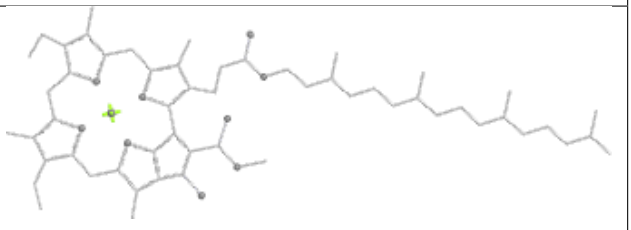


Bond angles

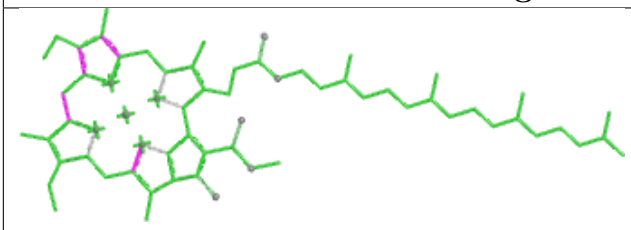


Torsions



Rings

Ligand CLA A 1106



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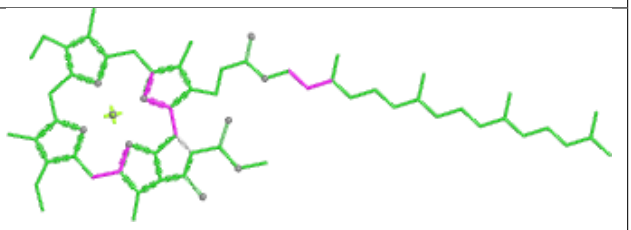
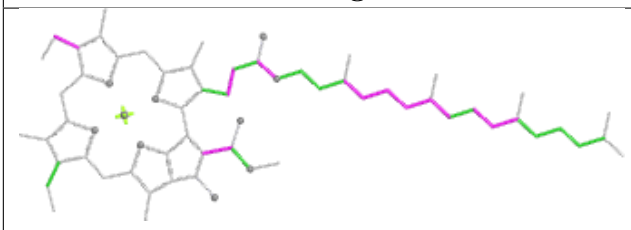
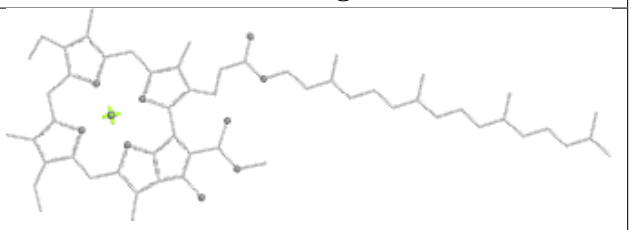


Bond angles

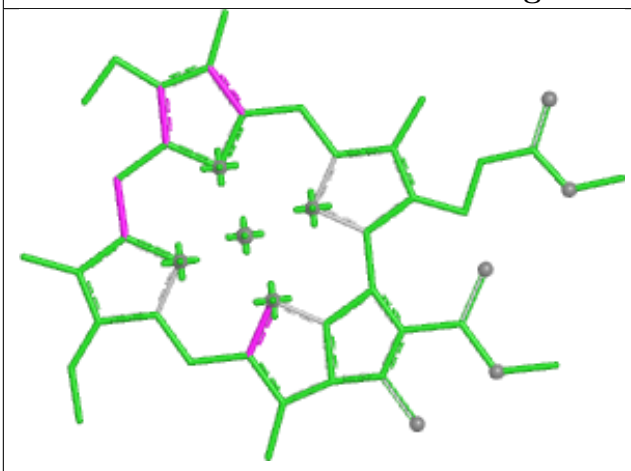


Torsions

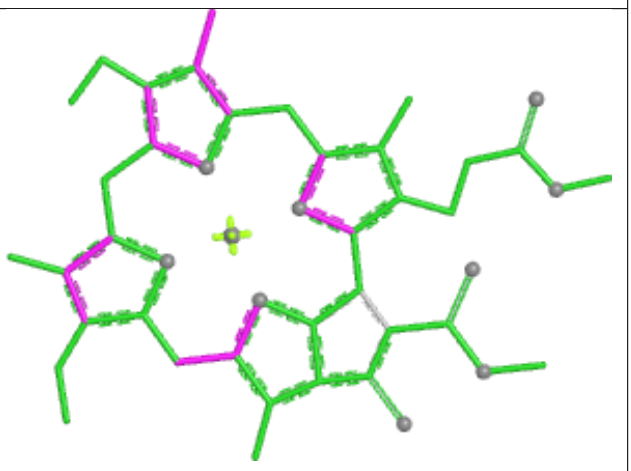


Rings

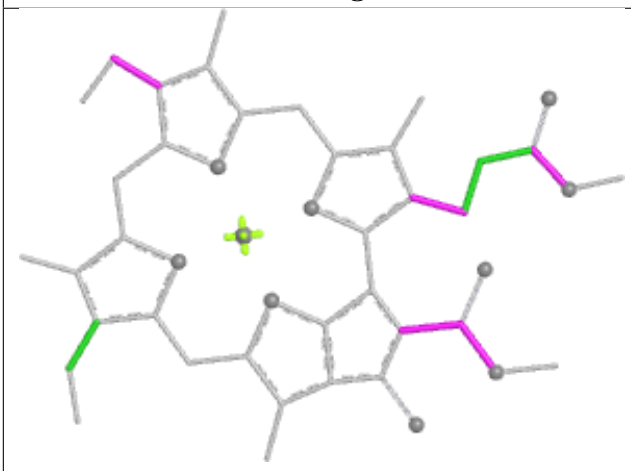
Ligand CLA Y 513



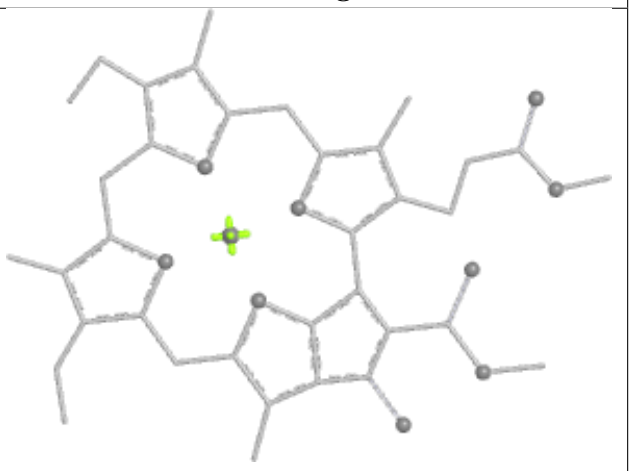
Bond lengths



Bond angles

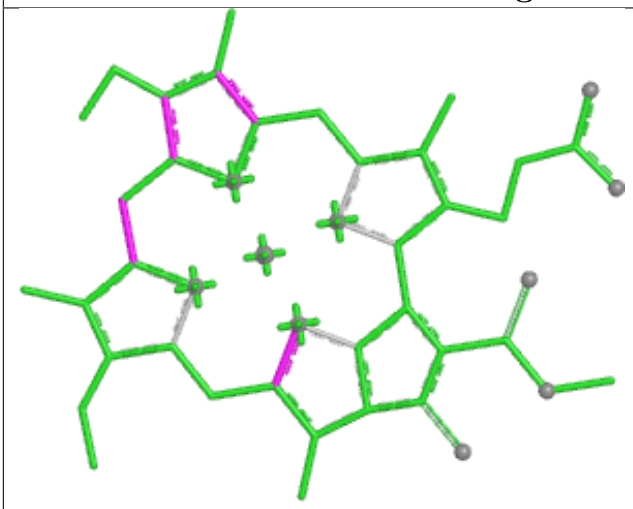


Torsions



Rings

Ligand CLA T 4002



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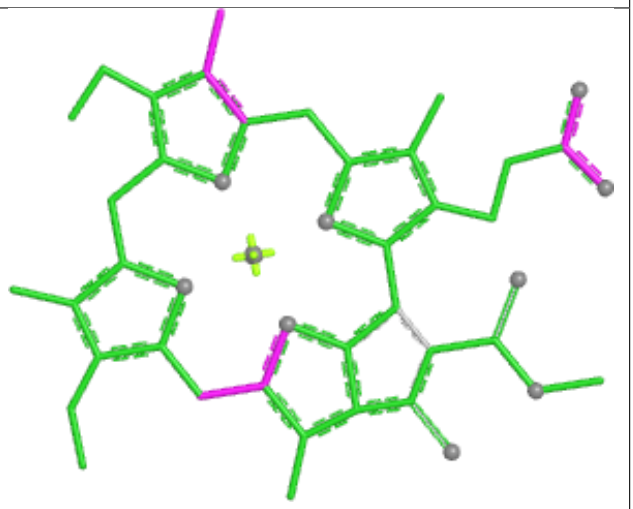
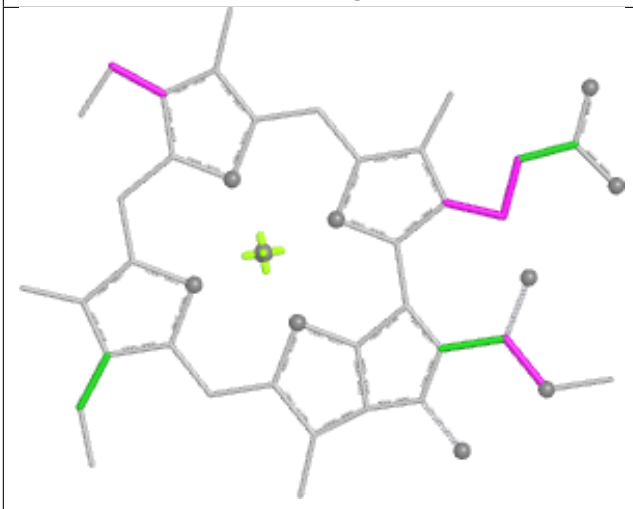


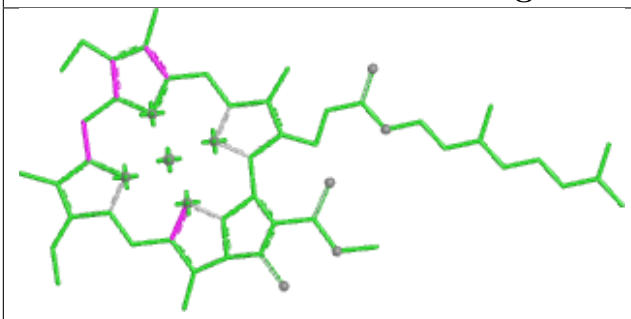
Bond angles



Torsions

Rings

Ligand CLA B 1012



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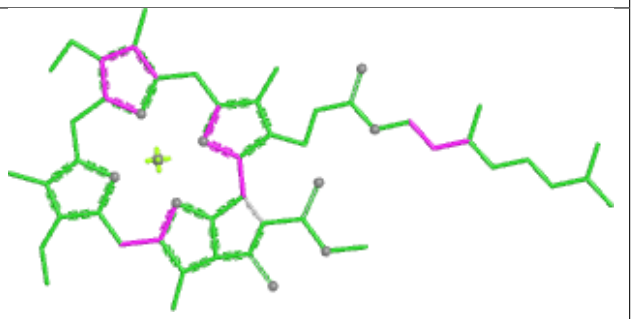

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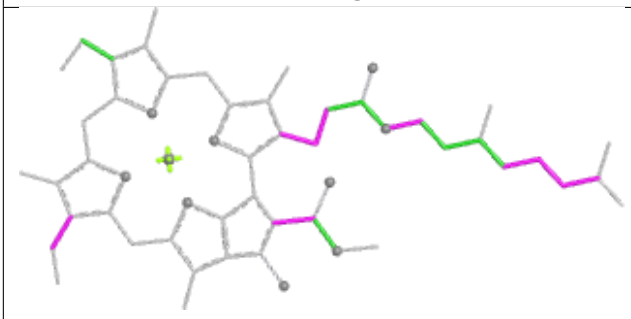

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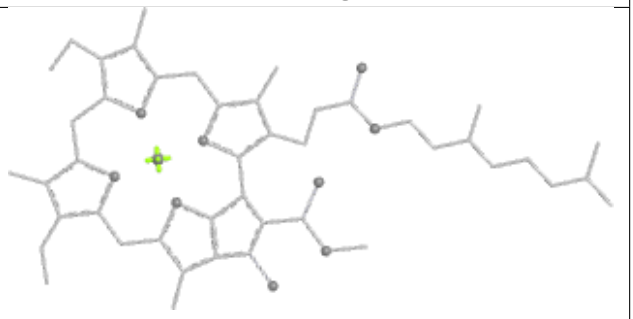
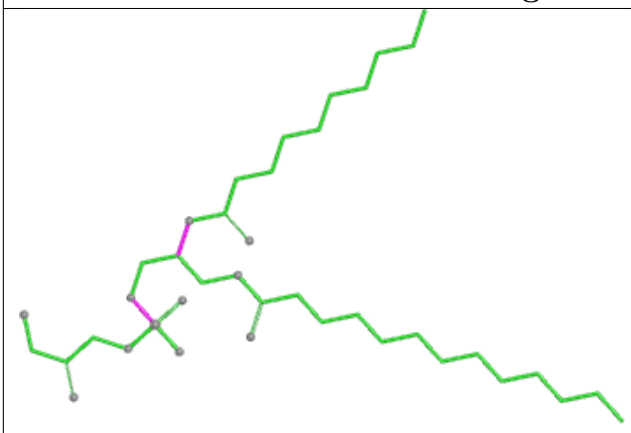


Rings

Ligand LHG R 103



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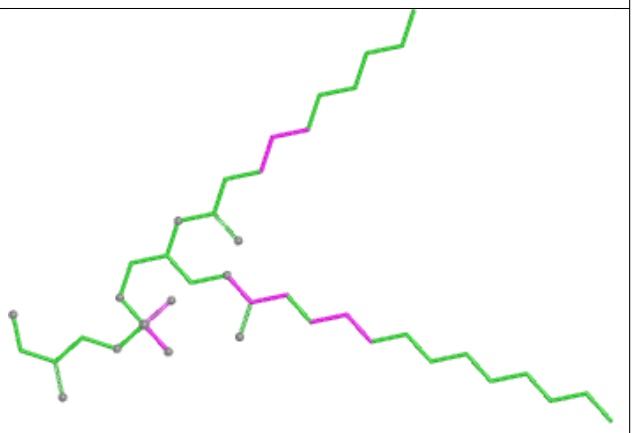
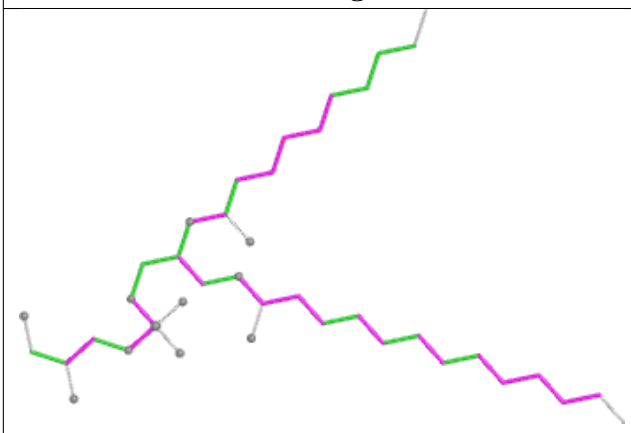


Bond angles



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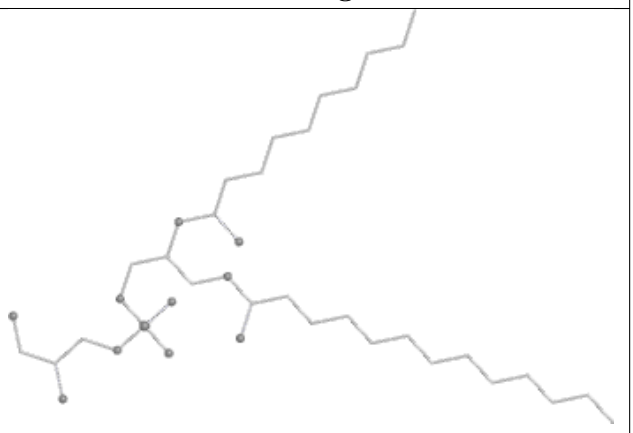
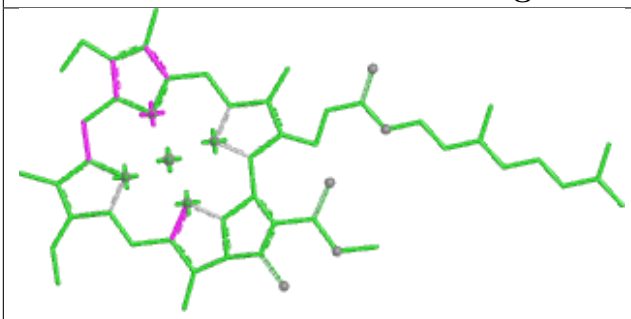


Rings

Ligand CLA G 1213



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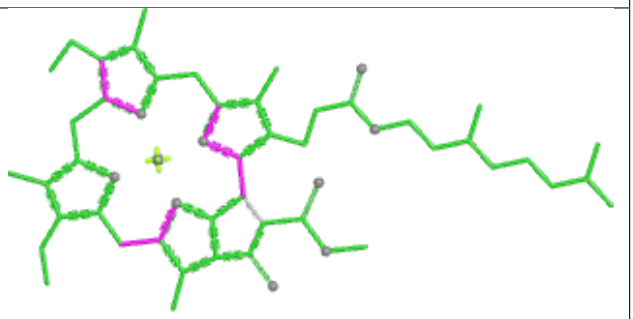

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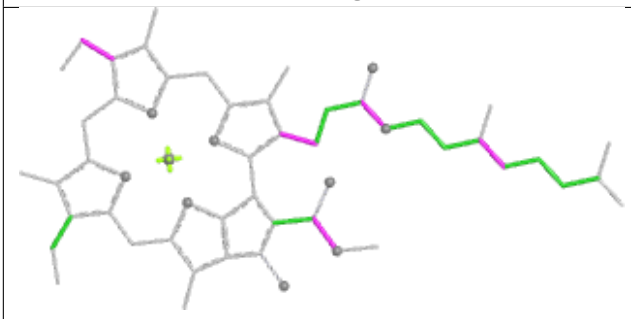

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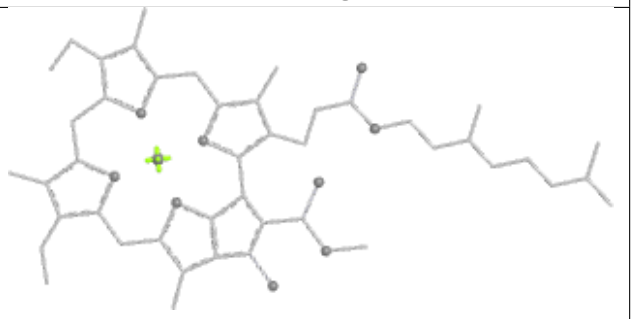
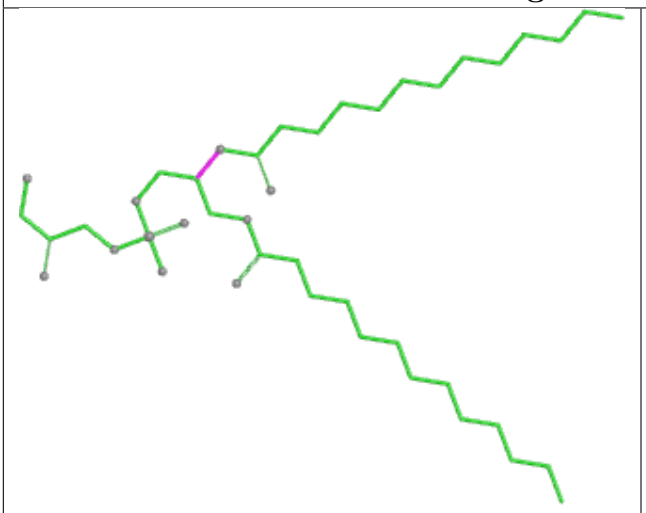


Rings

Ligand LHG a 849



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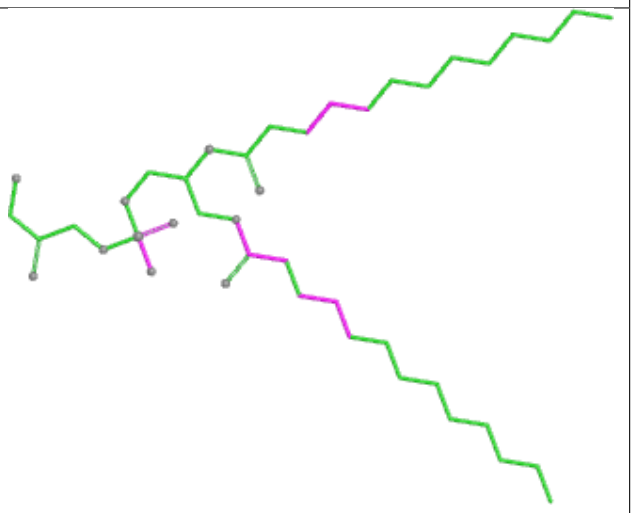
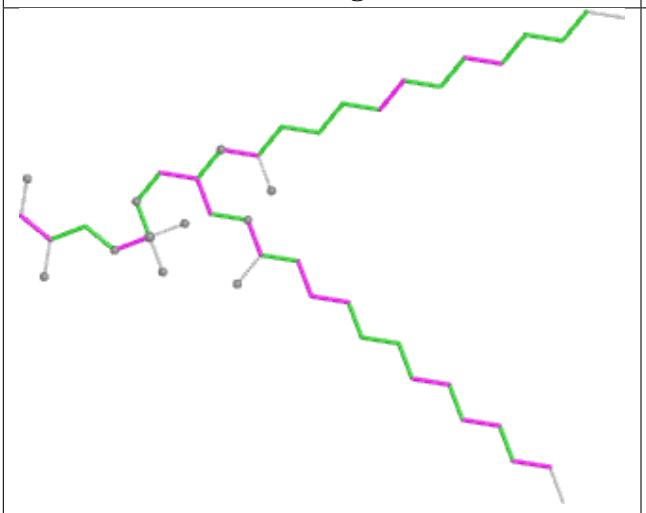


Bond angles



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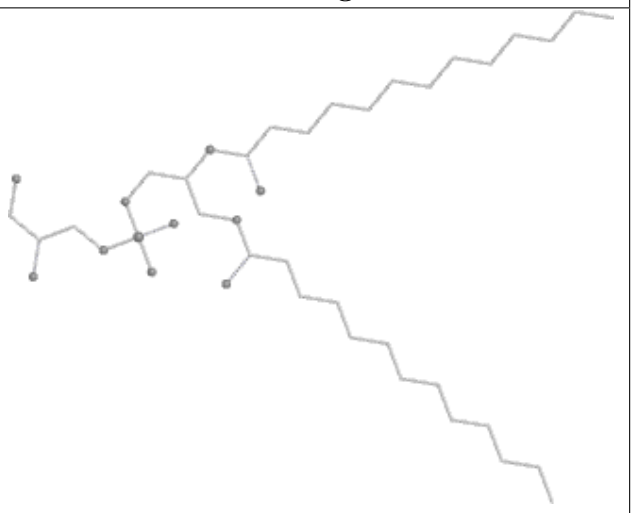
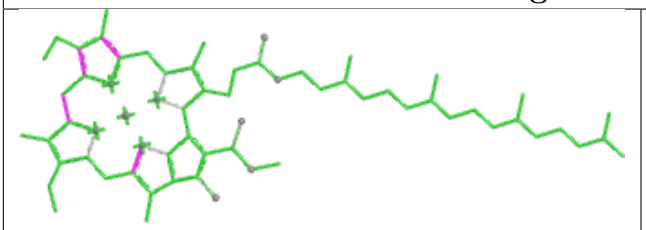


Rings

Ligand CLA s 504



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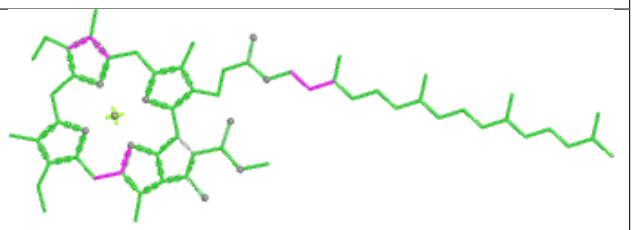
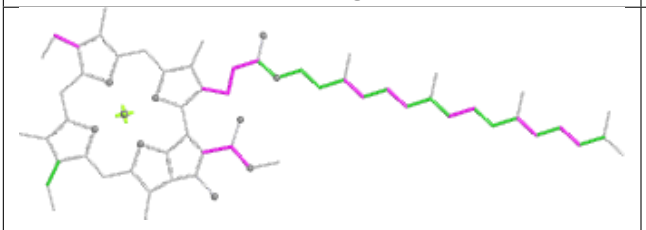


Bond angles



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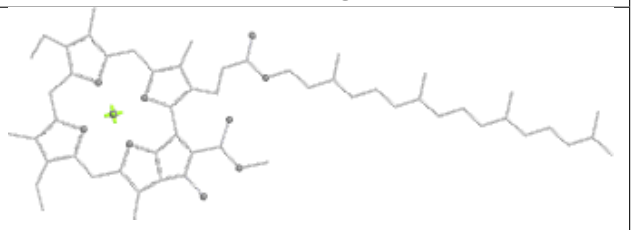
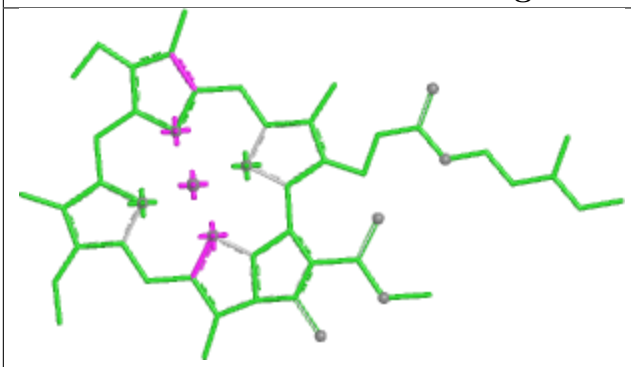


Rings

Ligand CLA H 1135



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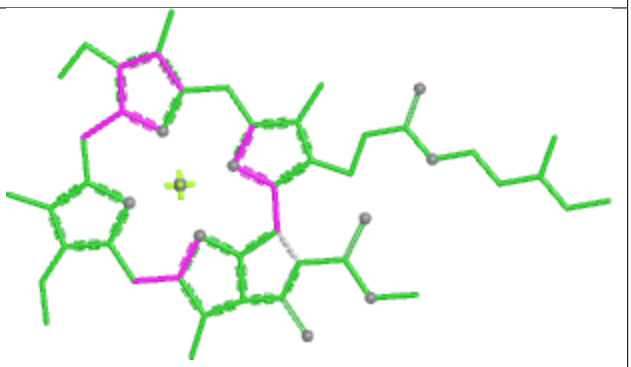
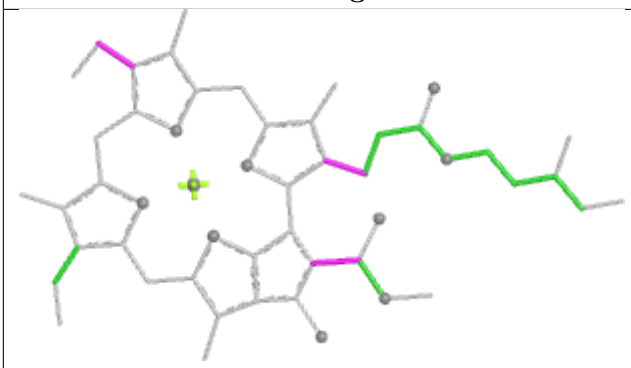


Bond angles



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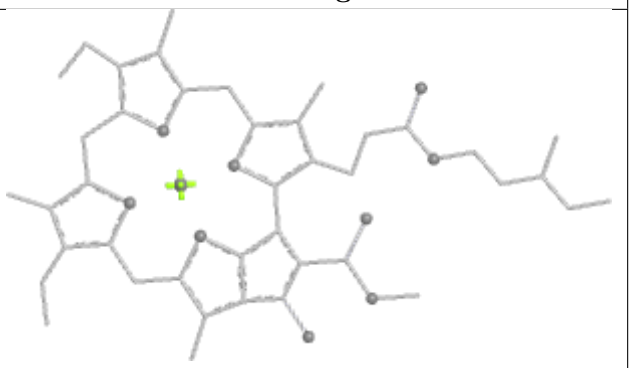
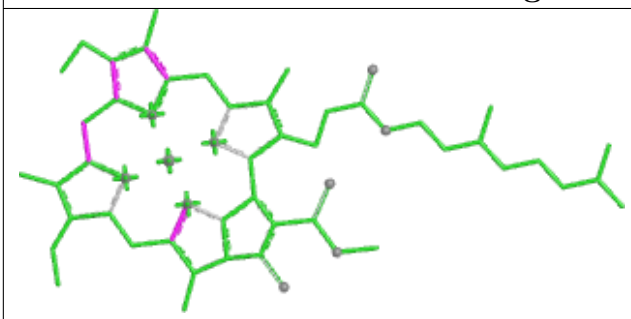


Rings

Ligand CLA Y 517



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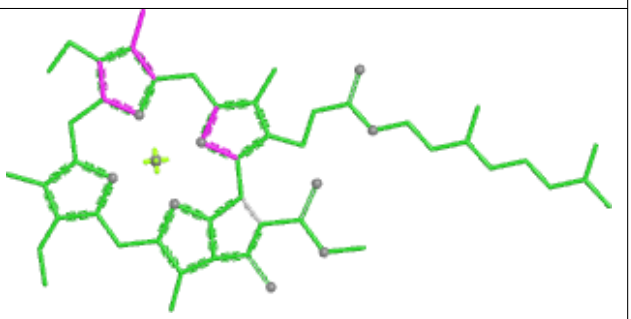
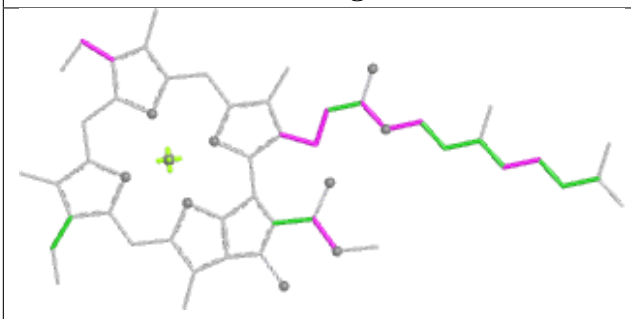
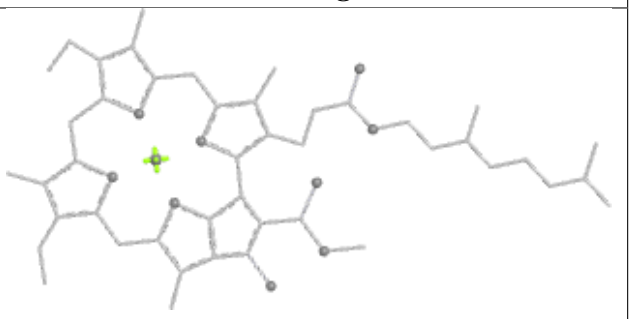


Bond angles

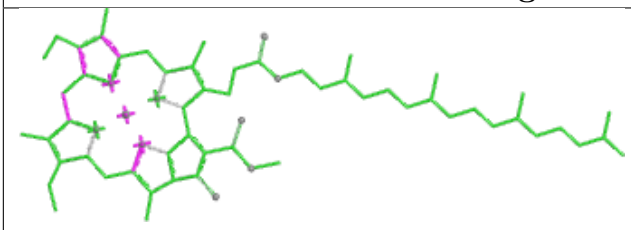


Torsions



Rings

Ligand CLA b 1225



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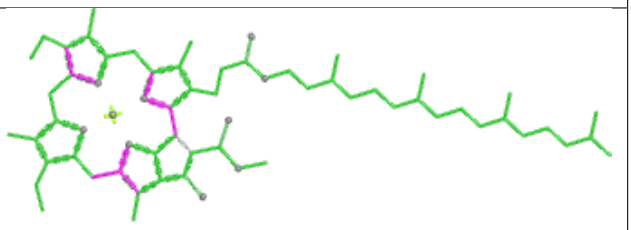
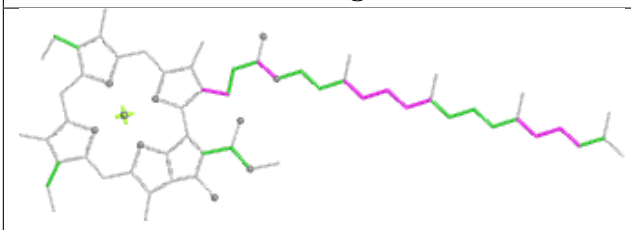


Bond angles



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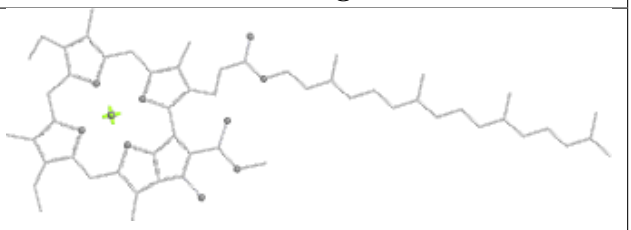
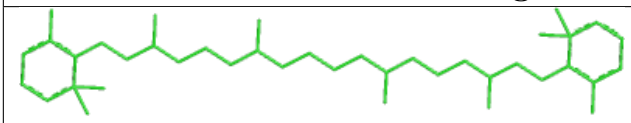


Rings

Ligand BCR H 4003



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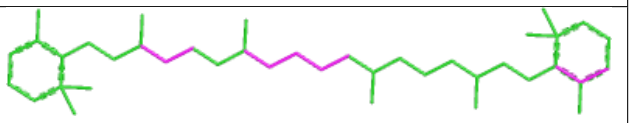
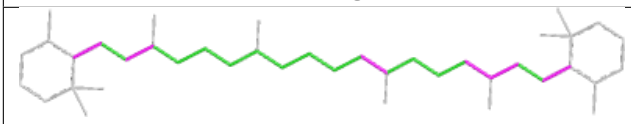
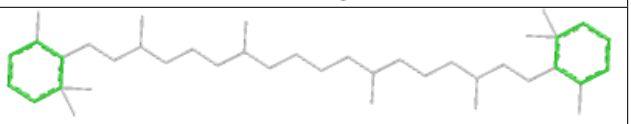


Bond angles

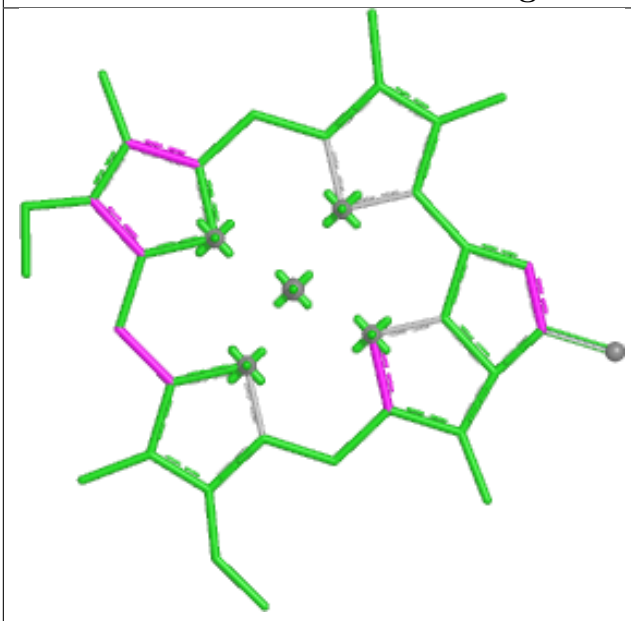


Torsions



Rings

Ligand CLA J 1303



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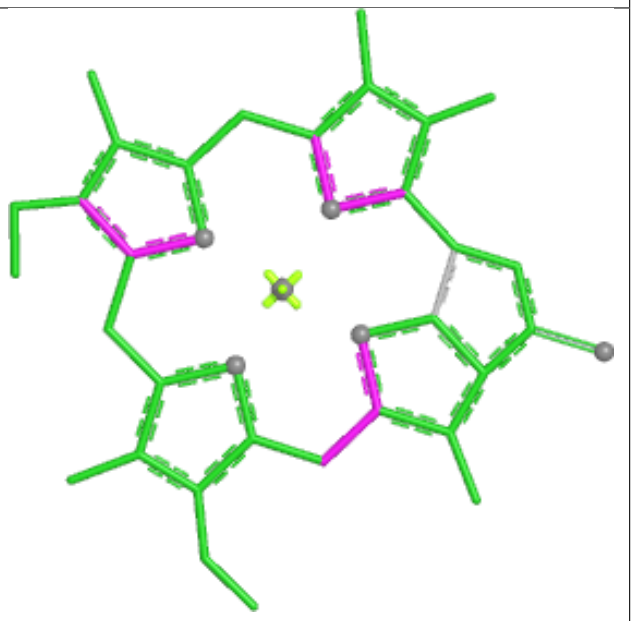
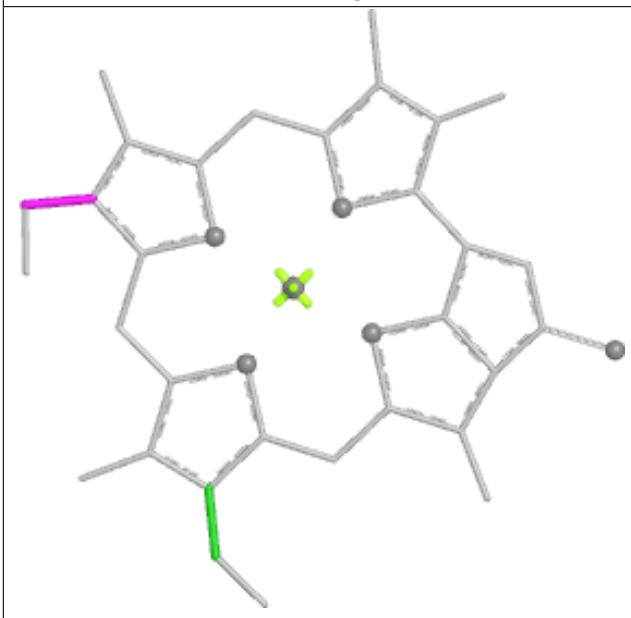
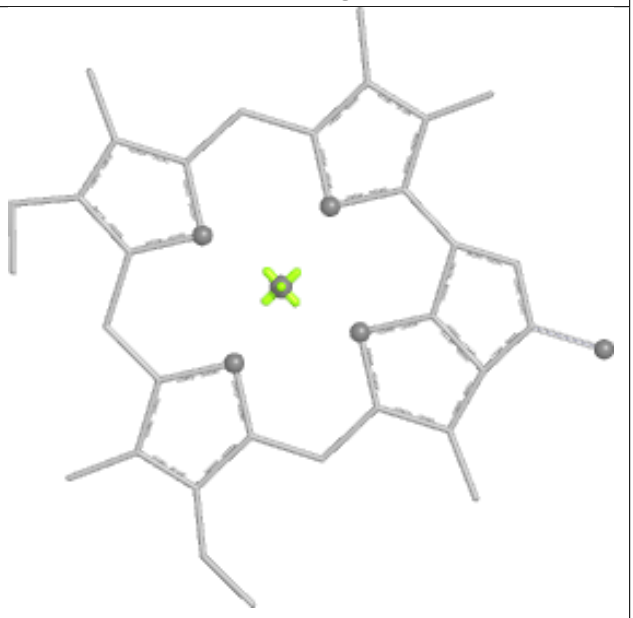


Bond angles

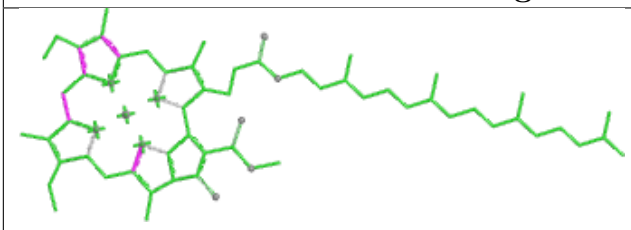


Torsions



Rings

Ligand CLA H 1123



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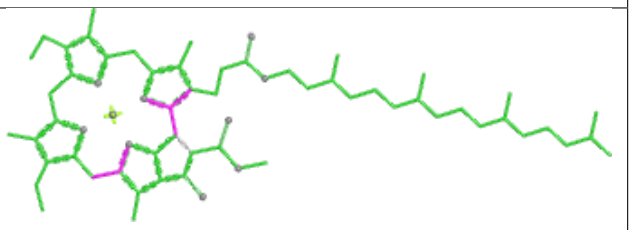
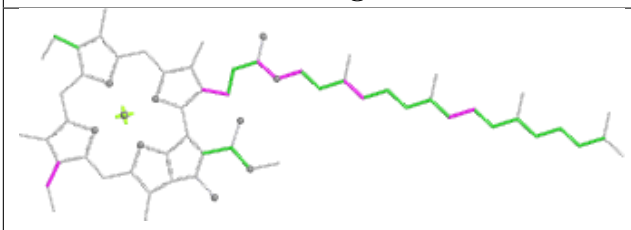
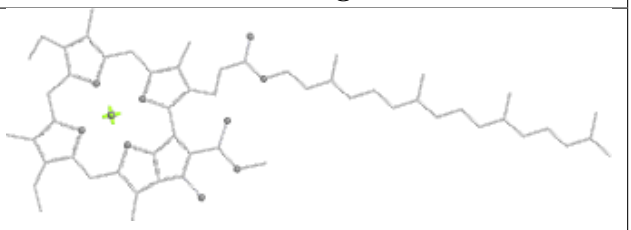


Bond angles

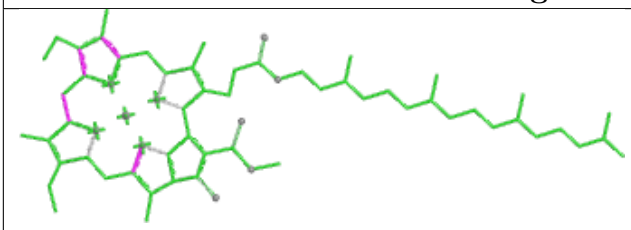


Torsions



Rings

Ligand CLA t 510



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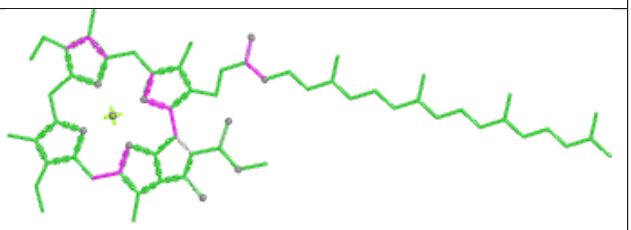
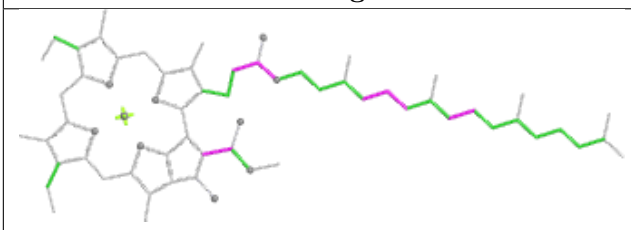
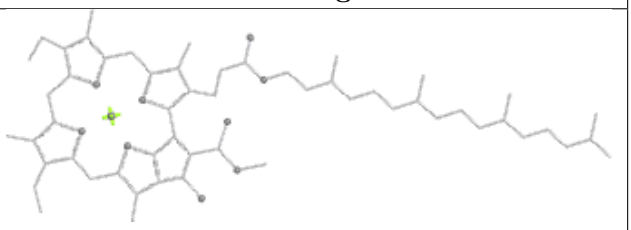


Bond angles

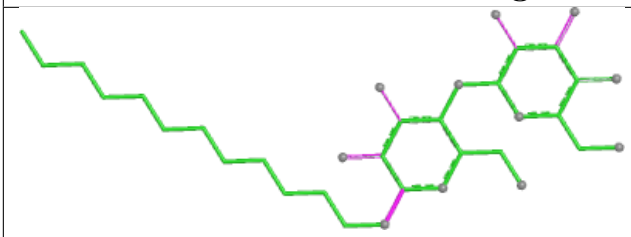


Torsions

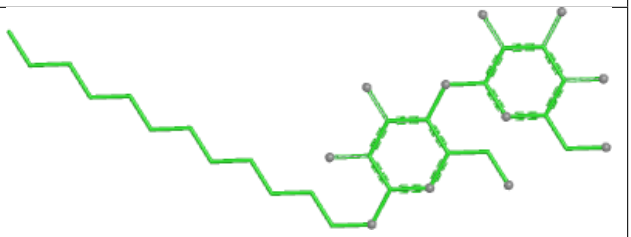


Rings

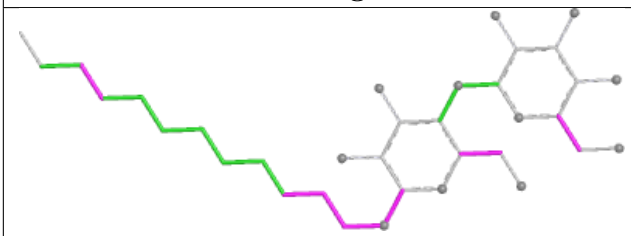
Ligand LMT H 4202



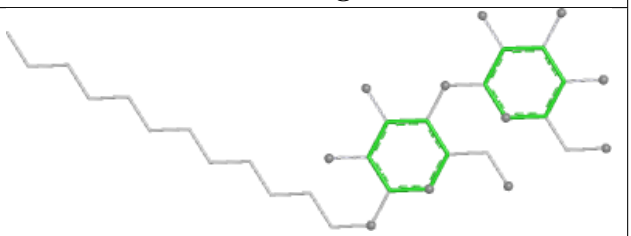
Bond lengths



Bond angles

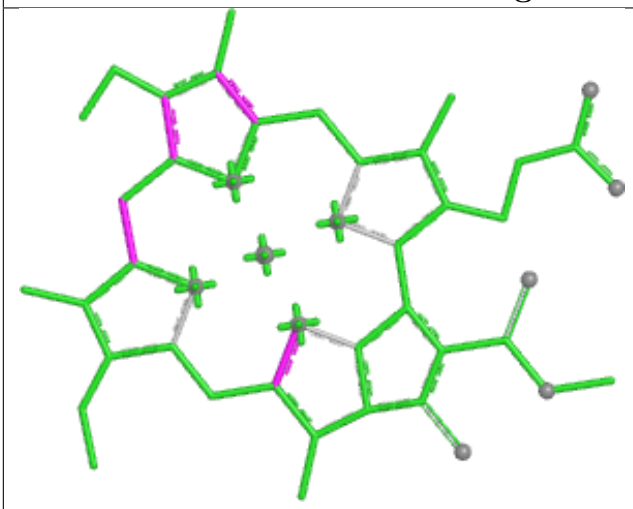


Torsions



Rings

Ligand CLA A 1113



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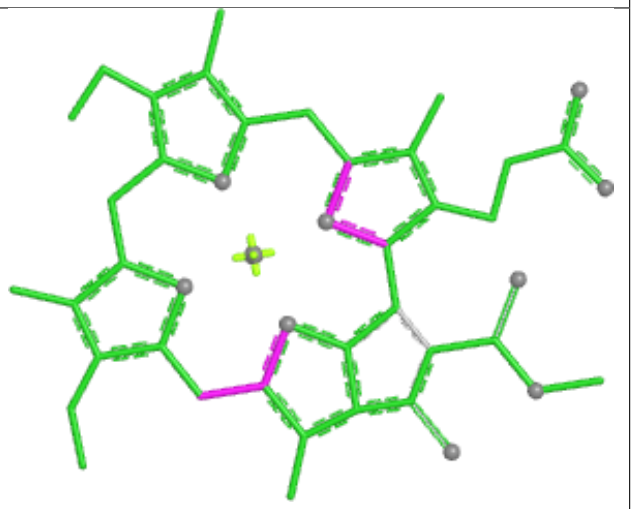
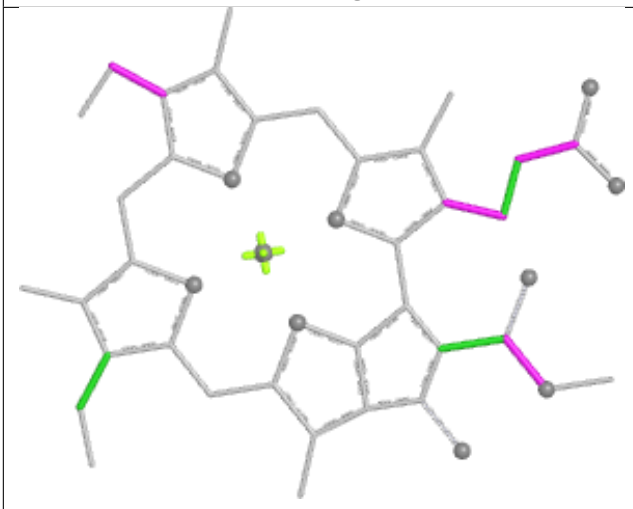


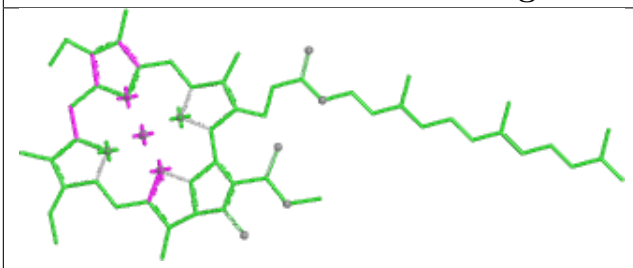
Bond angles



Torsions

Rings

Ligand CLA b 1224



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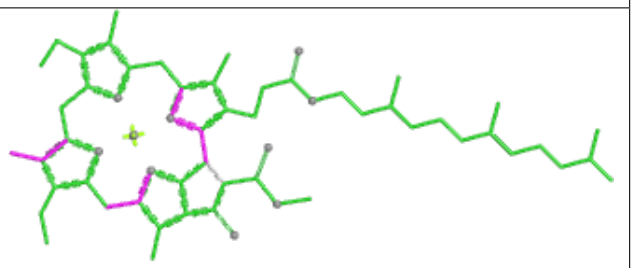
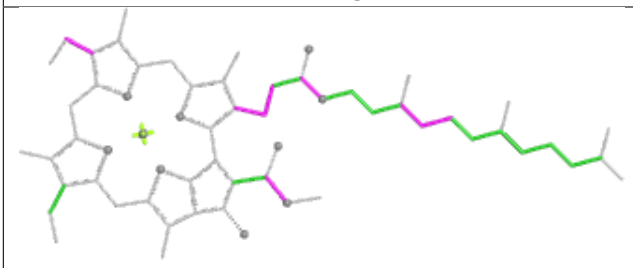
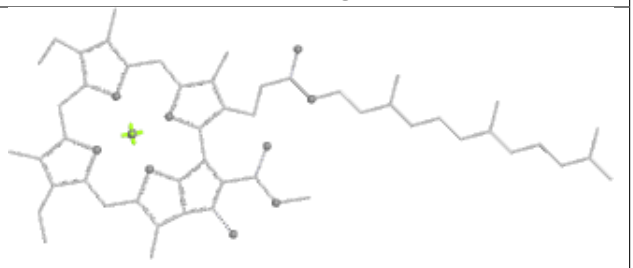


Bond angles

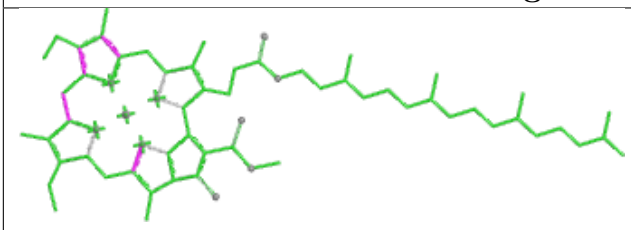


Torsions



Rings

Ligand CLA Y 515



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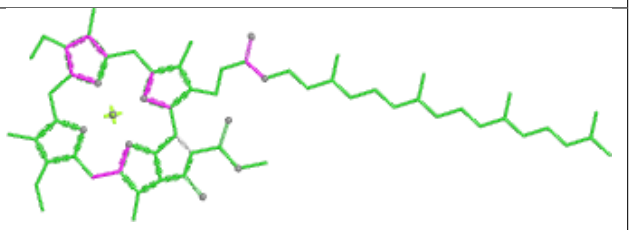
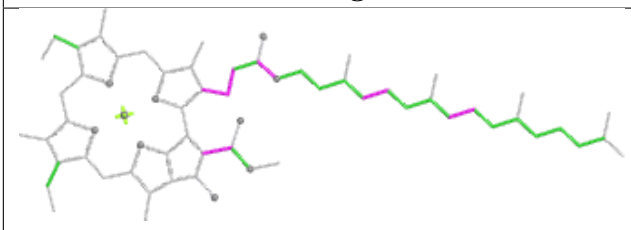
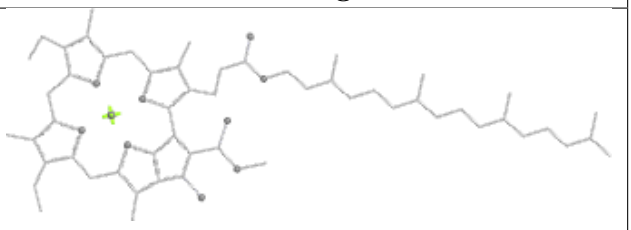


Bond angles

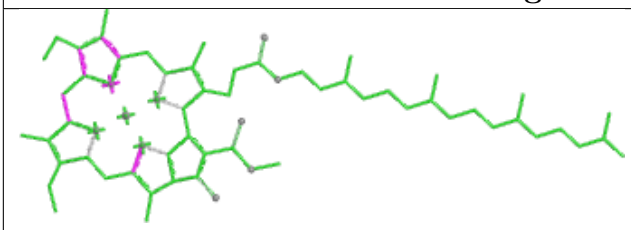


Torsions



Rings

Ligand CLA w 511



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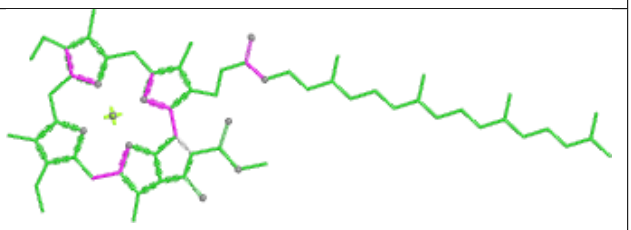
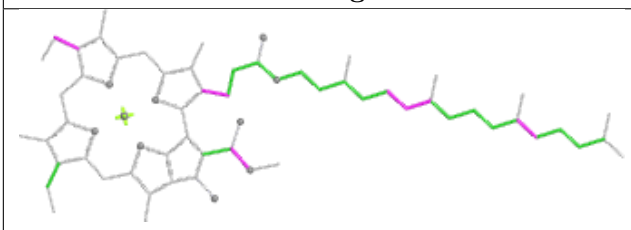


Bond angles



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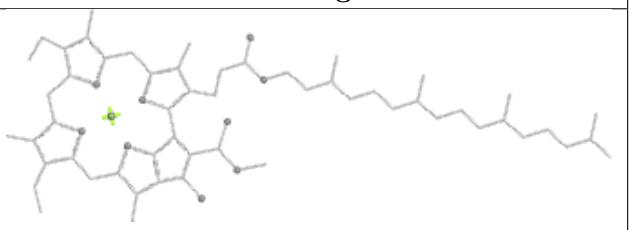
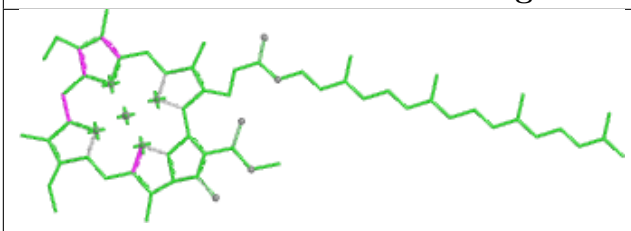


Rings

Ligand CLA B 1238



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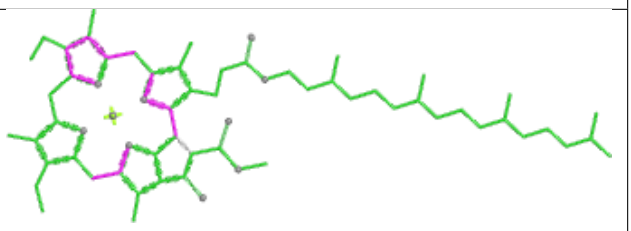
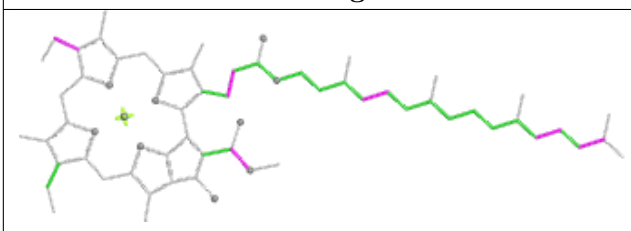


Bond angles



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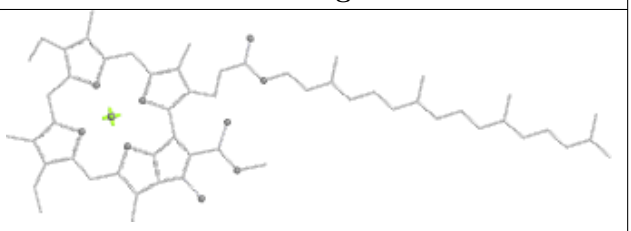
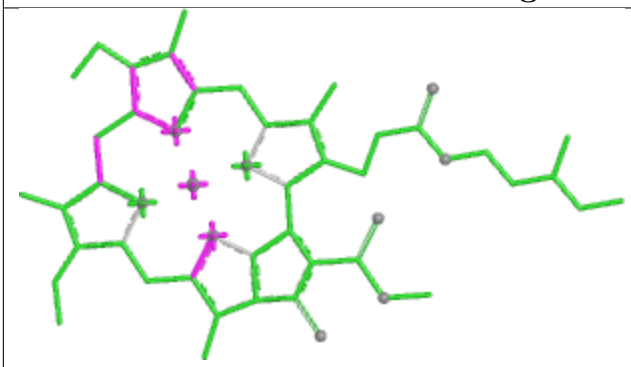


Rings

Ligand CLA a 1135



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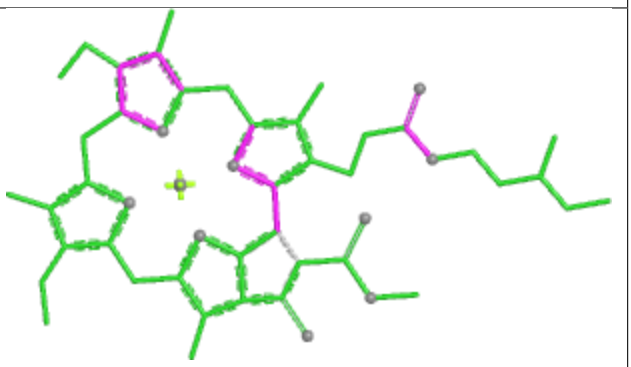
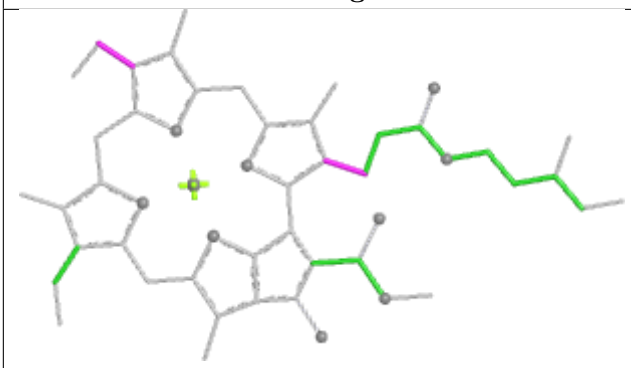
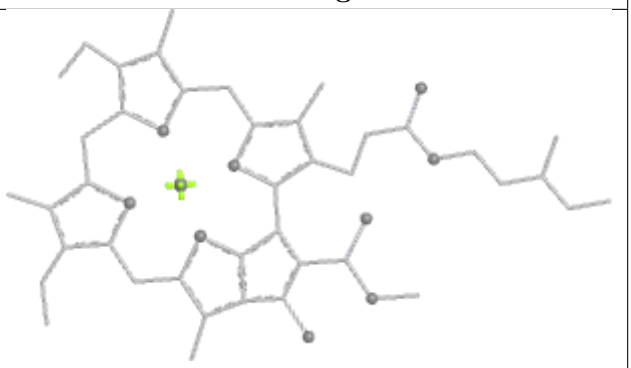


Bond angles

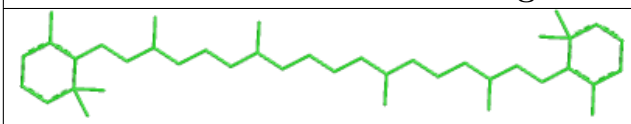


Torsions



Rings

Ligand BCR a 4002



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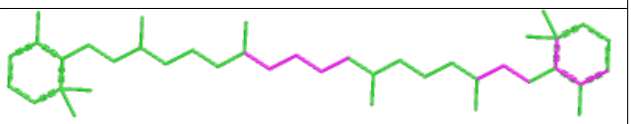
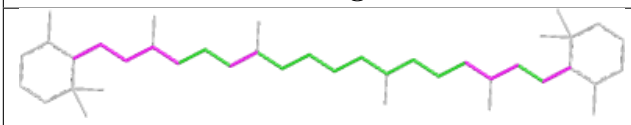
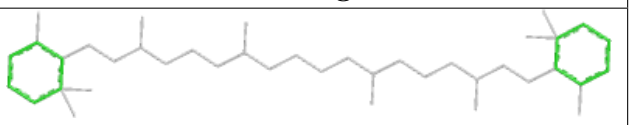


Bond angles

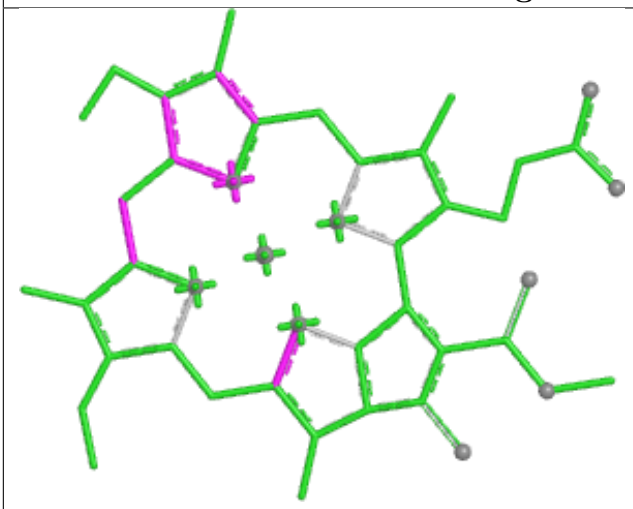


Torsions

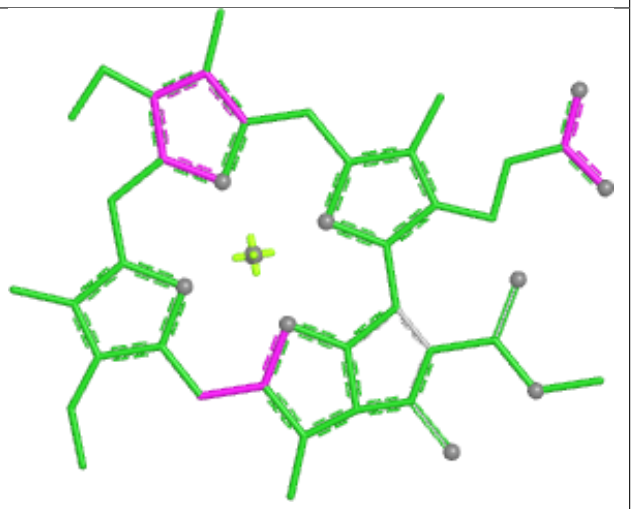


Rings

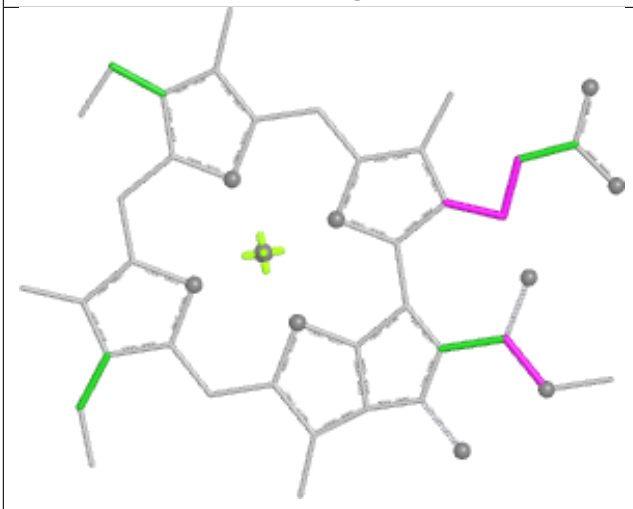
Ligand CLA B 1219



Bond lengths



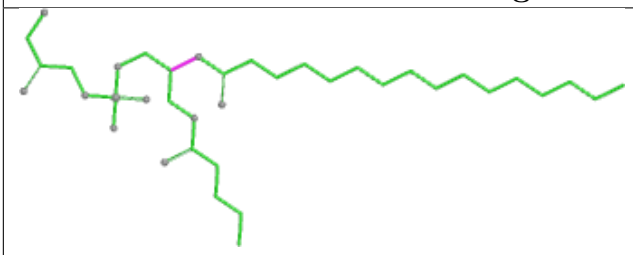
Bond angles



Torsions

Rings

Ligand LHG G 4018



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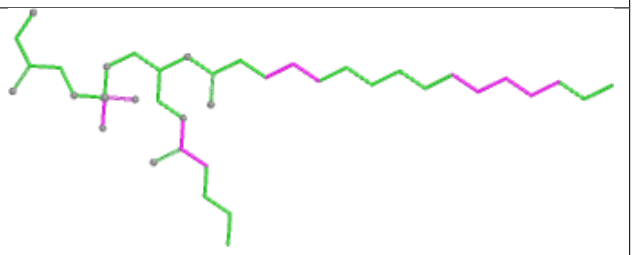
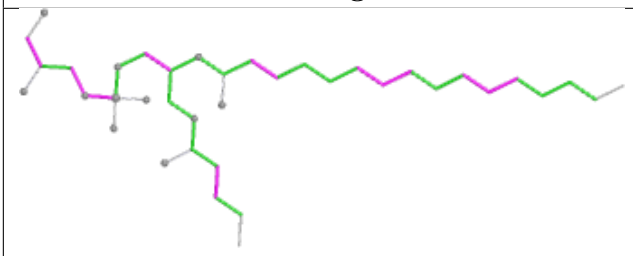
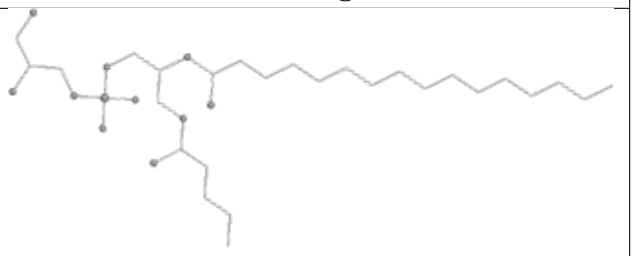


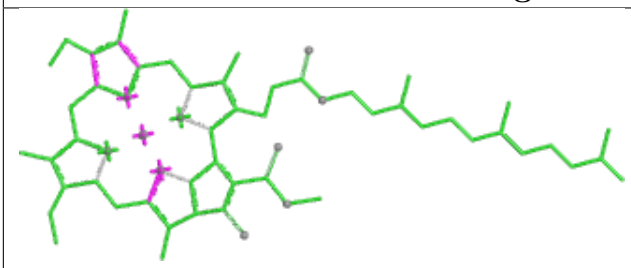
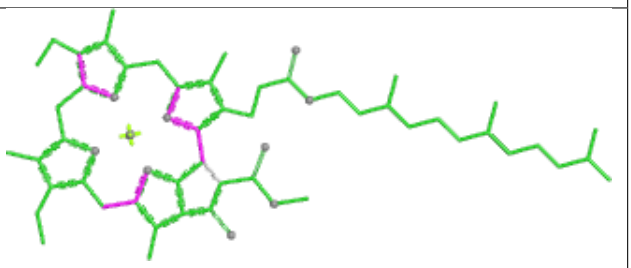
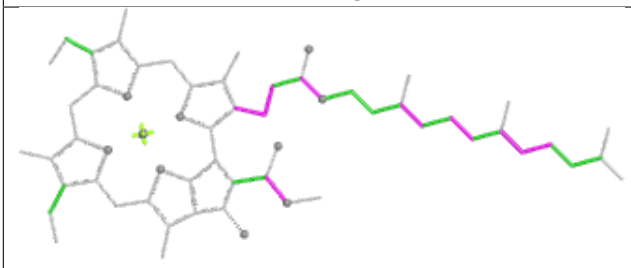
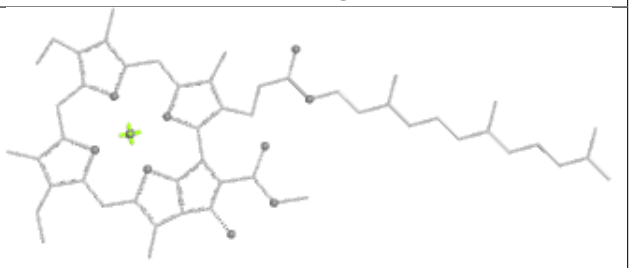
Bond angles

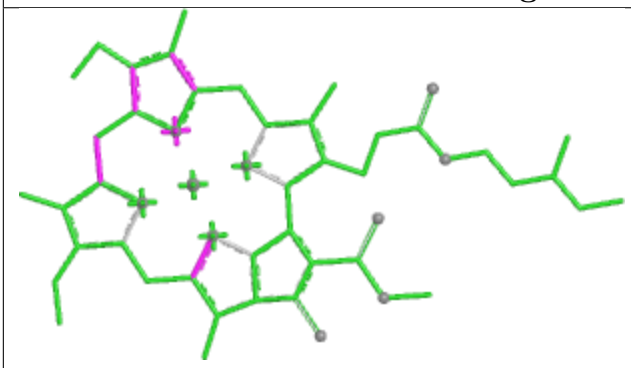
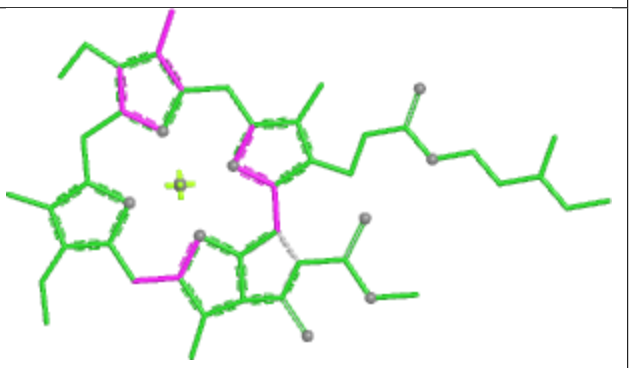
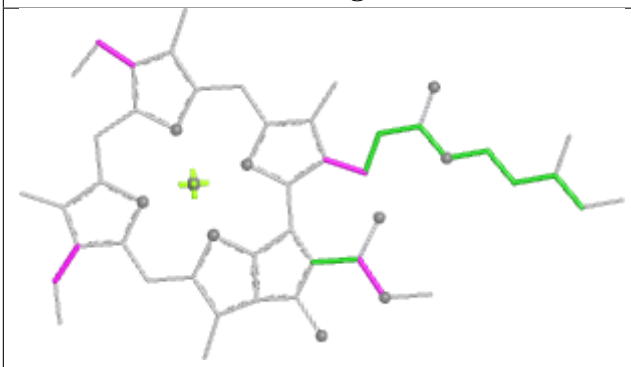
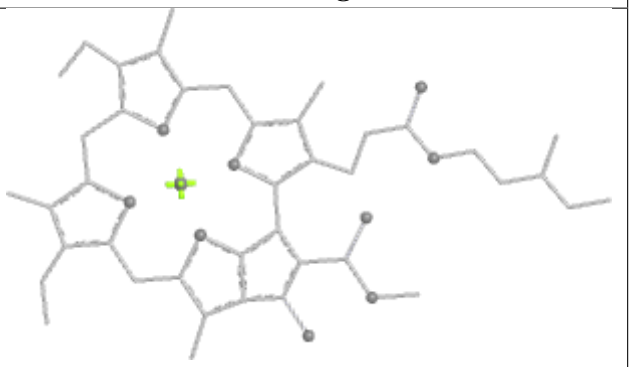


Torsions

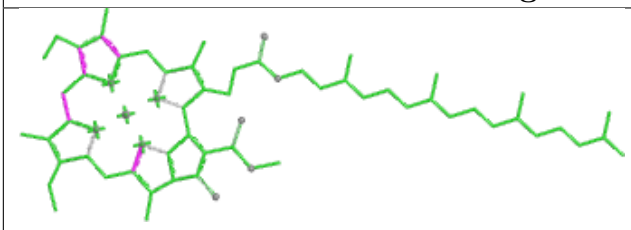


Rings

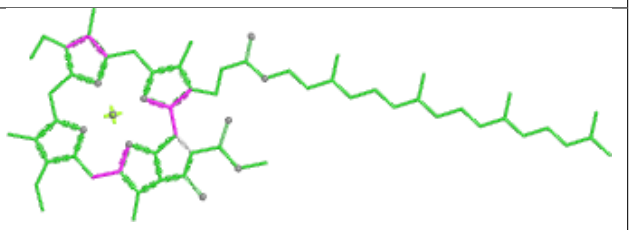
Ligand CLA G 1224	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1121	
	
Bond lengths	Bond angles
	
Torsions	Rings

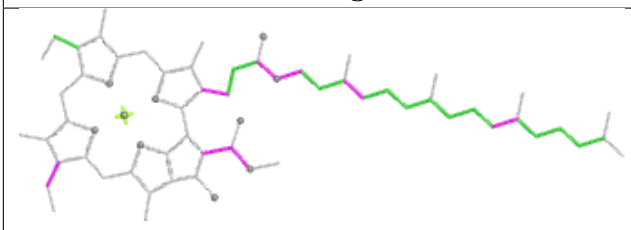
Ligand CLA a 1123



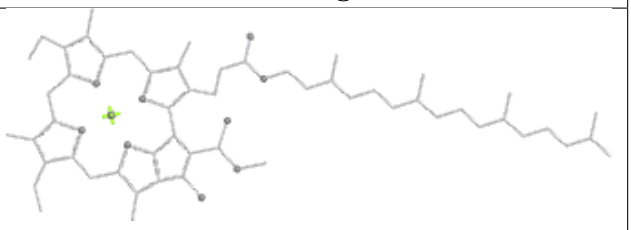
Bond lengths



Bond angles

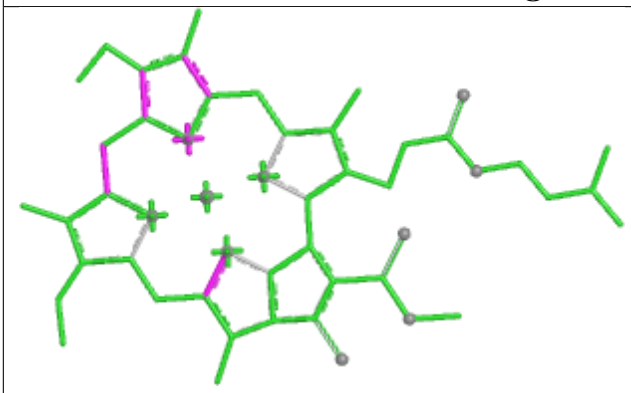


Torsions

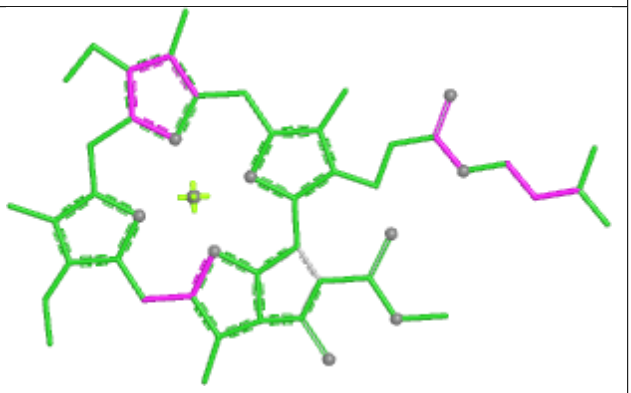


Rings

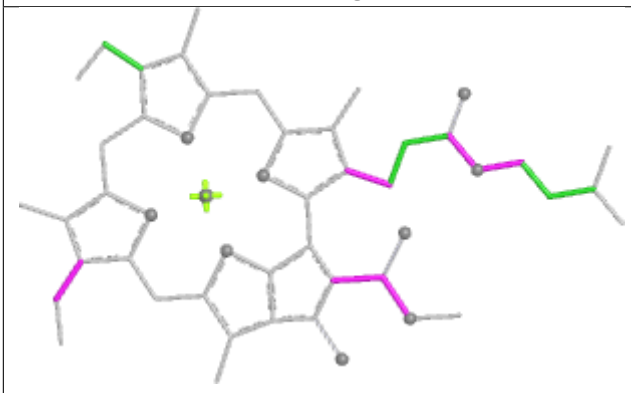
Ligand CLA w 501



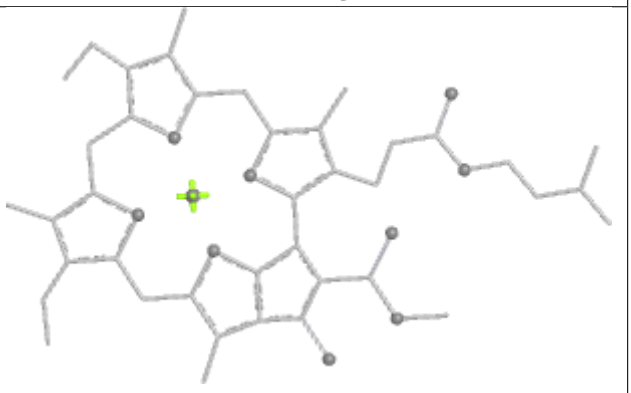
Bond lengths



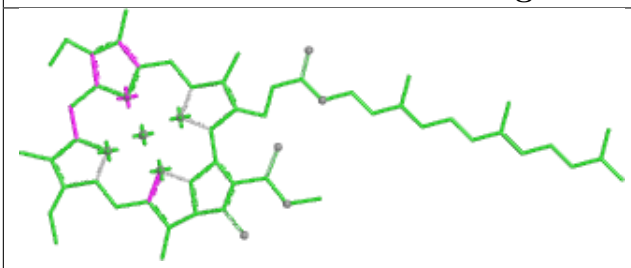
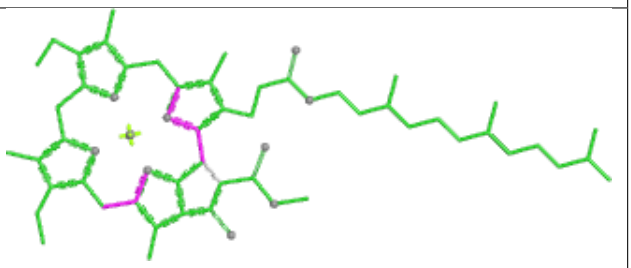
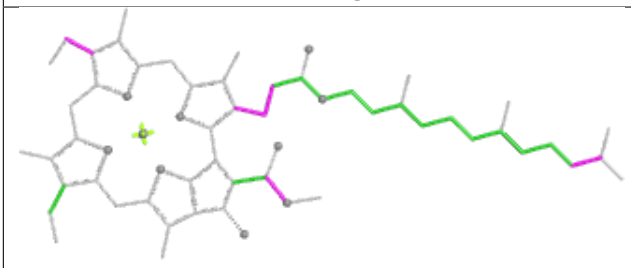
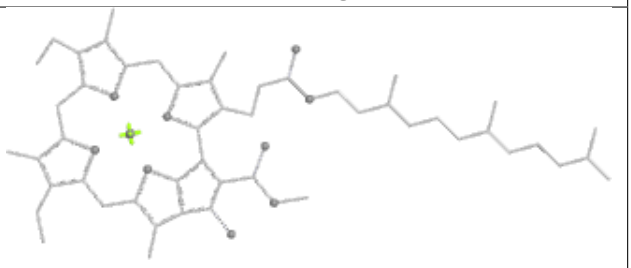
Bond angles

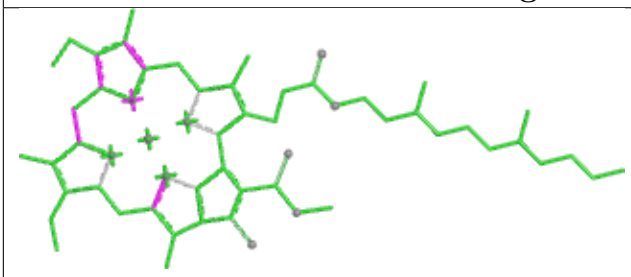
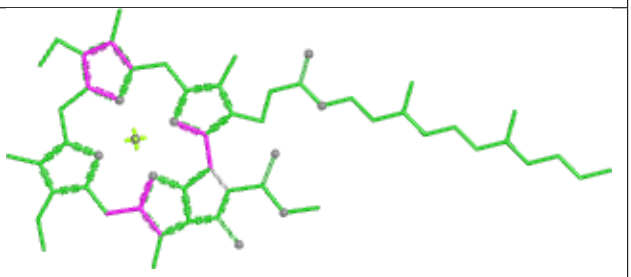
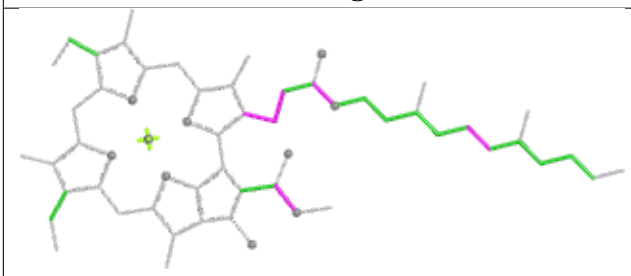
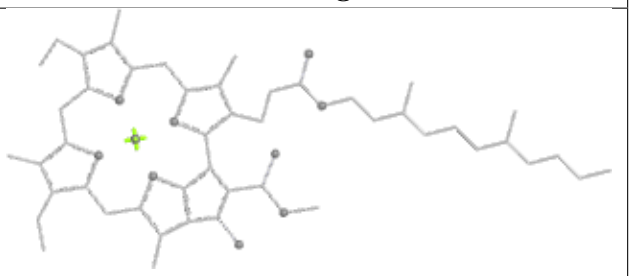


Torsions

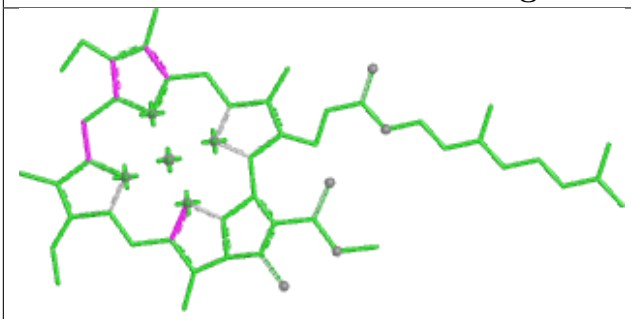


Rings

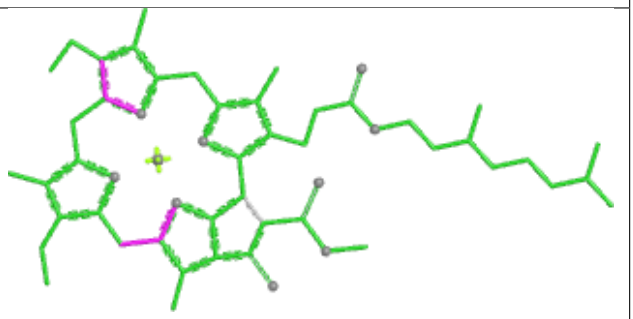
Ligand CLA B 1215	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1105	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1118



Bond lengths



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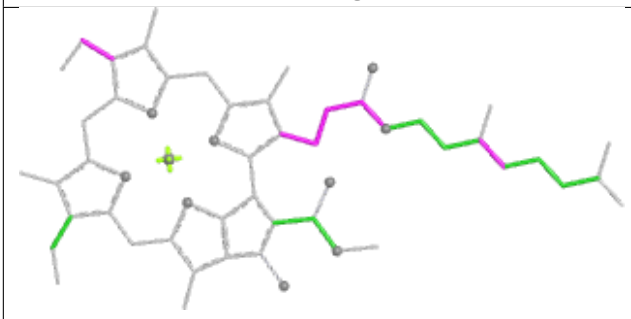
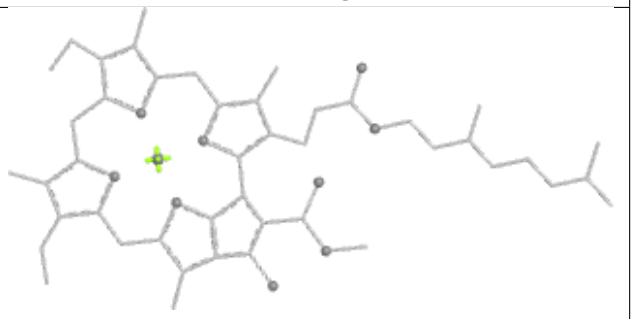
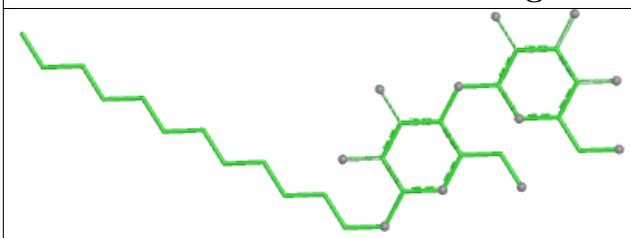


Torsions



Rings

Ligand LMU r 606



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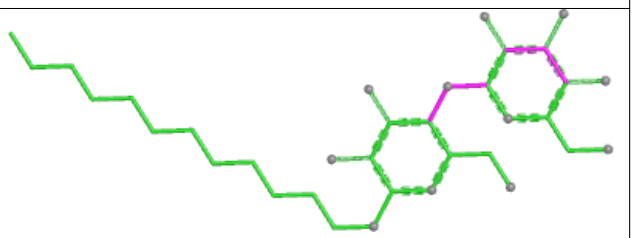

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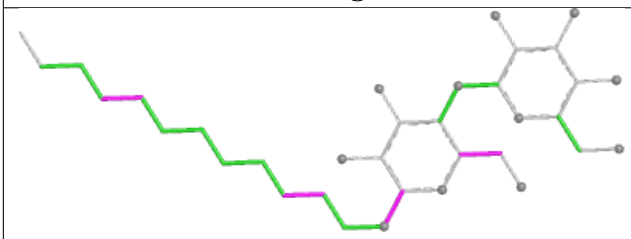

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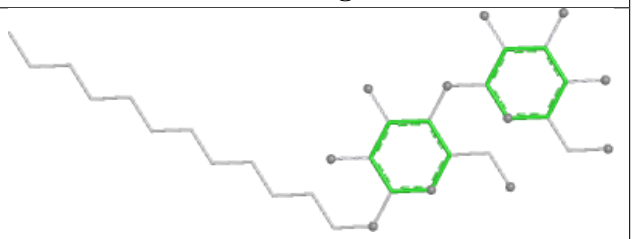
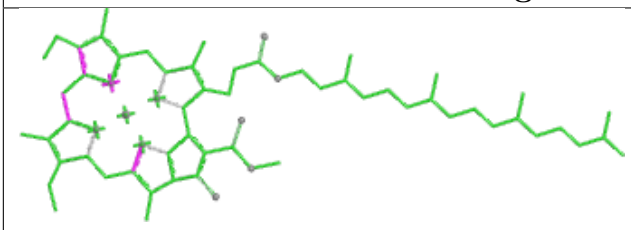


Rings

Ligand CLA A 1119



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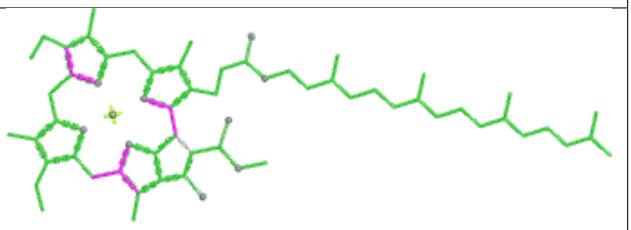
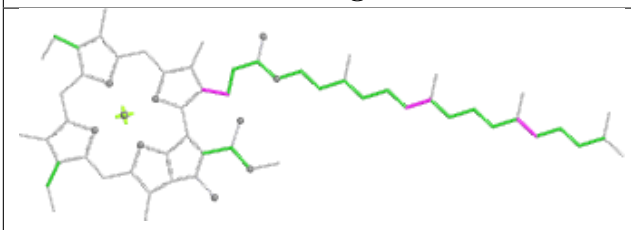


Bond angles



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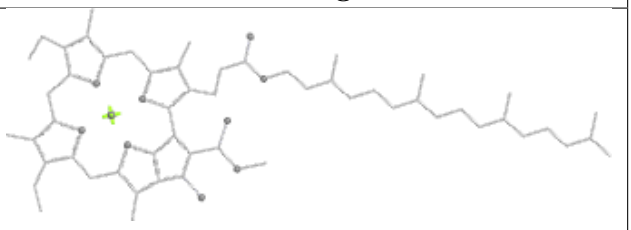
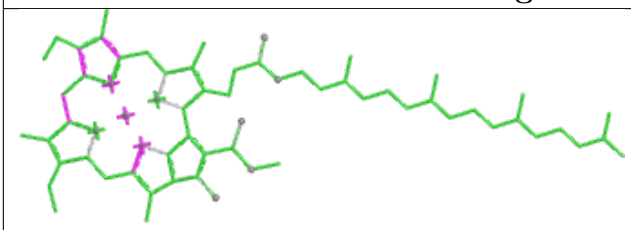


Rings

Ligand CLA B 1225



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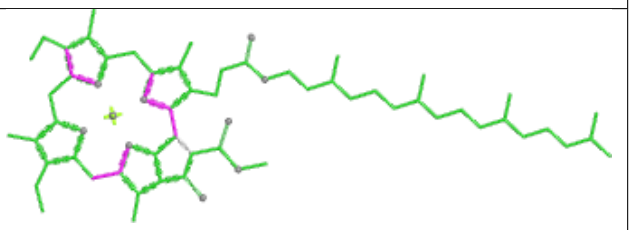
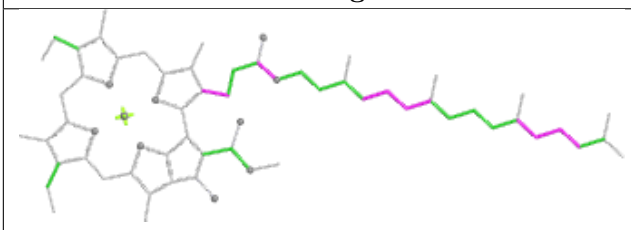


Bond angles



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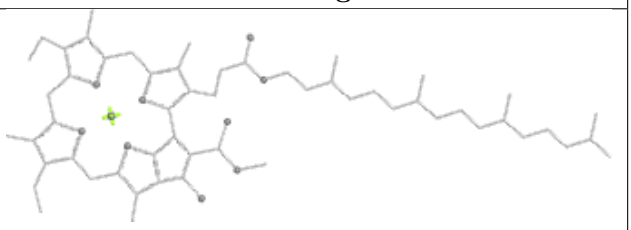
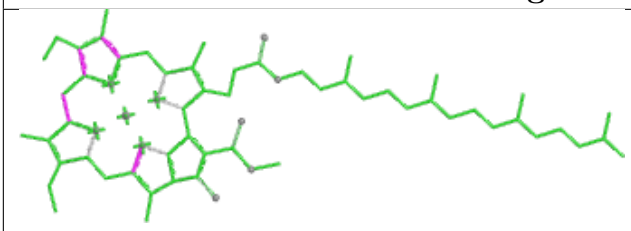


Rings

Ligand CLA p 511



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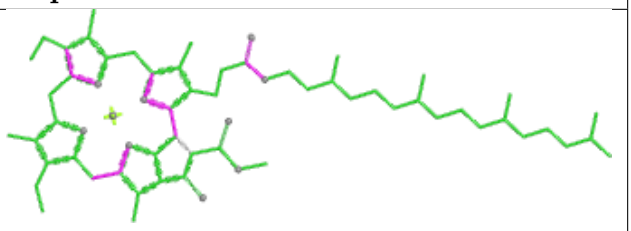

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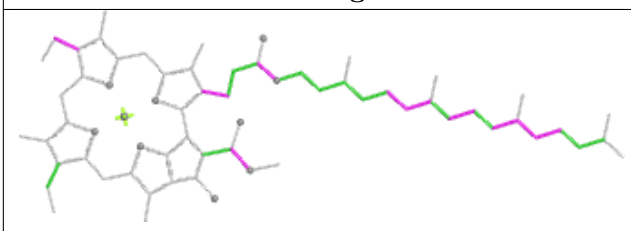

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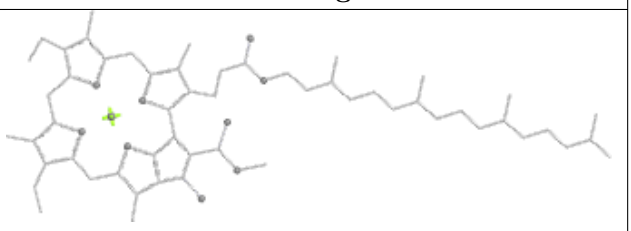
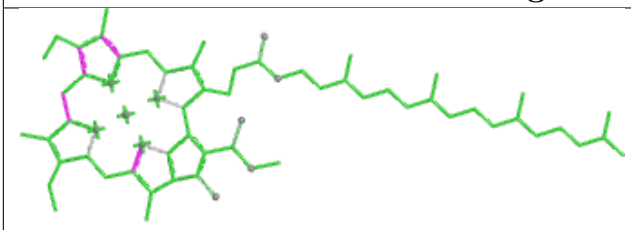


Rings

Ligand CLA p 515



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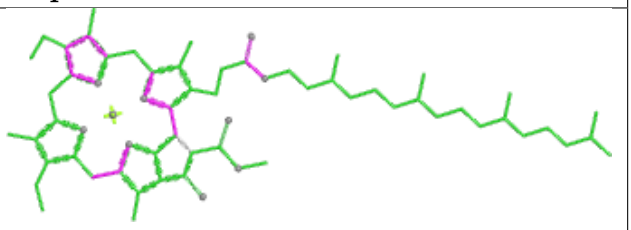

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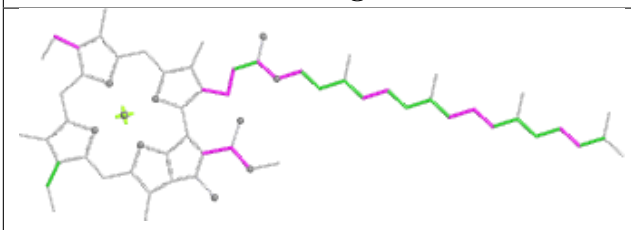

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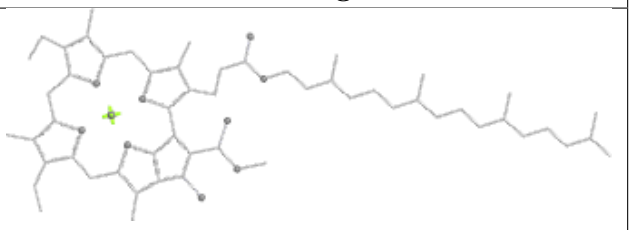
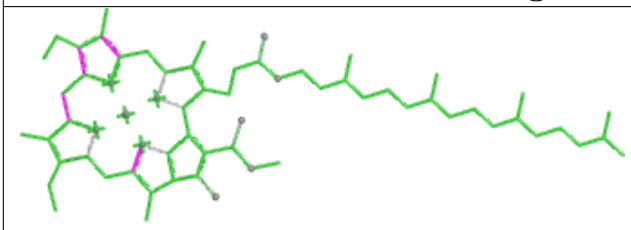


Rings

Ligand CLA q 507



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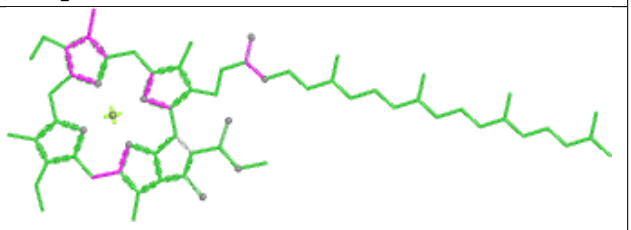
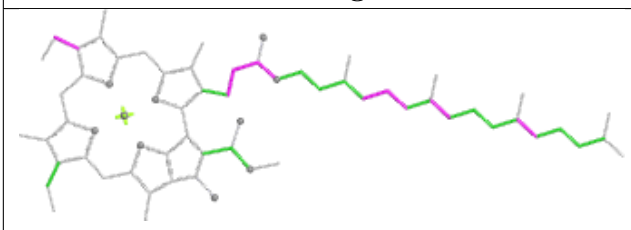
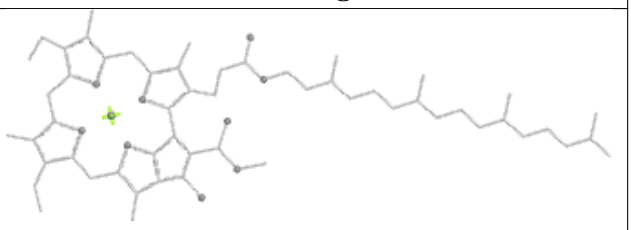


Bond angles

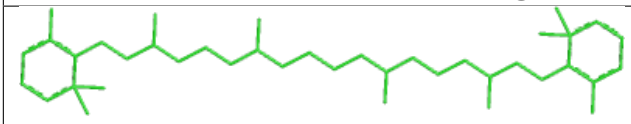


Torsions

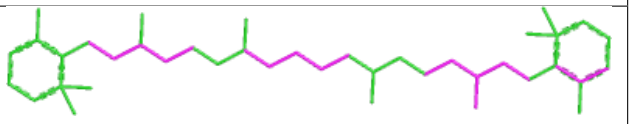


Rings

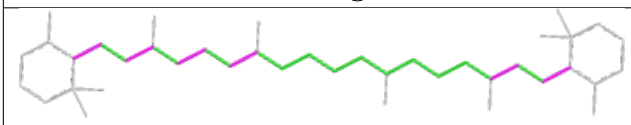
Ligand BCR U 4019



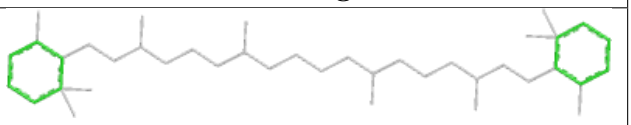
Bond lengths



Bond angles

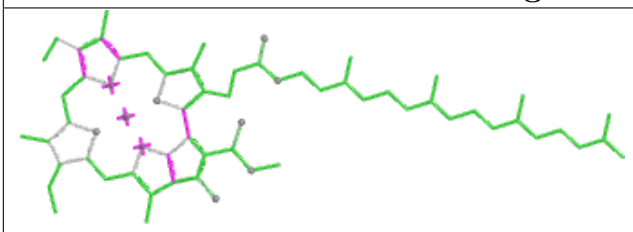


Torsions



Rings

Ligand CL0 a 1011



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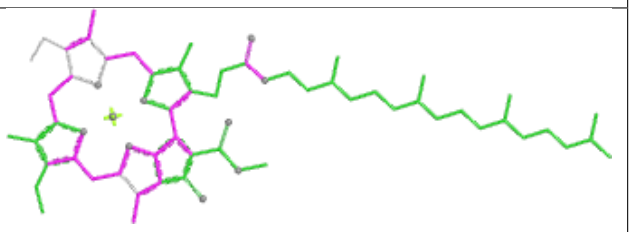
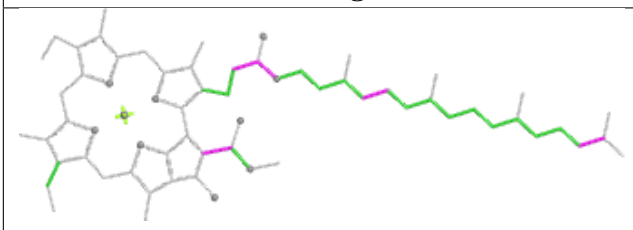
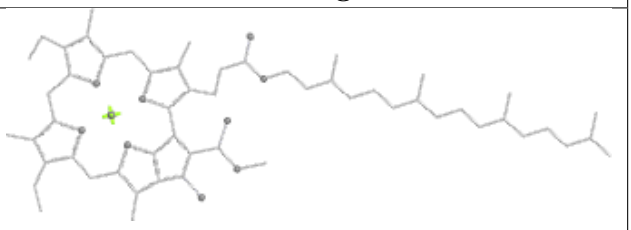


Bond angles

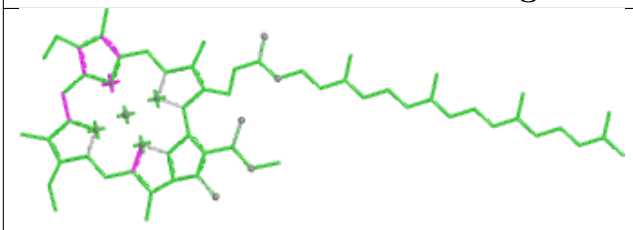


Torsions

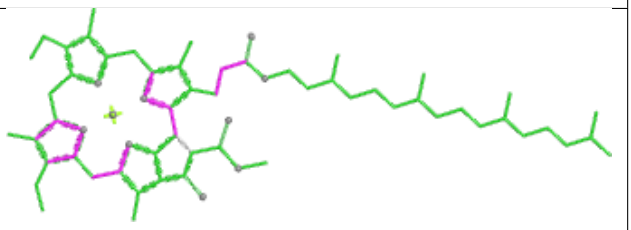


Rings

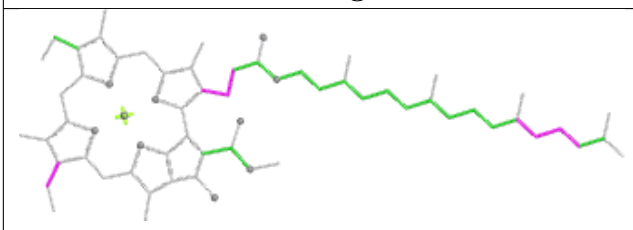
Ligand CLA a 1022



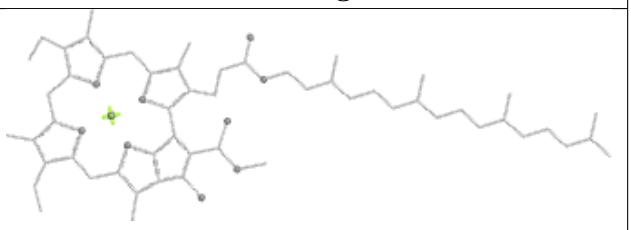
Bond lengths



Bond angles

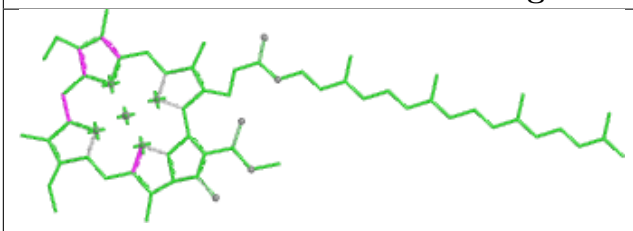


Torsions



Rings

Ligand CLA p 504



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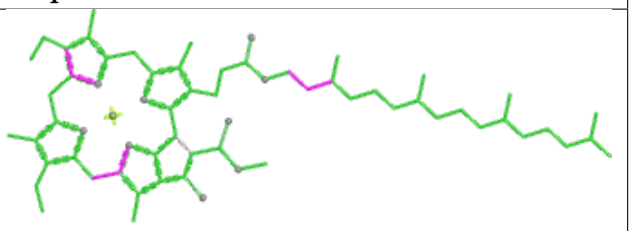
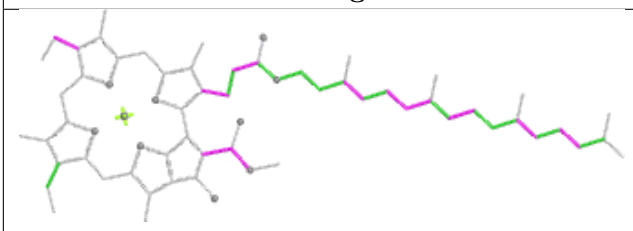
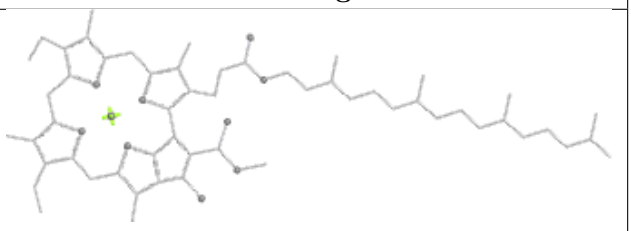


Bond angles

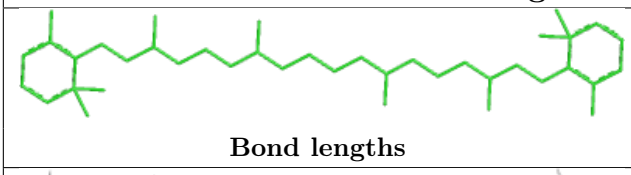


Torsions

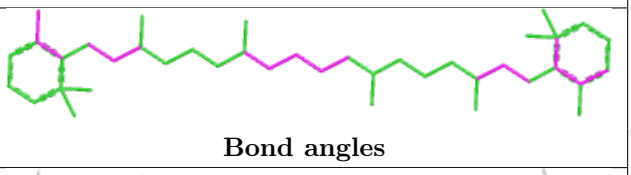


Rings

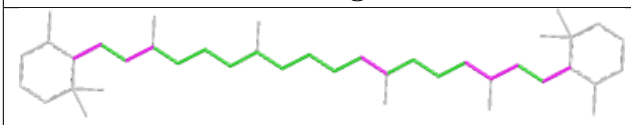
Ligand BCR s 601



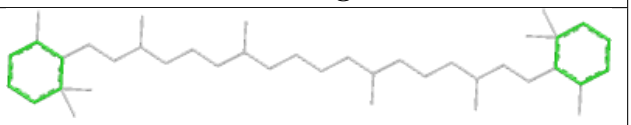
Bond lengths



Bond angles

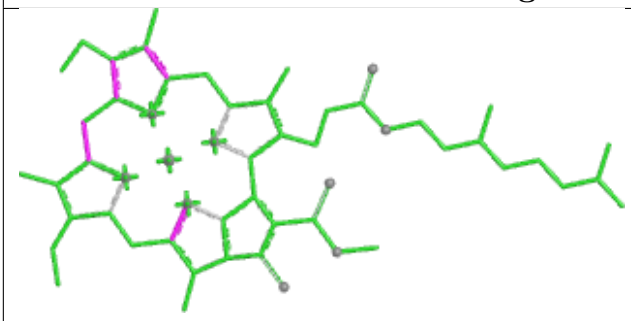


Torsions

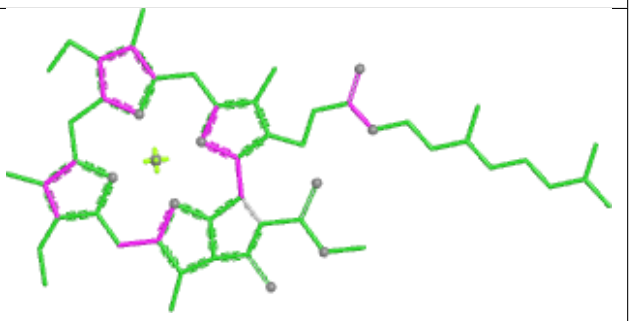


Rings

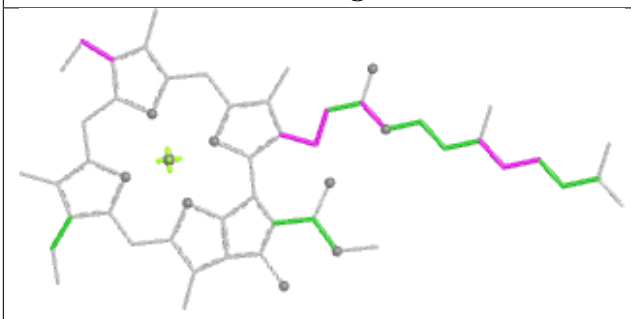
Ligand CLA b 1218



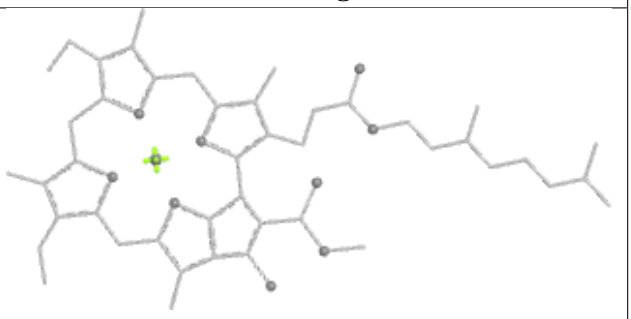
Bond lengths



Bond angles

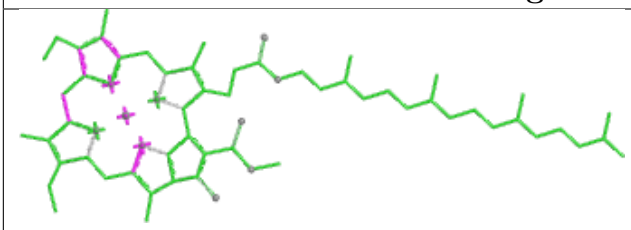


Torsions



Rings

Ligand CLA Z 512



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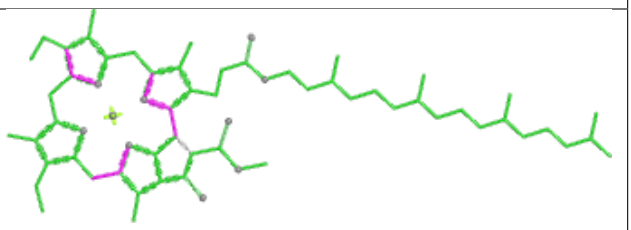
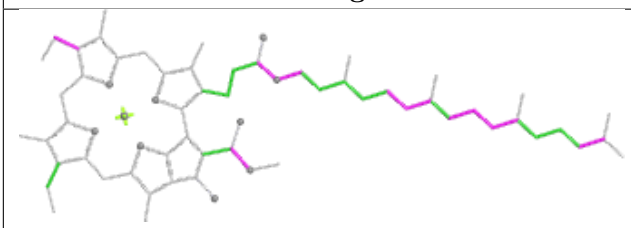
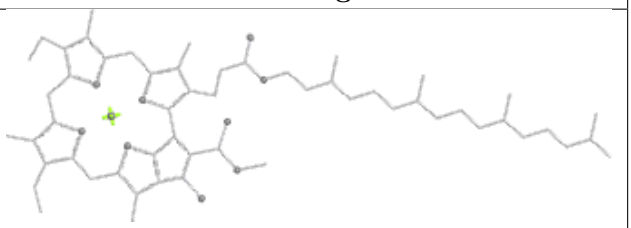


Bond angles

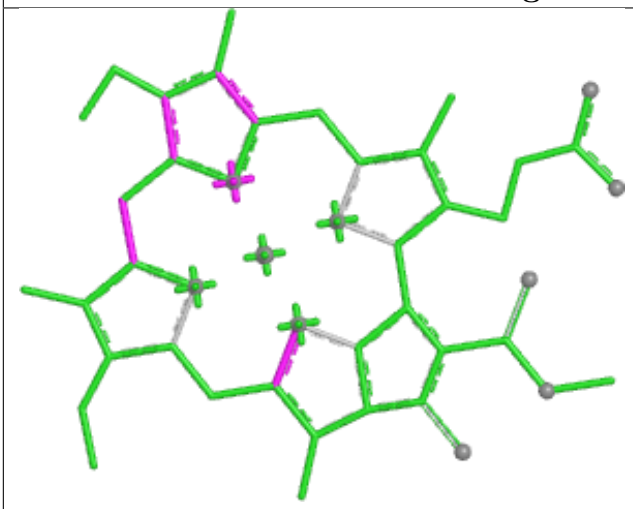


Torsions



Rings

Ligand CLA j 1302



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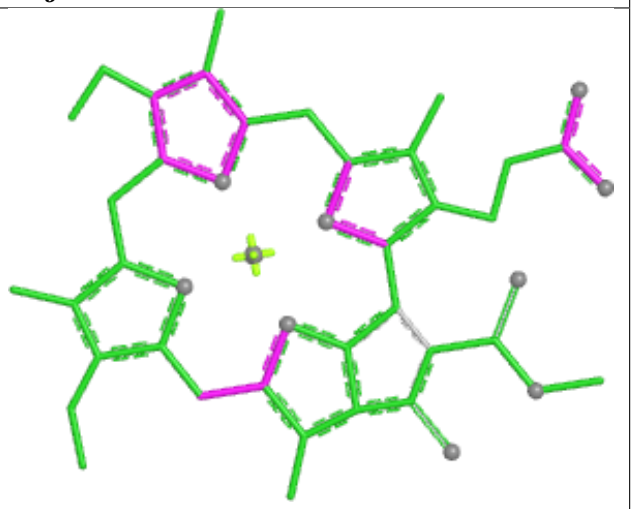

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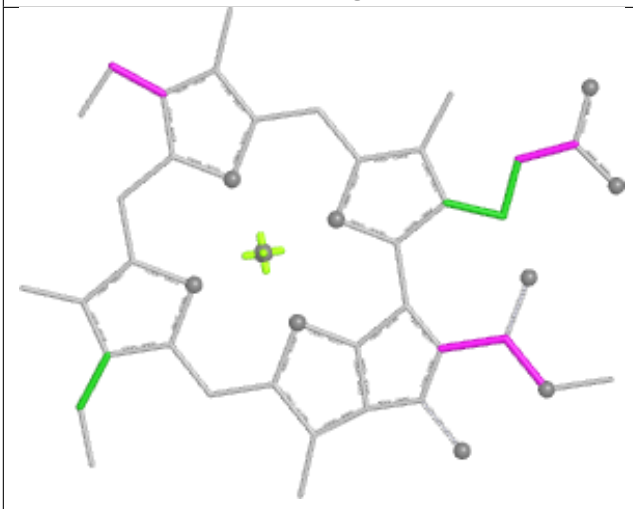
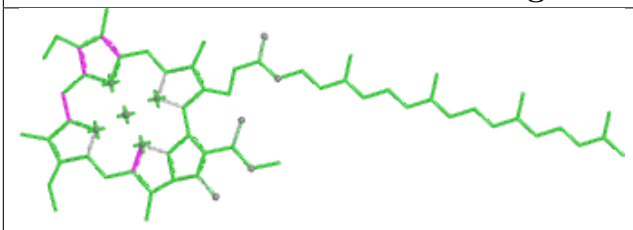


Torsions

Rings

Ligand CLA h 515



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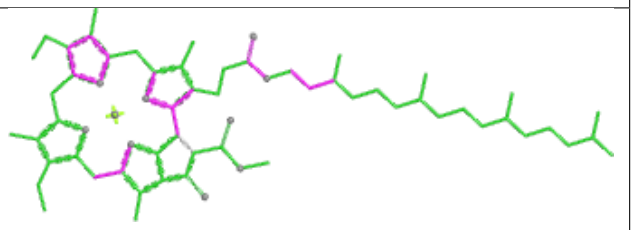
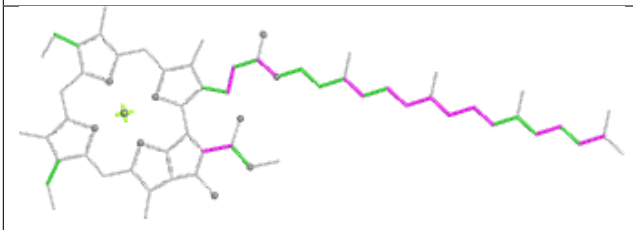
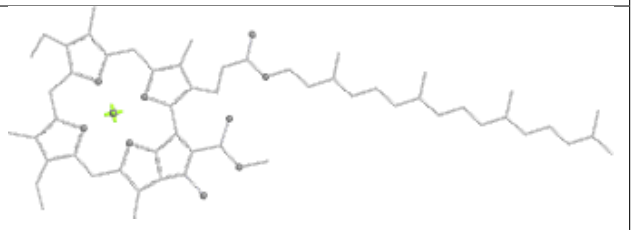


Bond angles

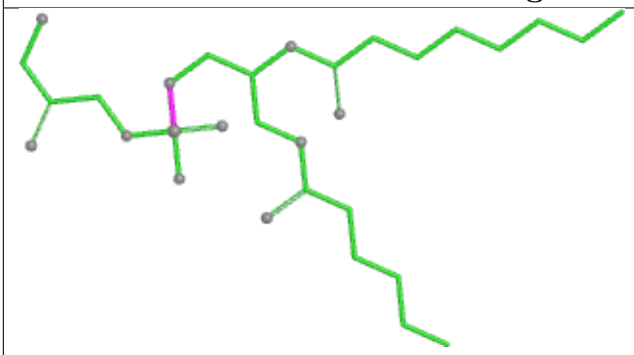


Torsions



Rings

Ligand LHG x 605



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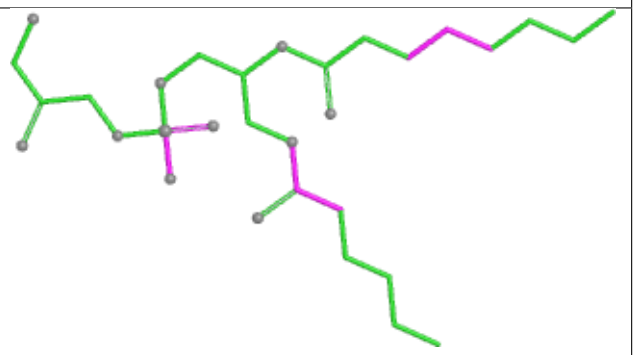
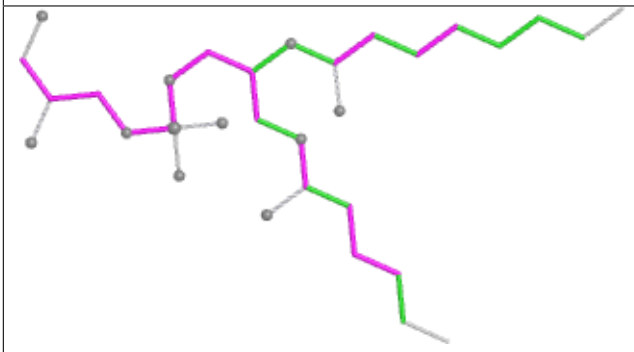


Bond angles



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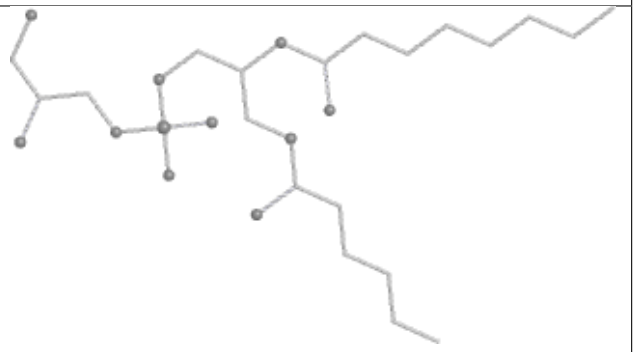
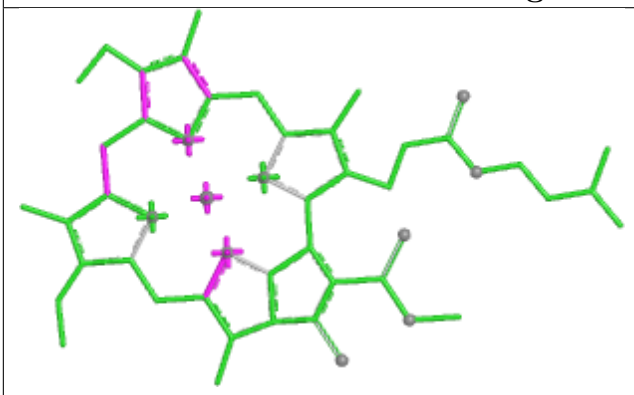


Rings

Ligand CLA Z 502



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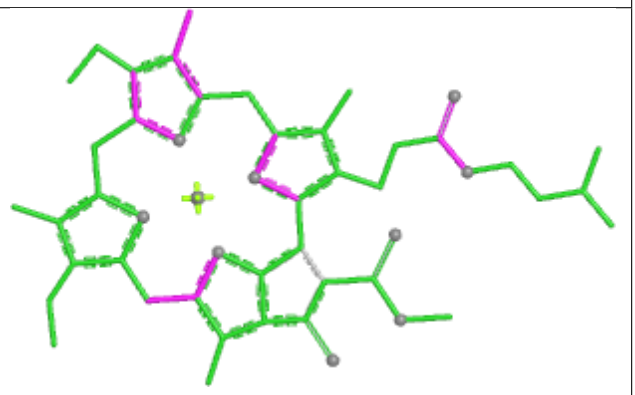
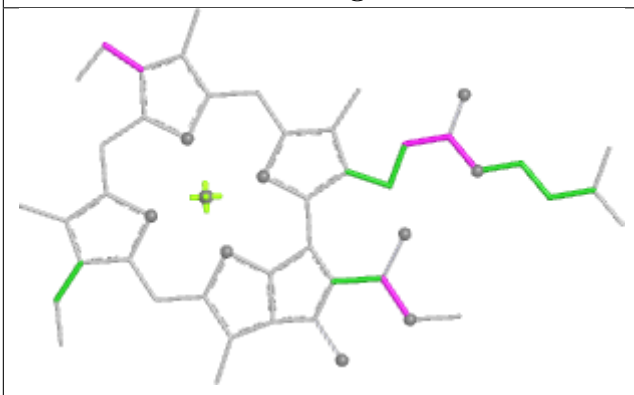
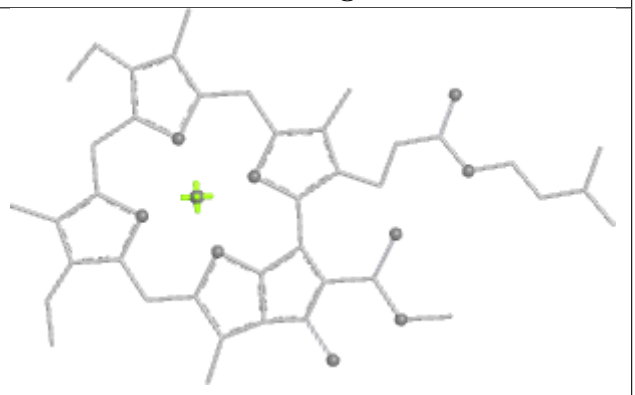


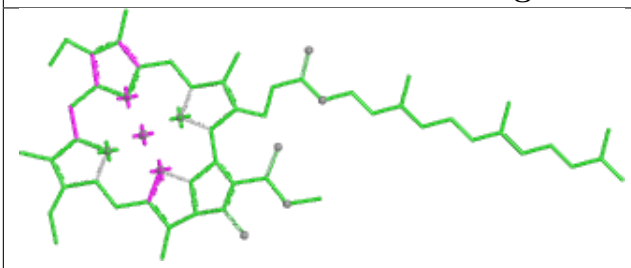
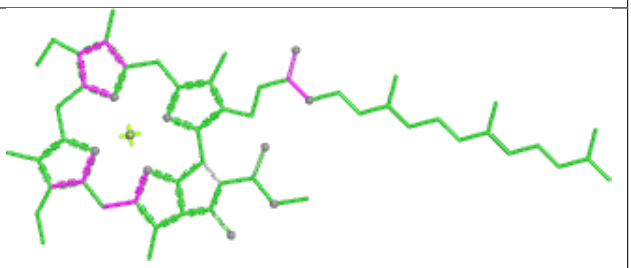
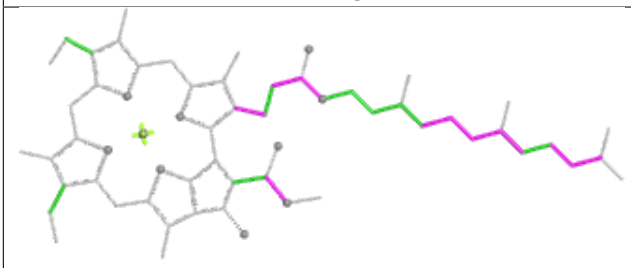
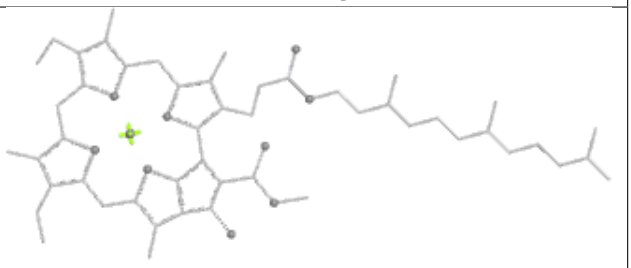
Bond angles

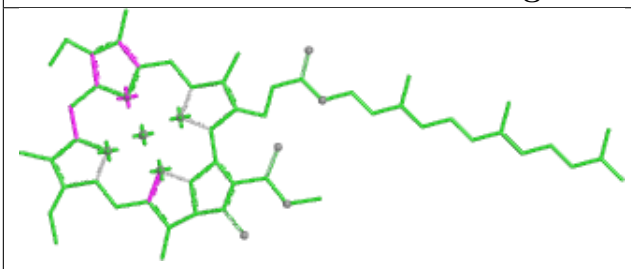
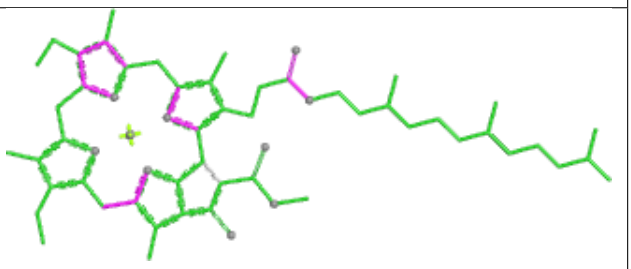
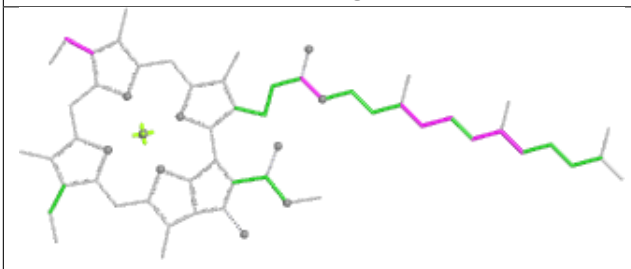
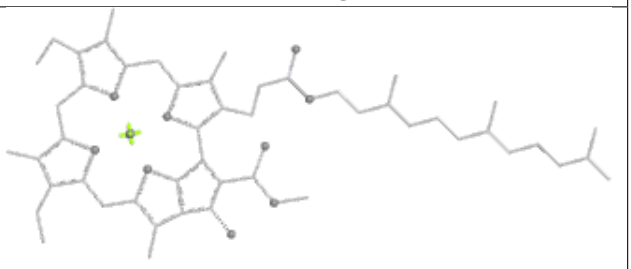


Torsions

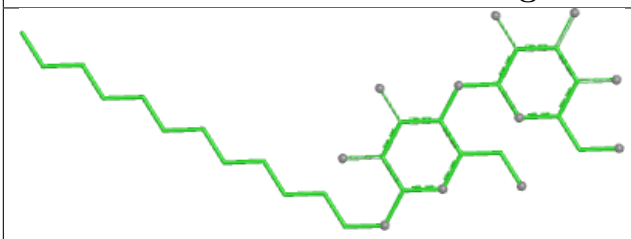


Rings

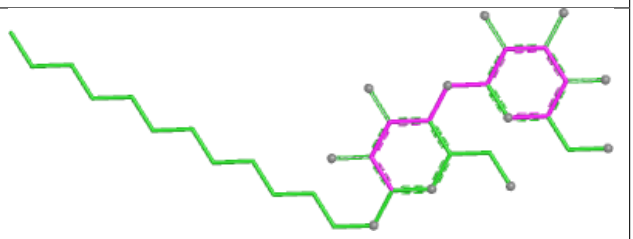
Ligand CLA G 1226	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA l 1502	
	
Bond lengths	Bond angles
	
Torsions	Rings

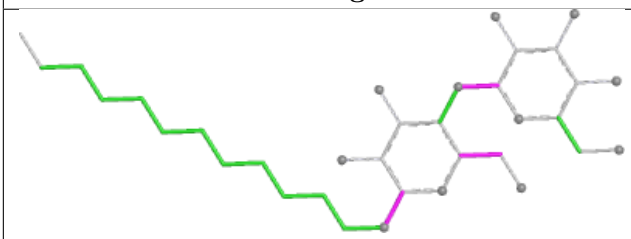
Ligand LMU Y 606



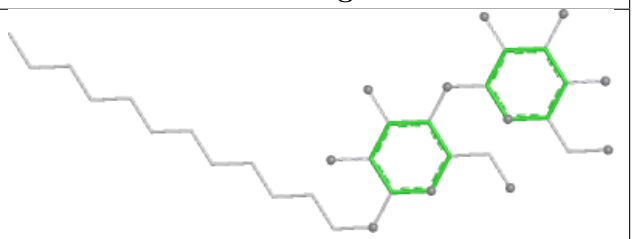
Bond lengths



Bond angles

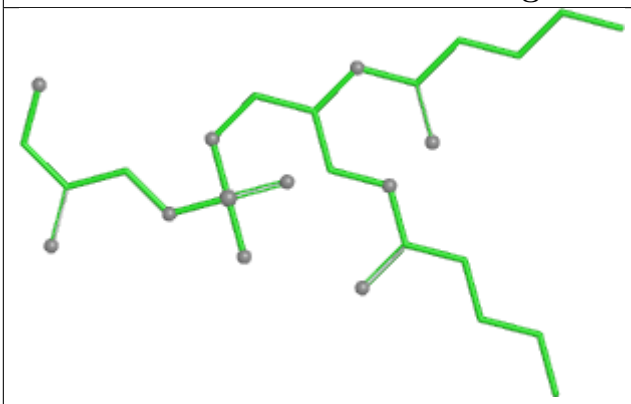


Torsions



Rings

Ligand LHG X 605



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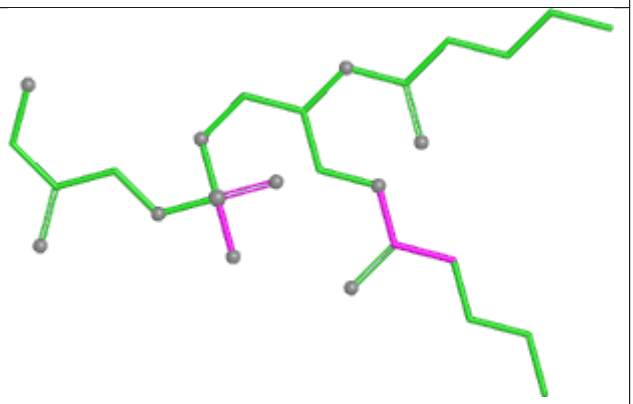
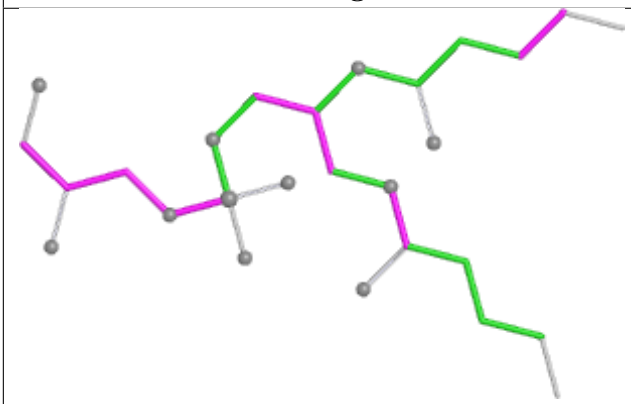
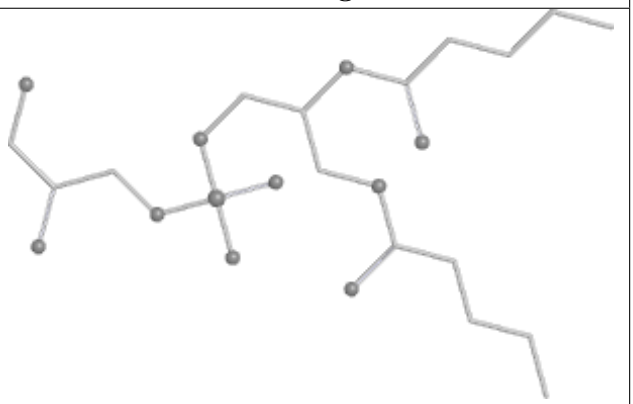


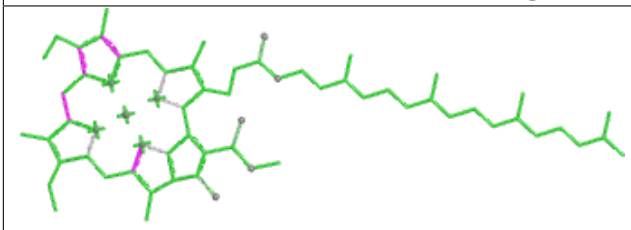
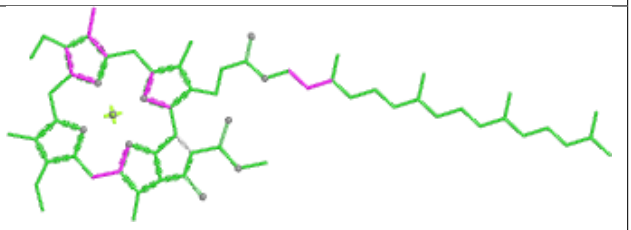
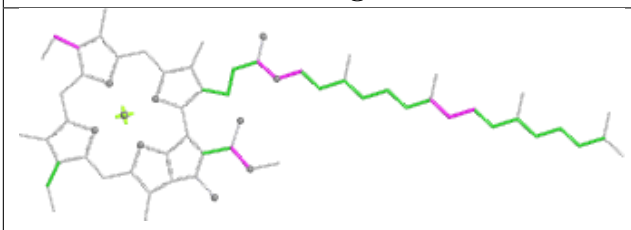
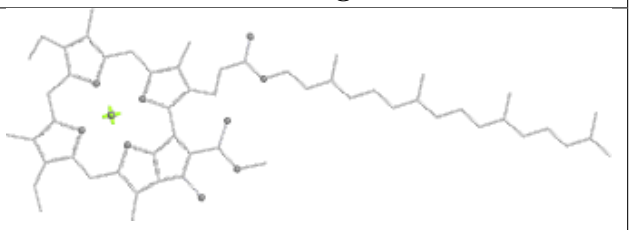
Bond angles

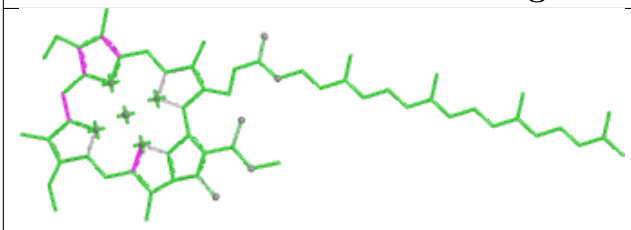
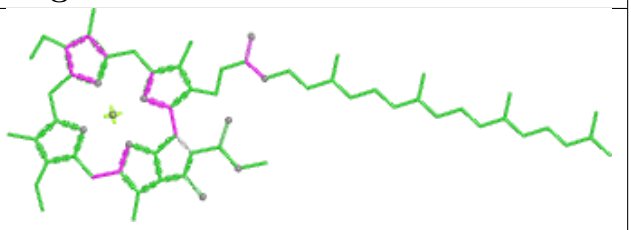
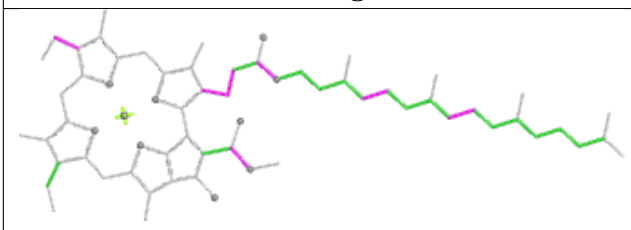
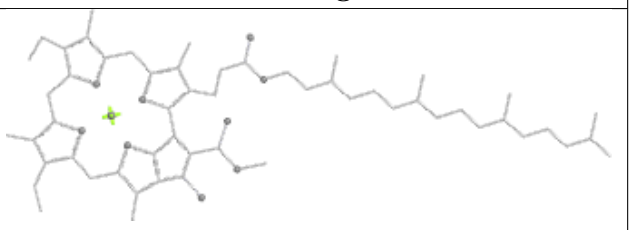


Torsions

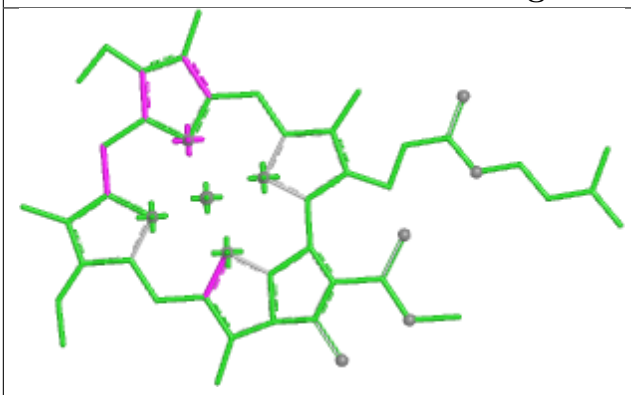


Rings

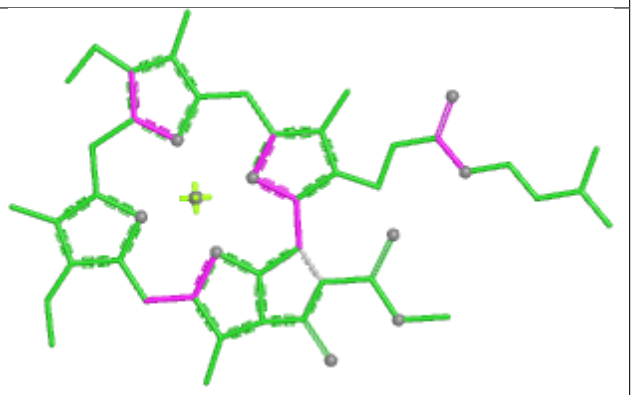
Ligand CLA Y 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA g 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

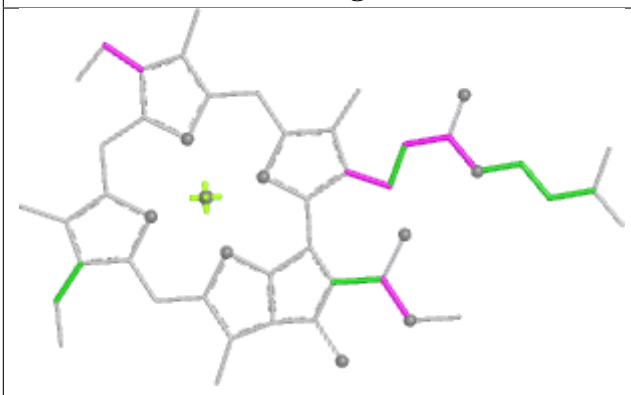
Ligand CLA x 514



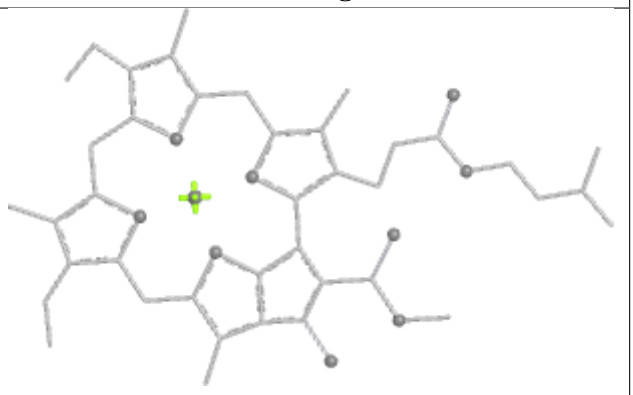
Bond lengths



Bond angles

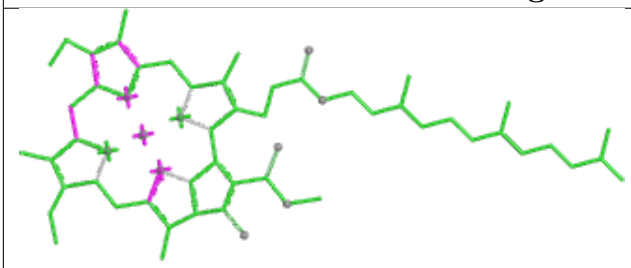


Torsions

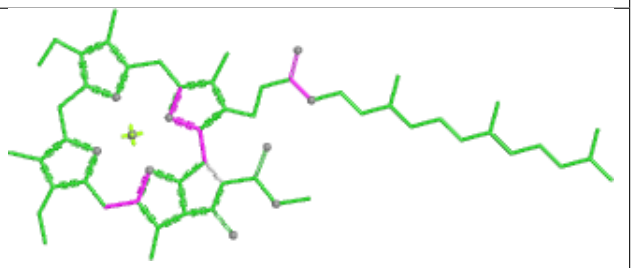


Rings

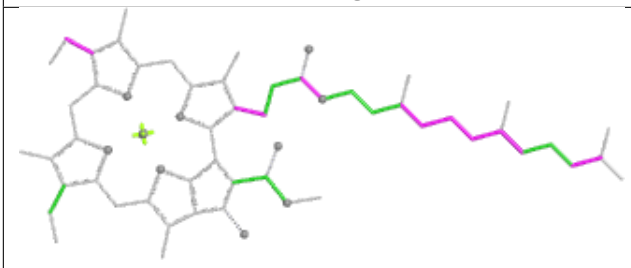
Ligand CLA x 506



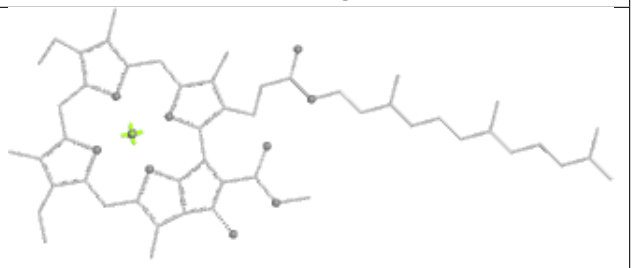
Bond lengths



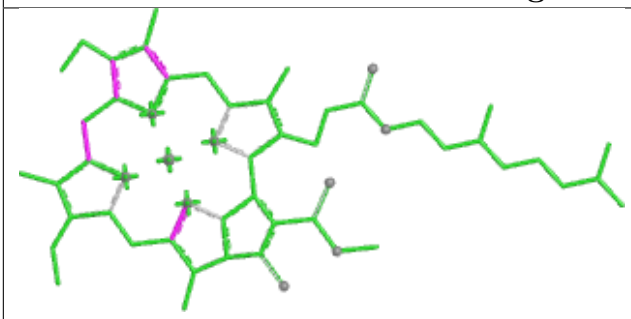
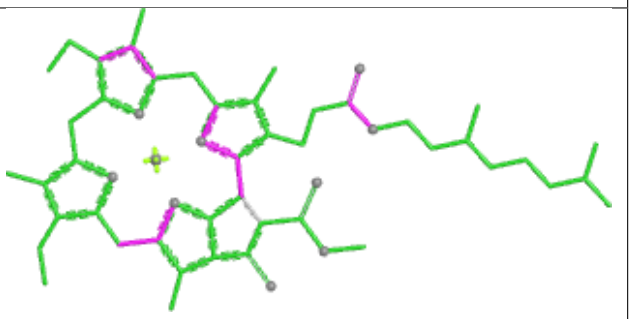
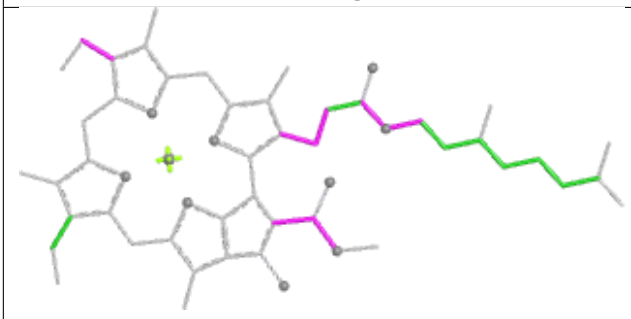
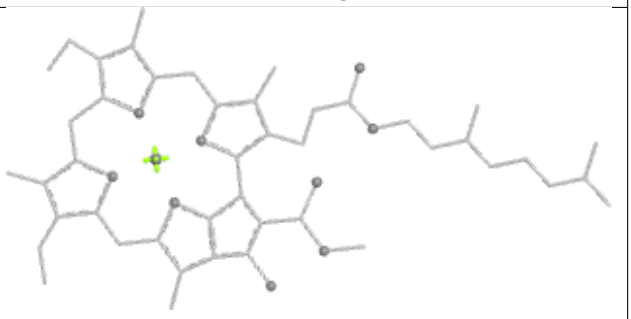
Bond angles

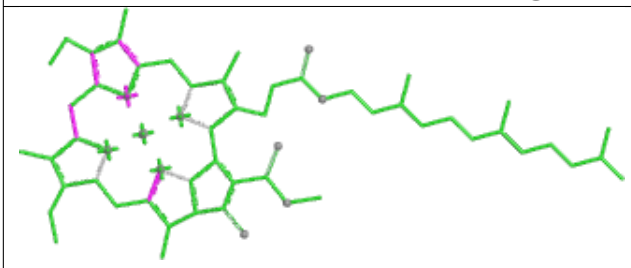
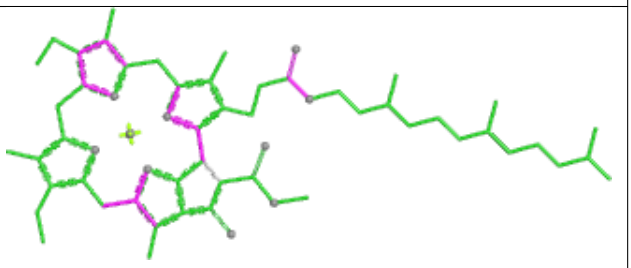
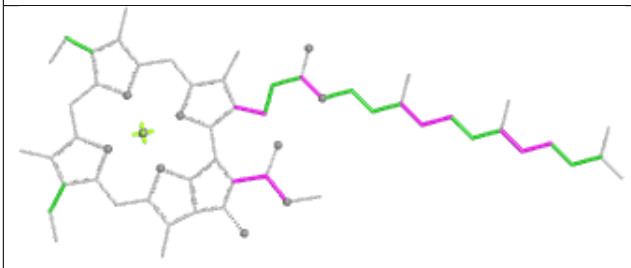
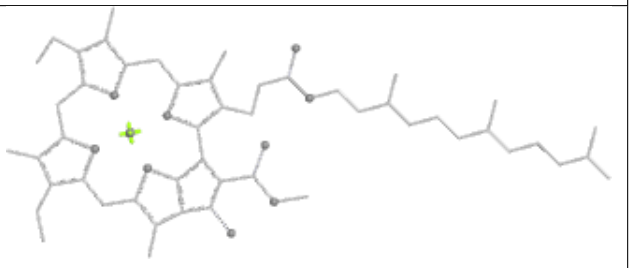


Torsions

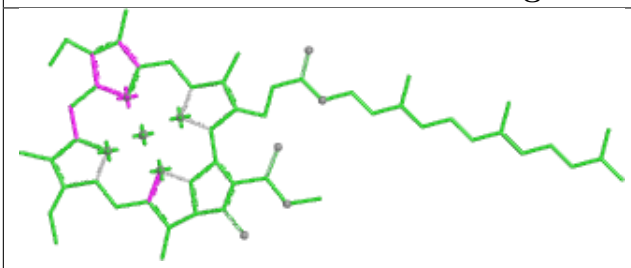


Rings

Ligand CLA h 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA h 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA X 504



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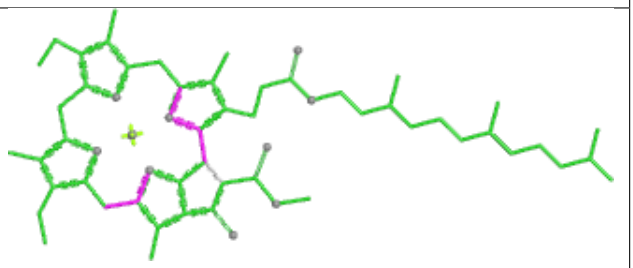
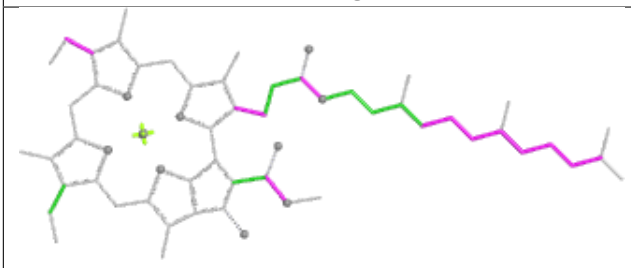
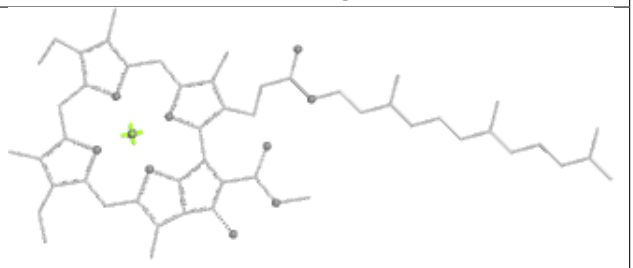


Bond angles

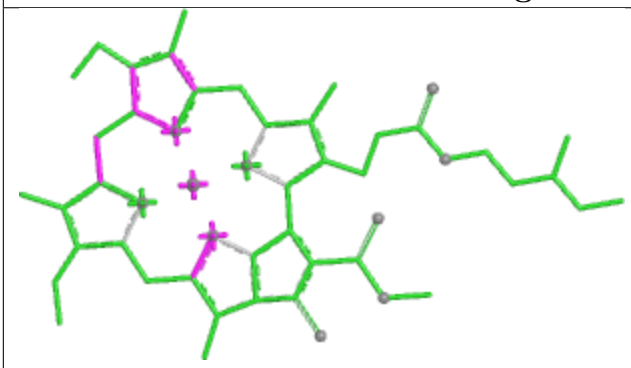


Torsions



Rings

Ligand CLA A 1135



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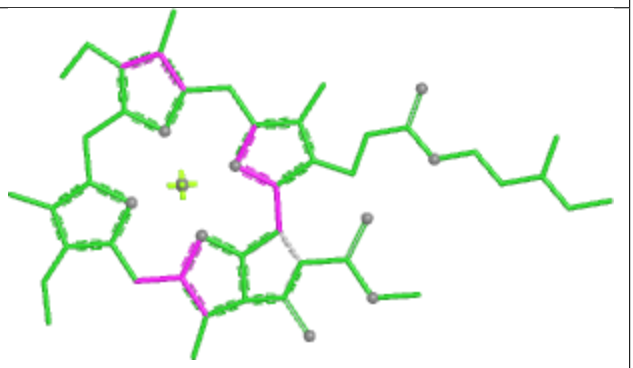
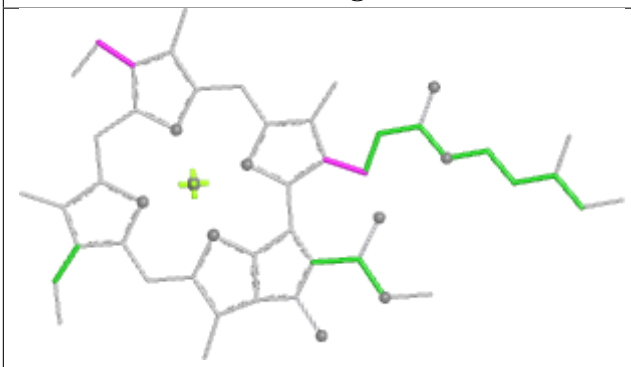


Bond angles



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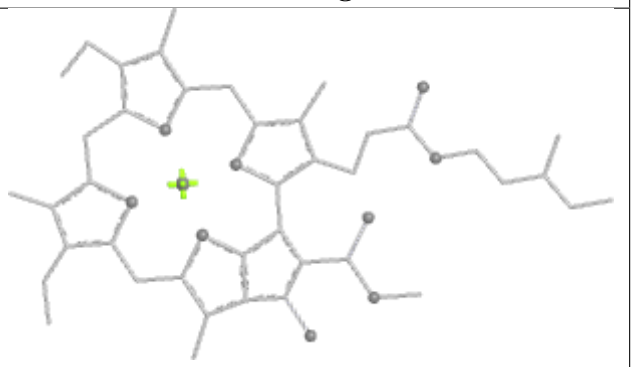
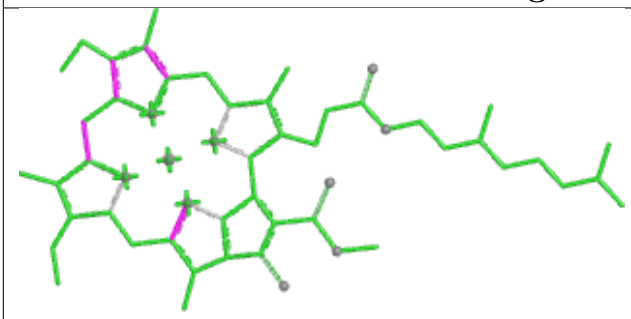


Rings

Ligand CLA o 517



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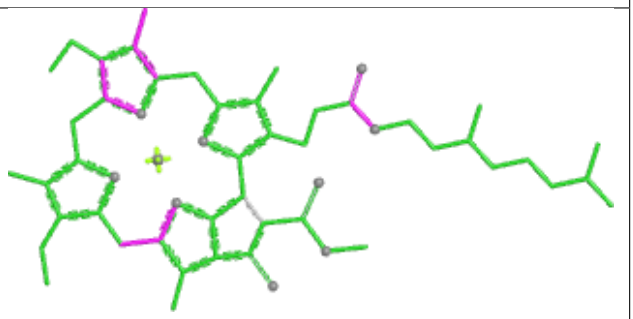
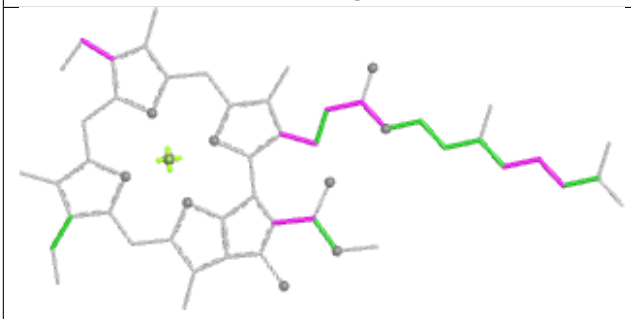


Bond angles



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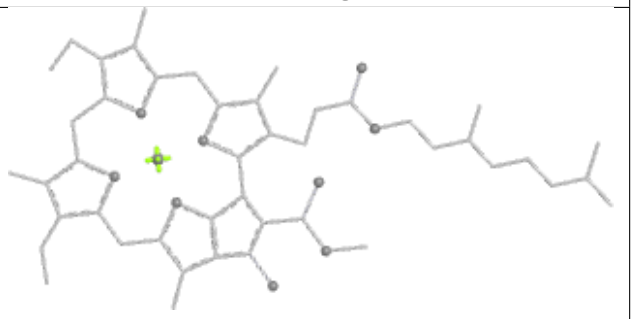
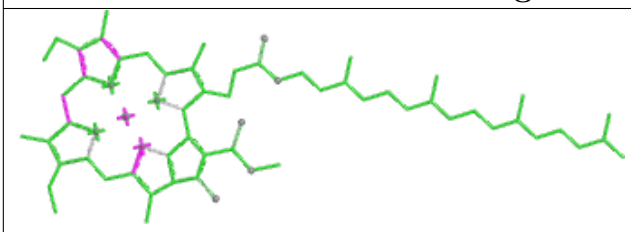


Rings

Ligand CLA H 1140



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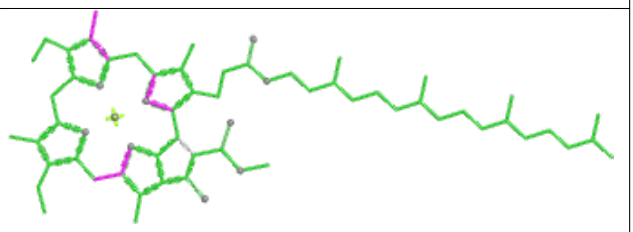
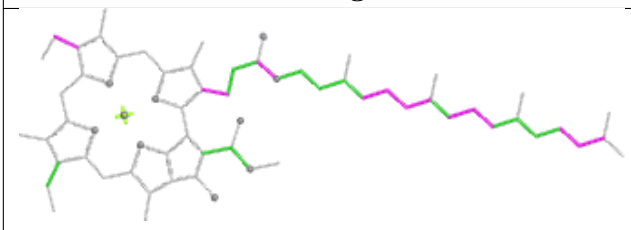


Bond angles



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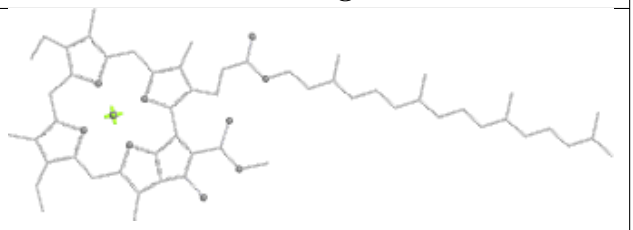
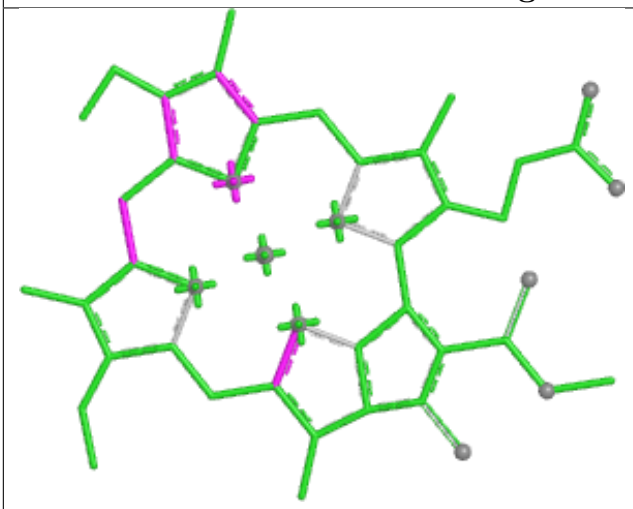


Rings

Ligand CLA b 1230



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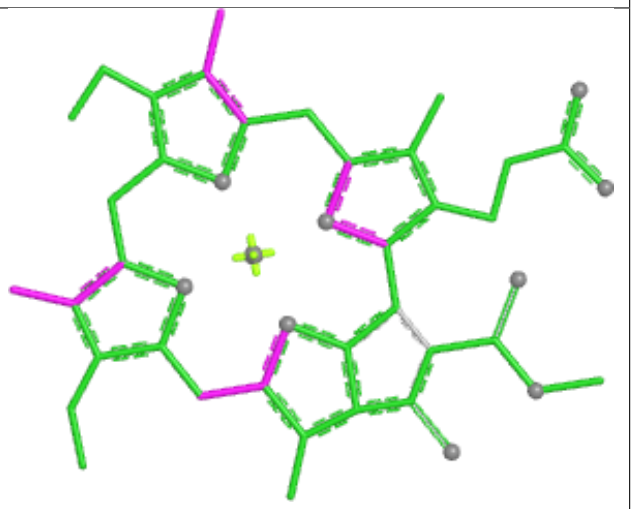
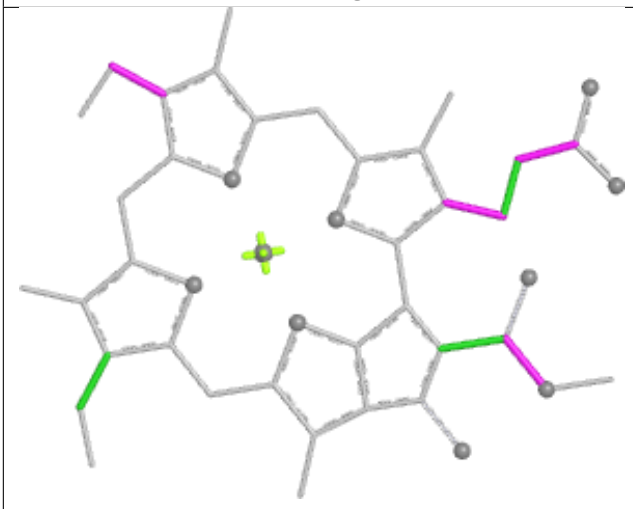


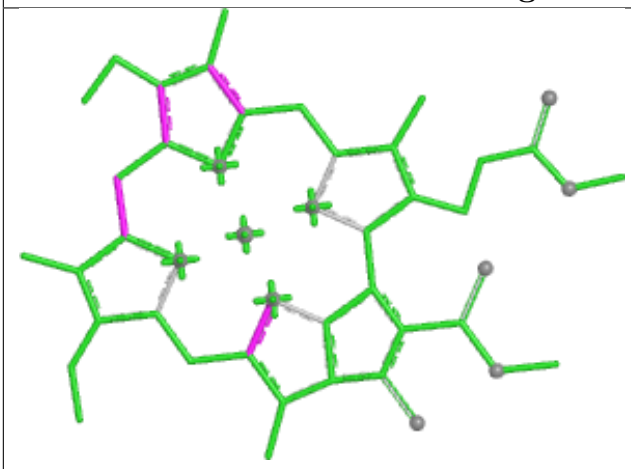
Bond angles



Torsions

Rings

Ligand CLA b 1240



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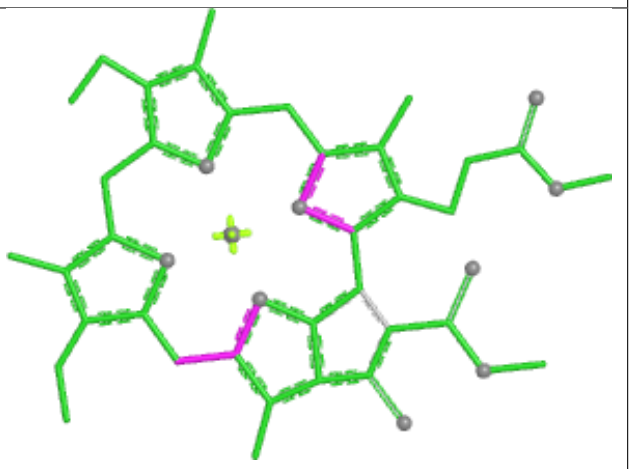
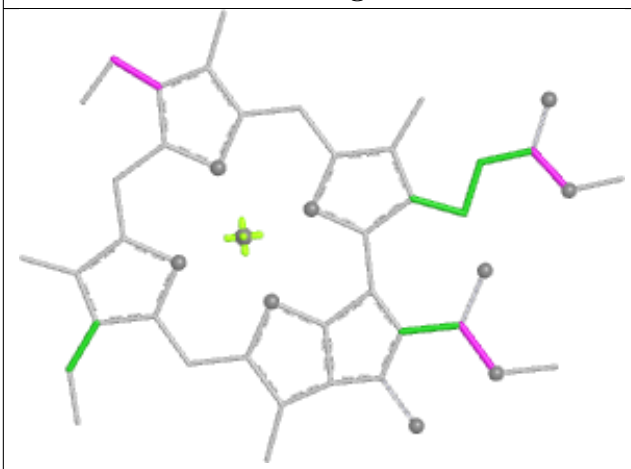


Bond angles



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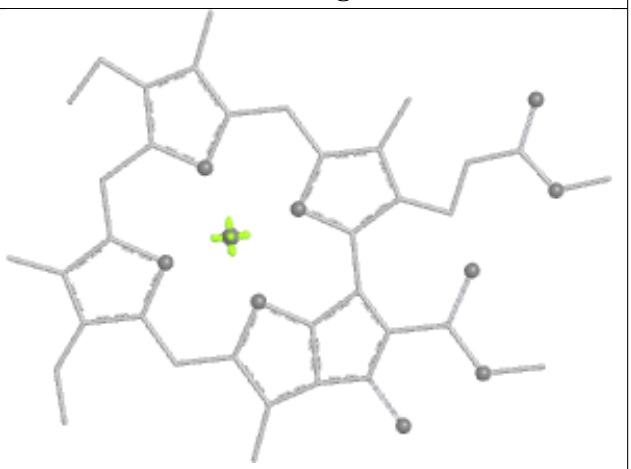
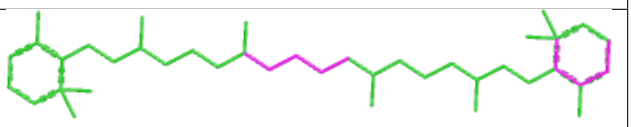


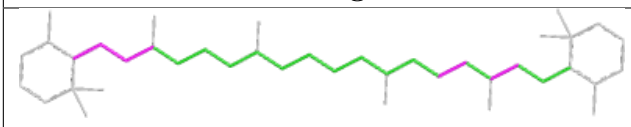
Rings

Ligand BCR B 4005

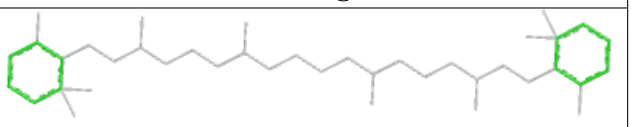
Bond lengths



Bond angles

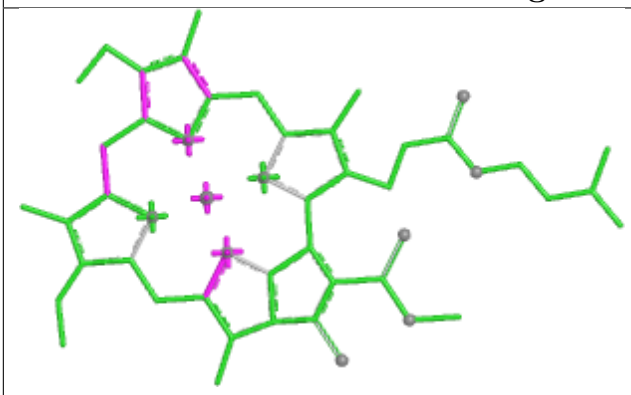


Torsions



Rings

Ligand CLA o 514



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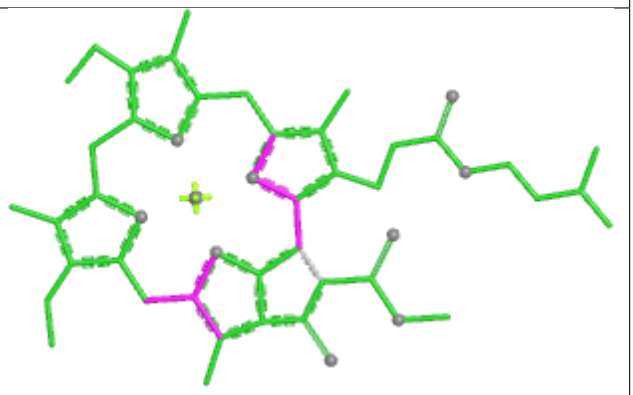
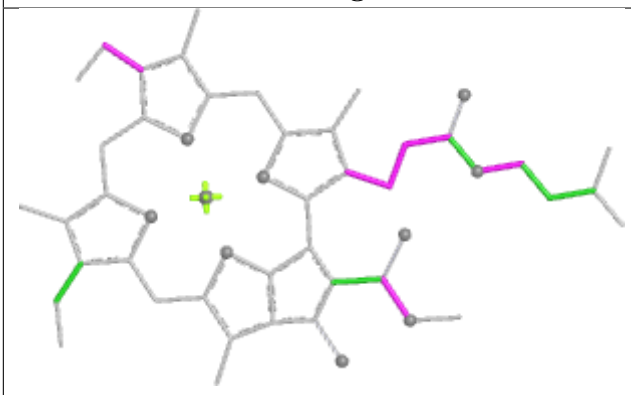


Bond angles



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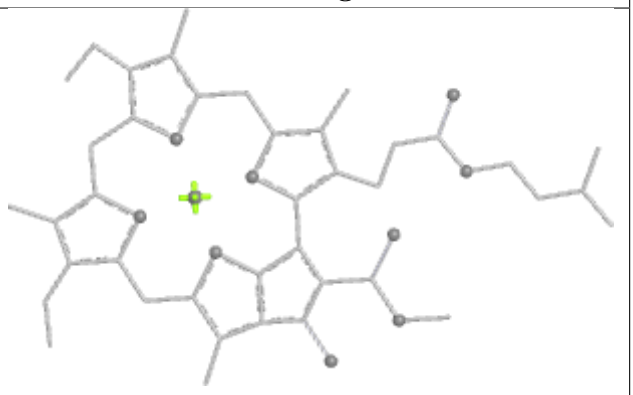
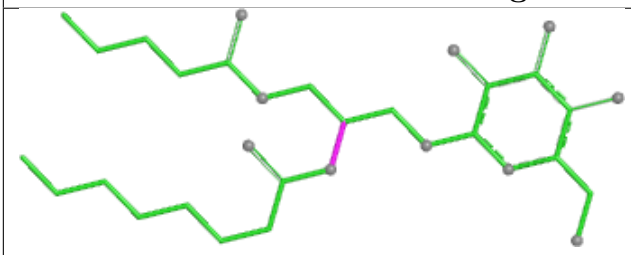
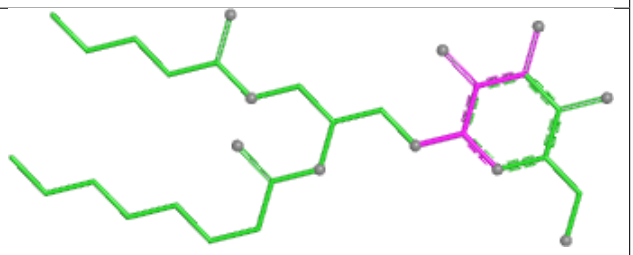


Rings

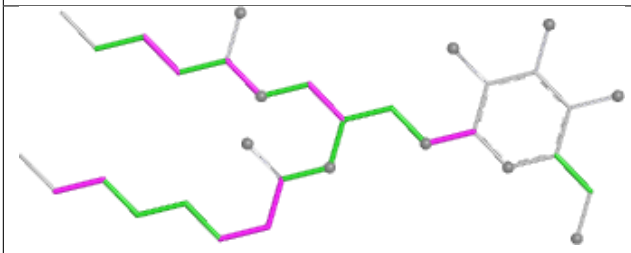
Ligand LMG H 4201



Bond lengths



Bond angles



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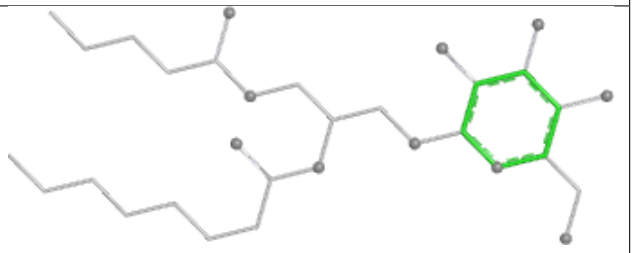
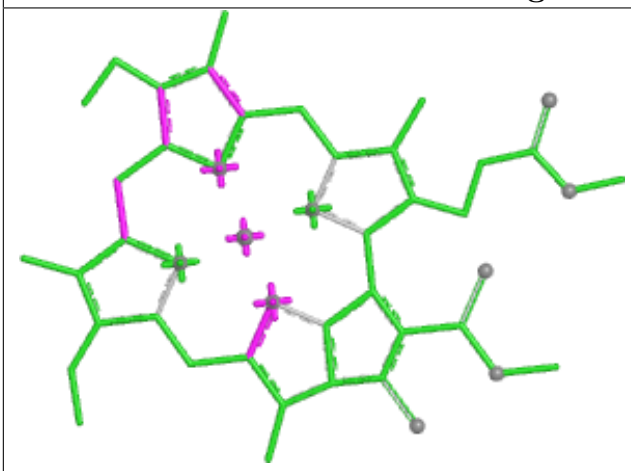


Rings

Ligand CLA q 503



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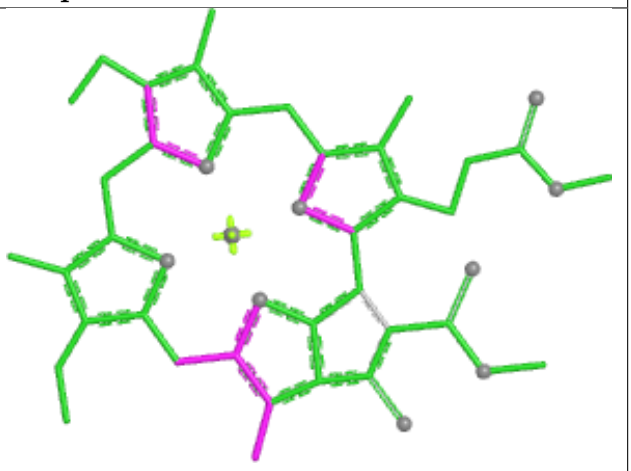
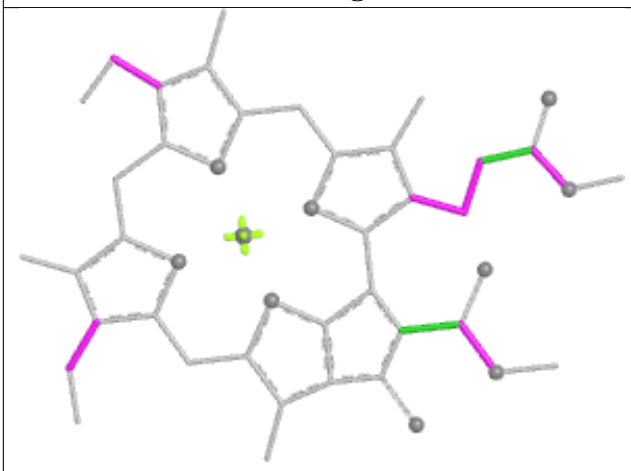
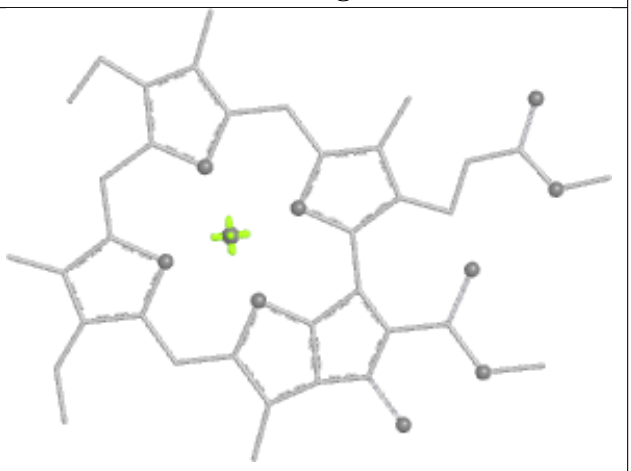


Bond angles

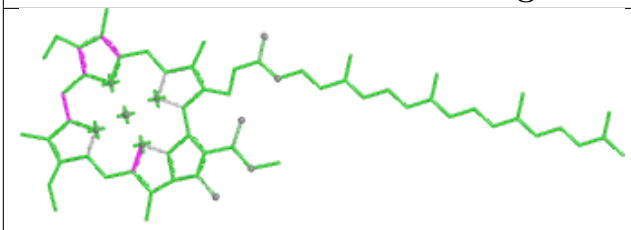


Torsions

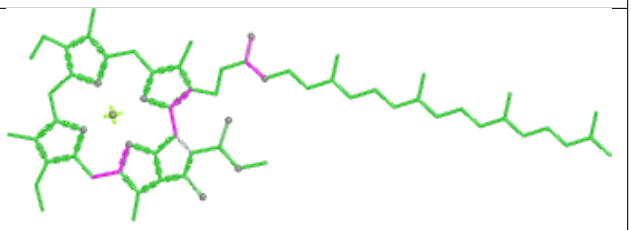


Rings

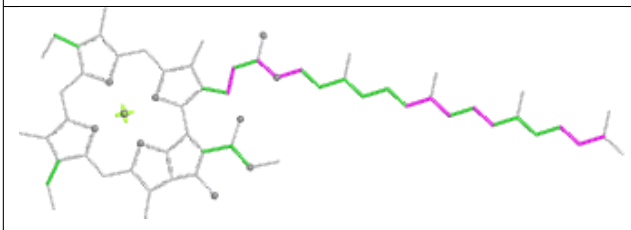
Ligand CLA L 1503



Bond lengths



Bond angles



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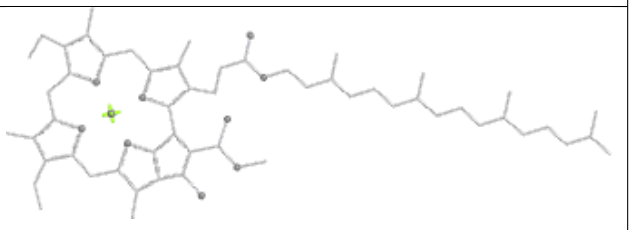
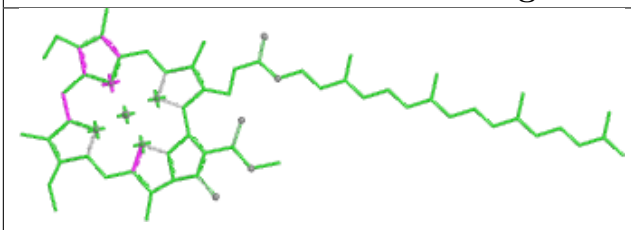
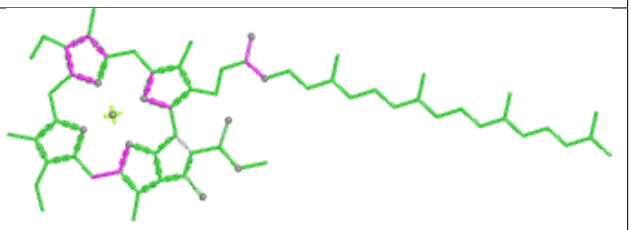
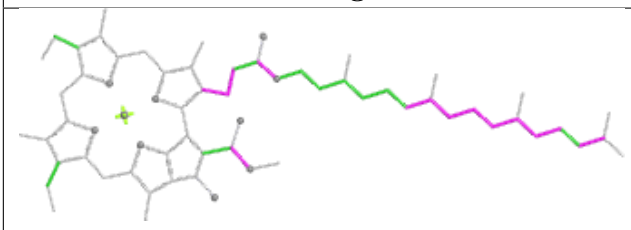
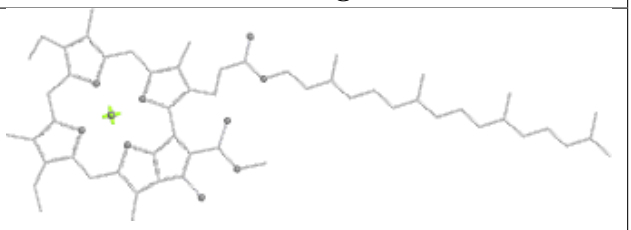
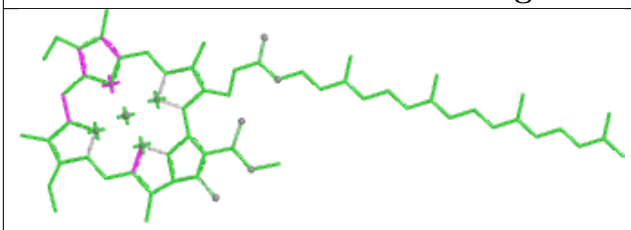
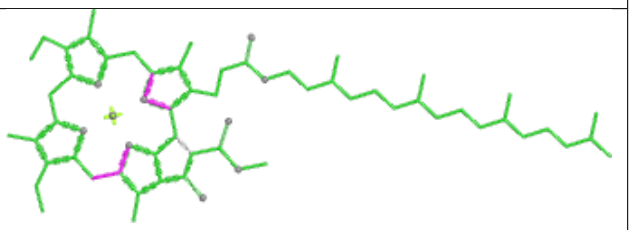
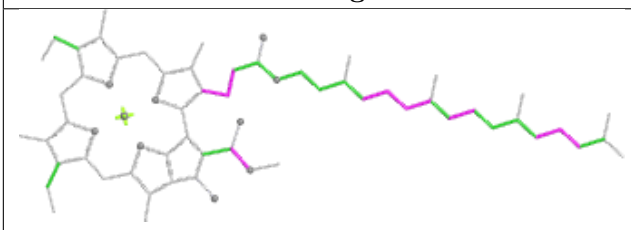
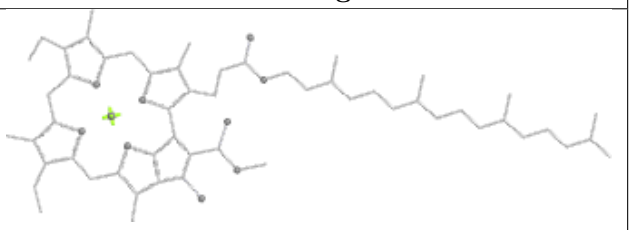
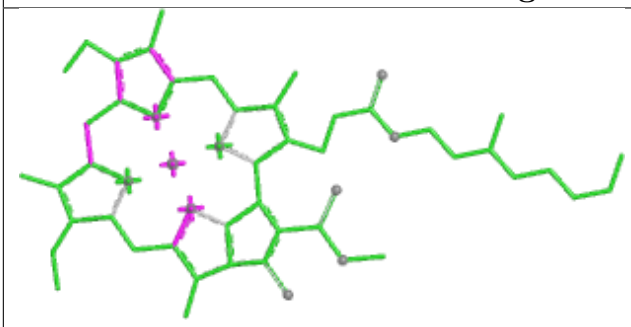


Rings

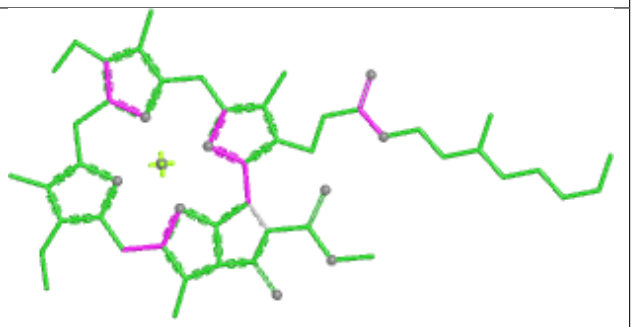
Ligand CLA b 1221	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1126	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1220



Bond lengths



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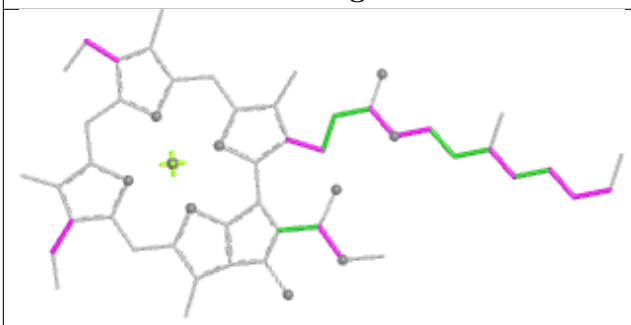

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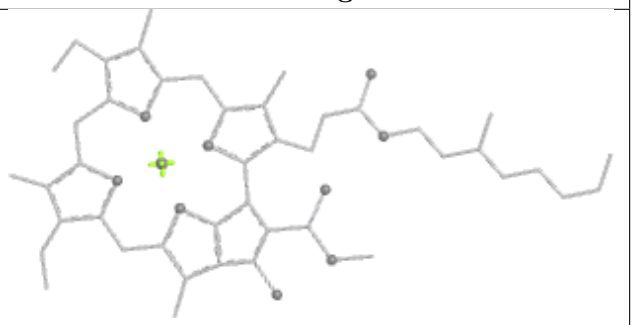

Rings

Ligand BCR L 4022

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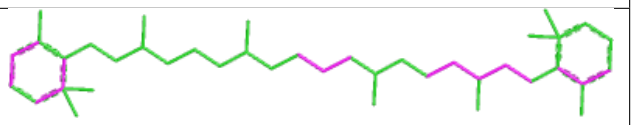

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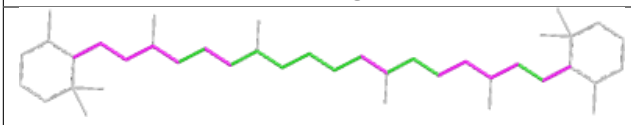

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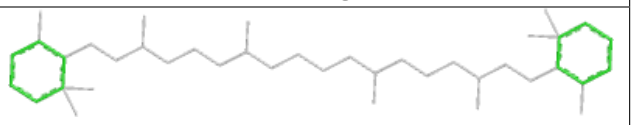
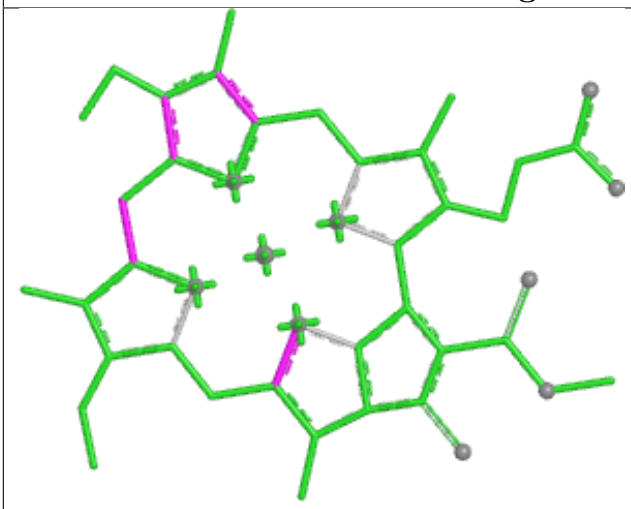


Rings

Ligand CLA k 4002



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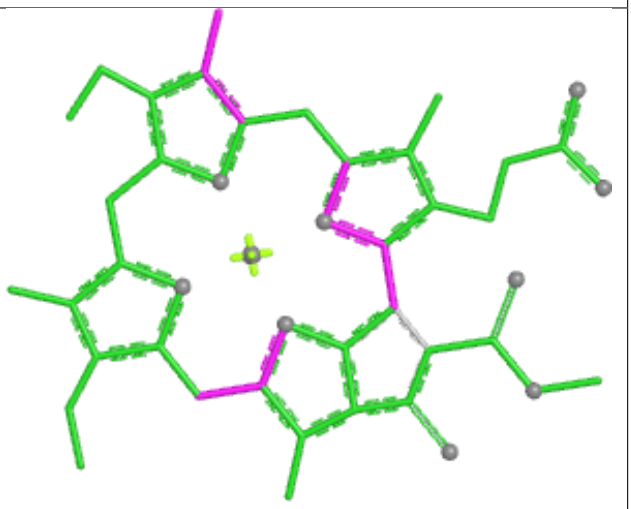

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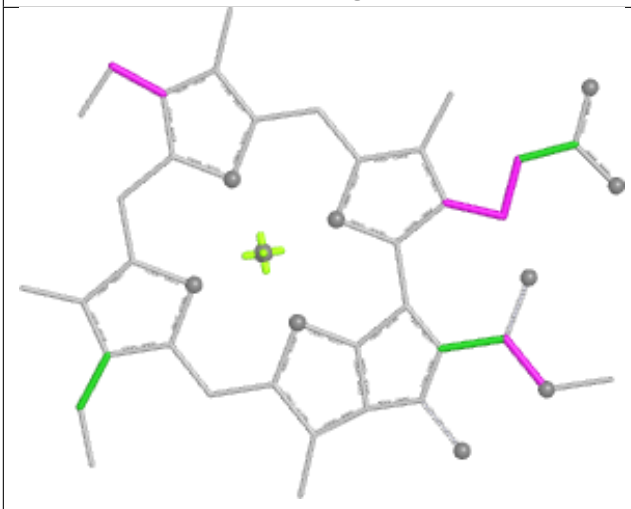
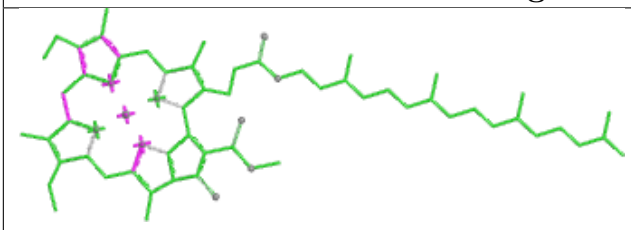


Torsions

Rings

Ligand CLA x 511



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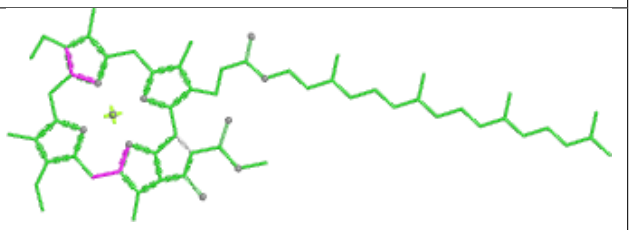

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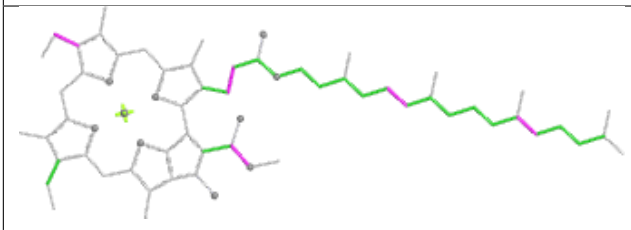

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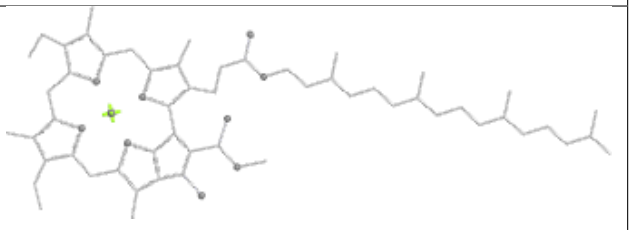
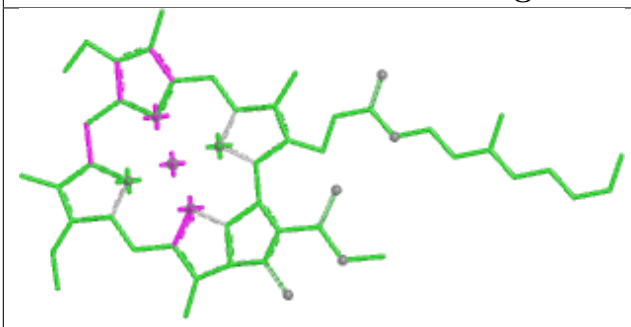


Rings

Ligand CLA H 1133



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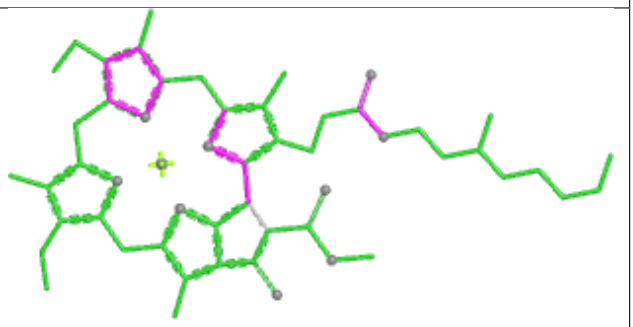

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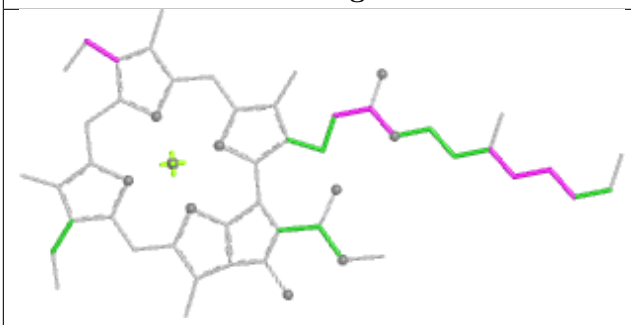

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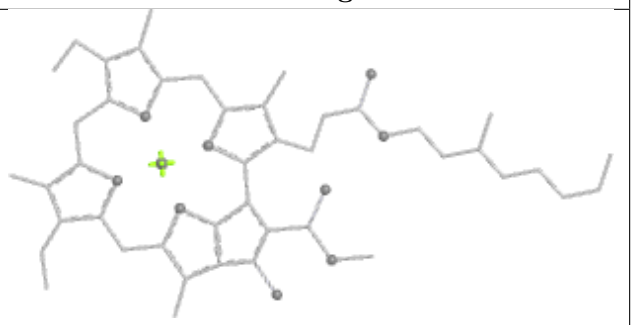

Rings

Ligand BCR i 4018

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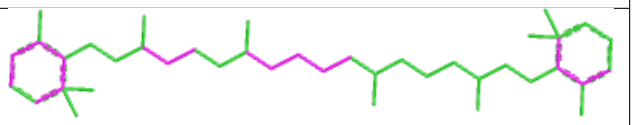

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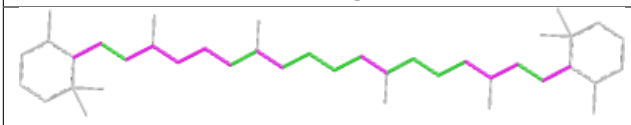

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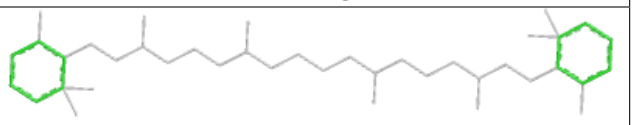
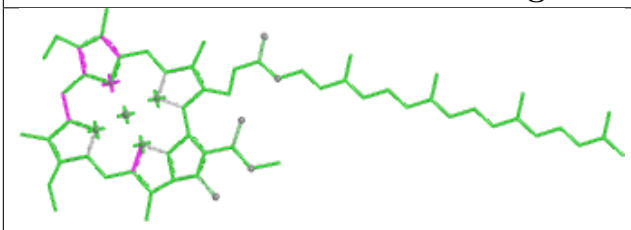


Rings

Ligand CLA y 512



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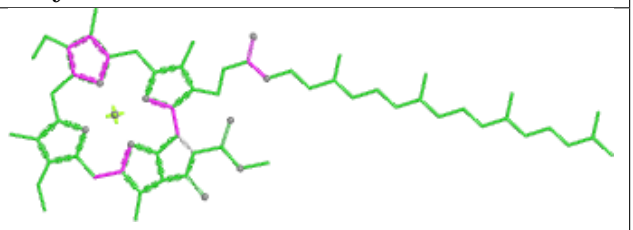

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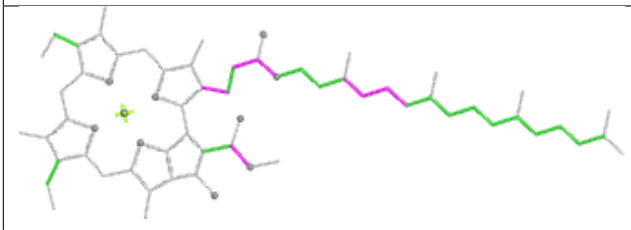

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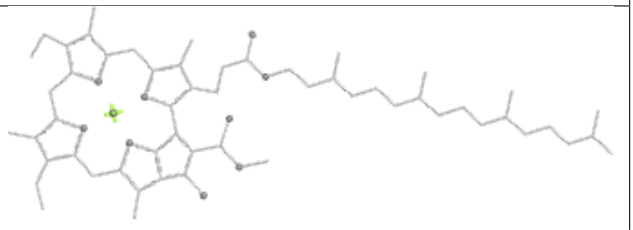
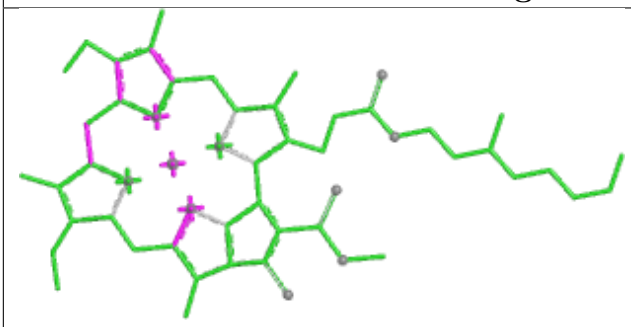


Rings

Ligand CLA A 1115



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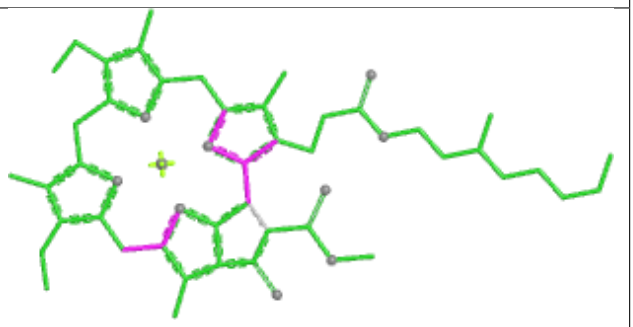

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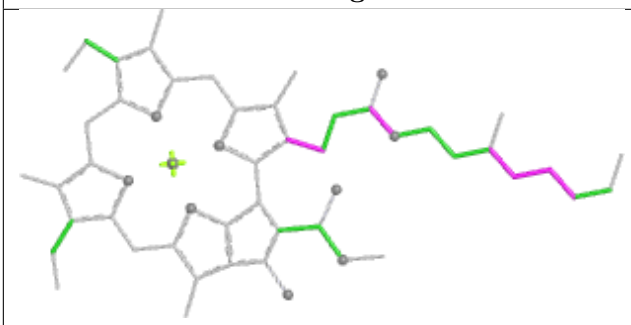

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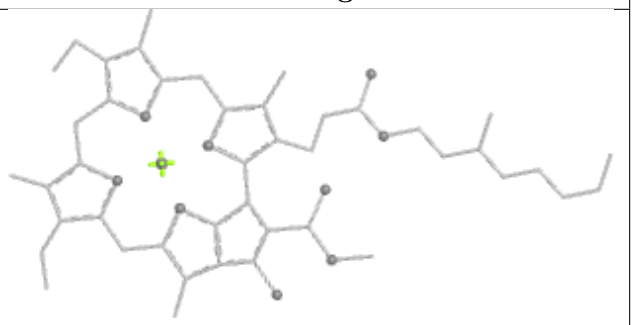
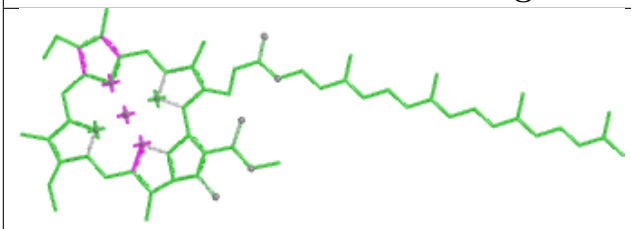


Rings

Ligand CLA A 1128



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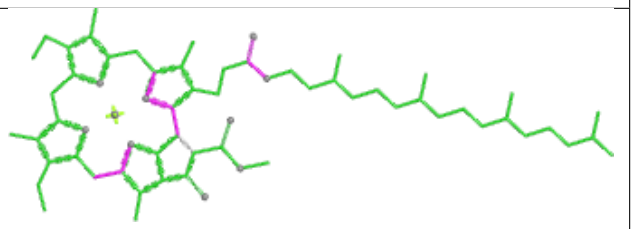

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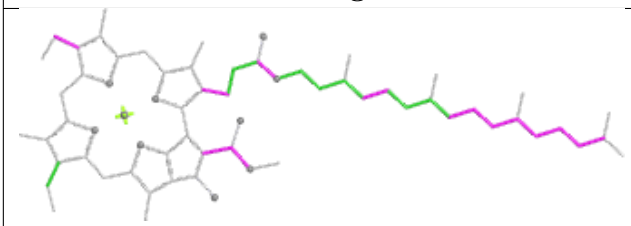

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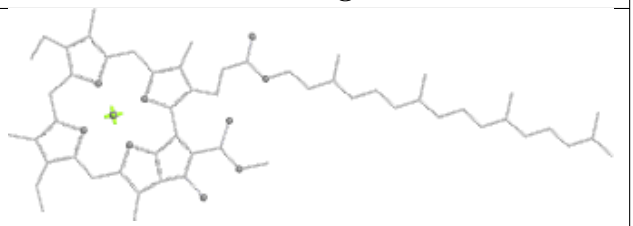
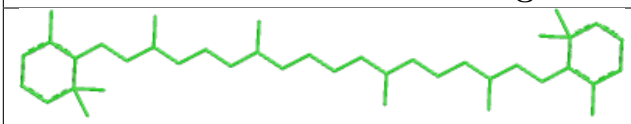


Rings

Ligand BCR b 4004



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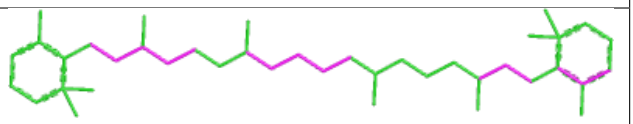
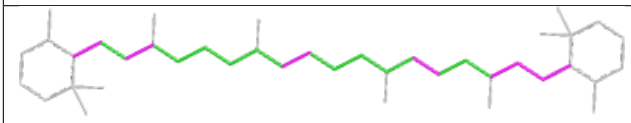


Bond angles



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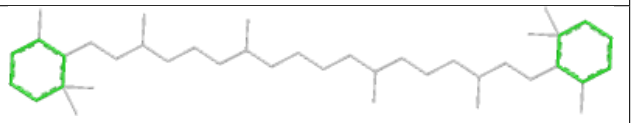
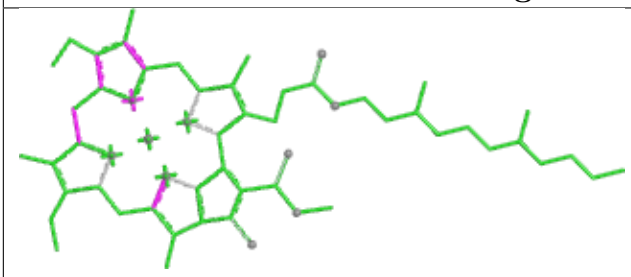


Rings

Ligand CLA H 1105



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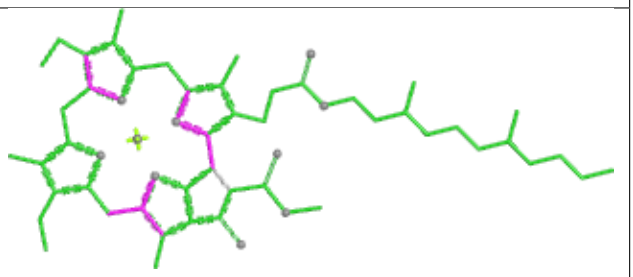

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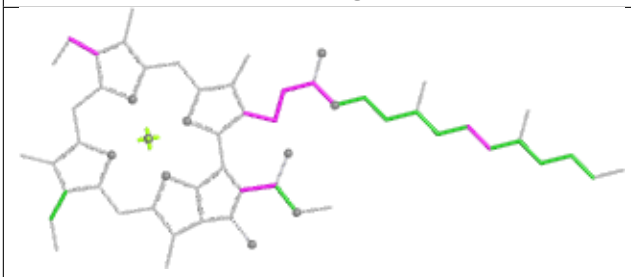

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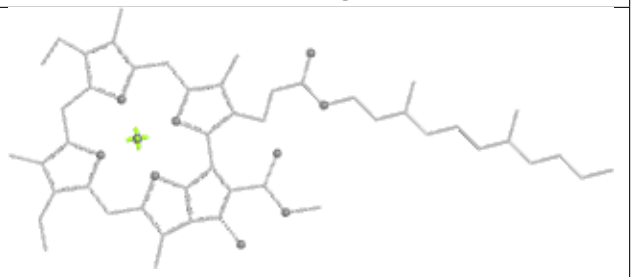
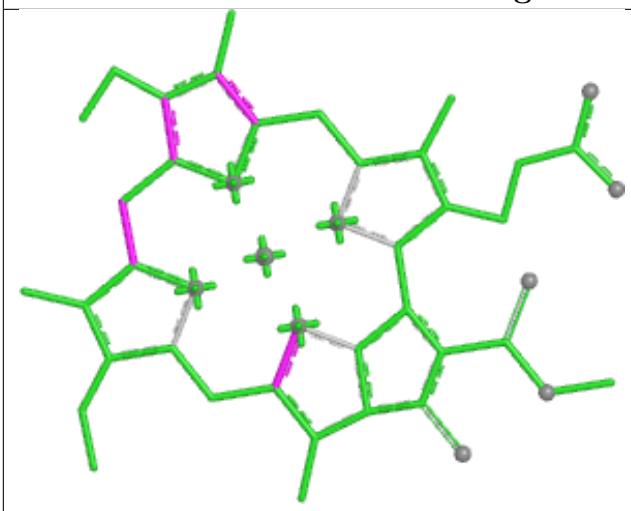


Rings

Ligand CLA G 1231



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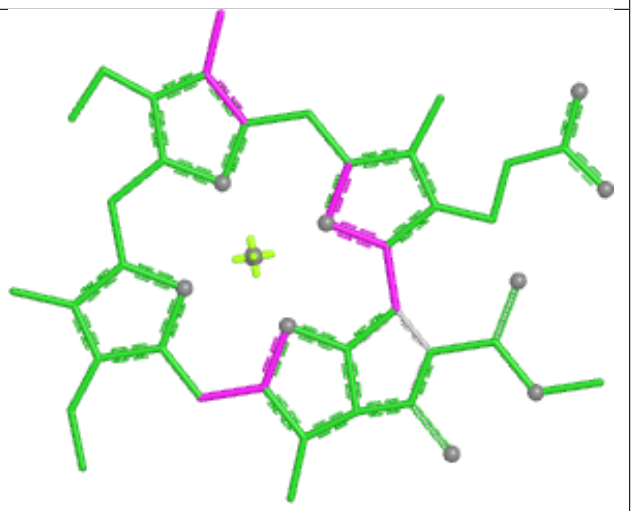

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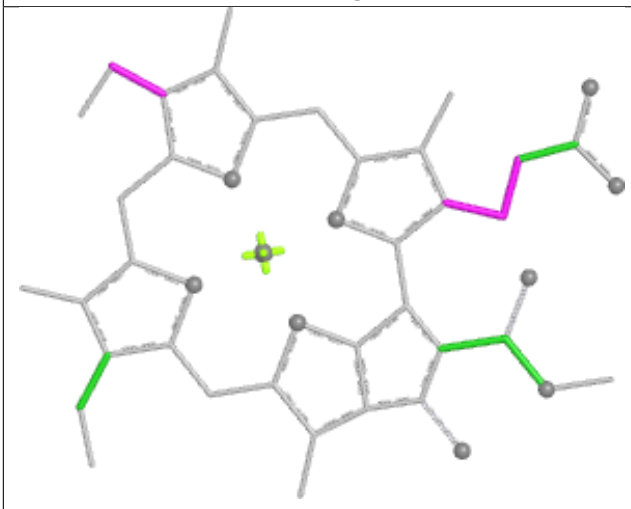
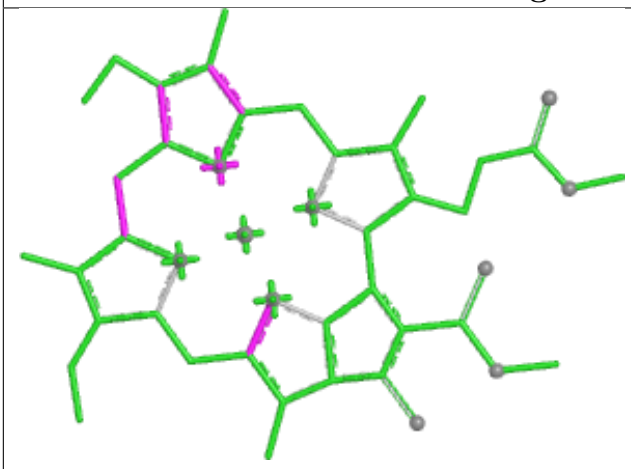


Torsions

Rings

Ligand CLA r 516



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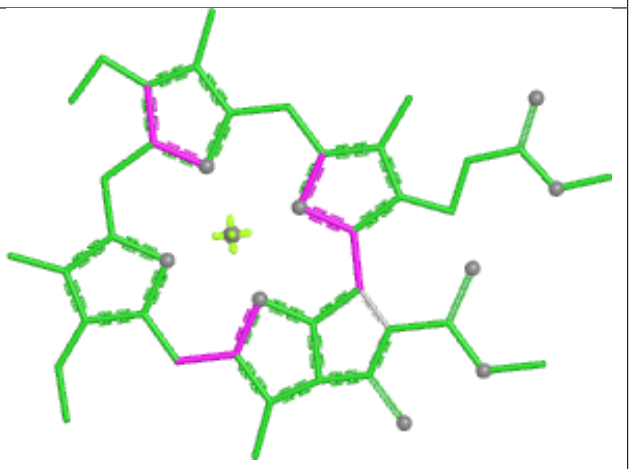

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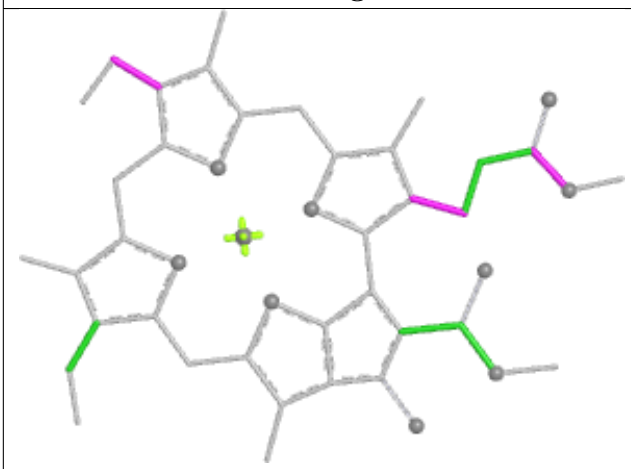

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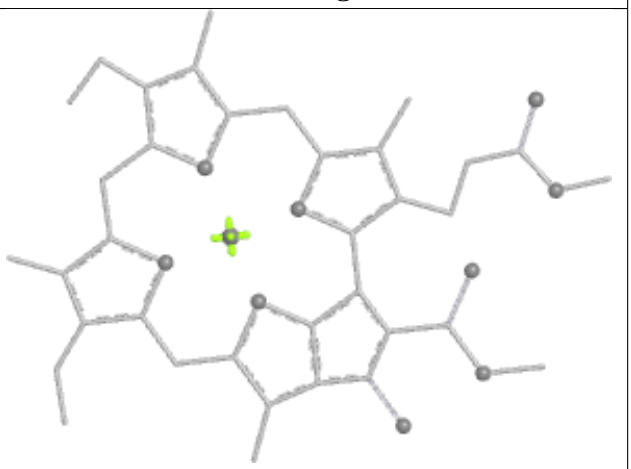
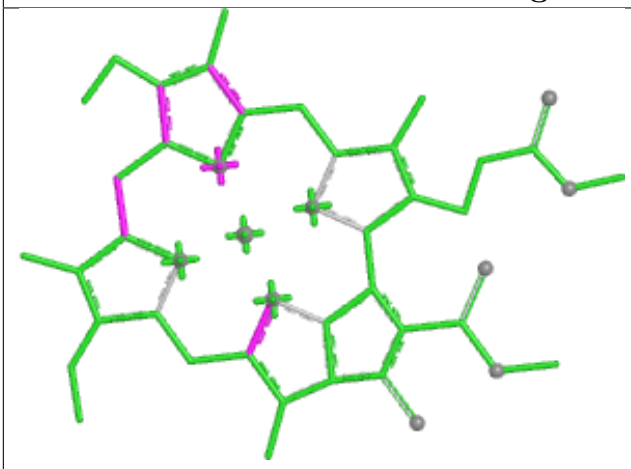


Rings

Ligand CLA t 513



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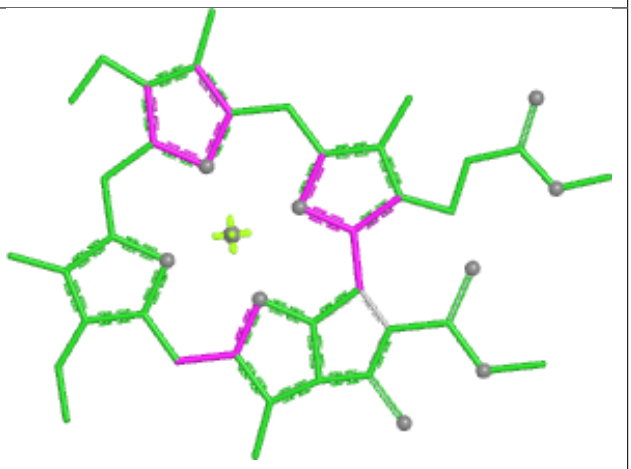
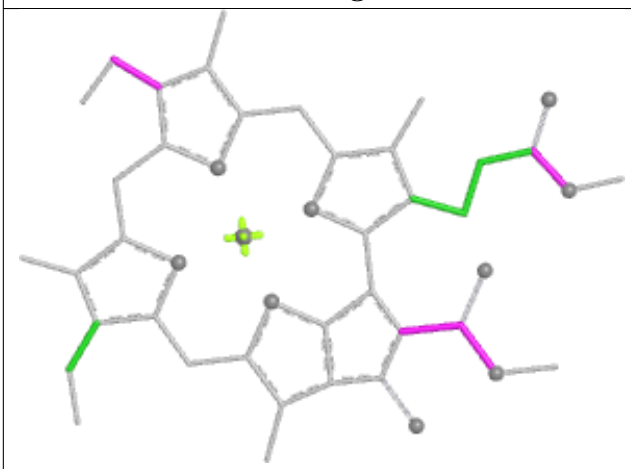


Bond angles



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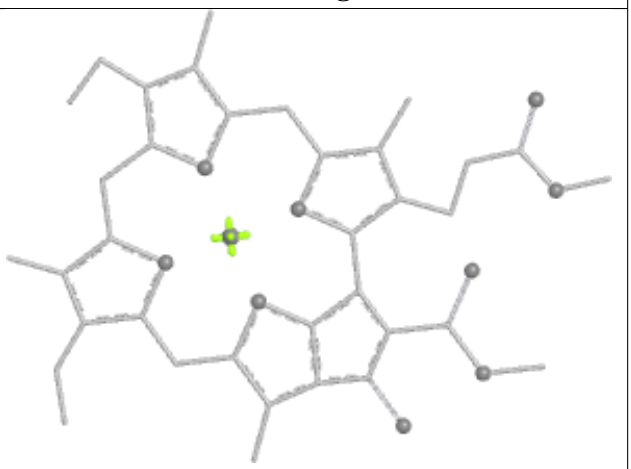
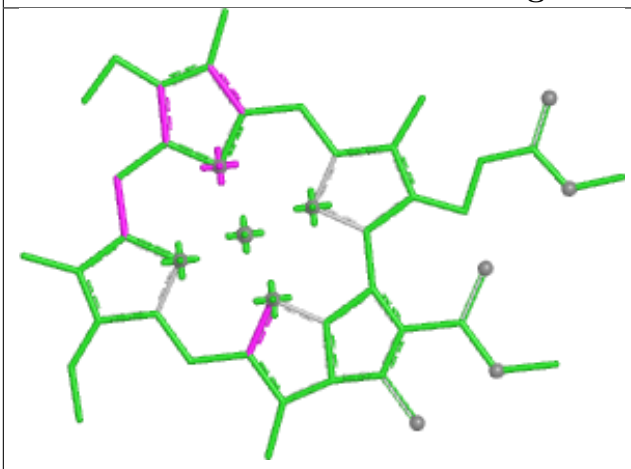
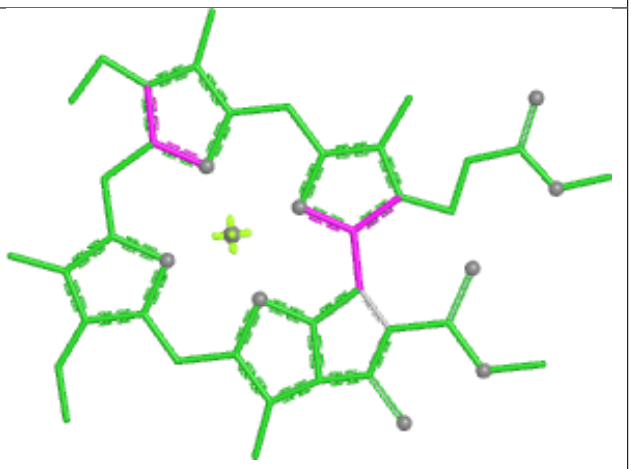


Rings

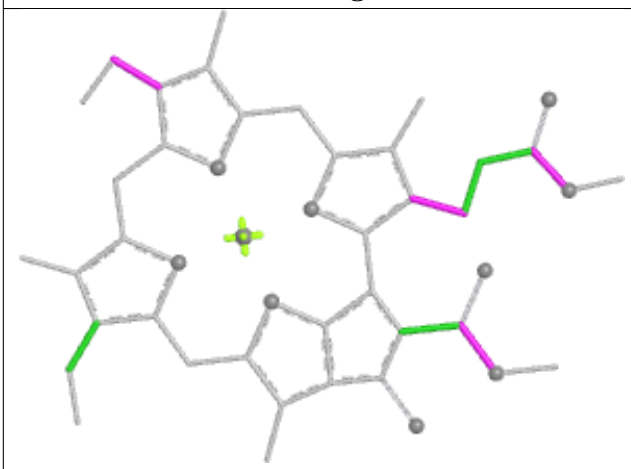
Ligand CLA u 513



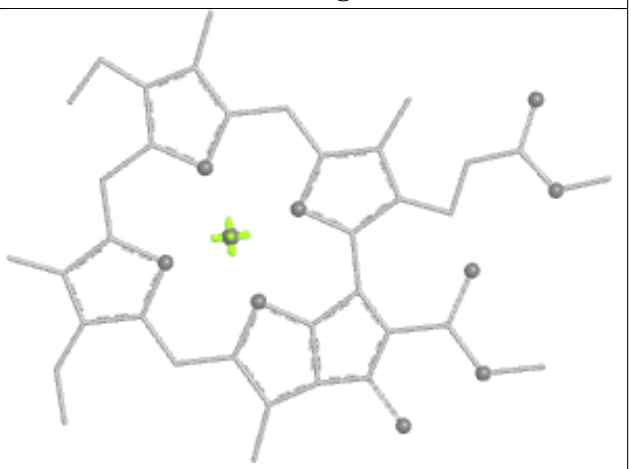
Bond lengths



Bond angles



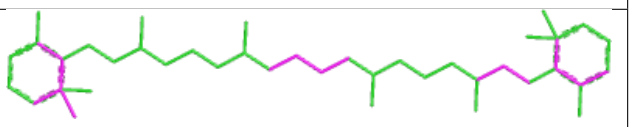
Torsions



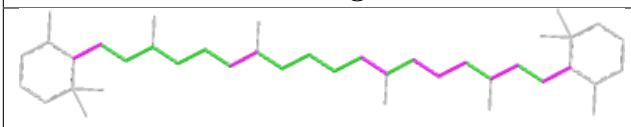
Rings

Ligand BCR J 4013

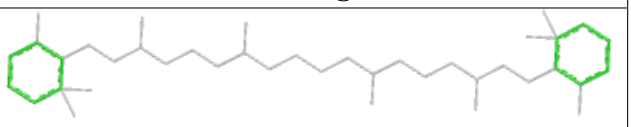
Bond lengths



Bond angles

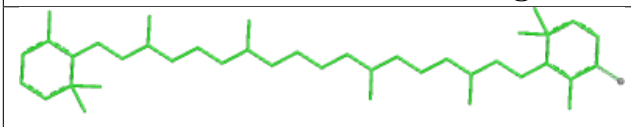


Torsions



Rings

Ligand ECH G 4006



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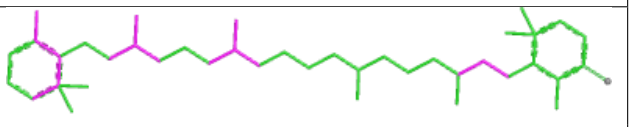
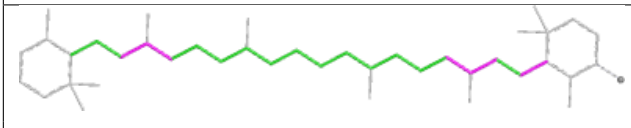
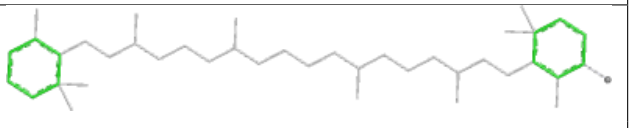


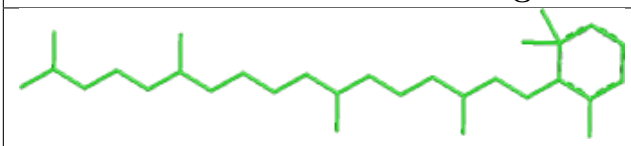
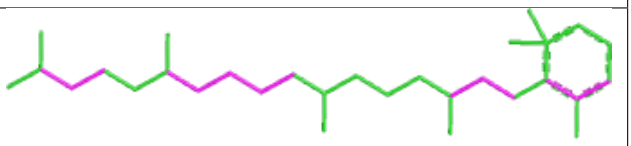
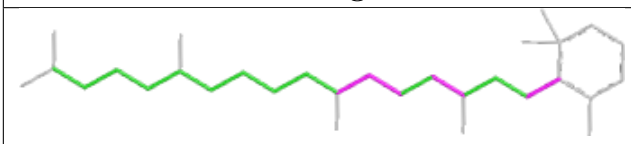
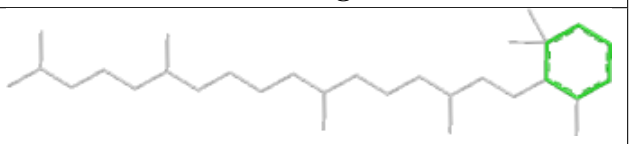
Bond angles

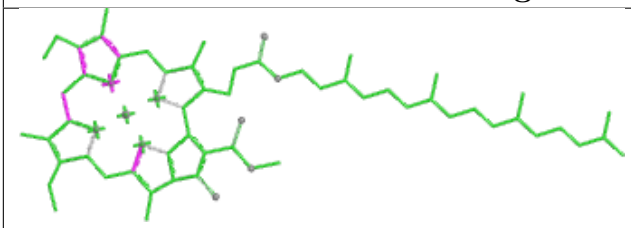
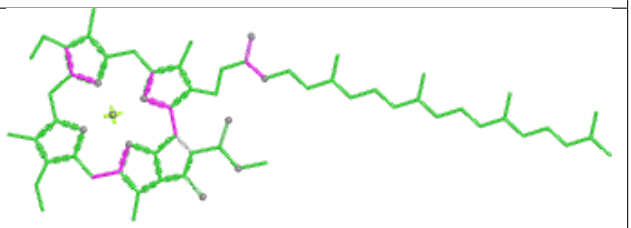
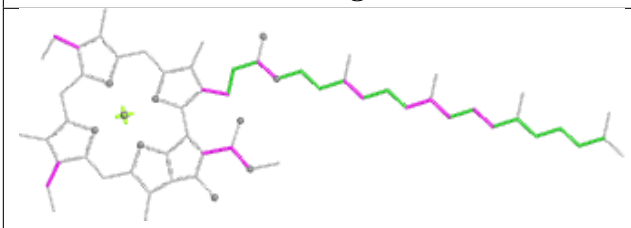
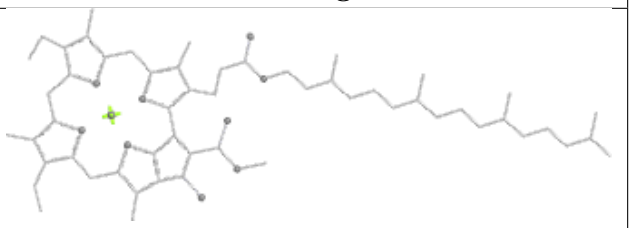


Torsions

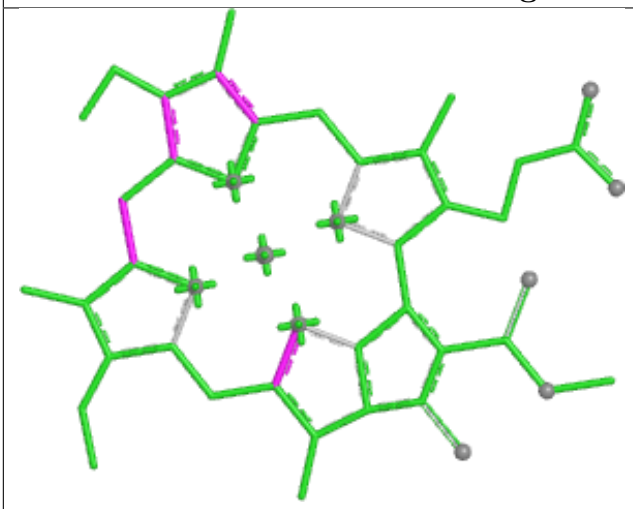


Rings

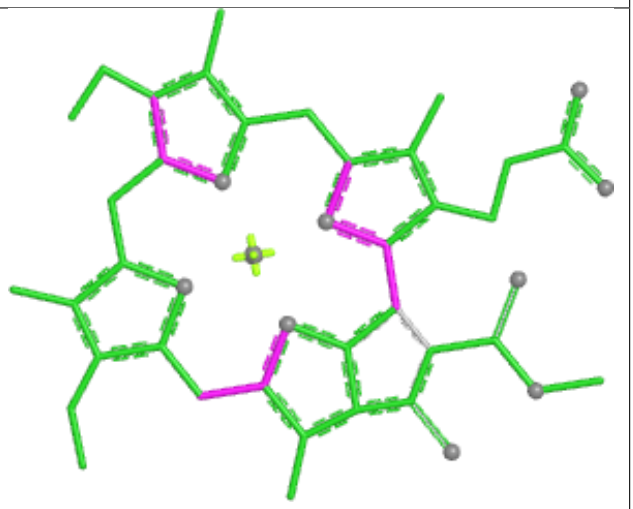
Ligand BCR B 4009	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1210	
 Bond lengths	 Bond angles
 Torsions	 Rings

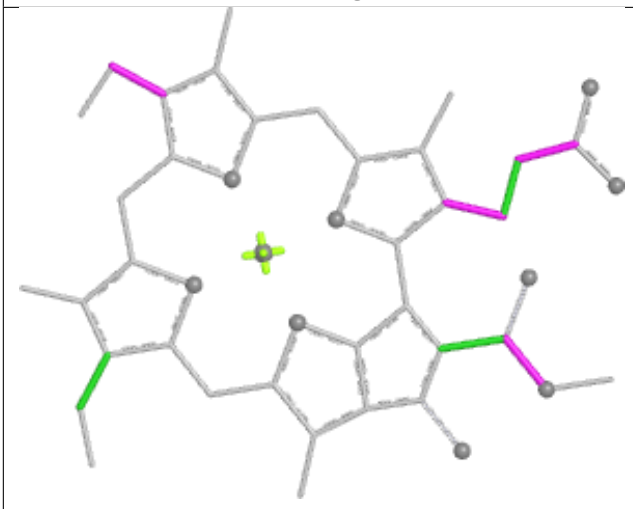
Ligand CLA a 1134



Bond lengths



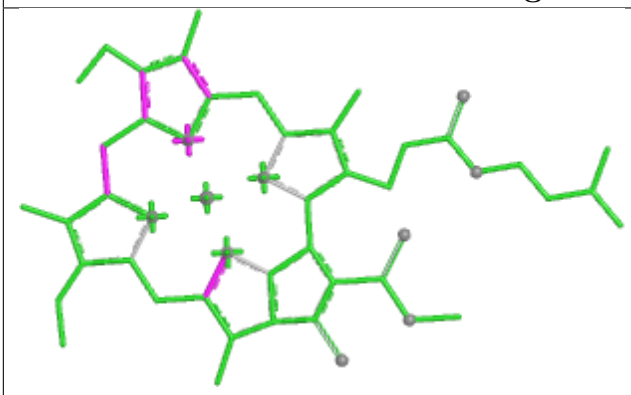
Bond angles



Torsions

Rings

Ligand CLA w 514



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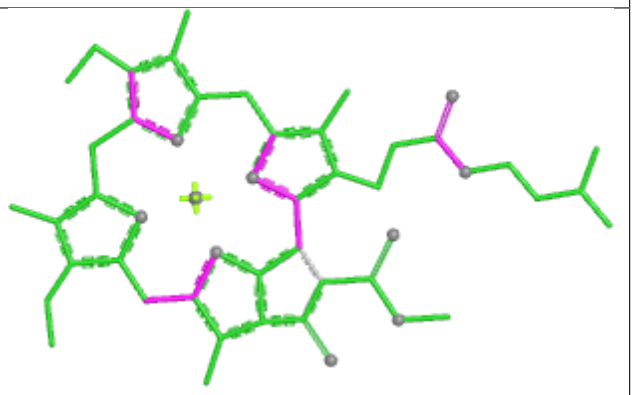

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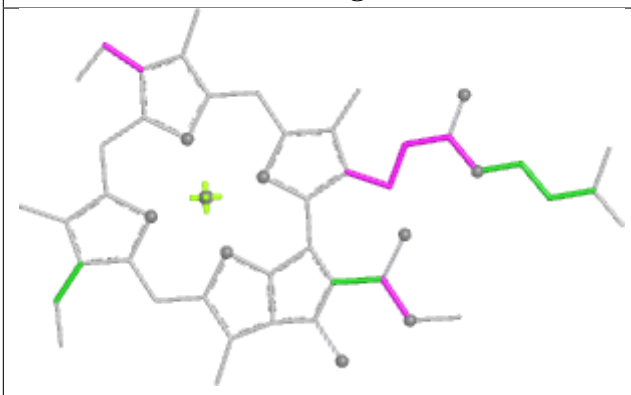

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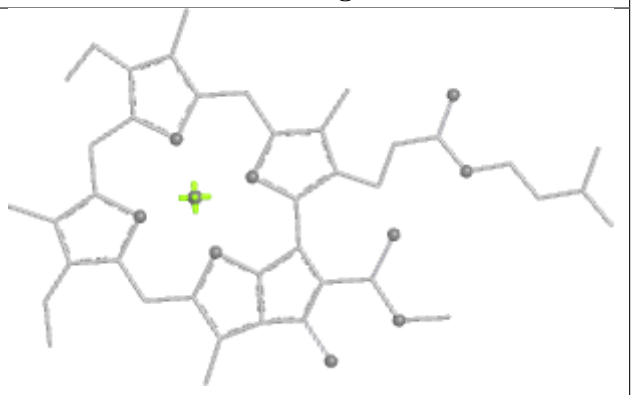
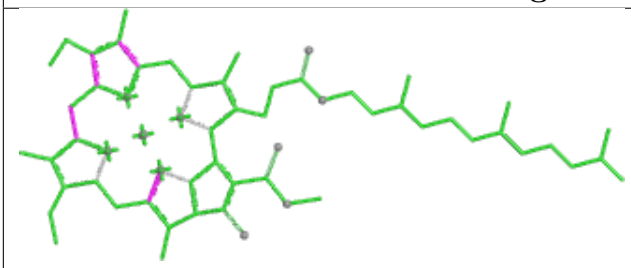


Rings

Ligand CLA s 509



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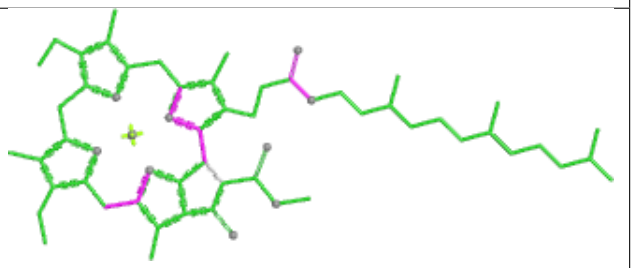
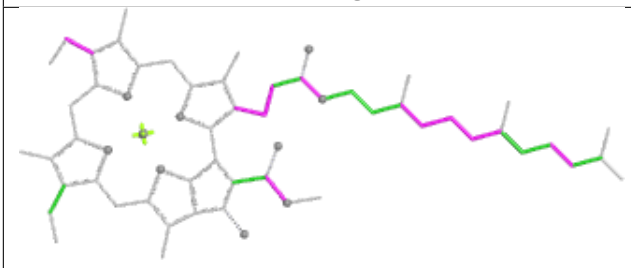
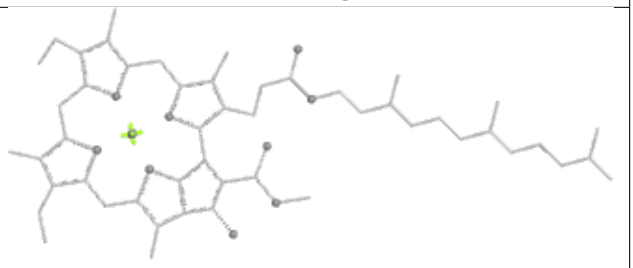


Bond angles

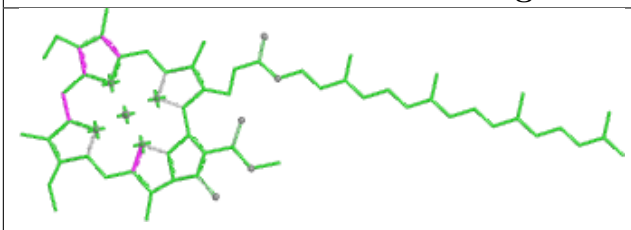


Torsions

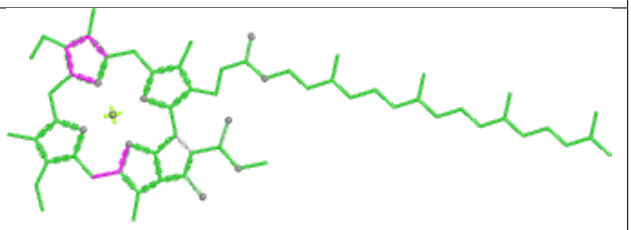


Rings

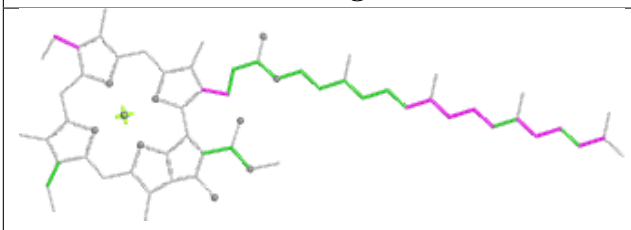
Ligand CLA B 1221



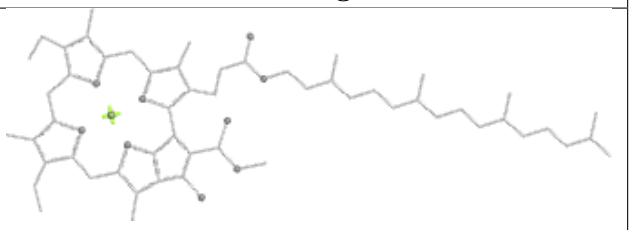
Bond lengths



Bond angles

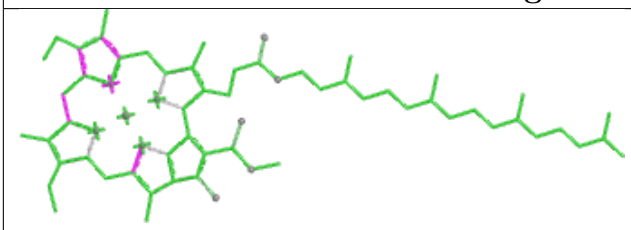


Torsions



Rings

Ligand CLA w 504



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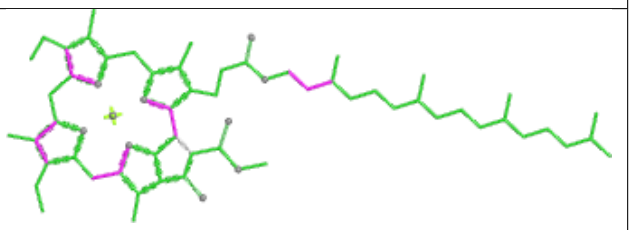
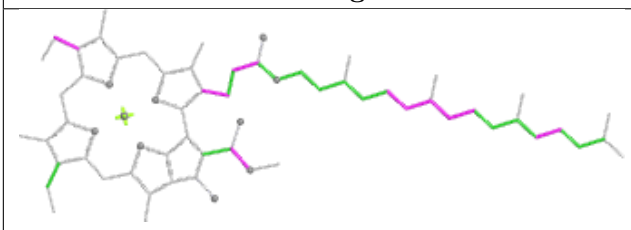


Bond angles



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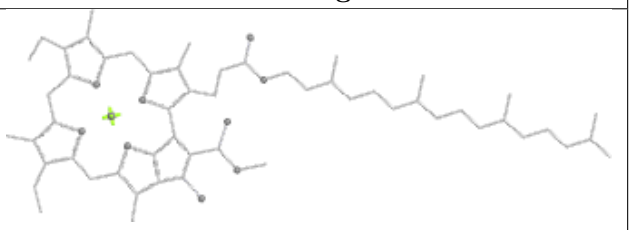
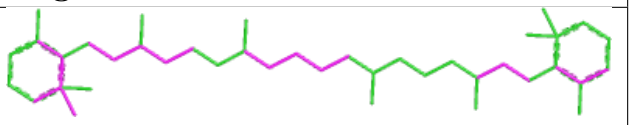


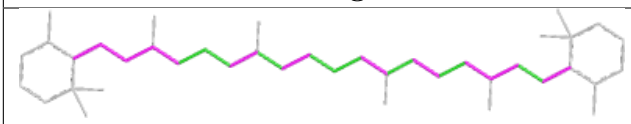
Rings

Ligand BCR g 601

Bond lengths



Bond angles



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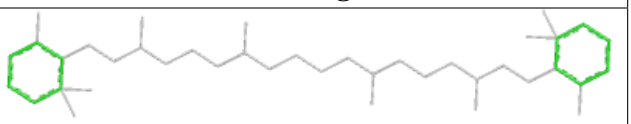
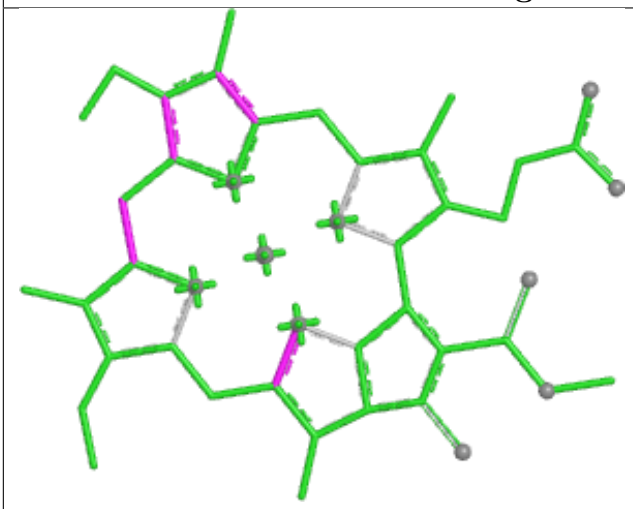


Rings

Ligand CLA B 1230



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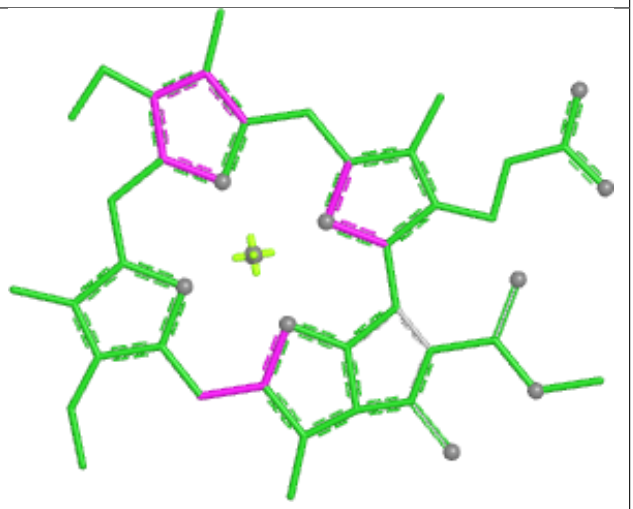
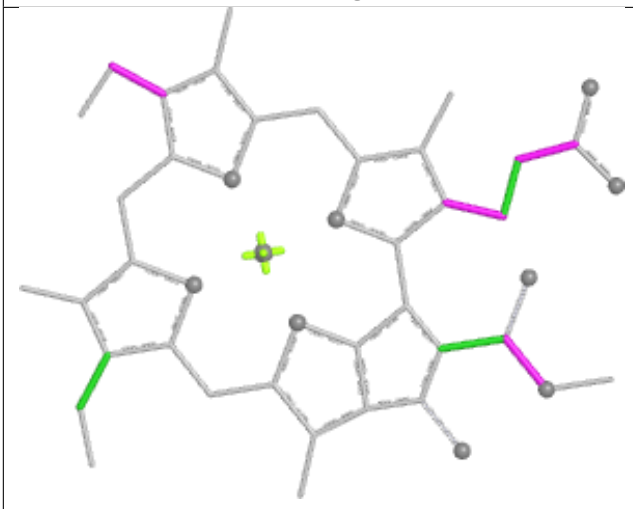


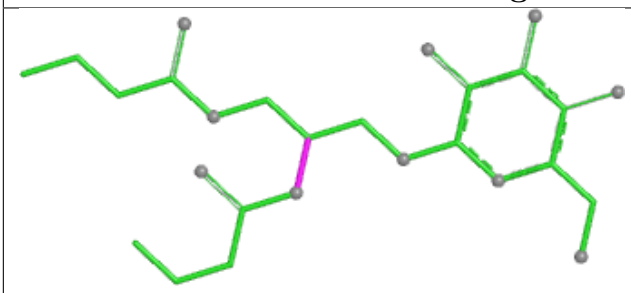
Bond angles



Torsions

Rings

Ligand LMG Q 4017



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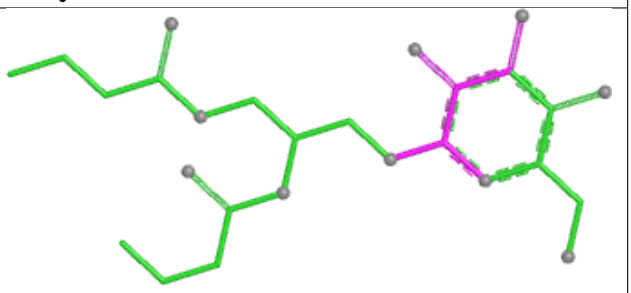
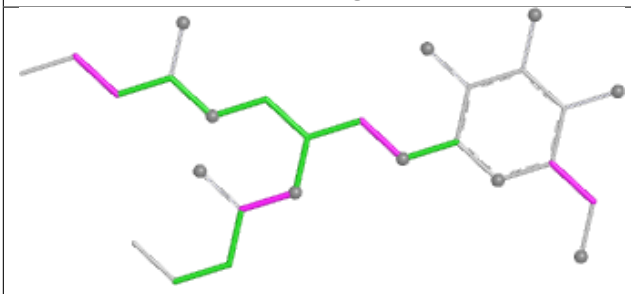
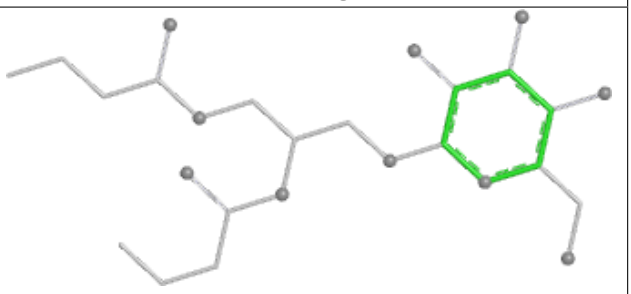


Bond angles

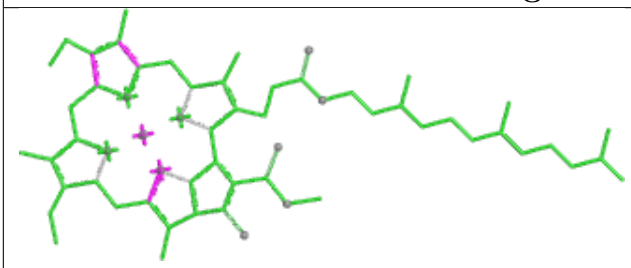


Torsions



Rings

Ligand CLA X 506



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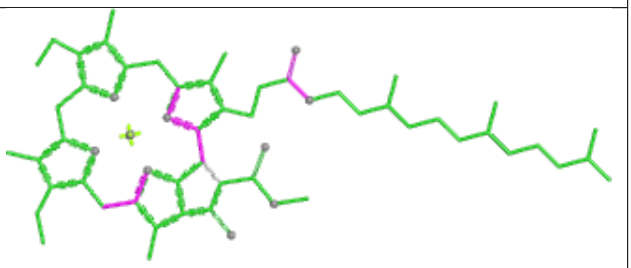
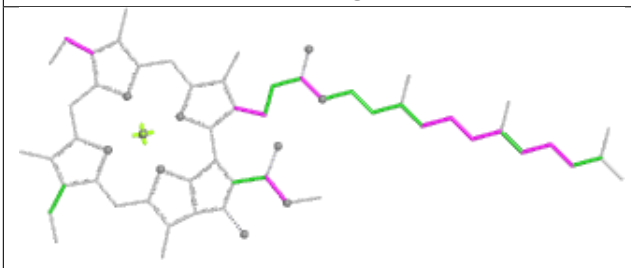
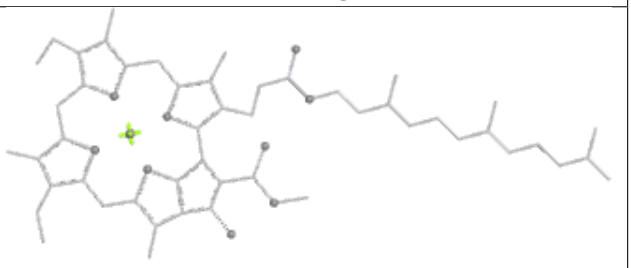


Bond angles

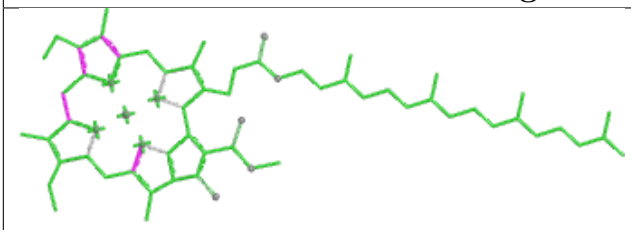


Torsions

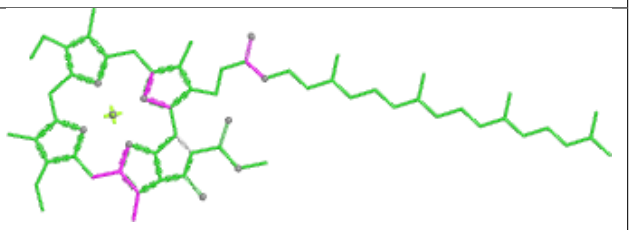


Rings

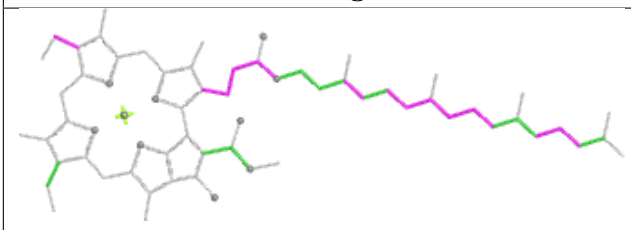
Ligand CLA a 1101



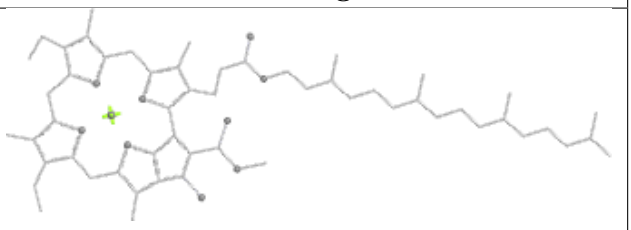
Bond lengths



Bond angles

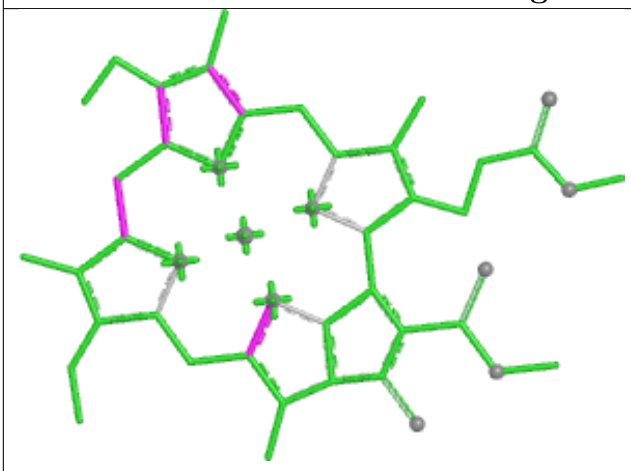


Torsions

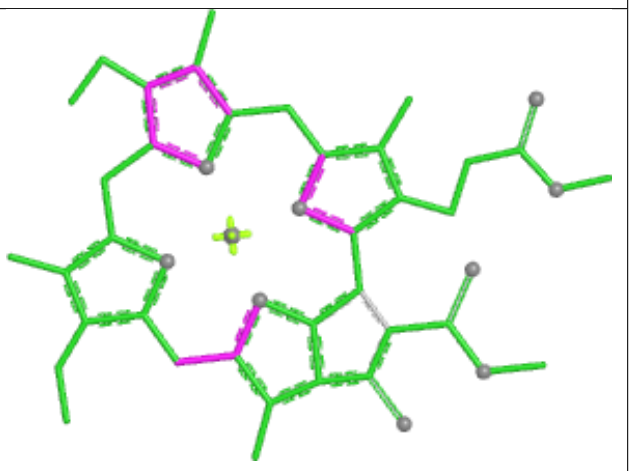


Rings

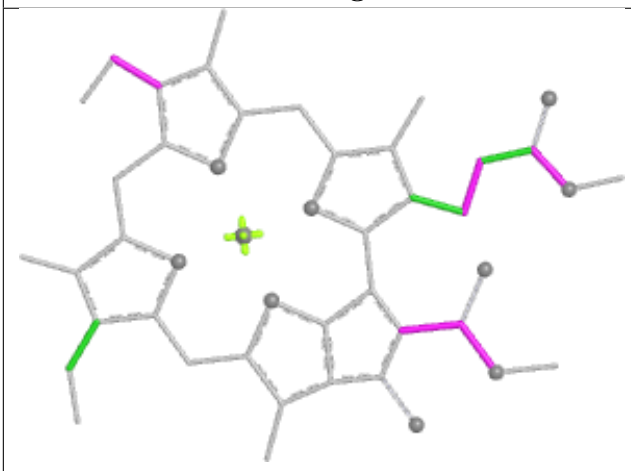
Ligand CLA t 516



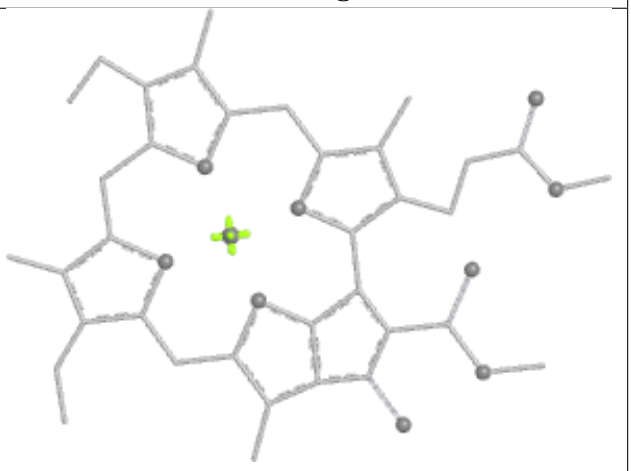
Bond lengths



Bond angles

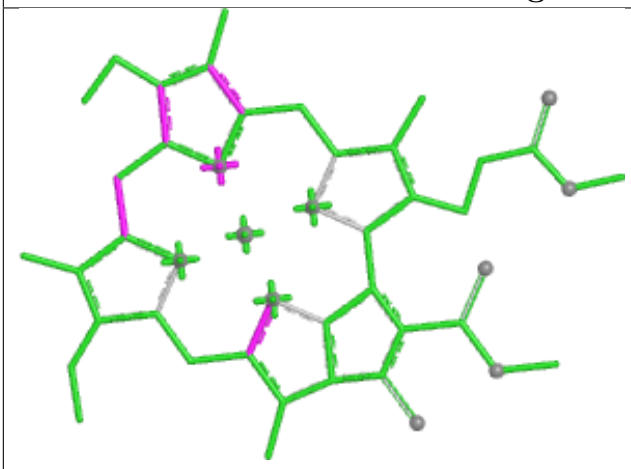


Torsions



Rings

Ligand CLA u 516



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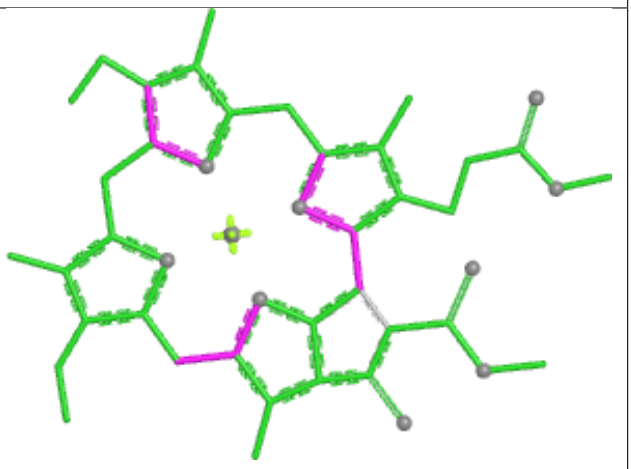

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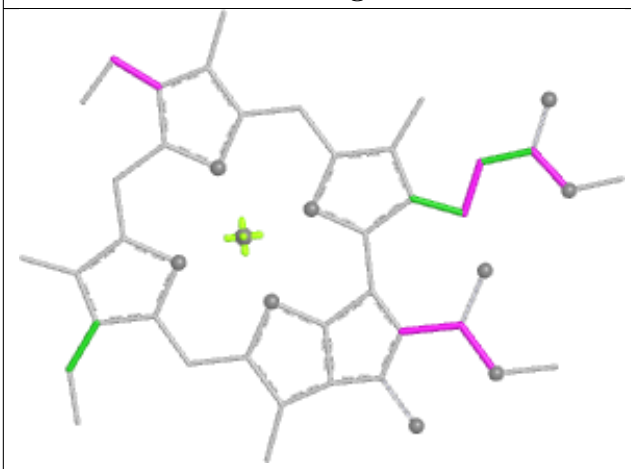

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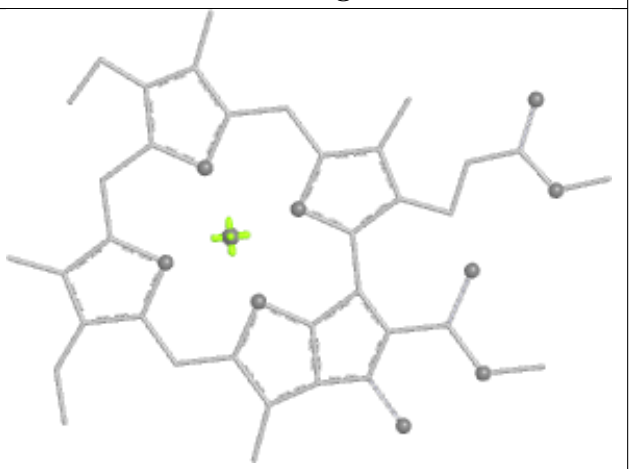
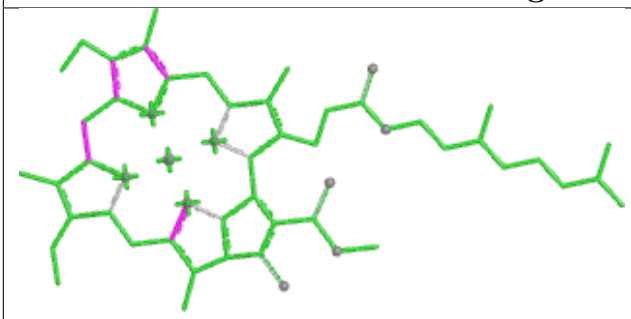


Rings

Ligand CLA p 517



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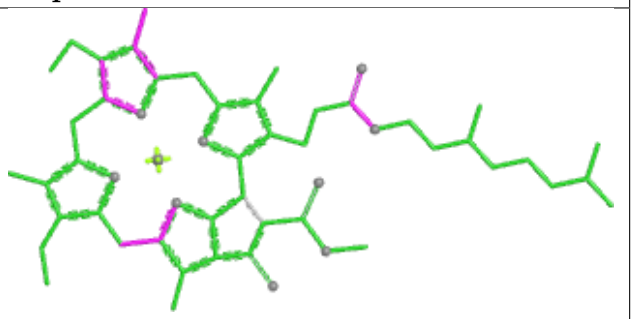

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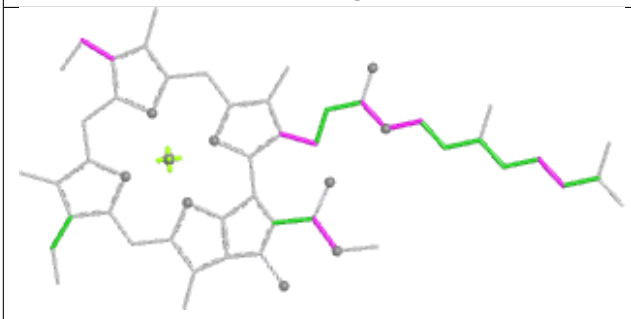

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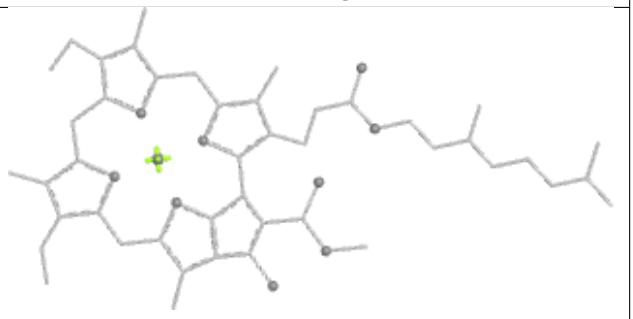
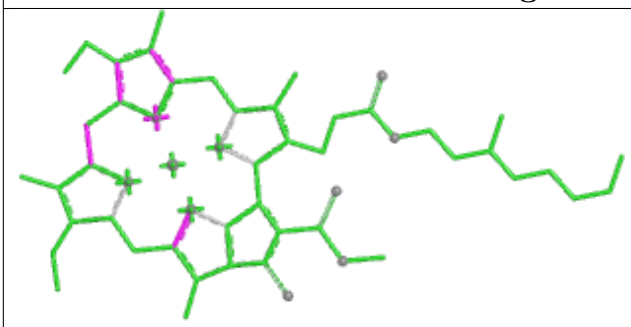


Rings

Ligand CLA a 1115



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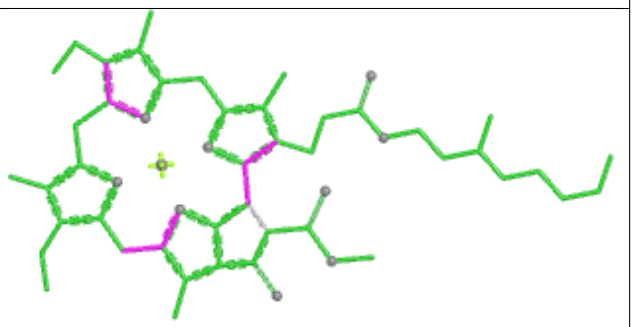

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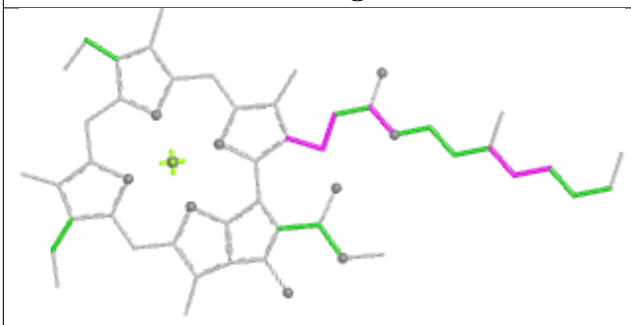

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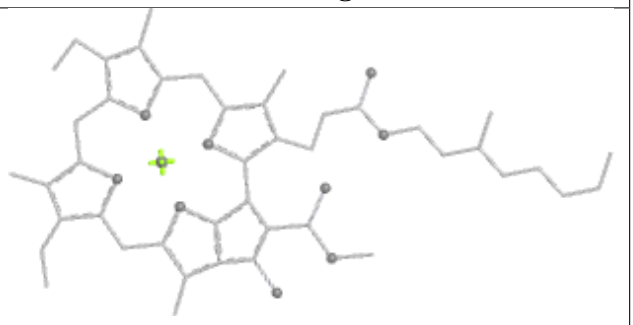
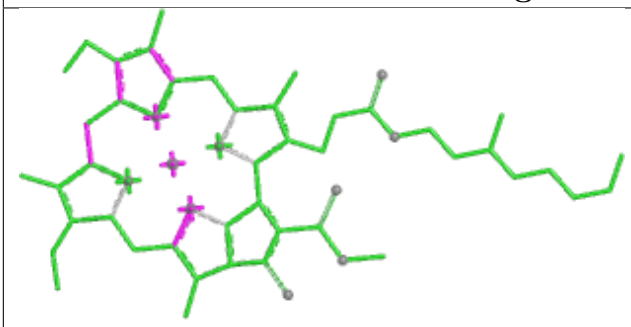


Rings

Ligand CLA A 1133



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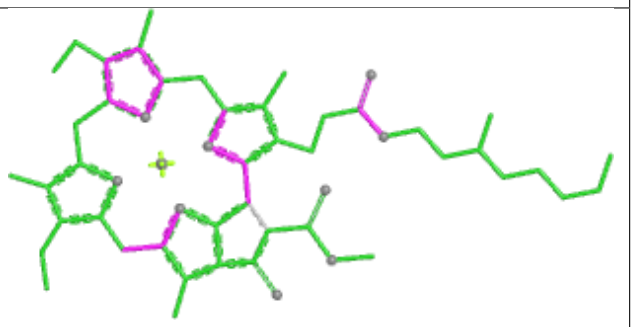
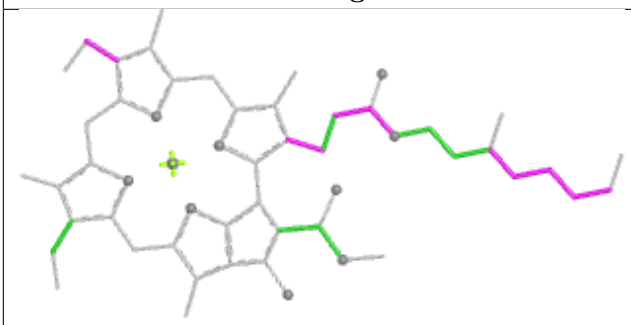


Bond angles



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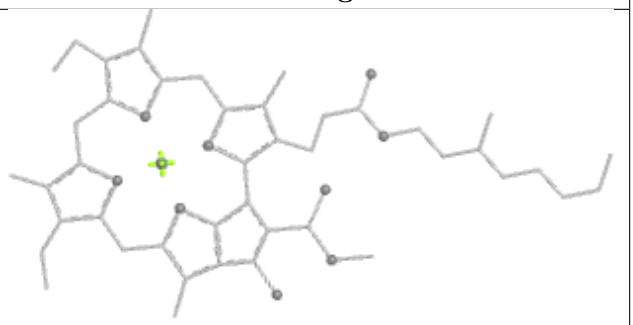
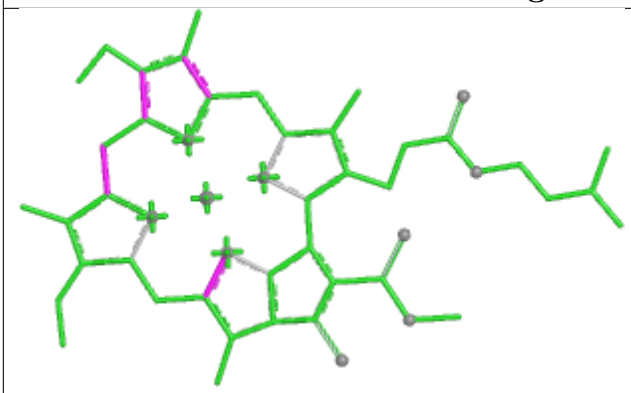


Rings

Ligand CLA q 513



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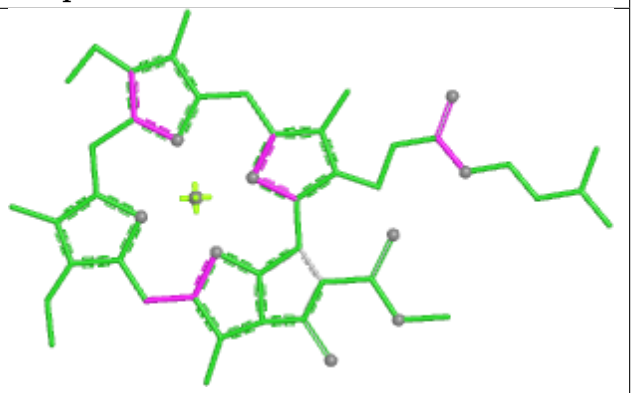
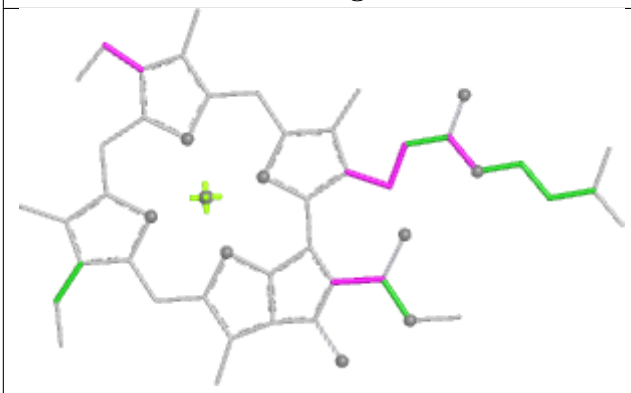


Bond angles



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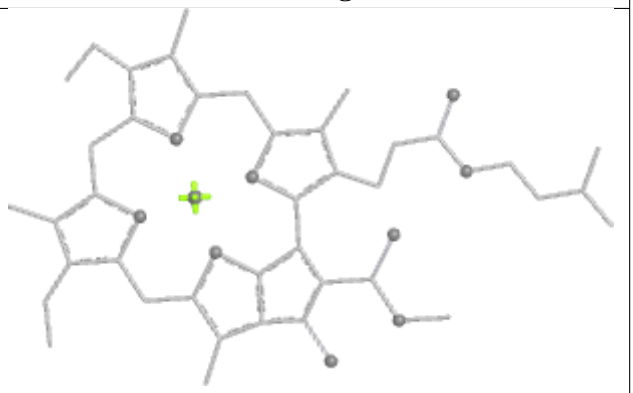
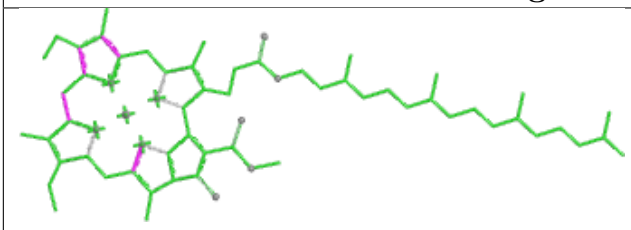


Rings

Ligand CLA g 504



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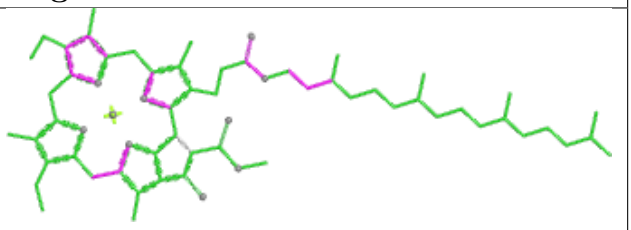
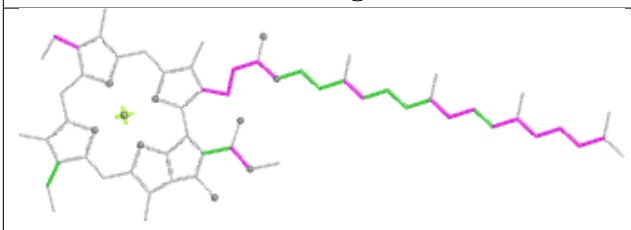


Bond angles



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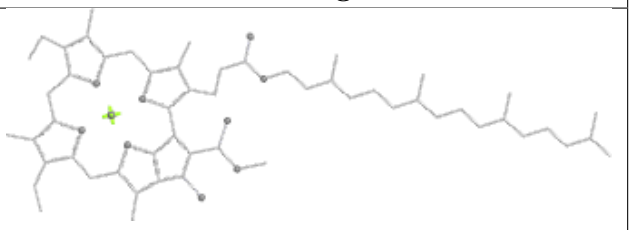
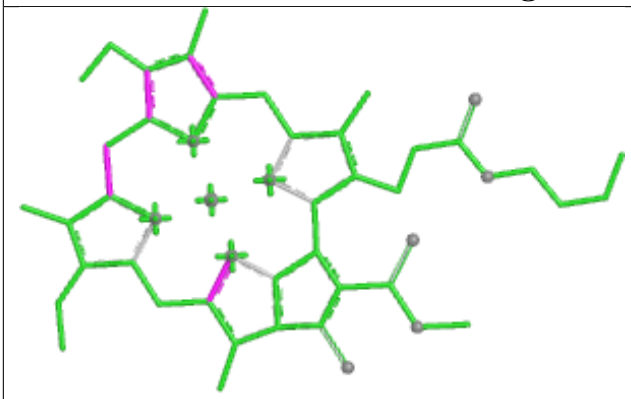


Rings

Ligand CLA a 1120



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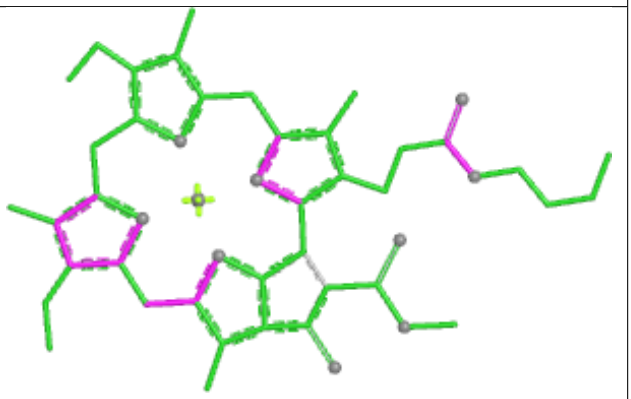

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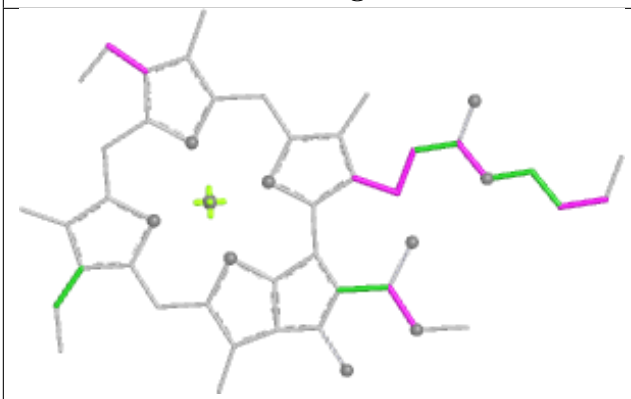

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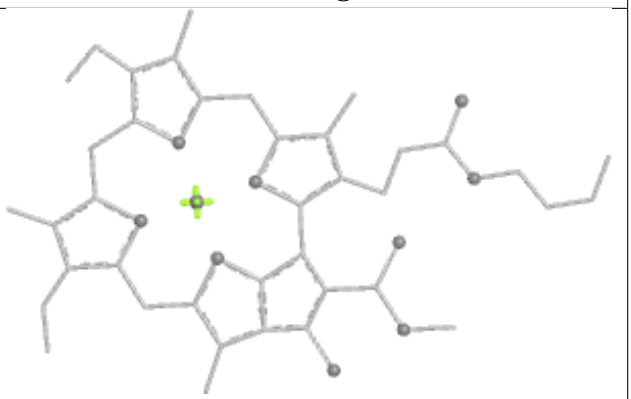
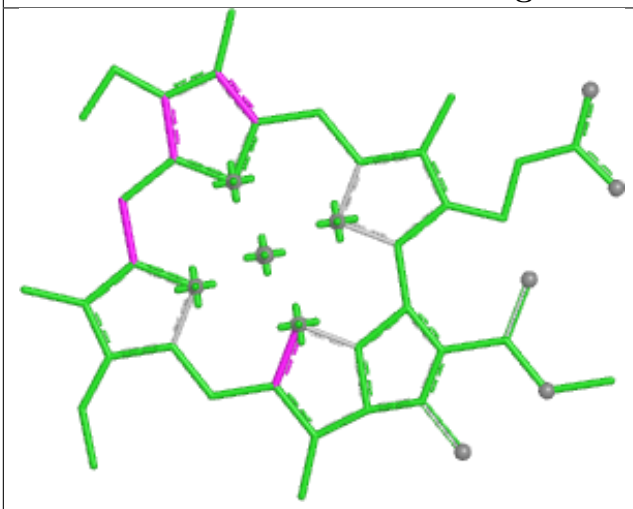


Rings

Ligand CLA B 1231



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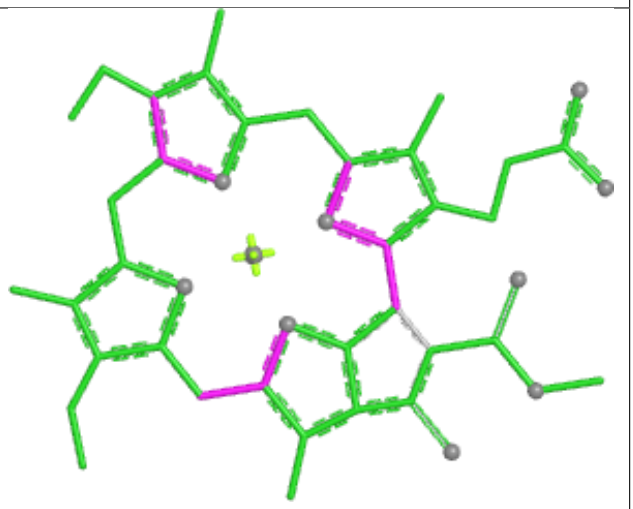

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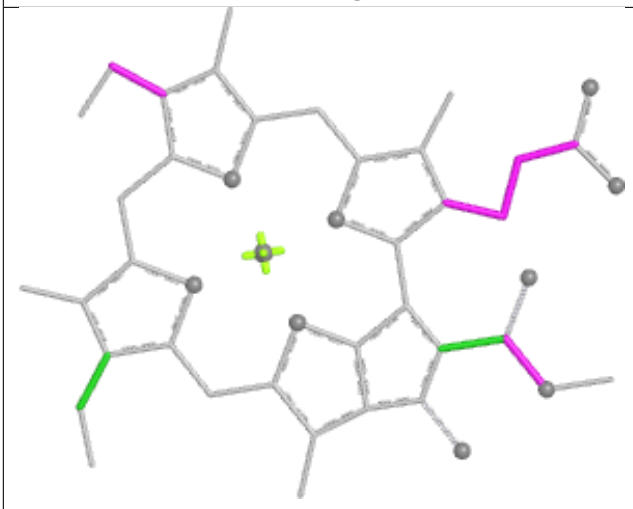
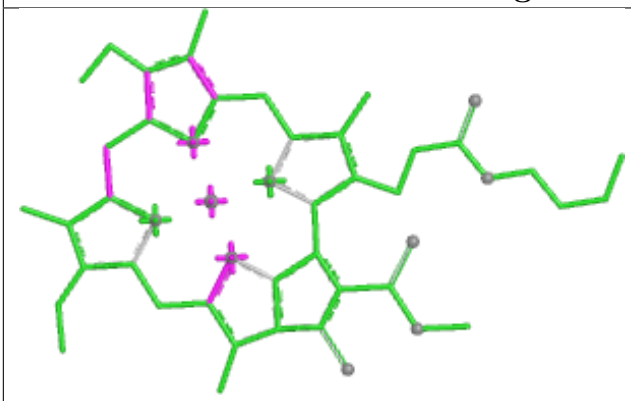


Torsions

Rings

Ligand CLA G 1227



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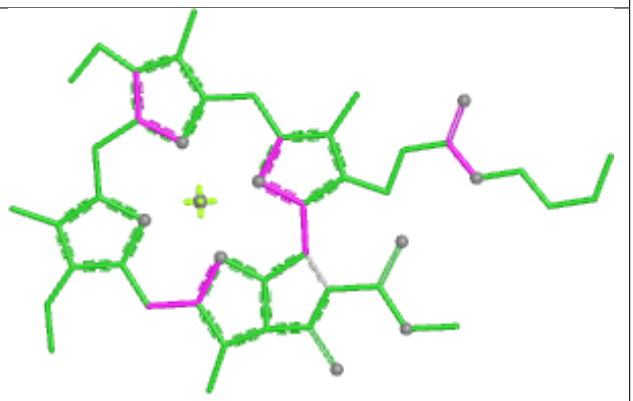

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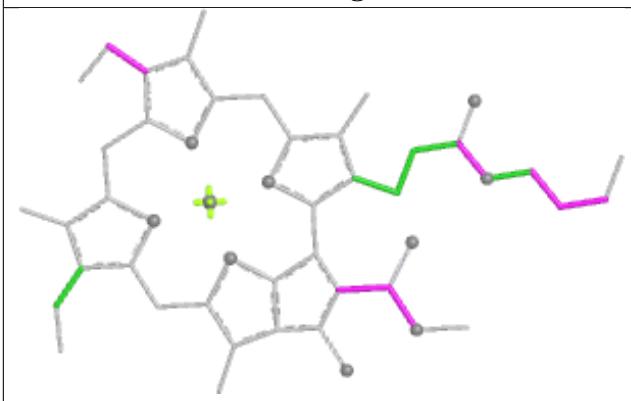

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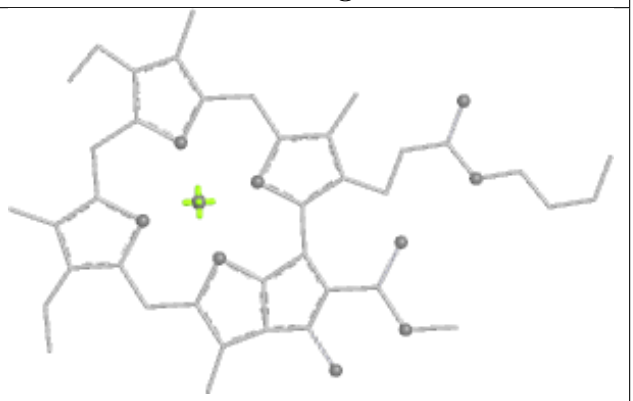
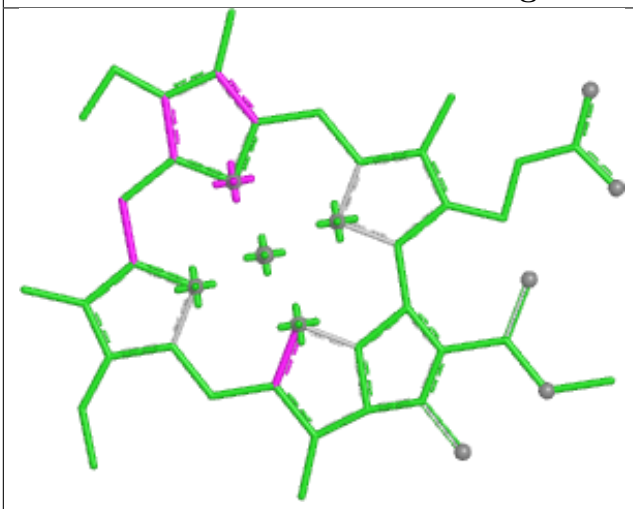


Rings

Ligand CLA a 1112



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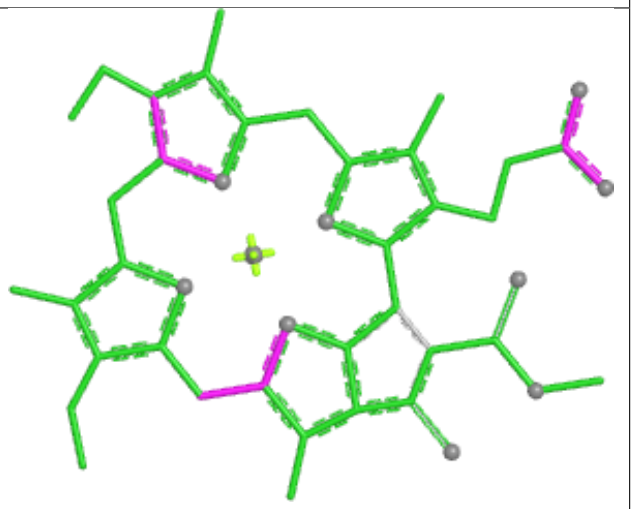

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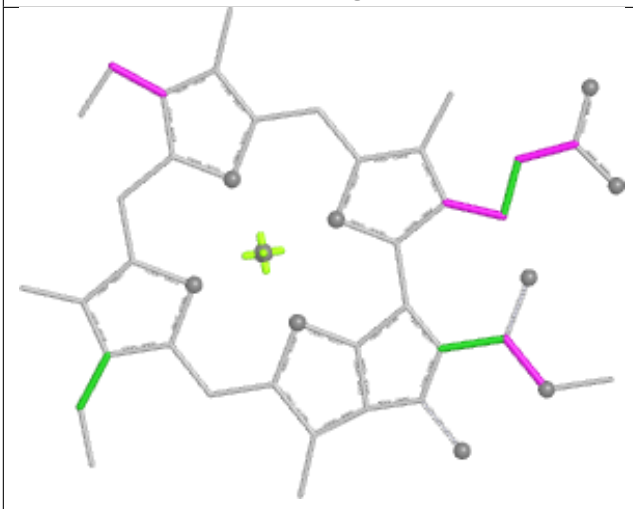
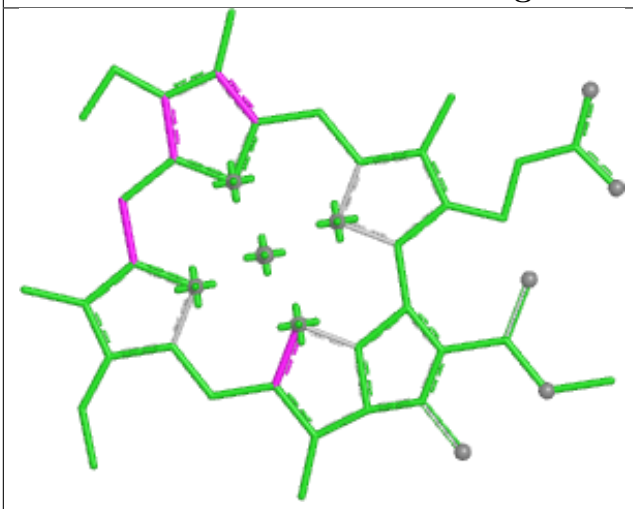


Torsions

Rings

Ligand CLA K 4002



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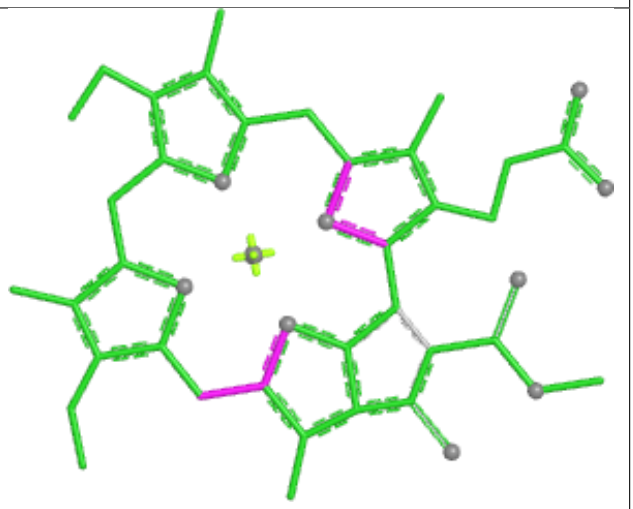

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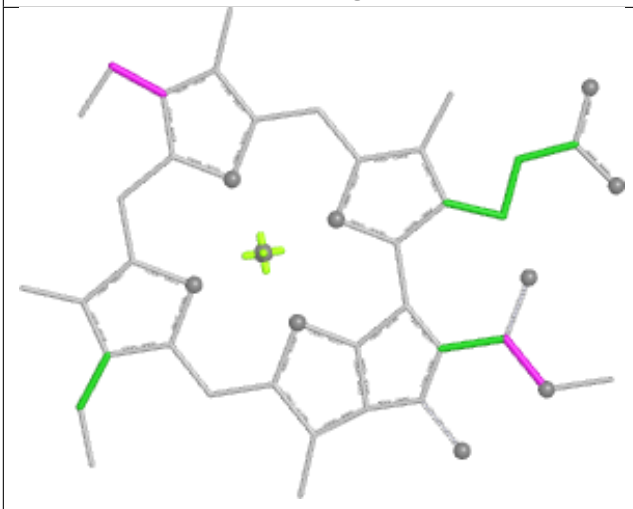
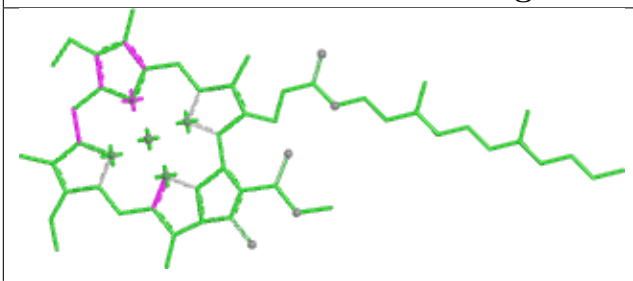


Torsions

Rings

Ligand CLA A 1105



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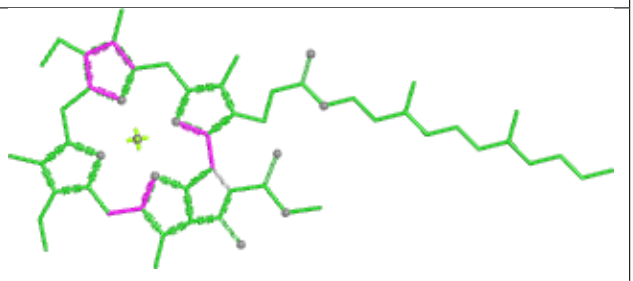

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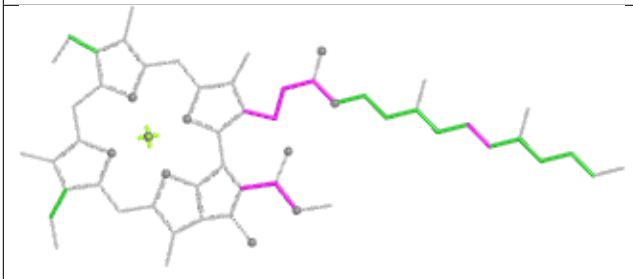

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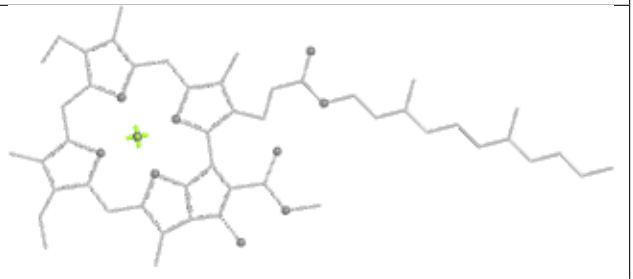
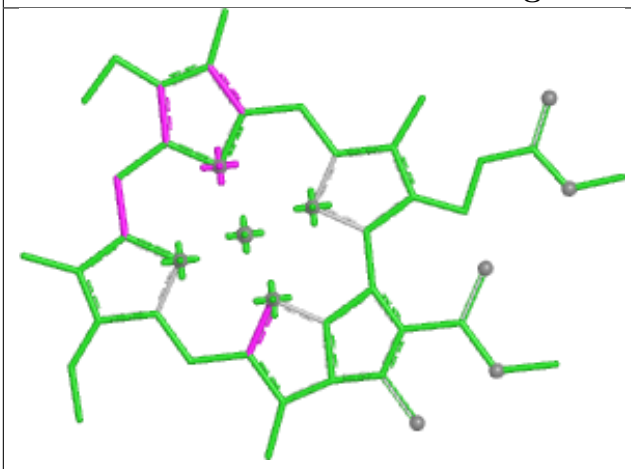


Rings

Ligand CLA X 516



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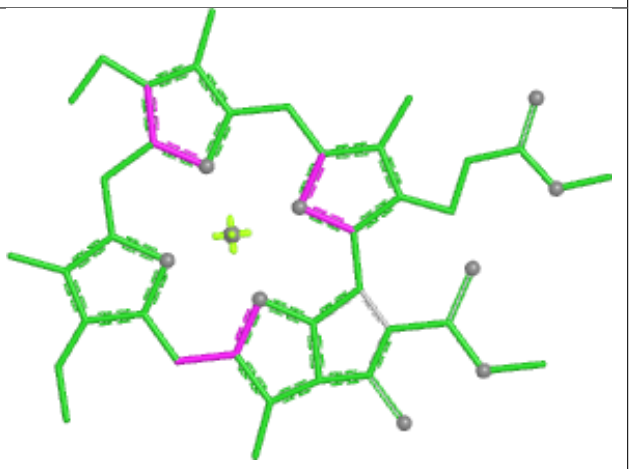
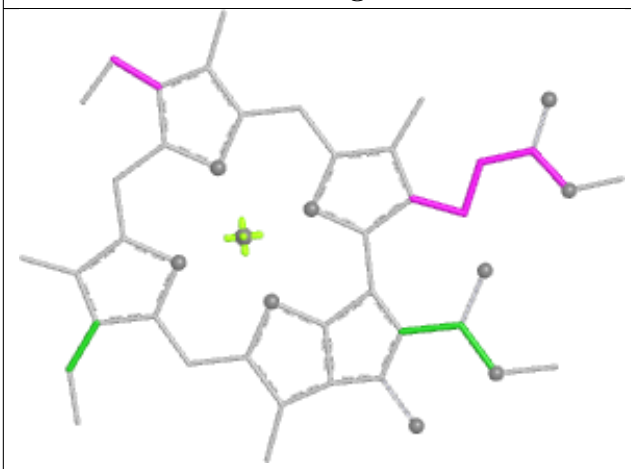


Bond angles



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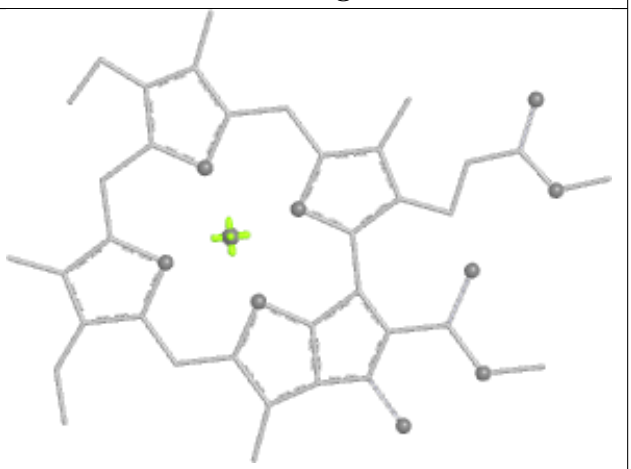
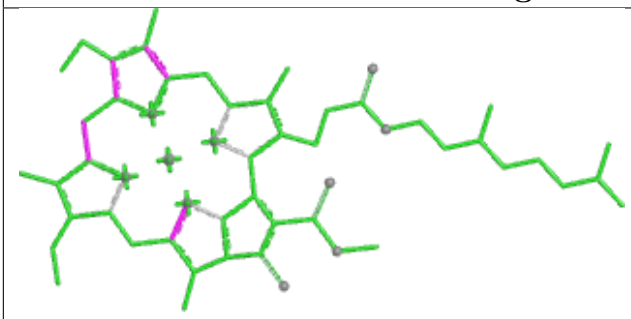
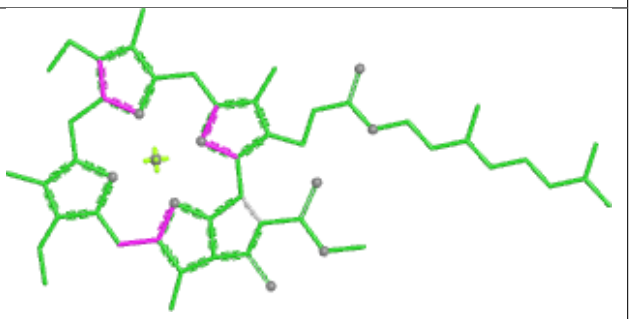
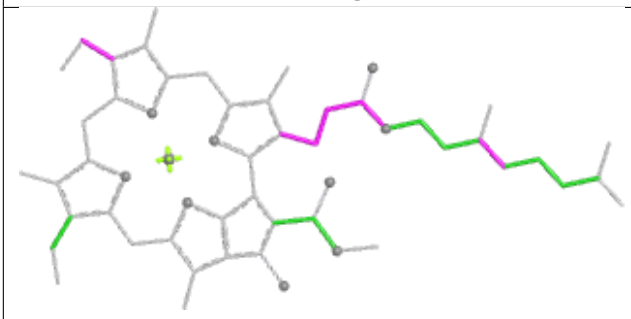
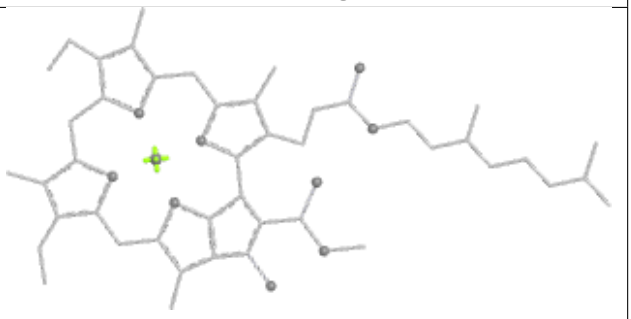
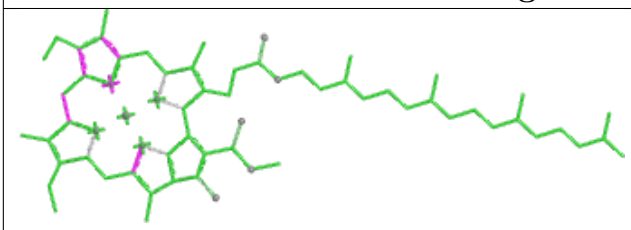
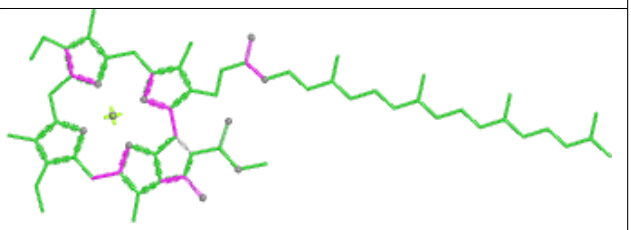
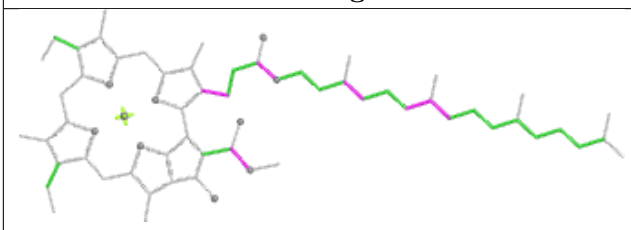
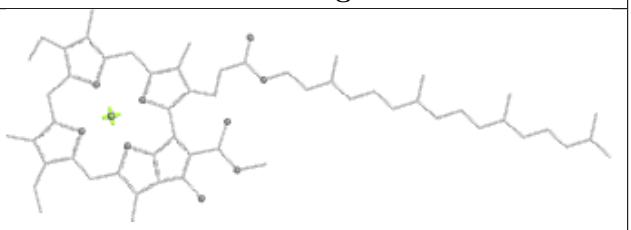
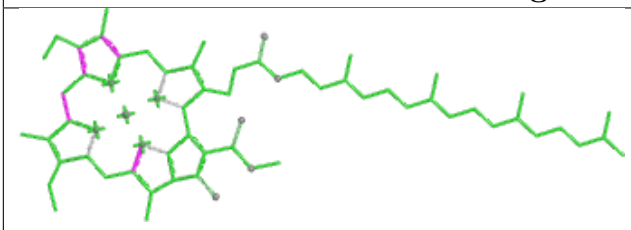


Rings

Ligand CLA A 1118	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1210	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s 515



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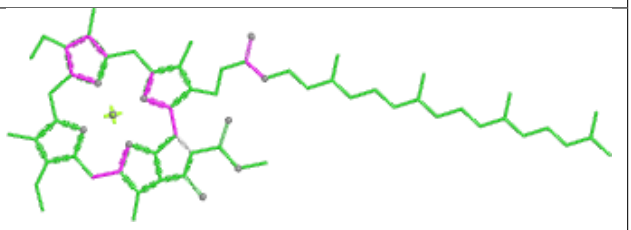
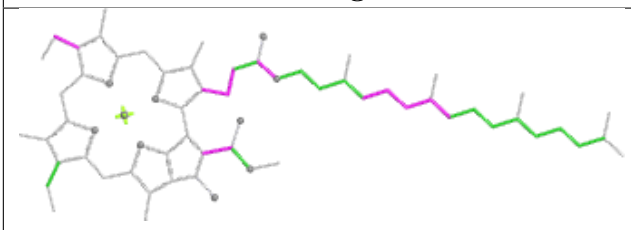
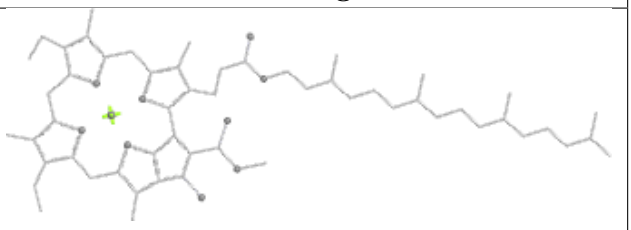


Bond angles

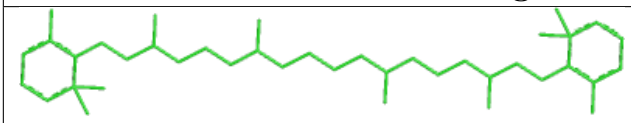


Torsions



Rings

Ligand BCR H 4011



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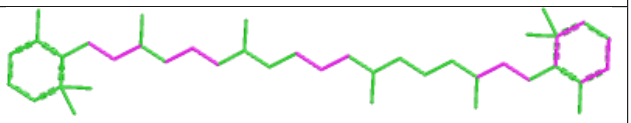

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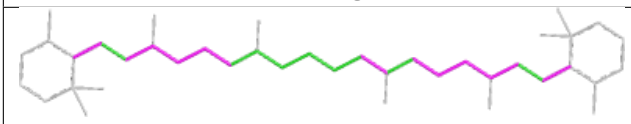

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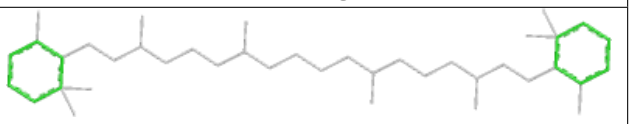
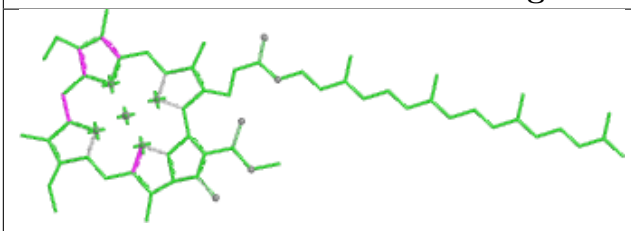


Rings

Ligand CLA p 510



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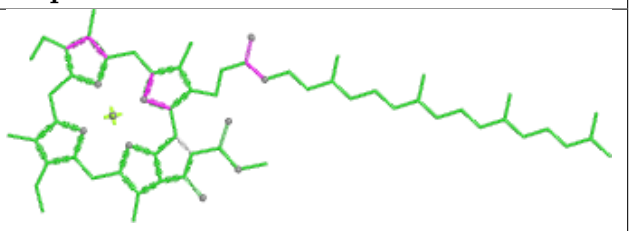
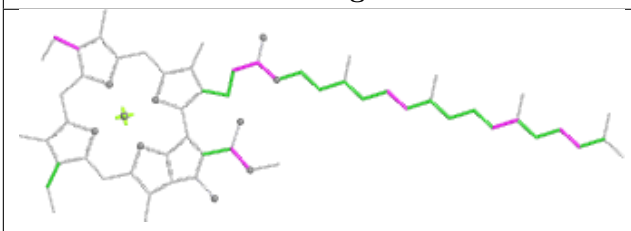
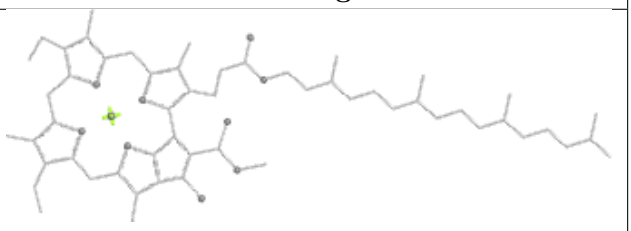


Bond angles

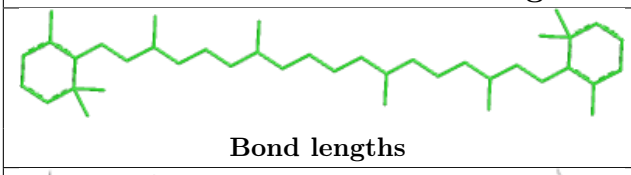


Torsions



Rings

Ligand BCR y 603



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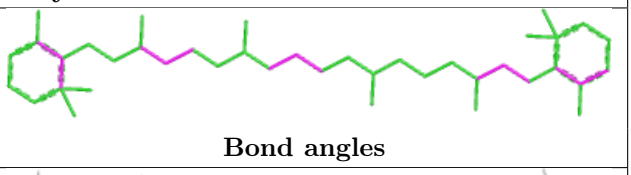

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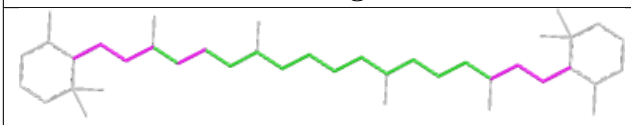

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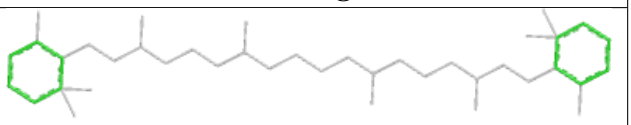
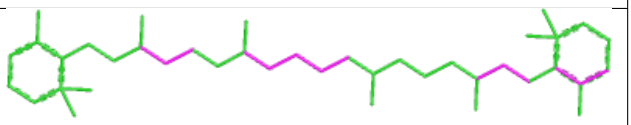


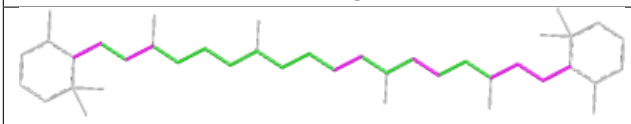
Rings

Ligand BCR B 4004

Bond lengths



Bond angles



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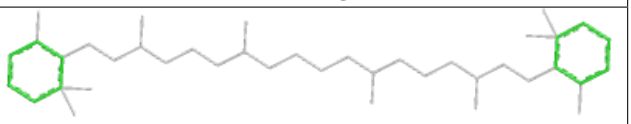
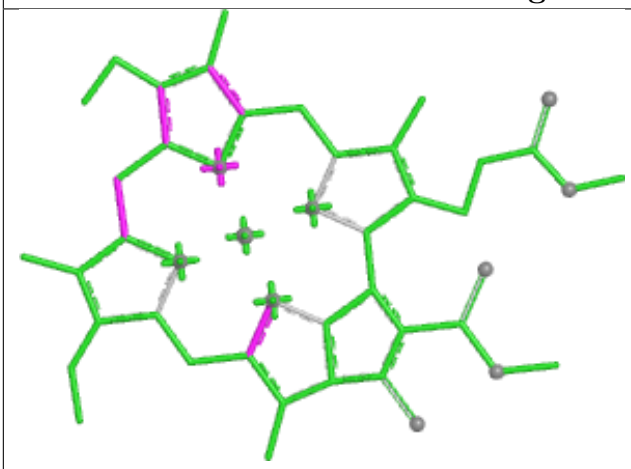


Rings

Ligand CLA o 503



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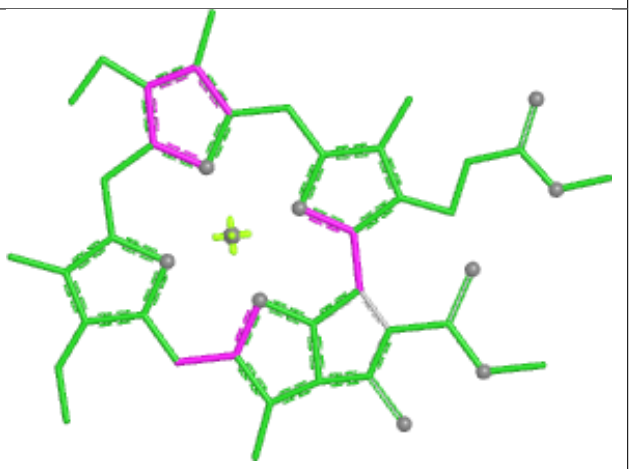
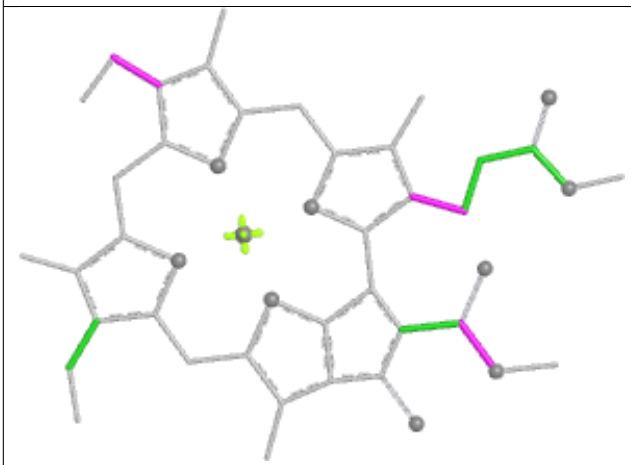


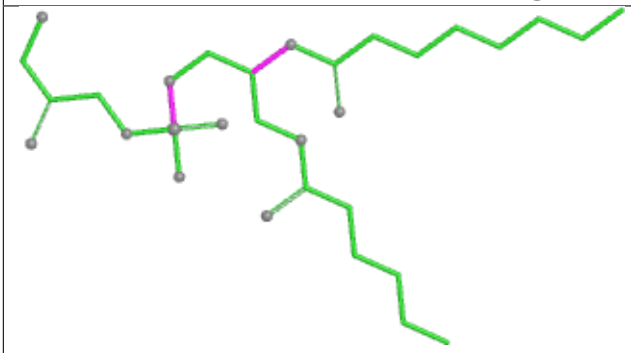
Bond angles



Torsions

Rings

Ligand LHG r 605



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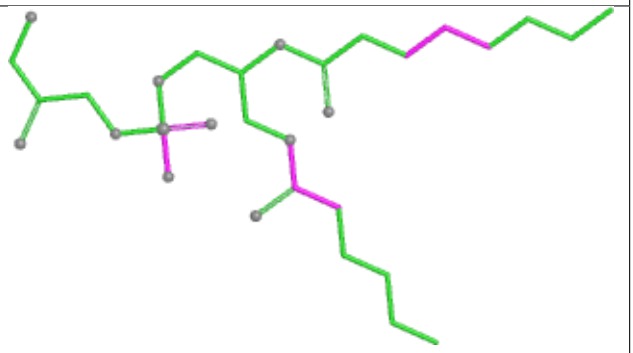
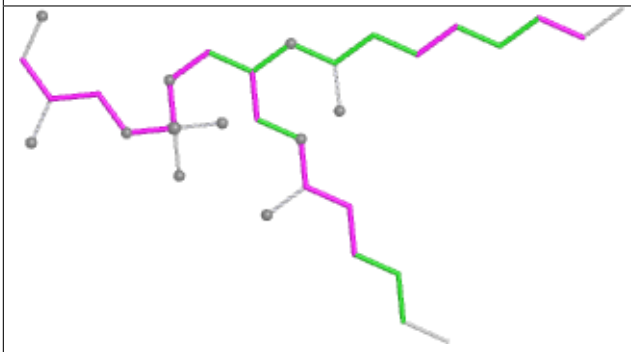


Bond angles



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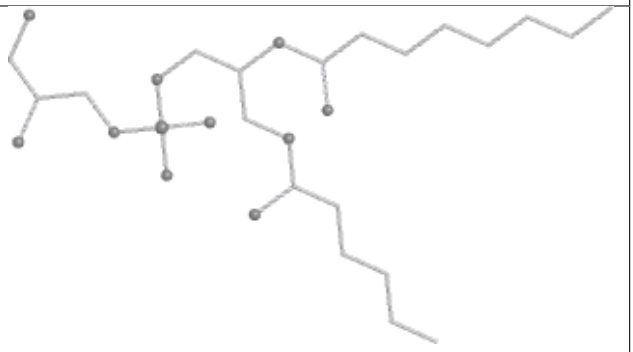
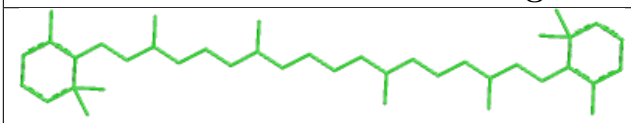


Rings

Ligand BCR v 601



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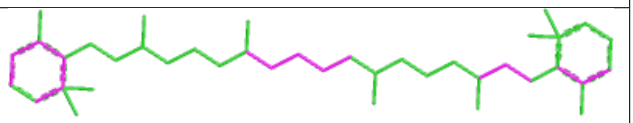
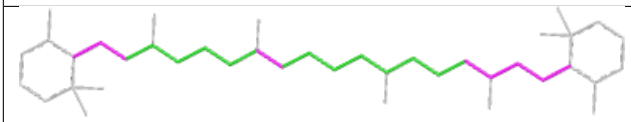


Bond angles



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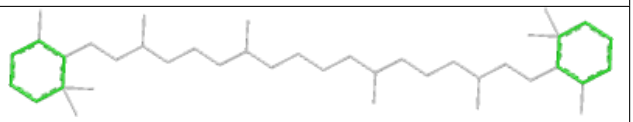
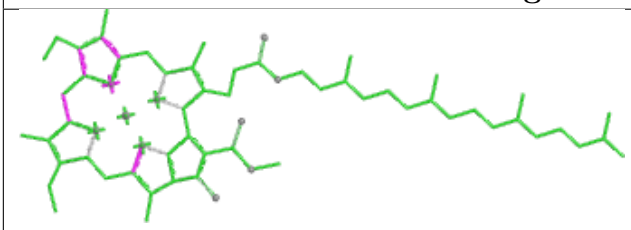


Rings

Ligand CLA Y 505



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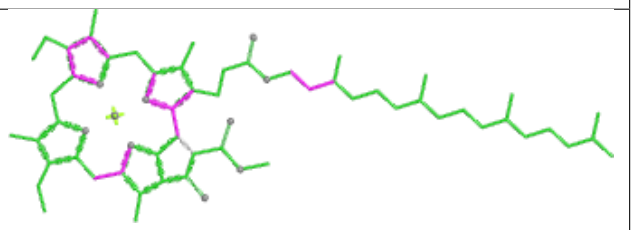
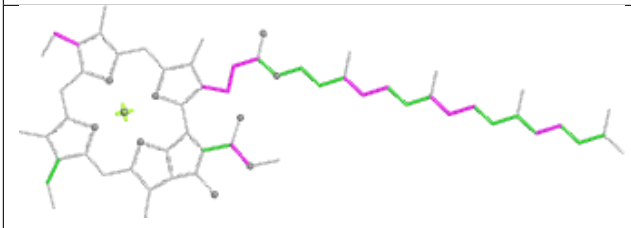


Bond angles



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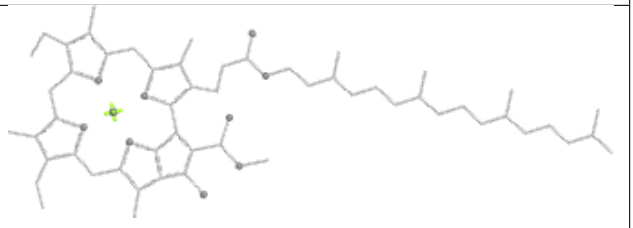
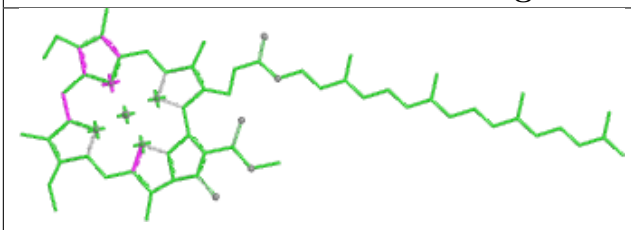


Rings

Ligand CLA A 1022



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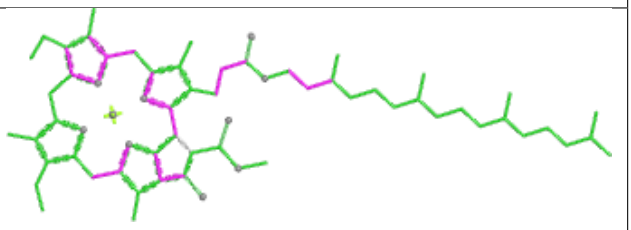
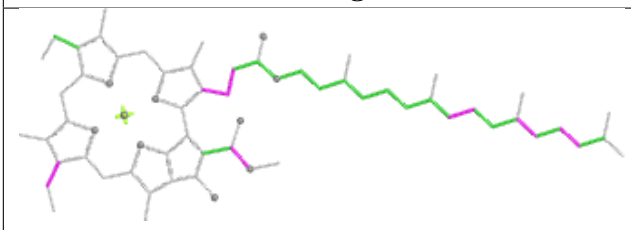


Bond angles



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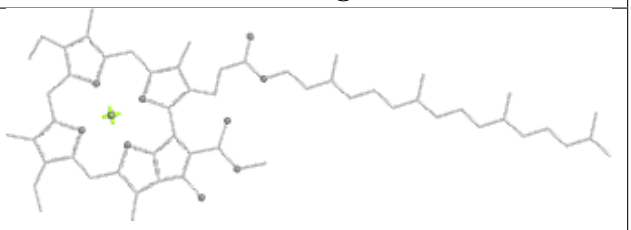
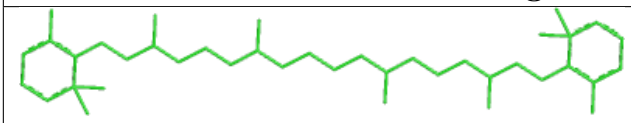


Rings

Ligand BCR p 604



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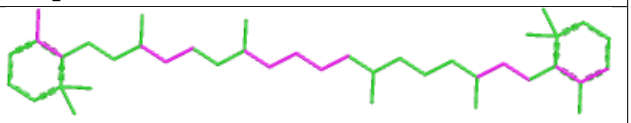
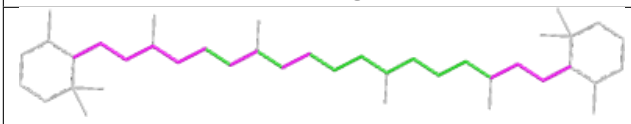


Bond angles



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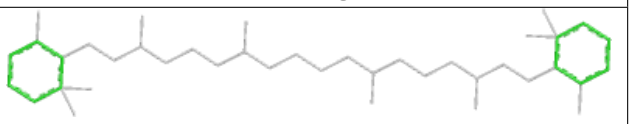
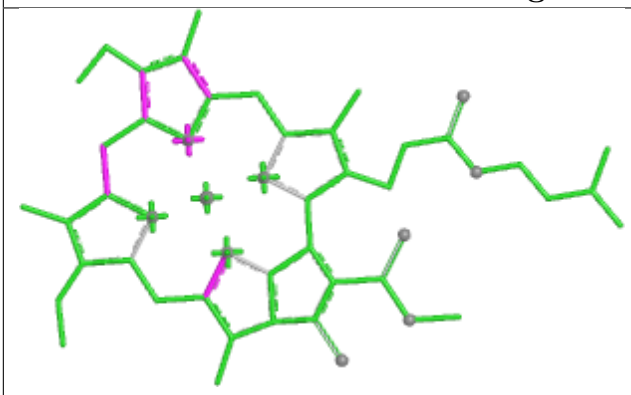


Rings

Ligand CLA q 514



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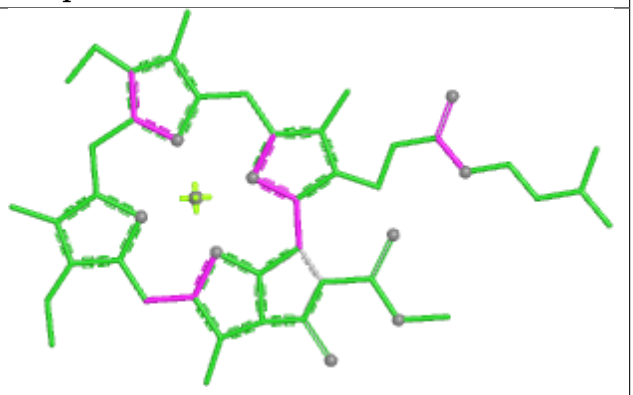
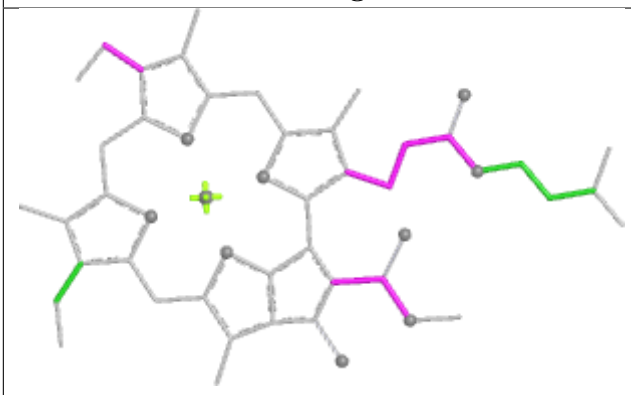


Bond angles



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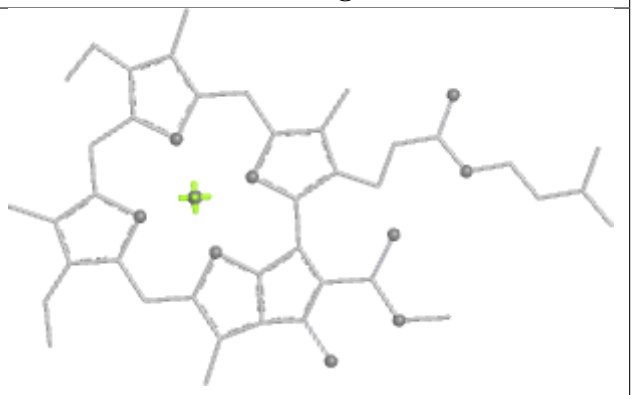
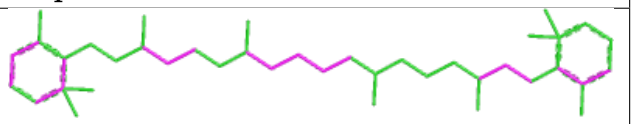


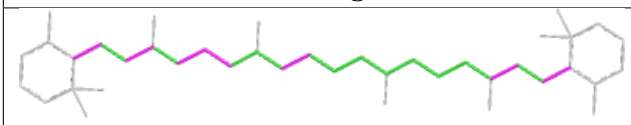
Rings

Ligand BCR p 602

Bond lengths



Bond angles



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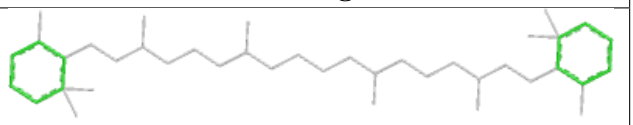
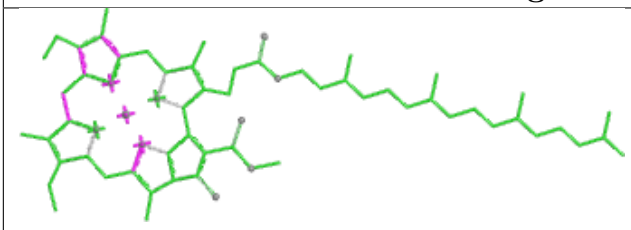
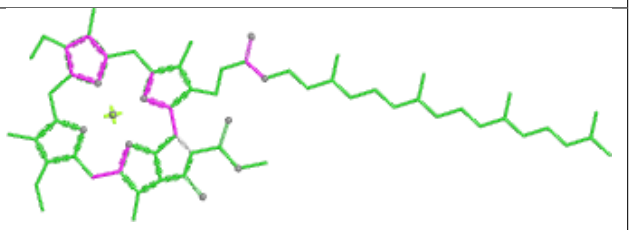


Rings

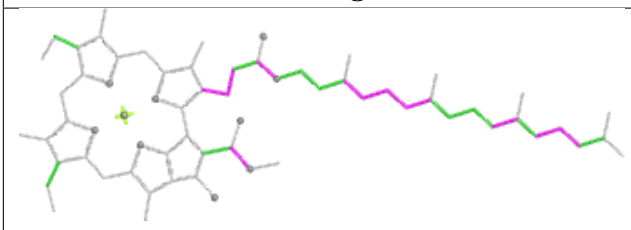
Ligand CLA h 512



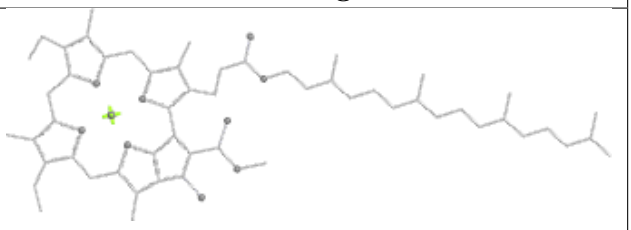
Bond lengths



Bond angles

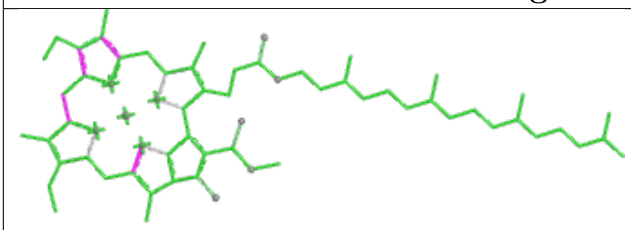


Torsions



Rings

Ligand CLA r 515



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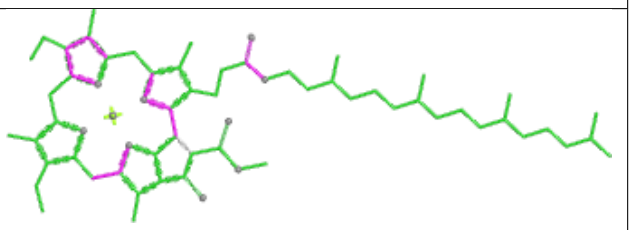
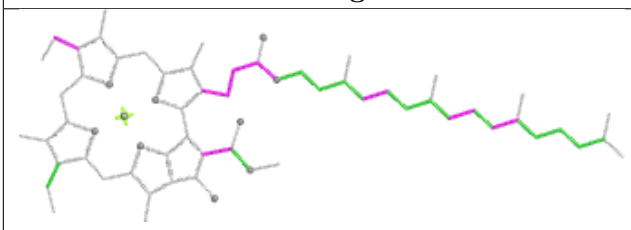
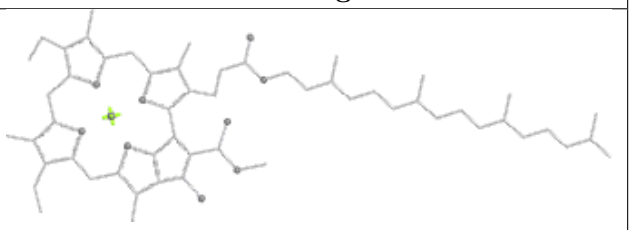


Bond angles

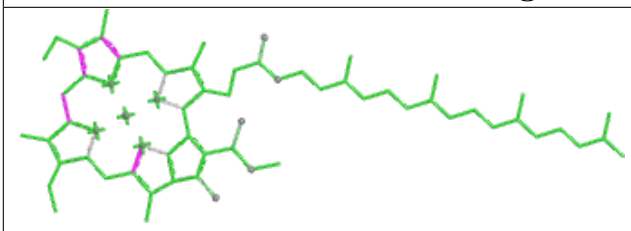


Torsions



Rings

Ligand CLA W 507



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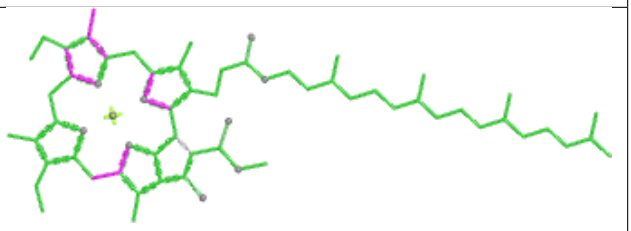
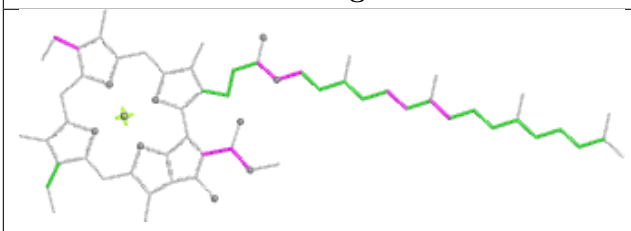
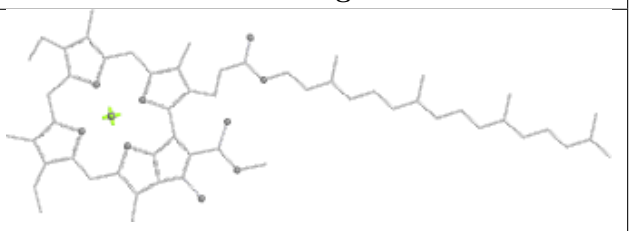


Bond angles

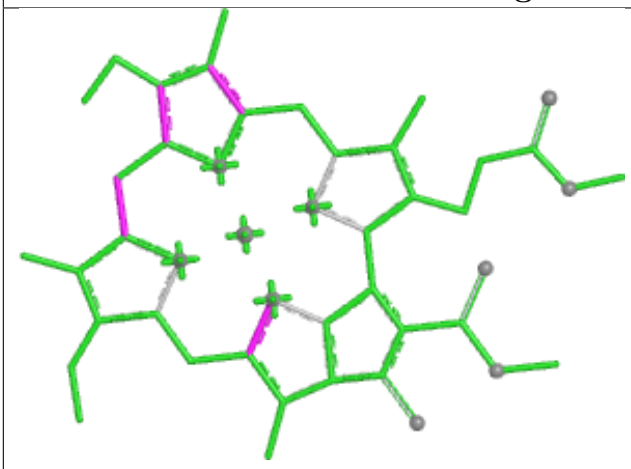


Torsions



Rings

Ligand CLA A 1129



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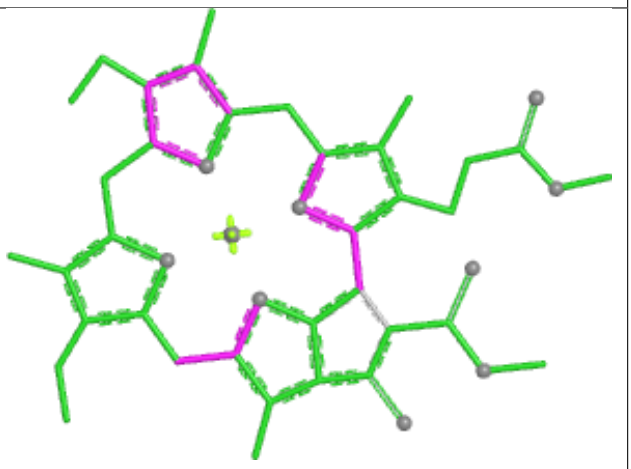

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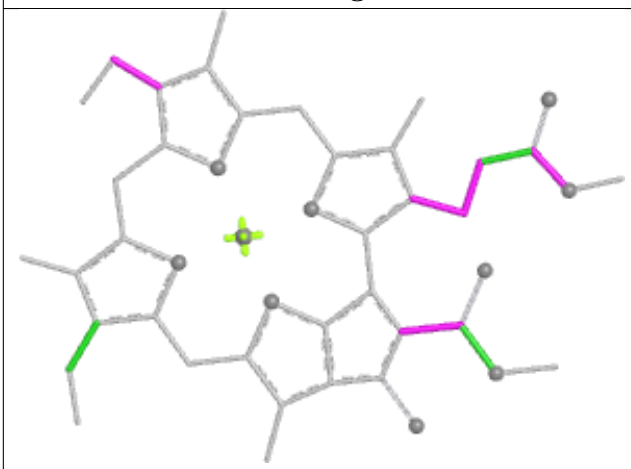

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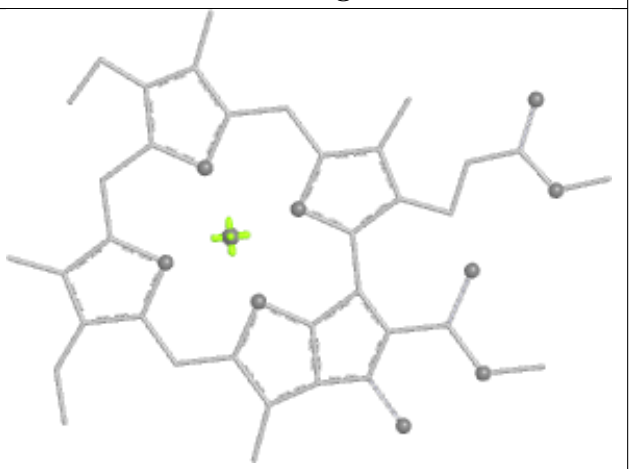
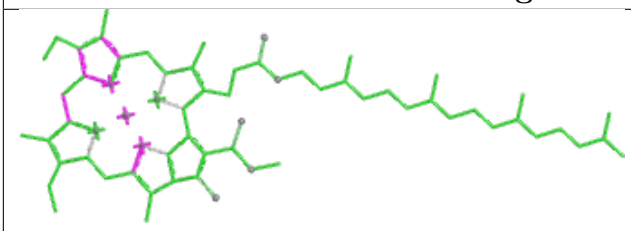


Rings

Ligand CLA B 1023



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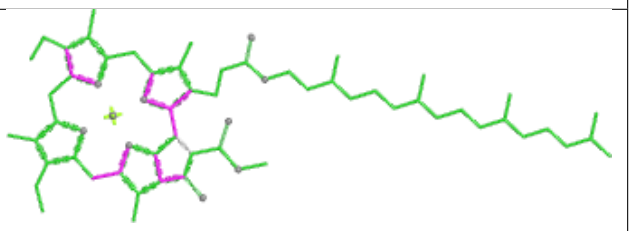
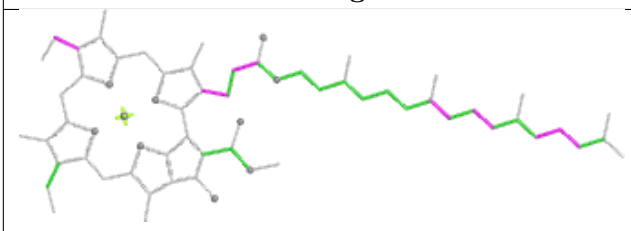


Bond angles



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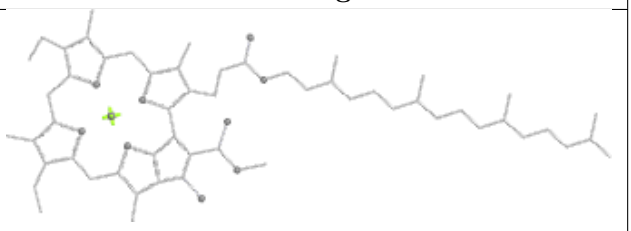
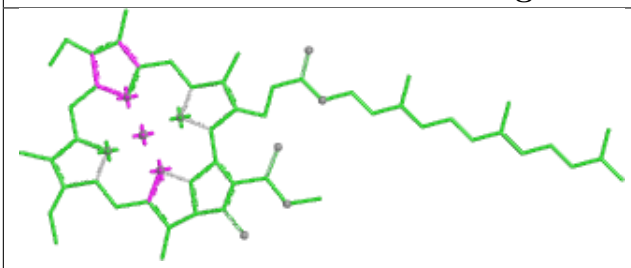
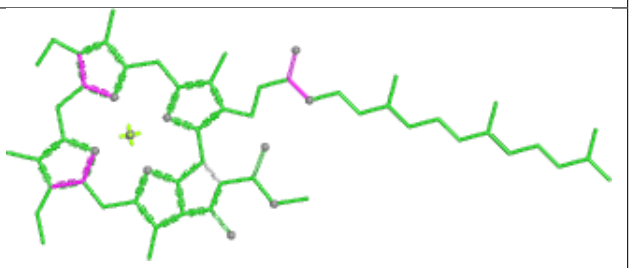
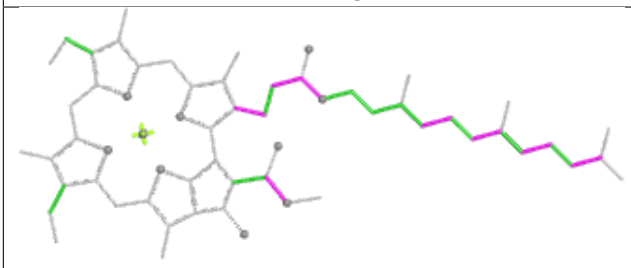
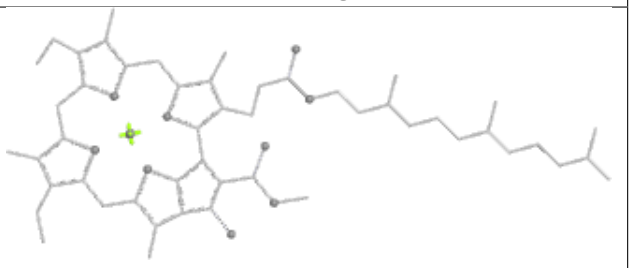


Rings

Ligand CLA B 1226	
	
Bond lengths	Bond angles
	
Torsions	Rings

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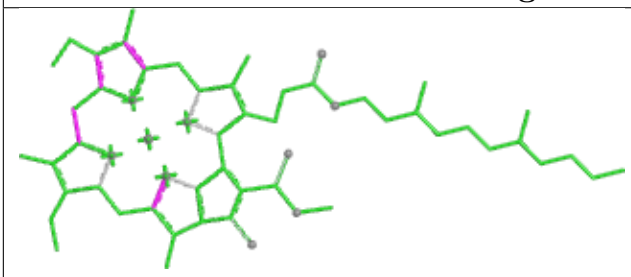
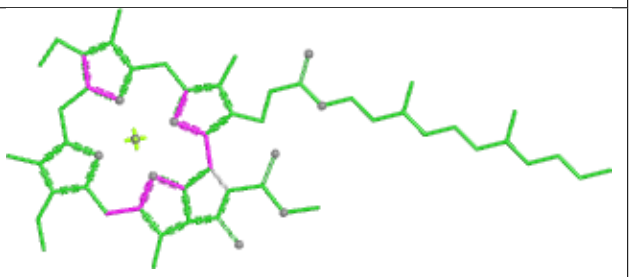
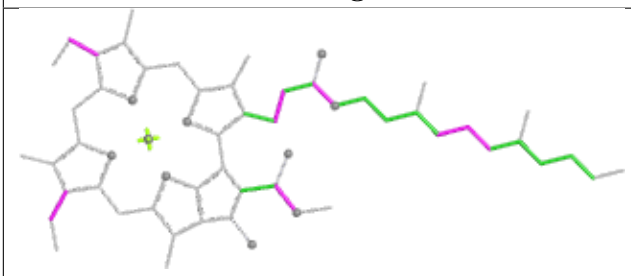
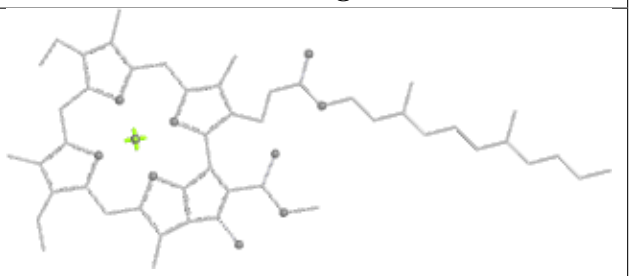
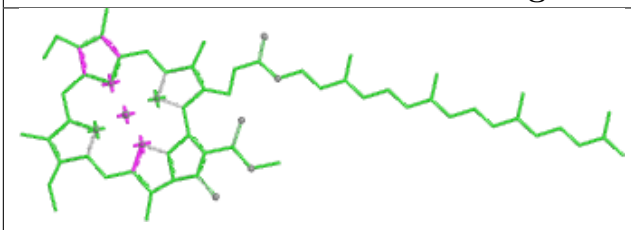
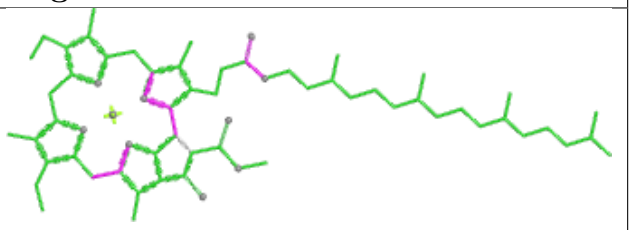
	
Bond lengths	Bond angles
	
Torsions	Rings

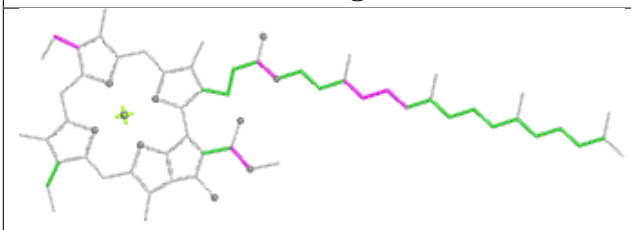
Ligand CLA g 512



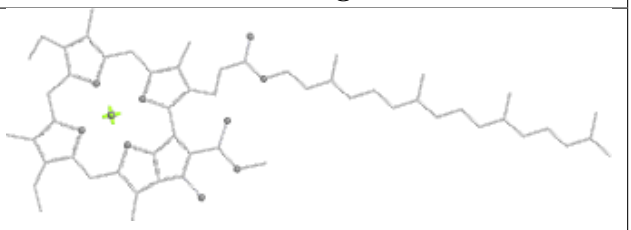
Bond lengths



Bond angles

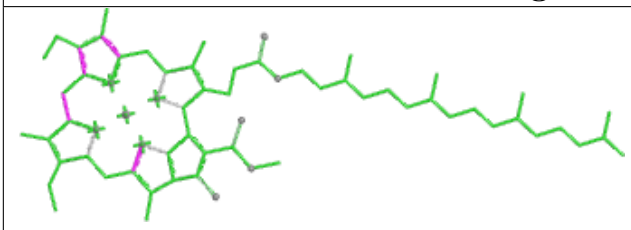


Torsions



Rings

Ligand CLA t 507



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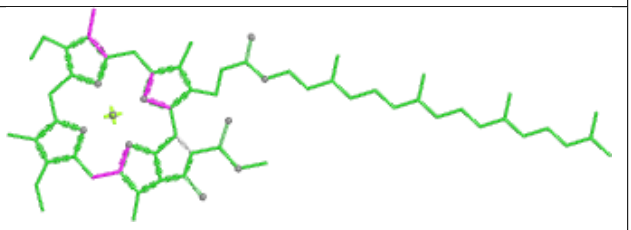
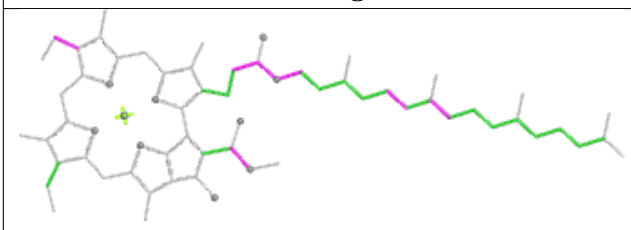
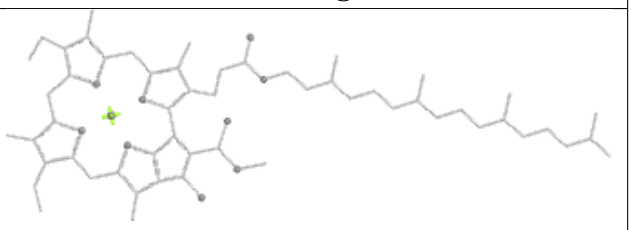


Bond angles

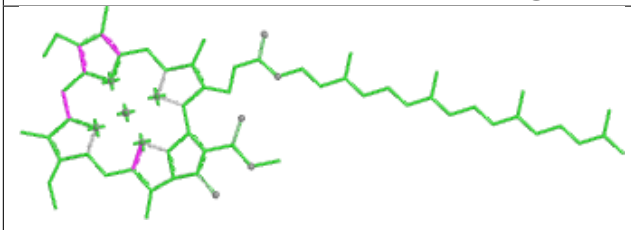


Torsions



Rings

Ligand CLA v 512



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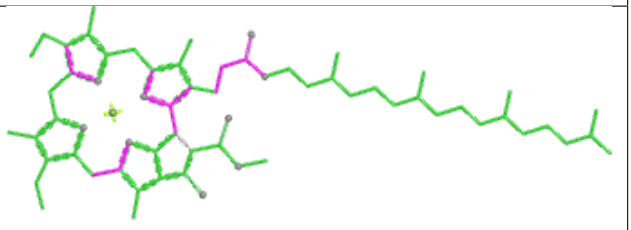
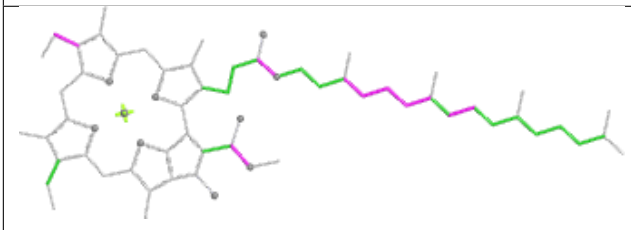


Bond angles



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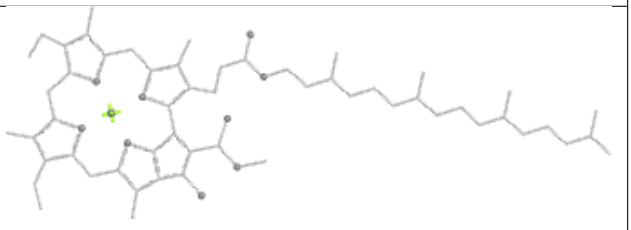
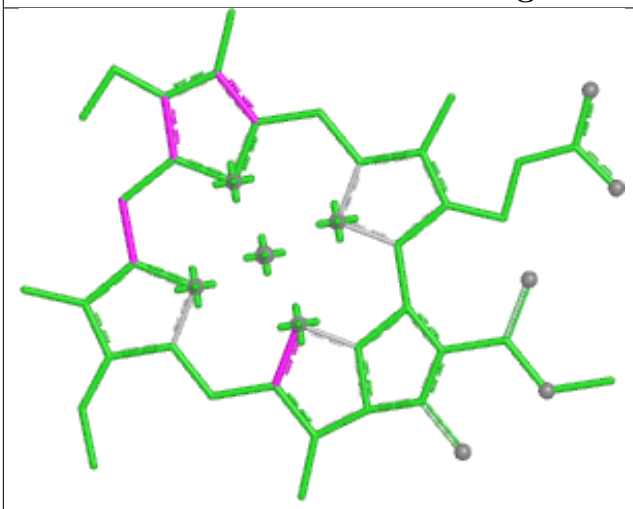
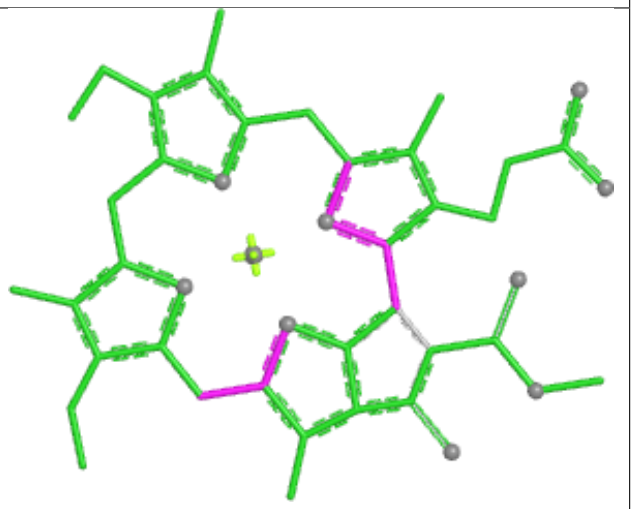


Rings

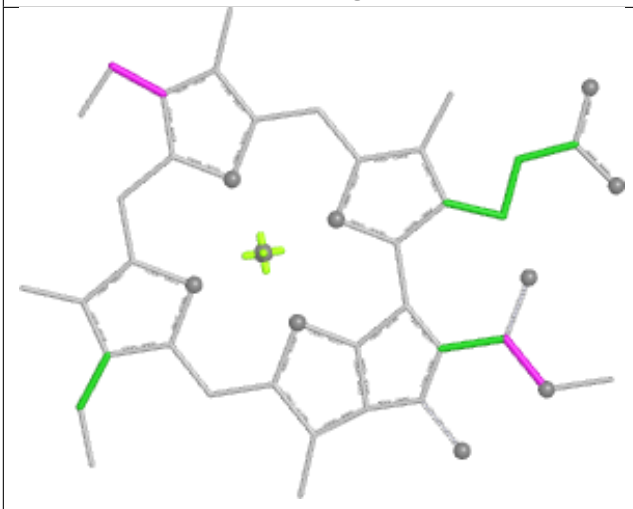
Ligand CLA F 1301



Bond lengths



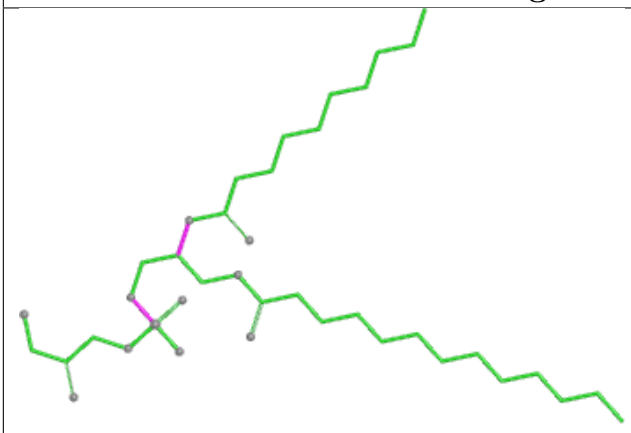
Bond angles



Torsions

Rings

Ligand LHG I 103



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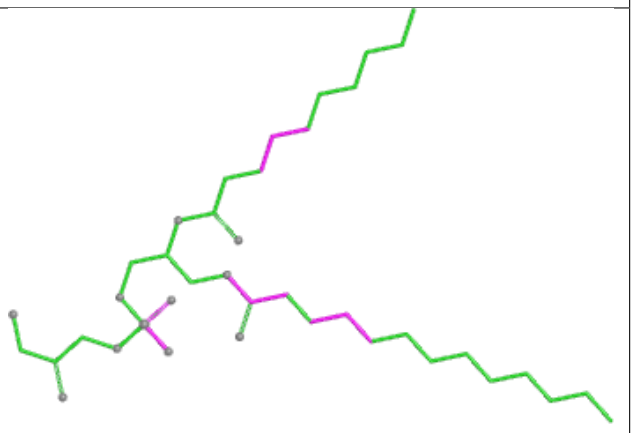

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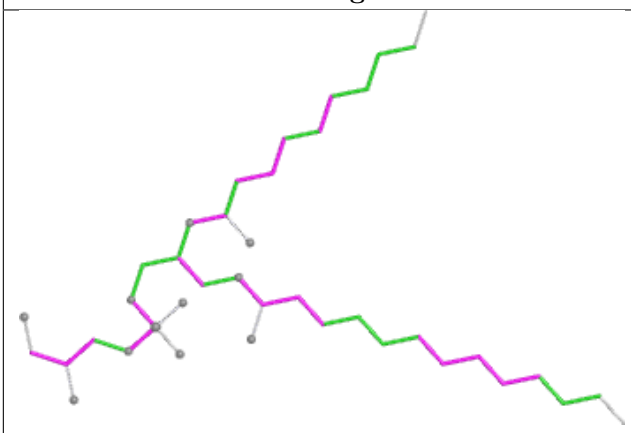
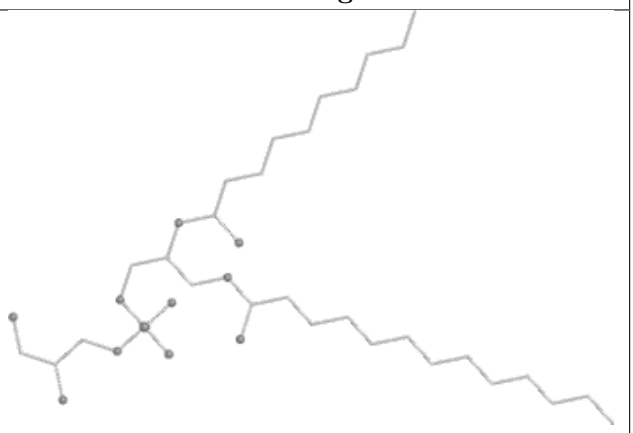
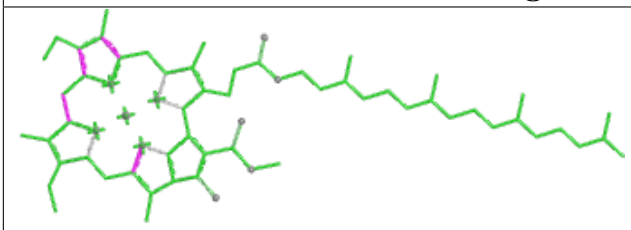


Torsions



Rings

Ligand CLA w 507



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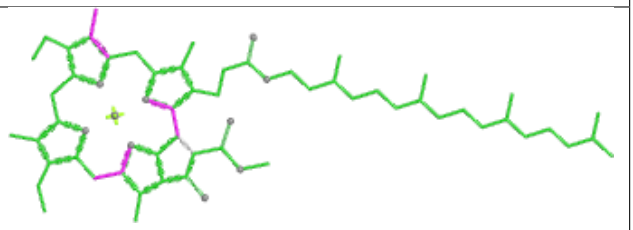
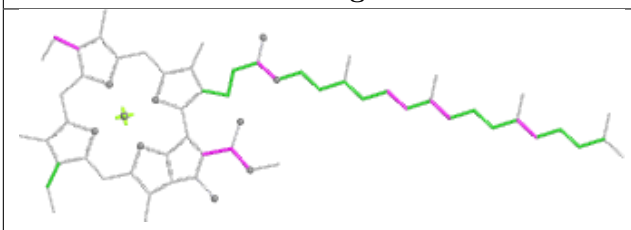
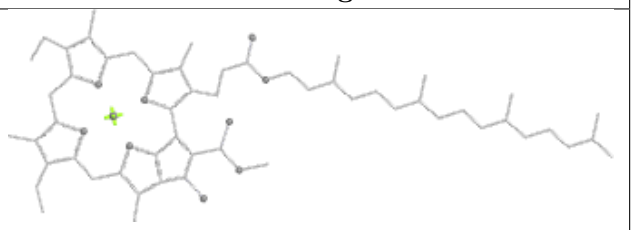


Bond angles

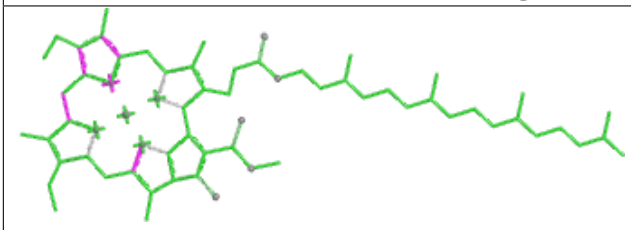


Torsions



Rings

Ligand CLA A 1131



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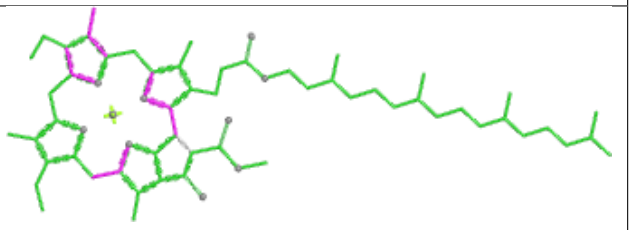
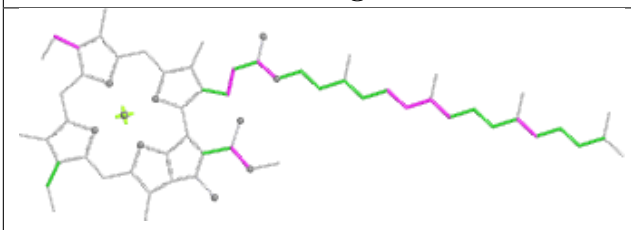
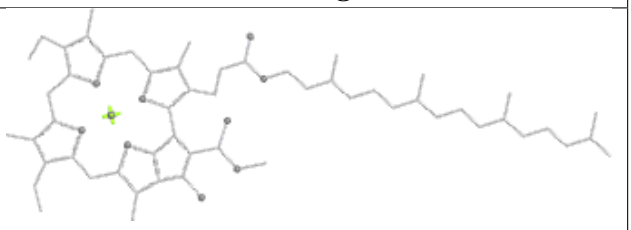


Bond angles

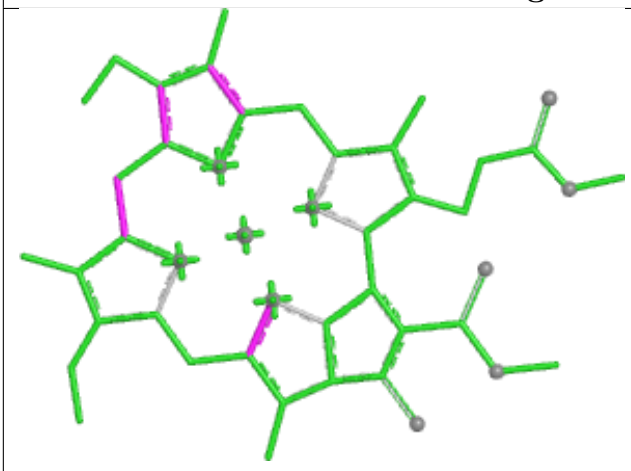


Torsions

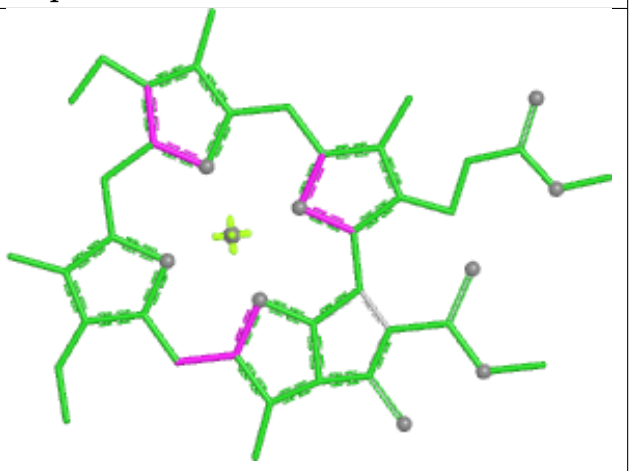


Rings

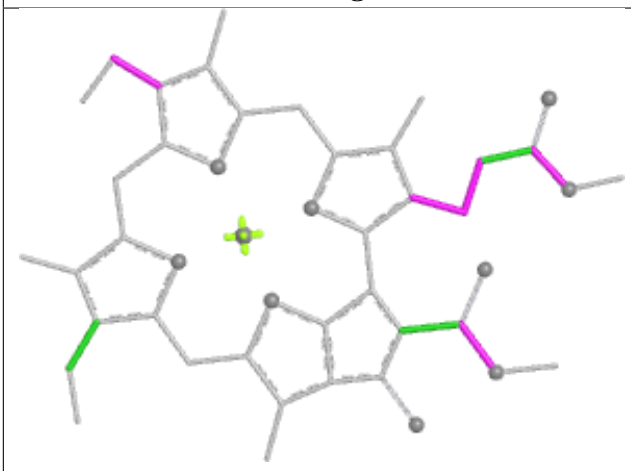
Ligand CLA p 516



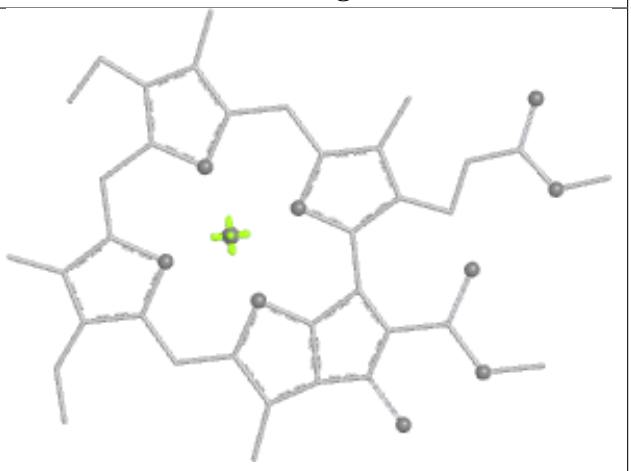
Bond lengths



Bond angles

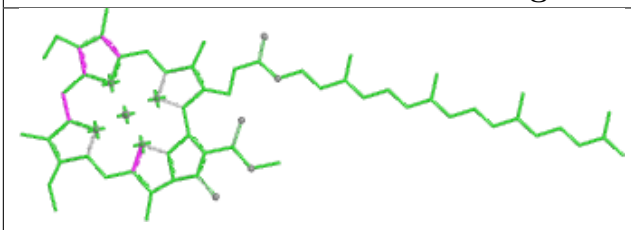


Torsions

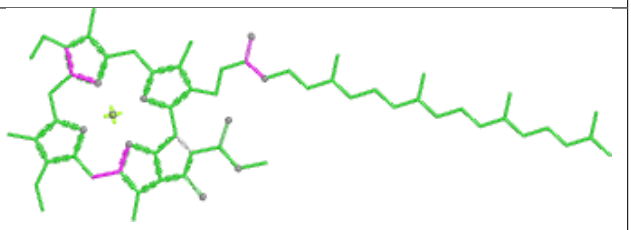


Rings

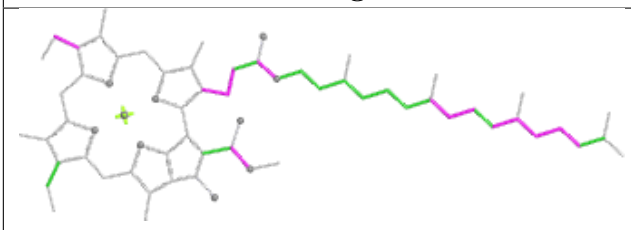
Ligand CLA r 504



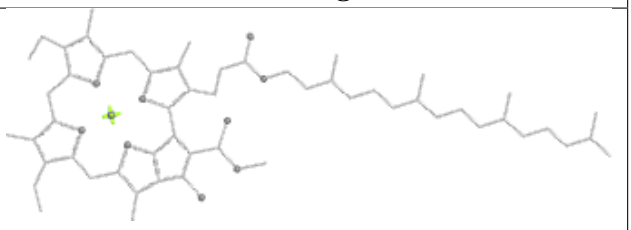
Bond lengths



Bond angles

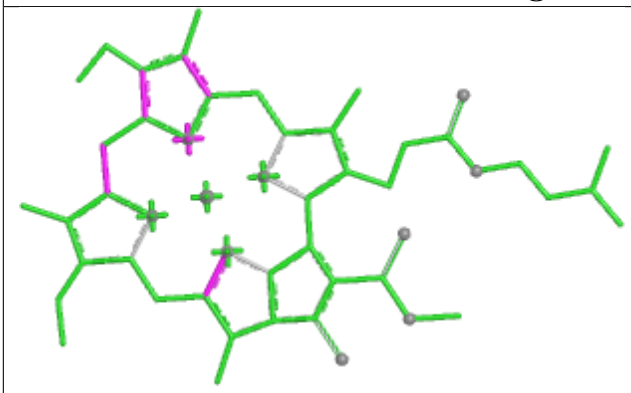


Torsions



Rings

Ligand CLA v 502



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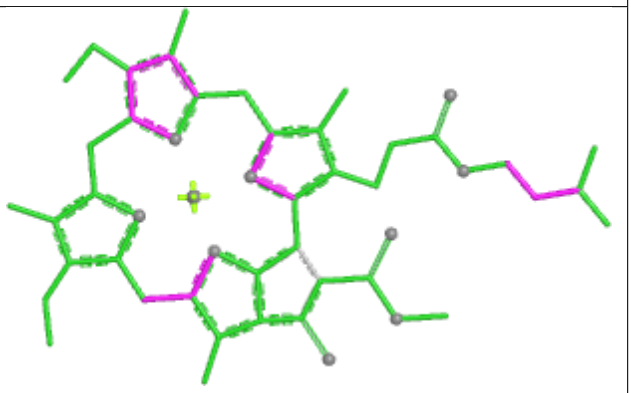
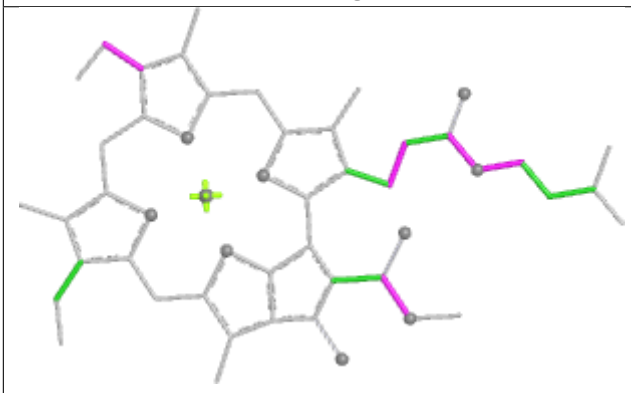
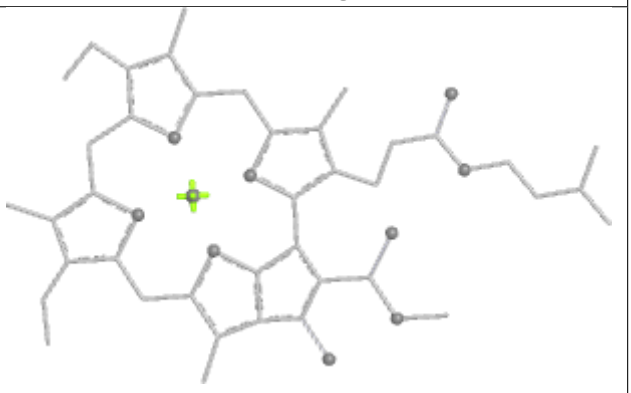


Bond angles

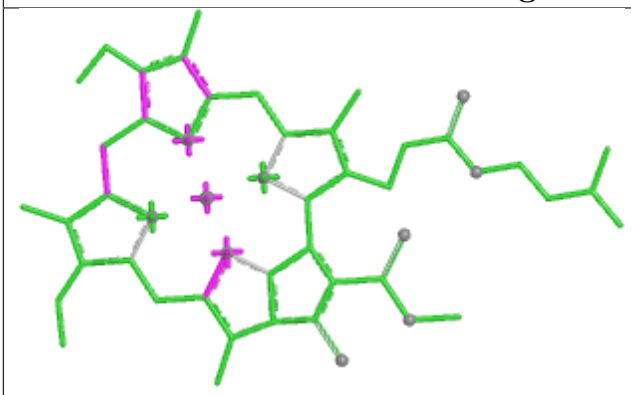


Torsions



Rings

Ligand CLA W 502



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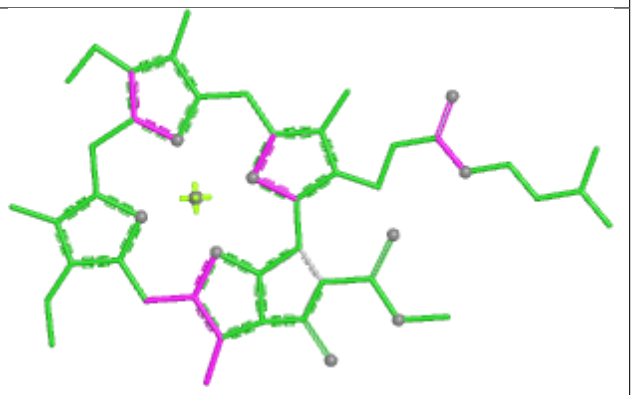
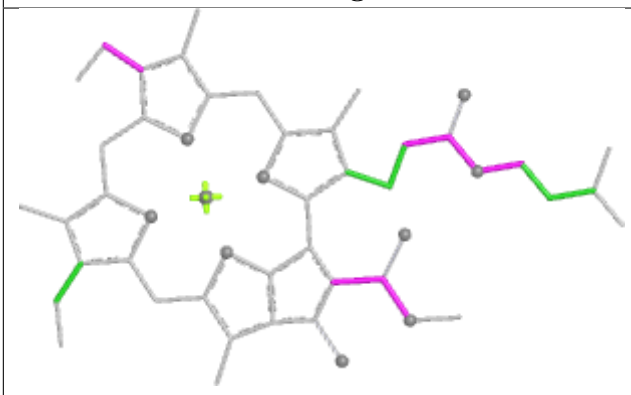
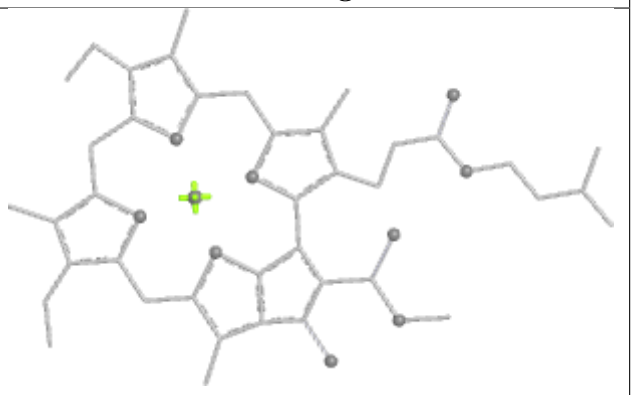


Bond angles

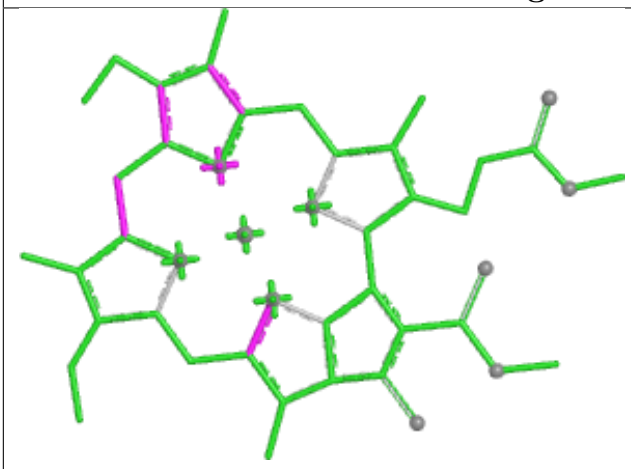


Torsions



Rings

Ligand CLA v 503



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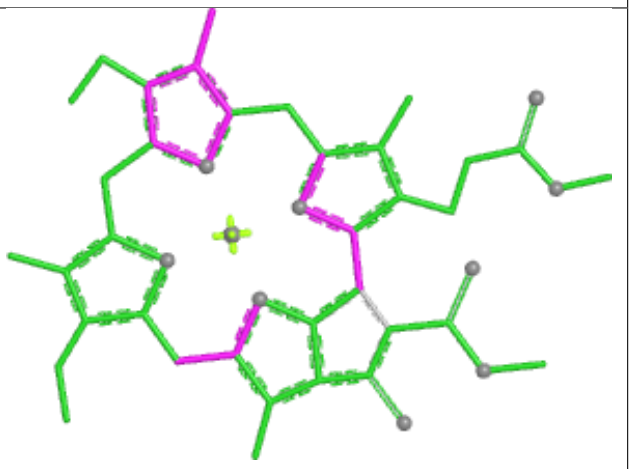
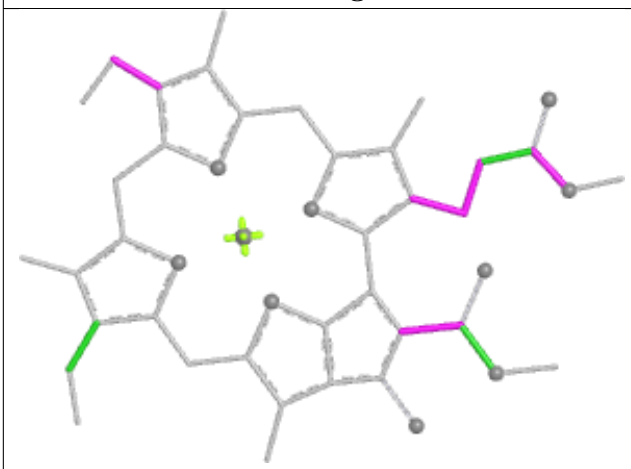


Bond angles



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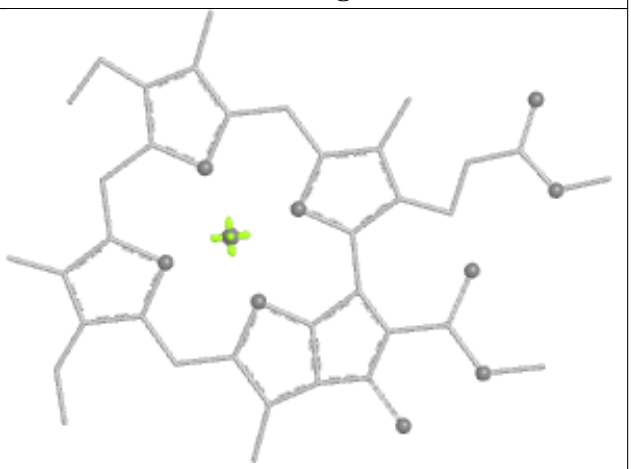
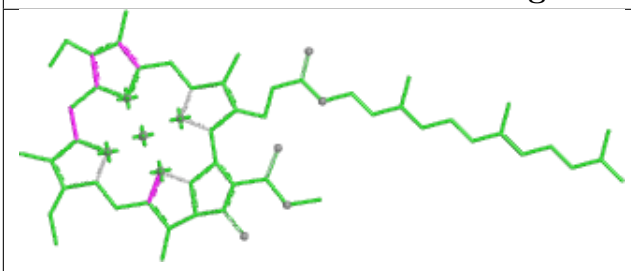


Rings

Ligand CLA o 509



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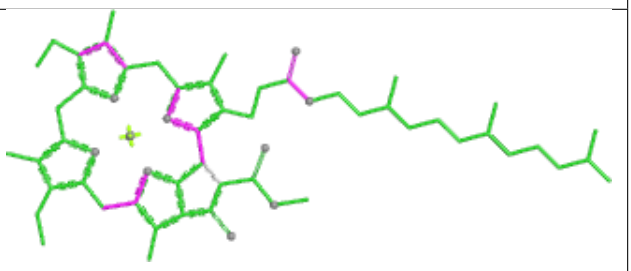
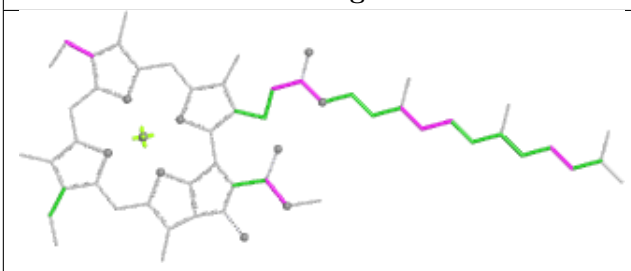


Bond angles



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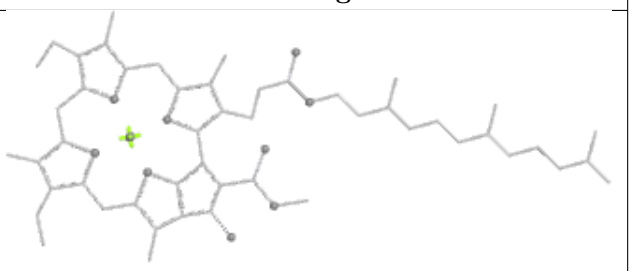
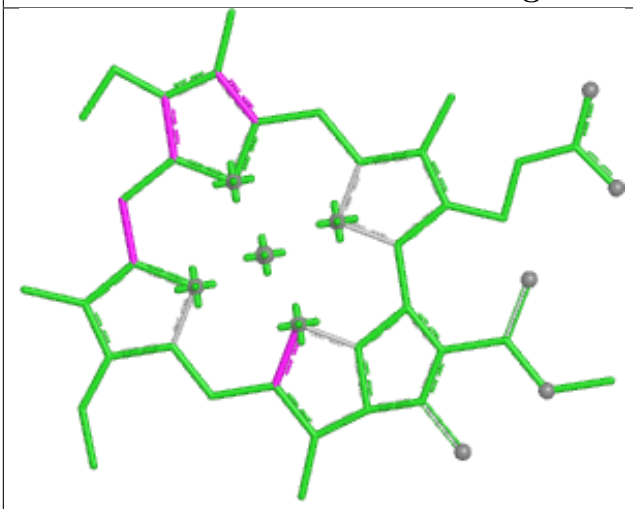


Rings

Ligand CLA f 1301



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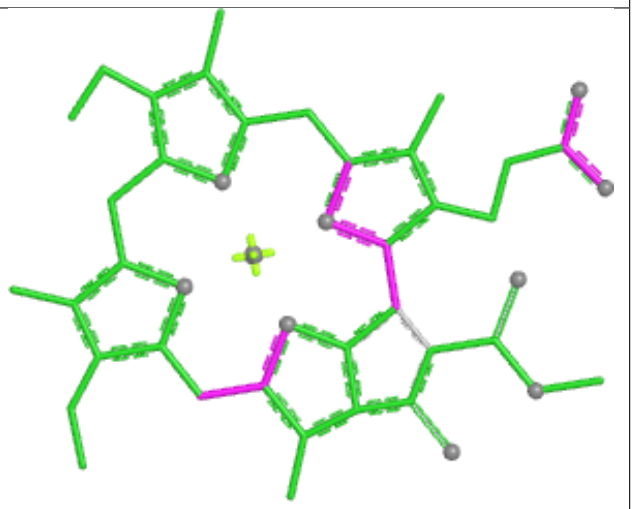
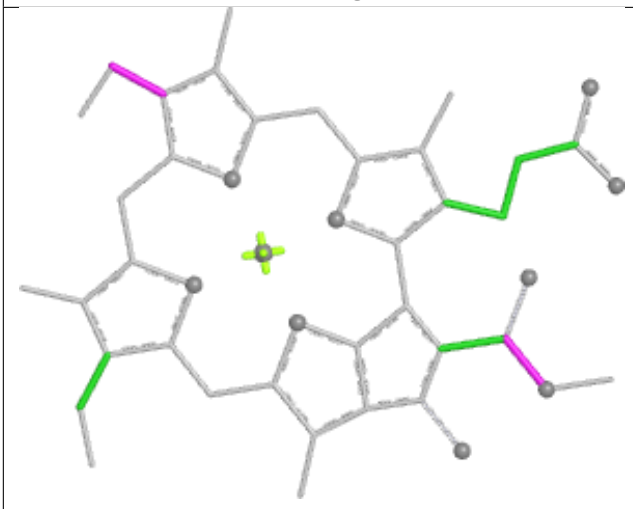


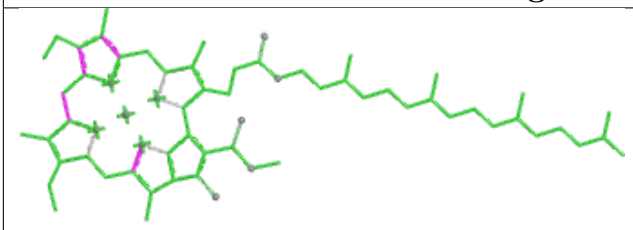
Bond angles



Torsions

Rings

Ligand CLA x 504



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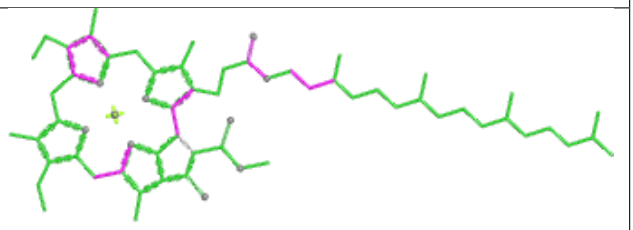
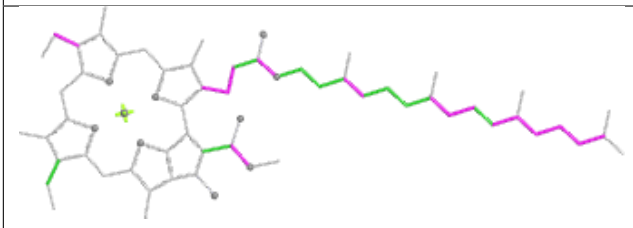
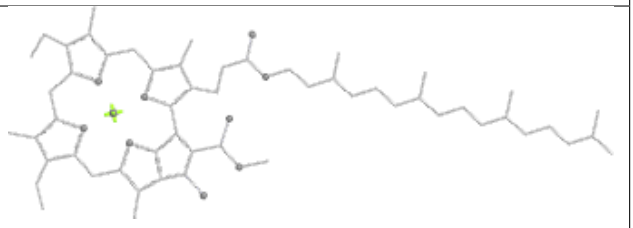


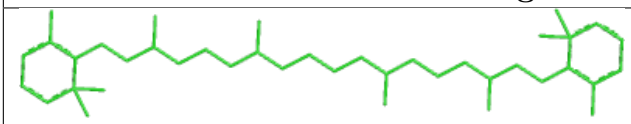
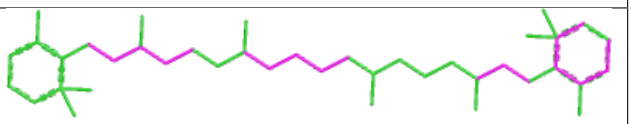
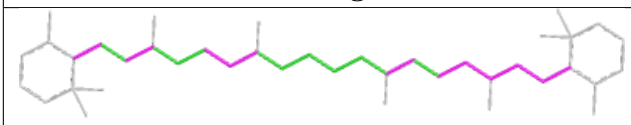
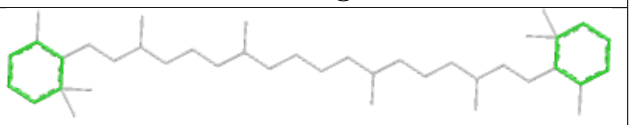
Bond angles

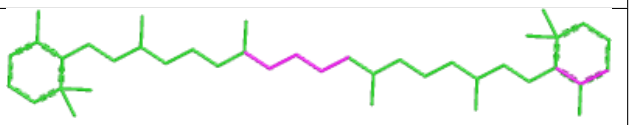
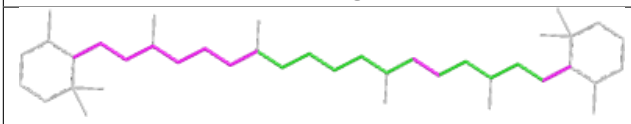
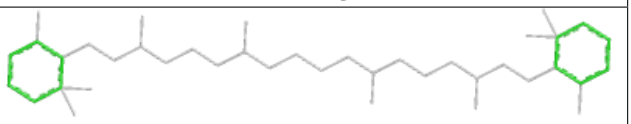


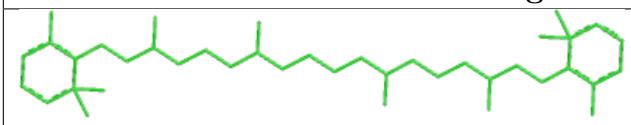
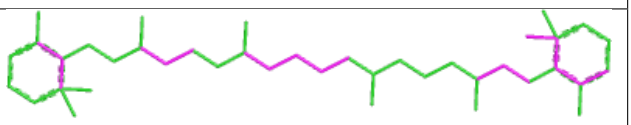
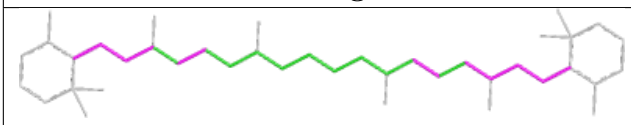
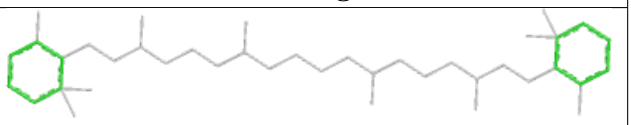
Torsions



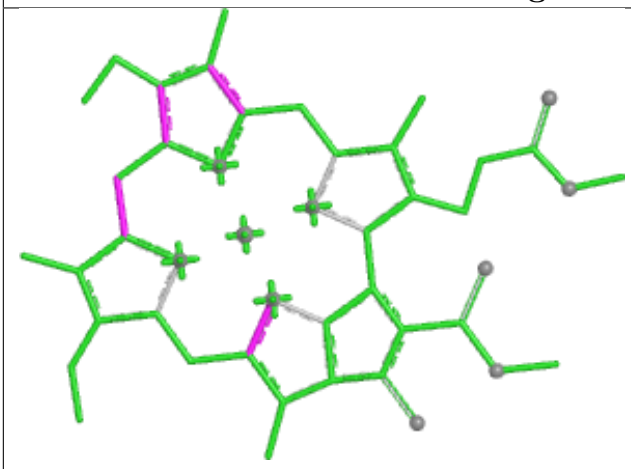
Rings

Ligand BCR W 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

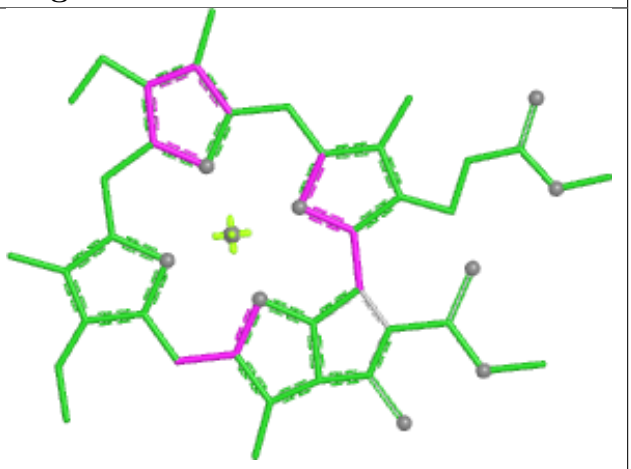
Ligand BCR W 603	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR v 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

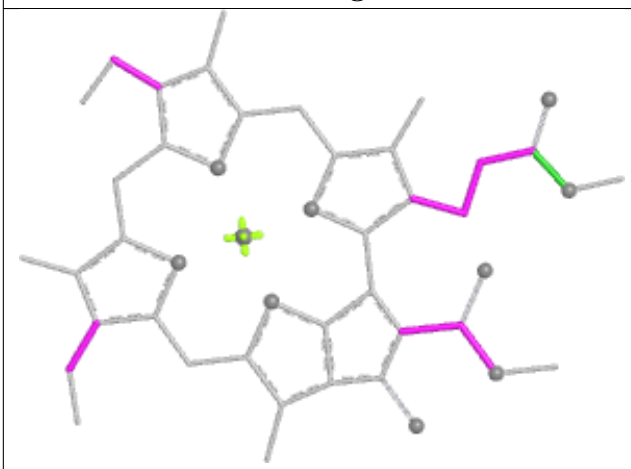
Ligand CLA g 513



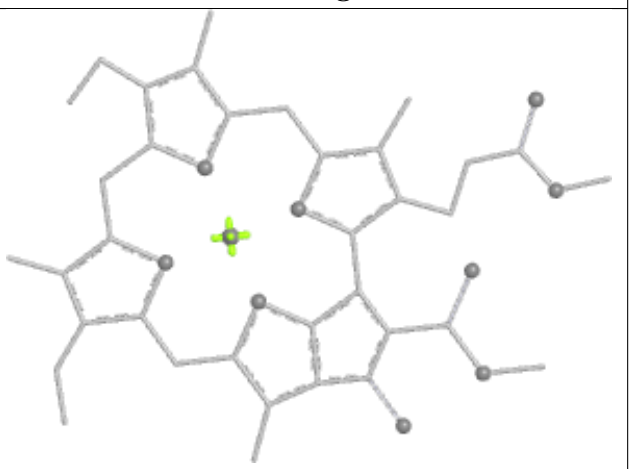
Bond lengths



Bond angles

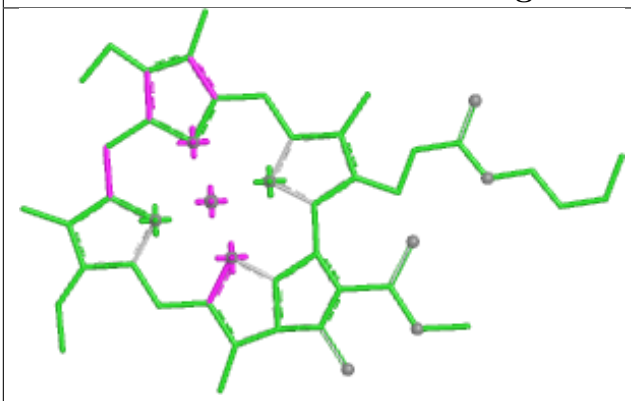


Torsions

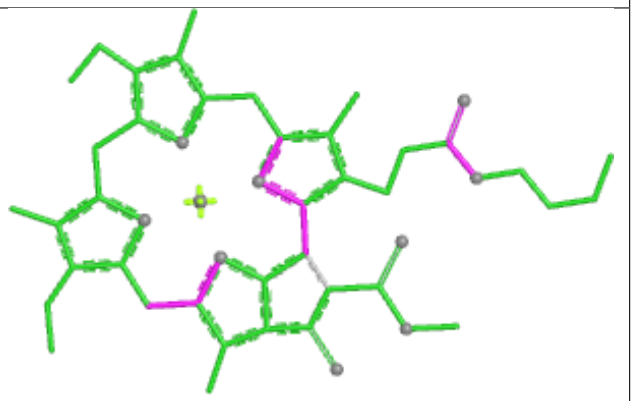


Rings

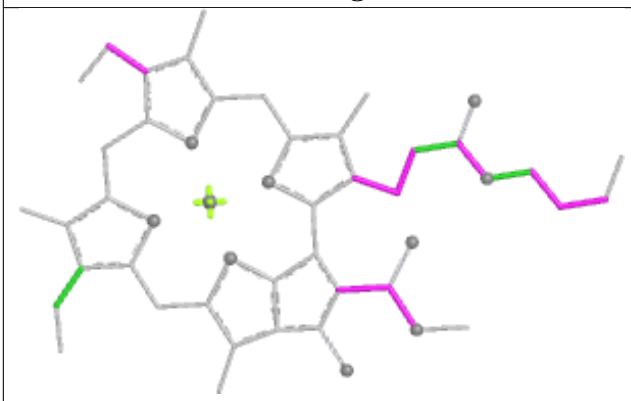
Ligand CLA B 1227



Bond lengths



Bond angles



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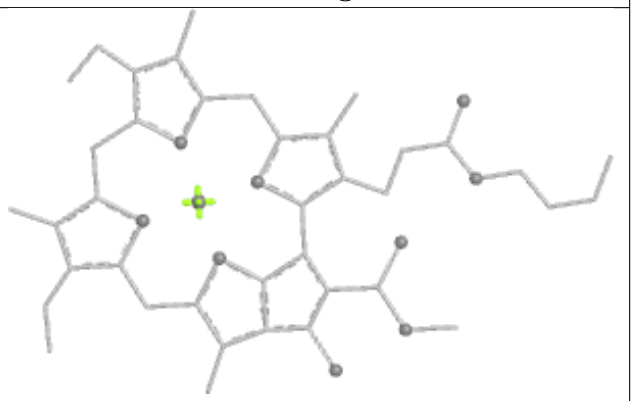
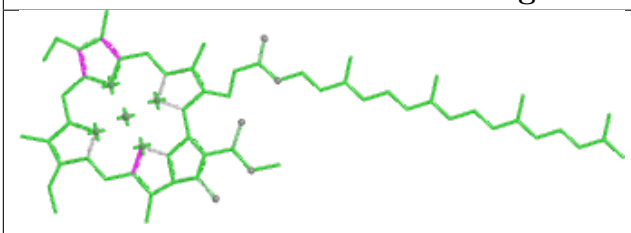
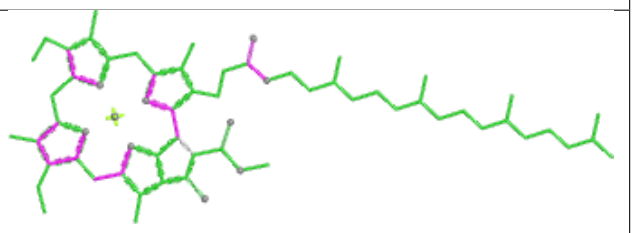


Rings

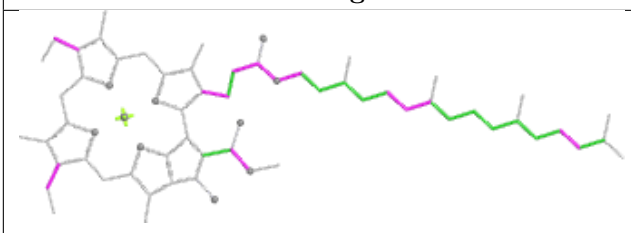
Ligand CLA b 1239



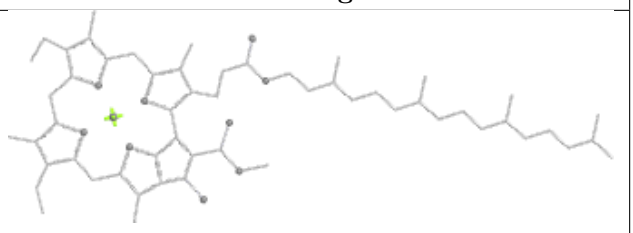
Bond lengths



Bond angles

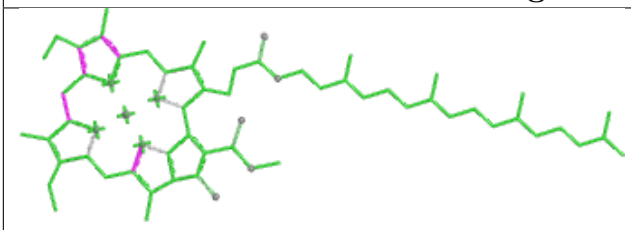


Torsions

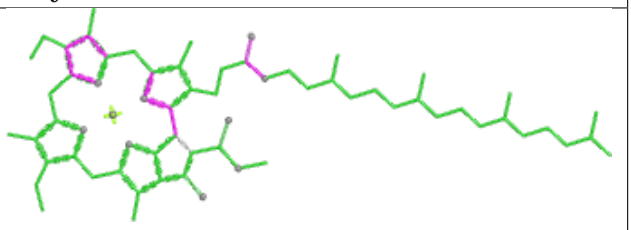


Rings

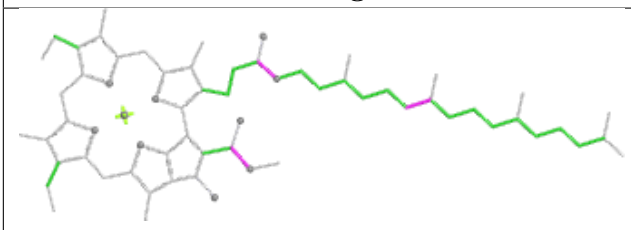
Ligand CLA y 510



Bond lengths



Bond angles



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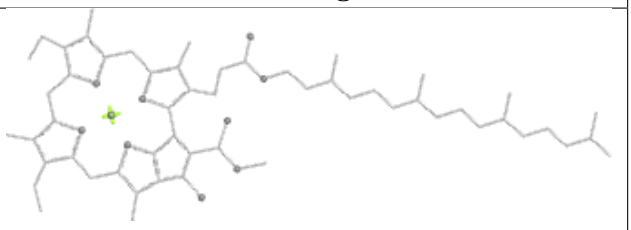
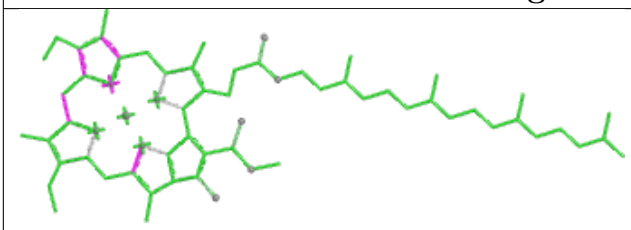
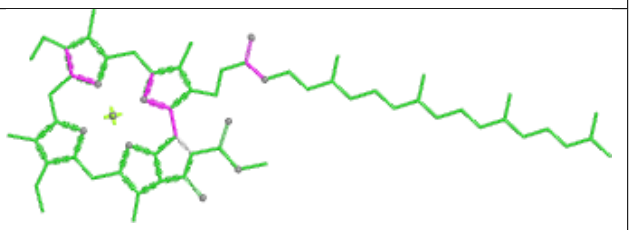


Rings

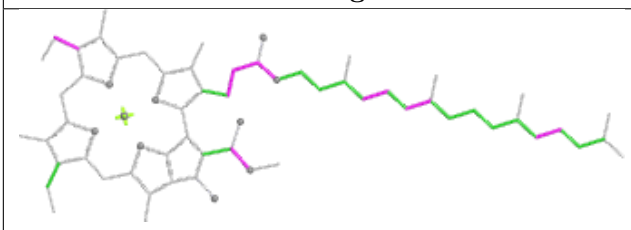
Ligand CLA x 510



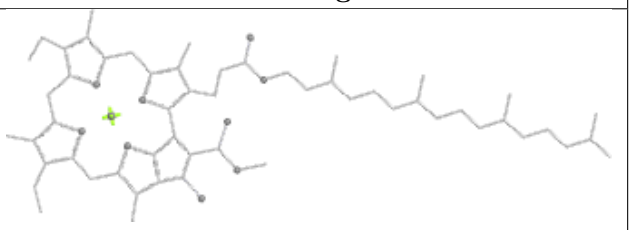
Bond lengths



Bond angles



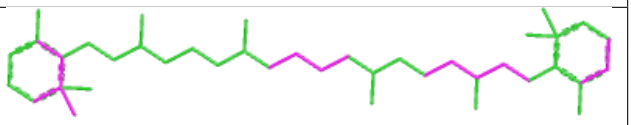
Torsions



Rings

Ligand BCR l 4022

Bond lengths



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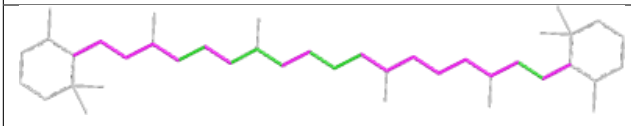
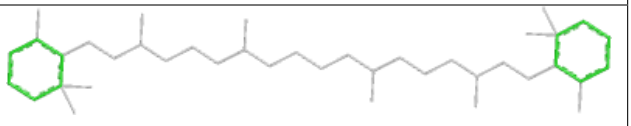
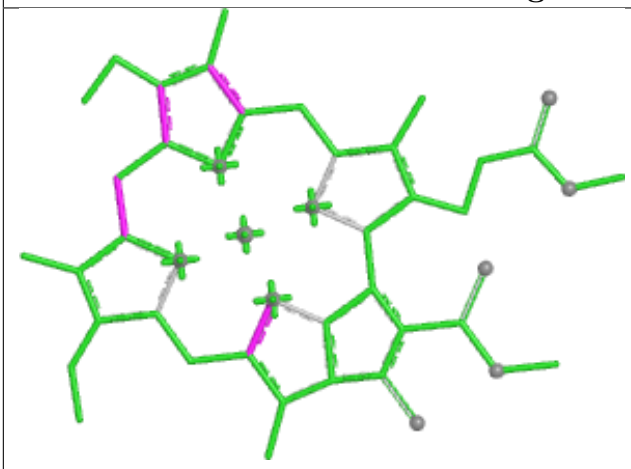


Torsions



Rings

Ligand CLA h 516



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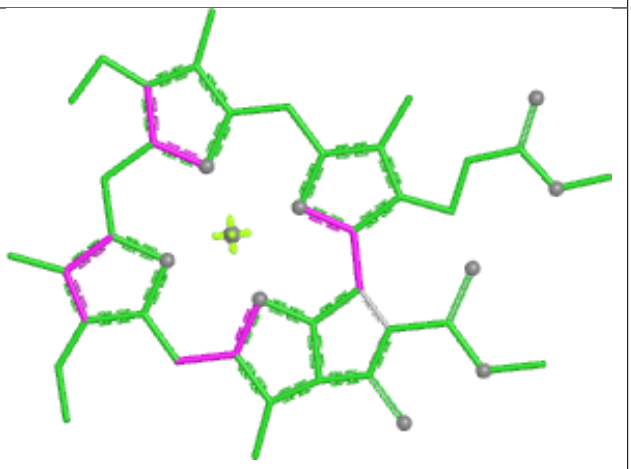

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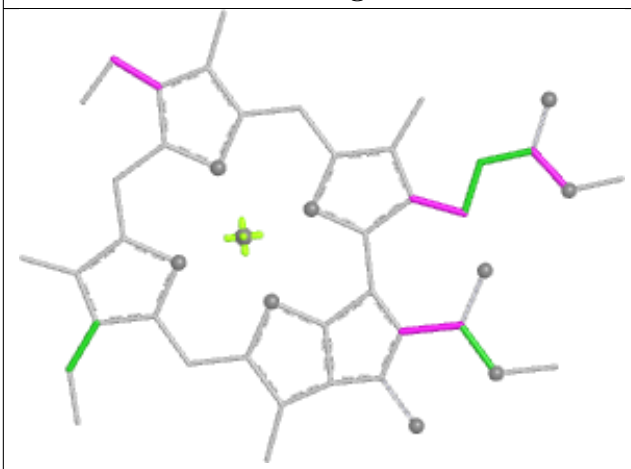
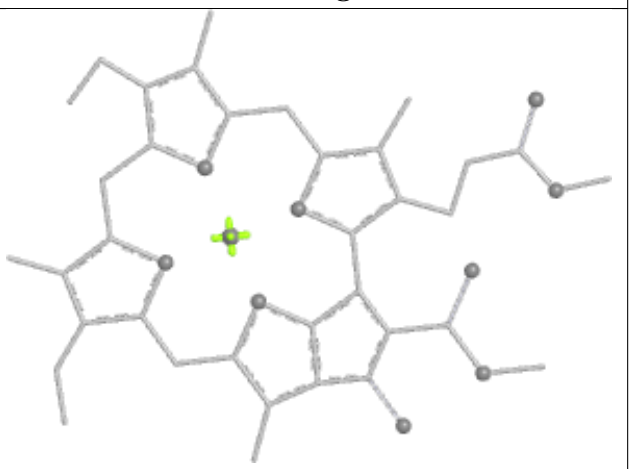
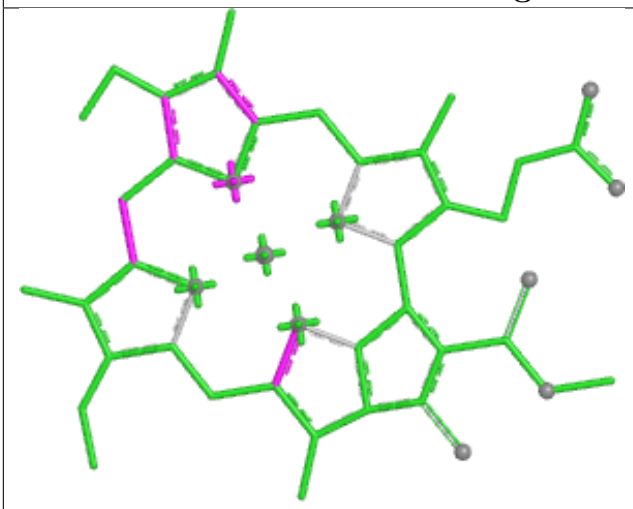


Torsions



Rings

Ligand CLA G 1212



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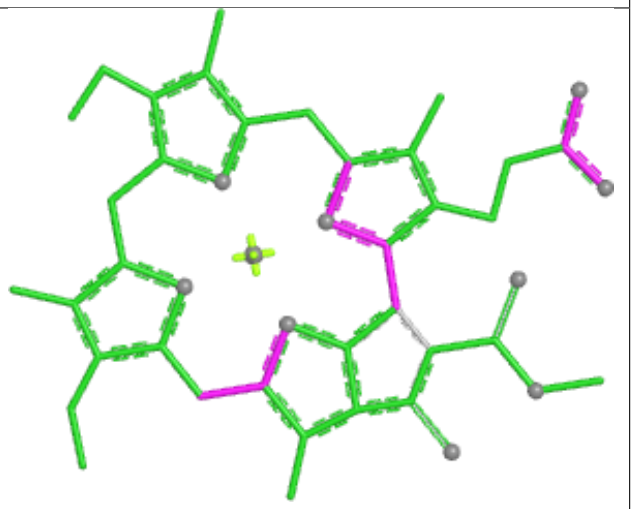
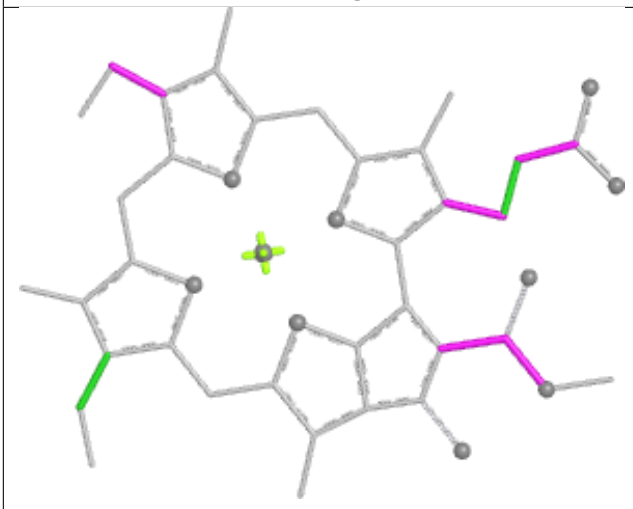
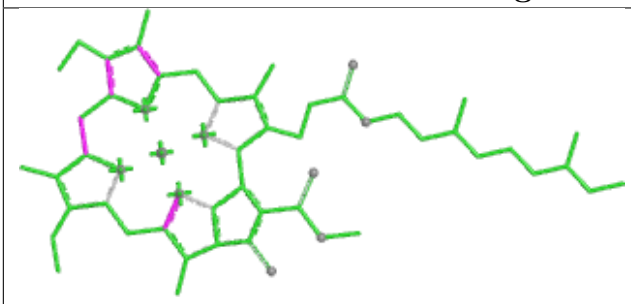
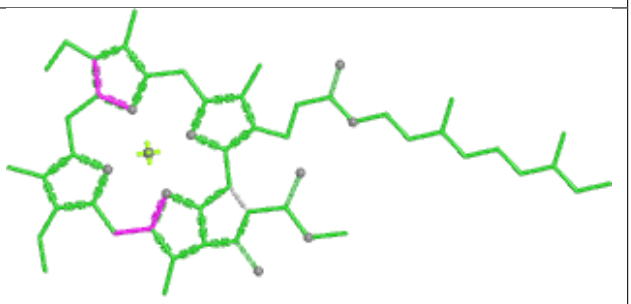


Bond angles



Torsions

Rings

Ligand CLA H 1102	
	
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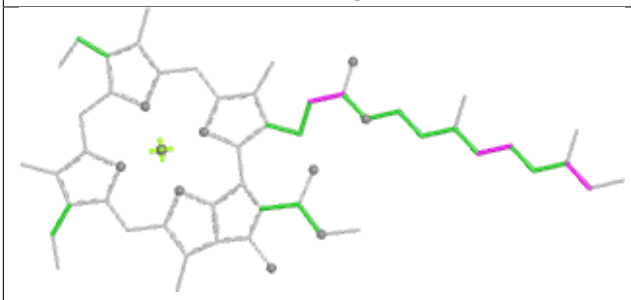
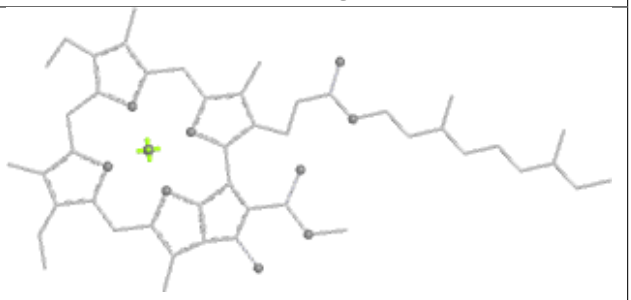
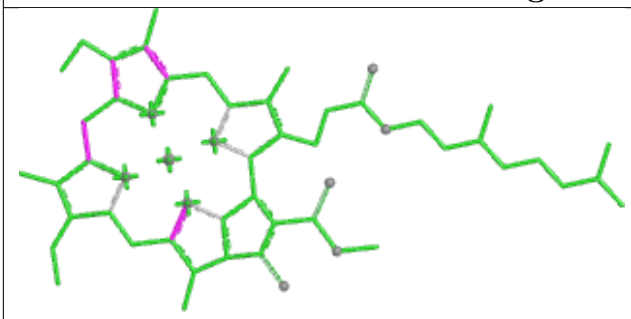
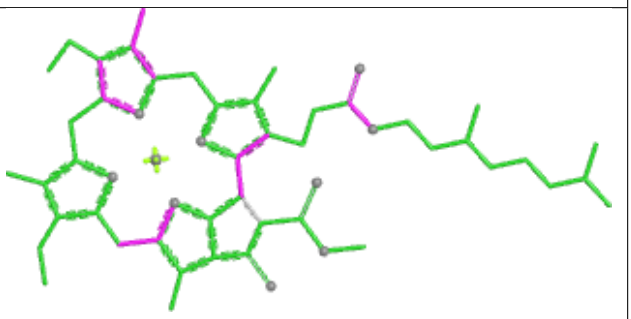
	
Torsions	Rings

Ligand CLA u 517	
	
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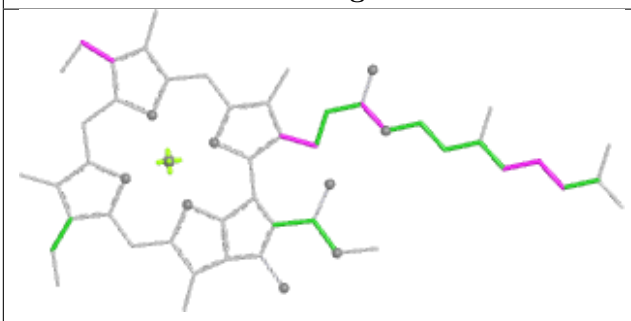	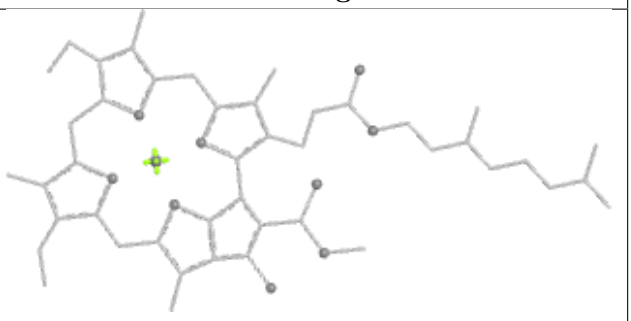
Torsions	Rings

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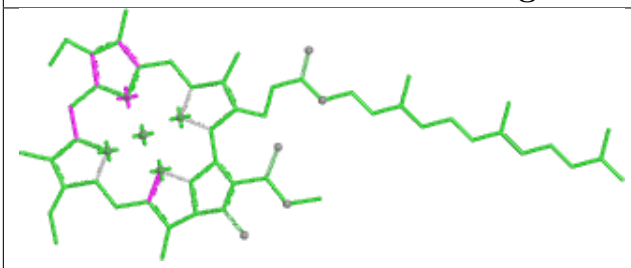
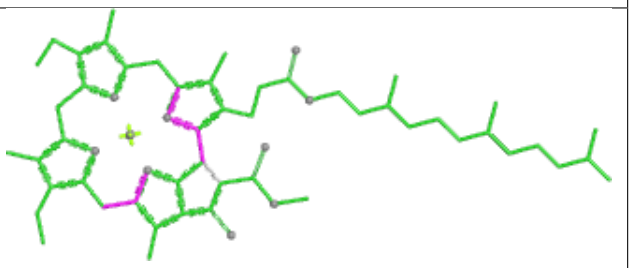
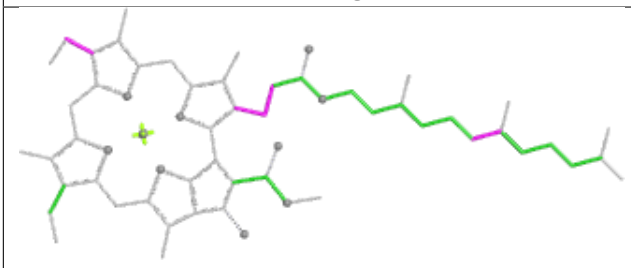
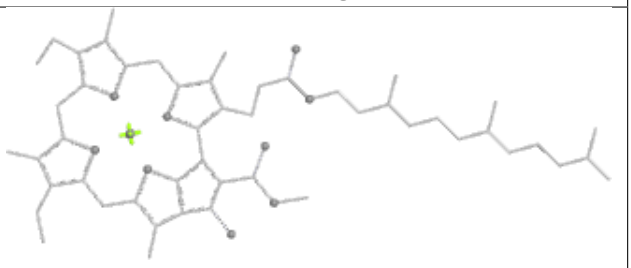
	
Bond lengths	Bond angles
	
Torsions	Rings

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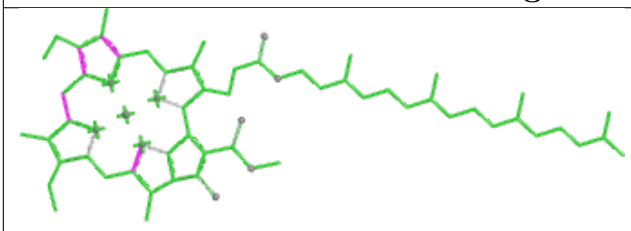	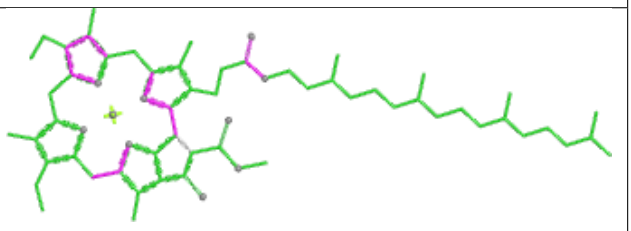
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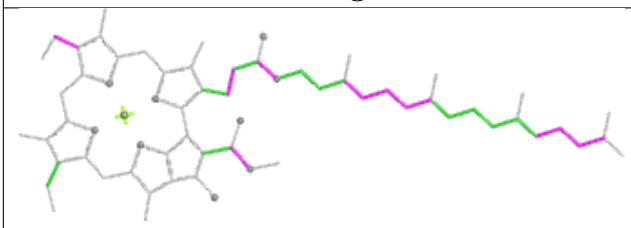	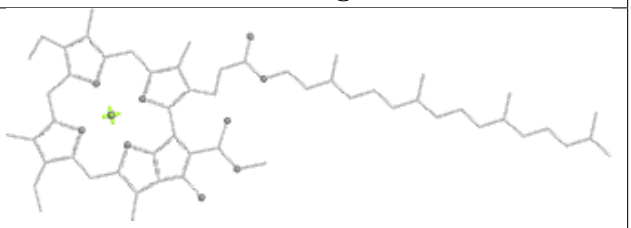
Torsions	Rings

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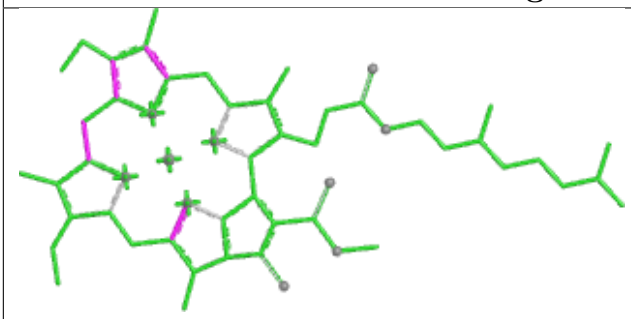

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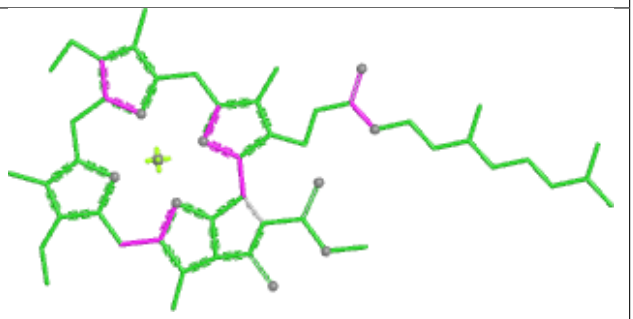
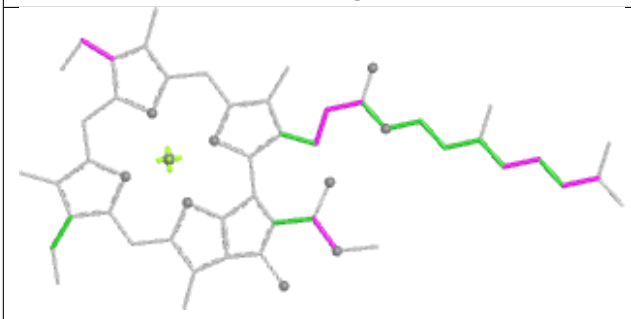
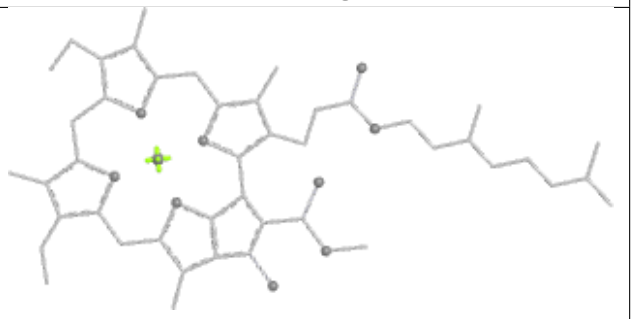


Bond angles

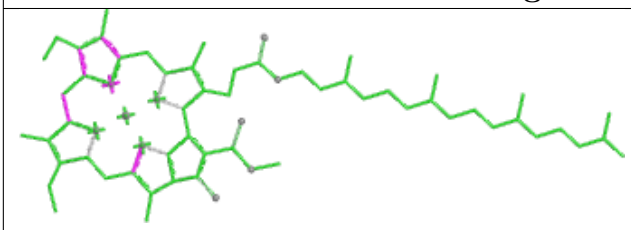


Torsions



Rings

Ligand CLA Y 504



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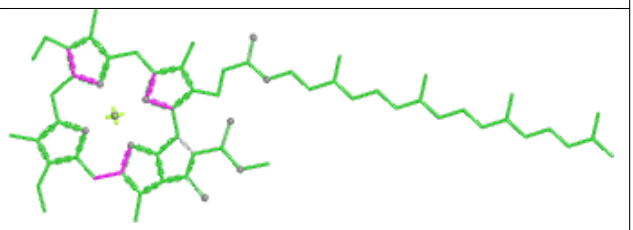

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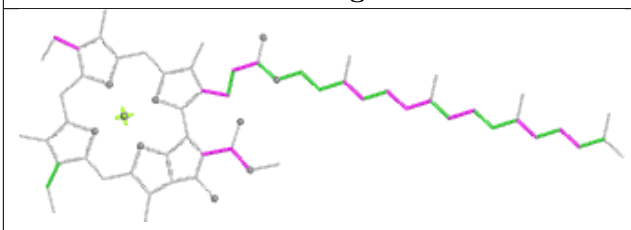
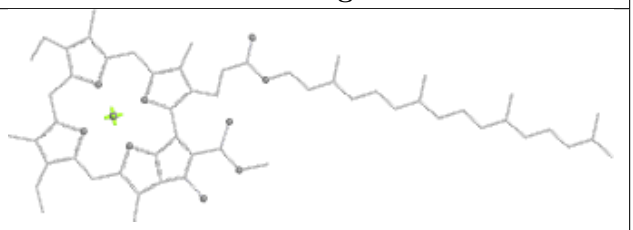
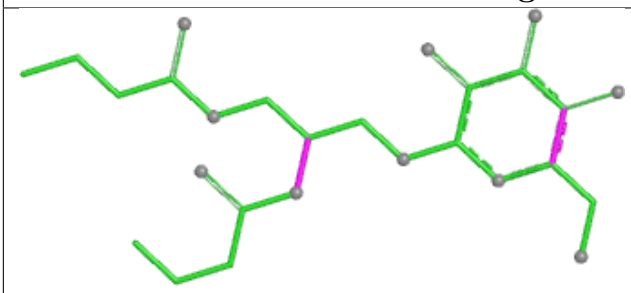


Torsions



Rings

Ligand LMG f 4017



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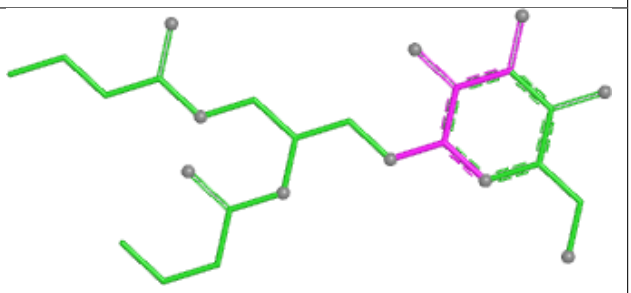
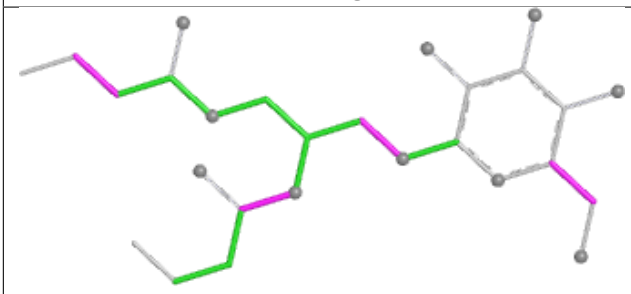


Bond angles



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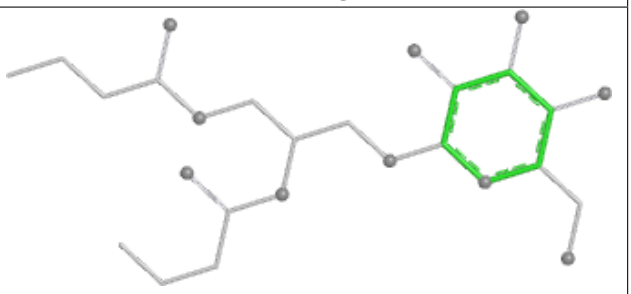
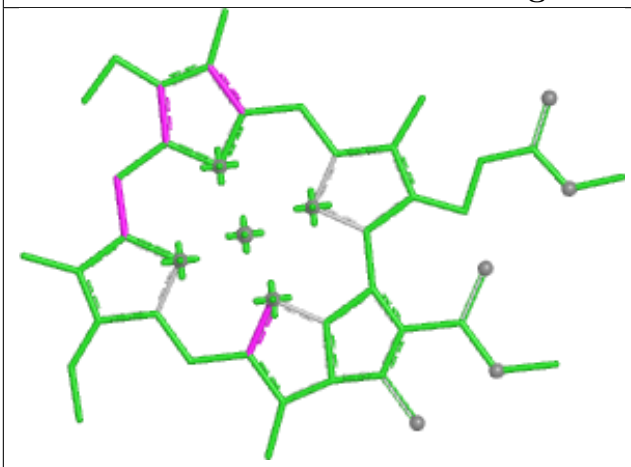


Rings

Ligand CLA g 516



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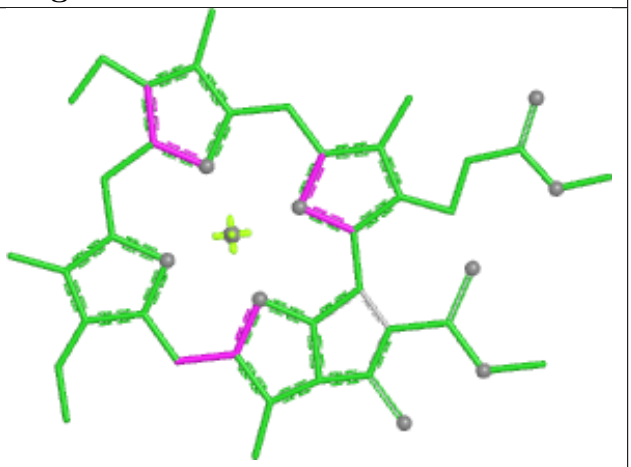
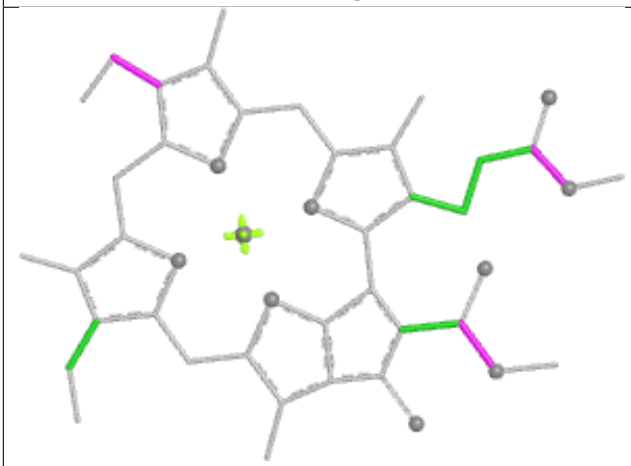


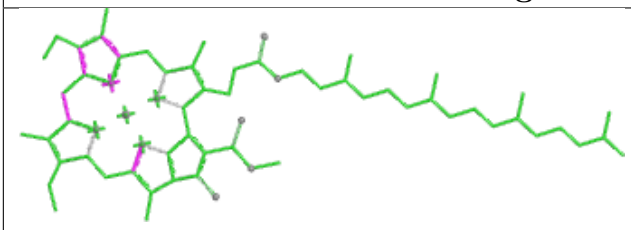
Bond angles



Torsions

Rings

Ligand CLA B 1210



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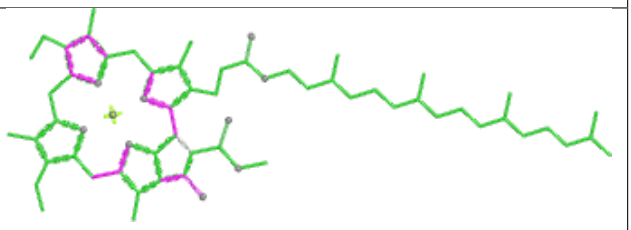
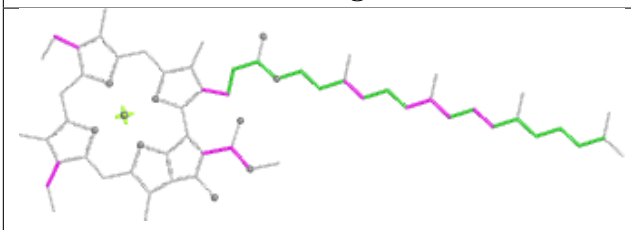
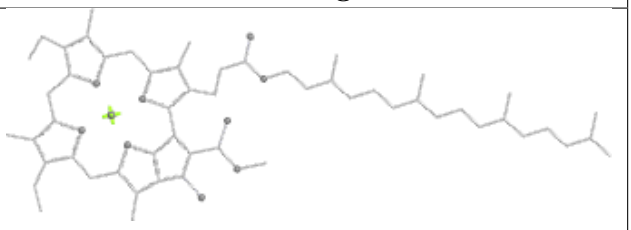


Bond angles

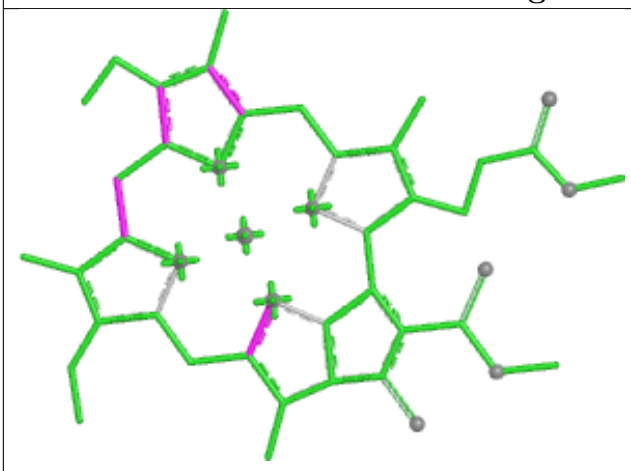


Torsions

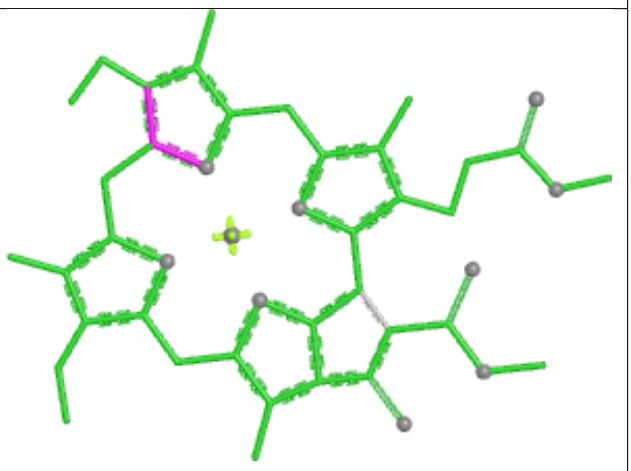


Rings

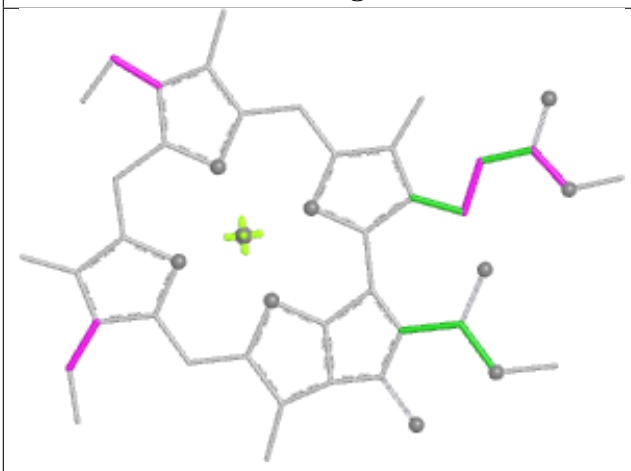
Ligand CLA o 513



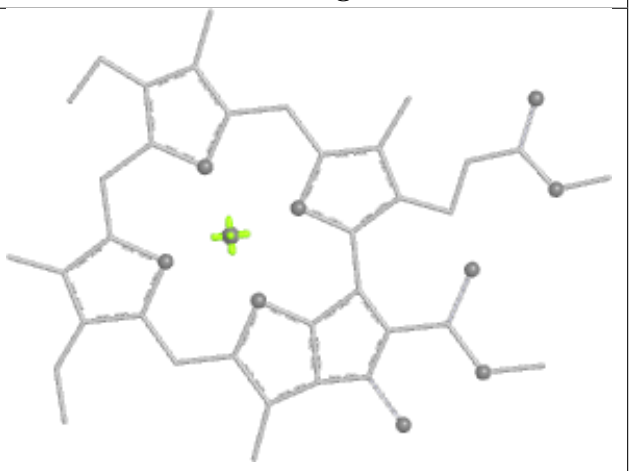
Bond lengths



Bond angles

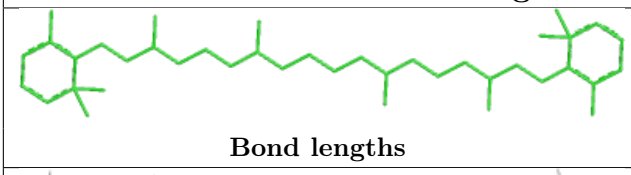


Torsions



Rings

Ligand BCR U 4022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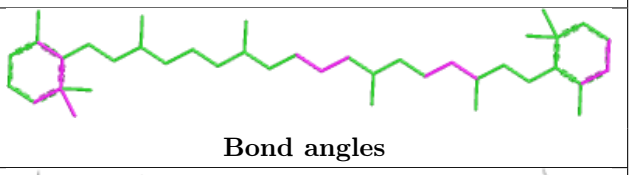
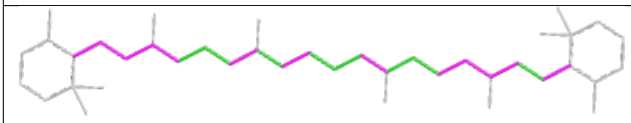
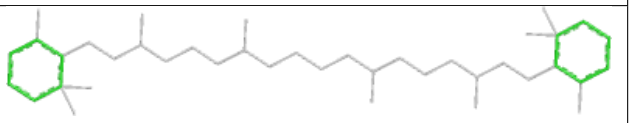
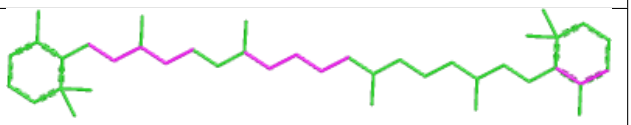

Bond angles

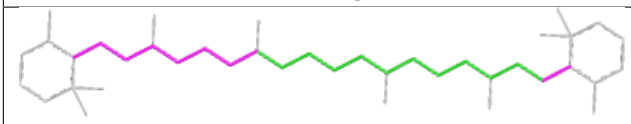

Torsions


Rings

Ligand BCR n 603

Bond lengths


Bond angles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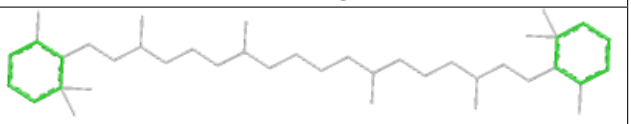
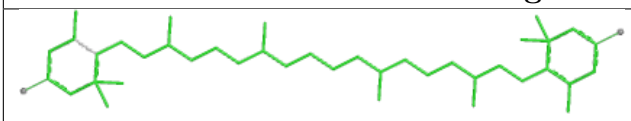

Rings

Ligand LUT w 601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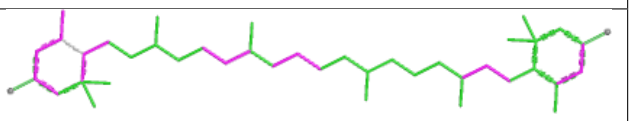
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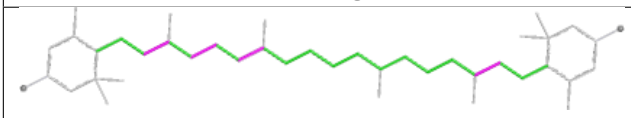
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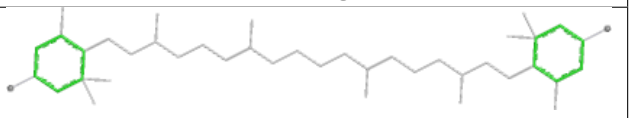
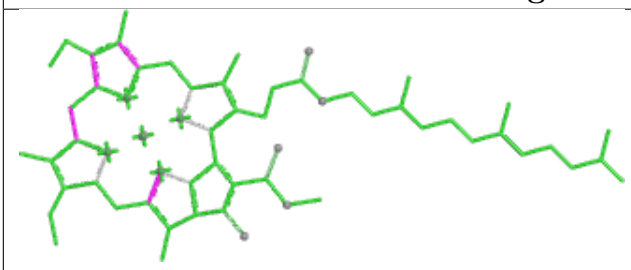

Rings

Ligand CLA q 510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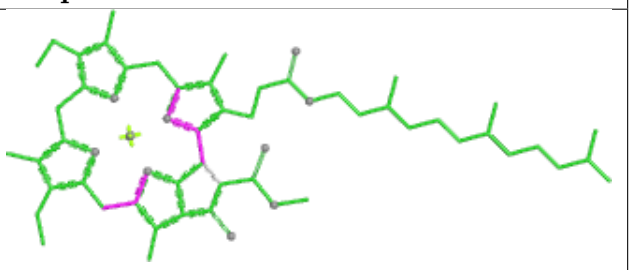
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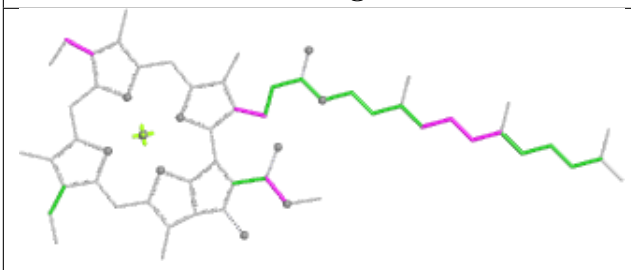
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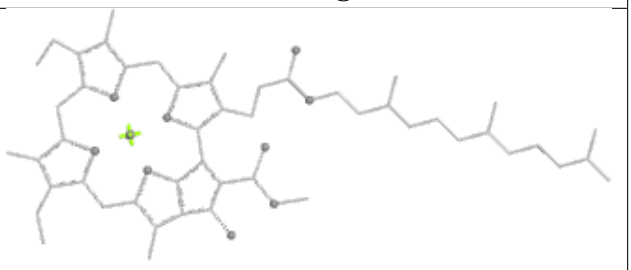
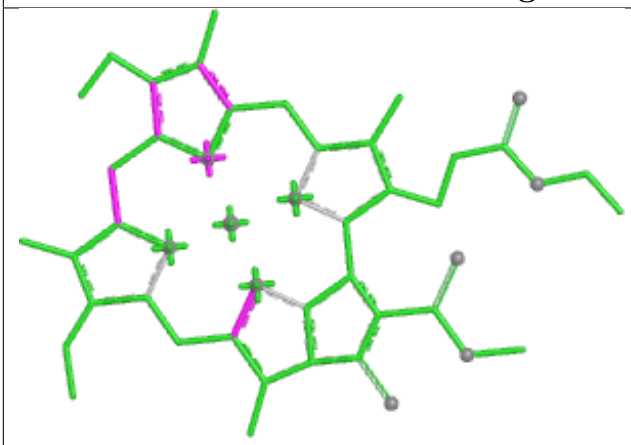

Rings

Ligand CLA b 1216



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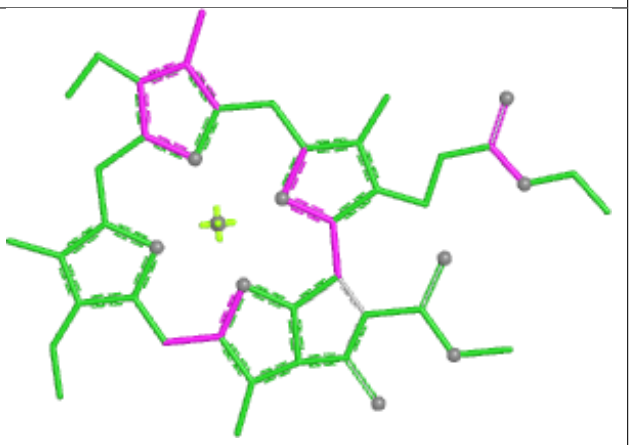
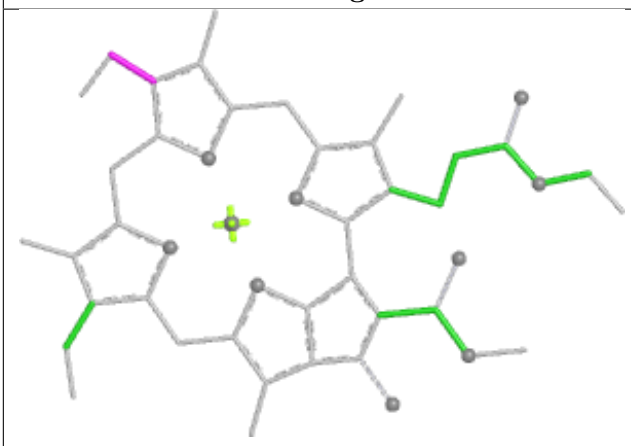


Bond angles



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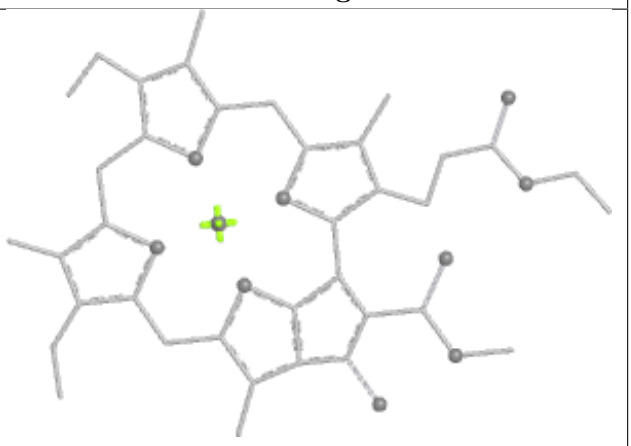
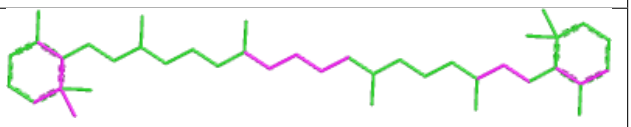


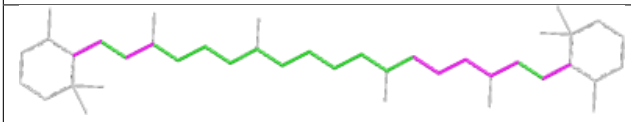
Rings

Ligand BCR S 4013

Bond lengths



Bond angles



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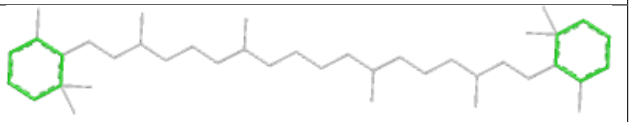
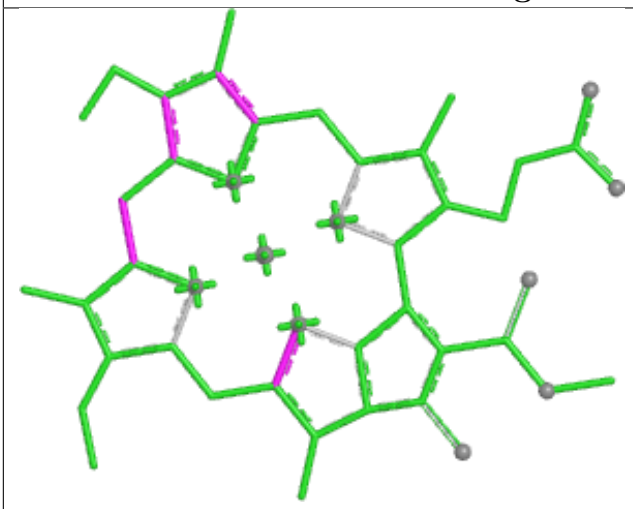


Rings

Ligand CLA G 1217



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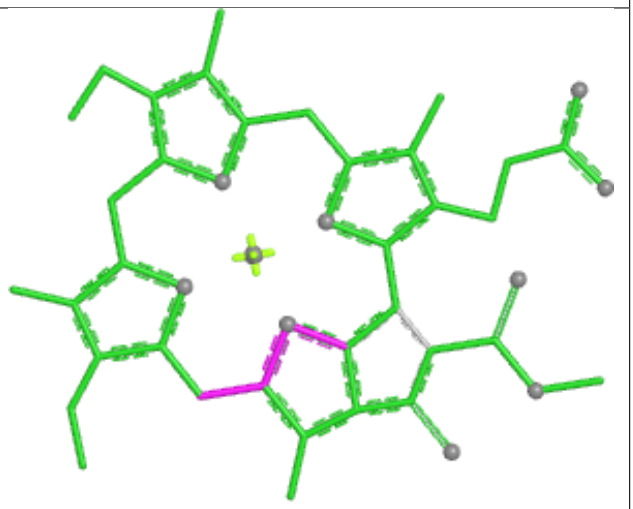

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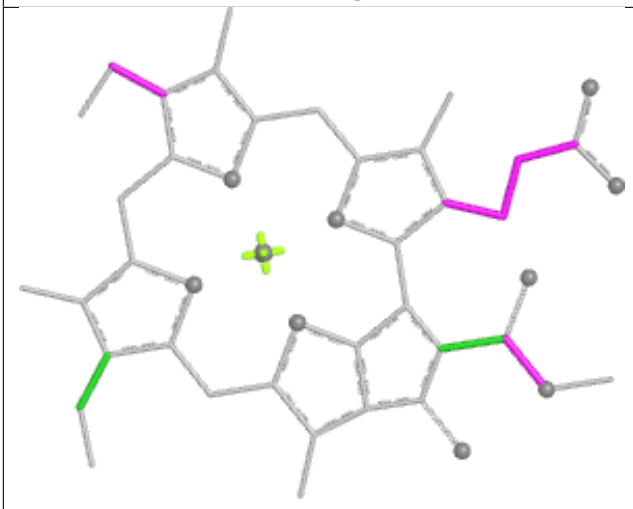
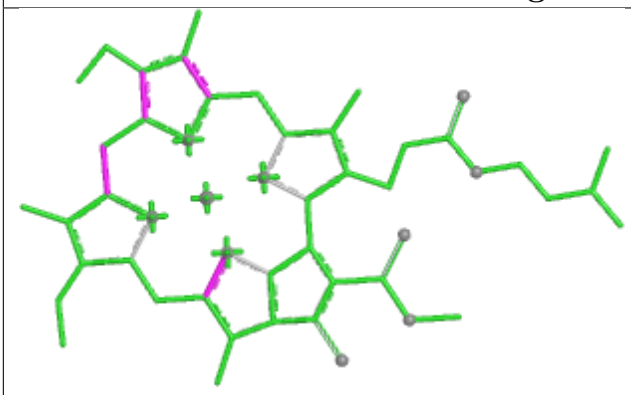


Torsions

Rings

Ligand CLA v 514



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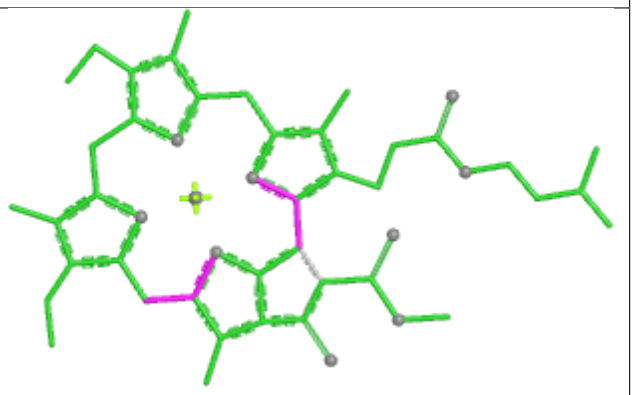

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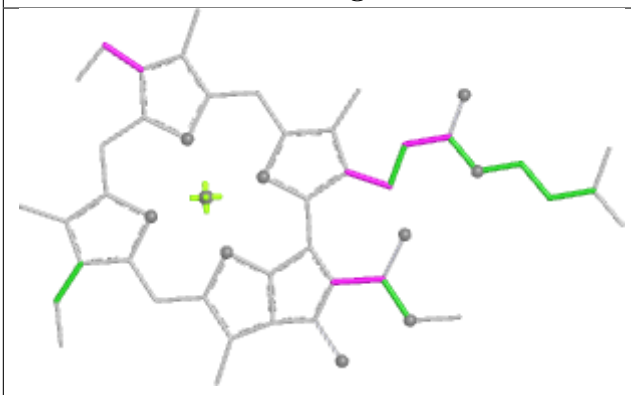

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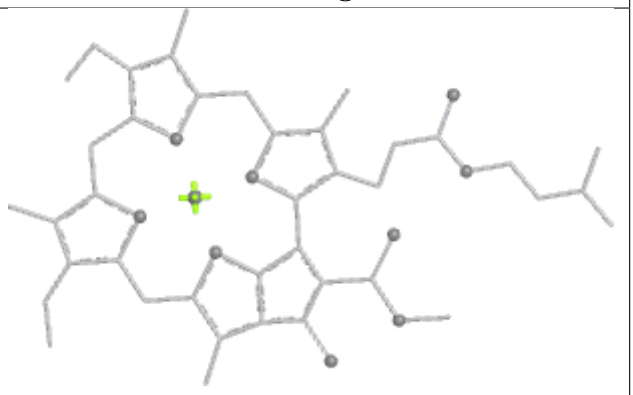
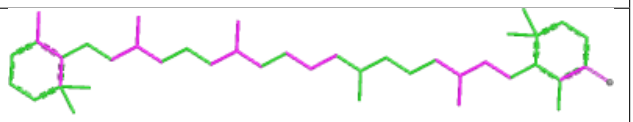


Rings

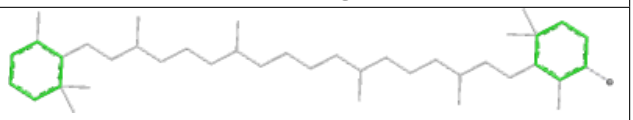
Ligand ECH B 4006

Bond lengths



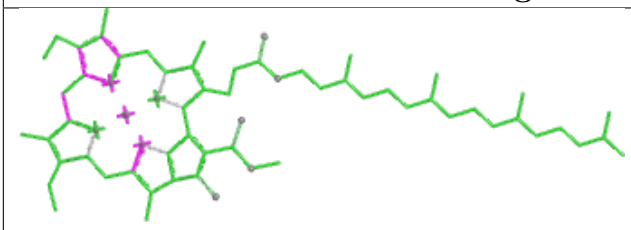
Bond angles

Torsions



Rings

Ligand CLA H 1013



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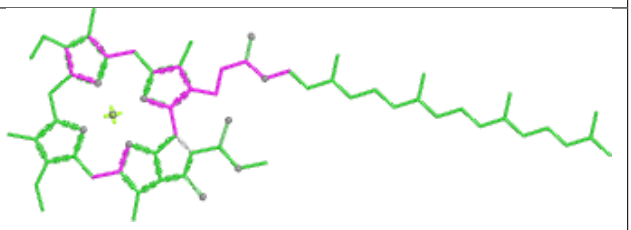

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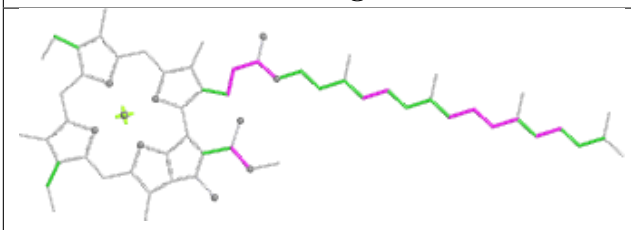

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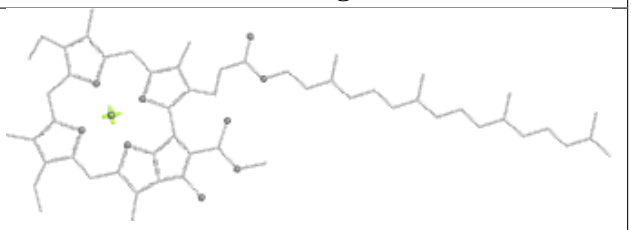
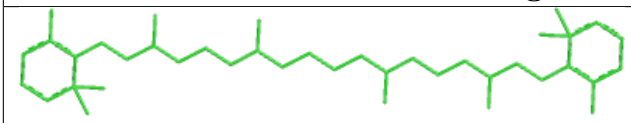


Rings

Ligand BCR u 604



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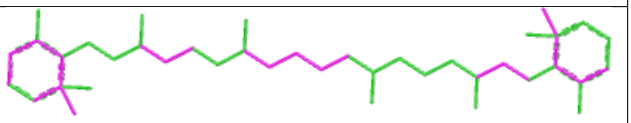

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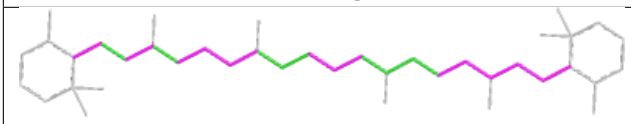

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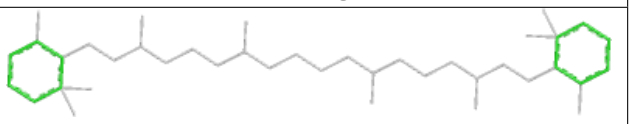

Rings

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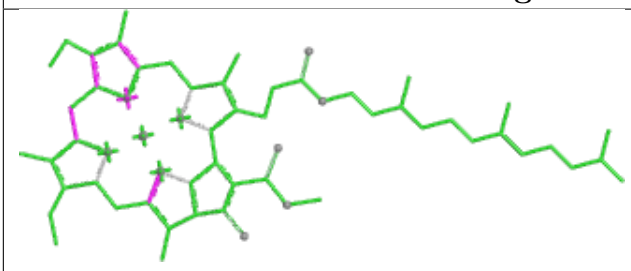

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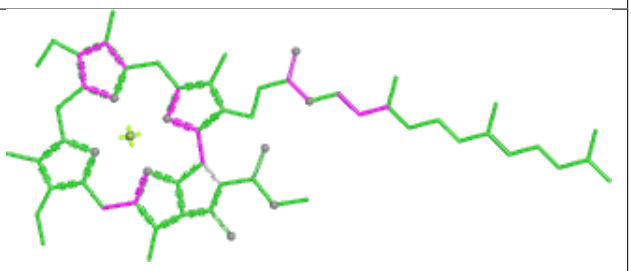

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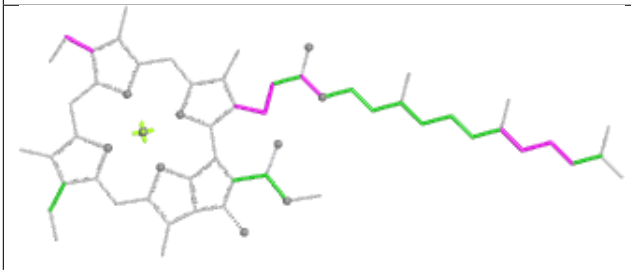

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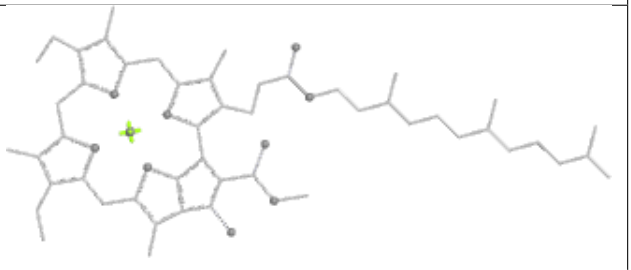
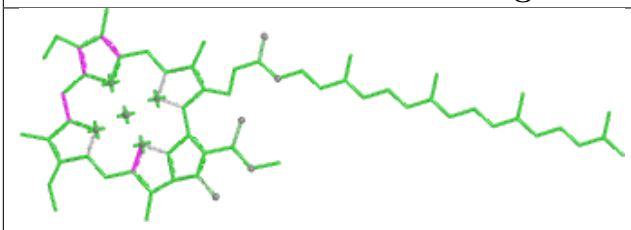
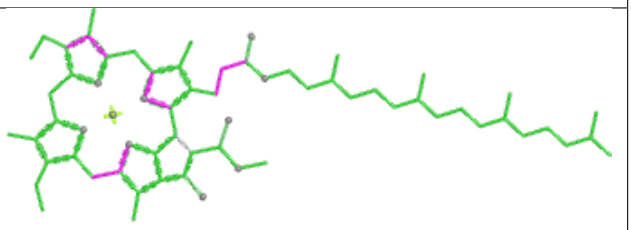


Rings

Ligand CLA H 1103	
	
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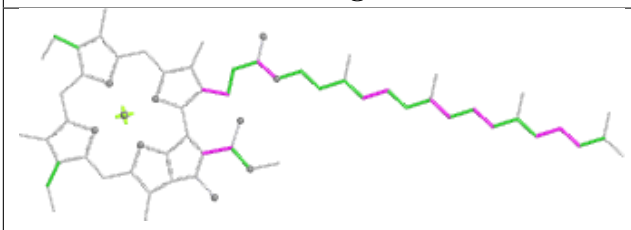
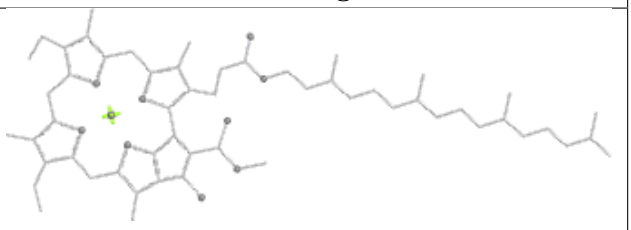
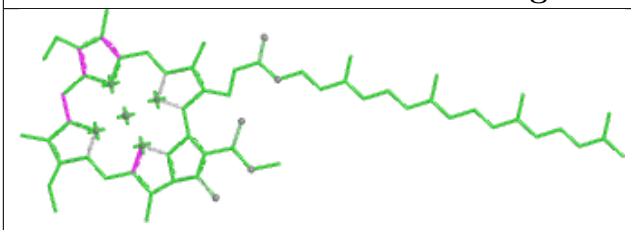
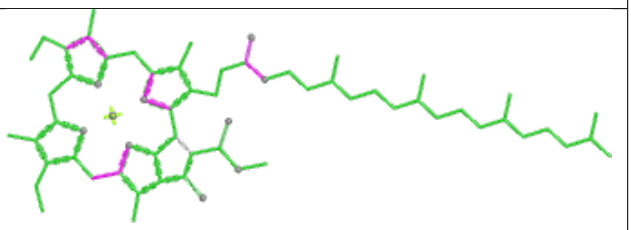
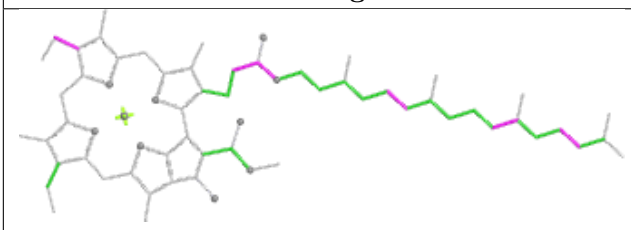
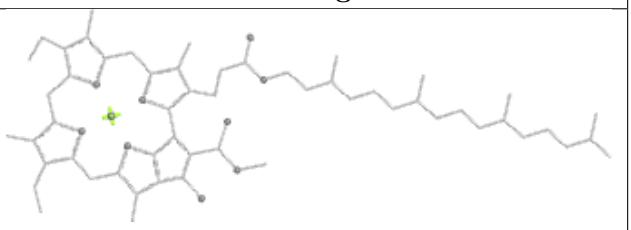
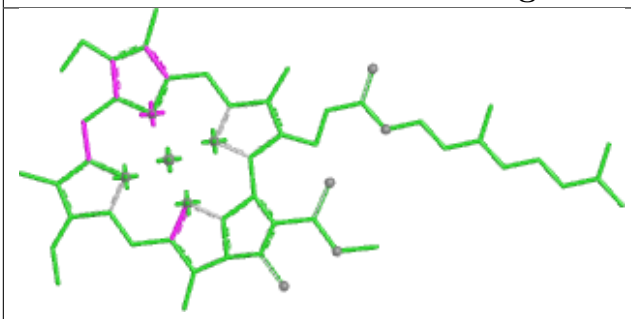
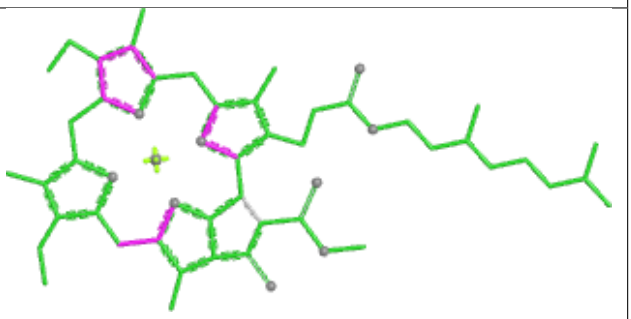
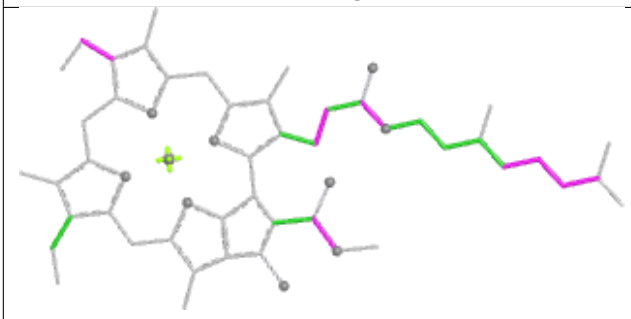
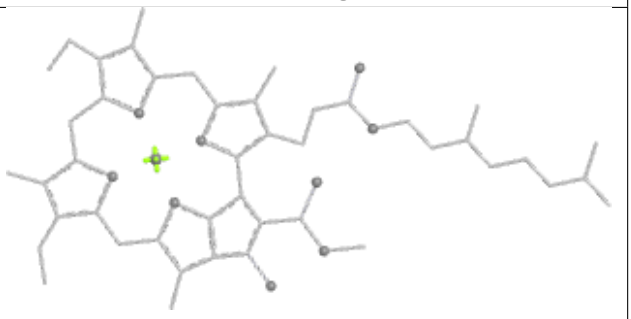
	
Torsions	Rings

Ligand CLA s 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

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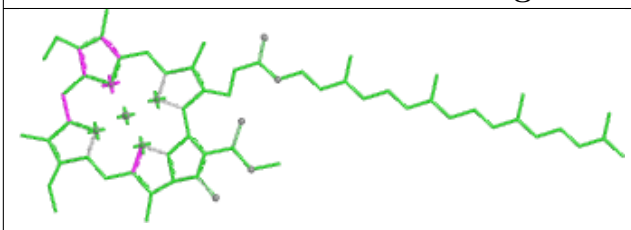
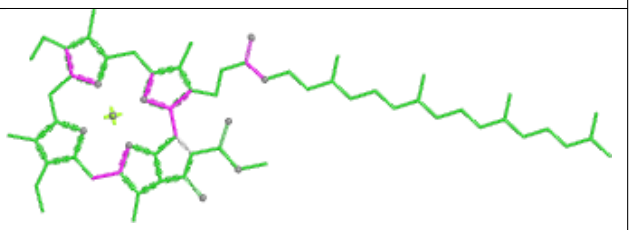
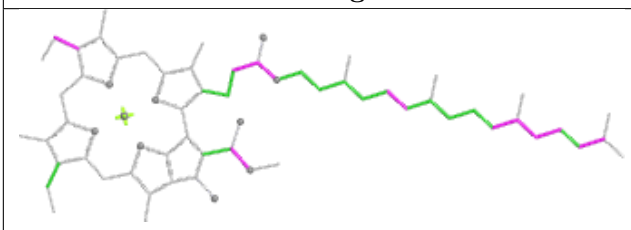
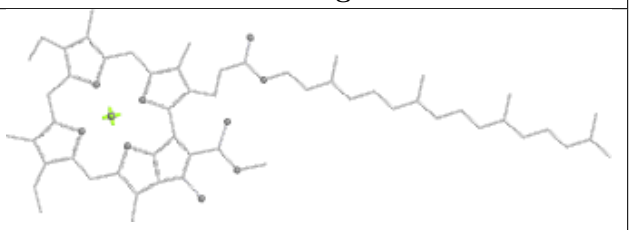
 Bond lengths	 Bond angles
 Torsions	 Rings

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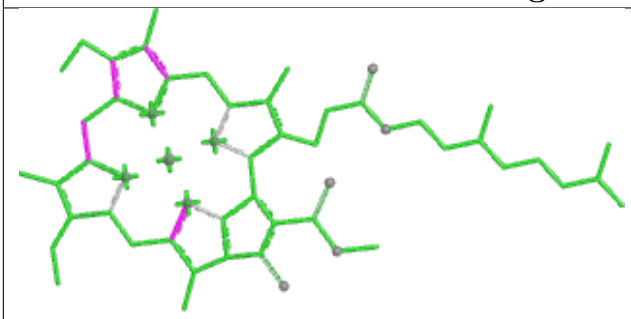
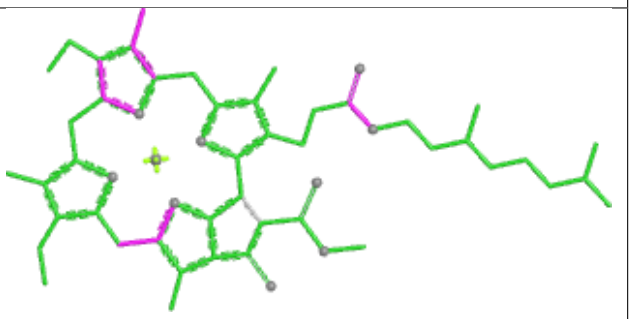
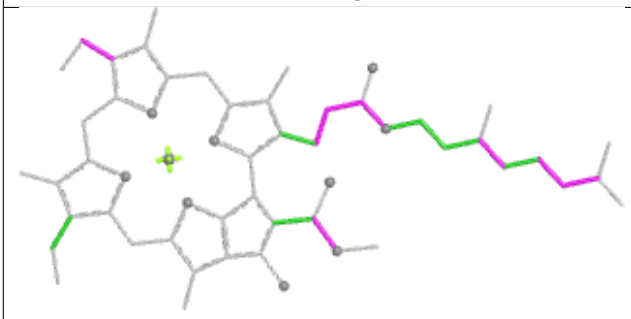
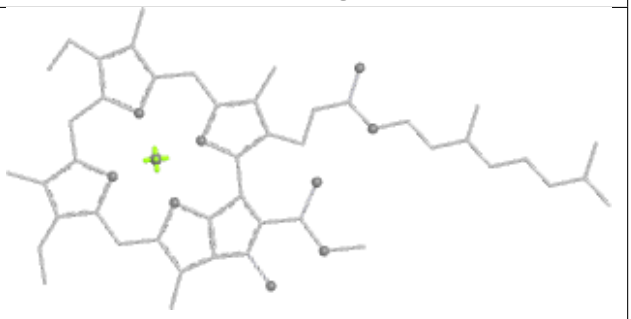
 Bond lengths	 Bond angles
 Torsions	 Rings

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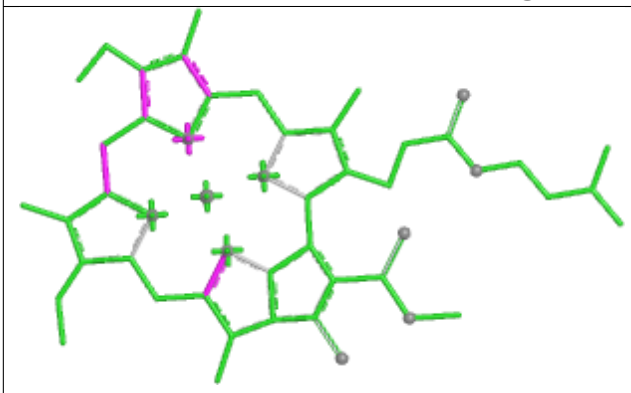
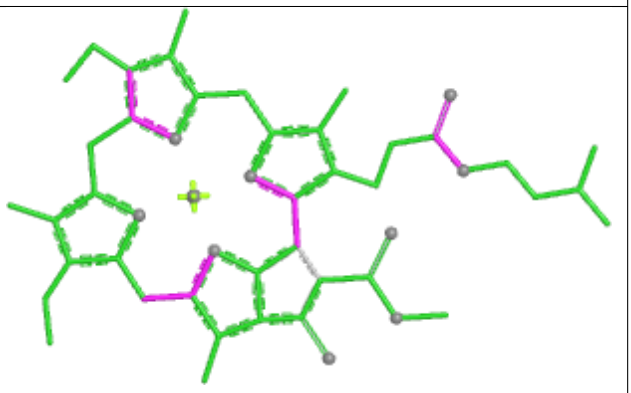
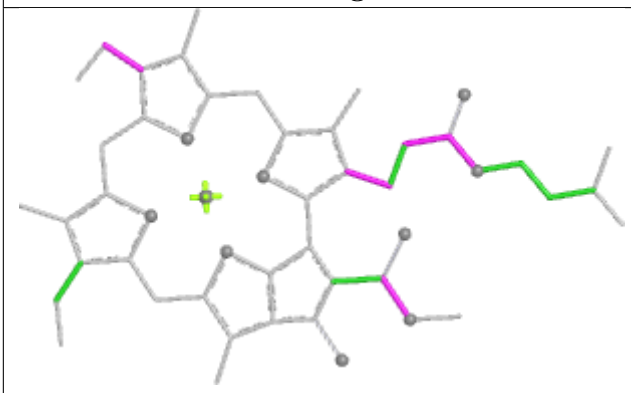
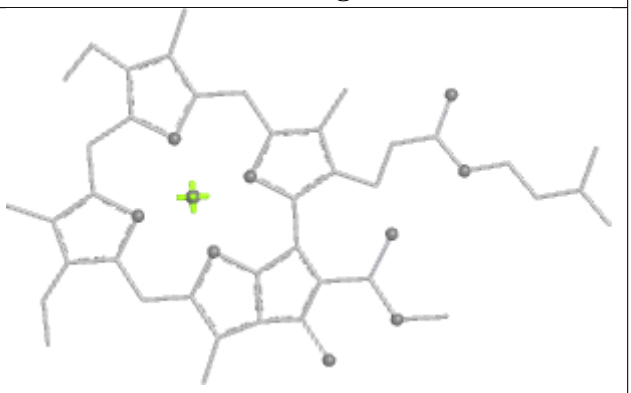
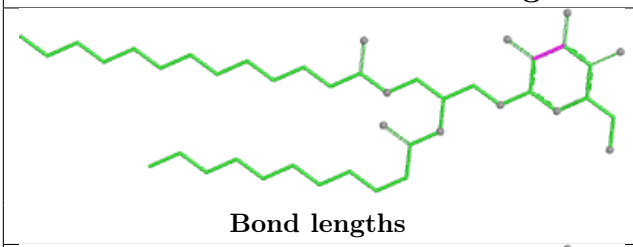
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG b 848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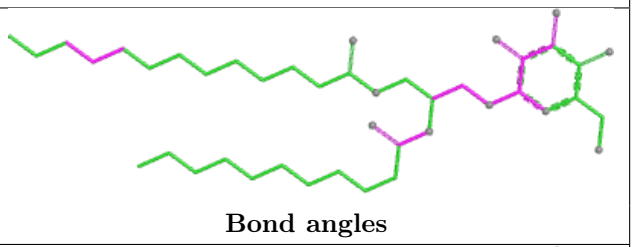
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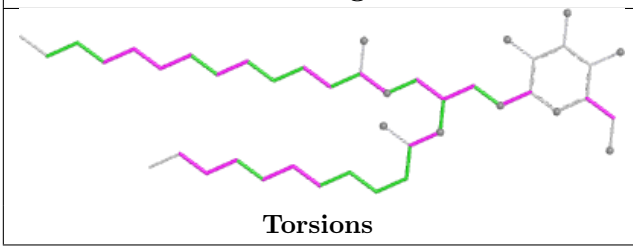
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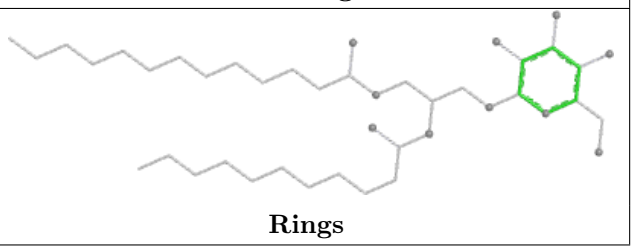
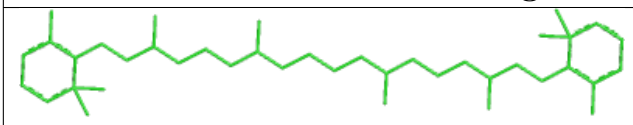

Rings

Ligand BCR j 4012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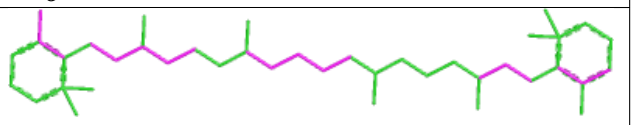
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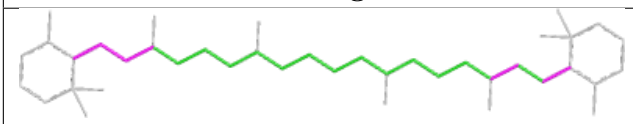
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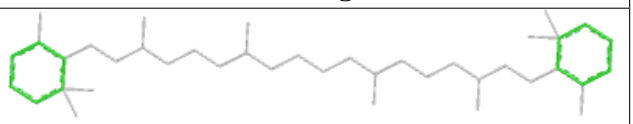
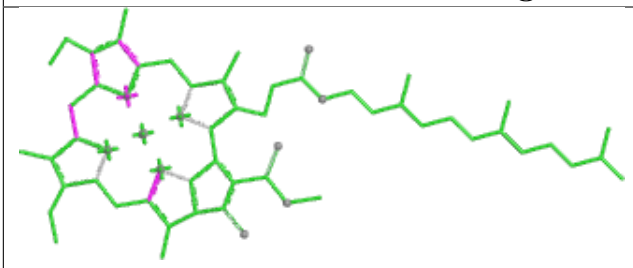

Rings

Ligand CLA L 1501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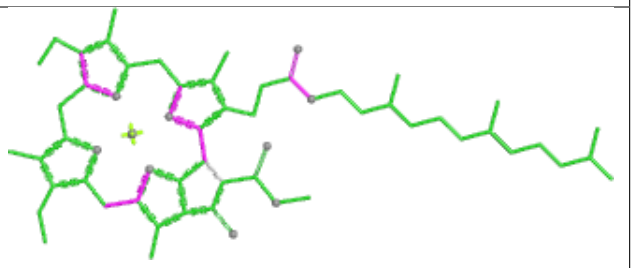
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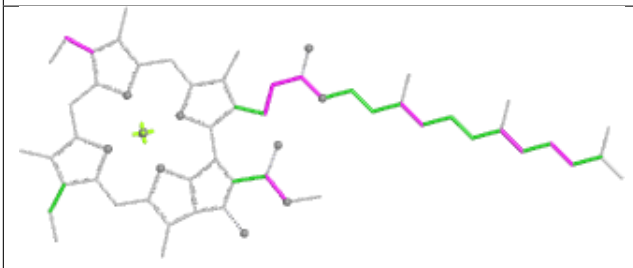
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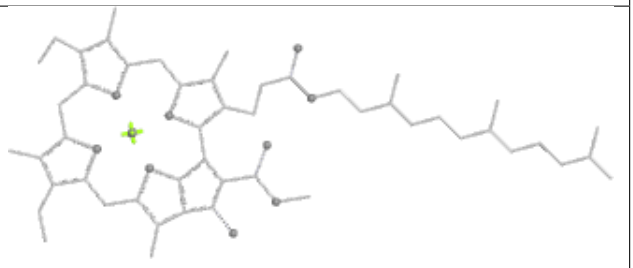
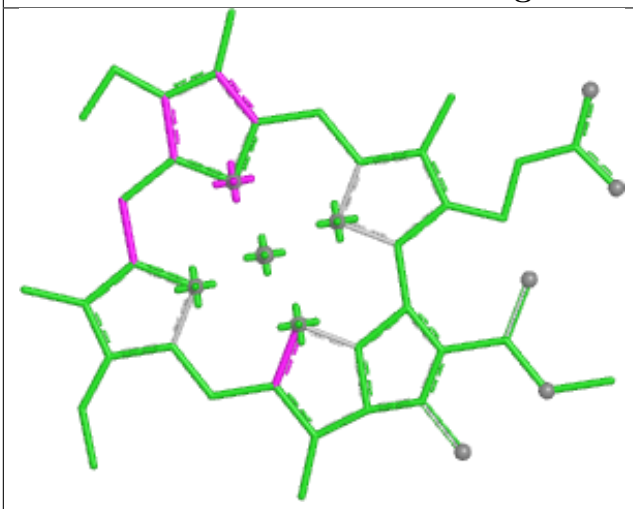

Rings

Ligand CLA H 1108



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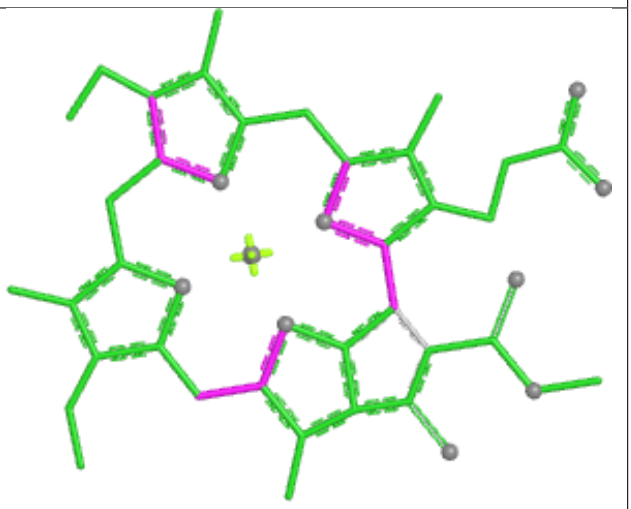

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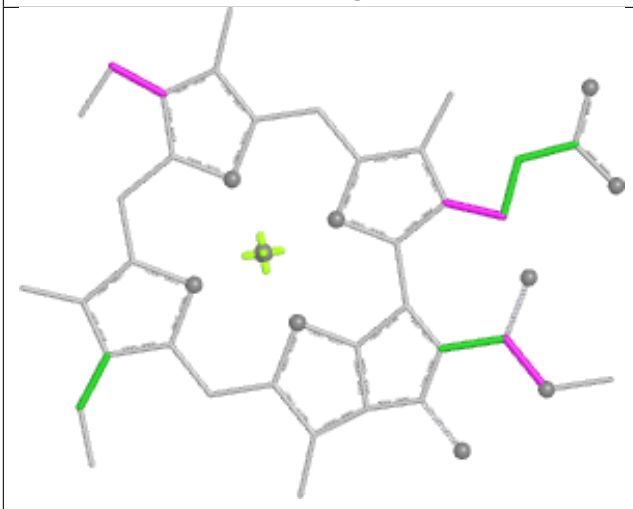
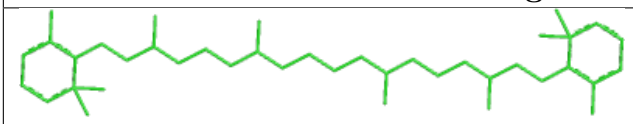


Torsions

Rings

Ligand BCR n 604



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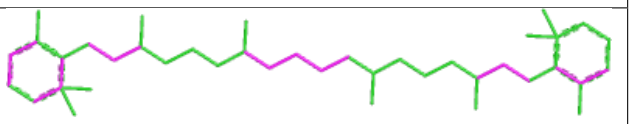

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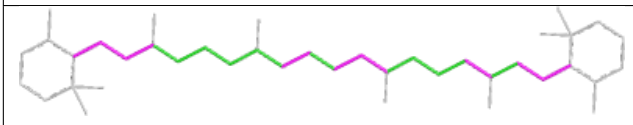
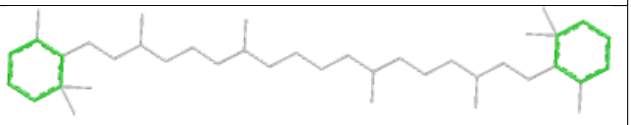
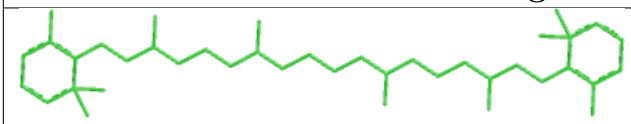
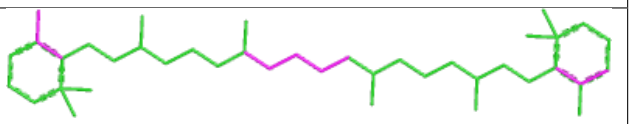
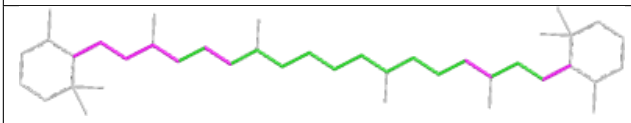
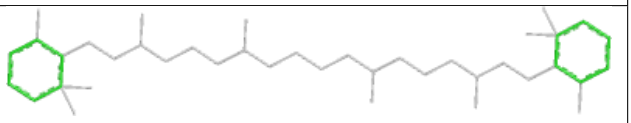


Torsions



Rings

Ligand BCR t 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

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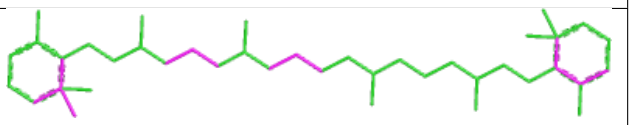
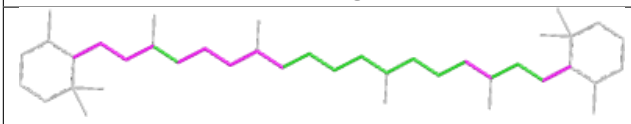
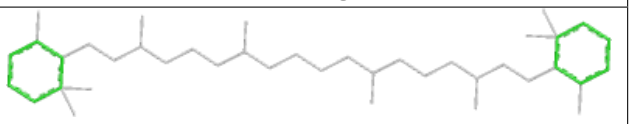
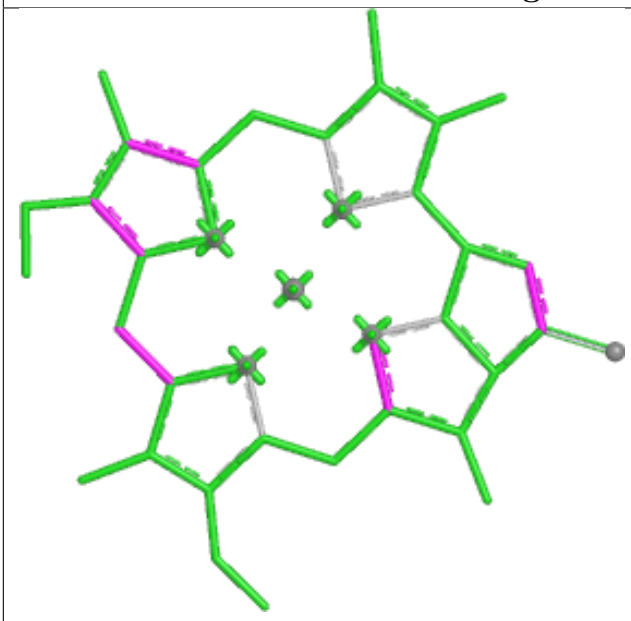
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 1303



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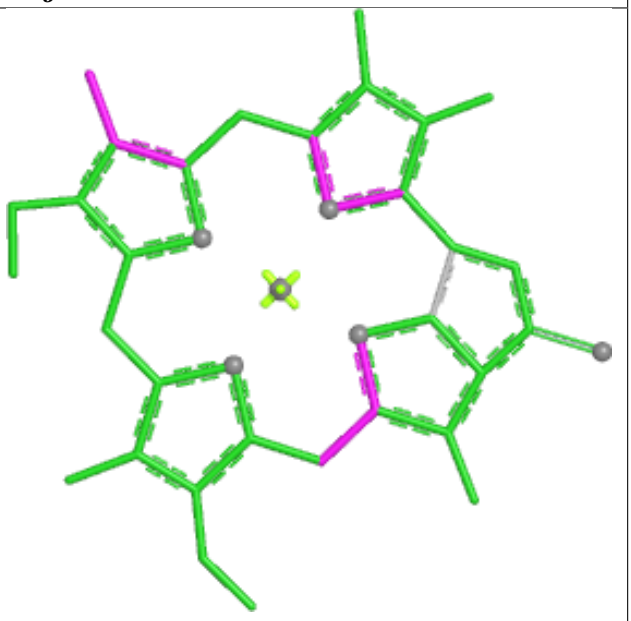
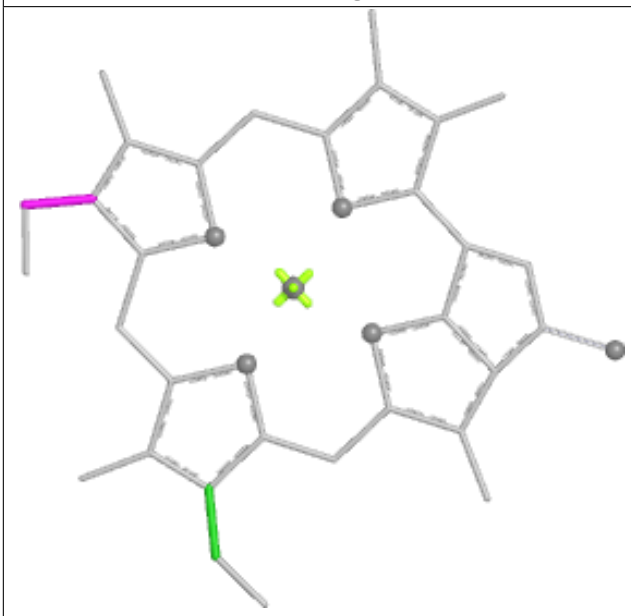
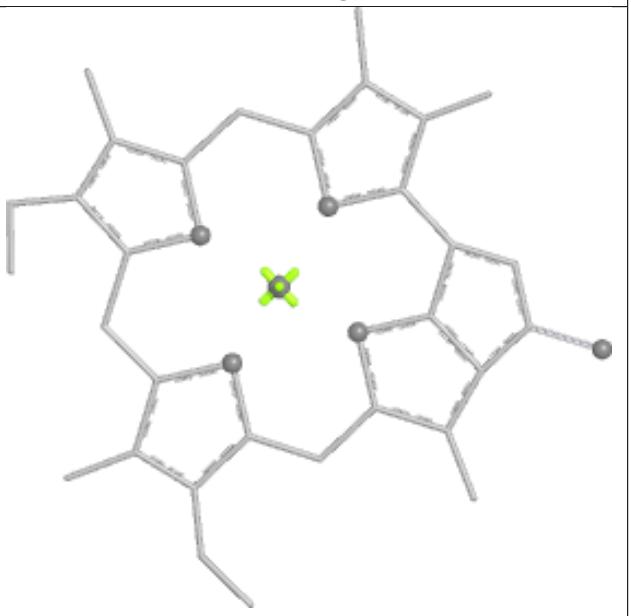


Bond angles

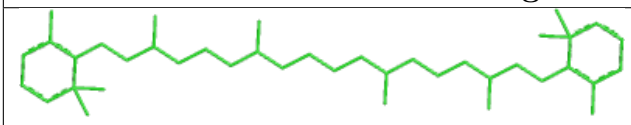


Torsions



Rings

Ligand BCR Y 602



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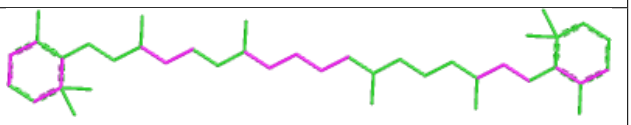

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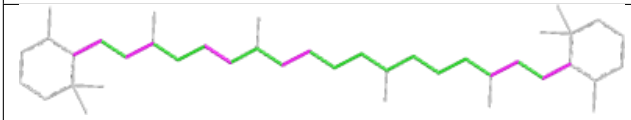

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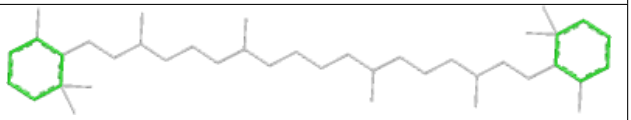
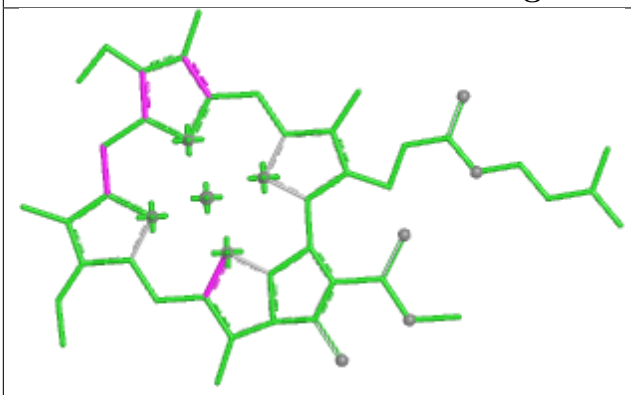


Rings

Ligand CLA Y 501



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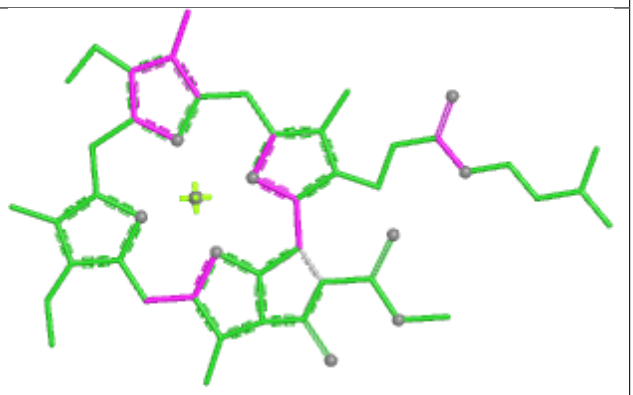

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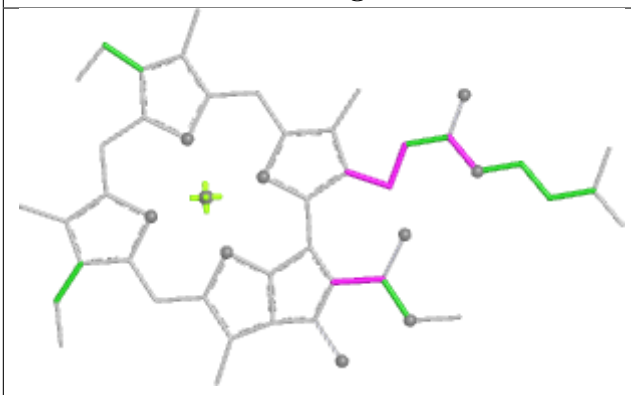

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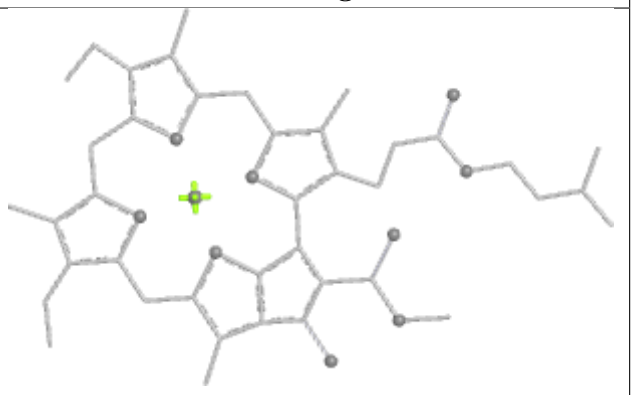
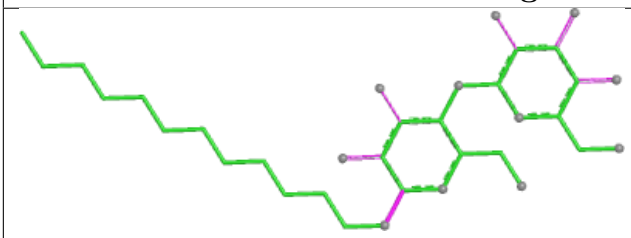


Rings

Ligand LMT l 4101



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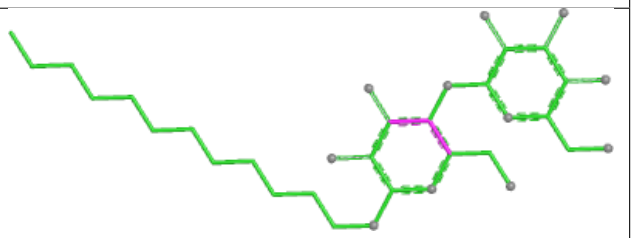
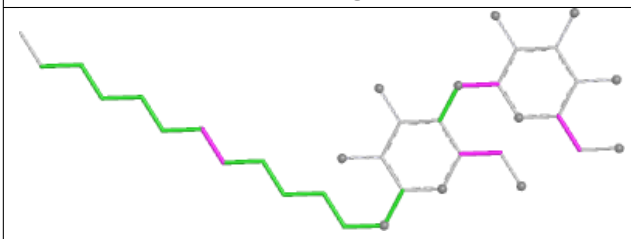


Bond angles



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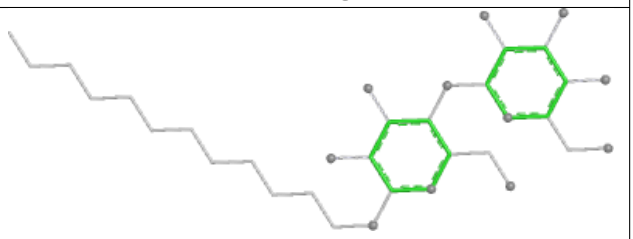
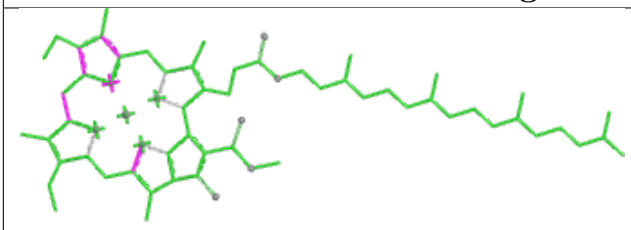


Rings

Ligand CLA a 1136



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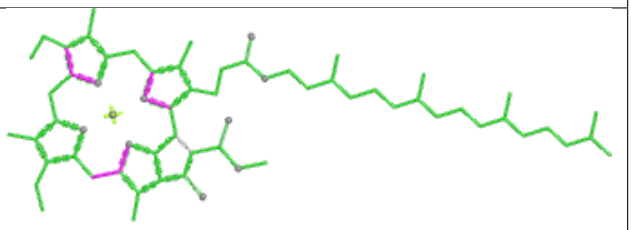
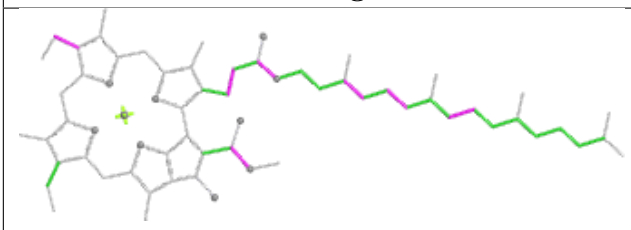
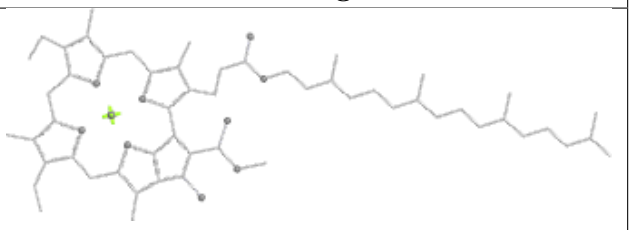


Bond angles

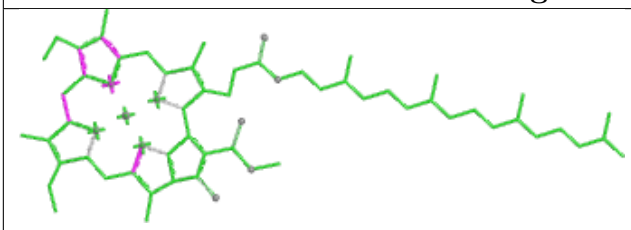


Torsions

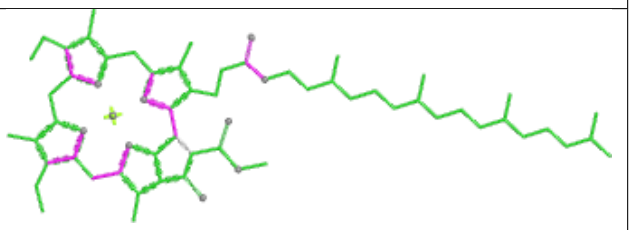


Rings

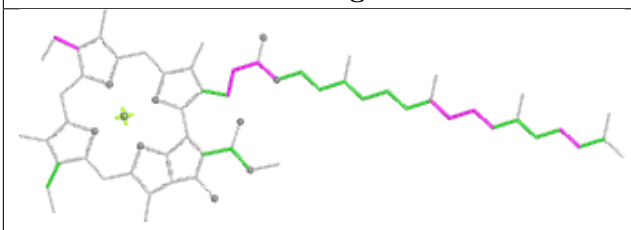
Ligand CLA t 505



Bond lengths



Bond angles



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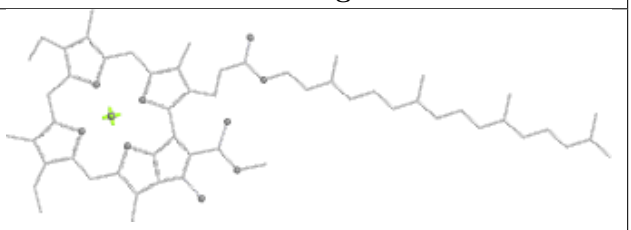
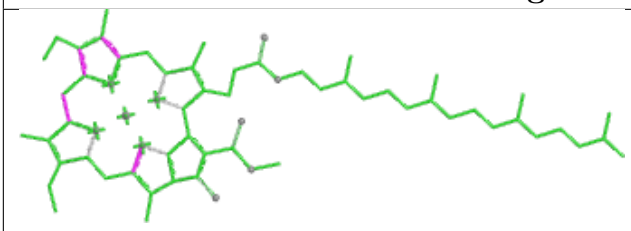


Rings

Ligand CLA u 505



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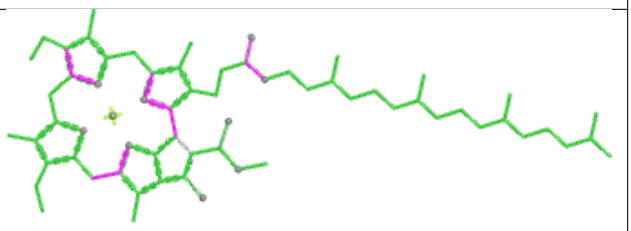
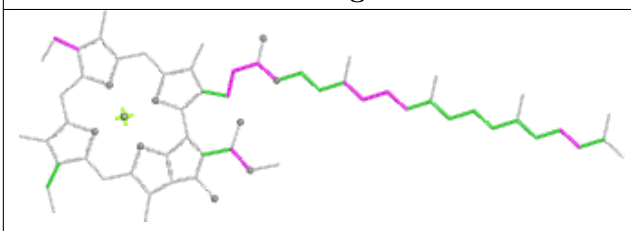
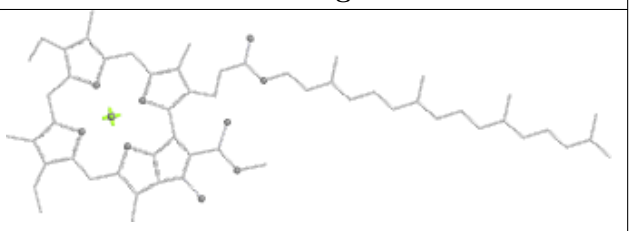


Bond angles

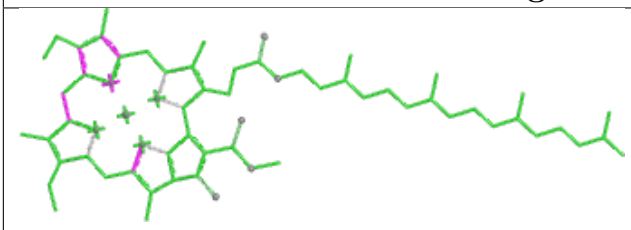


Torsions



Rings

Ligand CLA x 509



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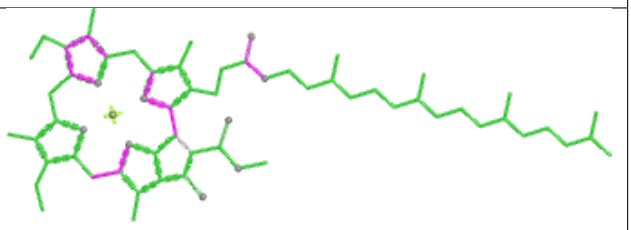
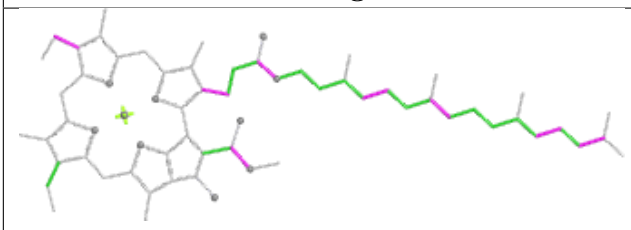


Bond angles



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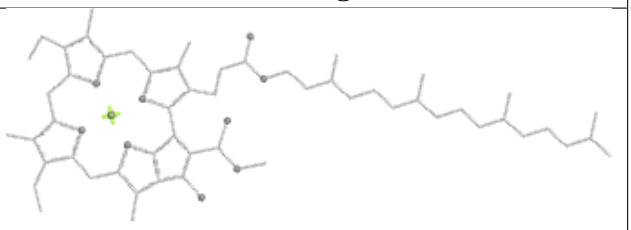
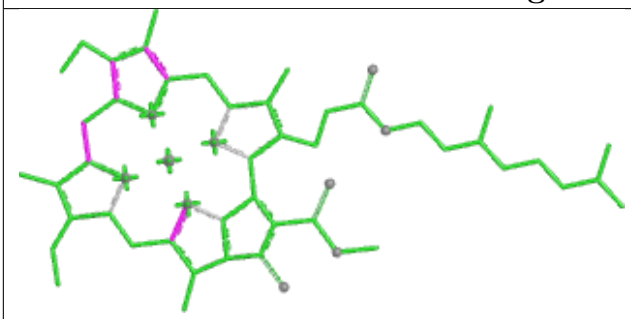


Rings

Ligand CLA y 508



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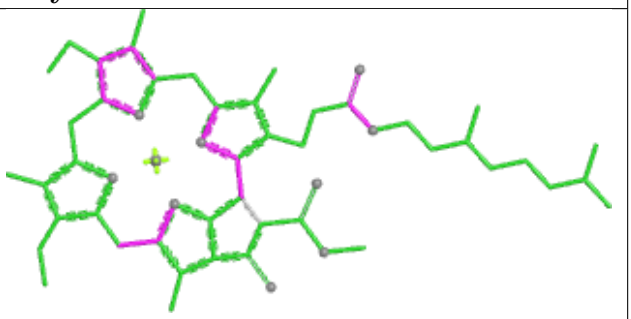
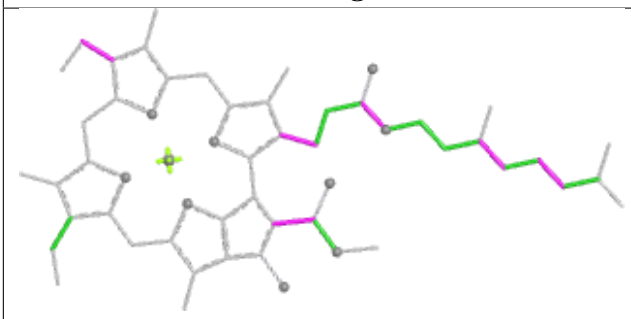


Bond angles



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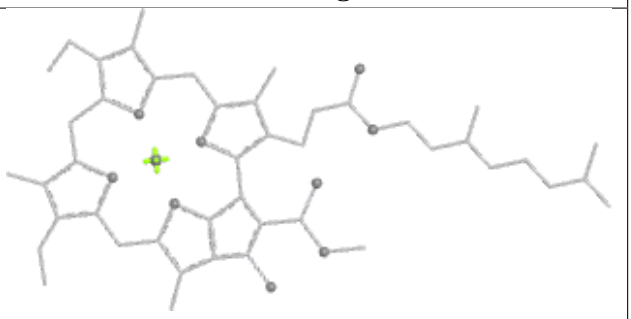
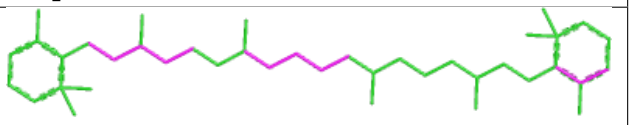


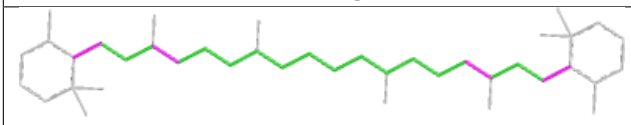
Rings

Ligand BCR p 603

Bond lengths



Bond angles



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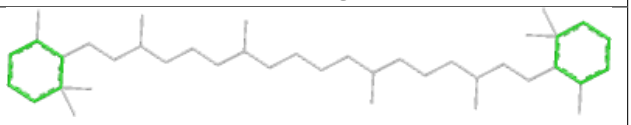
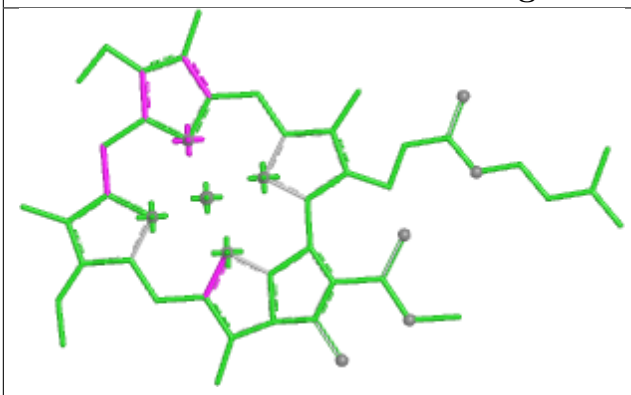
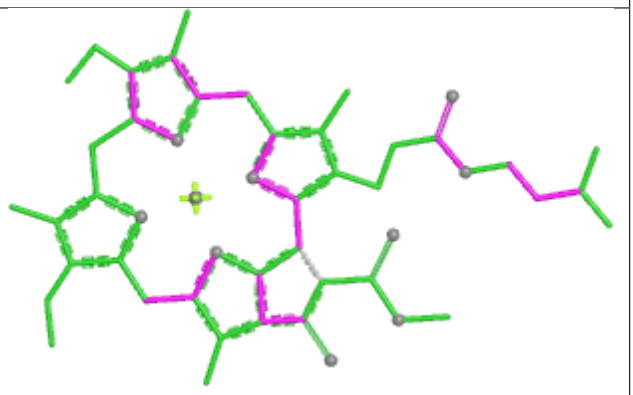


Rings

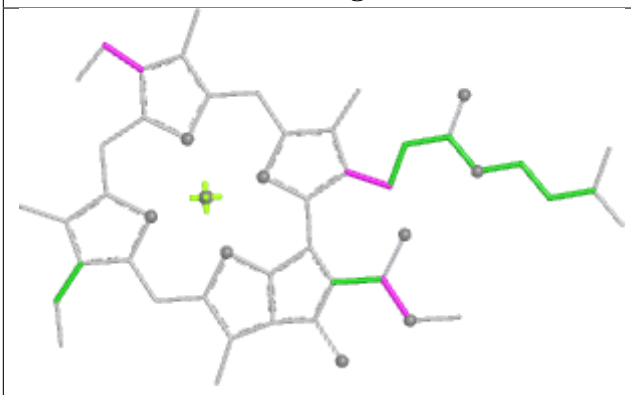
Ligand CLA b 1234



Bond lengths



Bond angles



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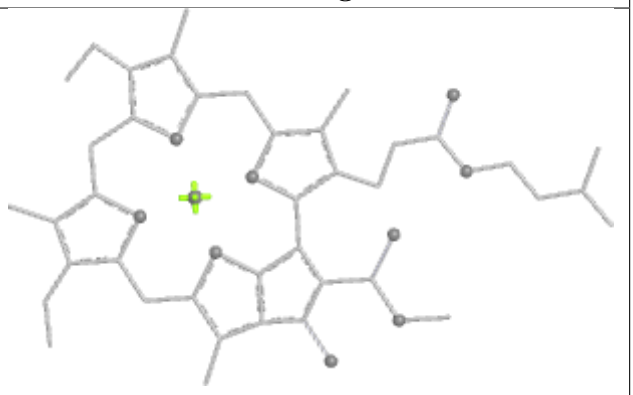
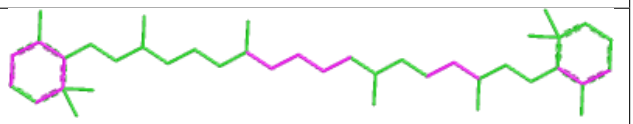


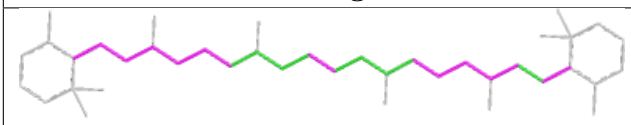
Rings

Ligand BCR X 602

Bond lengths



Bond angles



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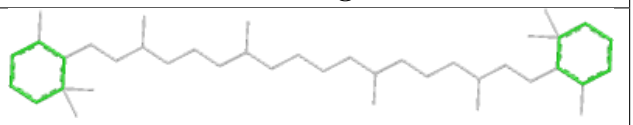
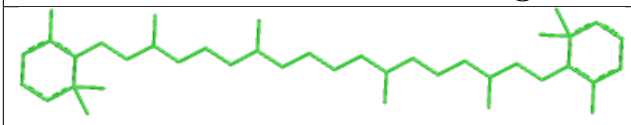


Rings

Ligand BCR T 4005



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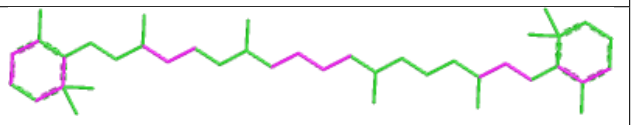
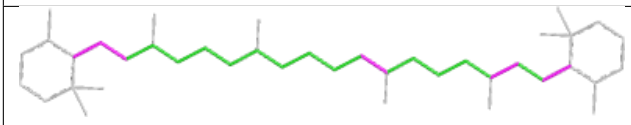


Bond angles



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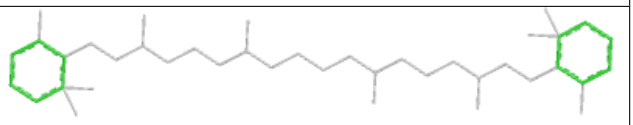
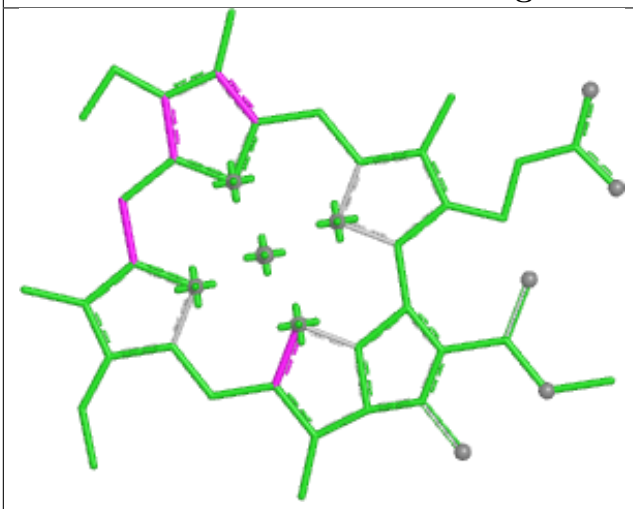


Rings

Ligand CLA B 1217



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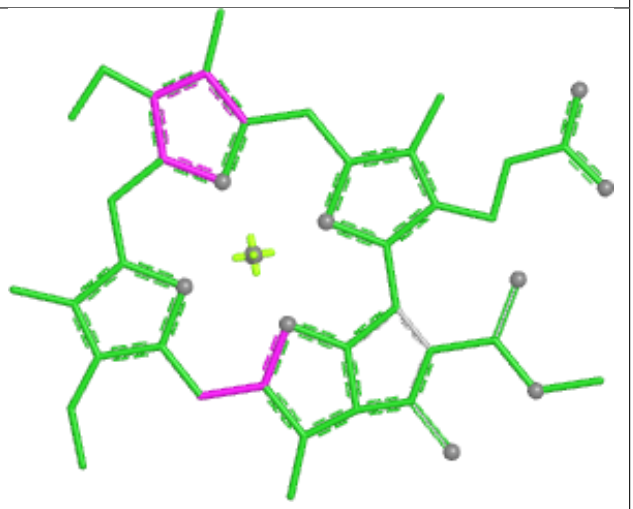
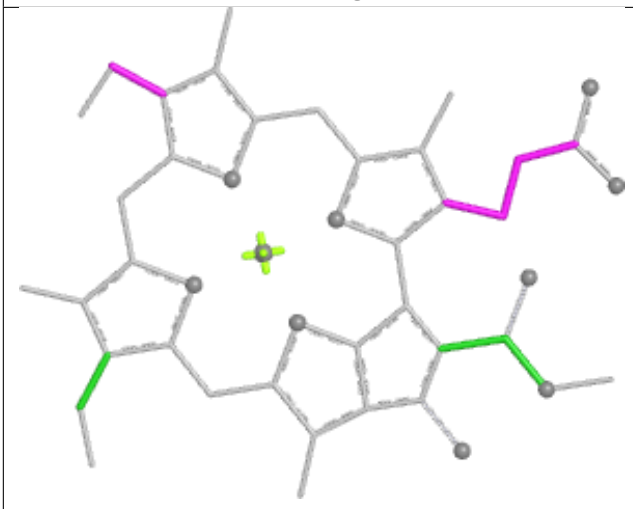


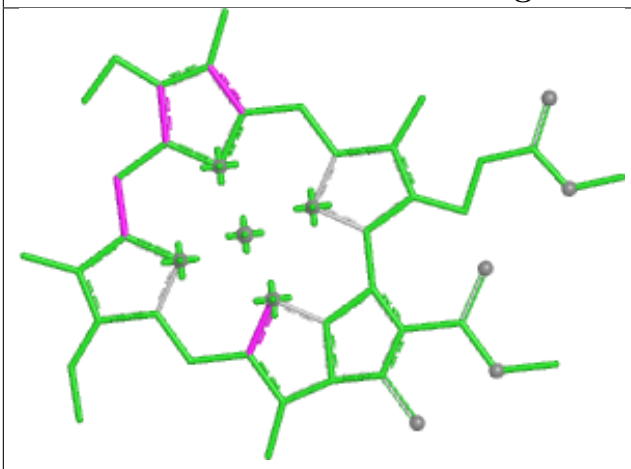
Bond angles



Torsions

Rings

Ligand CLA H 1801



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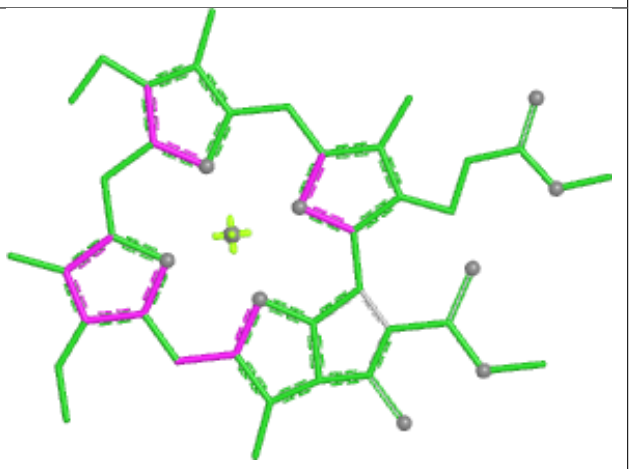

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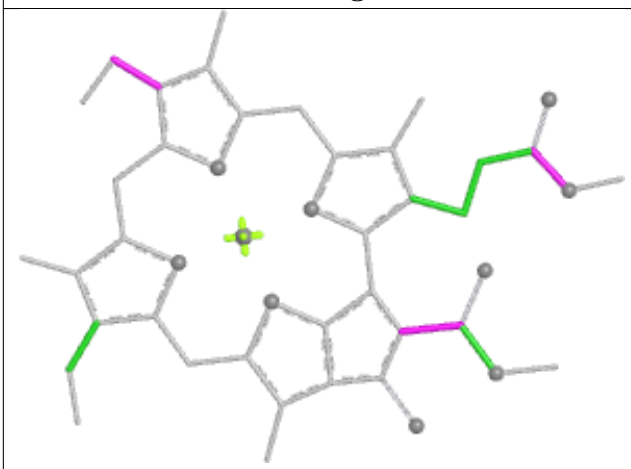

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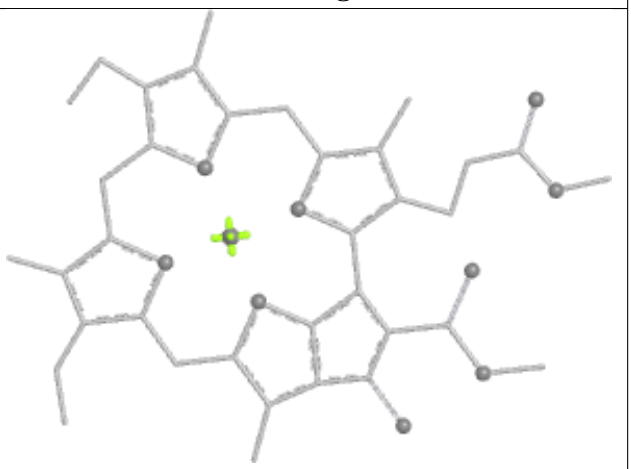
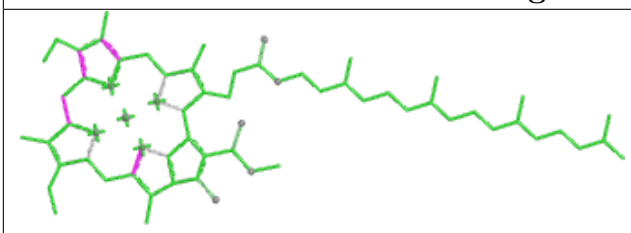


Rings

Ligand CLA o 507



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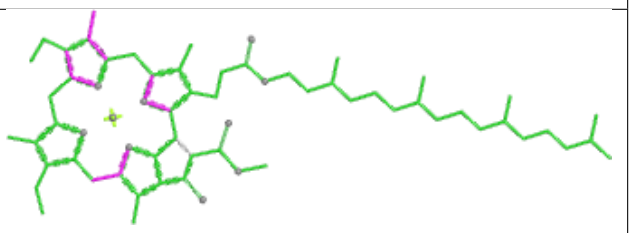
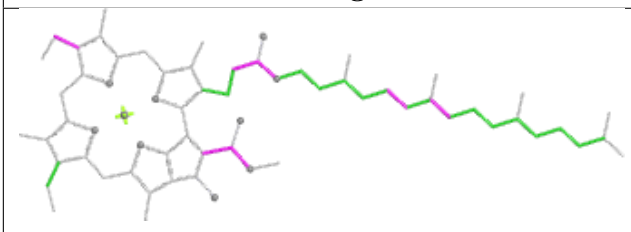


Bond angles



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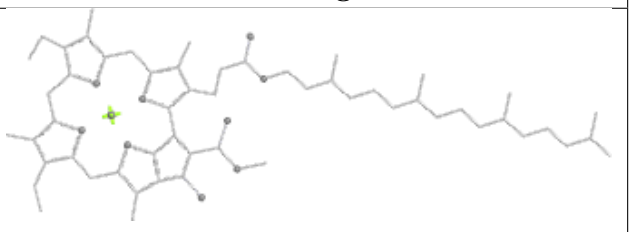
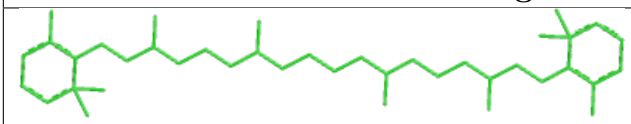


Rings

Ligand BCR F 4016



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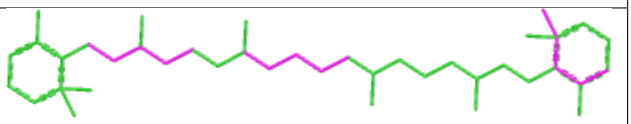
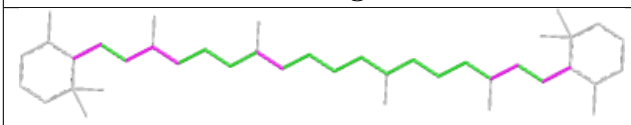


Bond angles



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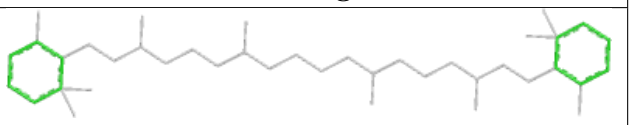
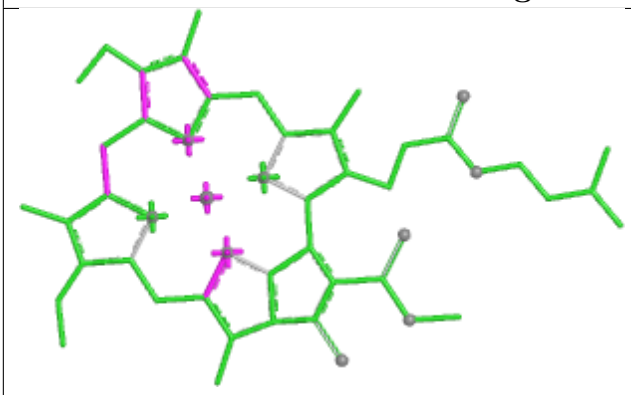


Rings

Ligand CLA G 1234



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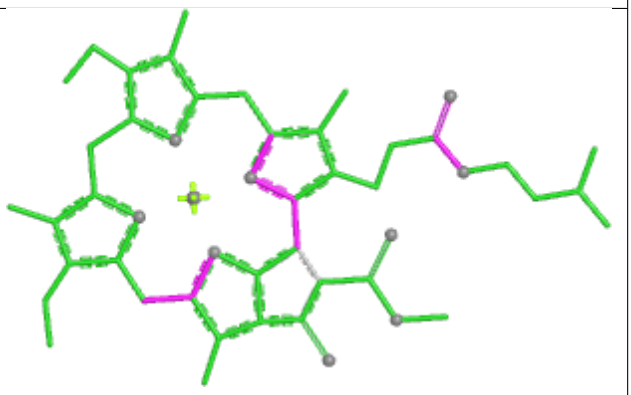
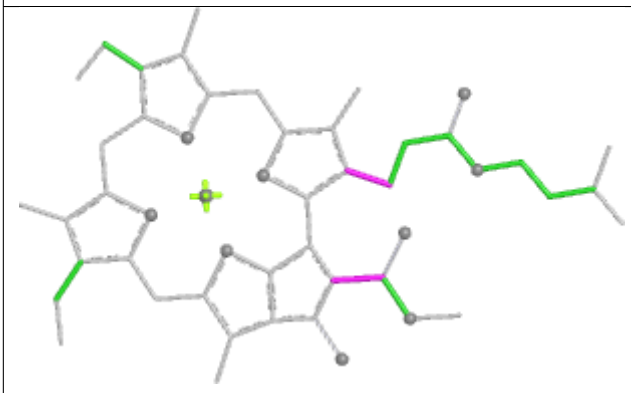


Bond angles



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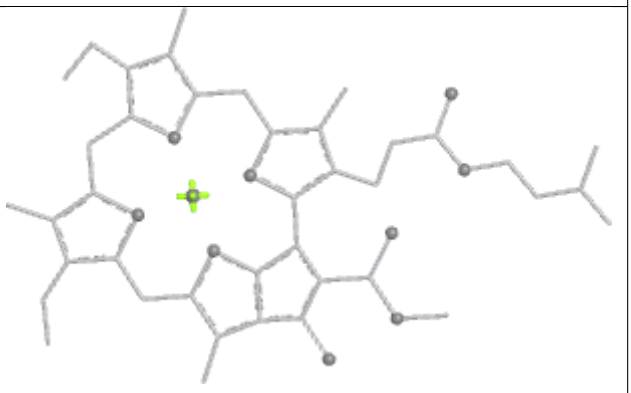
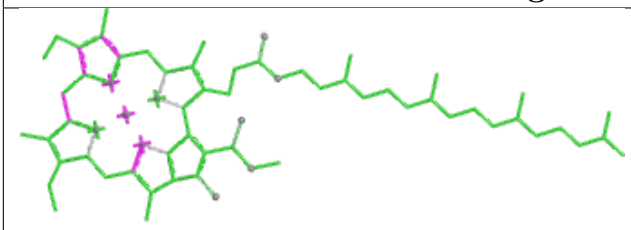
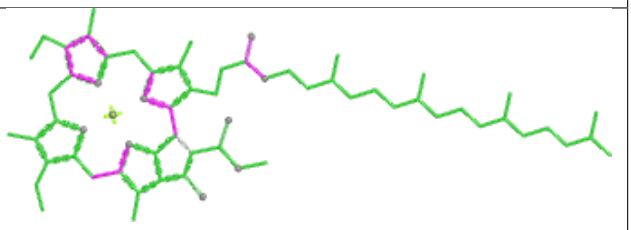


Rings

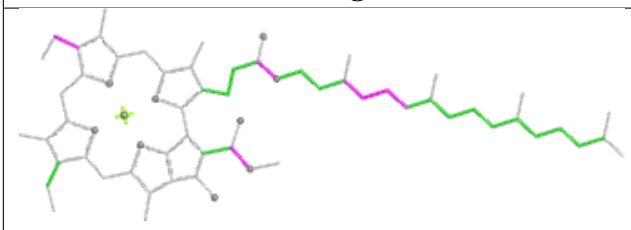
Ligand CLA x 512



Bond lengths



Bond angles



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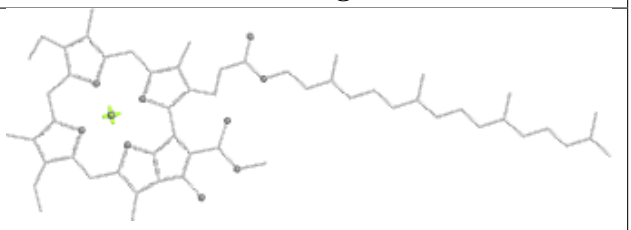
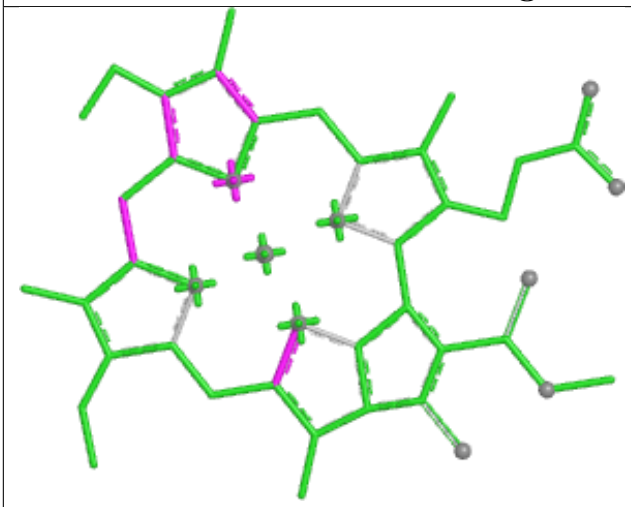
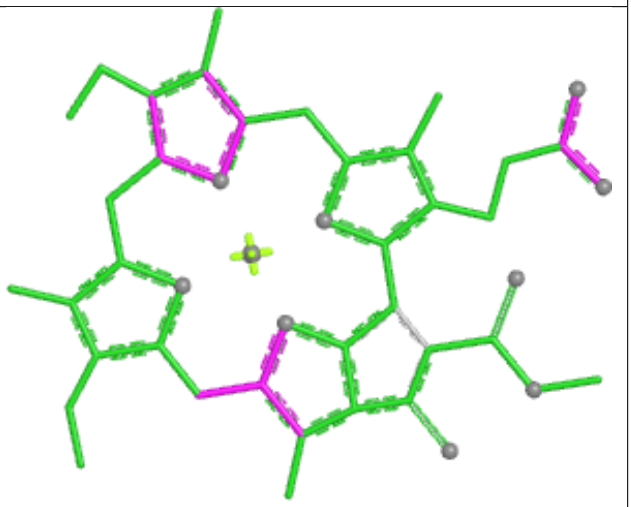


Rings

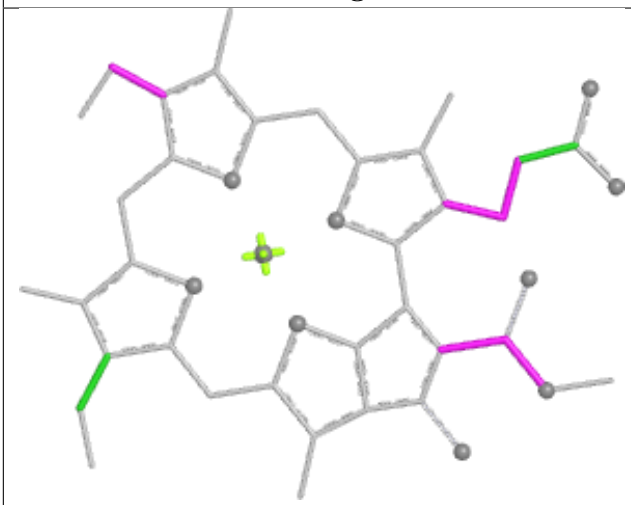
Ligand CLA b 1219



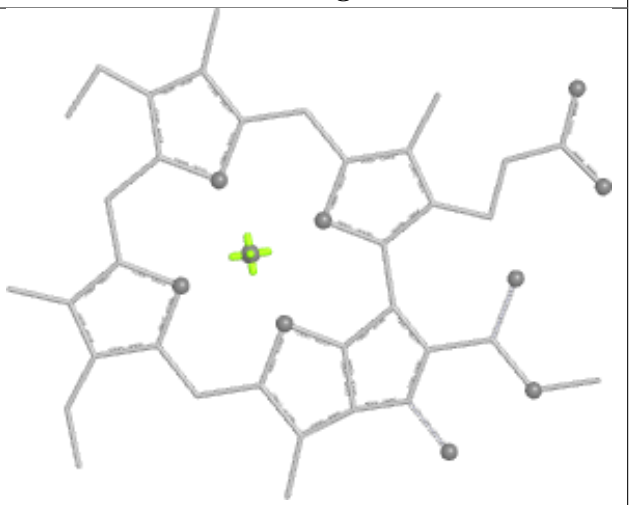
Bond lengths



Bond angles

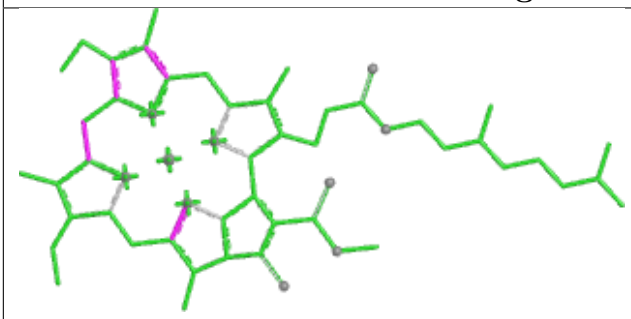


Torsions



Rings

Ligand CLA T 4004



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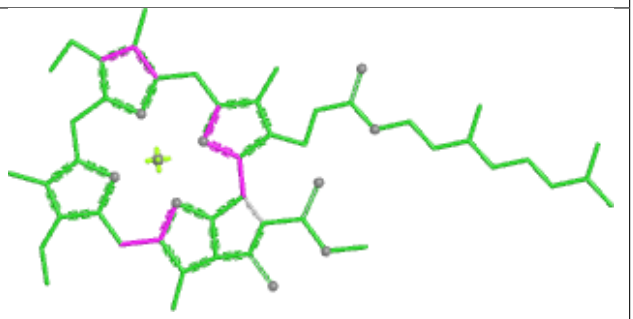

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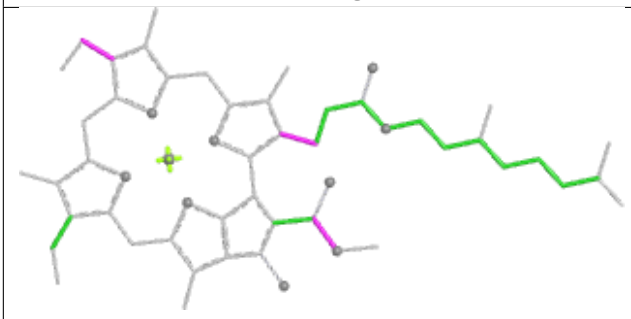

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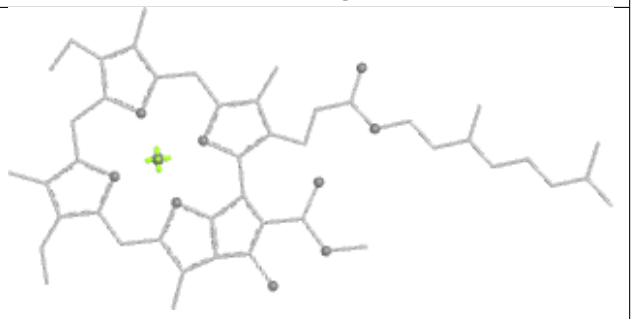
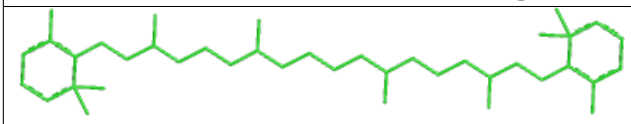


Rings

Ligand BCR H 4002



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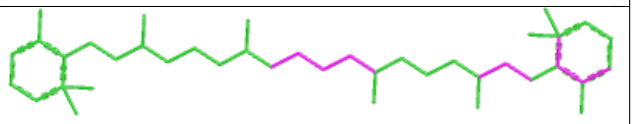

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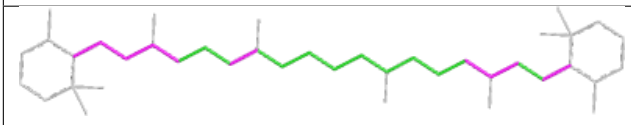

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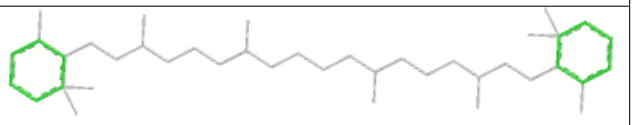
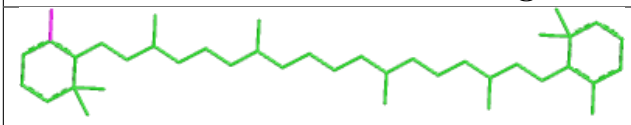


Rings

Ligand BCR a 4007



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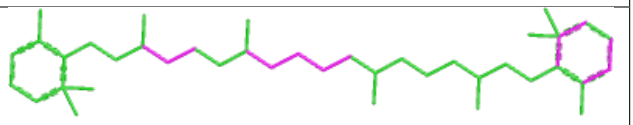
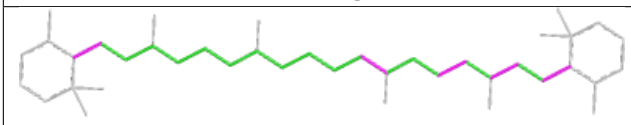


Bond angles



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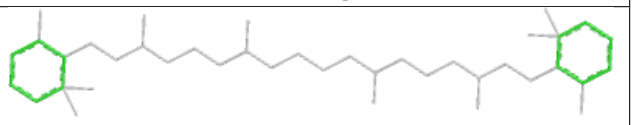
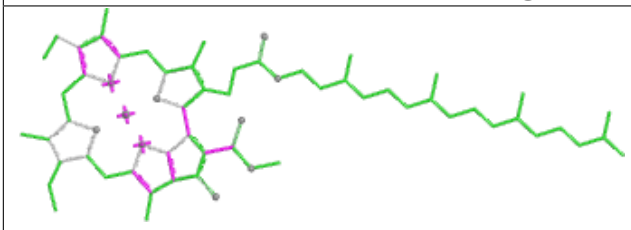


Rings

Ligand CL0 A 1011



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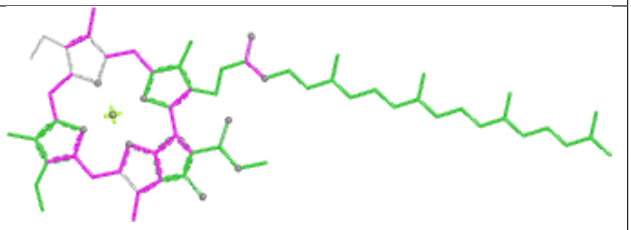
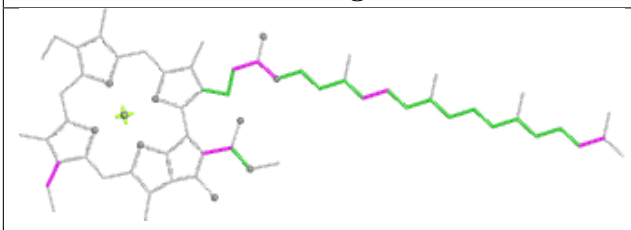


Bond angles



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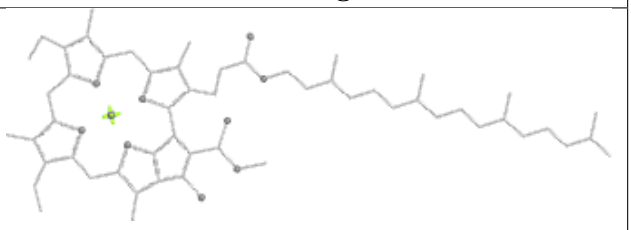
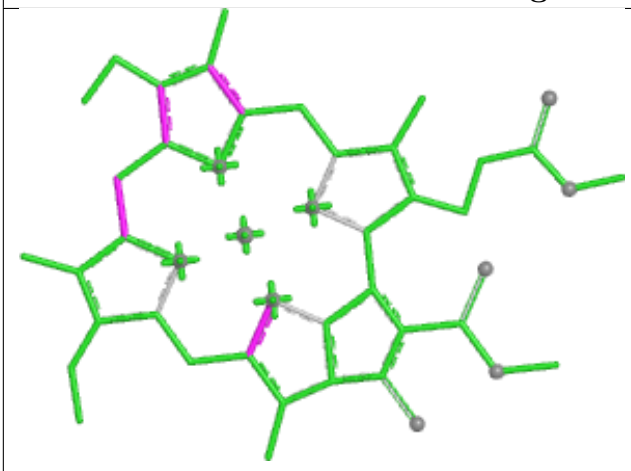


Rings

Ligand CLA s 513



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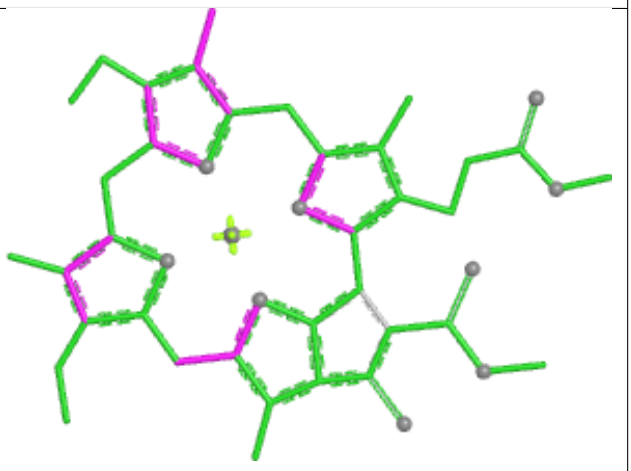
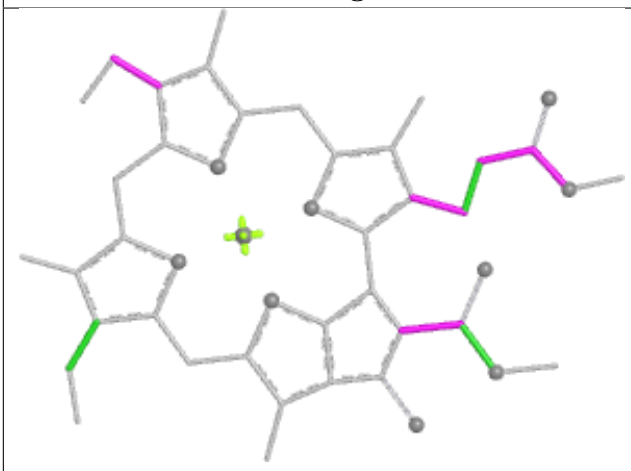


Bond angles



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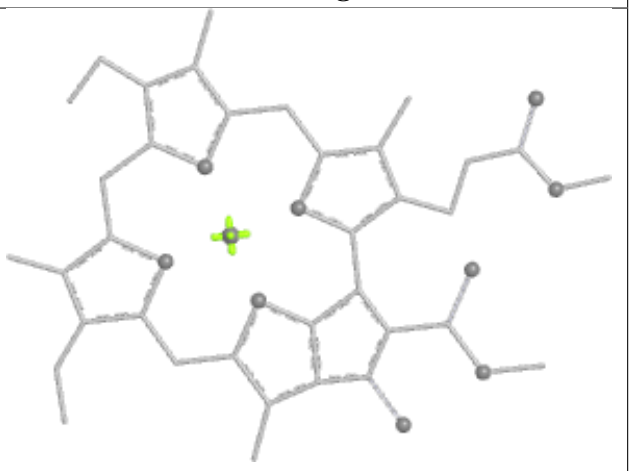
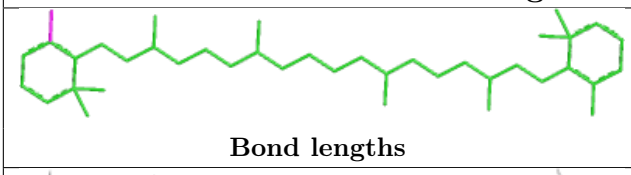


Rings

Ligand BCR o 601



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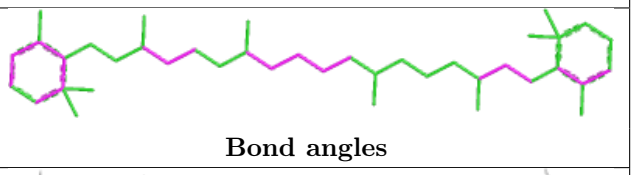
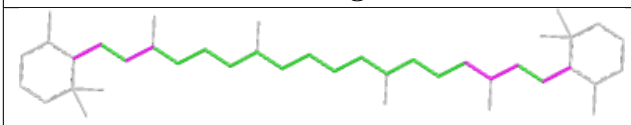


Bond angles



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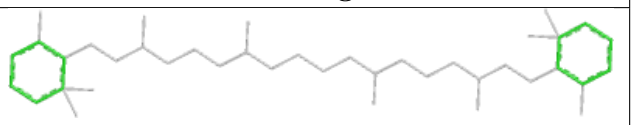
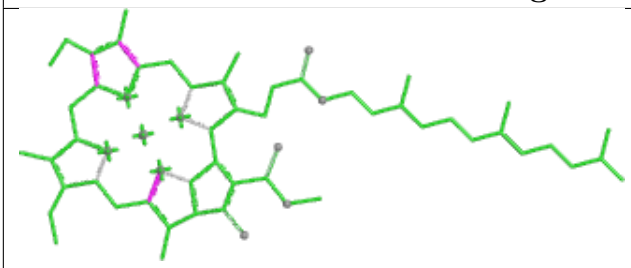


Rings

Ligand CLA r 506



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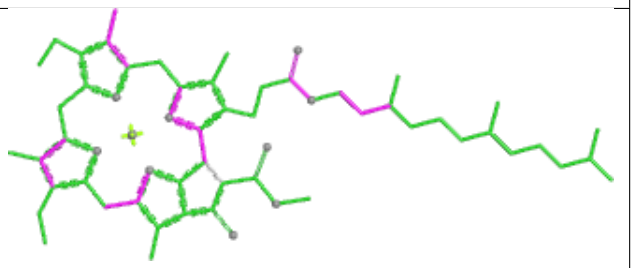
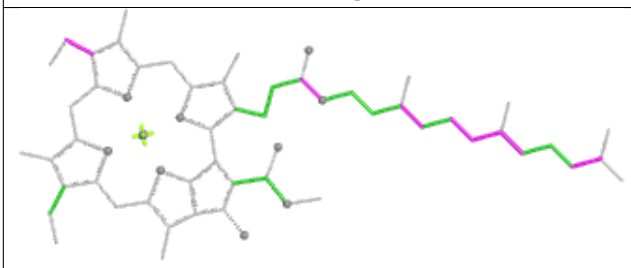


Bond angles



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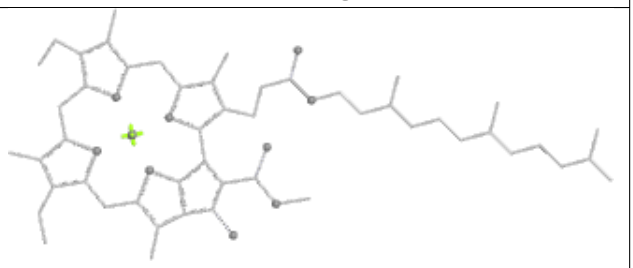
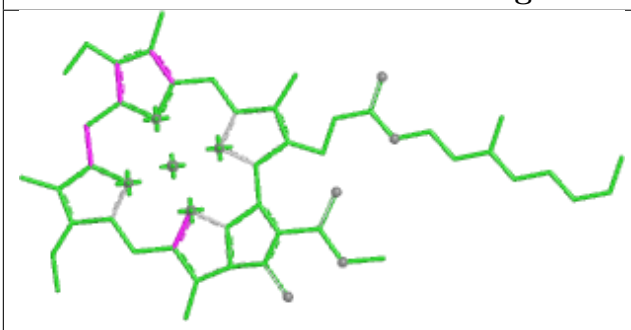


Rings

Ligand CLA A 1110



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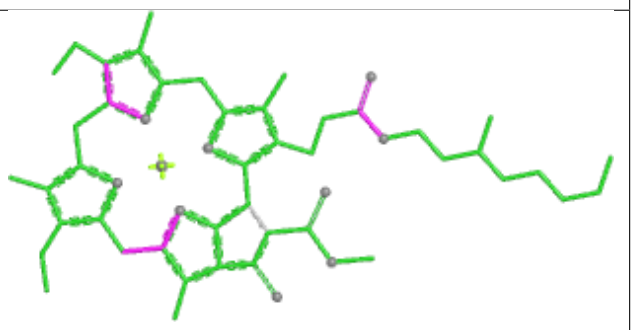
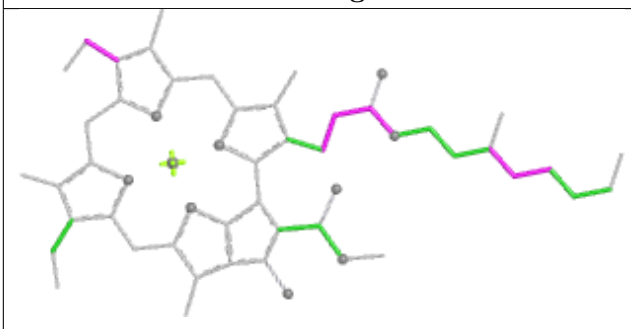


Bond angles



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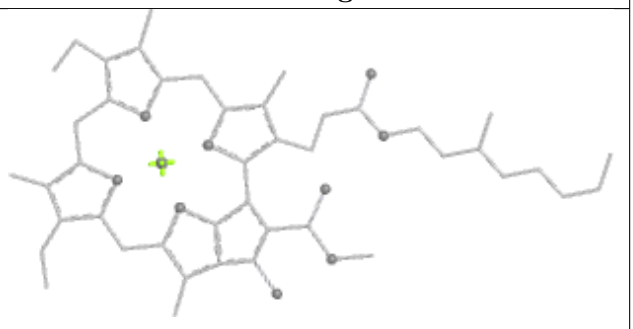
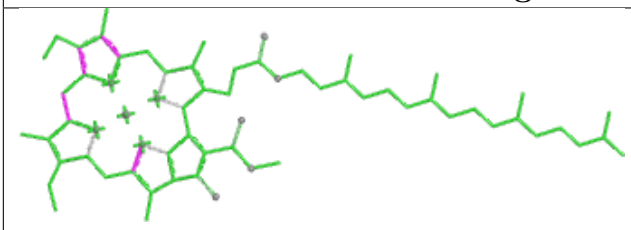


Rings

Ligand CLA H 1126



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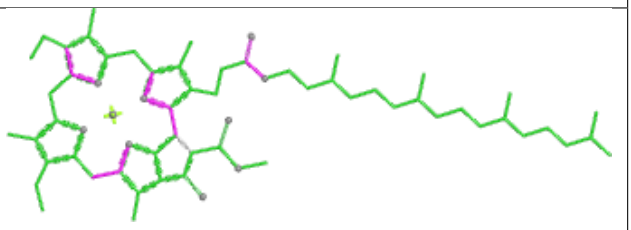
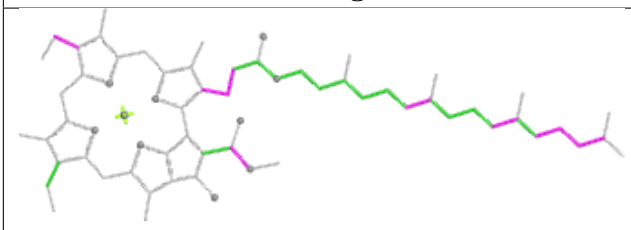


Bond angles



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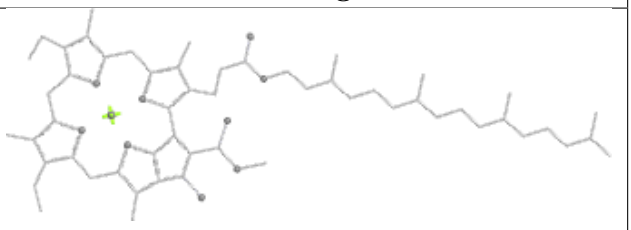
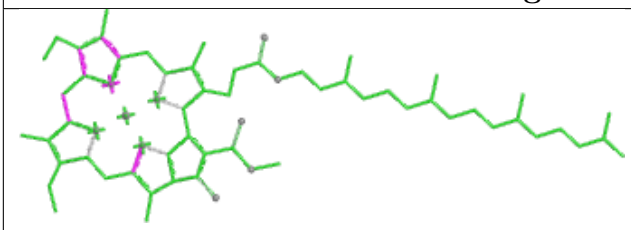


Rings

Ligand CLA X 505



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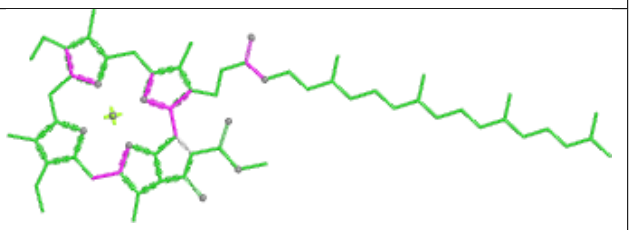
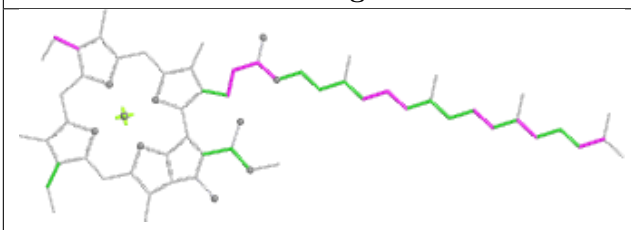


Bond angles



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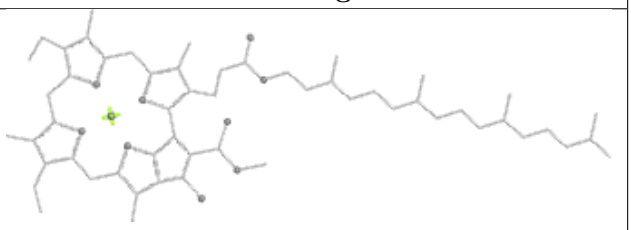
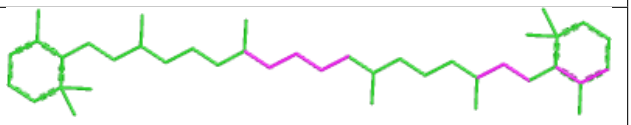


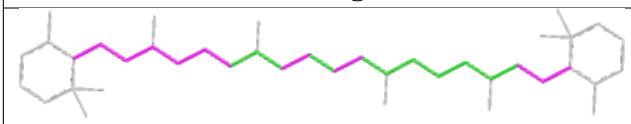
Rings

Ligand BCR t 604

Bond lengths



Bond angles



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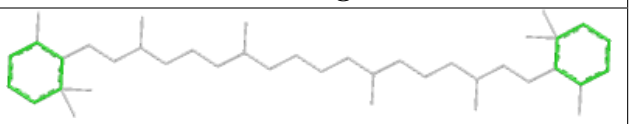
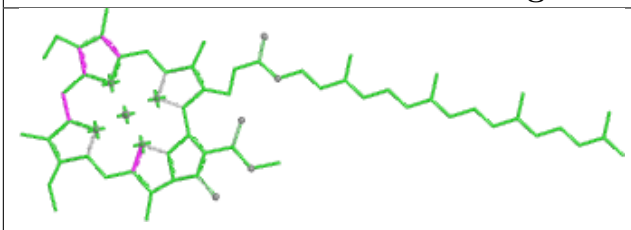


Rings

Ligand CLA u 511



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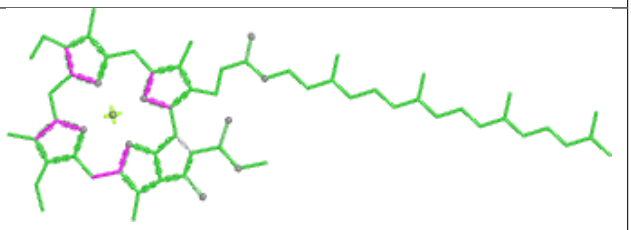
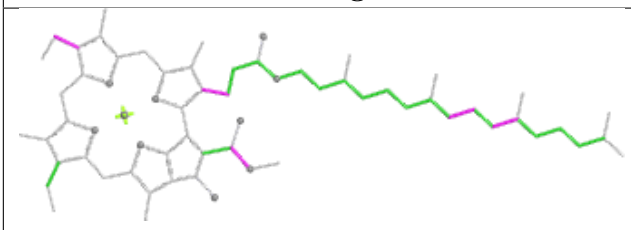


Bond angles



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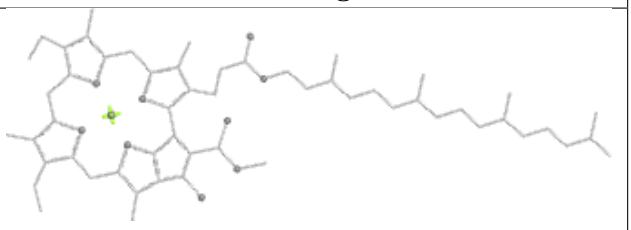
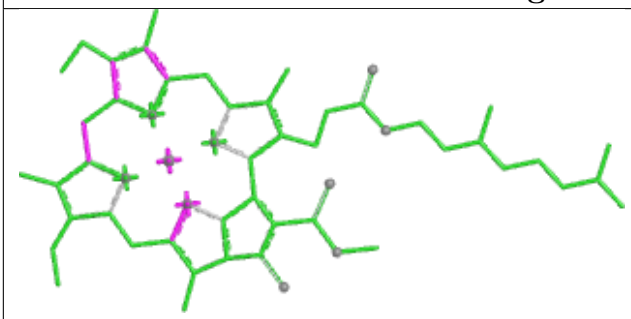


Rings

Ligand CLA v 508



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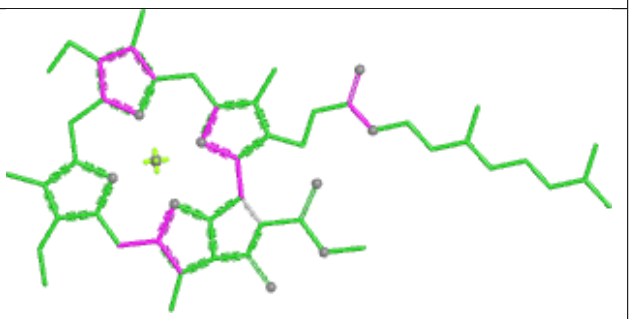
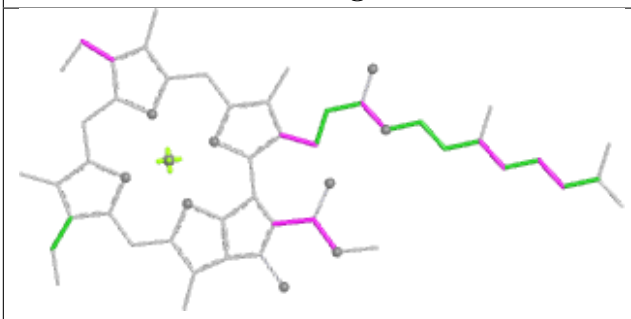
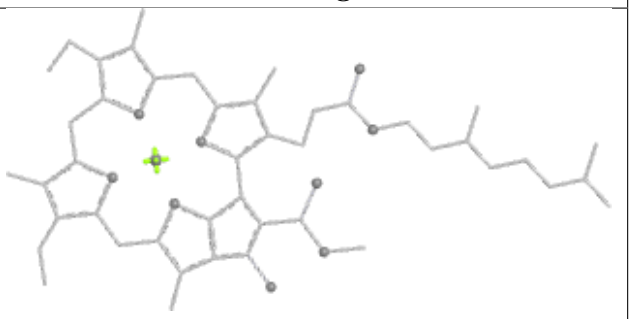


Bond angles

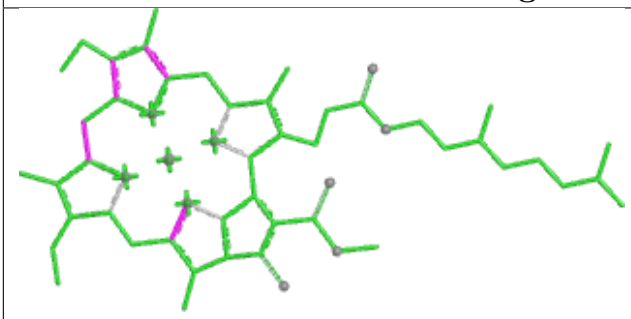


Torsions

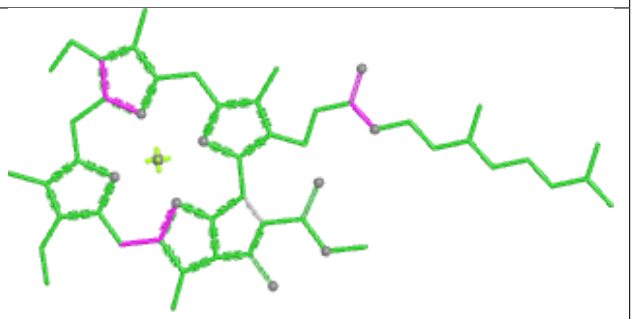


Rings

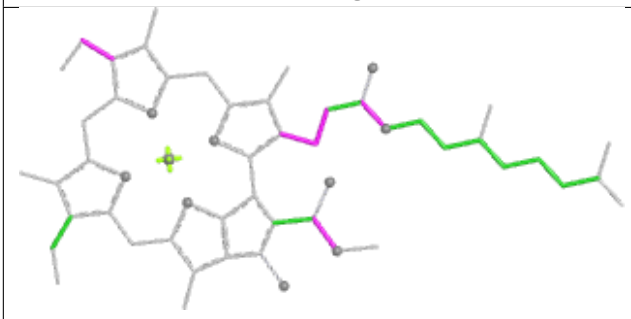
Ligand CLA W 508



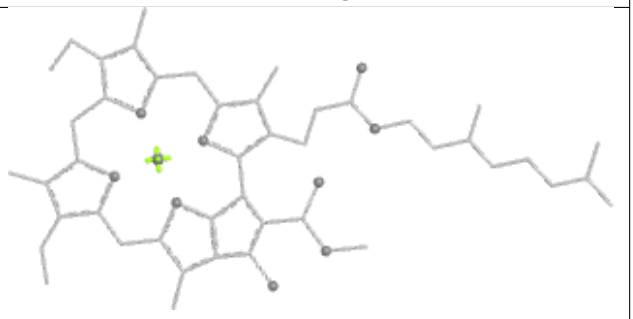
Bond lengths



Bond angles

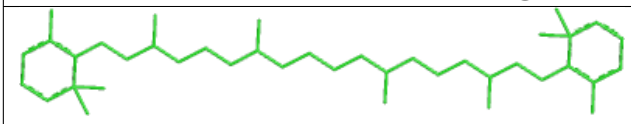


Torsions



Rings

Ligand BCR S 4015



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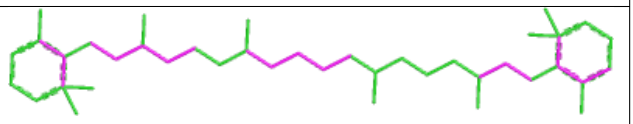
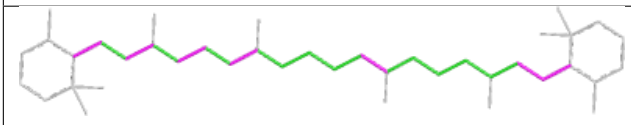


Bond angles



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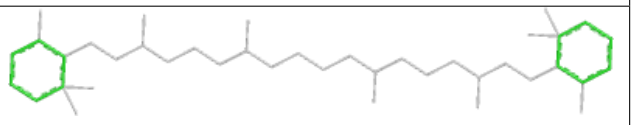
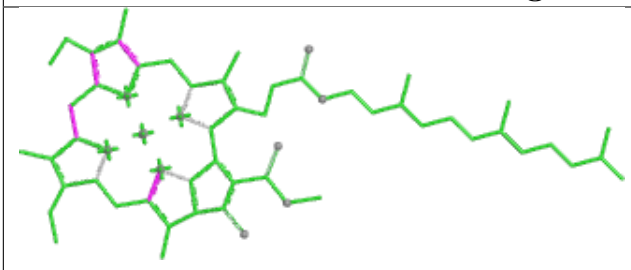


Rings

Ligand CLA Z 510



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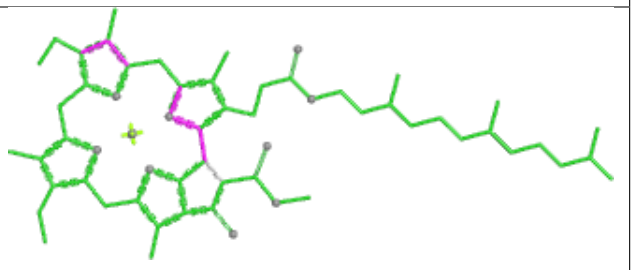
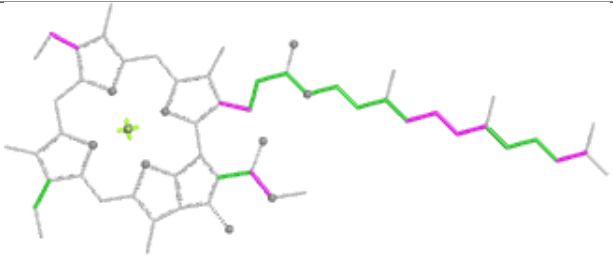


Bond angles



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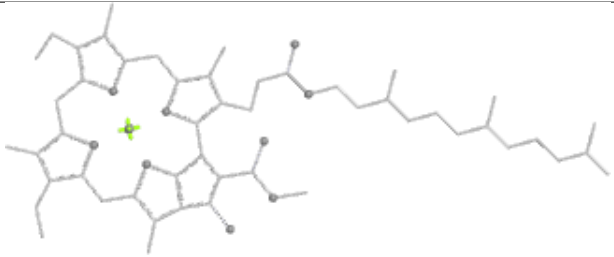
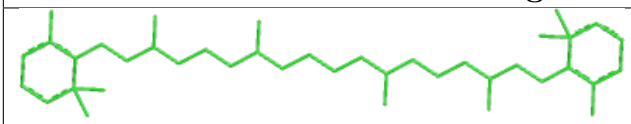


Rings

Ligand BCR q 604



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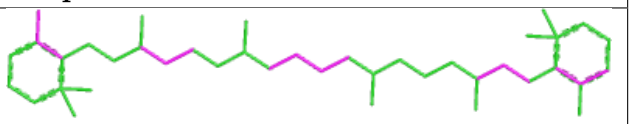
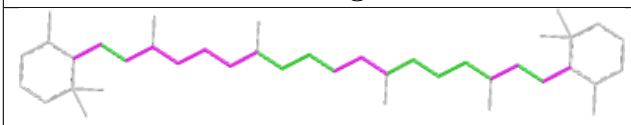


Bond angles



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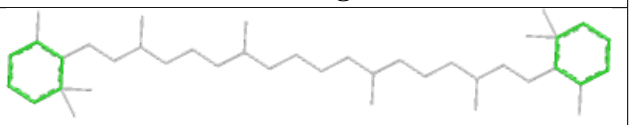
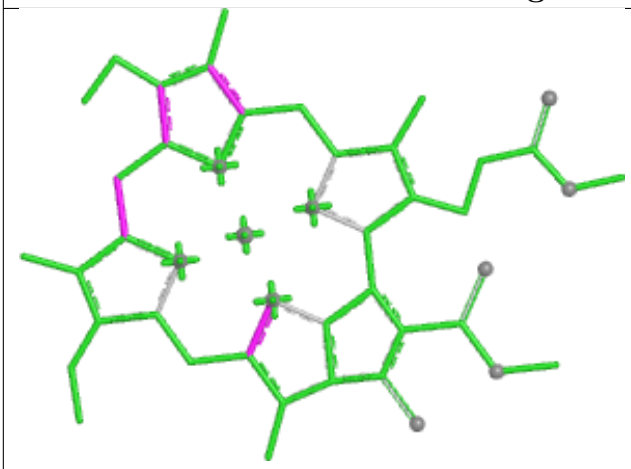
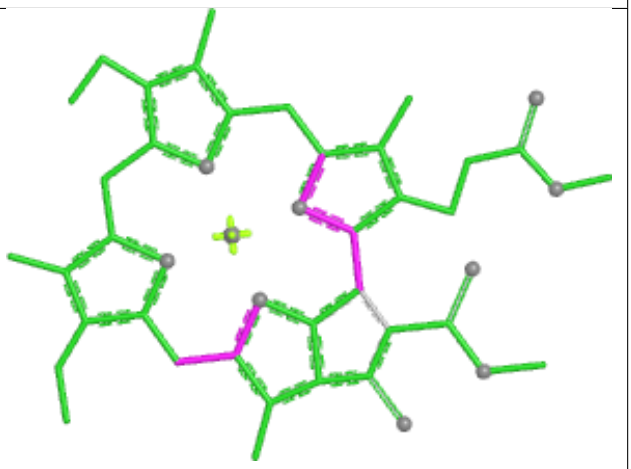


Rings

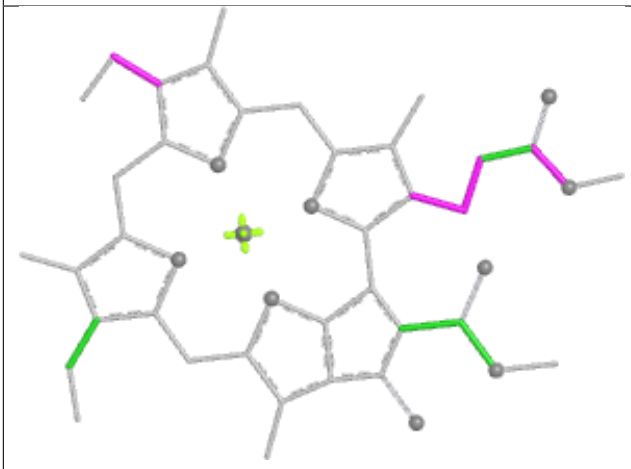
Ligand CLA u 501



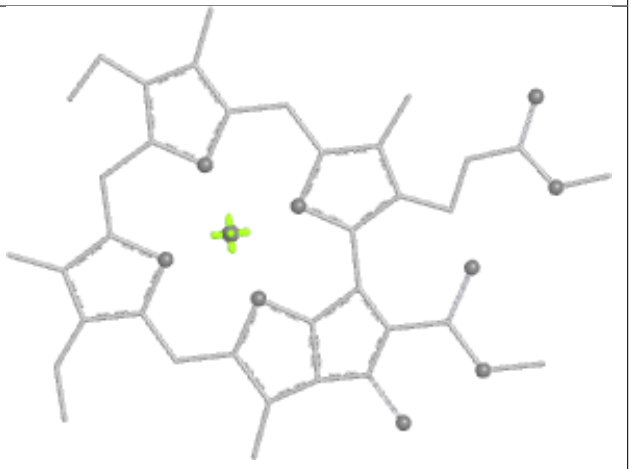
Bond lengths



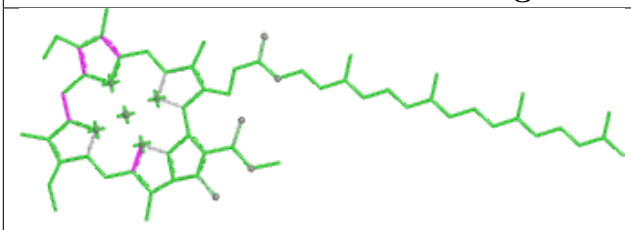
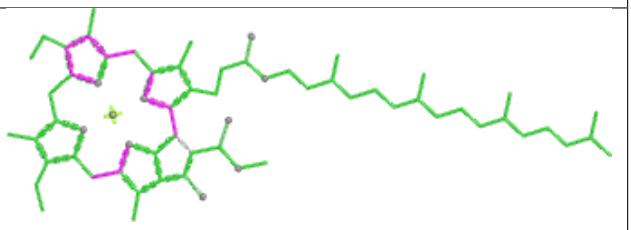
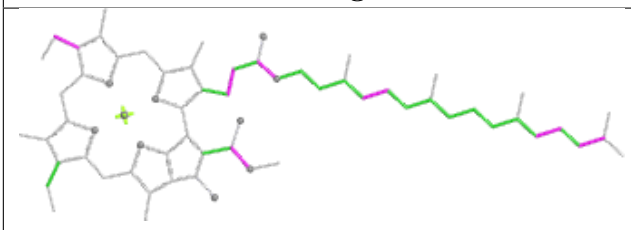
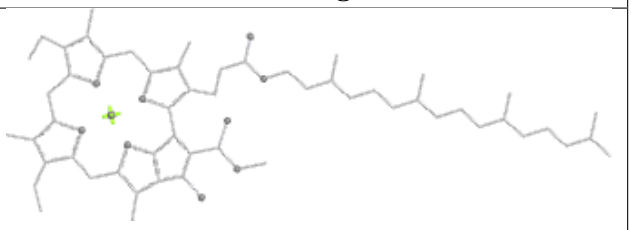
Bond angles

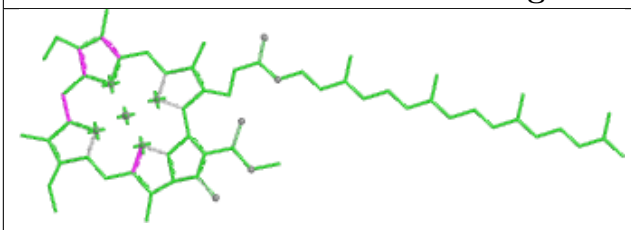
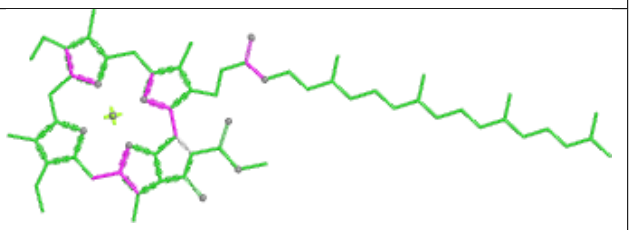
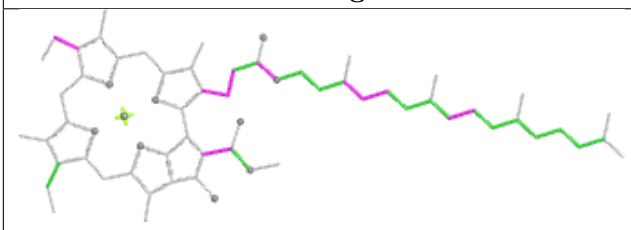
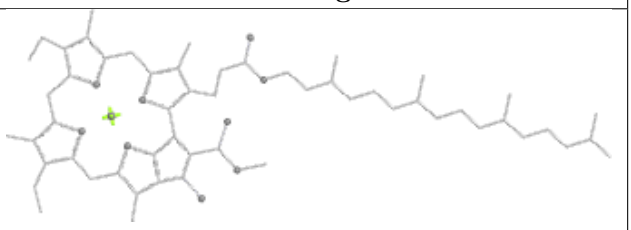


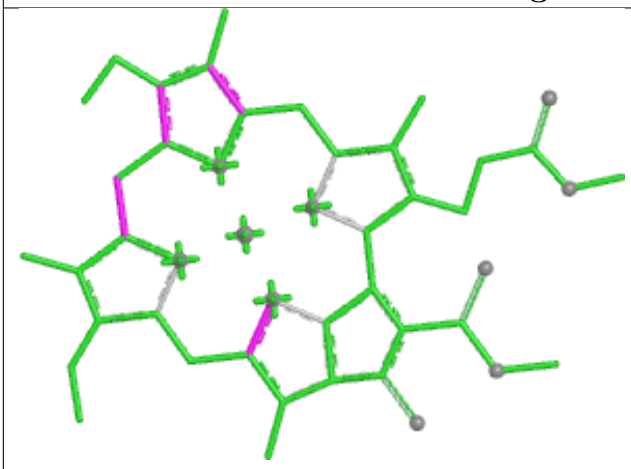
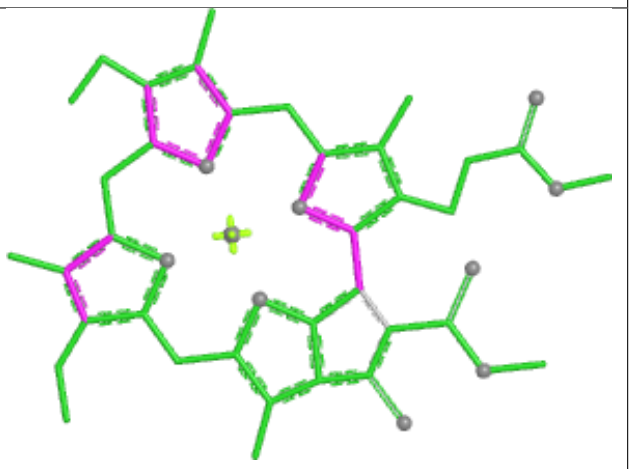
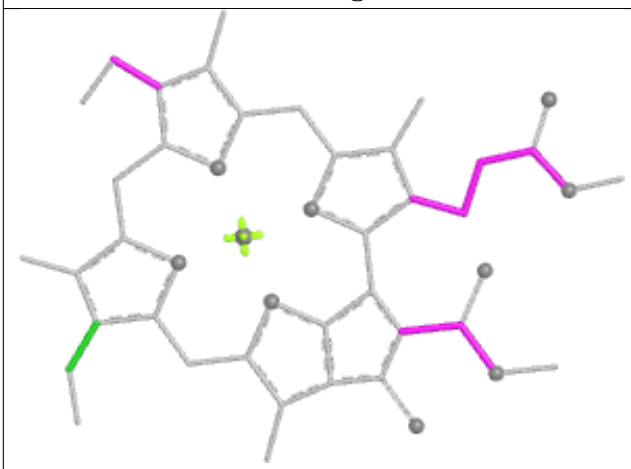
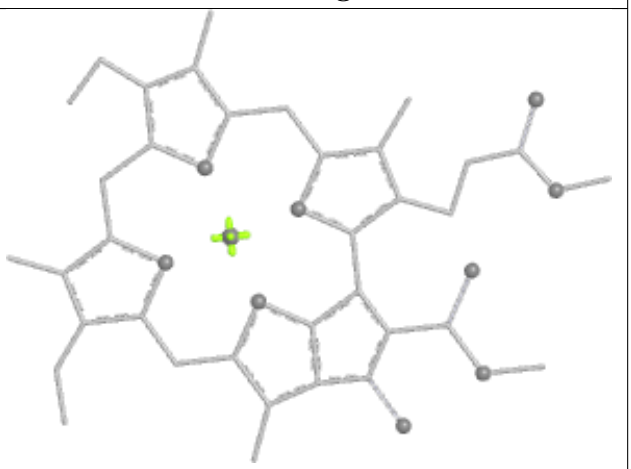
Torsions



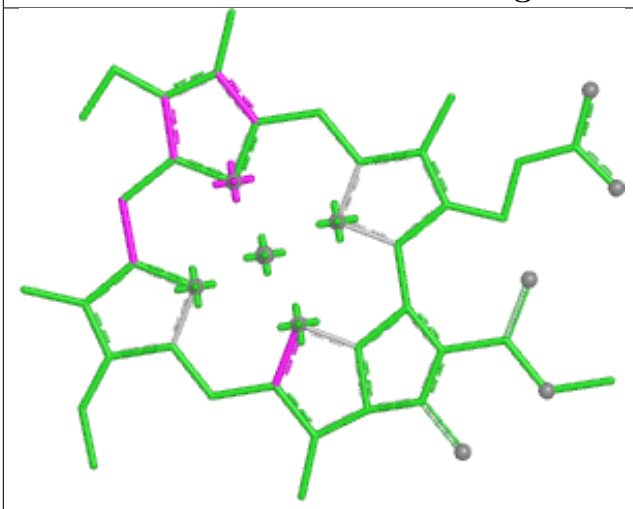
Rings

Ligand CLA G 1238	
	
Bond lengths	Bond angles
	
Torsions	Rings

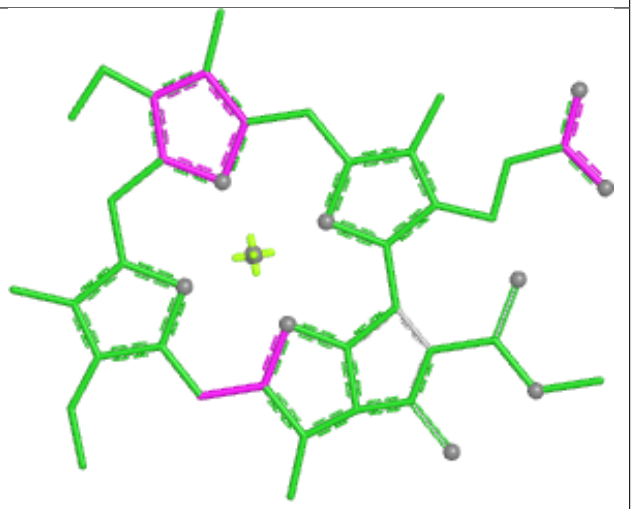
Ligand CLA x 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

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

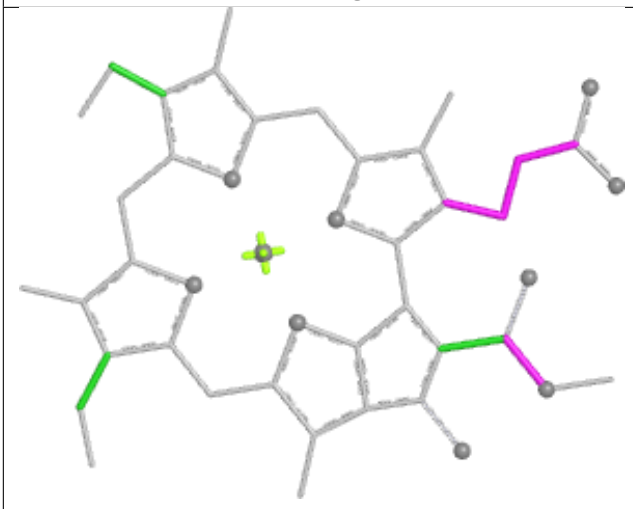
Ligand CLA G 1219



Bond lengths



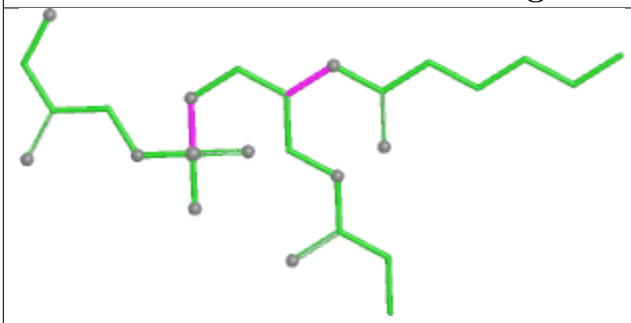
Bond angles



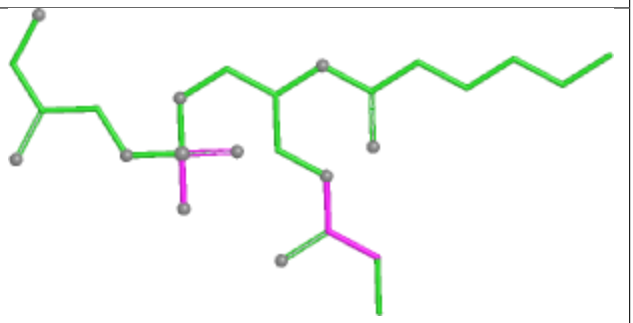
Torsions

Rings

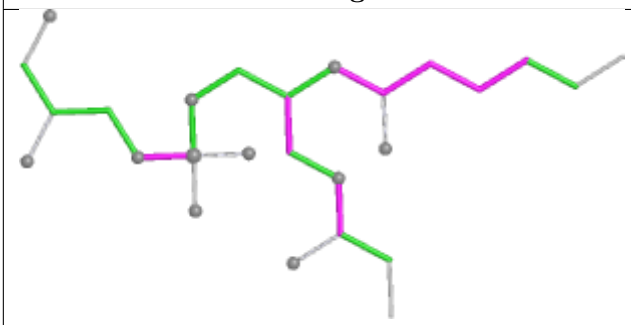
Ligand LHG a 851



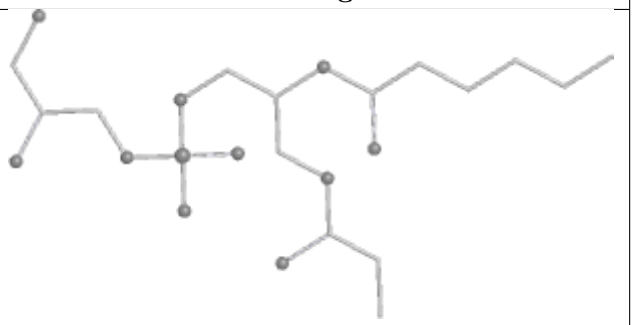
Bond lengths



Bond angles

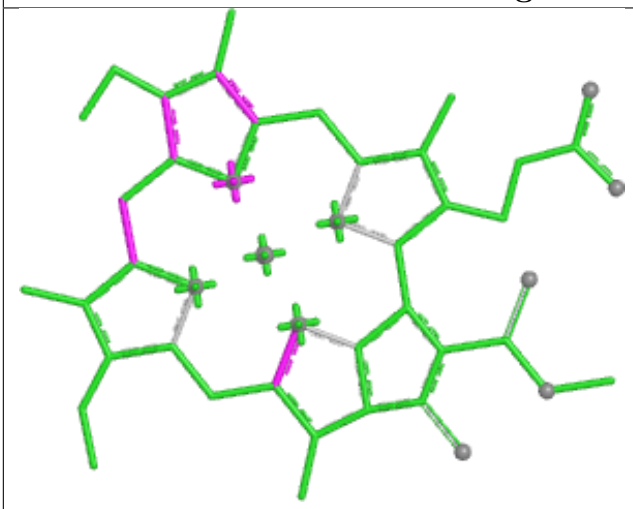


Torsions

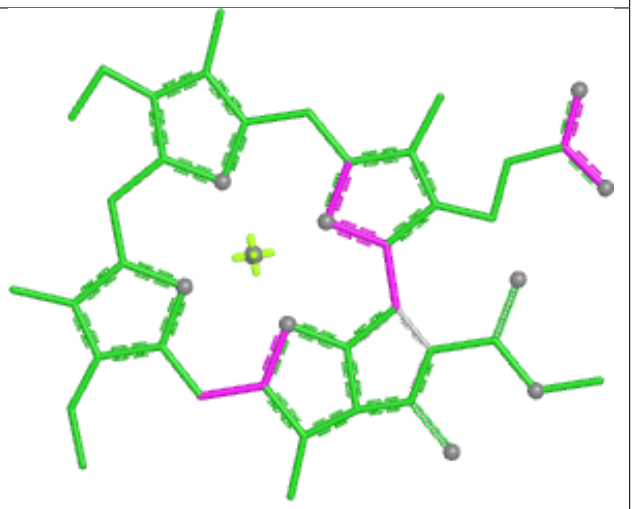


Rings

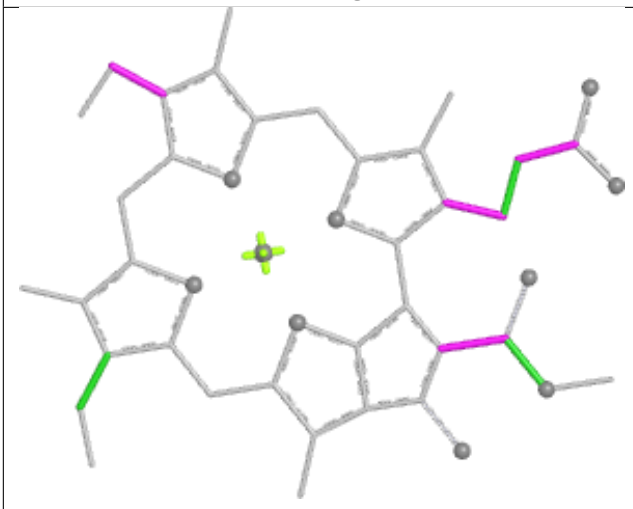
Ligand CLA B 1212



Bond lengths



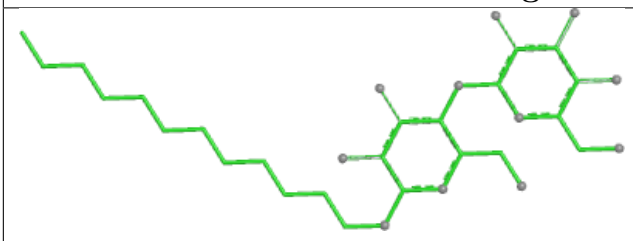
Bond angles



Torsions

Rings

Ligand LMU Z 605



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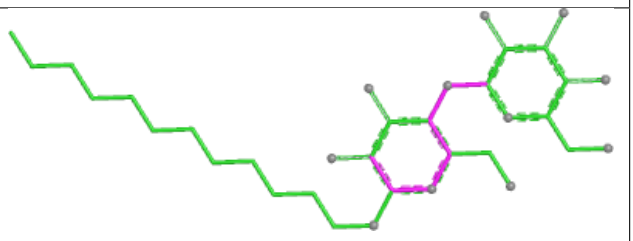
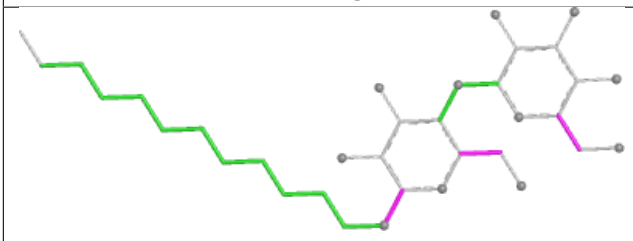
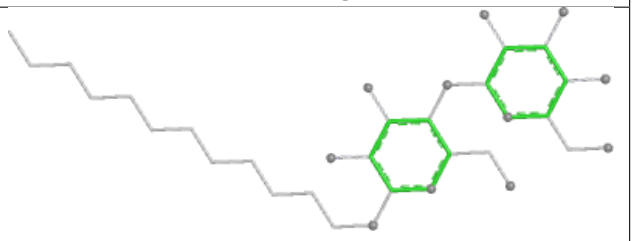


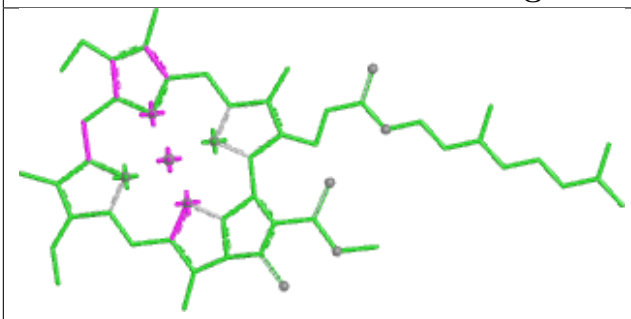
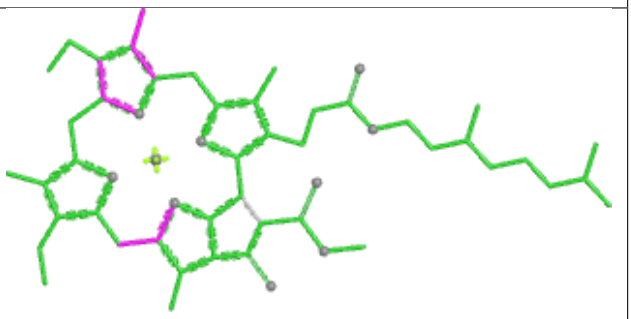
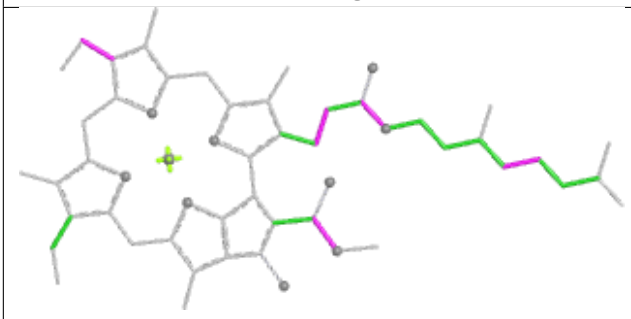
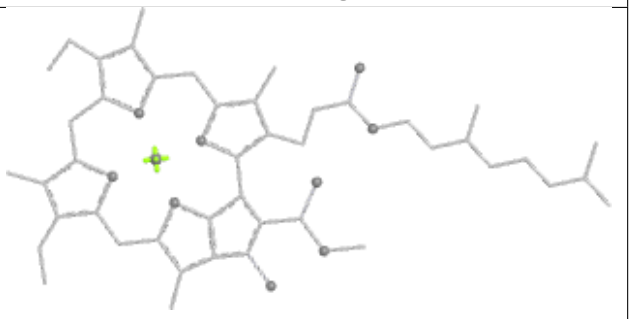
Bond angles

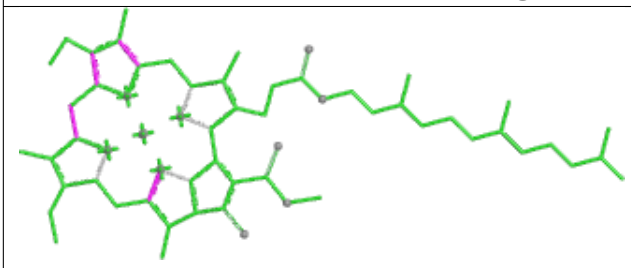
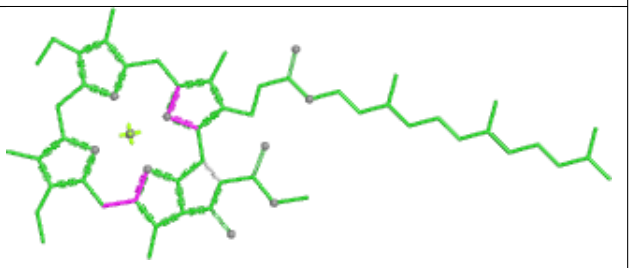
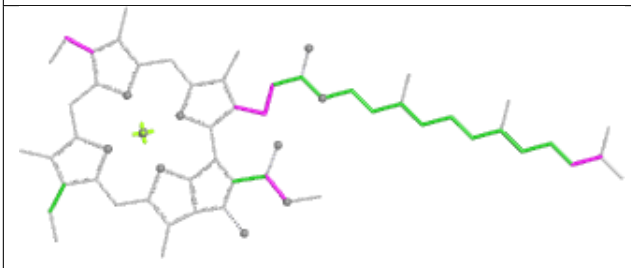
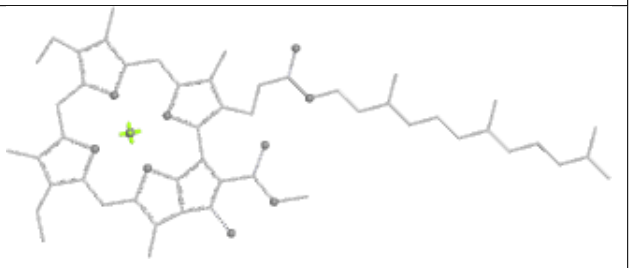


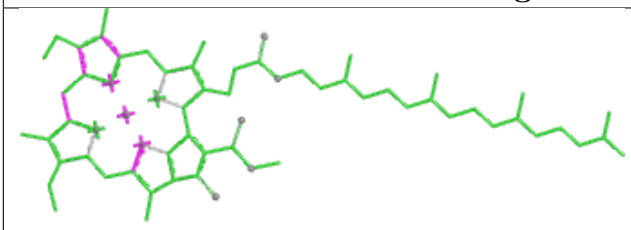
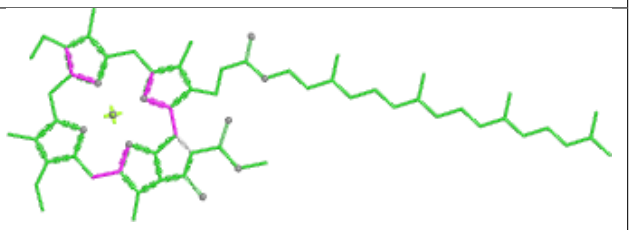
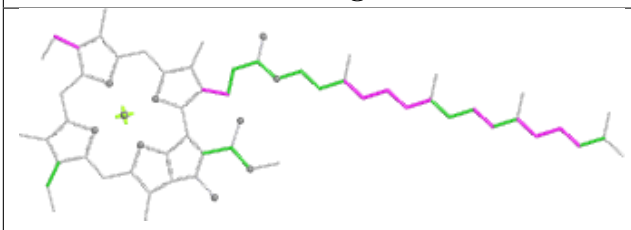
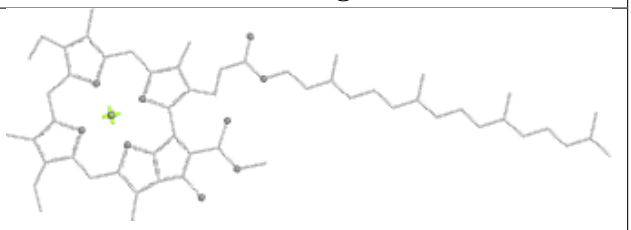
Torsions

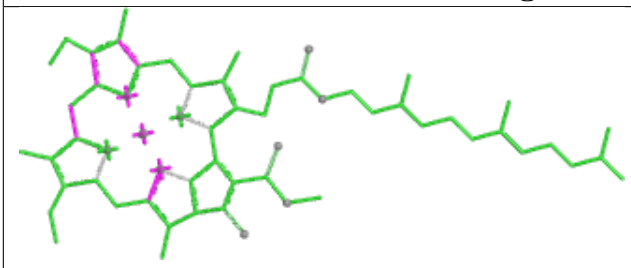
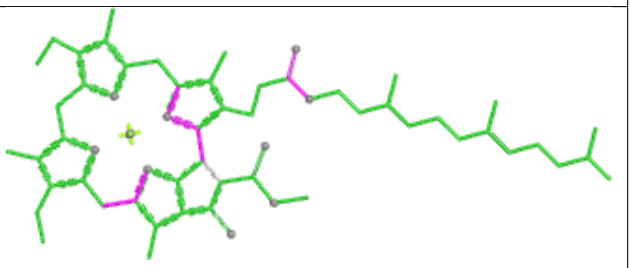


Rings

Ligand CLA w 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1215	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1225	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 512	
	
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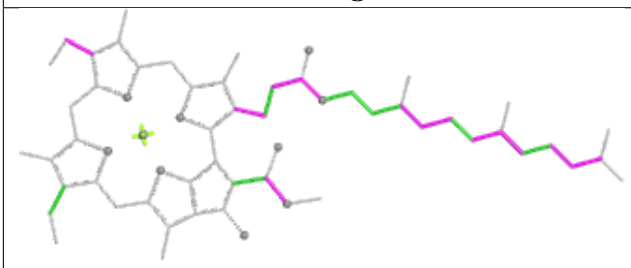
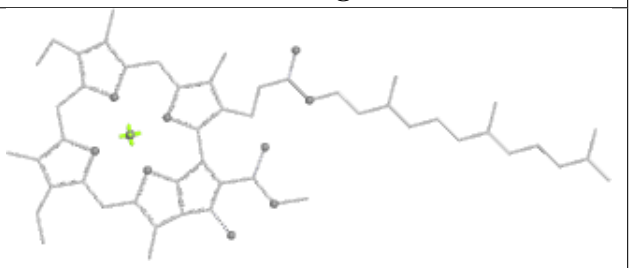
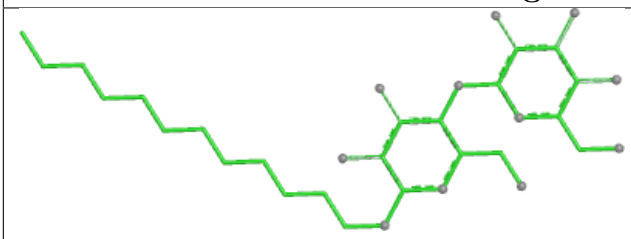
	
Torsions	Rings

Ligand LMU q 605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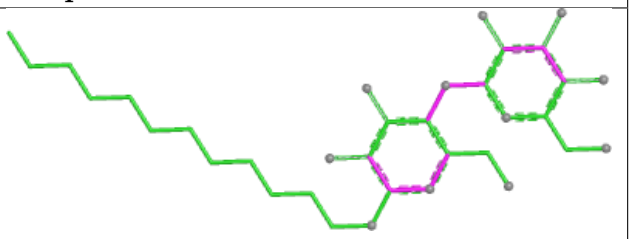
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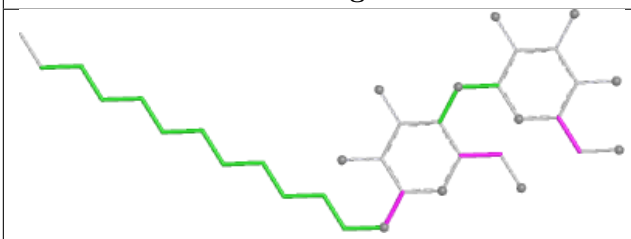
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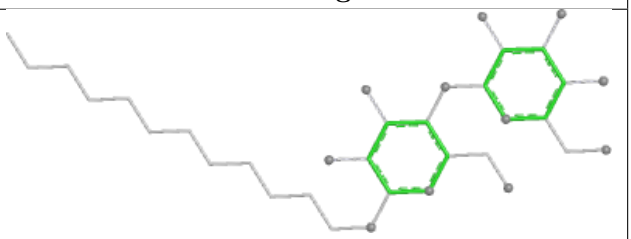
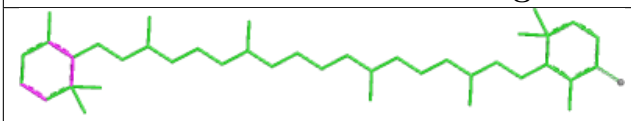

Rings

Ligand ECH R 4020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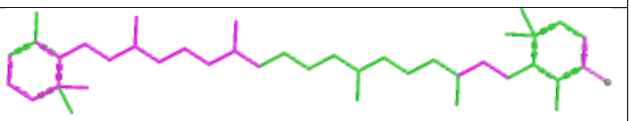
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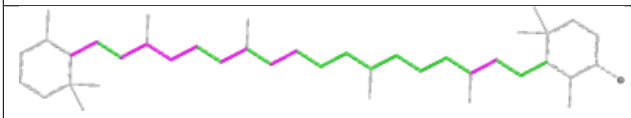
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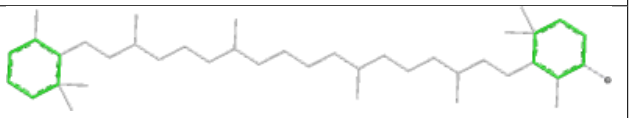
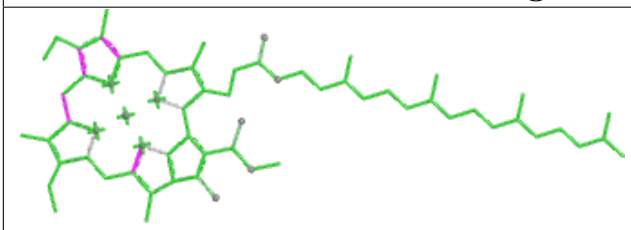

Rings

Ligand CLA p 507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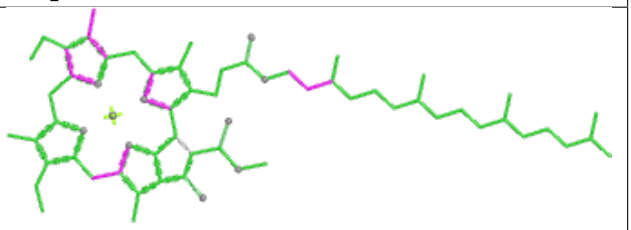
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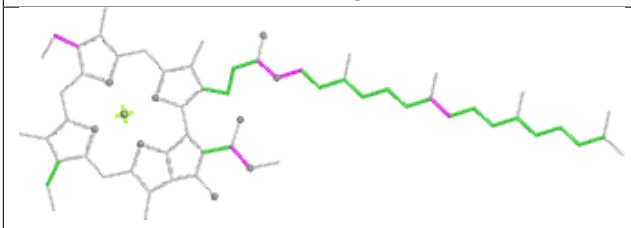
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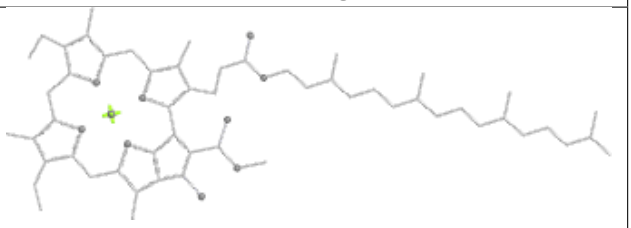
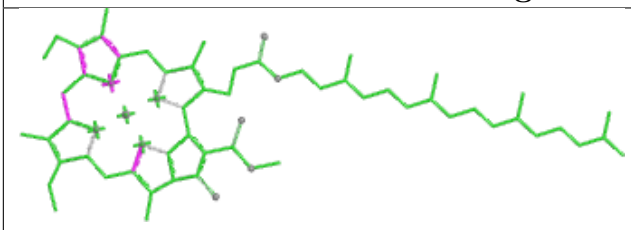

Rings

Ligand CLA A 1101



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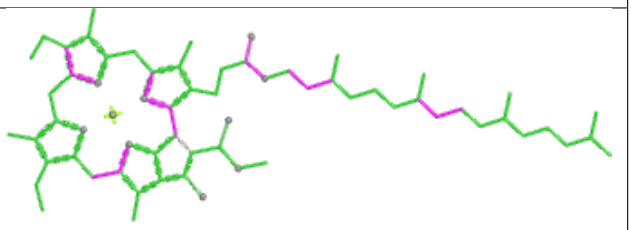

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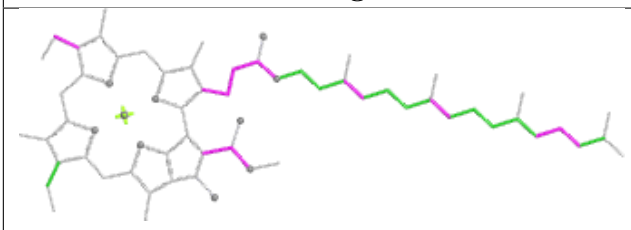

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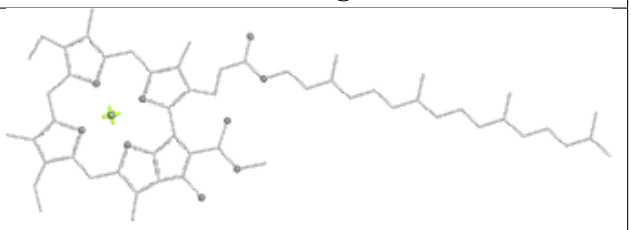
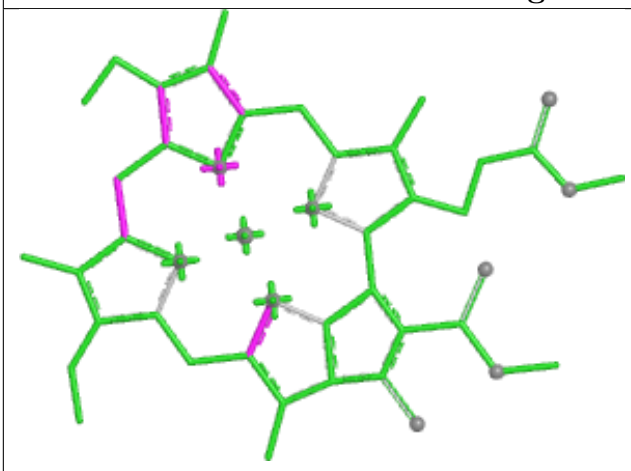


Rings

Ligand CLA q 516



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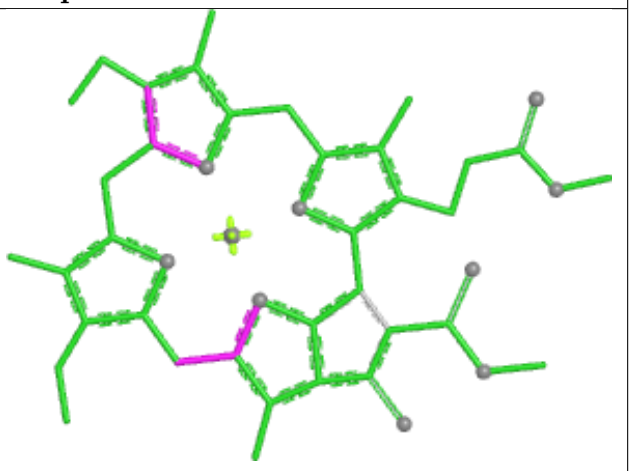

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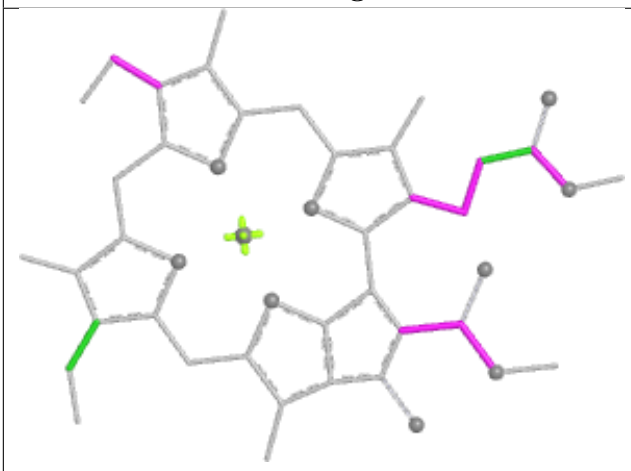

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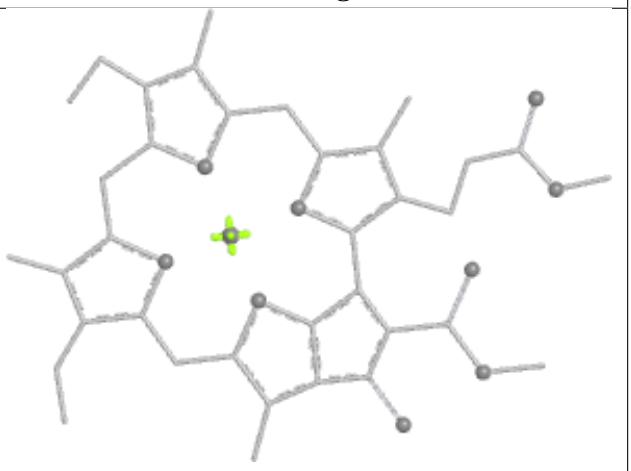
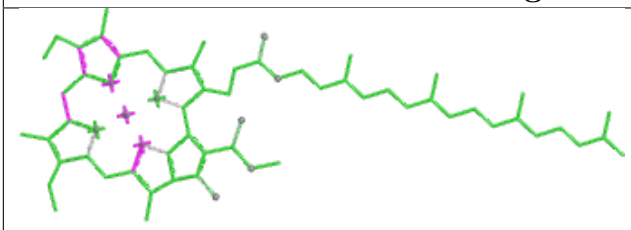


Rings

Ligand CLA w 512



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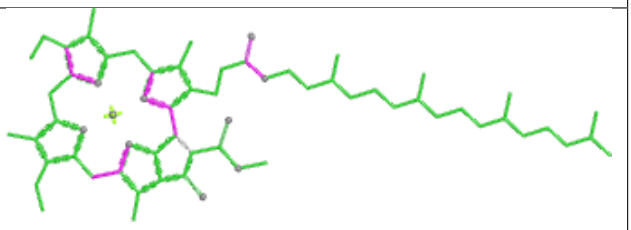

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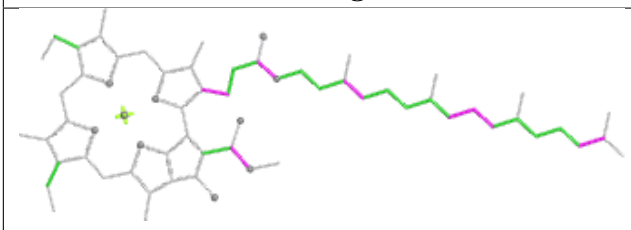

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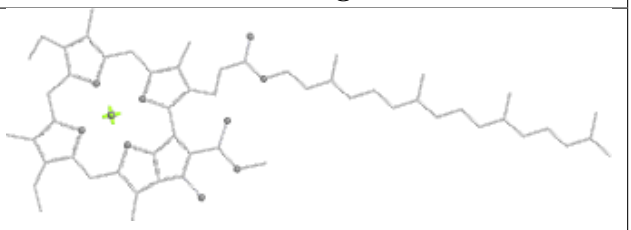
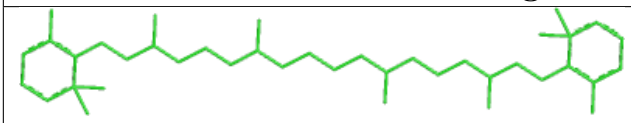


Rings

Ligand BCR Y 604



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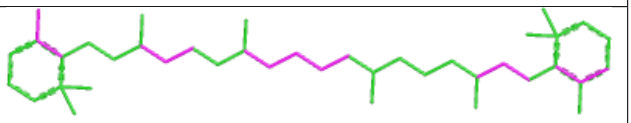

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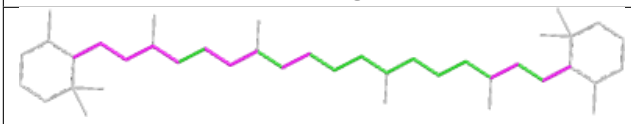
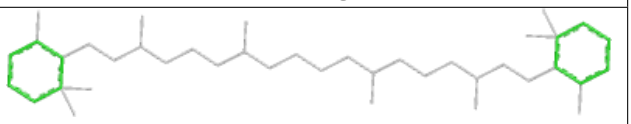
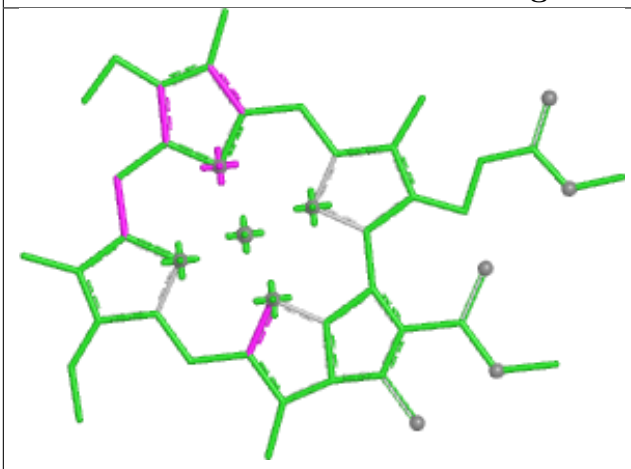


Torsions



Rings

Ligand CLA t 503



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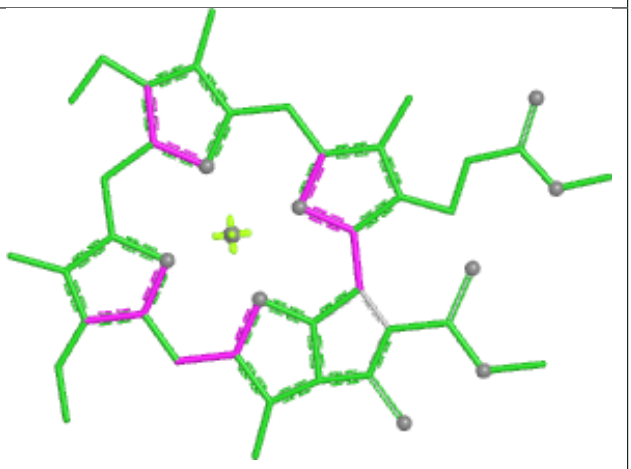

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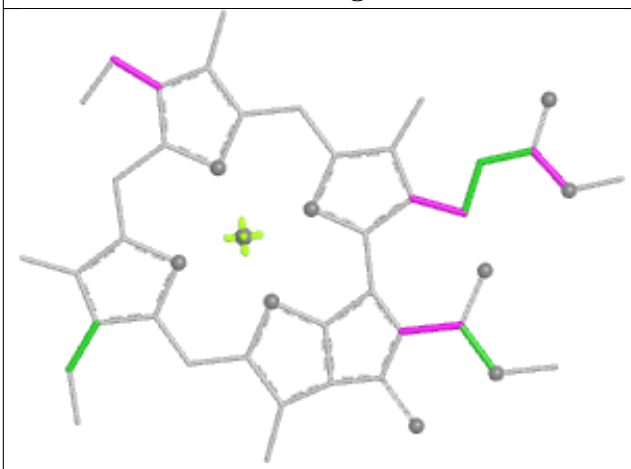

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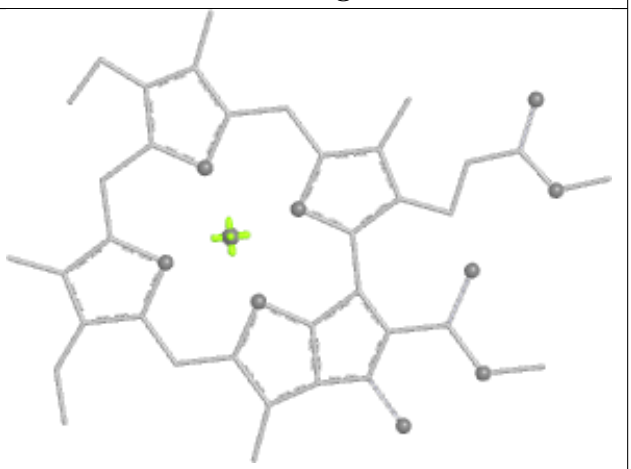
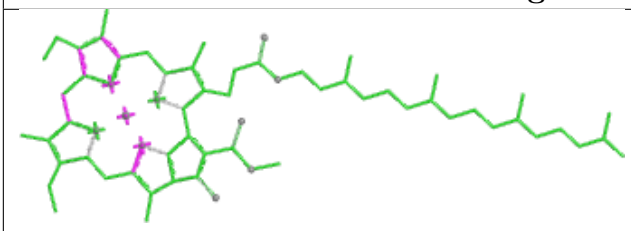


Rings

Ligand CLA q 512



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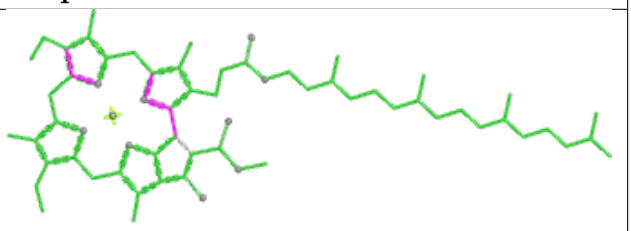

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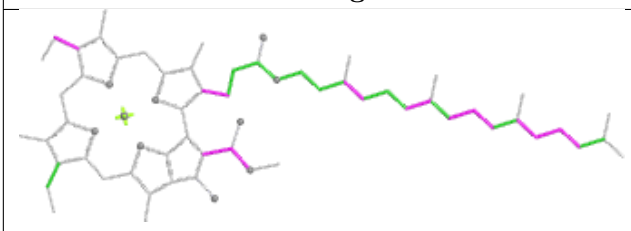

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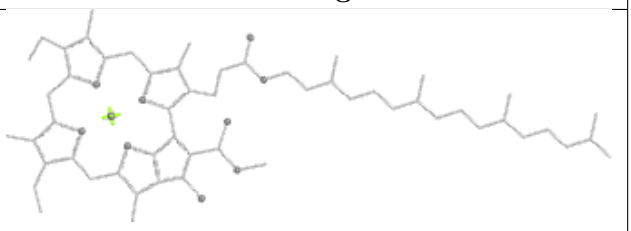
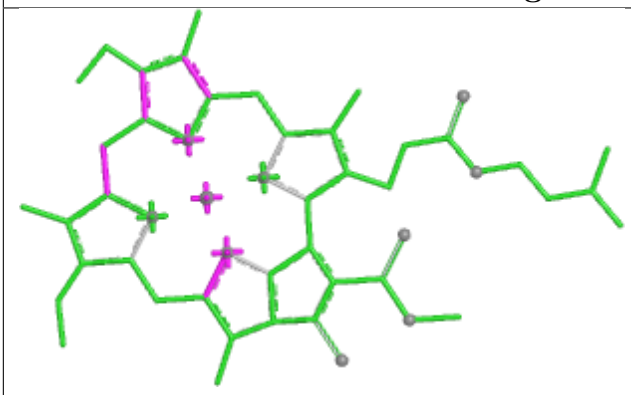


Rings

Ligand CLA w 502



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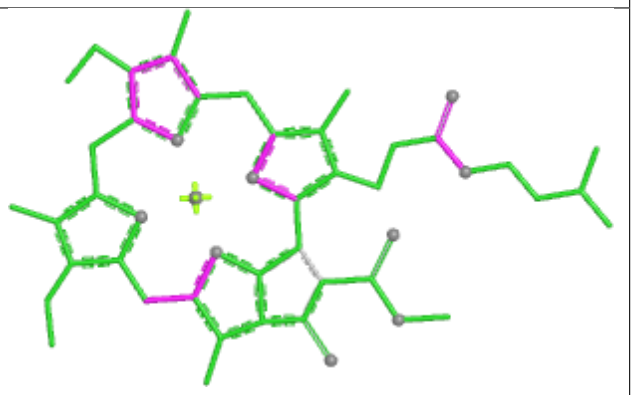

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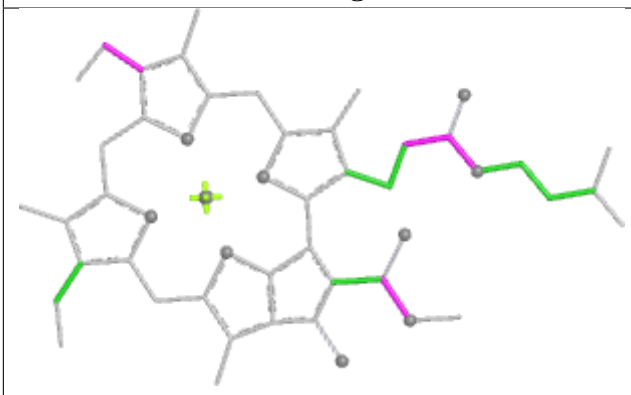

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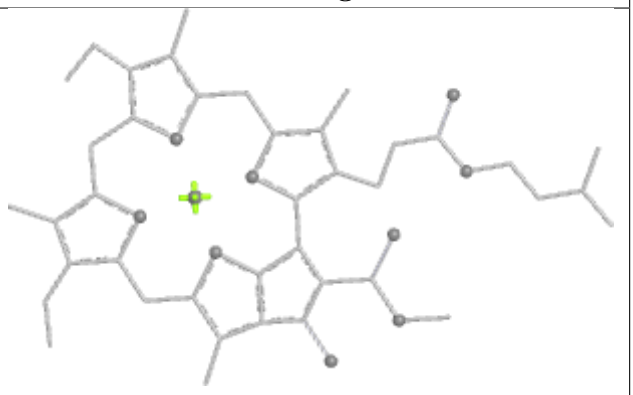
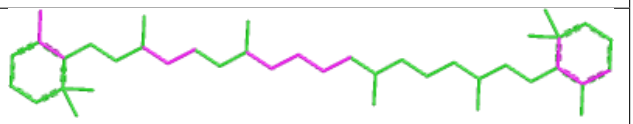


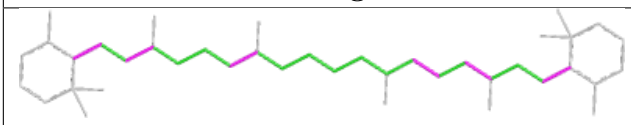
Rings

Ligand BCR r 603

Bond lengths



Bond angles



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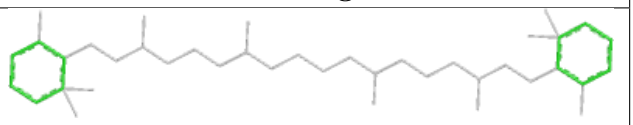
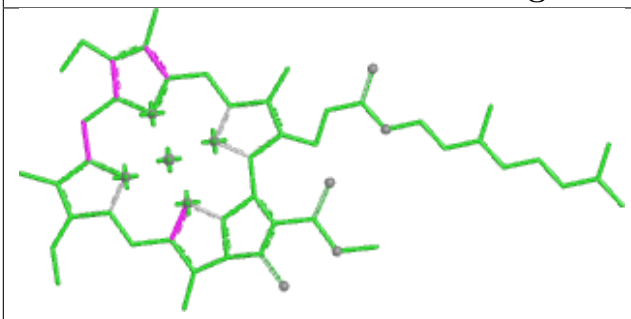


Rings

Ligand CLA g 517



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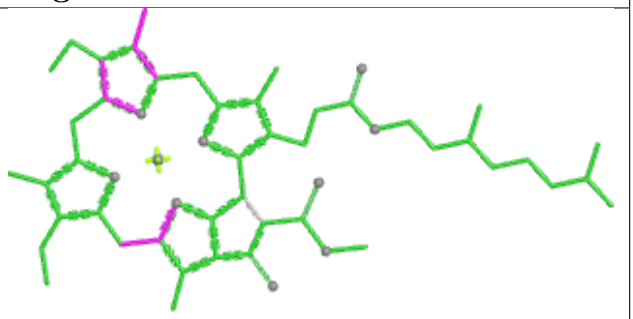
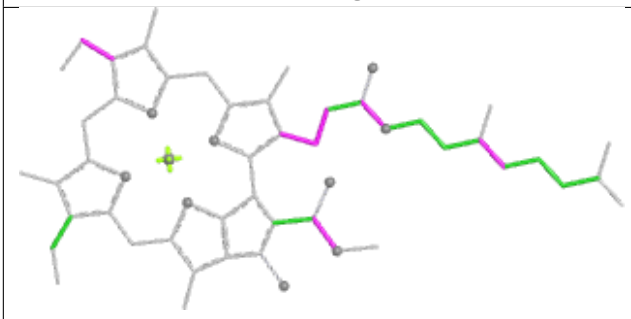


Bond angles



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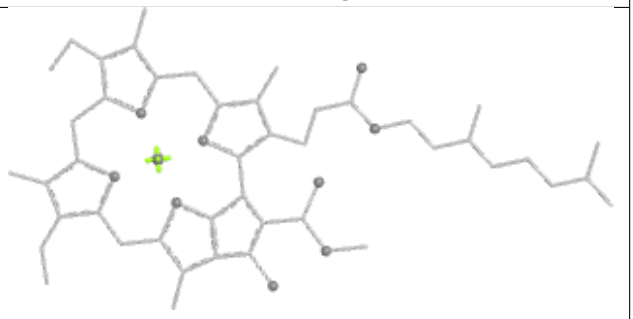
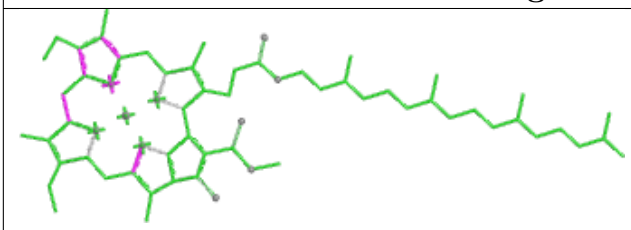


Rings

Ligand CLA p 505



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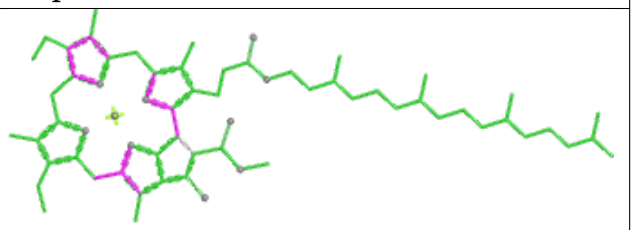
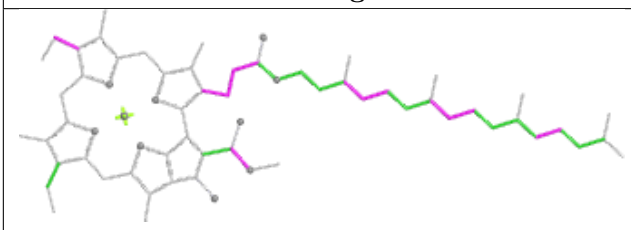
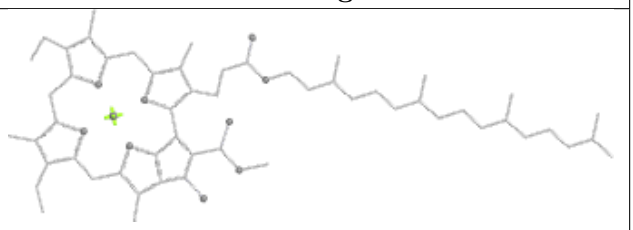


Bond angles

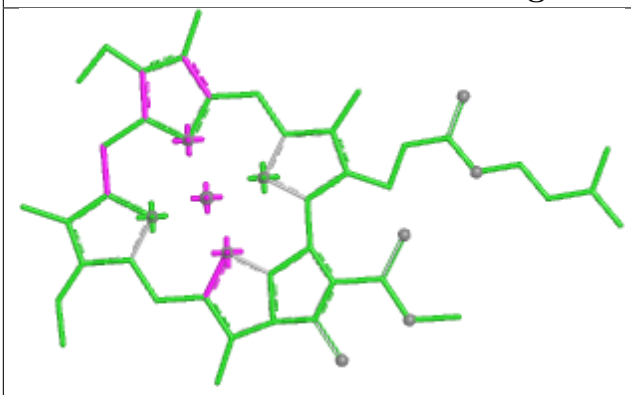


Torsions



Rings

Ligand CLA q 502



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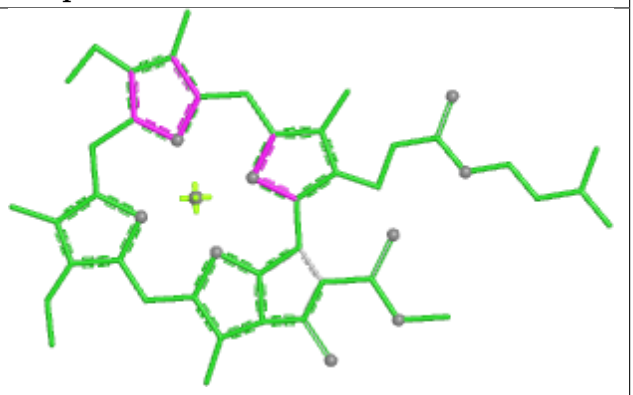

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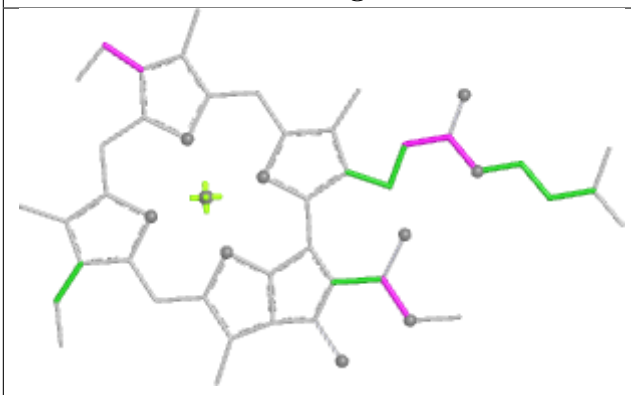

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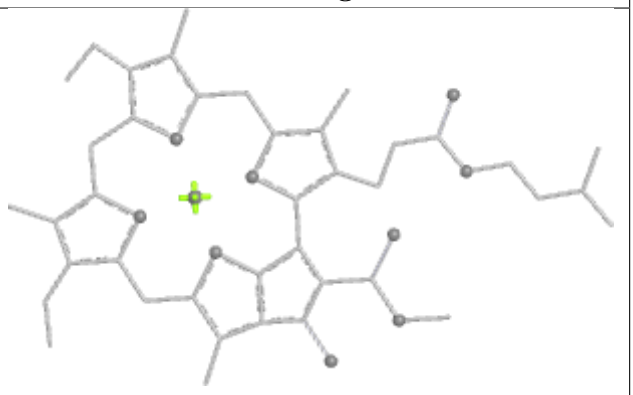
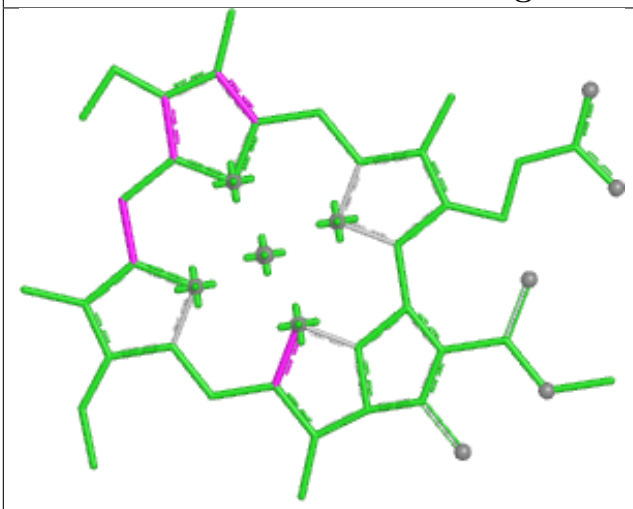


Rings

Ligand CLA A 1112



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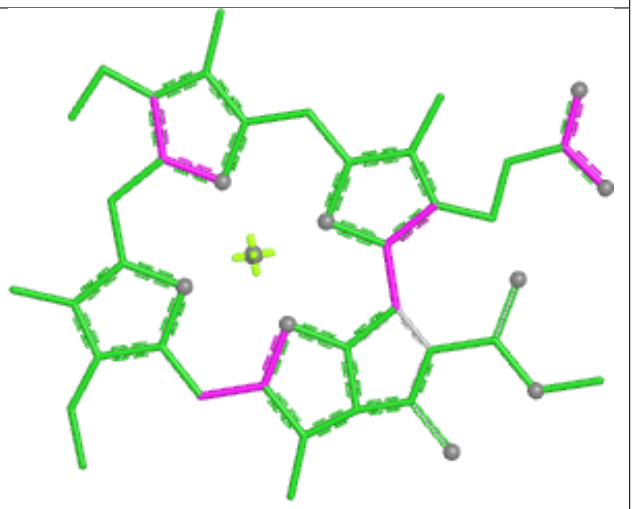

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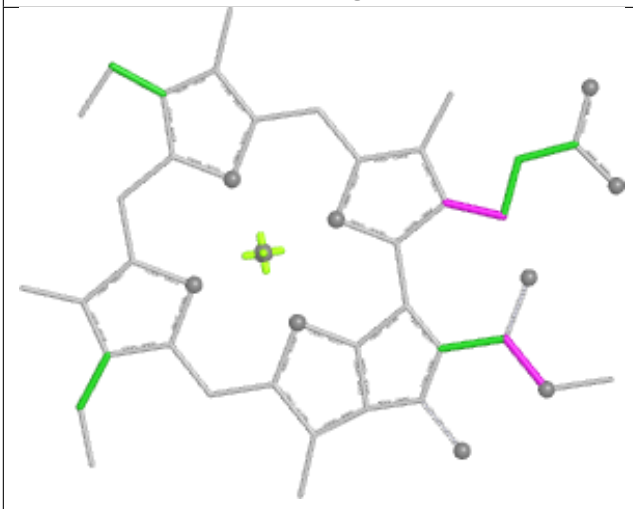
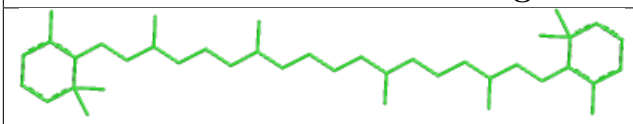


Torsions

Rings

Ligand BCR B 4014



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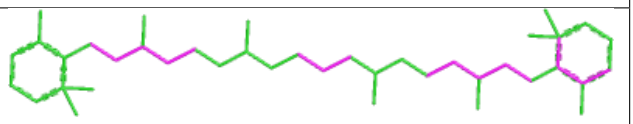

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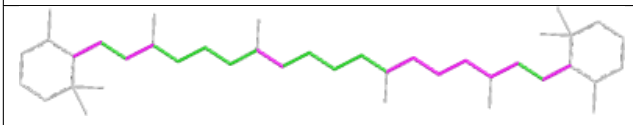
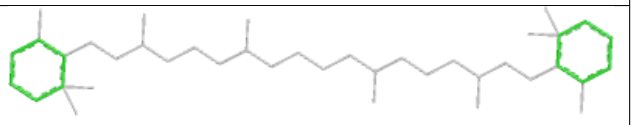
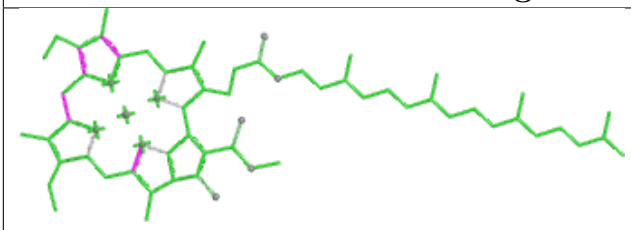


Torsions



Rings

Ligand CLA H 1109



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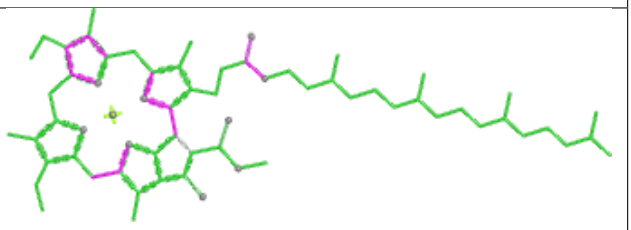

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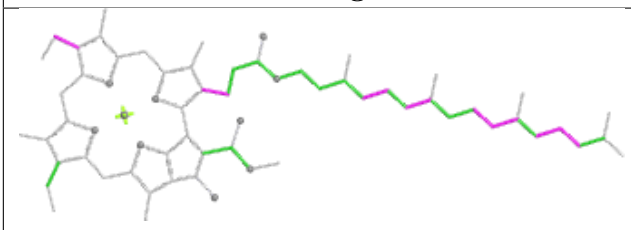

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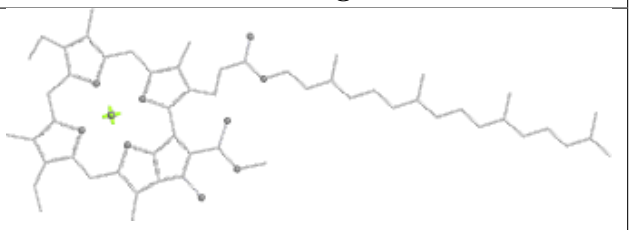
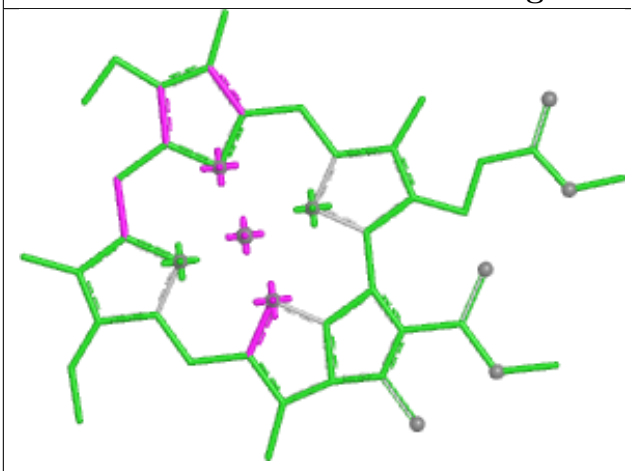


Rings

Ligand CLA Z 503



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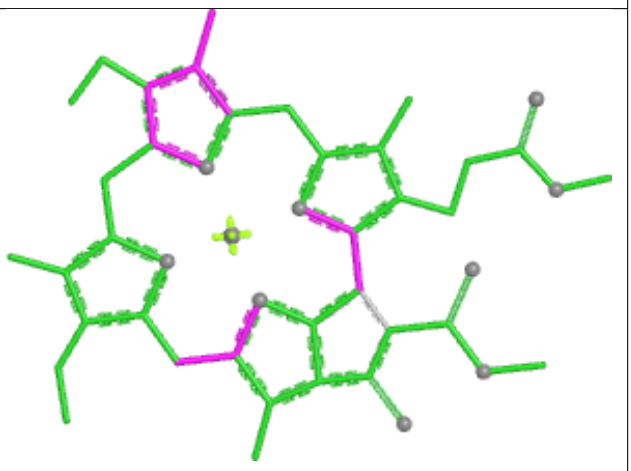

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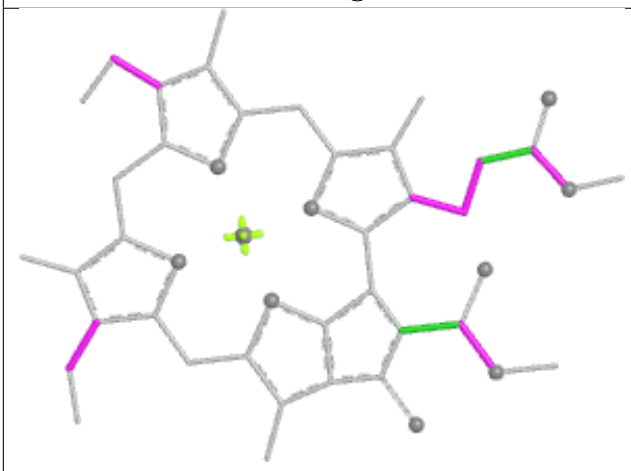

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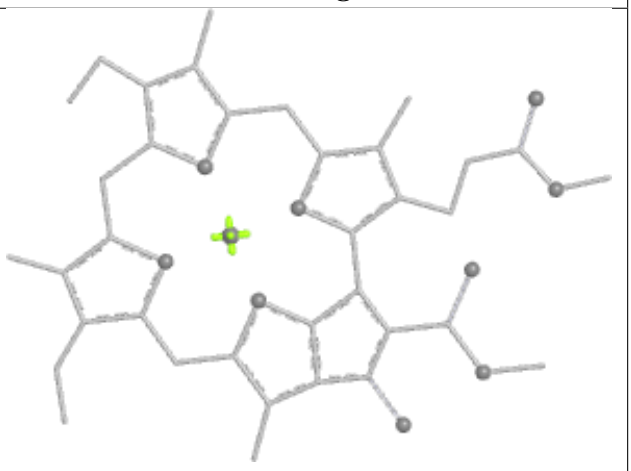
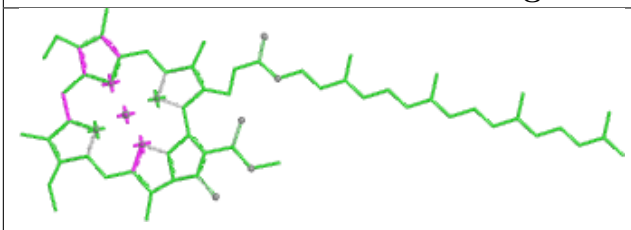


Rings

Ligand CLA Y 512



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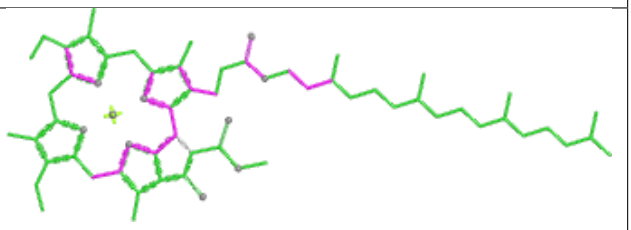

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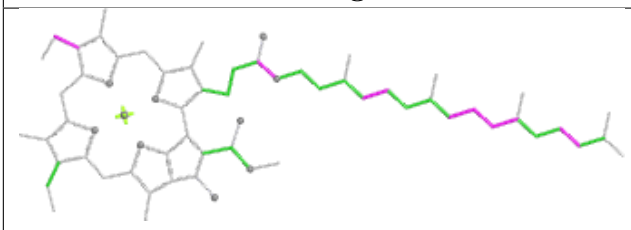

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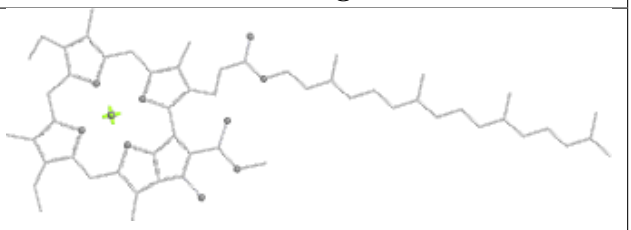
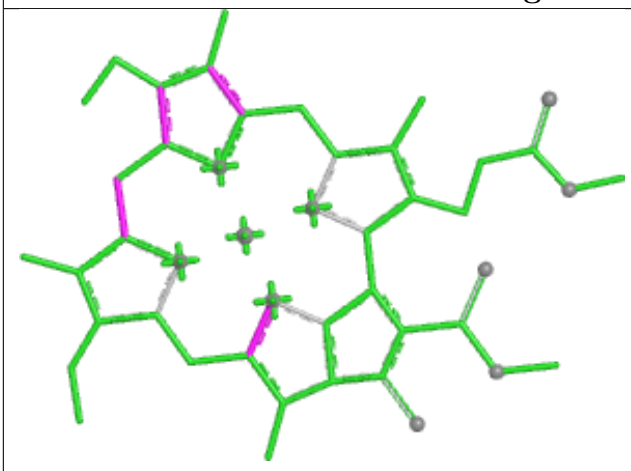


Rings

Ligand CLA X 513



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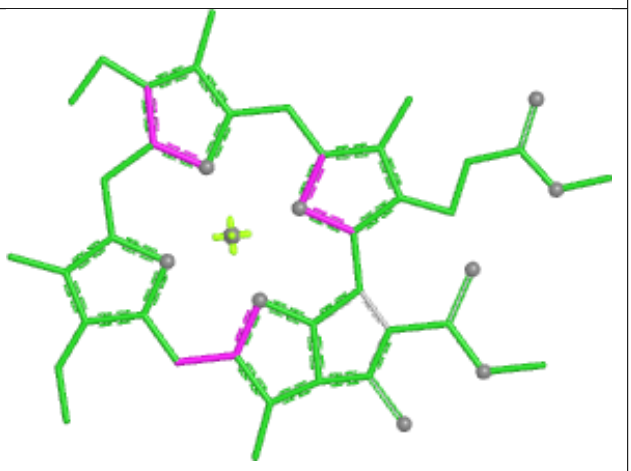
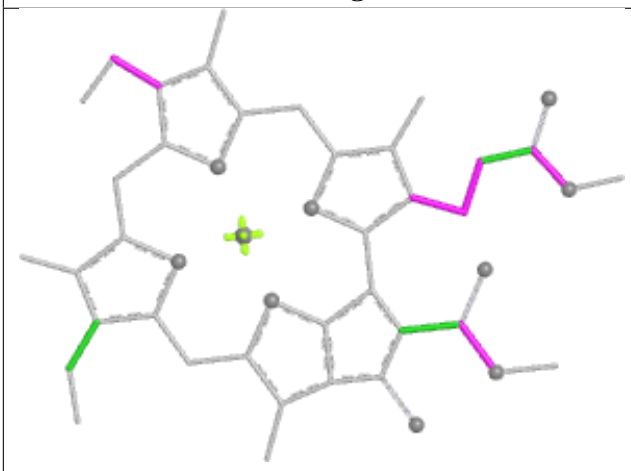


Bond angles



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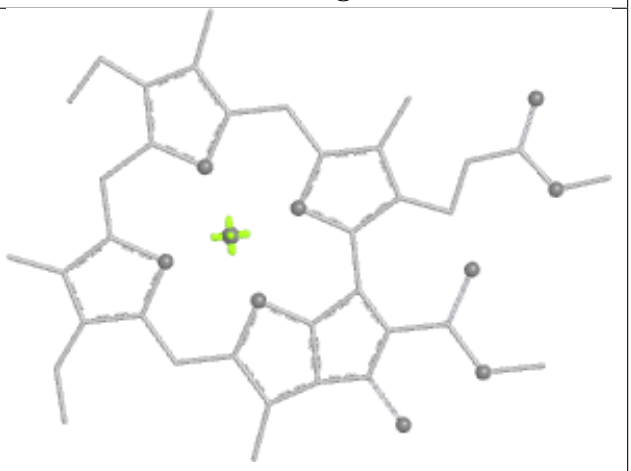
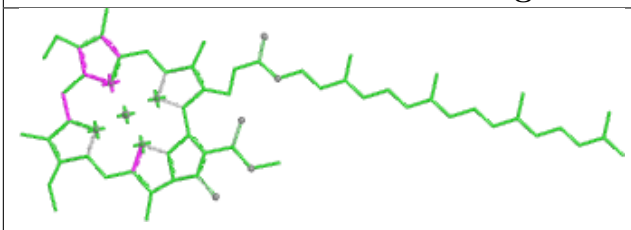
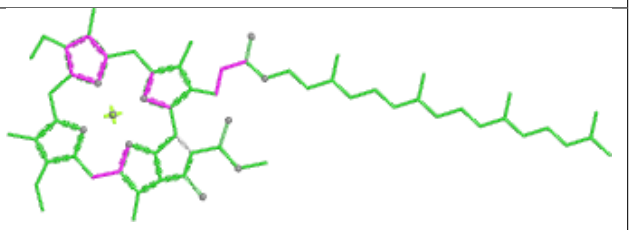
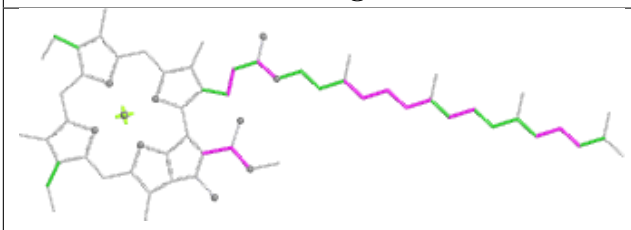
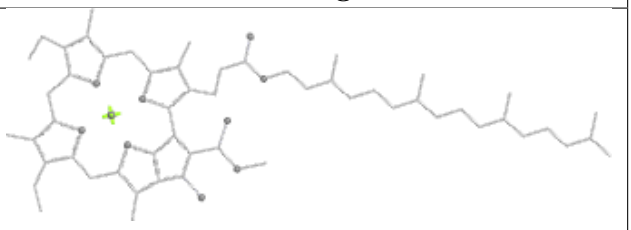
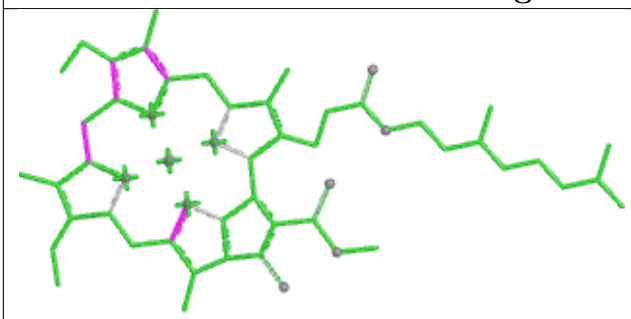
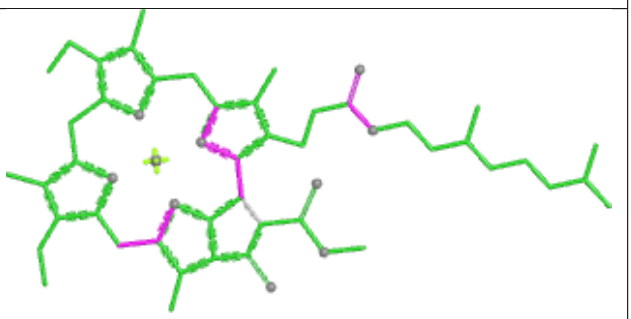
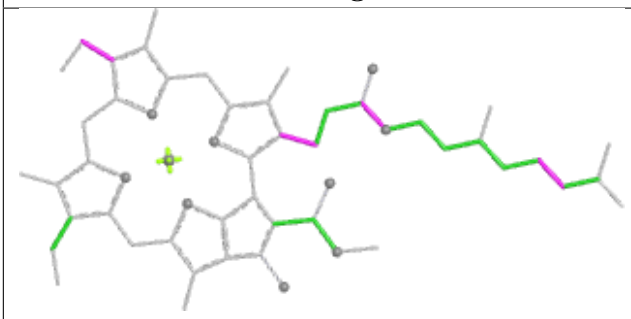
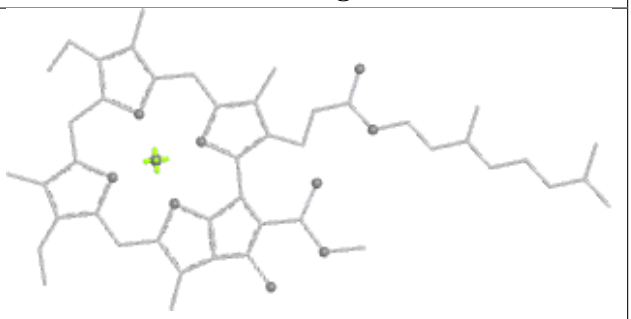
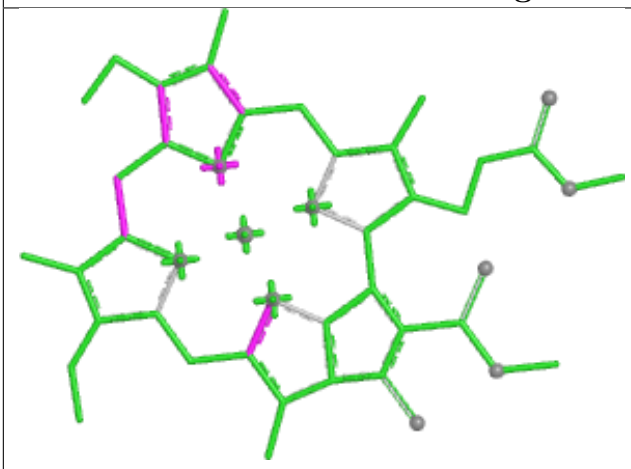


Rings

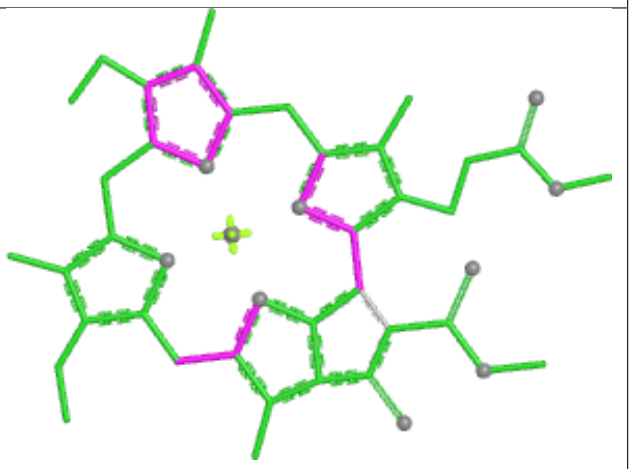
Ligand CLA A 1132	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 4004	
 Bond lengths	 Bond angles
 Torsions	 Rings

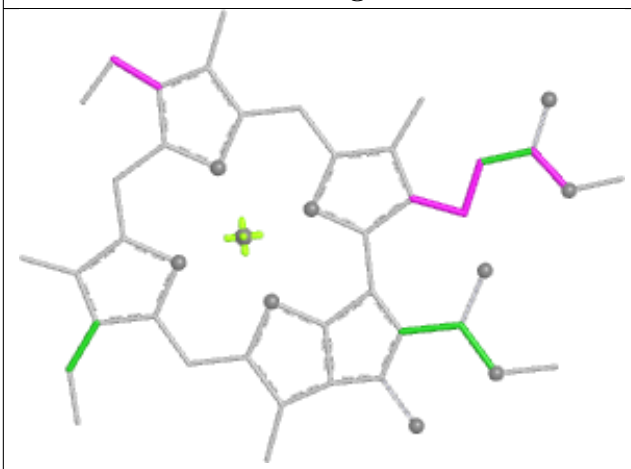
Ligand CLA H 1129



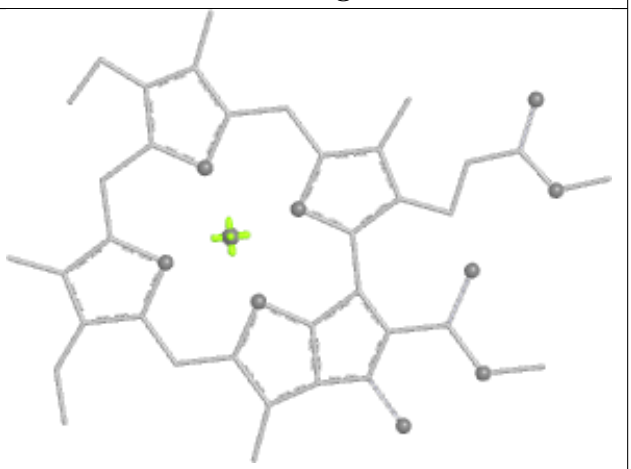
Bond lengths



Bond angles

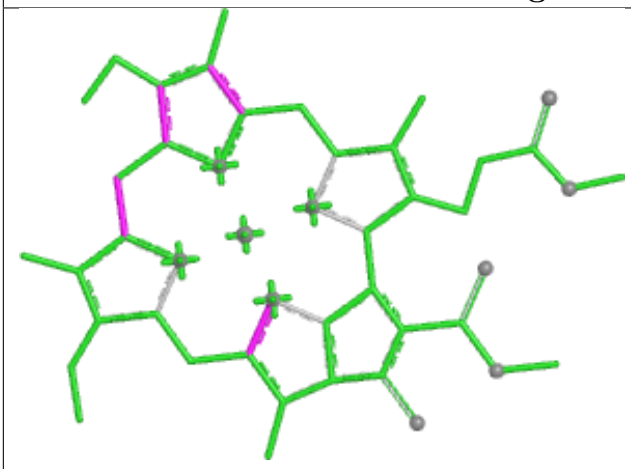


Torsions



Rings

Ligand CLA g 503



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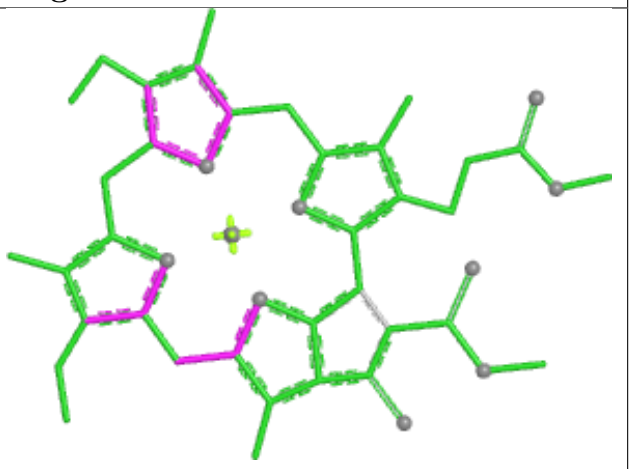
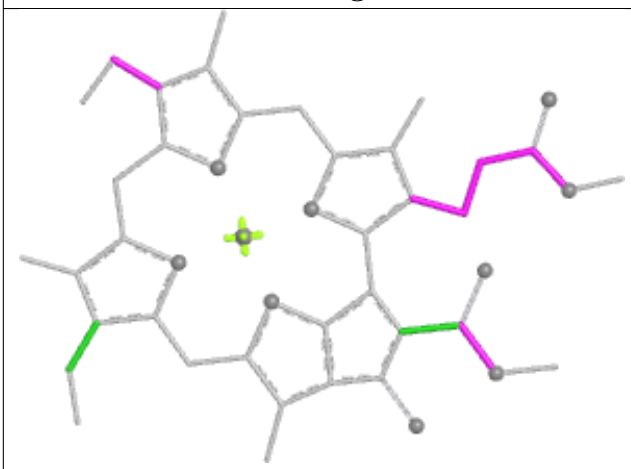


Bond angles



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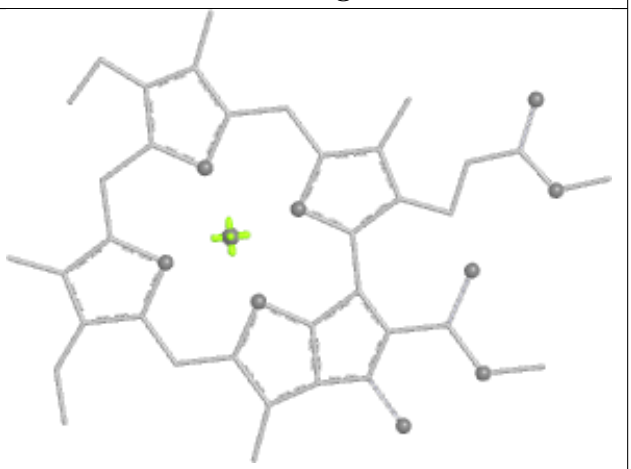
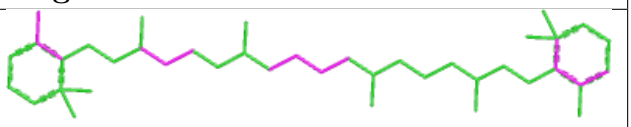


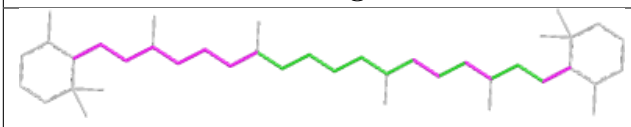
Rings

Ligand BCR g 603

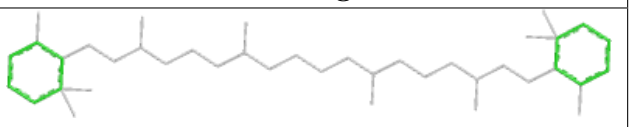
Bond lengths



Bond angles

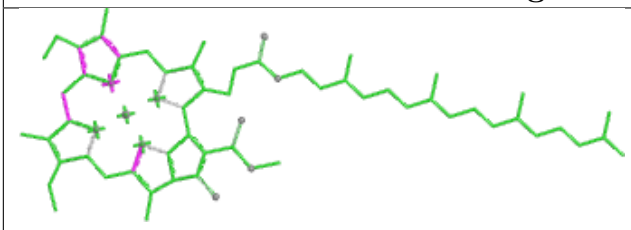


Torsions

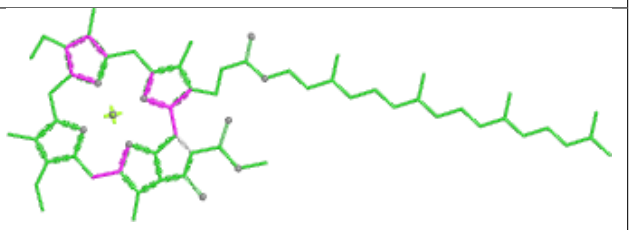


Rings

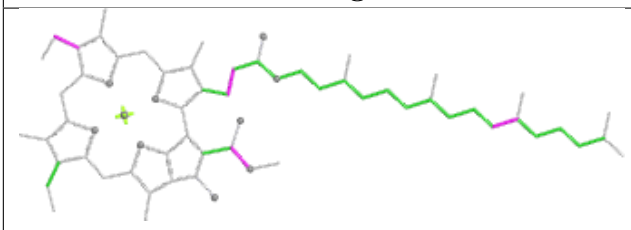
Ligand CLA h 505



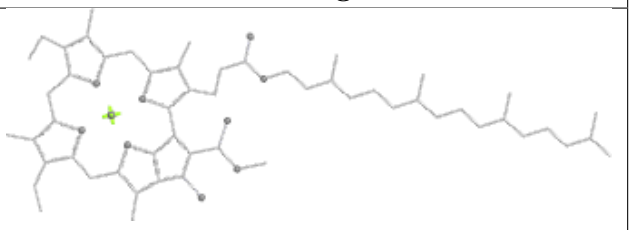
Bond lengths



Bond angles

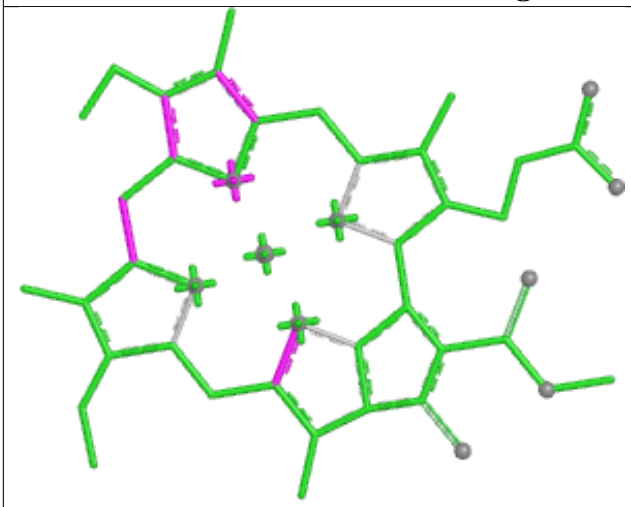


Torsions



Rings

Ligand CLA A 1134



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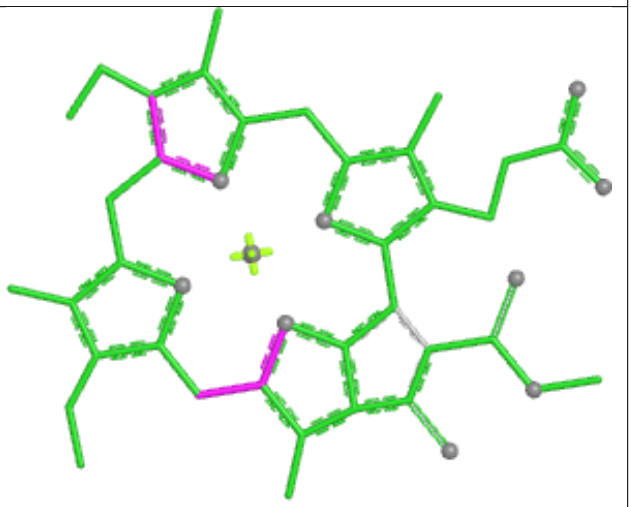
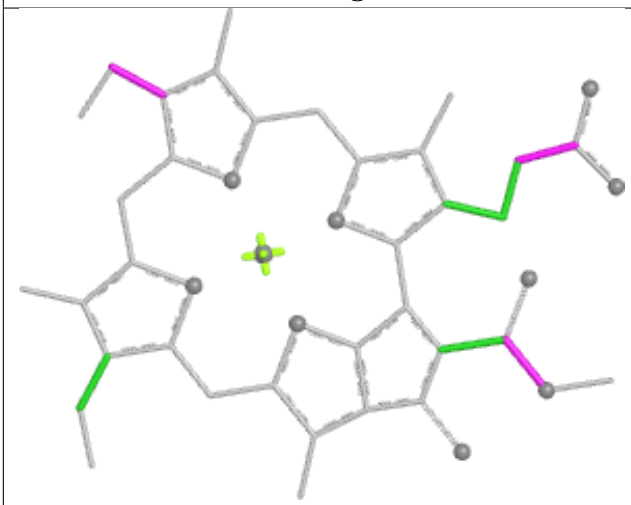
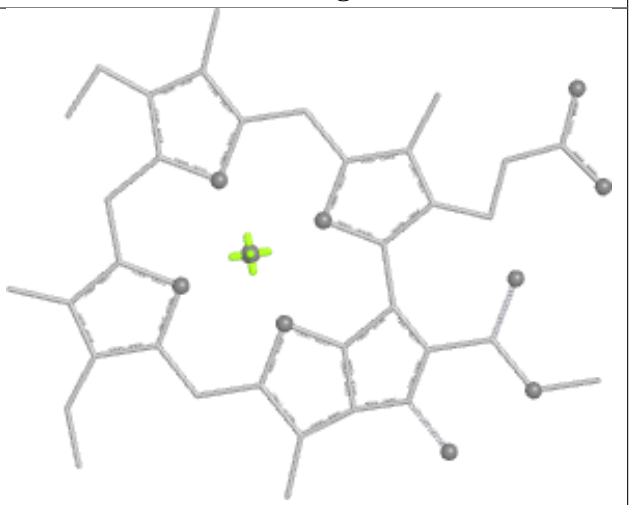


Bond angles

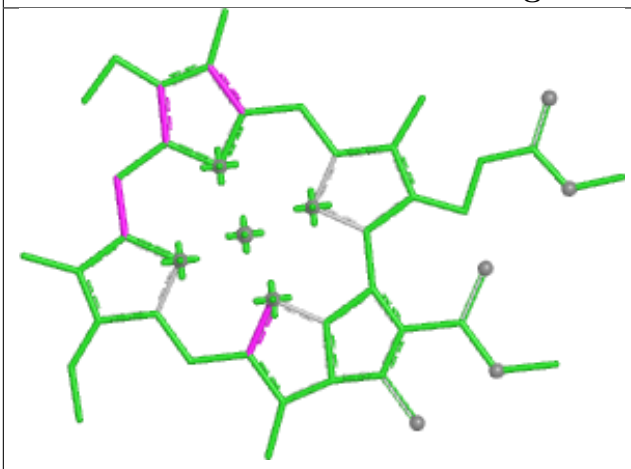


Torsions

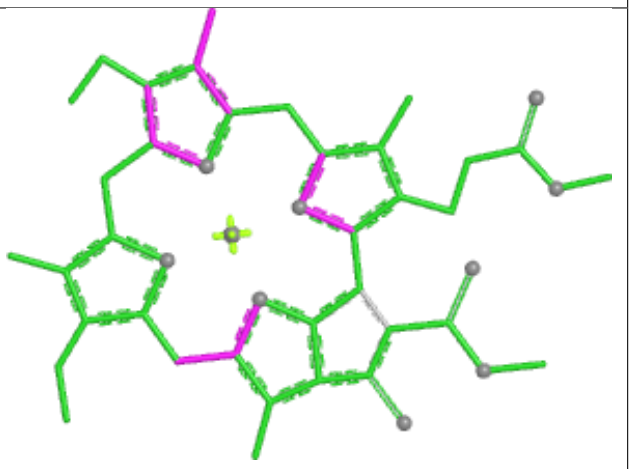


Rings

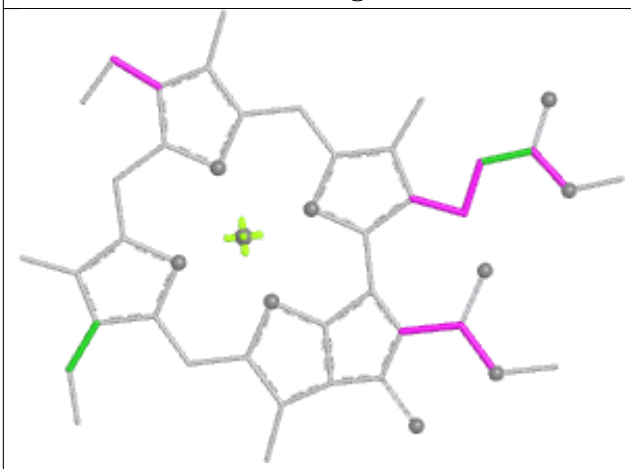
Ligand CLA Y 516



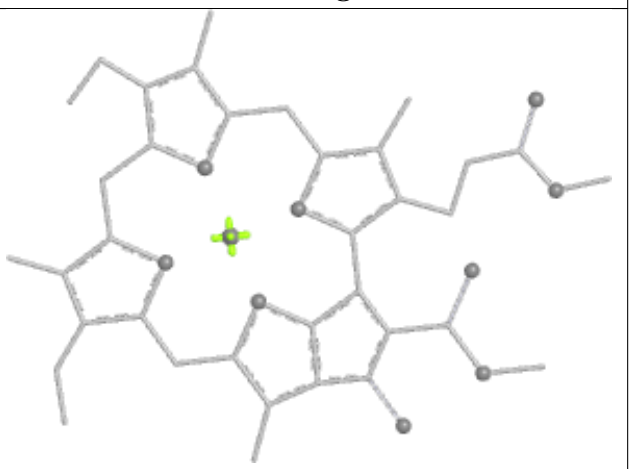
Bond lengths



Bond angles



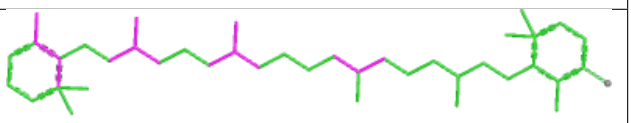
Torsions



Rings

Ligand ECH V 4021

Bond lengths



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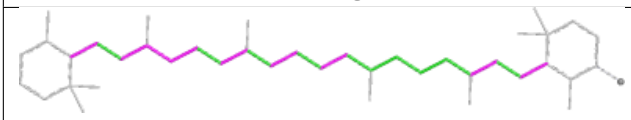

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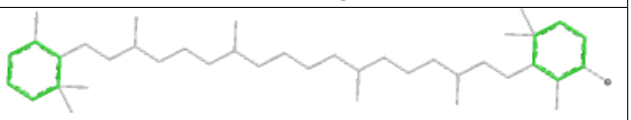
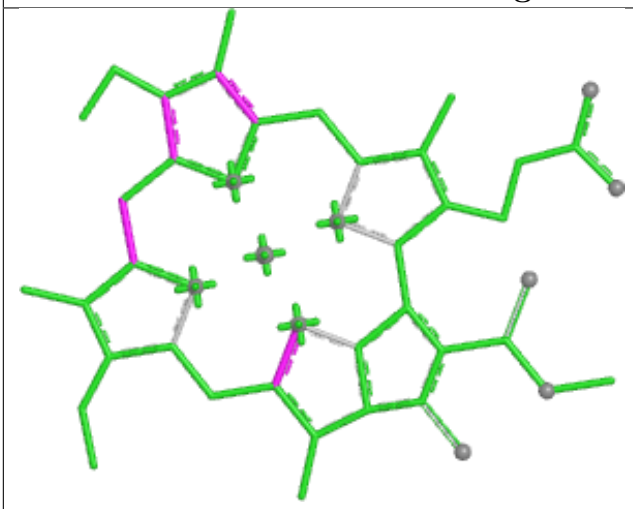


Rings

Ligand CLA G 1209



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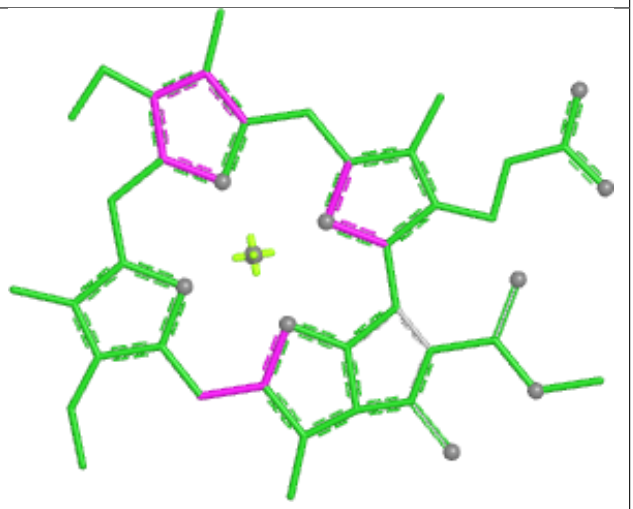

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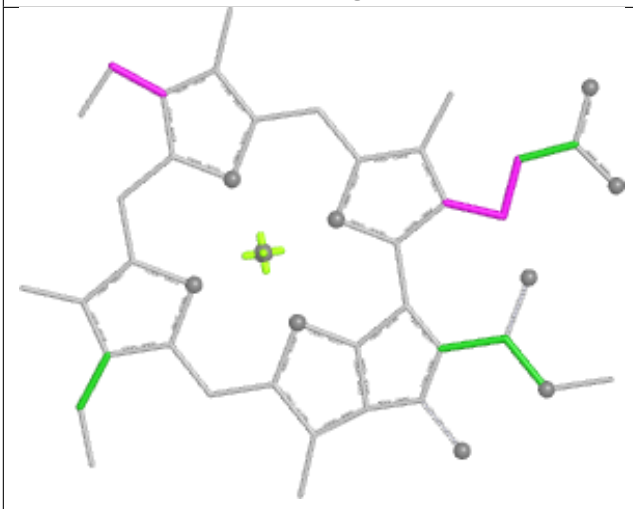
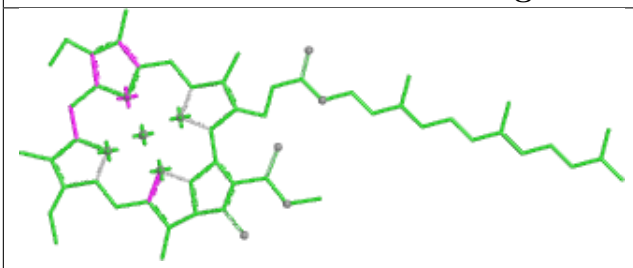


Torsions

Rings

Ligand CLA A 1139



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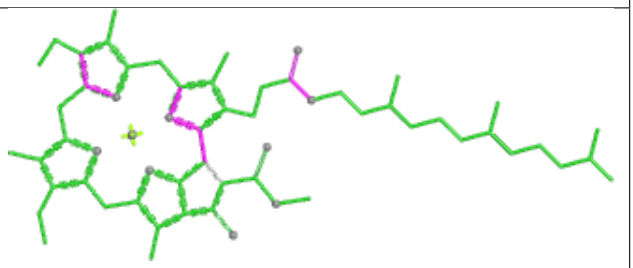

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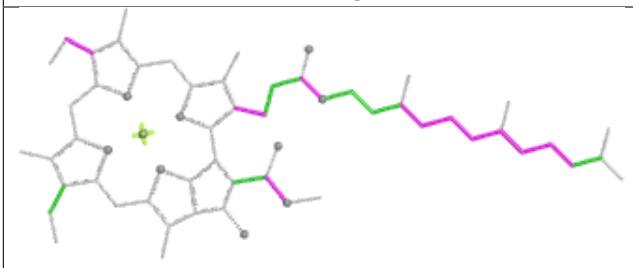

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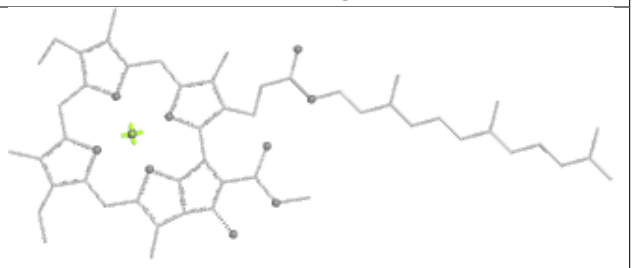
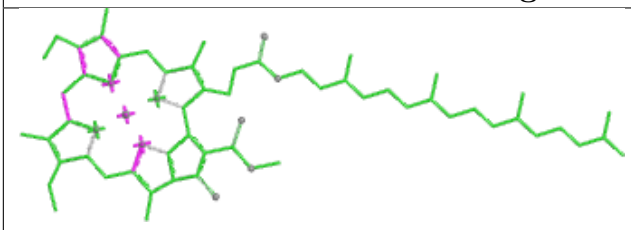


Rings

Ligand CLA a 1127



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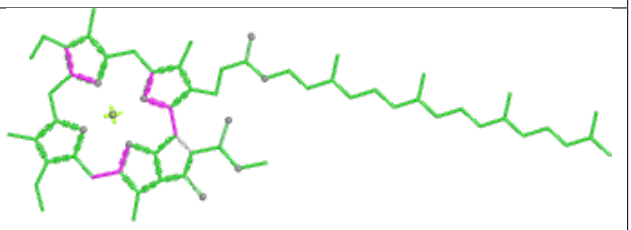
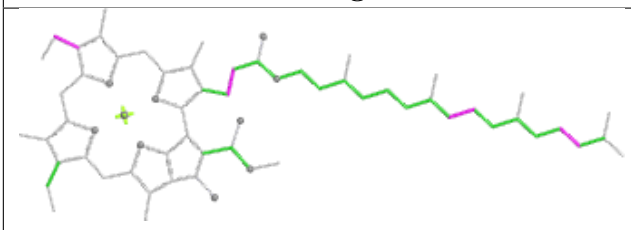


Bond angles



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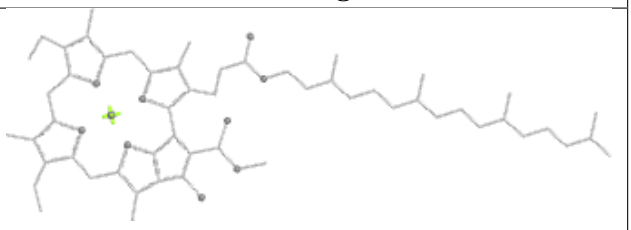
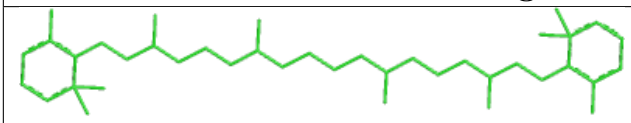


Rings

Ligand BCR a 4011



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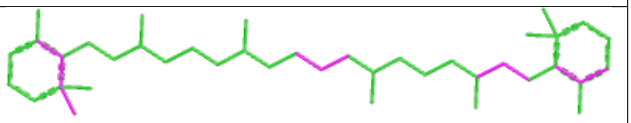
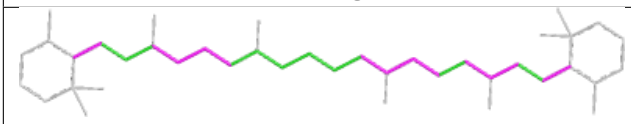


Bond angles



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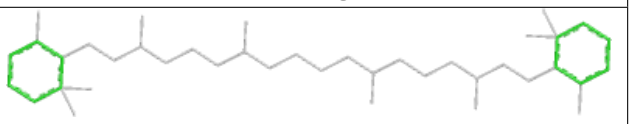
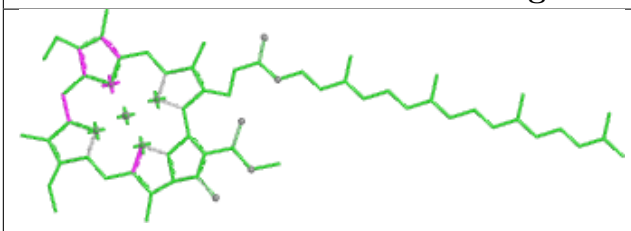


Rings

Ligand CLA g 505



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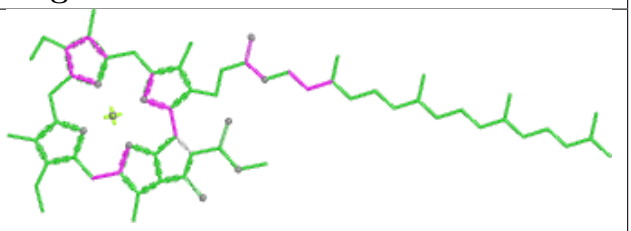

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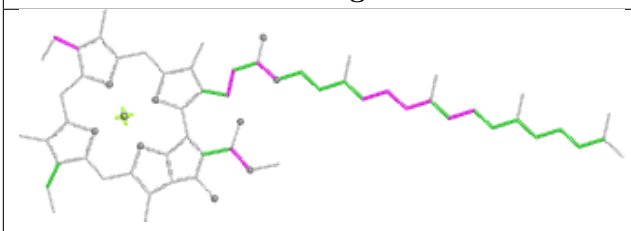

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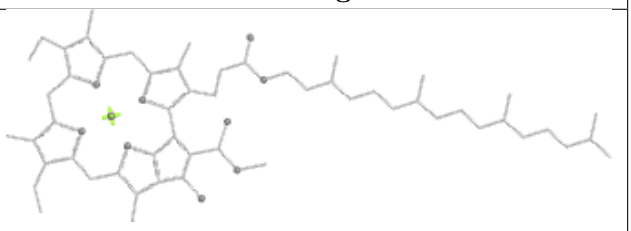
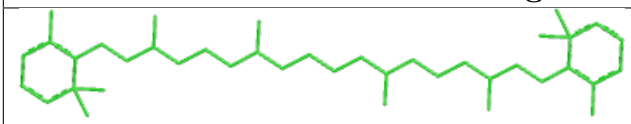


Rings

Ligand BCR h 604



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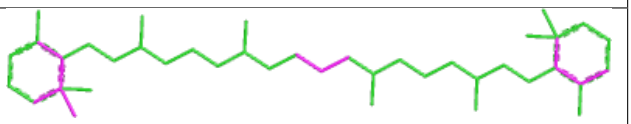

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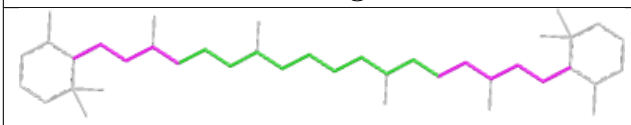

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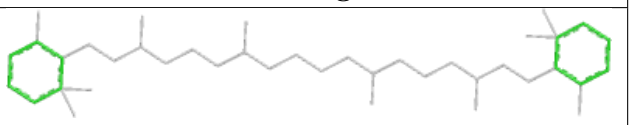
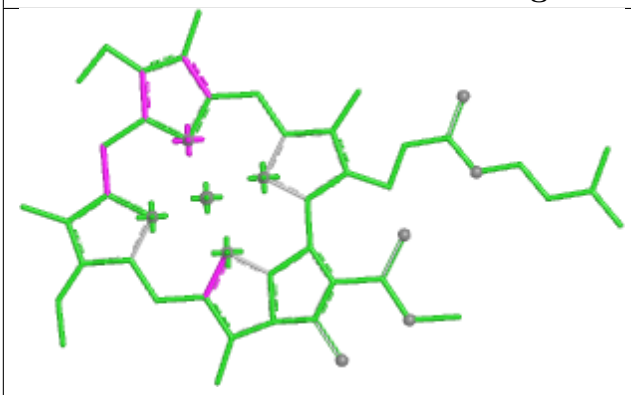
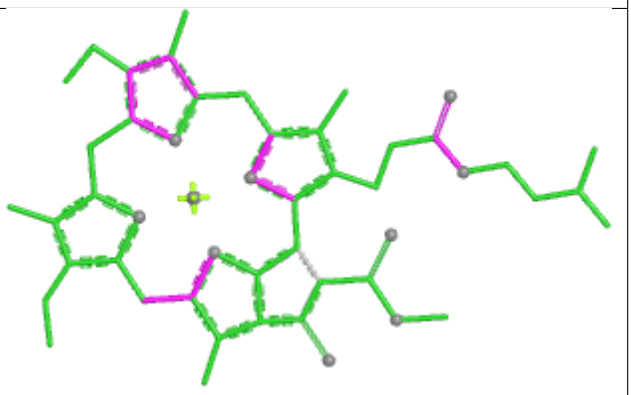


Rings

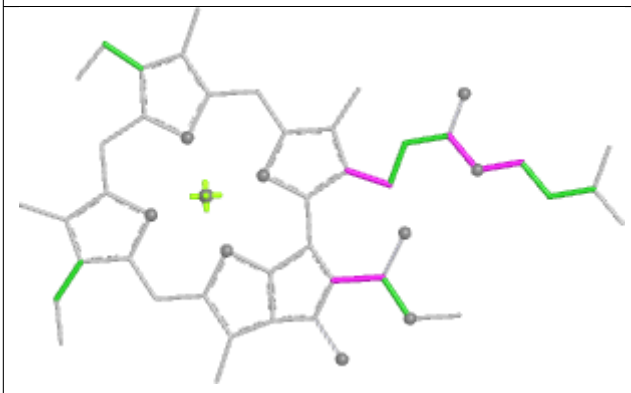
Ligand CLA t 501



Bond lengths



Bond angles



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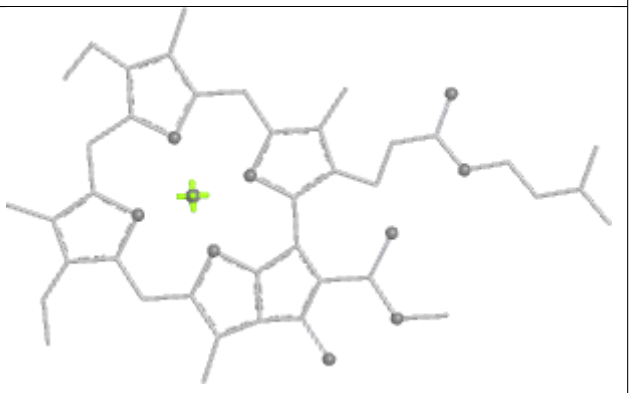
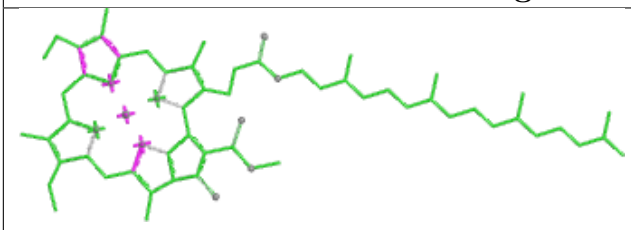
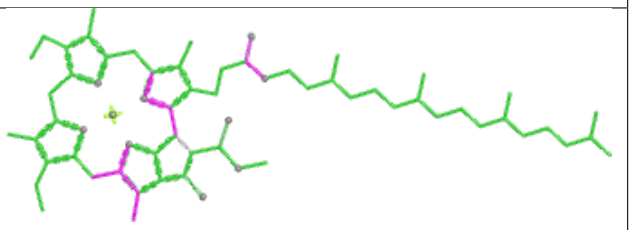
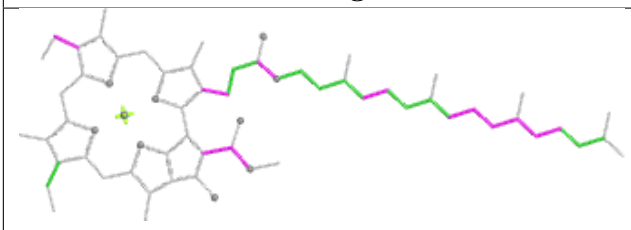
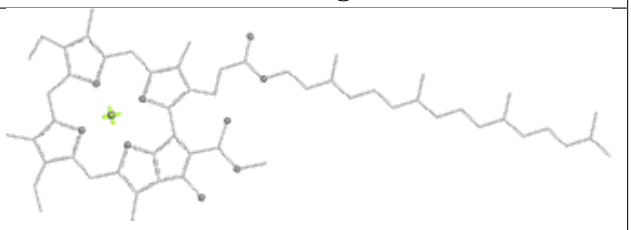
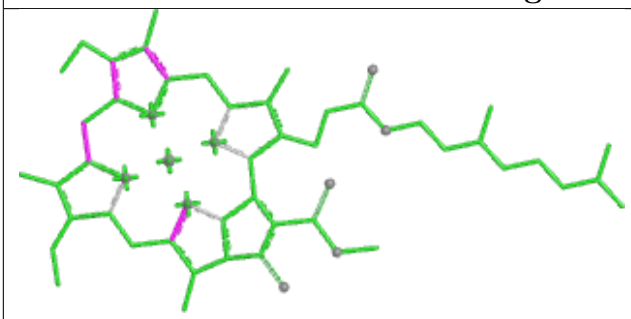
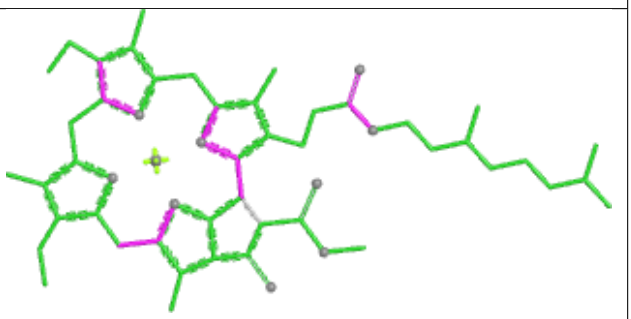
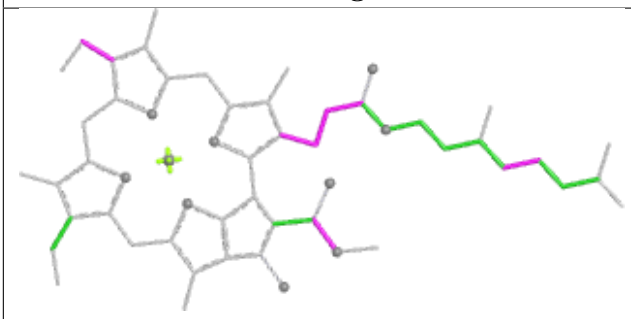
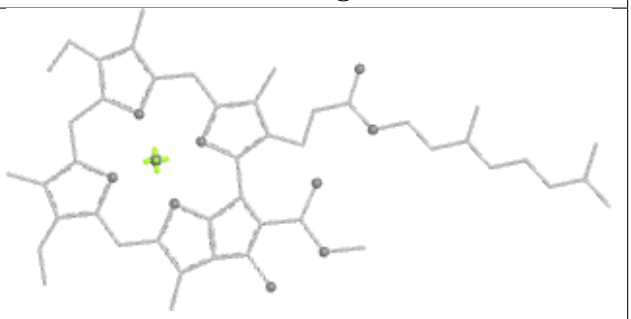
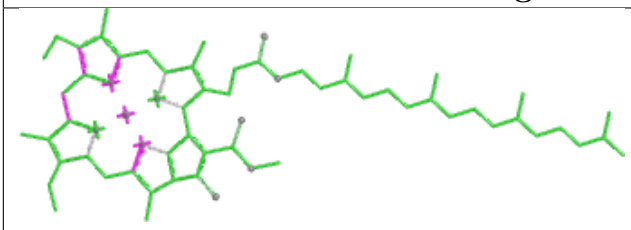


Rings

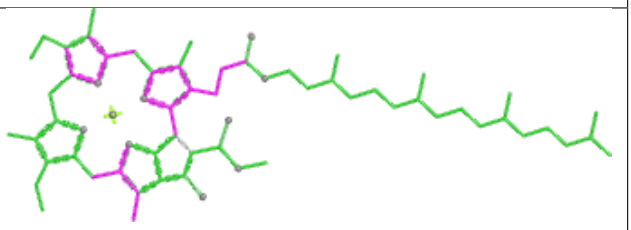
Ligand CLA H 1128	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA w 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

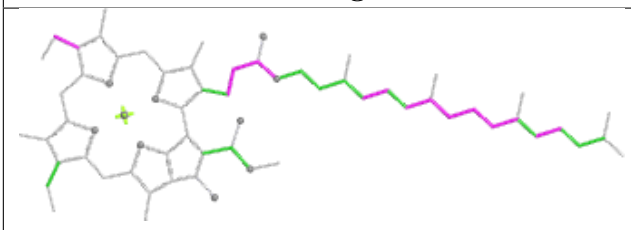
Ligand CLA A 1013



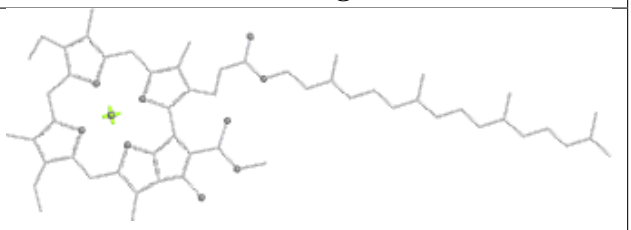
Bond lengths



Bond angles

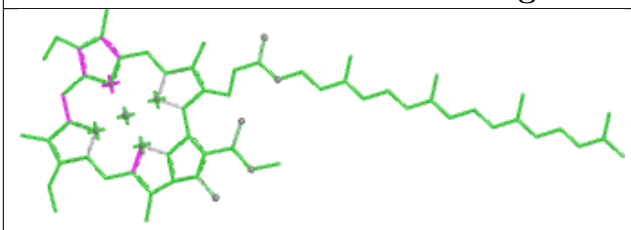


Torsions



Rings

Ligand CLA b 1206



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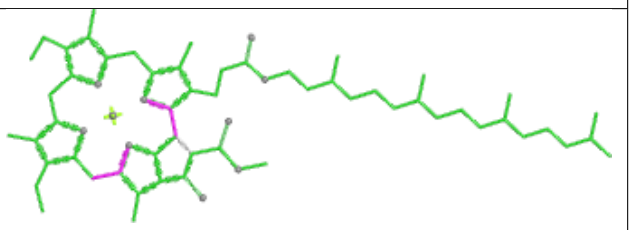
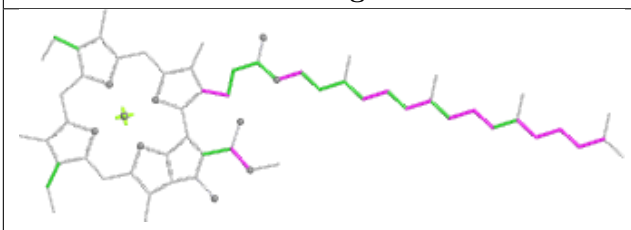


Bond angles



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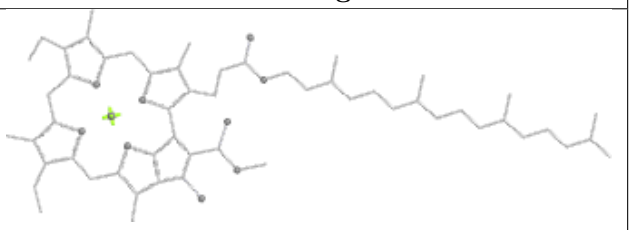
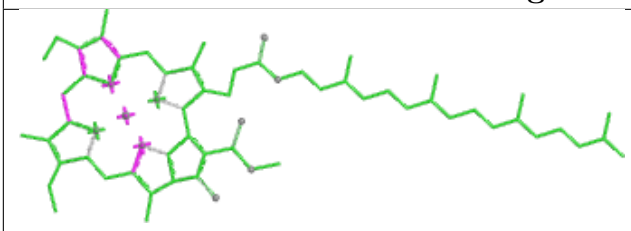
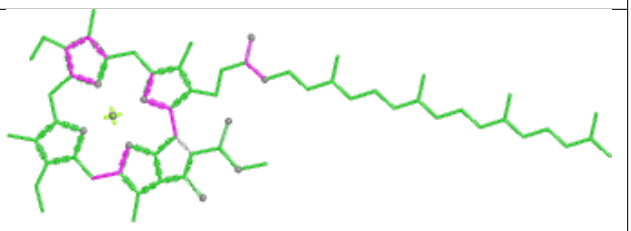


Rings

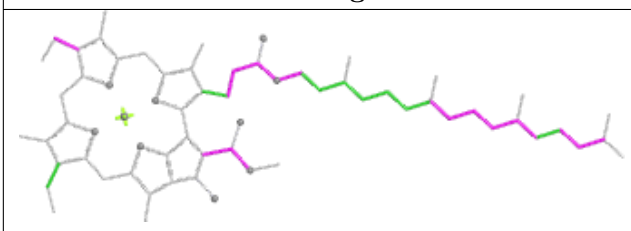
Ligand CLA n 505



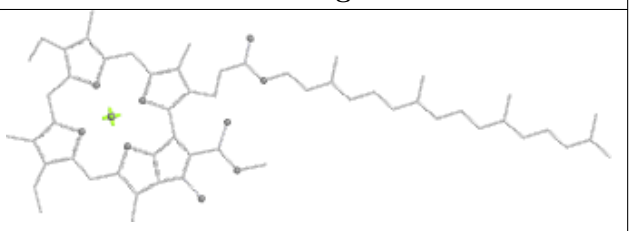
Bond lengths



Bond angles

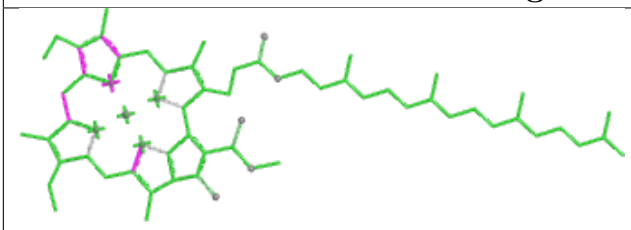


Torsions

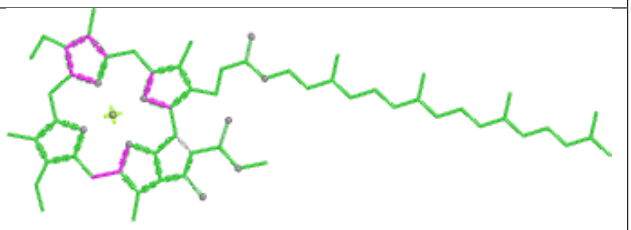


Rings

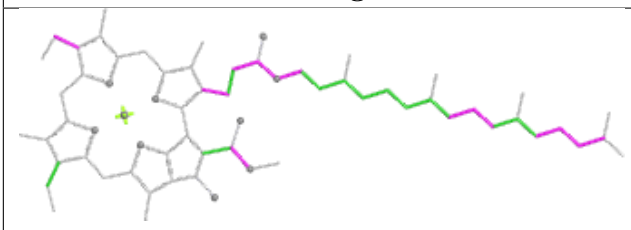
Ligand CLA Z 509



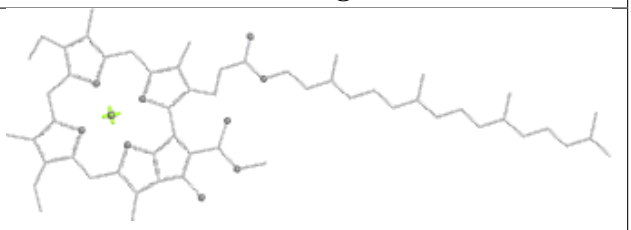
Bond lengths



Bond angles

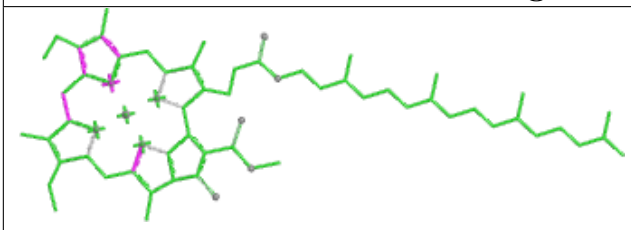


Torsions

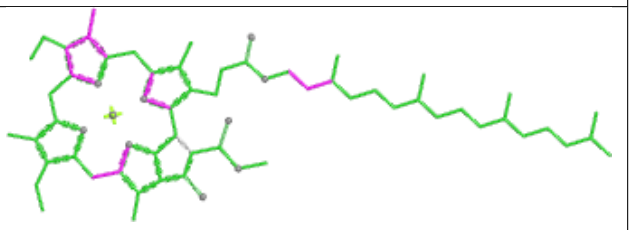


Rings

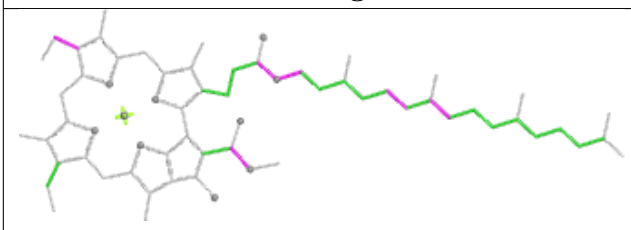
Ligand CLA x 507



Bond lengths



Bond angles



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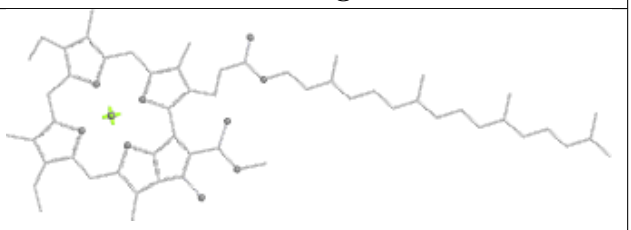
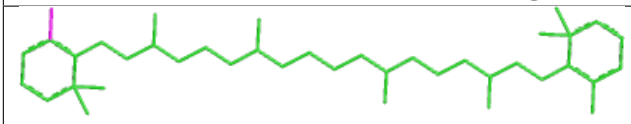
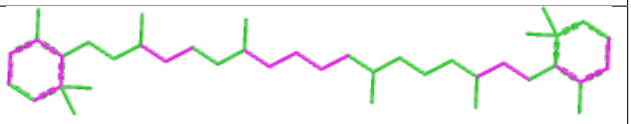


Rings

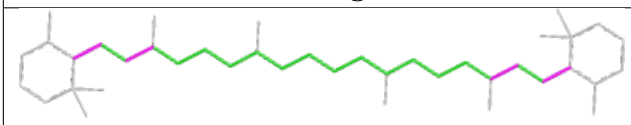
Ligand BCR u 601



Bond lengths



Bond angles



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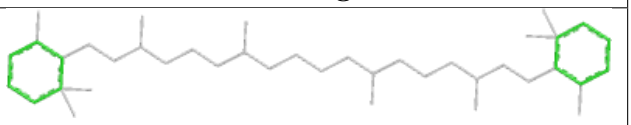
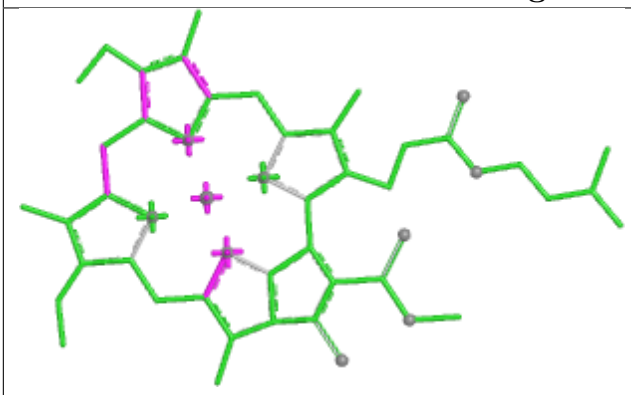


Rings

Ligand CLA o 502



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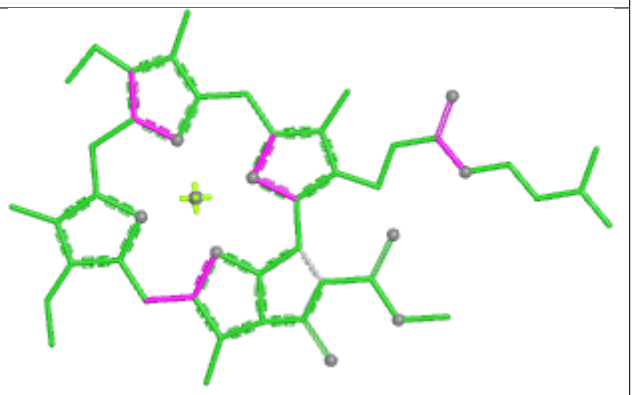
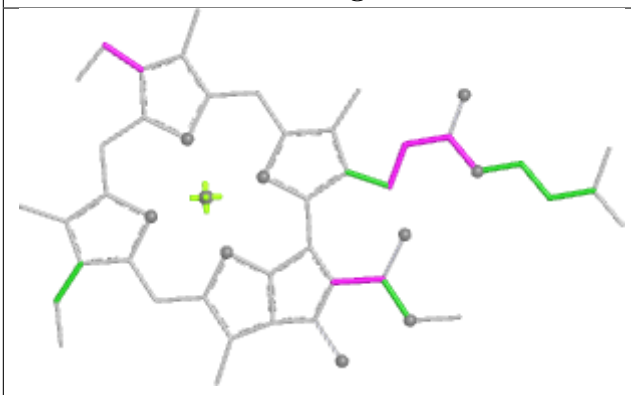
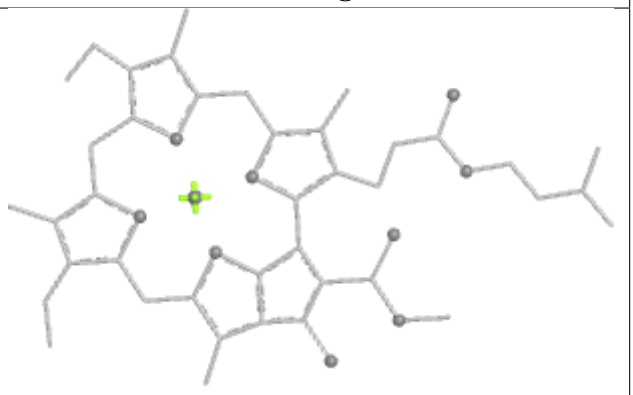


Bond angles

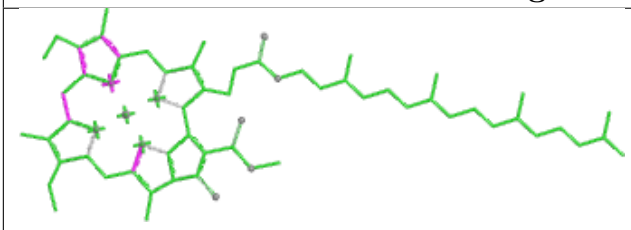


Torsions



Rings

Ligand CLA g 511



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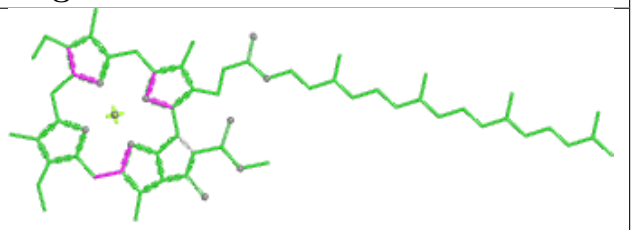
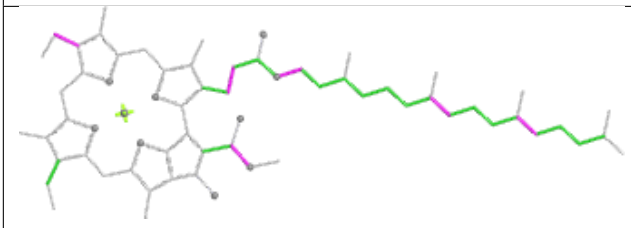


Bond angles



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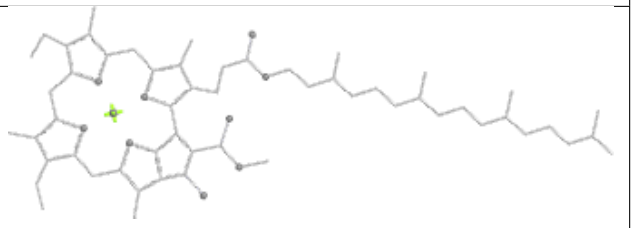
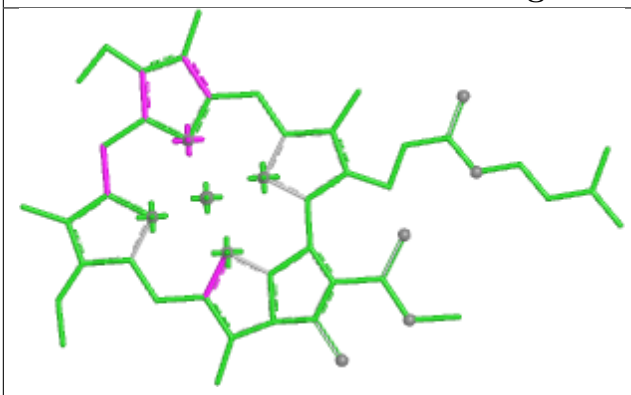


Rings

Ligand CLA p 501



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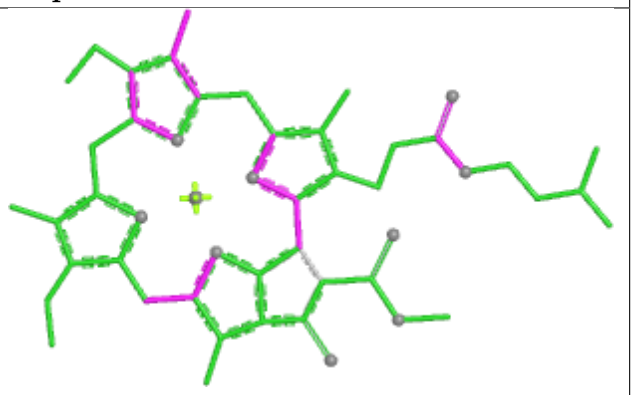
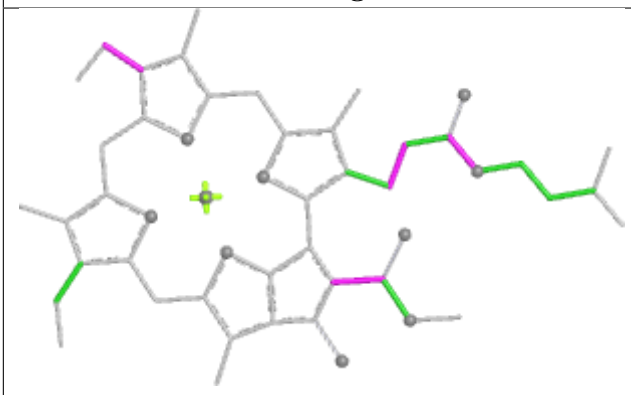
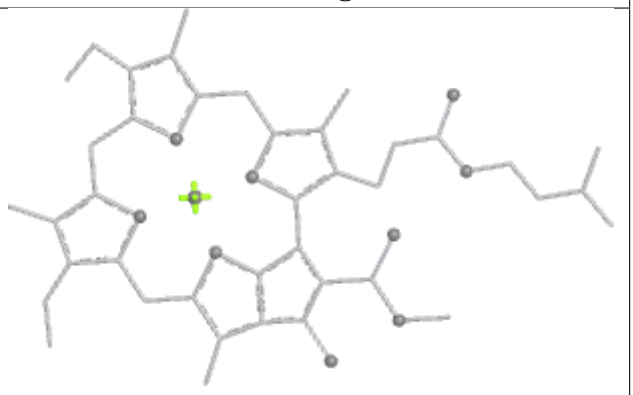


Bond angles



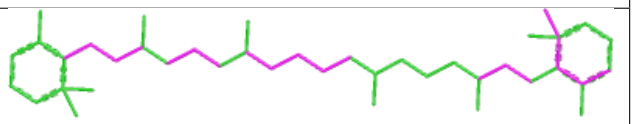
Torsions



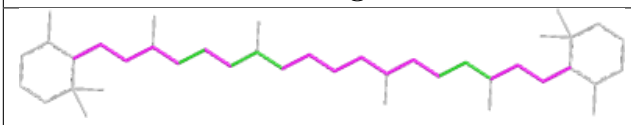
Rings

Ligand BCR G 4010

Bond lengths



Bond angles



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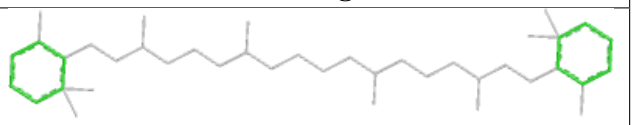
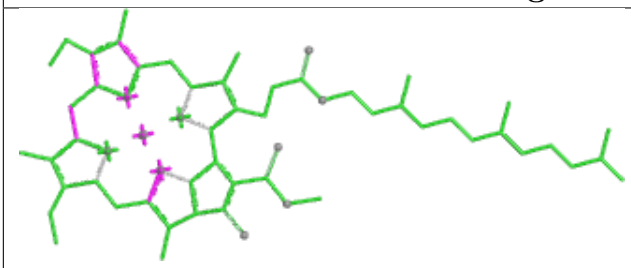
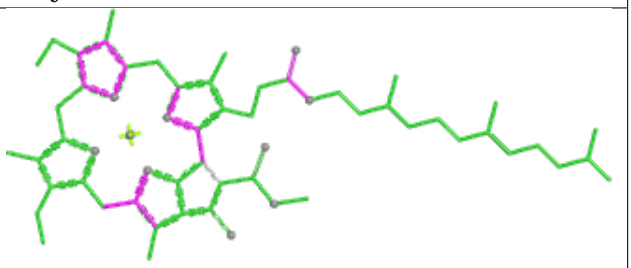
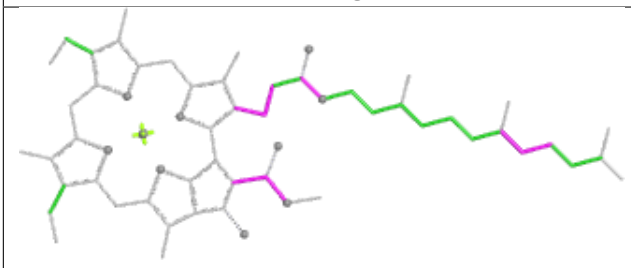
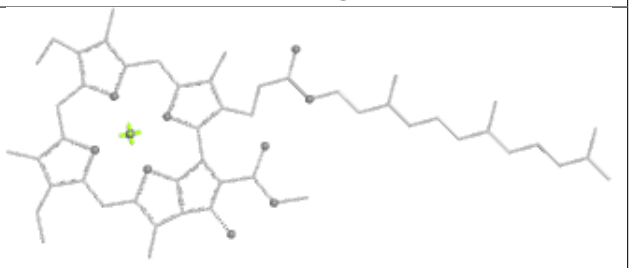
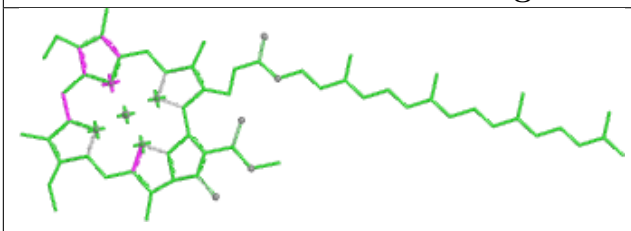
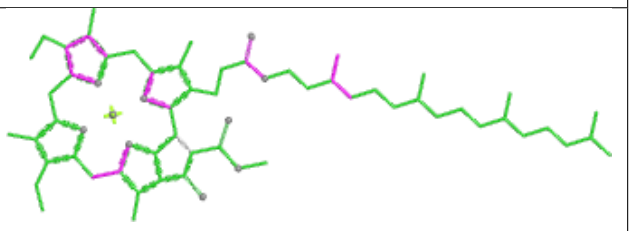
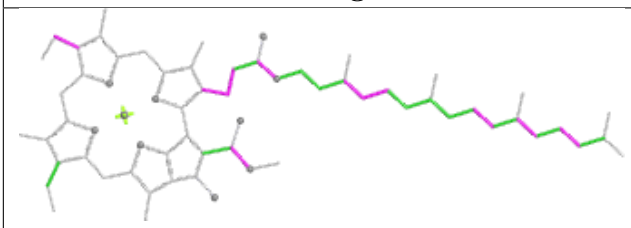
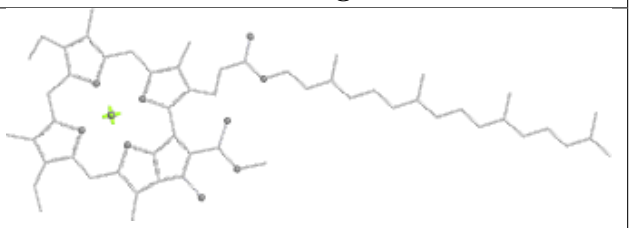
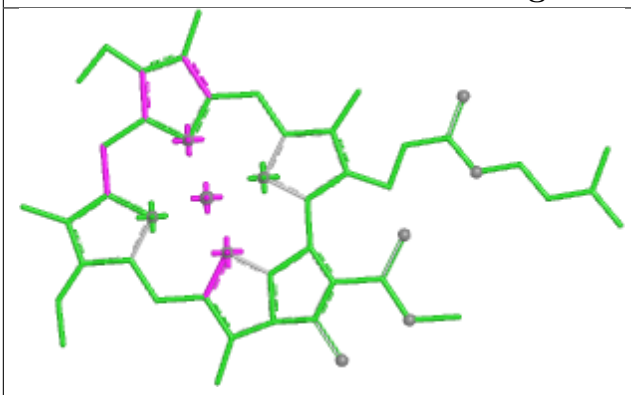


Rings

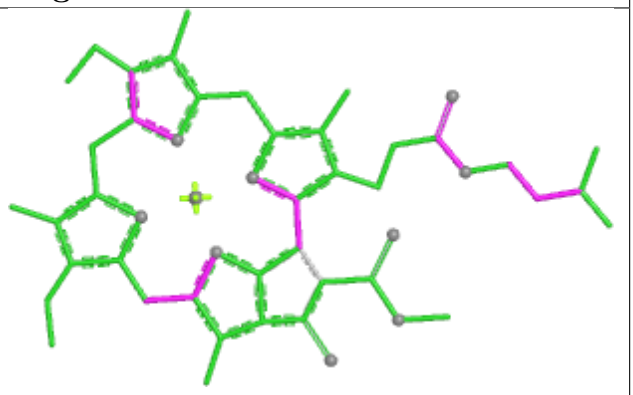
Ligand CLA y 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1203	
	
Bond lengths	Bond angles
	
Torsions	Rings

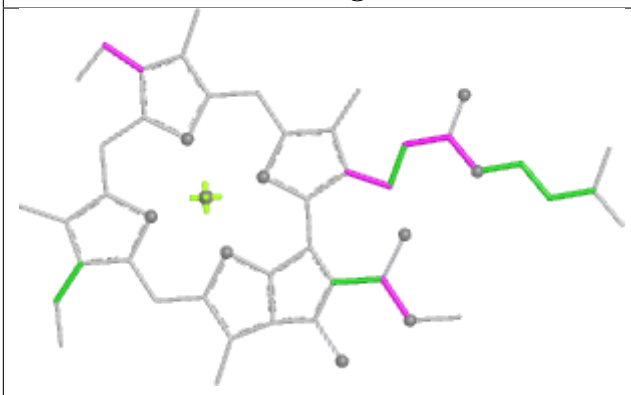
Ligand CLA g 514



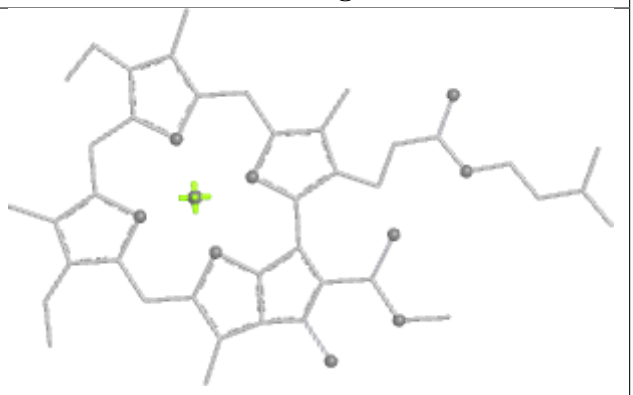
Bond lengths



Bond angles

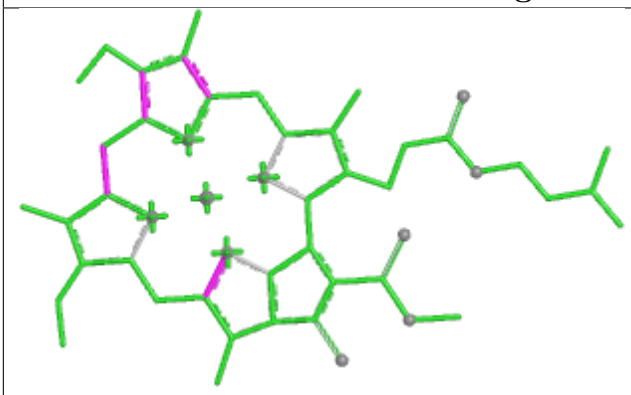


Torsions

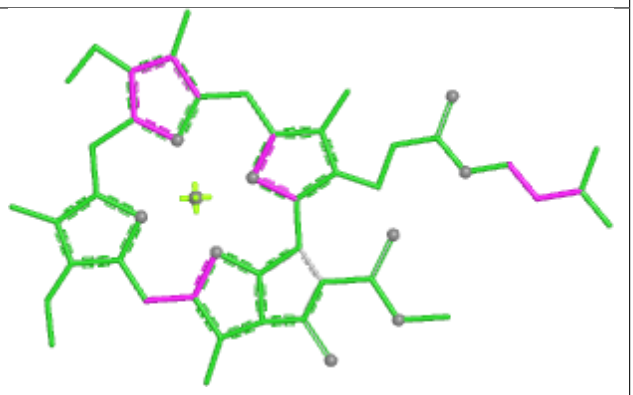


Rings

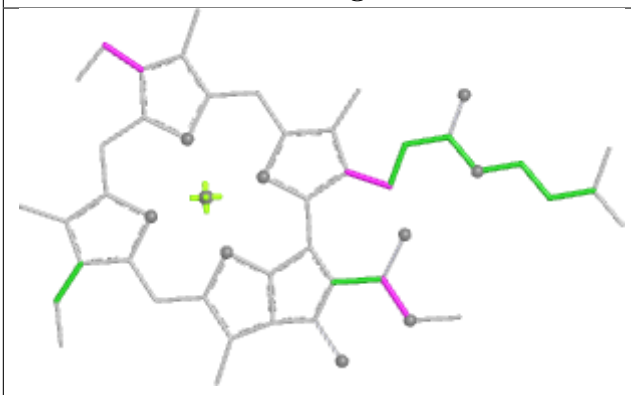
Ligand CLA A 1107



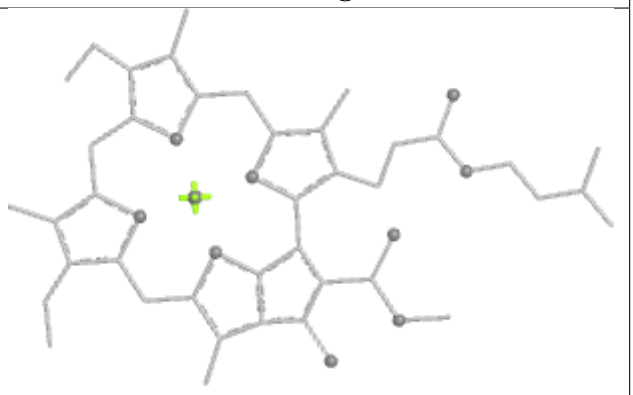
Bond lengths



Bond angles

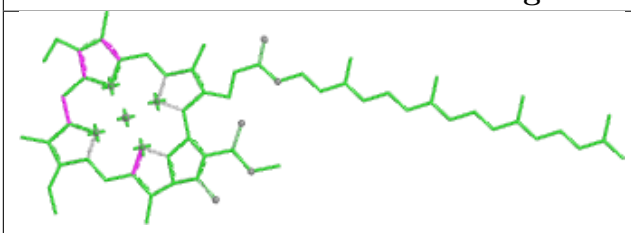


Torsions



Rings

Ligand CLA l 1503



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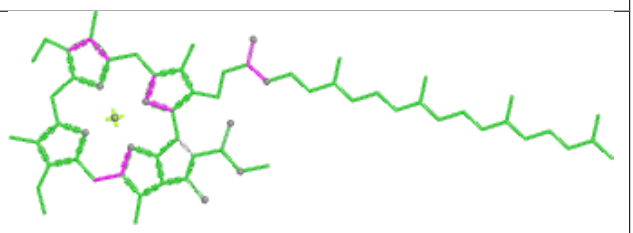
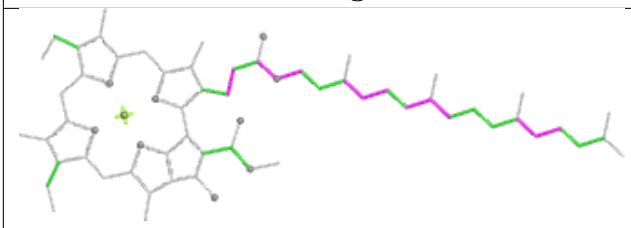
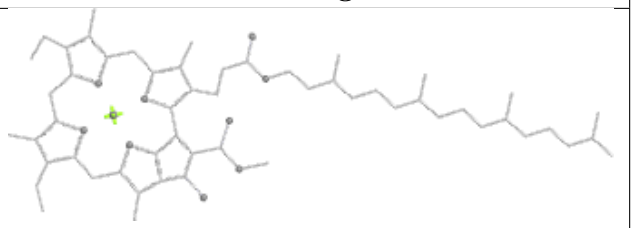


Bond angles

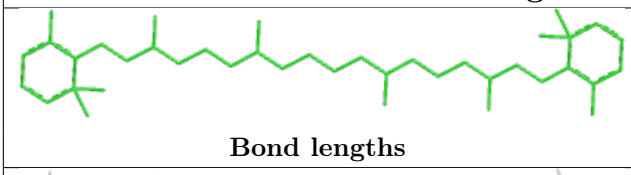


Torsions

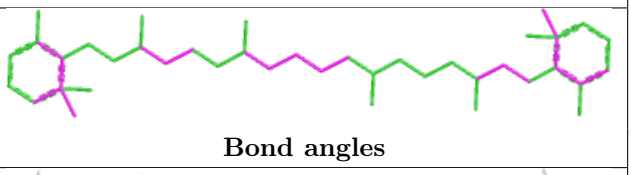


Rings

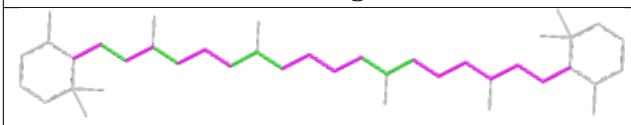
Ligand BCR o 604



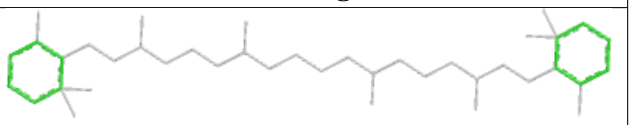
Bond lengths



Bond angles

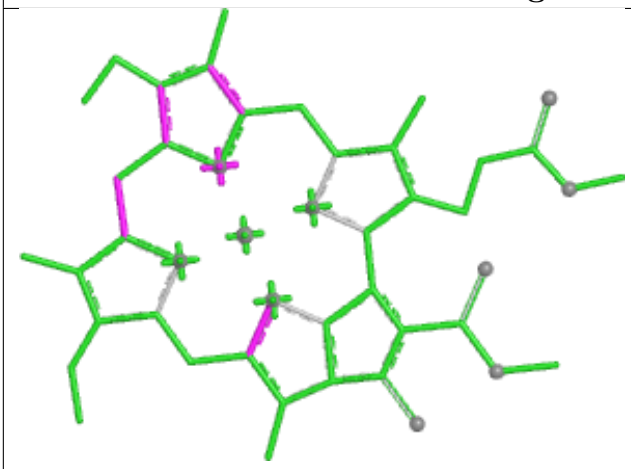


Torsions

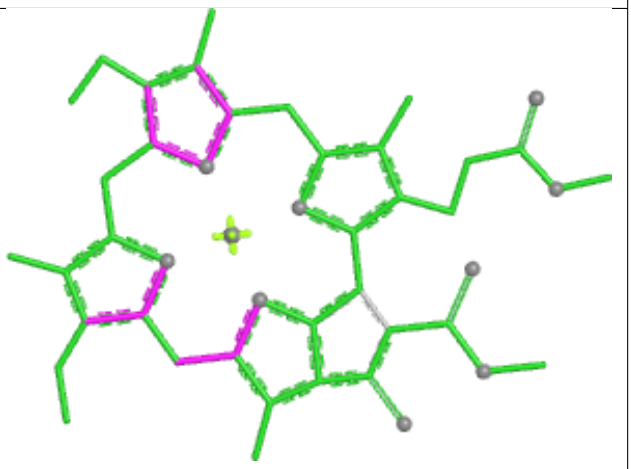


Rings

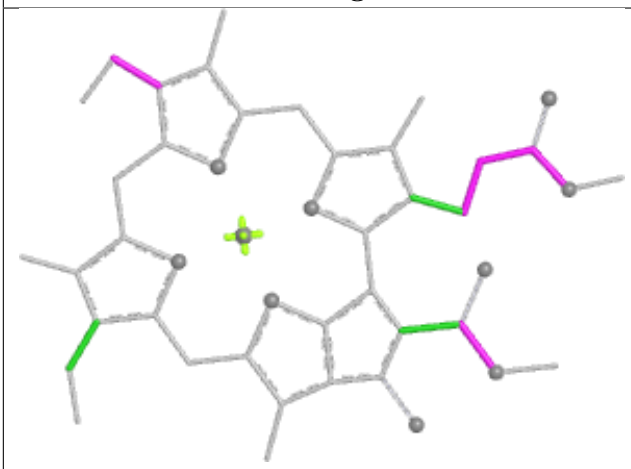
Ligand CLA x 503



Bond lengths



Bond angles



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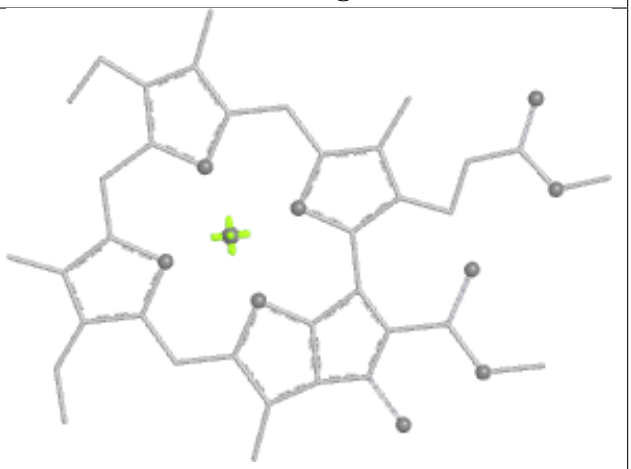
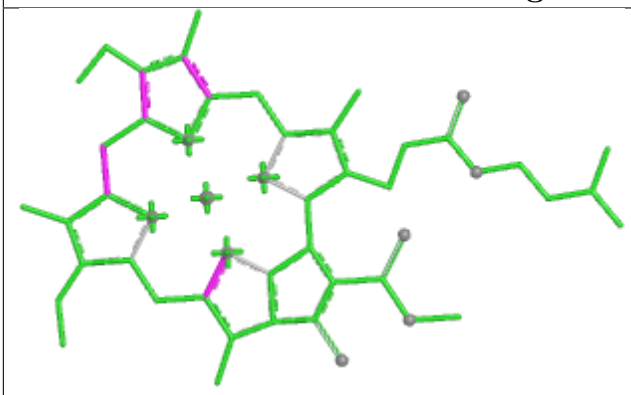
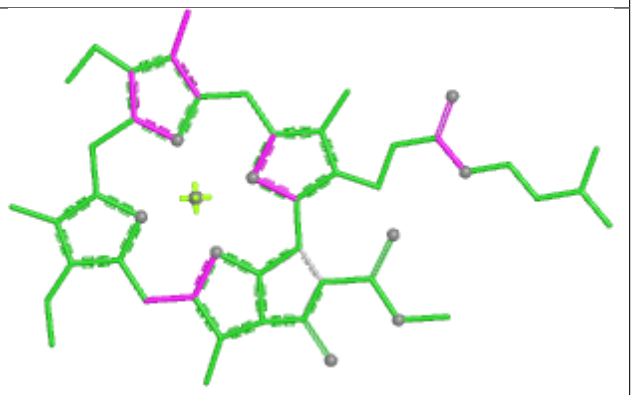


Rings

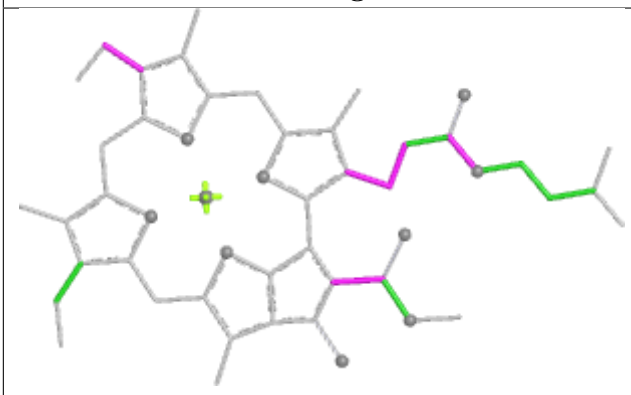
Ligand CLA Z 513



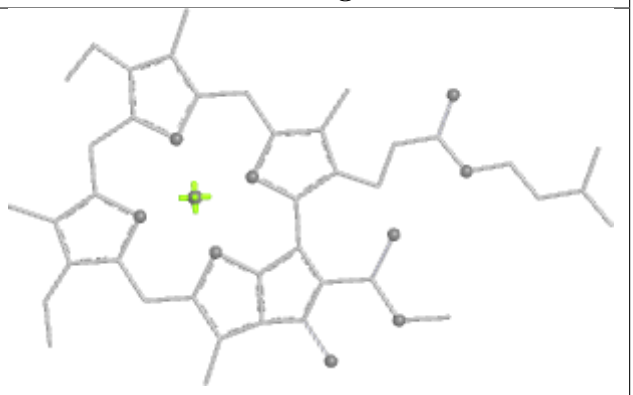
Bond lengths



Bond angles

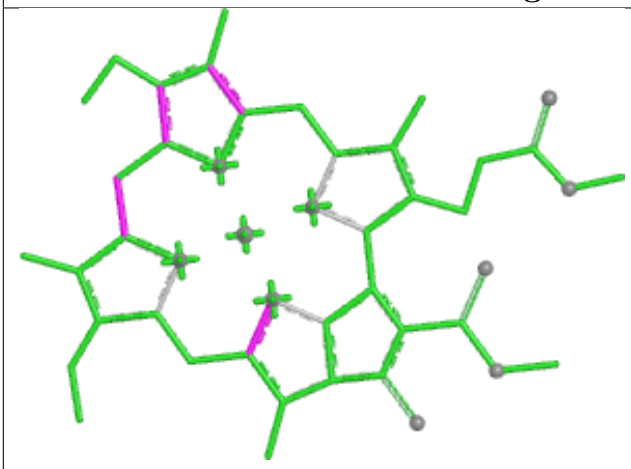


Torsions

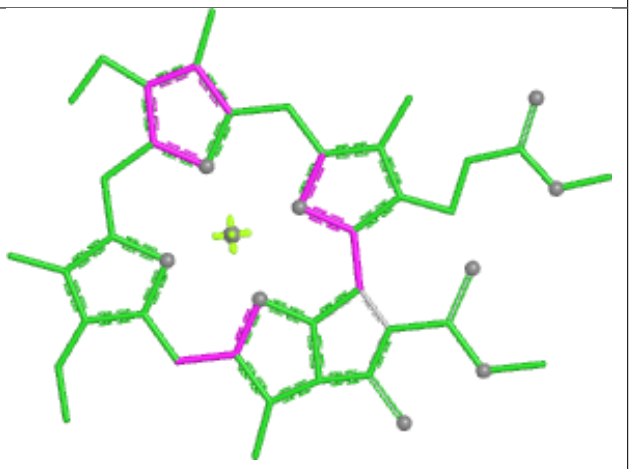


Rings

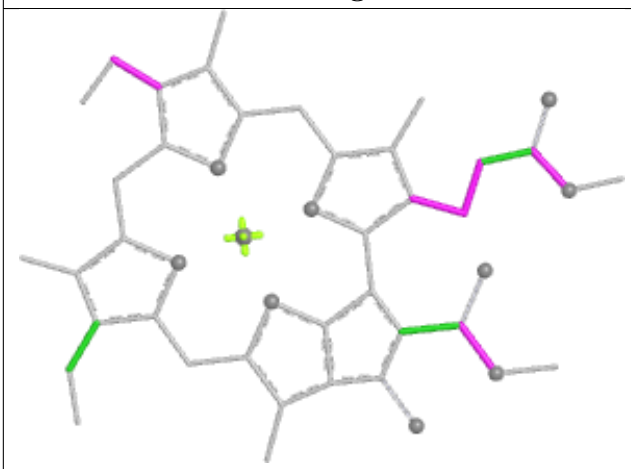
Ligand CLA X 501



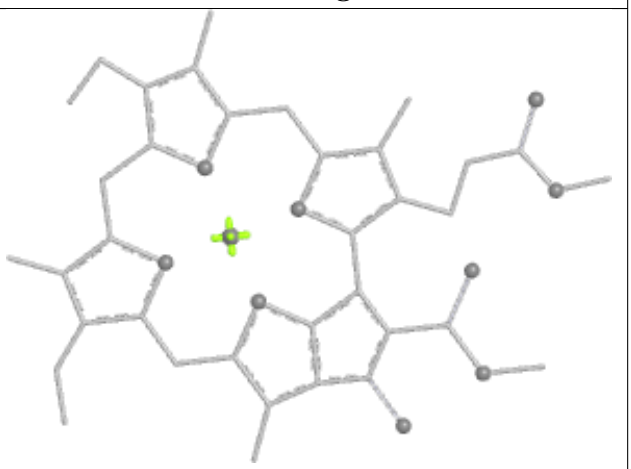
Bond lengths



Bond angles

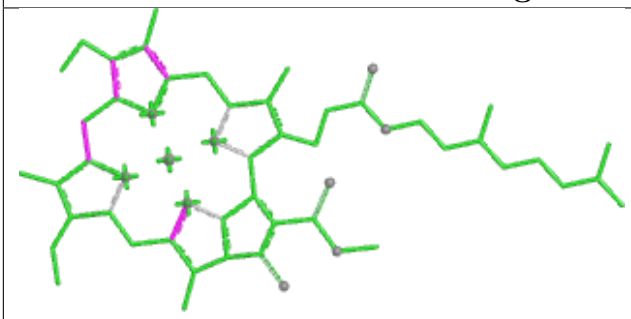


Torsions



Rings

Ligand CLA G 1218



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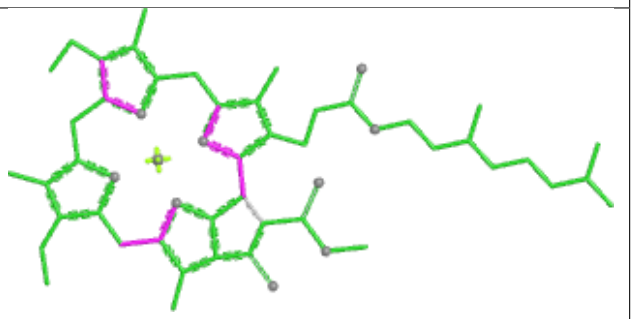
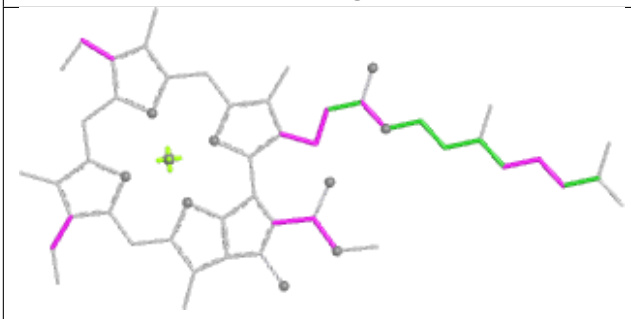
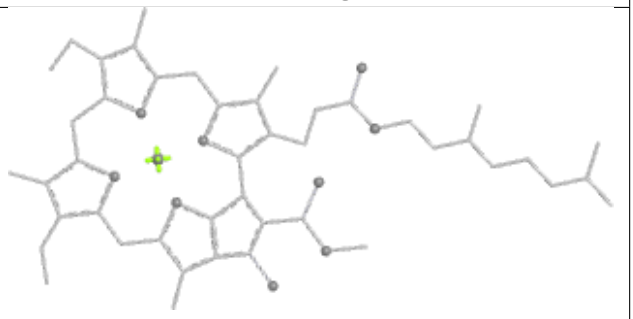


Bond angles

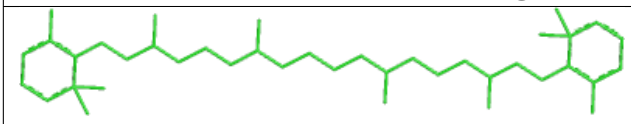


Torsions



Rings

Ligand BCR Q 4016



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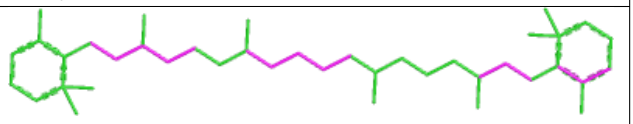
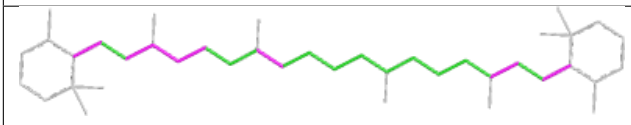
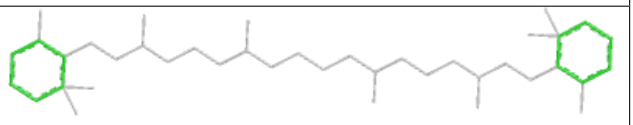


Bond angles

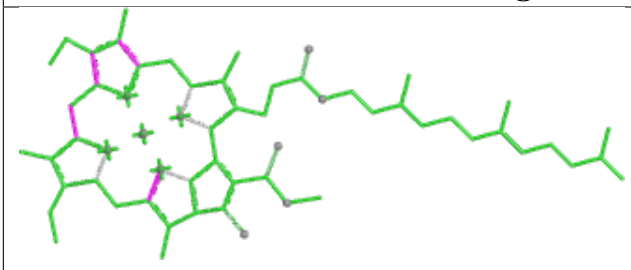


Torsions



Rings

Ligand CLA A 1124



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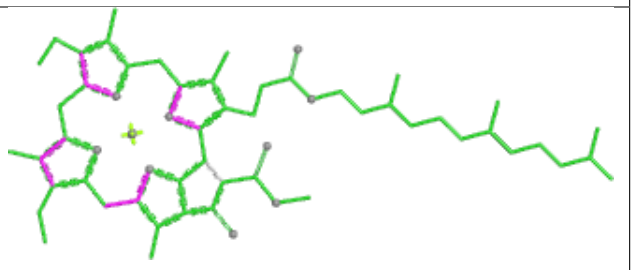
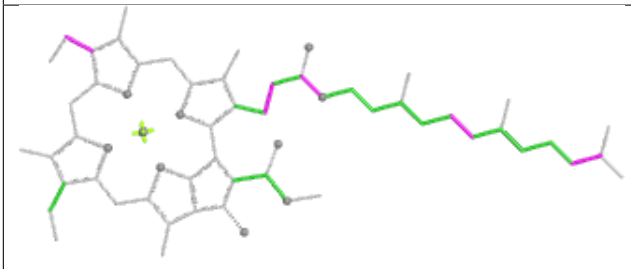


Bond angles



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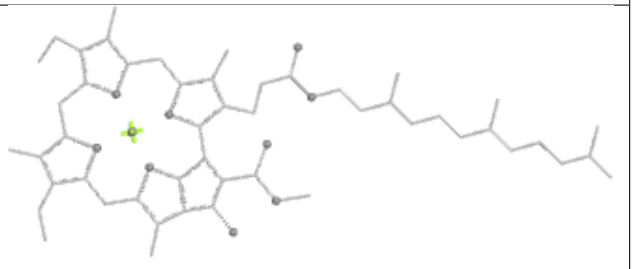
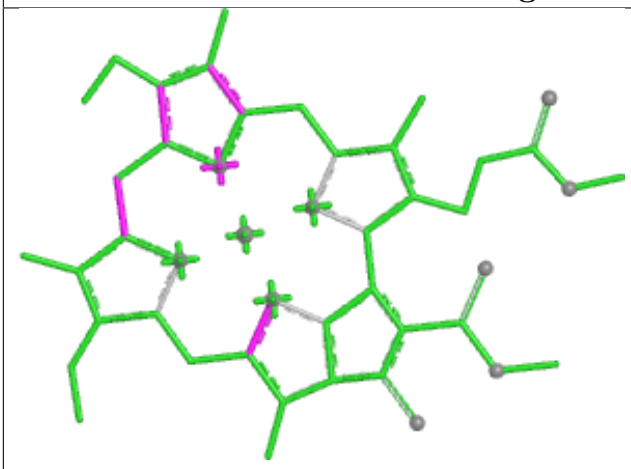


Rings

Ligand CLA W 503



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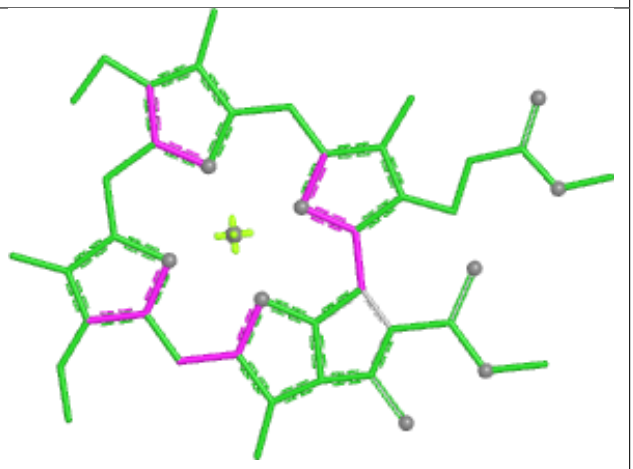
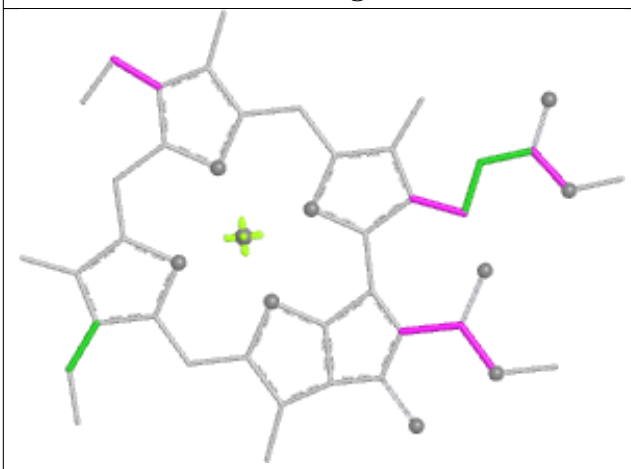


Bond angles



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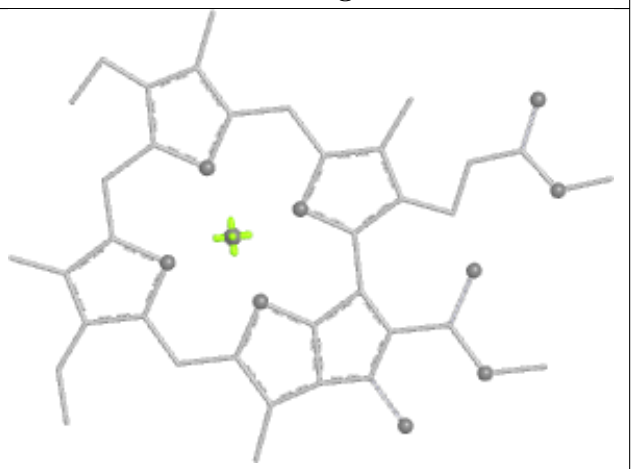
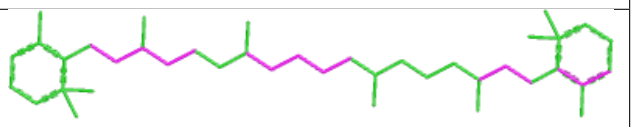


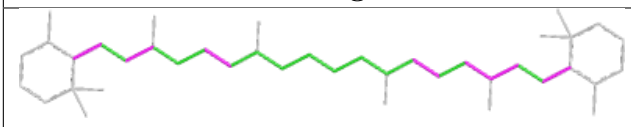
Rings

Ligand BCR G 4004

Bond lengths



Bond angles



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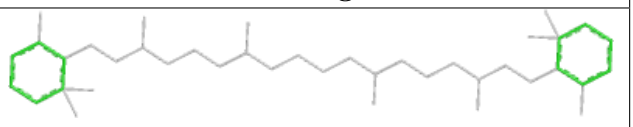
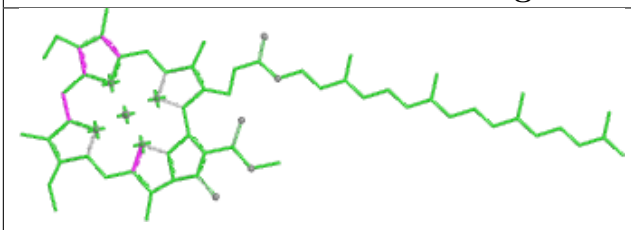


Rings

Ligand CLA U 1503



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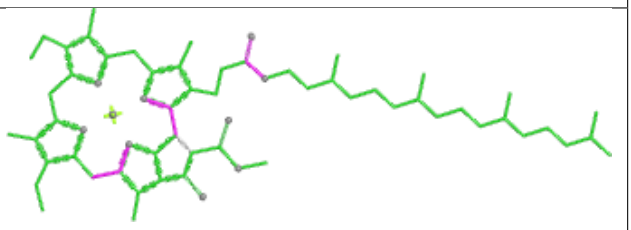
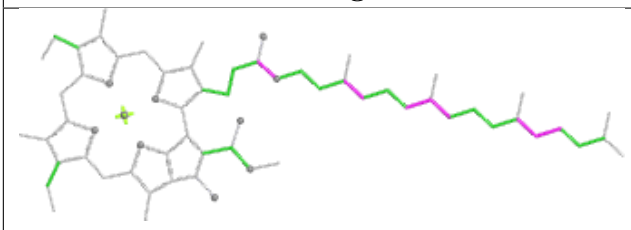
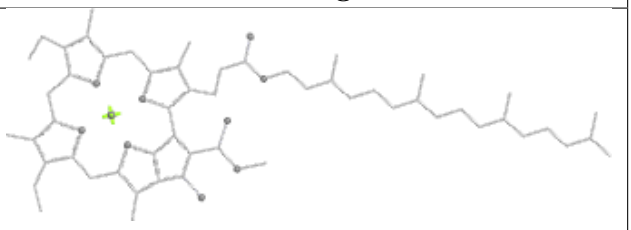


Bond angles

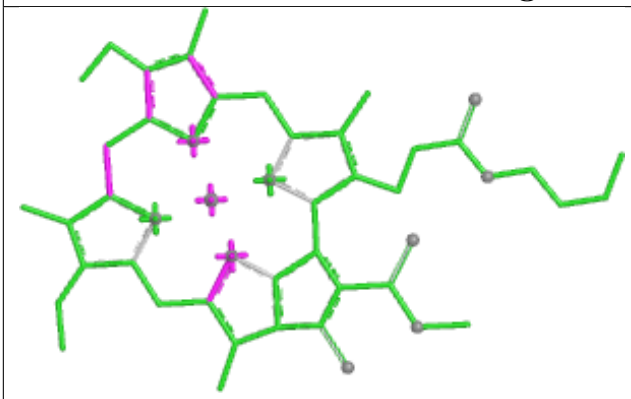


Torsions



Rings

Ligand CLA b 1227



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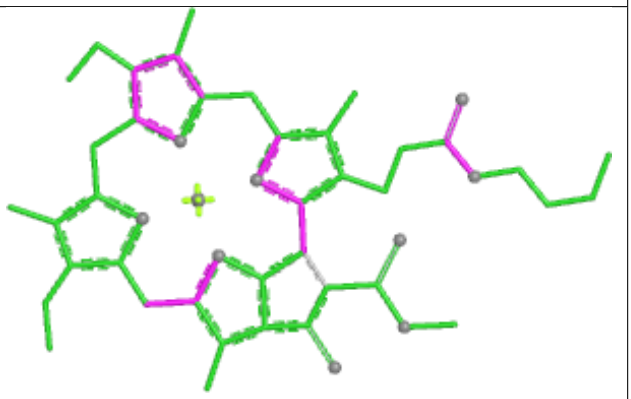
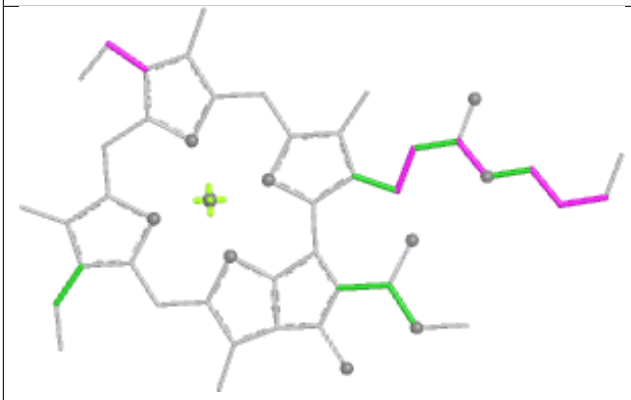
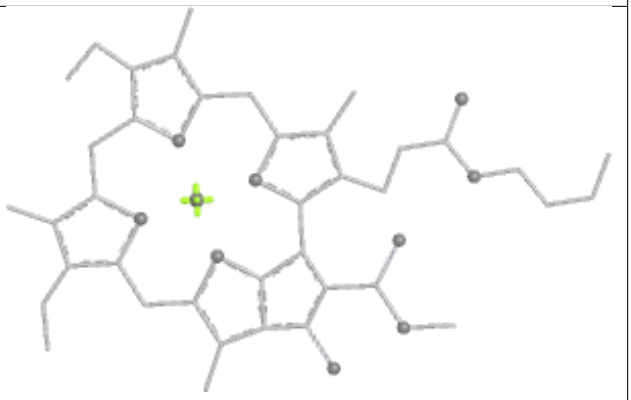


Bond angles

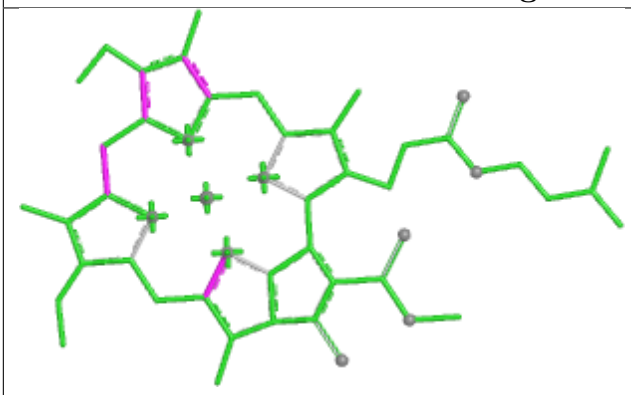


Torsions



Rings

Ligand CLA a 1107



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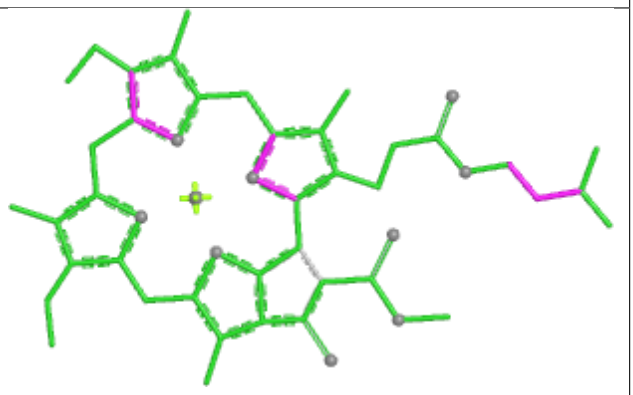
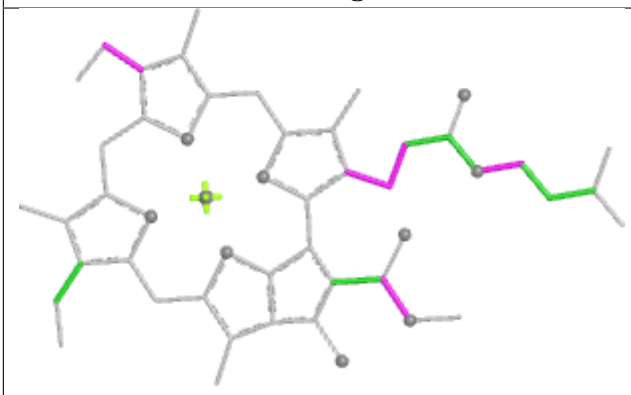


Bond angles



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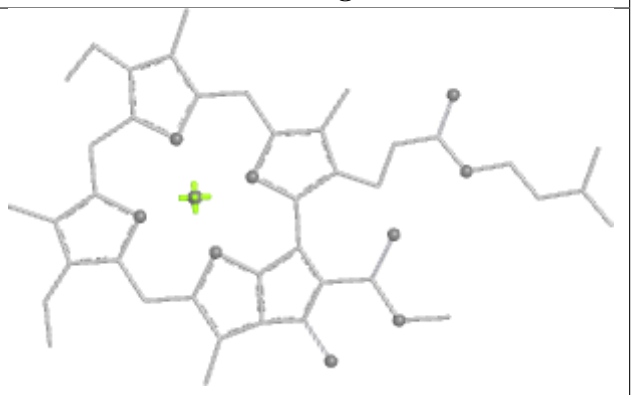
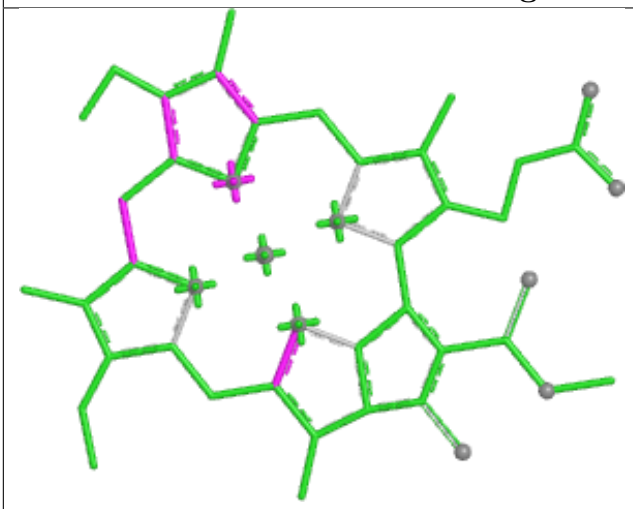


Rings

Ligand CLA a 1108



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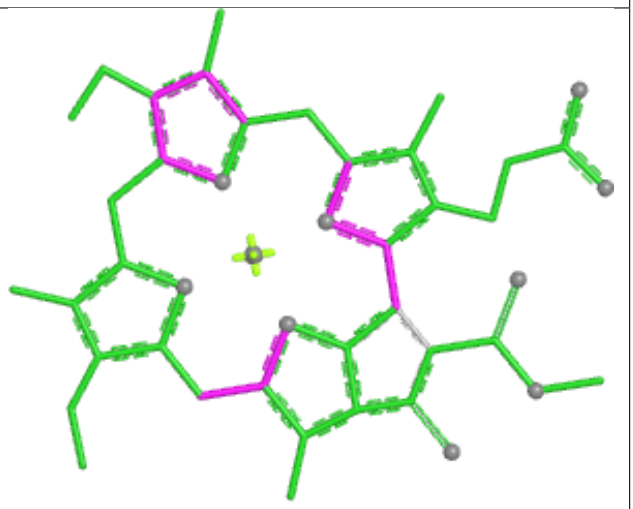
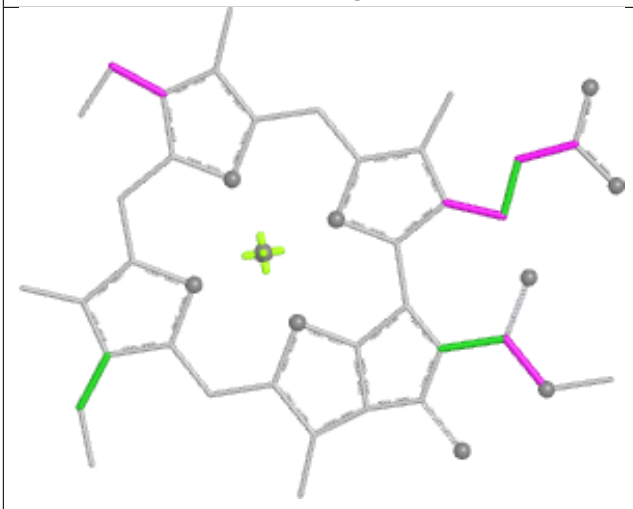


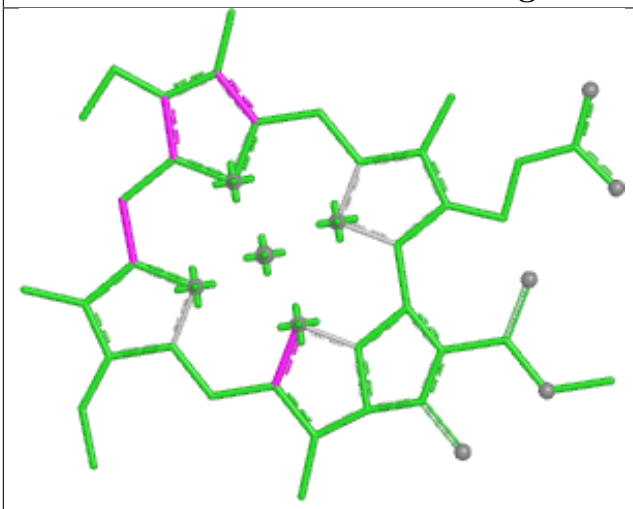
Bond angles



Torsions

Rings

Ligand CLA b 1231



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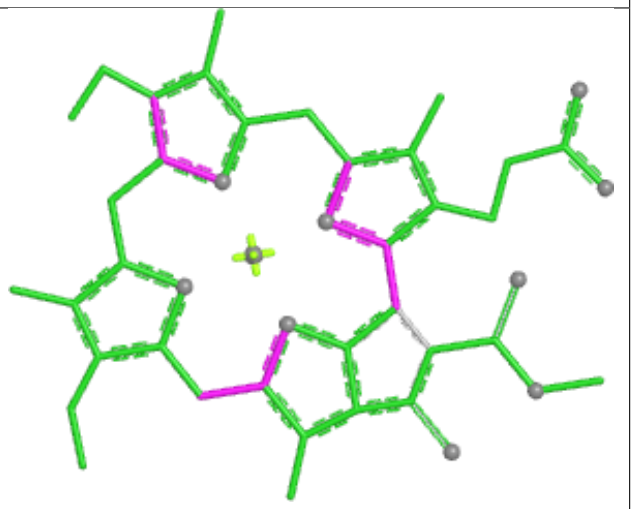
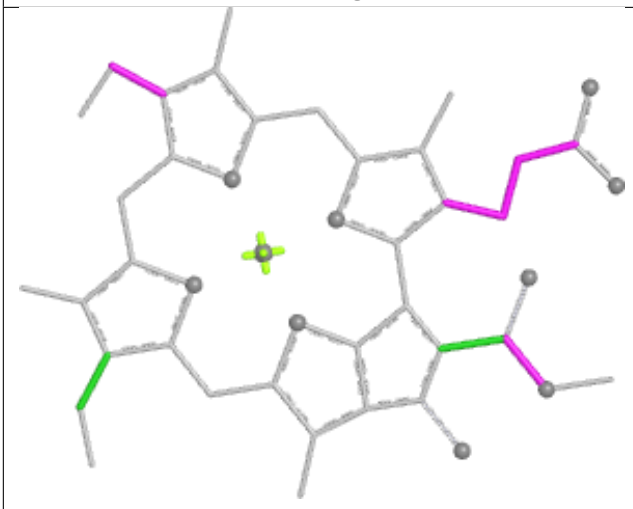


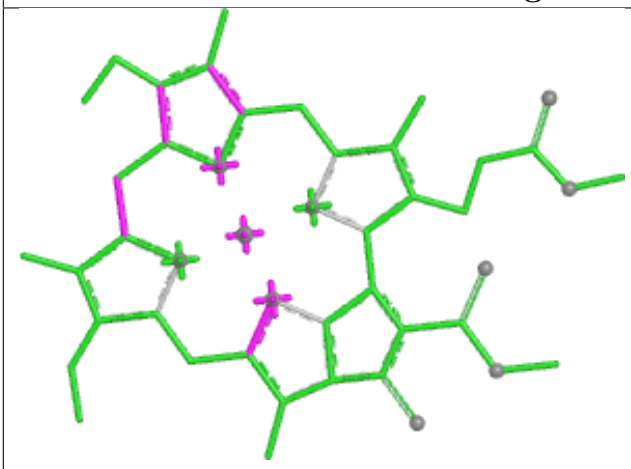
Bond angles



Torsions

Rings

Ligand CLA w 503



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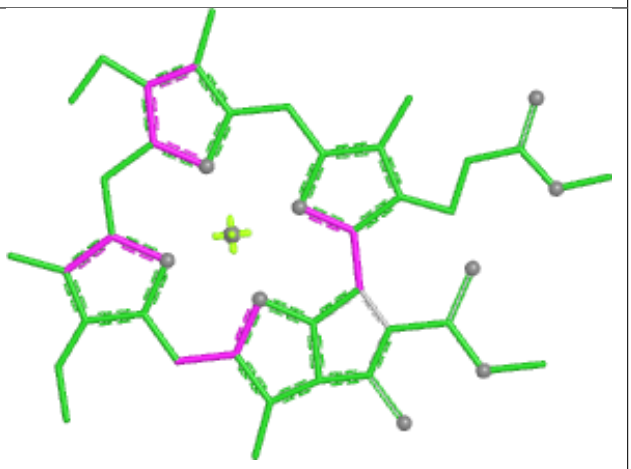
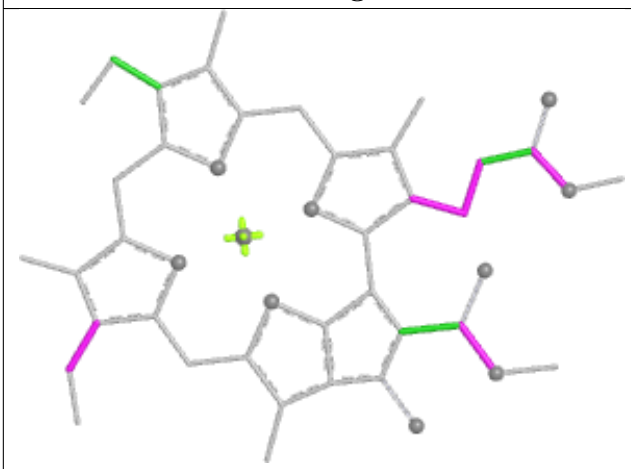


Bond angles



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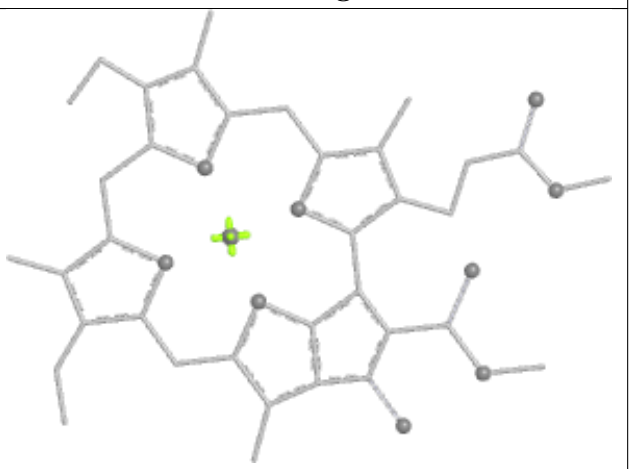
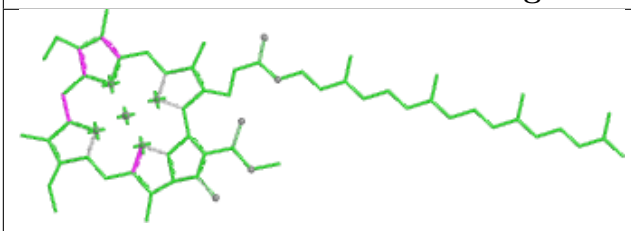
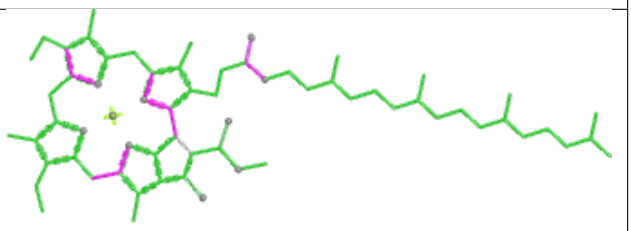


Rings

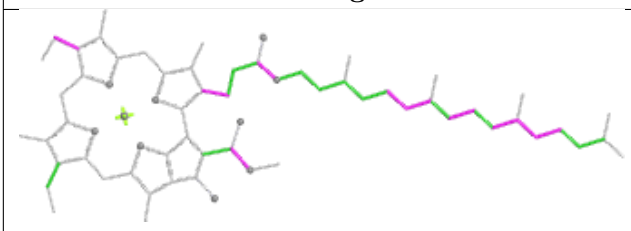
Ligand CLA Y 511



Bond lengths



Bond angles



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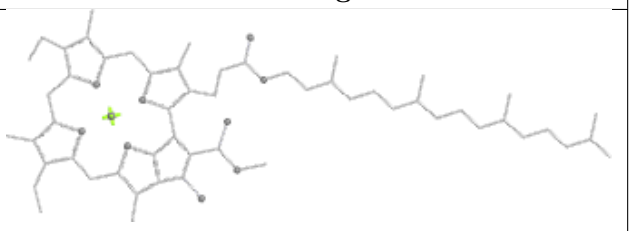
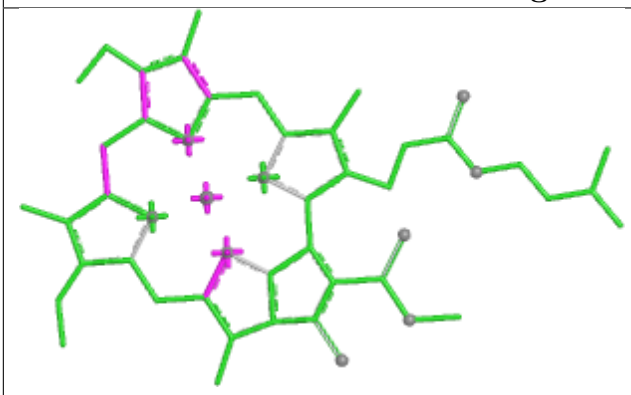
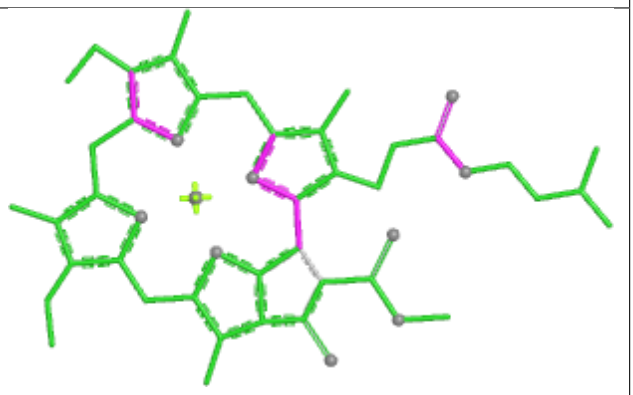


Rings

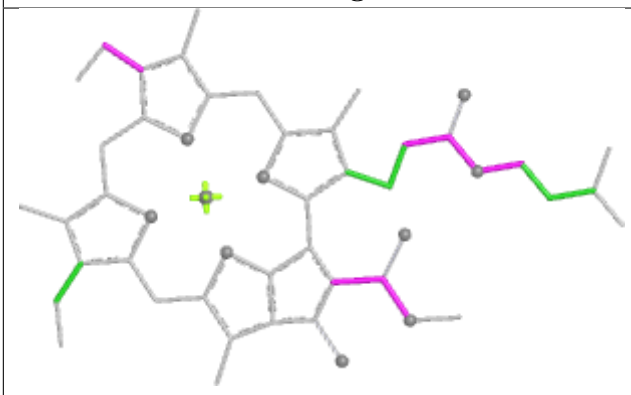
Ligand CLA t 502



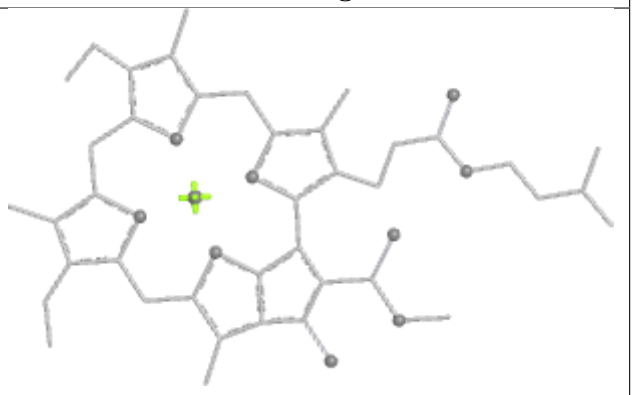
Bond lengths



Bond angles



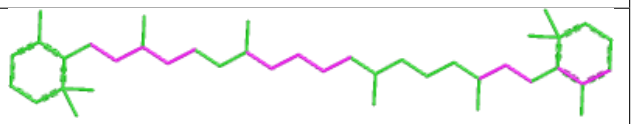
Torsions



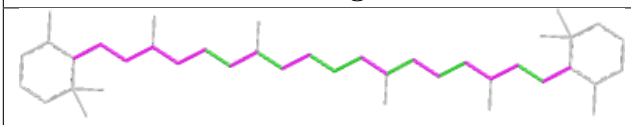
Rings

Ligand BCR r 604

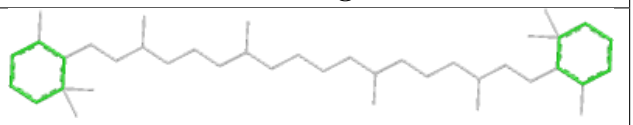
Bond lengths



Bond angles

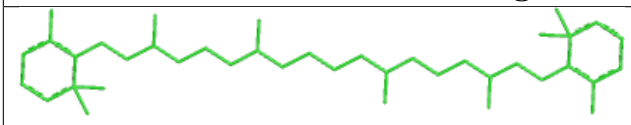


Torsions

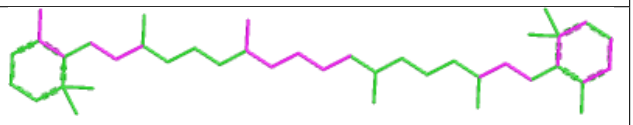


Rings

Ligand BCR A 4008

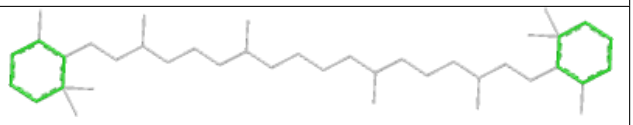


Bond lengths



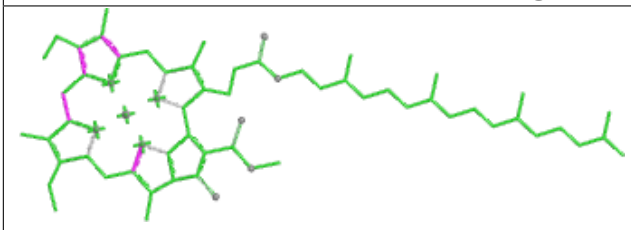
Bond angles

Torsions



Rings

Ligand CLA s 507



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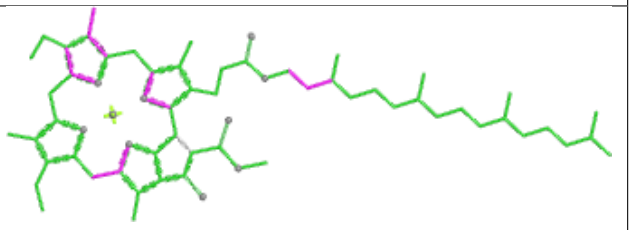
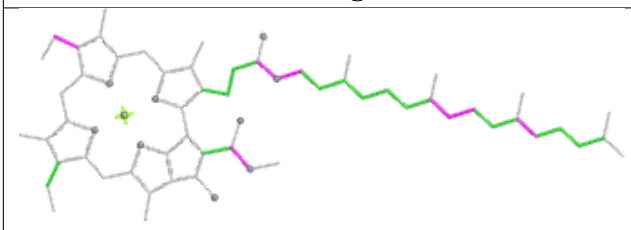
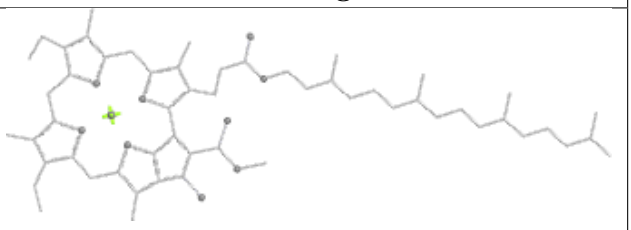


Bond angles

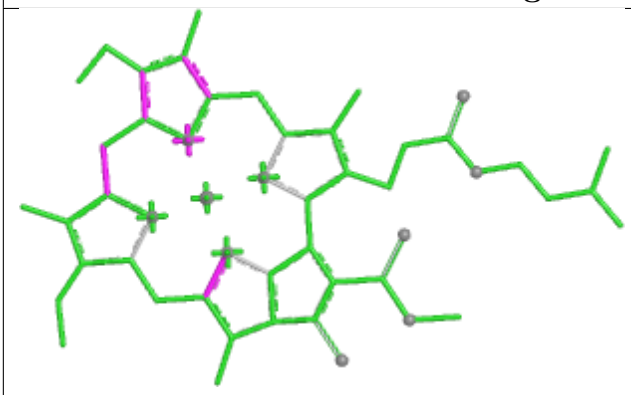


Torsions



Rings

Ligand CLA Y 514



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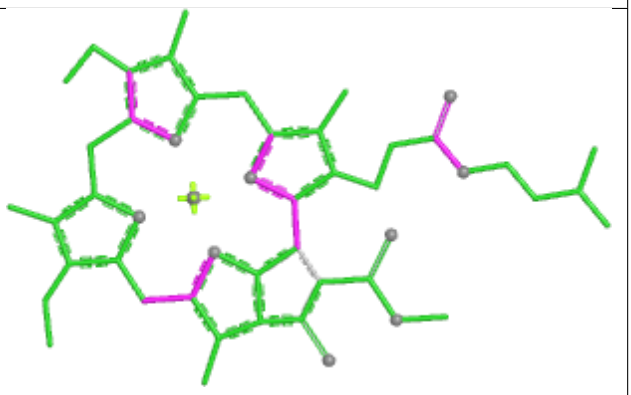
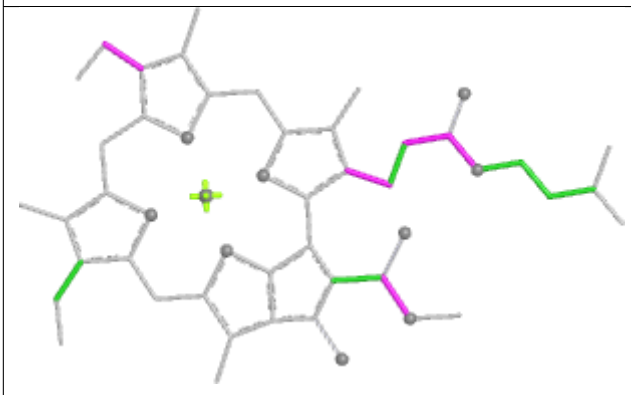
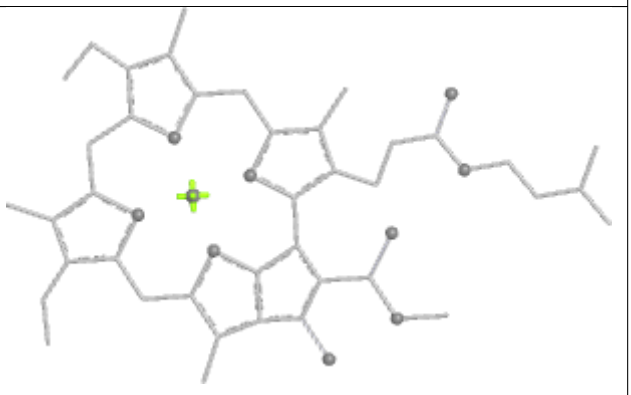


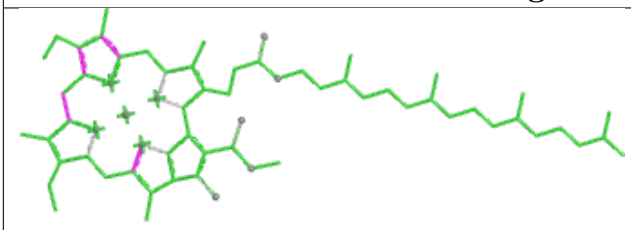
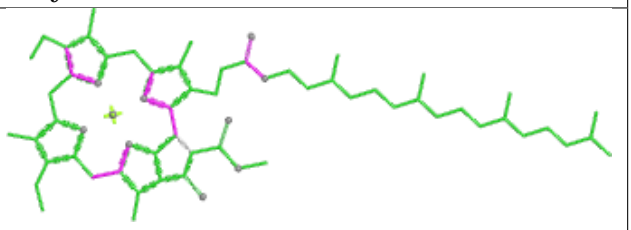
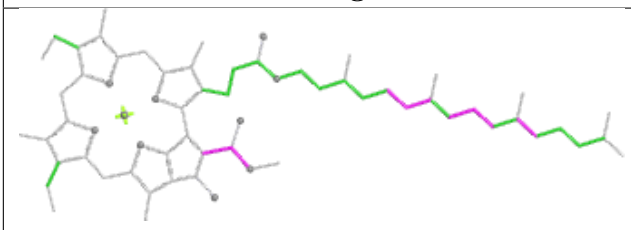
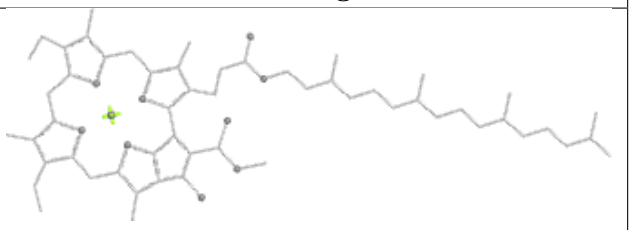
Bond angles

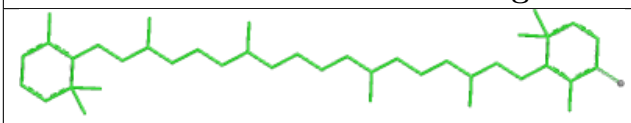
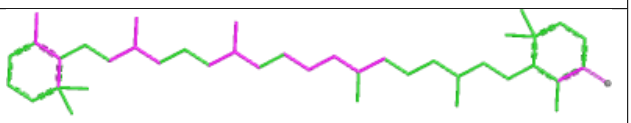
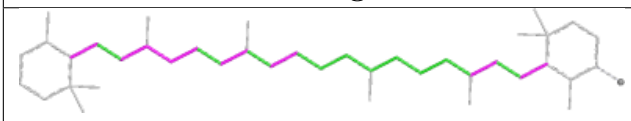
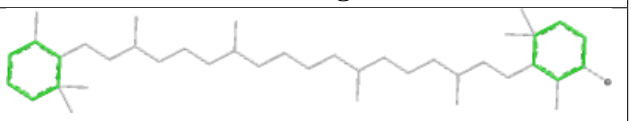


Torsions

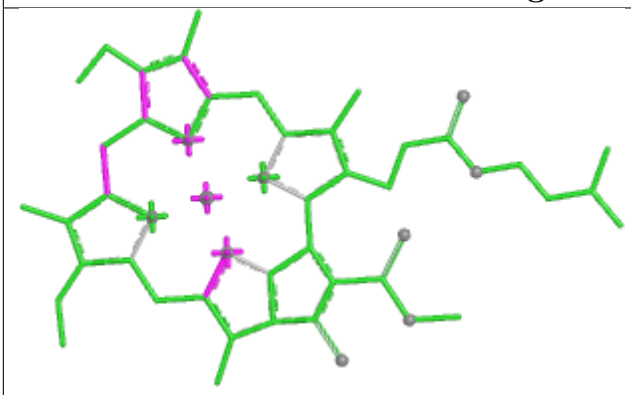


Rings

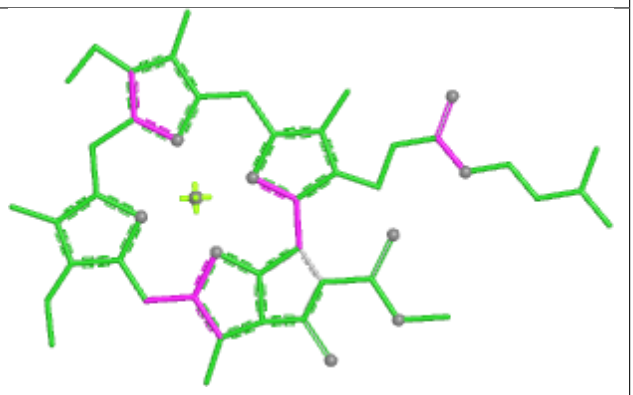
Ligand CLA y 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ECH m 4021	
	
Bond lengths	Bond angles
	
Torsions	Rings

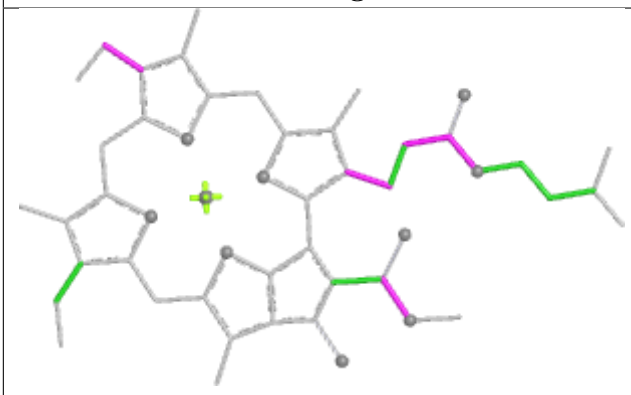
Ligand CLA n 514



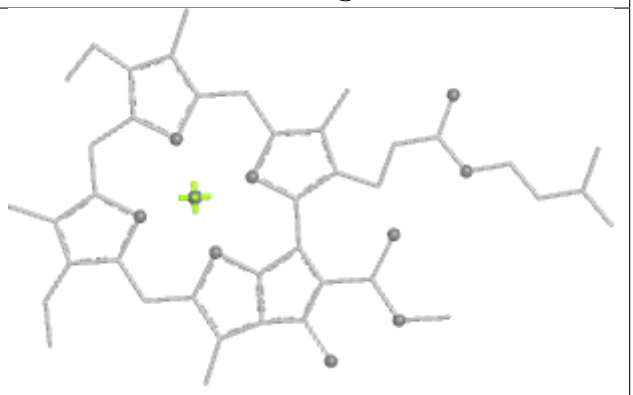
Bond lengths



Bond angles



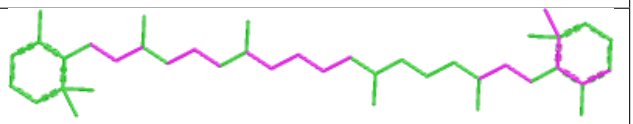
Torsions



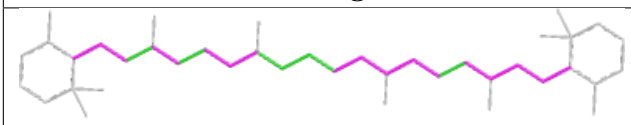
Rings

Ligand BCR B 4010

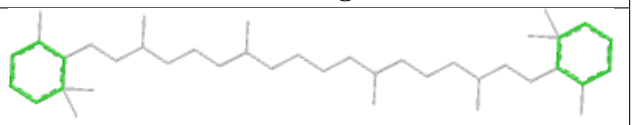
Bond lengths



Bond angles

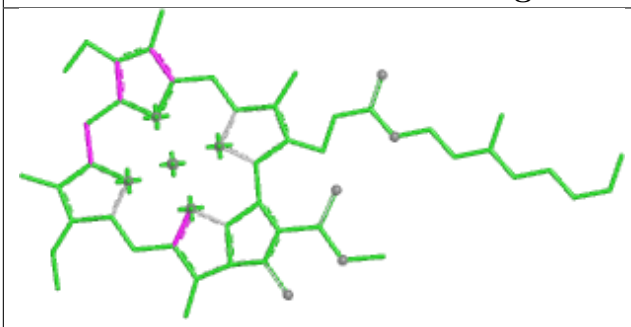


Torsions

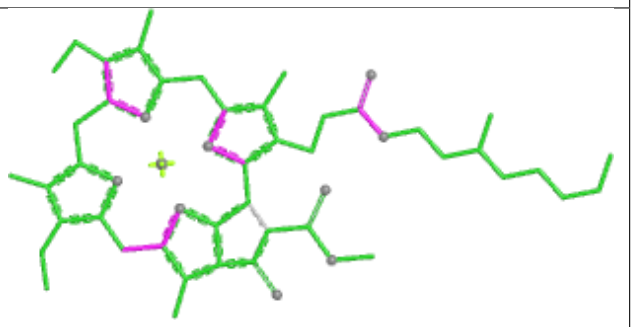


Rings

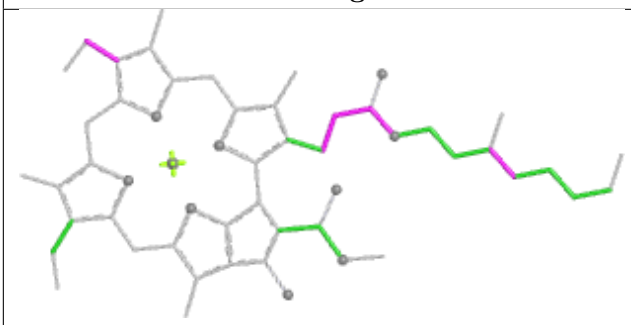
Ligand CLA H 1110



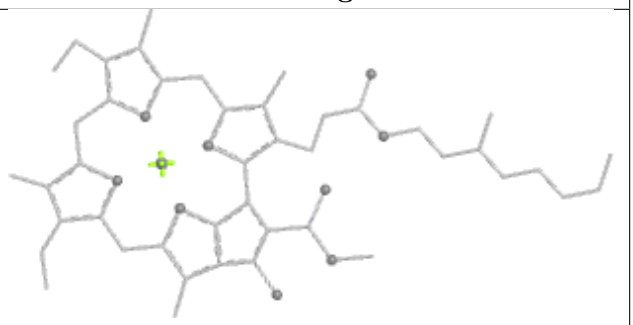
Bond lengths



Bond angles

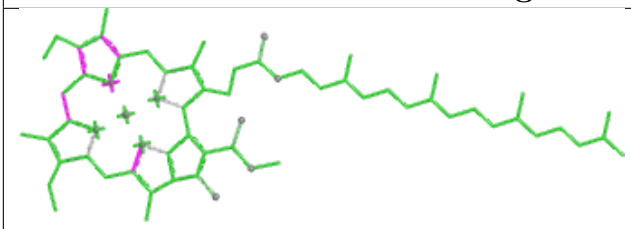


Torsions

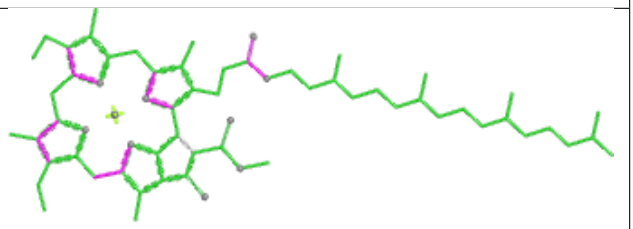


Rings

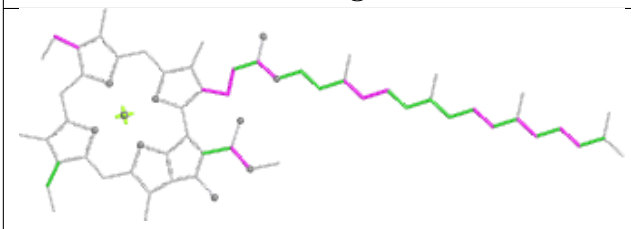
Ligand CLA B 1203



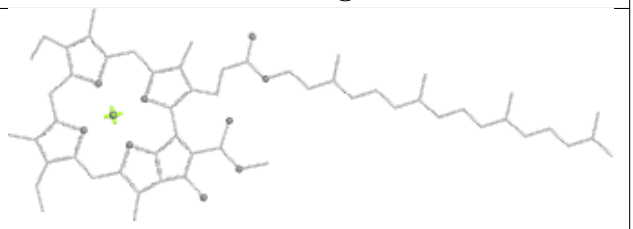
Bond lengths



Bond angles

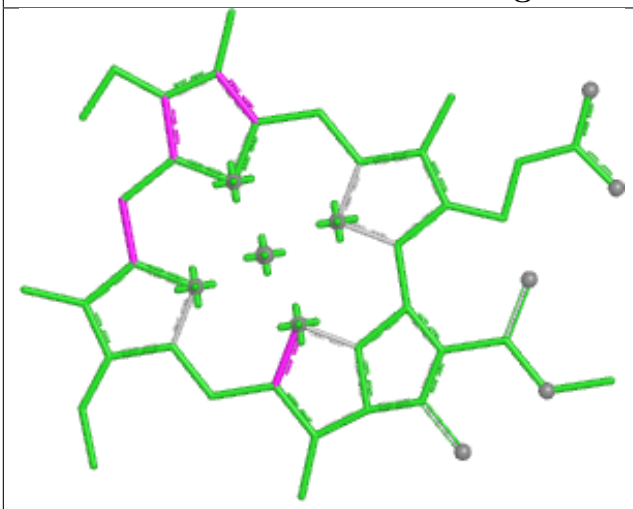


Torsions



Rings

Ligand CLA G 1230



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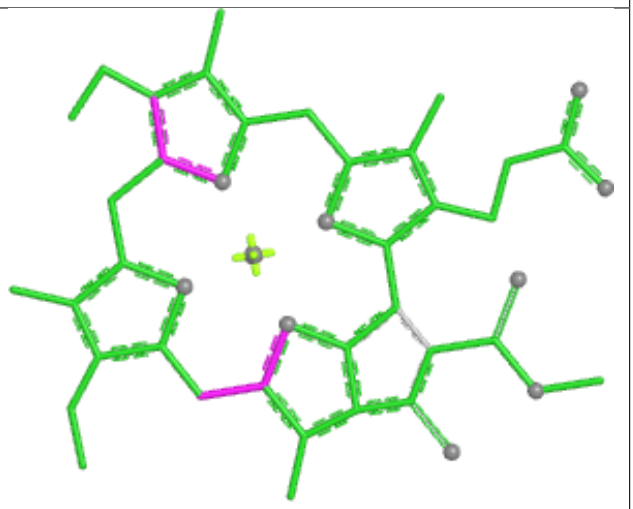
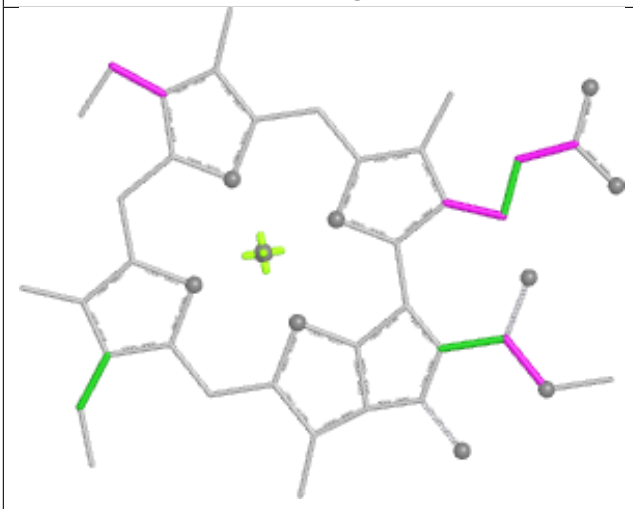


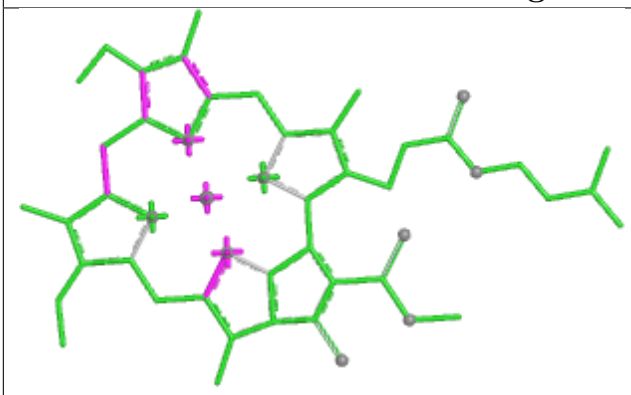
Bond angles



Torsions

Rings

Ligand CLA y 514



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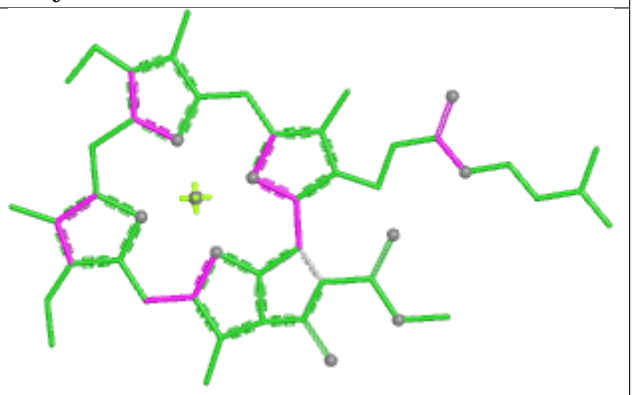
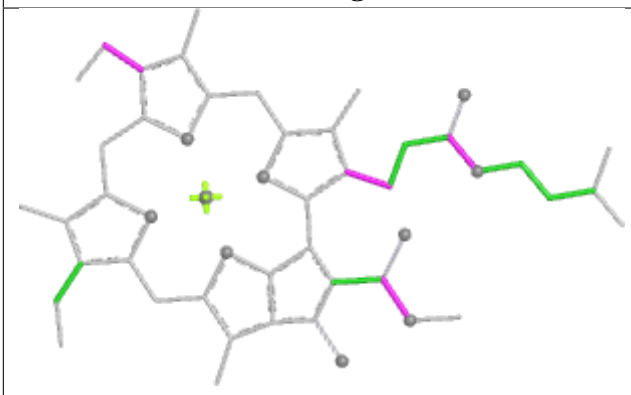


Bond angles



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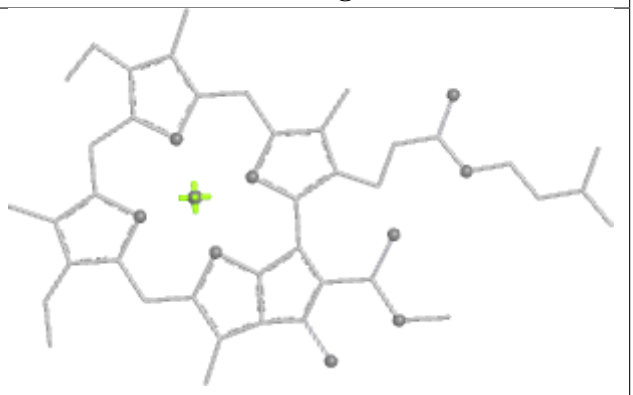
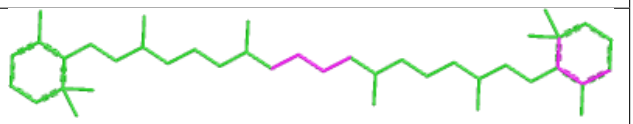


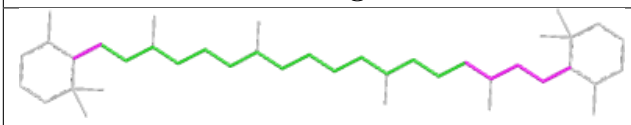
Rings

Ligand BCR Y 603

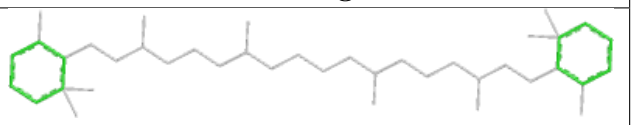
Bond lengths



Bond angles

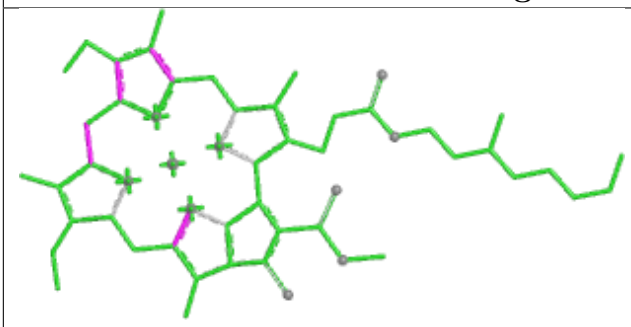


Torsions

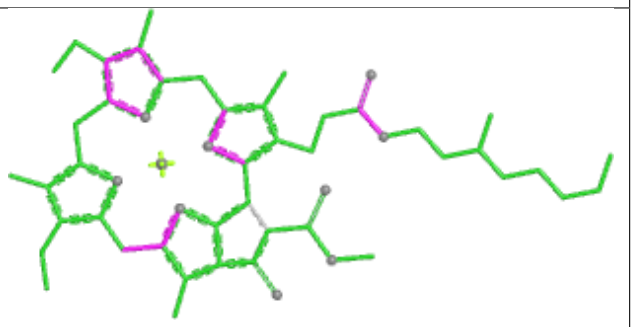


Rings

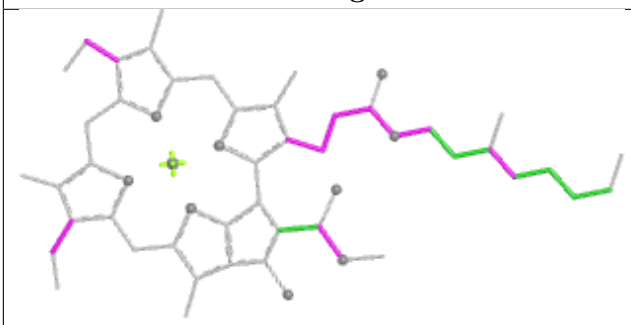
Ligand CLA G 1220



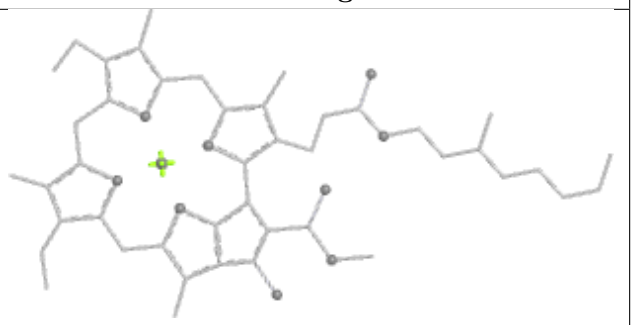
Bond lengths



Bond angles

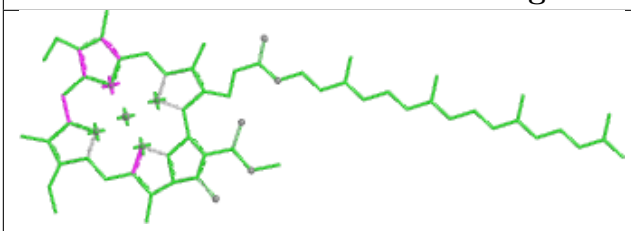


Torsions

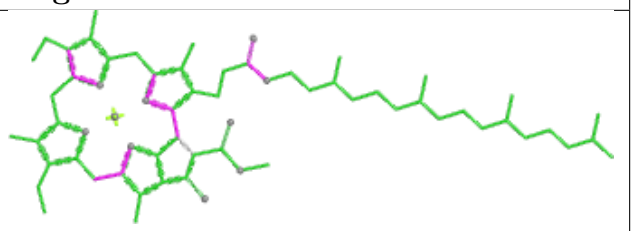


Rings

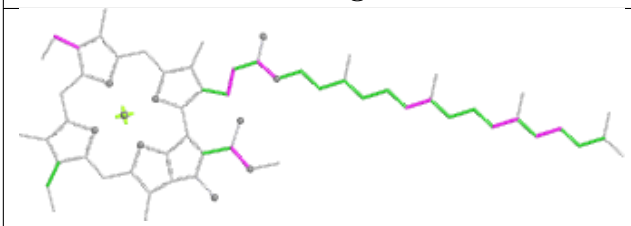
Ligand CLA g 510



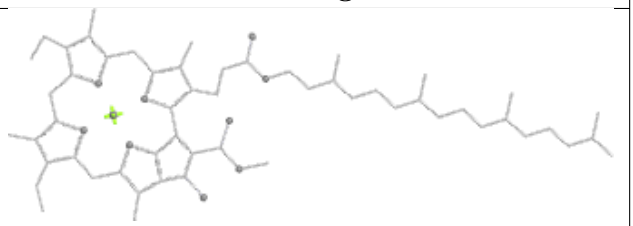
Bond lengths



Bond angles

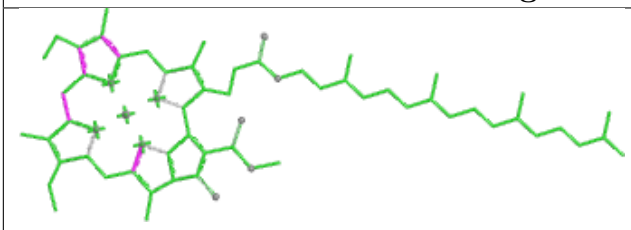


Torsions

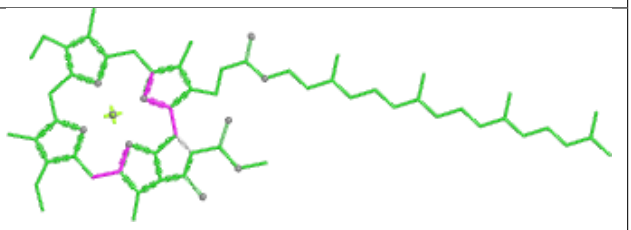


Rings

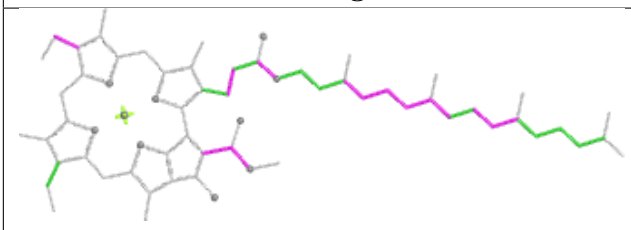
Ligand CLA a 1106



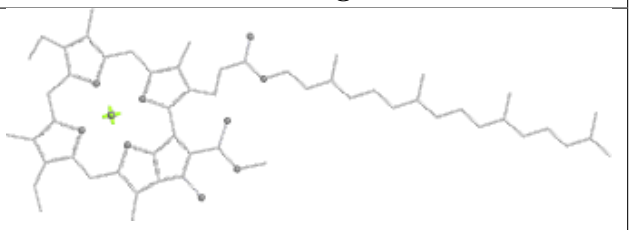
Bond lengths



Bond angles

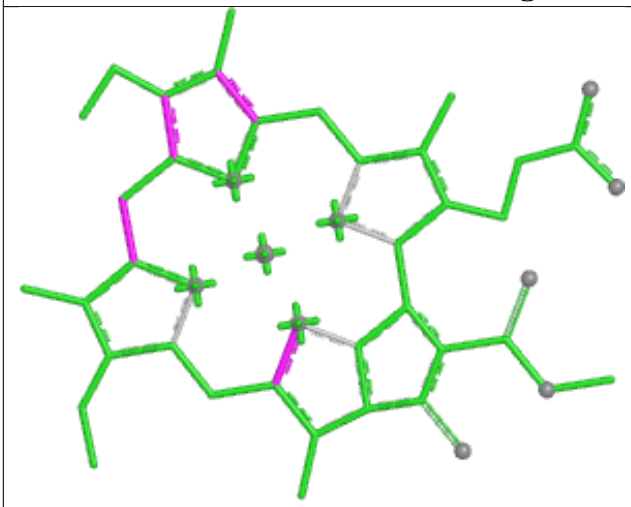


Torsions

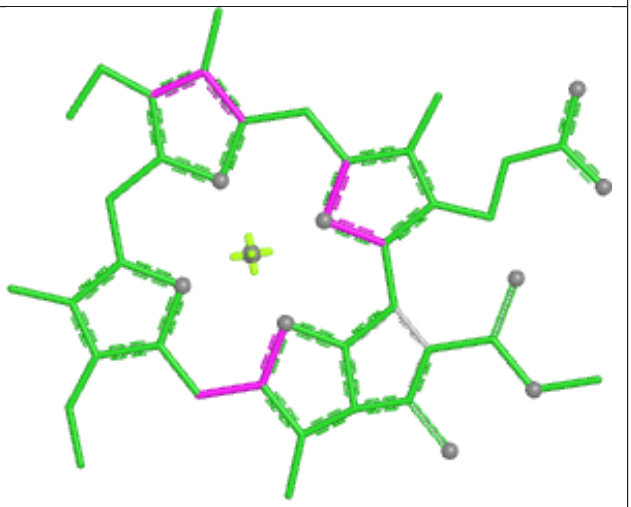


Rings

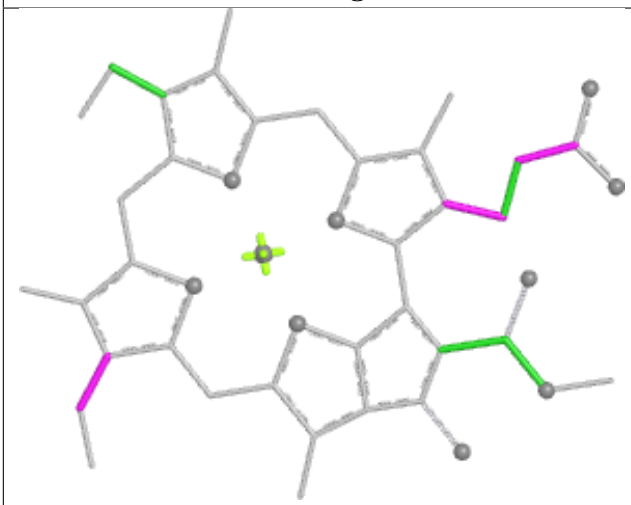
Ligand CLA k 4003



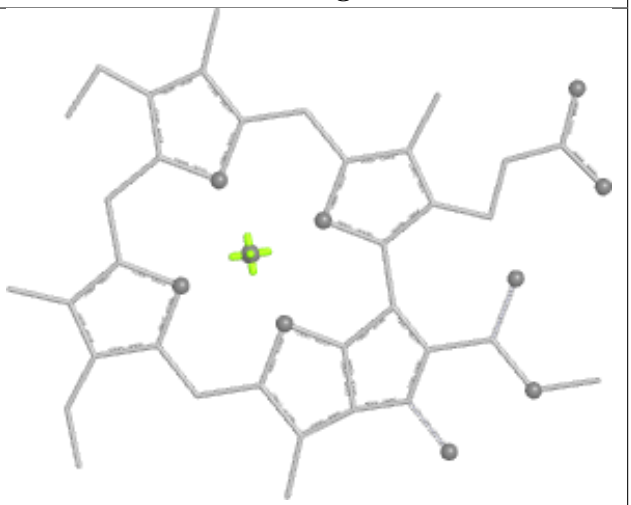
Bond lengths



Bond angles

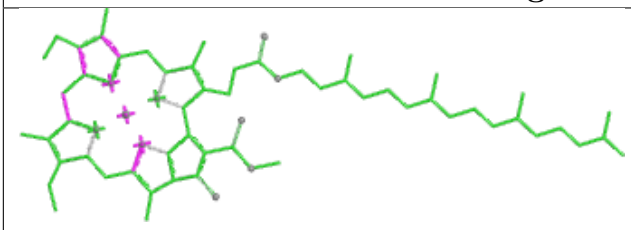


Torsions



Rings

Ligand CLA h 511



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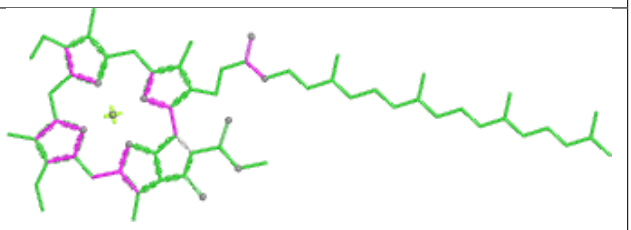
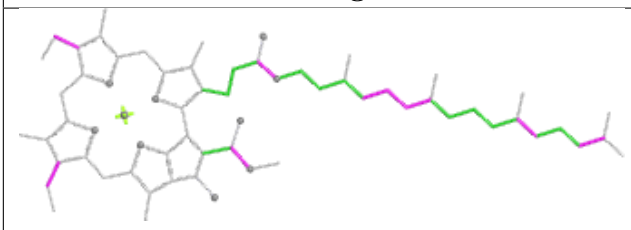
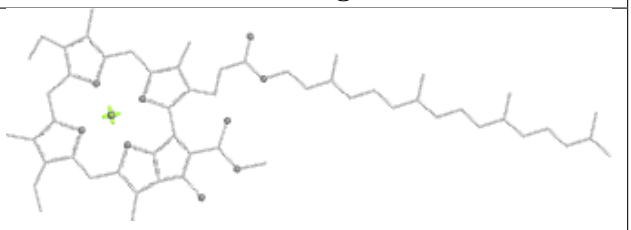


Bond angles

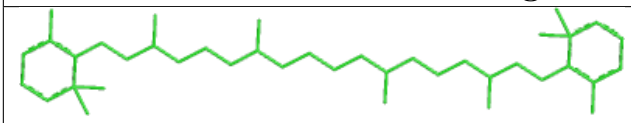


Torsions



Rings

Ligand BCR X 603



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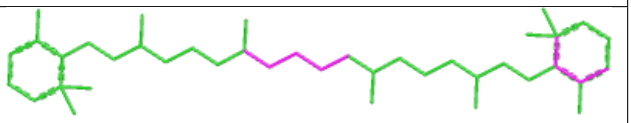
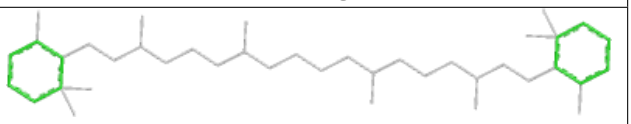


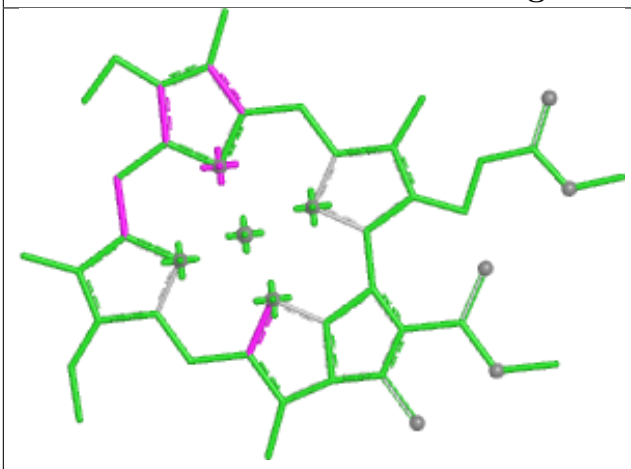
Bond angles

Torsions

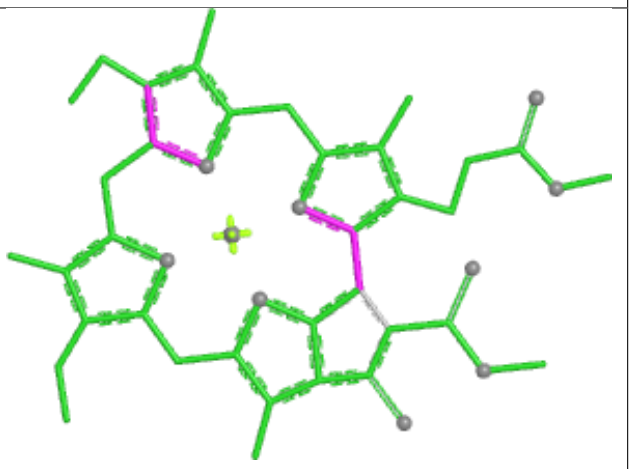


Rings

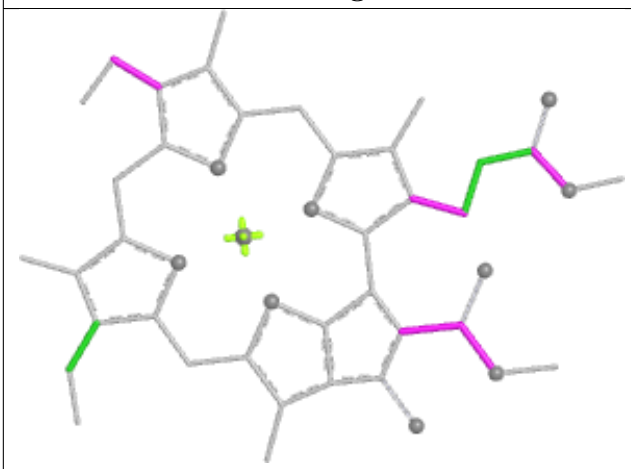
Ligand CLA x 513



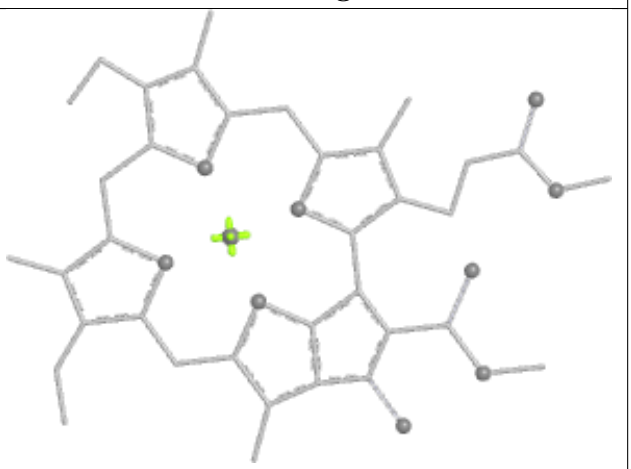
Bond lengths



Bond angles

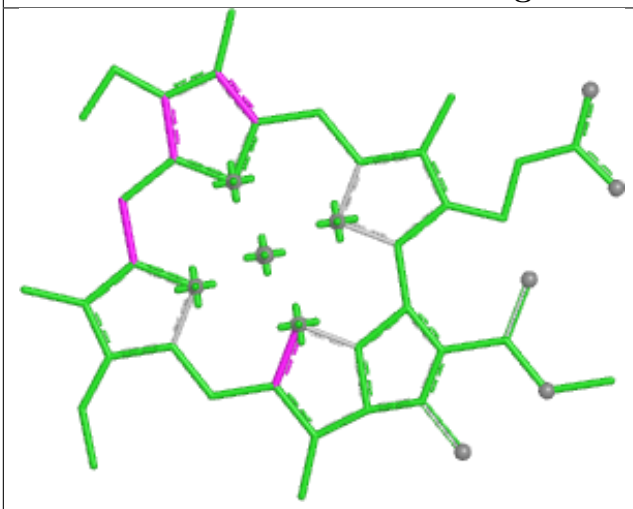


Torsions



Rings

Ligand CLA H 1134



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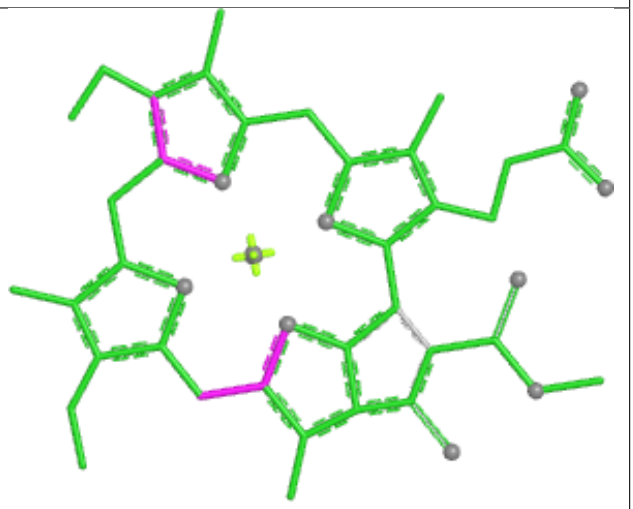
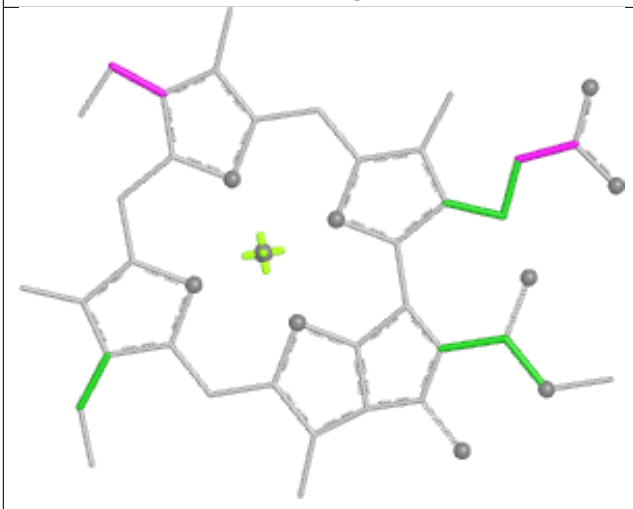


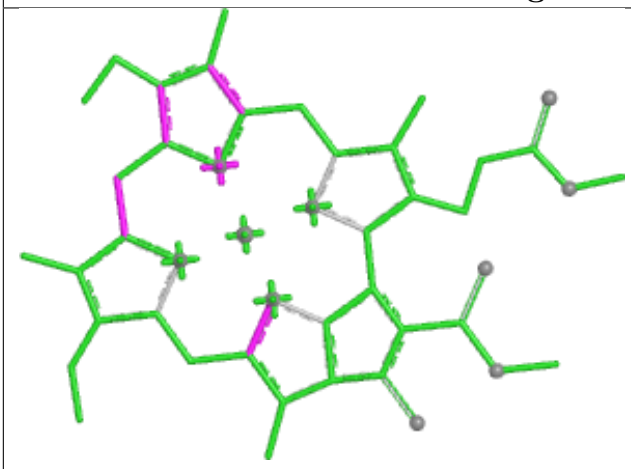
Bond angles



Torsions

Rings

Ligand CLA h 501



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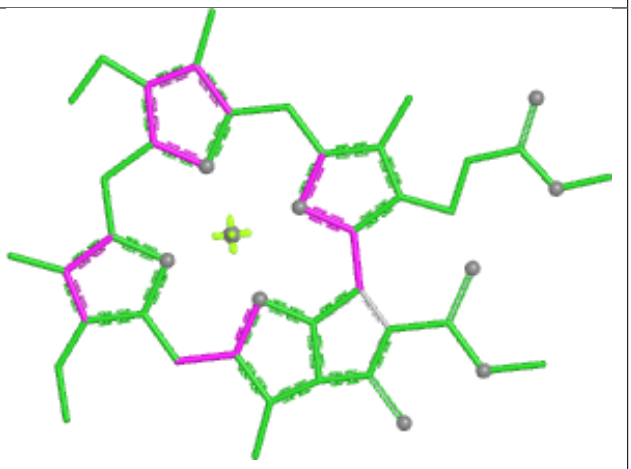
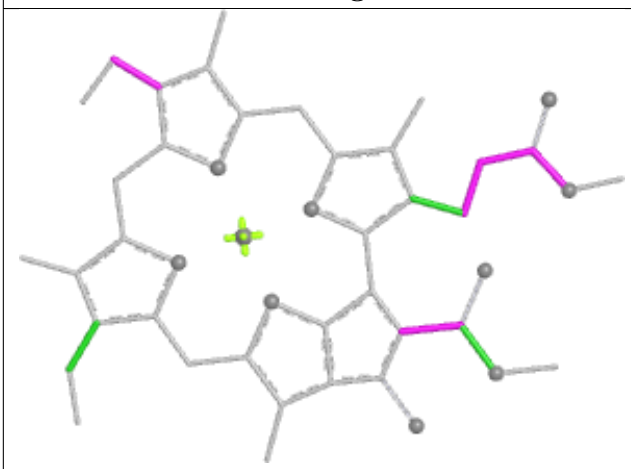
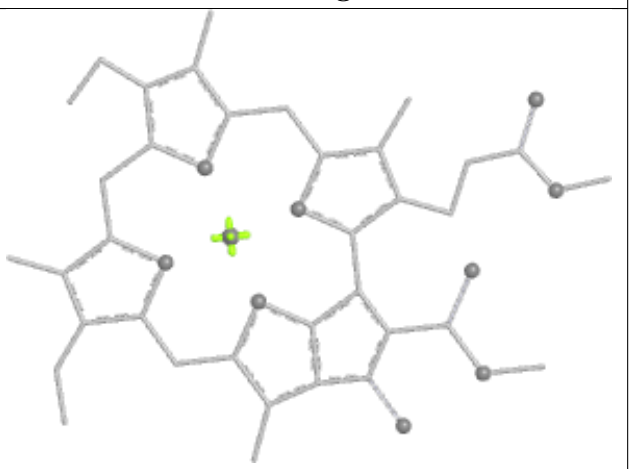


Bond angles



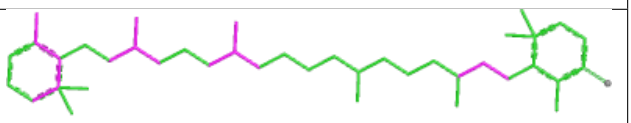
Torsions



Rings

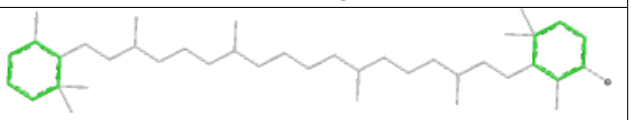
Ligand ECH b 4006

Bond lengths



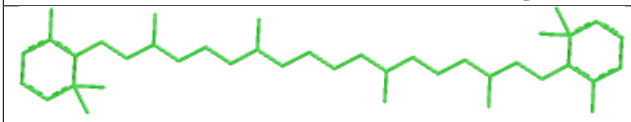
Bond angles

Torsions



Rings

Ligand BCR a 4003



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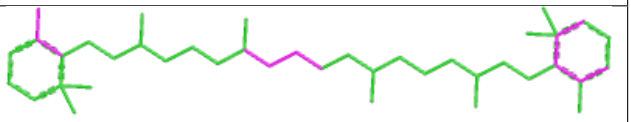
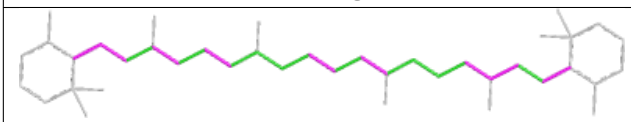


Bond angles



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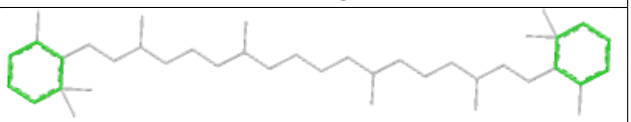
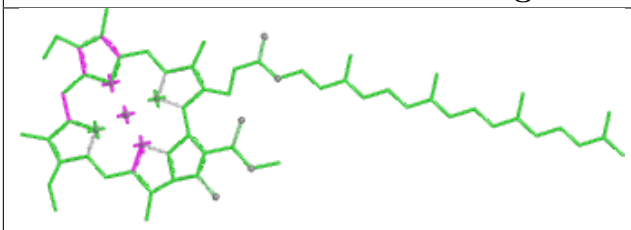
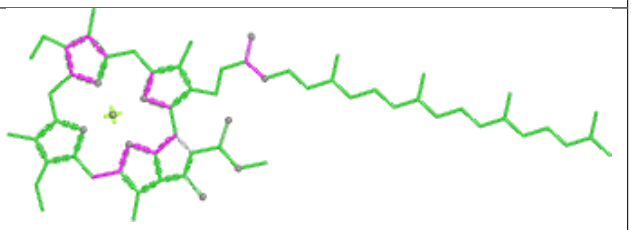
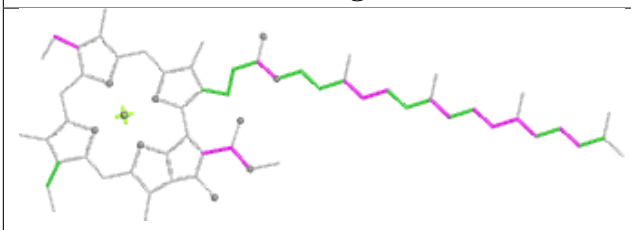
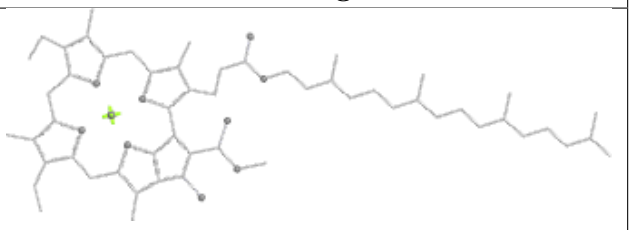
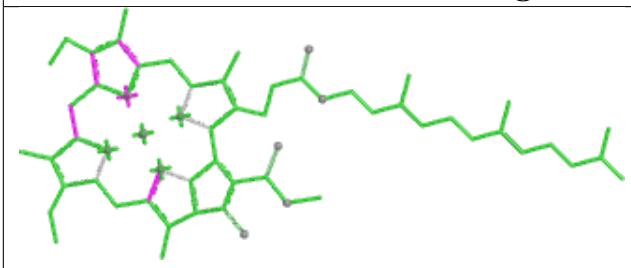
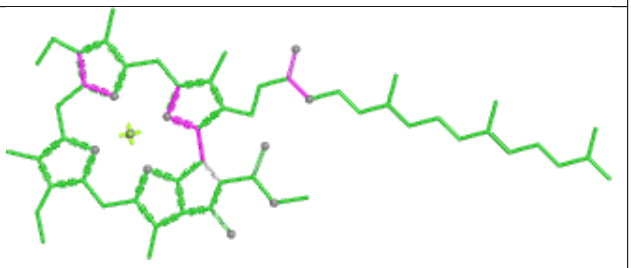
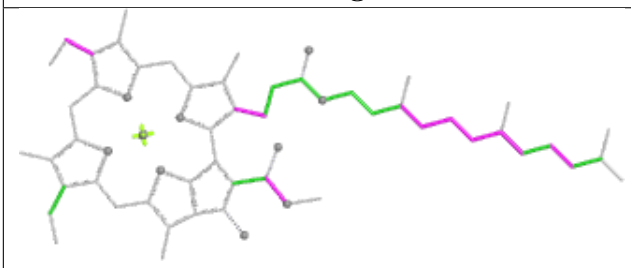
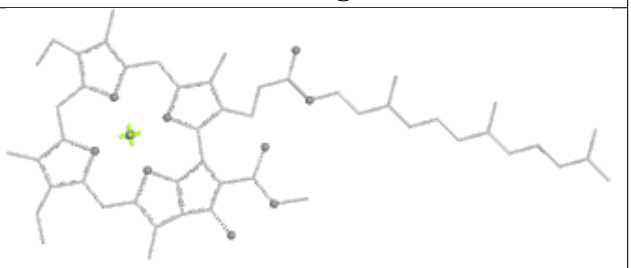
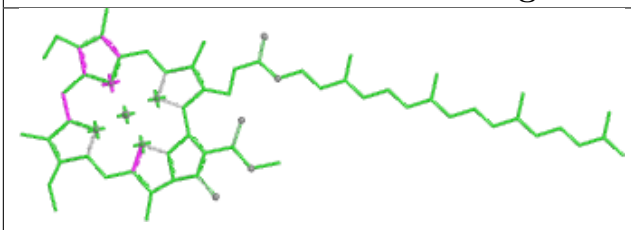


Rings

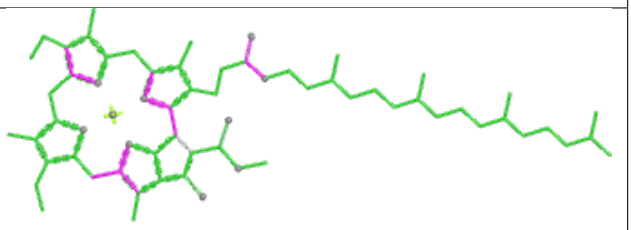
Ligand CLA H 1104	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1139	
	
Bond lengths	Bond angles
	
Torsions	Rings

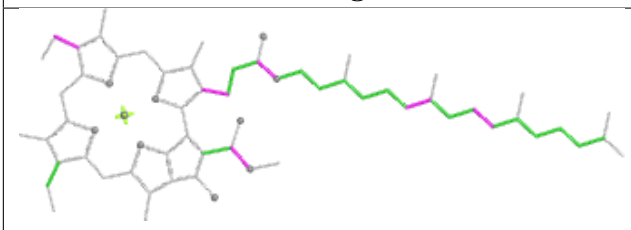
Ligand CLA W 511



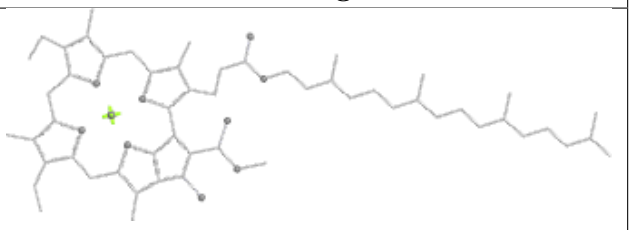
Bond lengths



Bond angles

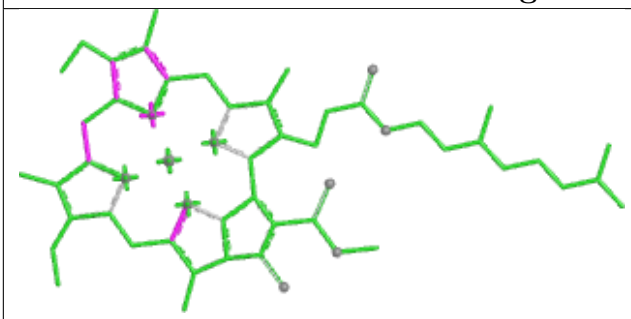


Torsions



Rings

Ligand CLA a 1139



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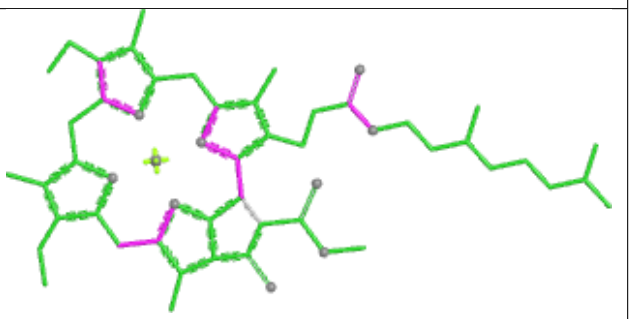
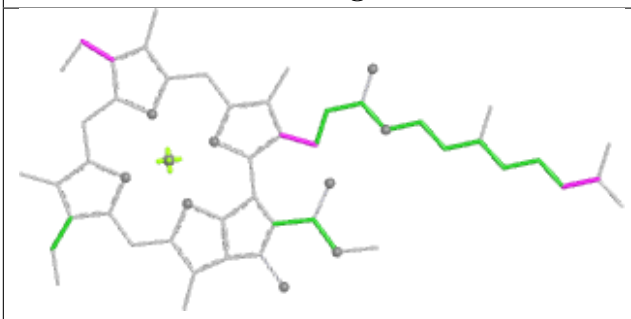


Bond angles



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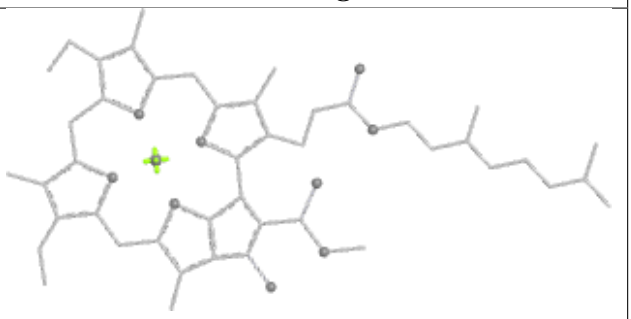
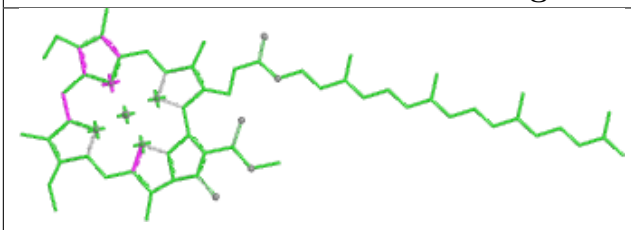
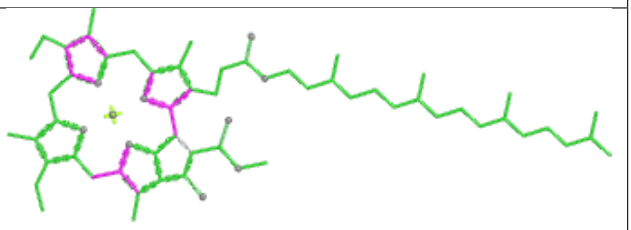


Rings

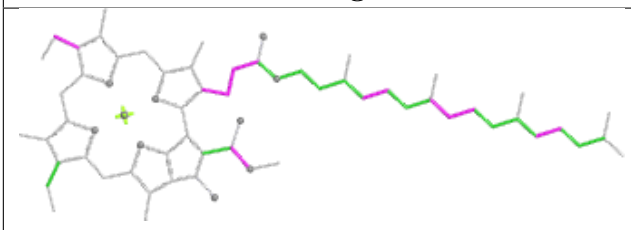
Ligand CLA s 505



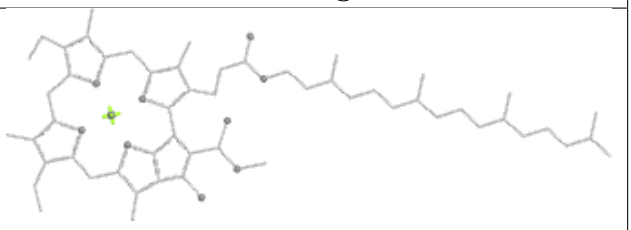
Bond lengths



Bond angles

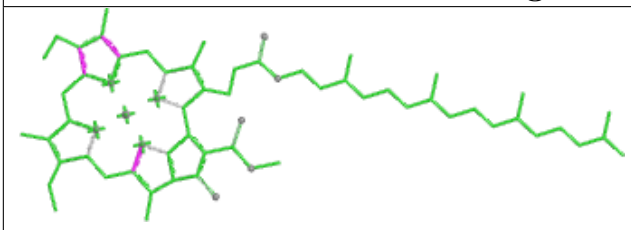


Torsions

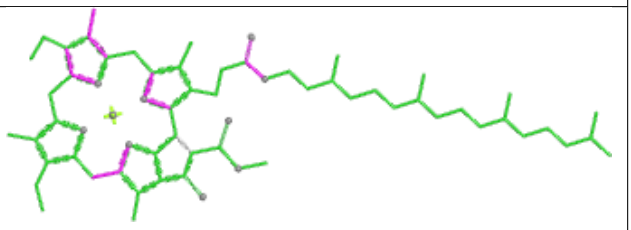


Rings

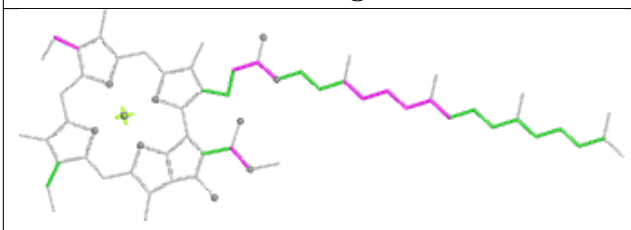
Ligand CLA Z 507



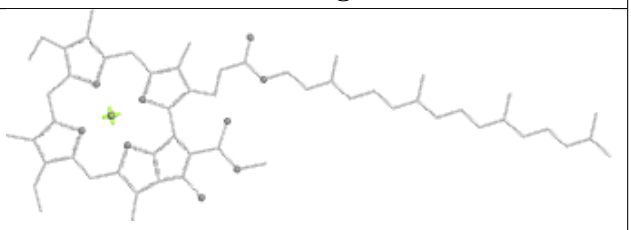
Bond lengths



Bond angles

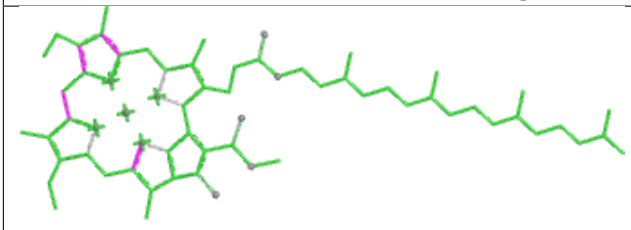


Torsions

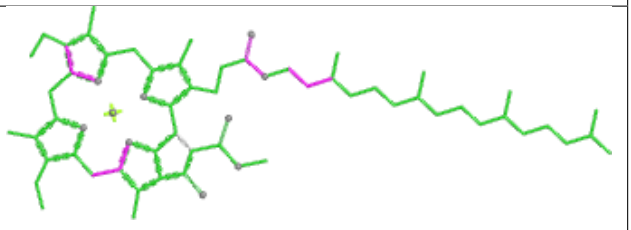


Rings

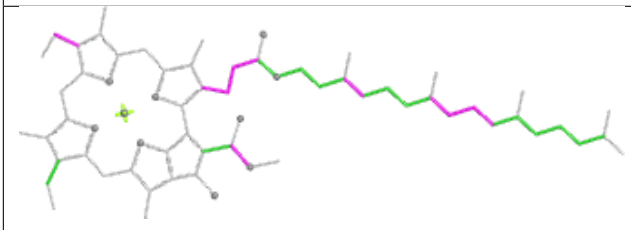
Ligand CLA A 1138



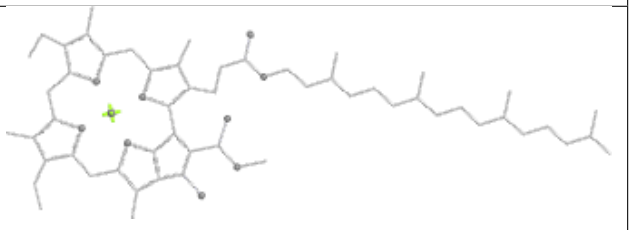
Bond lengths



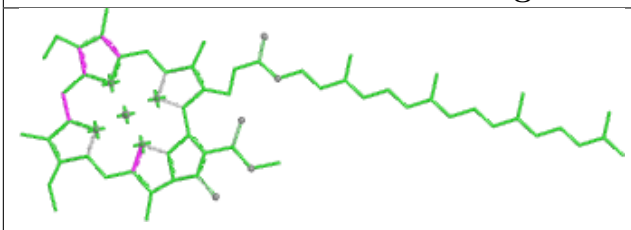
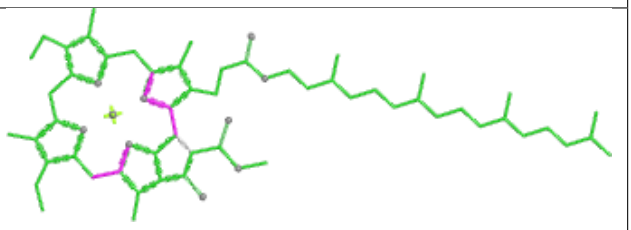
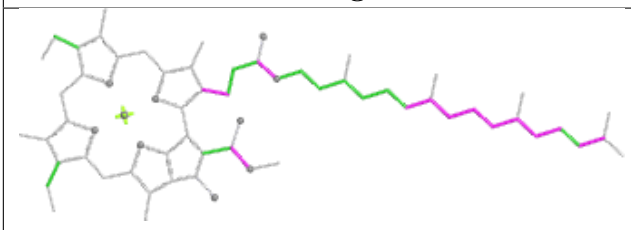
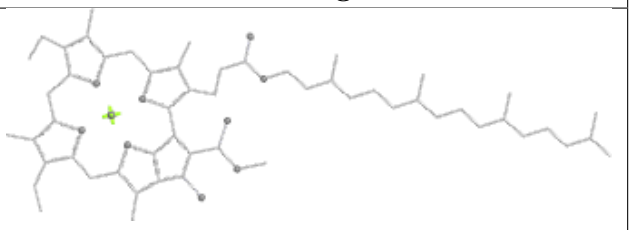
Bond angles

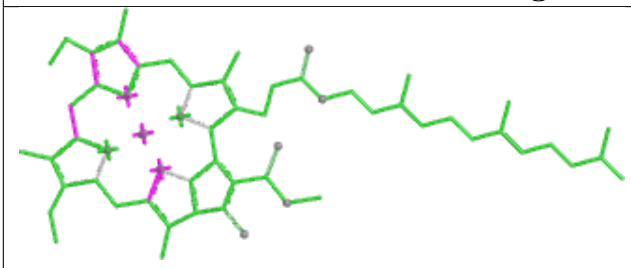
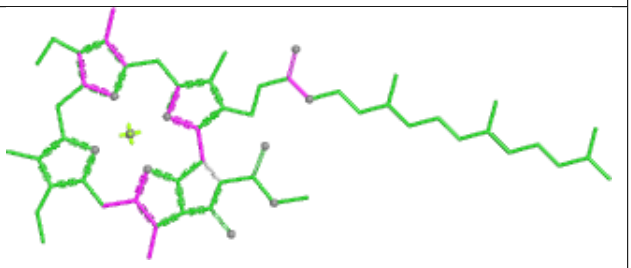
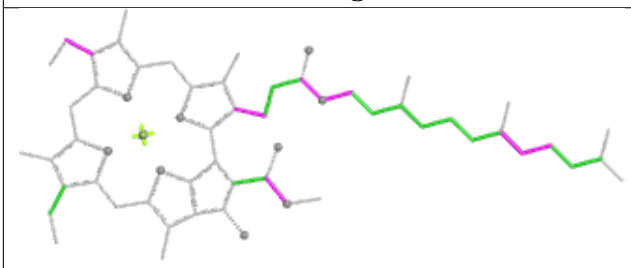
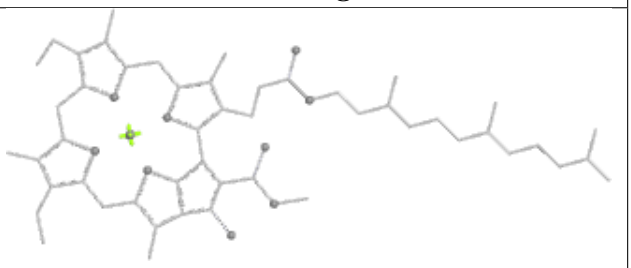


Torsions

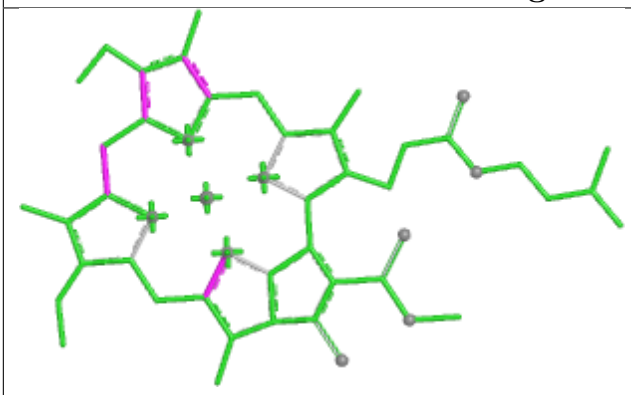


Rings

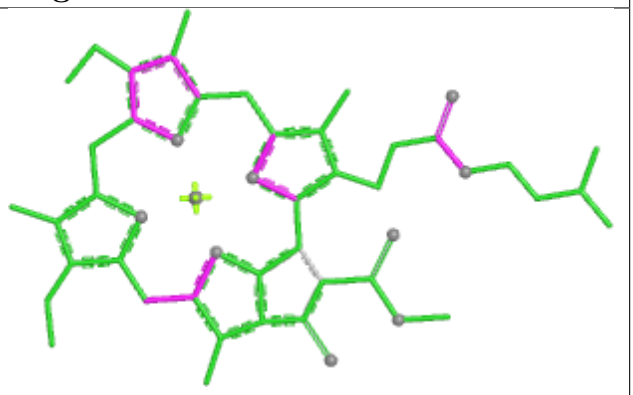
Ligand CLA G 1221	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

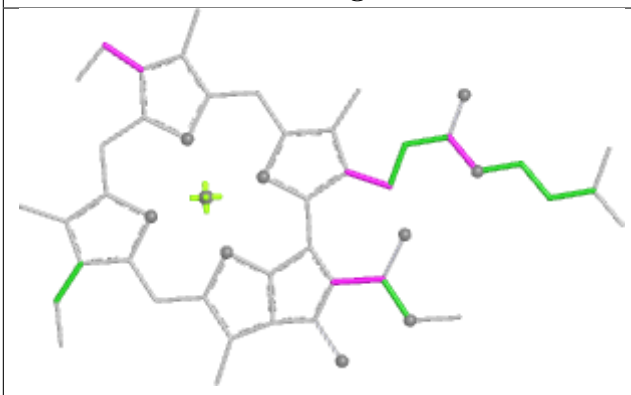
Ligand CLA g 501



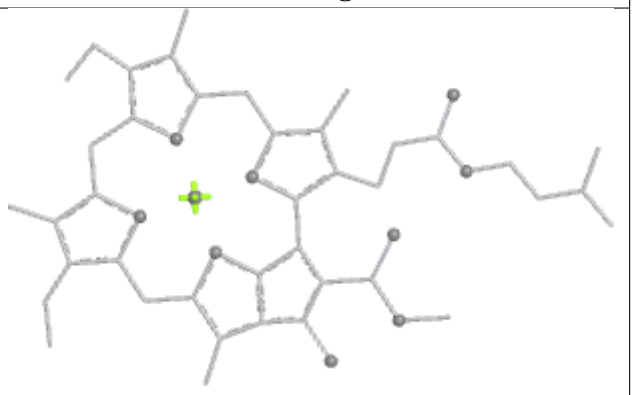
Bond lengths



Bond angles



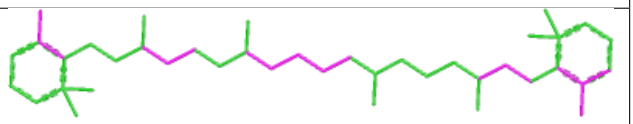
Torsions



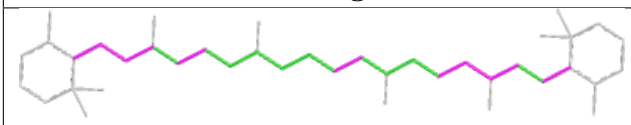
Rings

Ligand BCR h 601

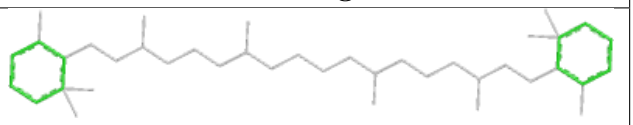
Bond lengths



Bond angles

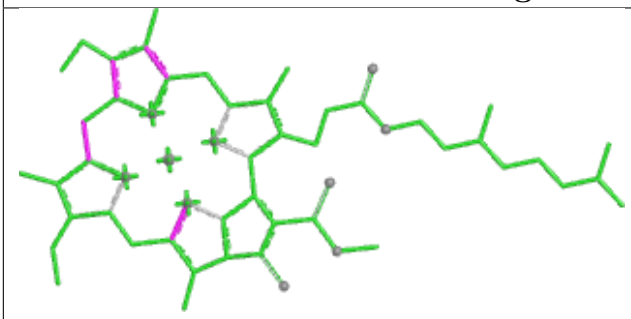


Torsions



Rings

Ligand CLA H 1111



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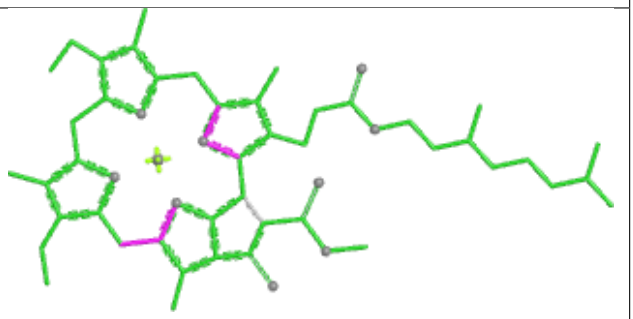
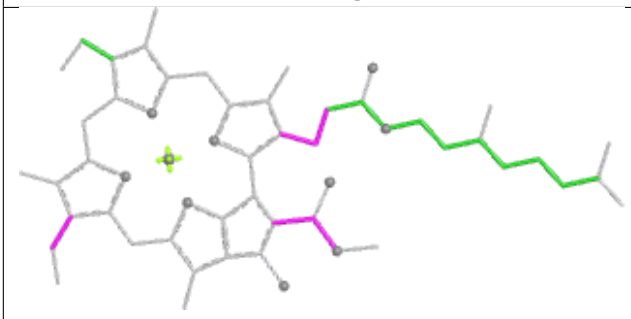
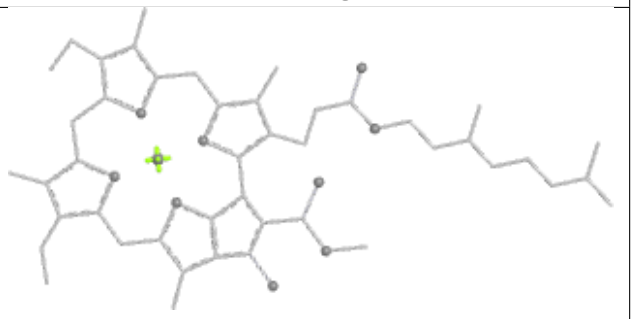


Bond angles

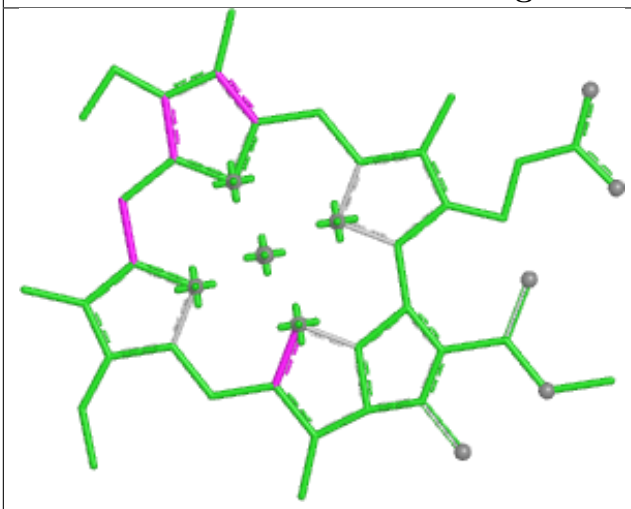


Torsions



Rings

Ligand CLA B 1209



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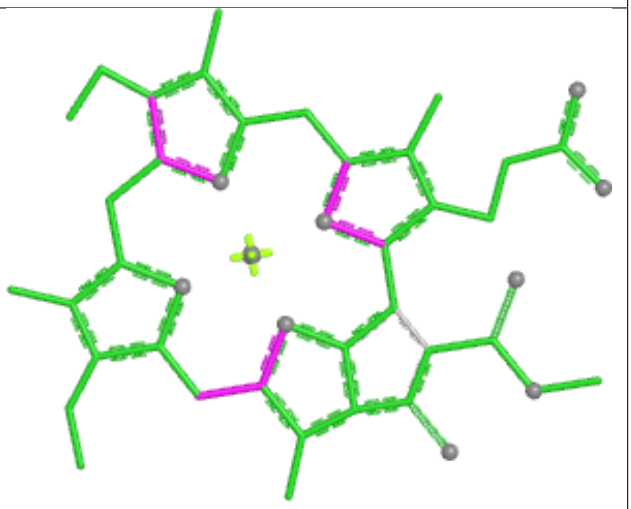
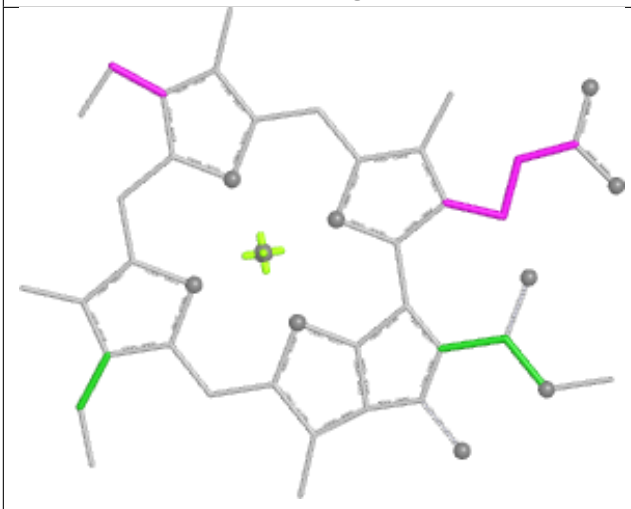


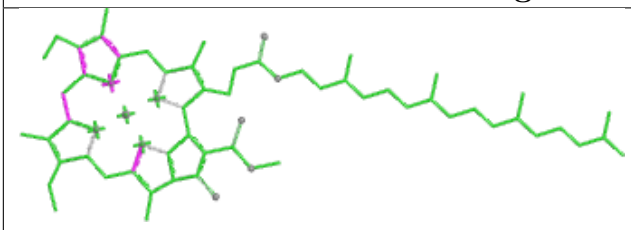
Bond angles



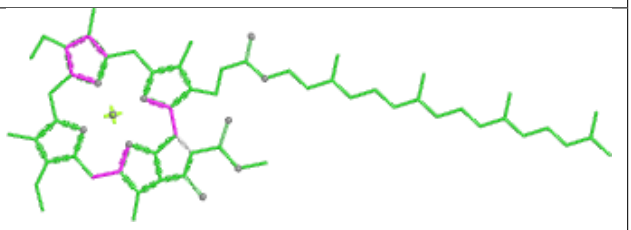
Torsions

Rings

Ligand CLA H 1119



Bond lengths



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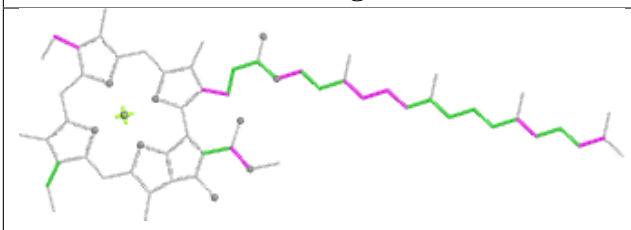
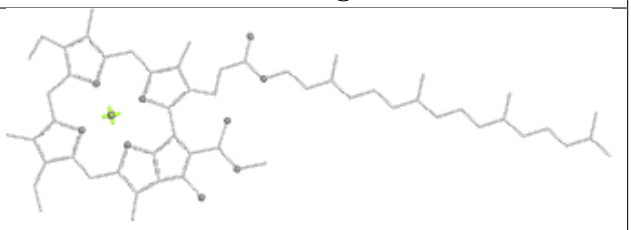
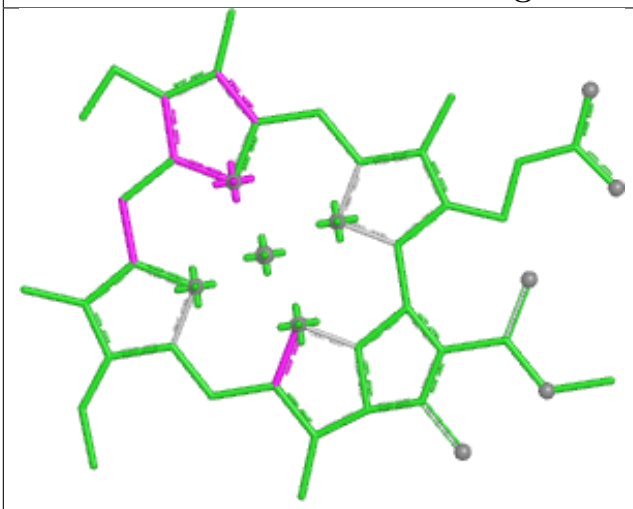


Torsions

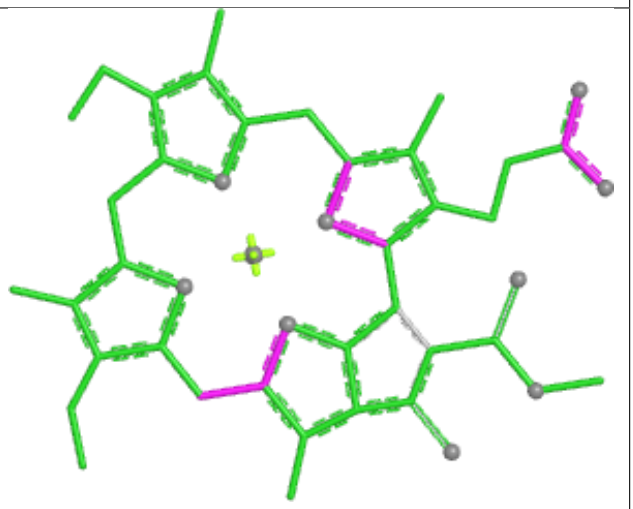


Rings

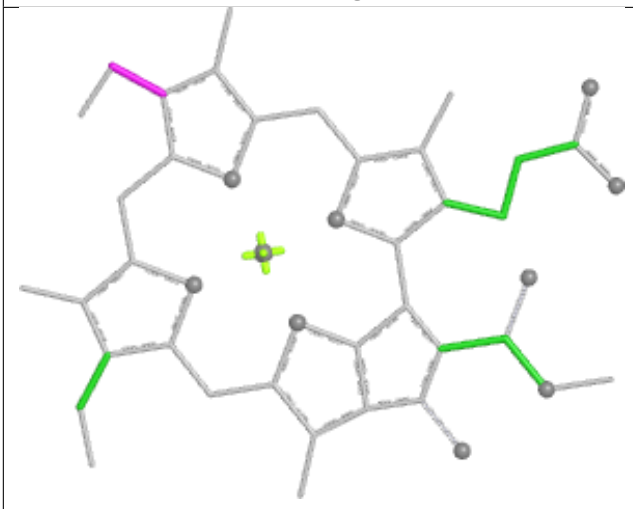
Ligand CLA H 1113



Bond lengths



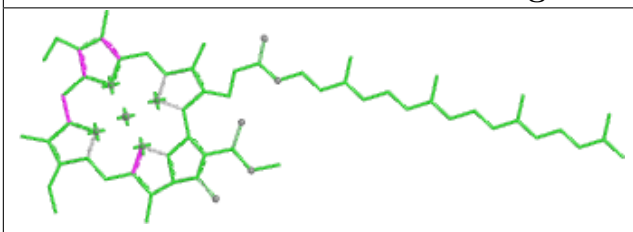
Bond angles



Torsions

Rings

Ligand CLA g 507



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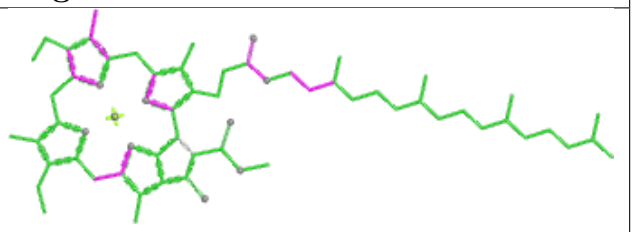
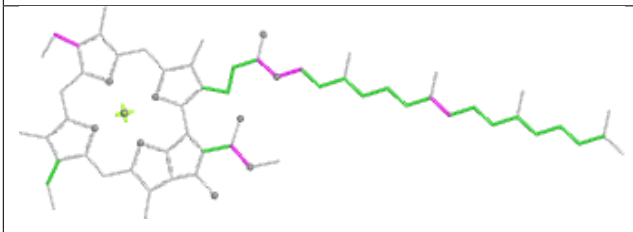
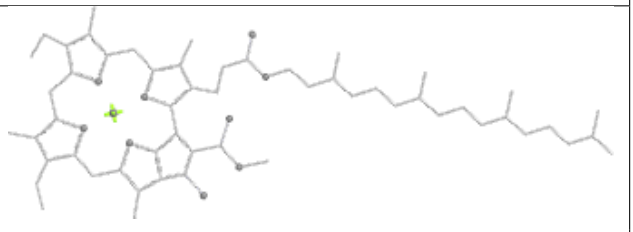


Bond angles

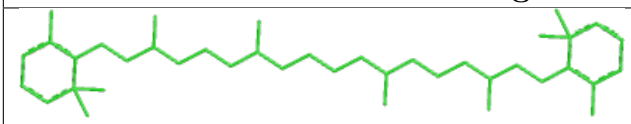


Torsions



Rings

Ligand BCR G 4005



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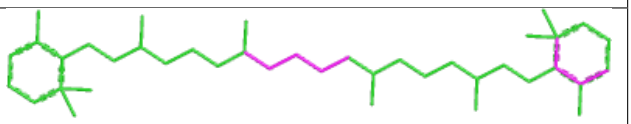
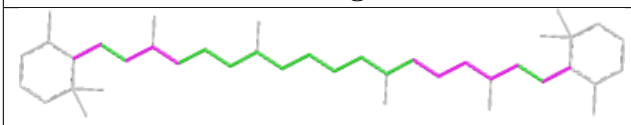
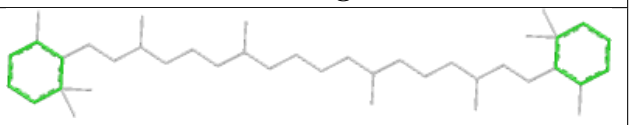


Bond angles

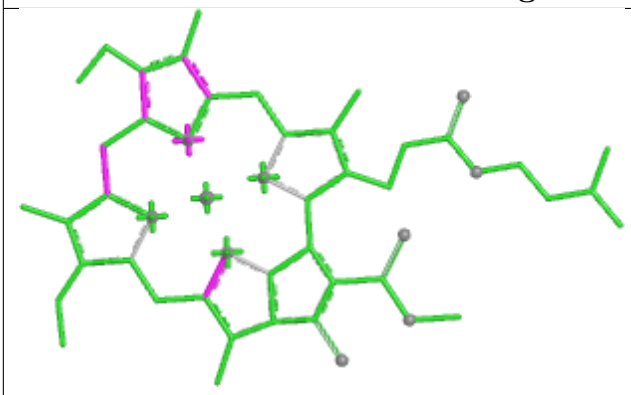


Torsions



Rings

Ligand CLA b 1222



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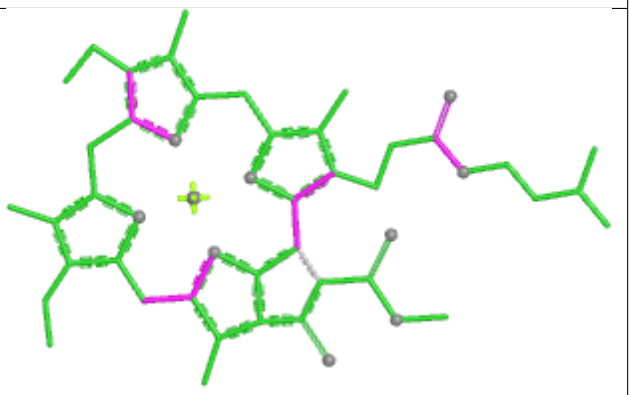
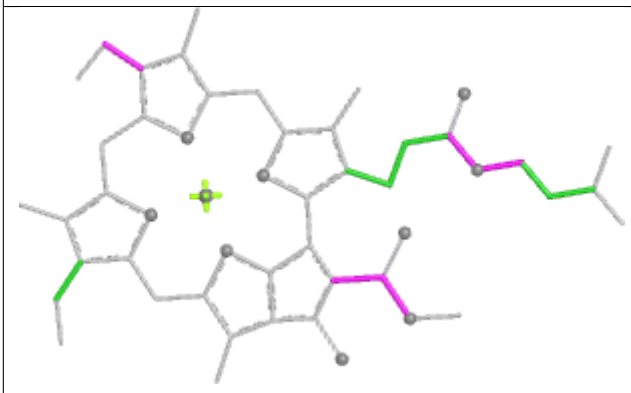
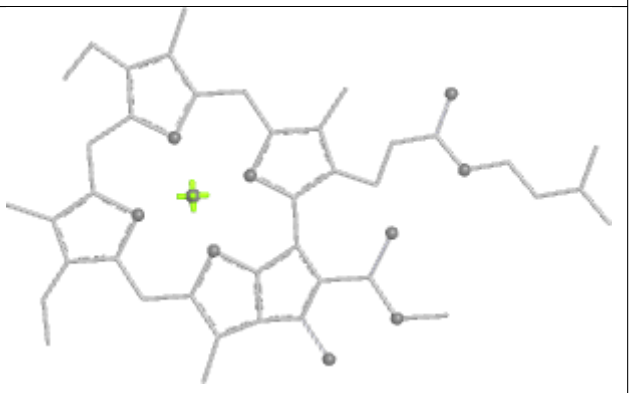


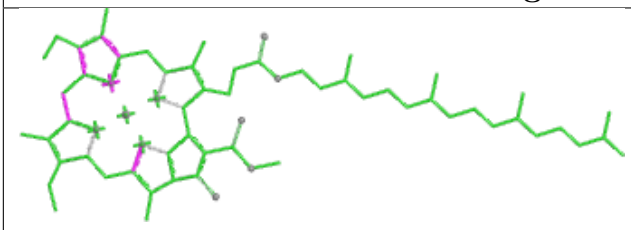
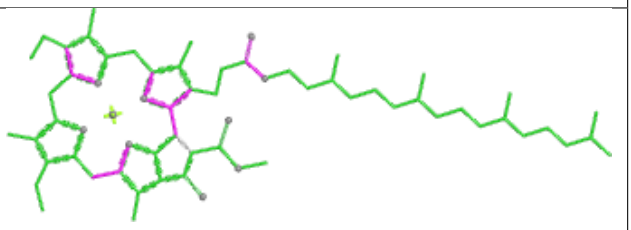
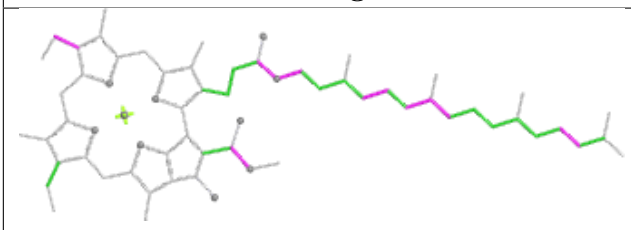
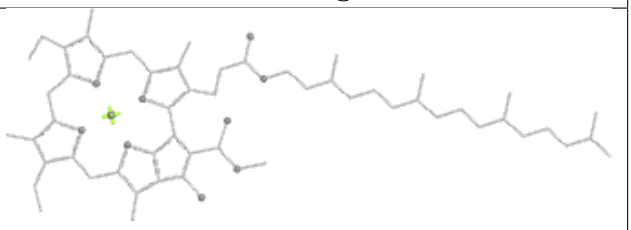
Bond angles

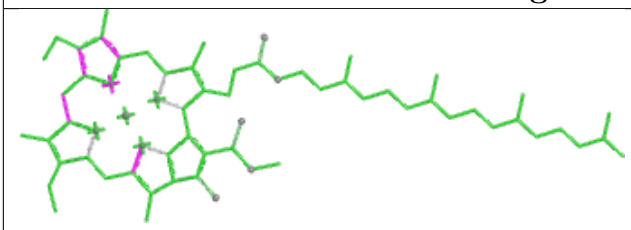
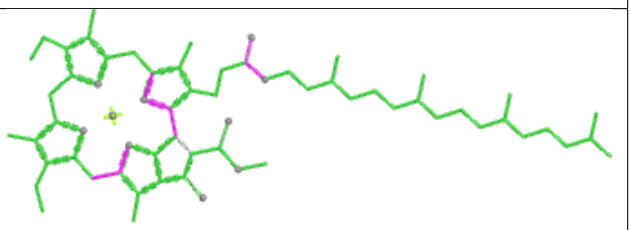
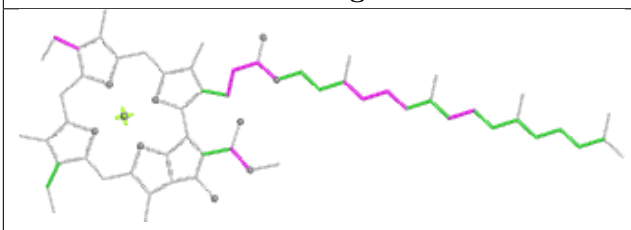
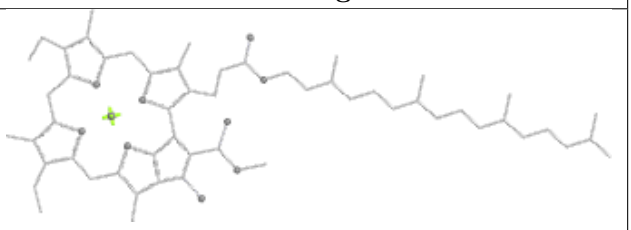


Torsions

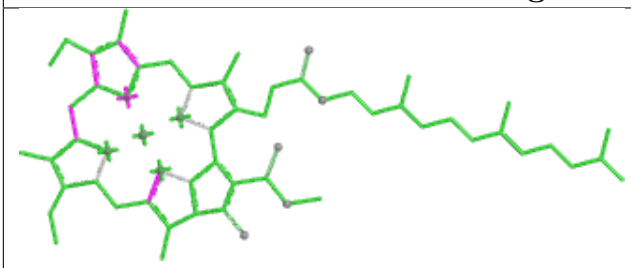


Rings

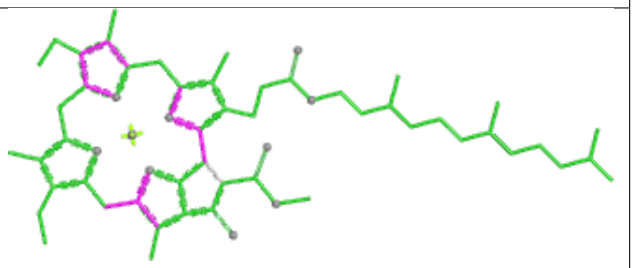
Ligand CLA X 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

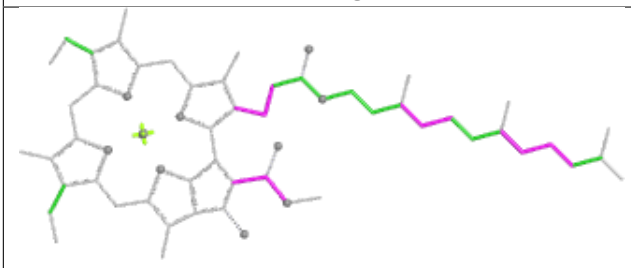
Ligand CLA v 504



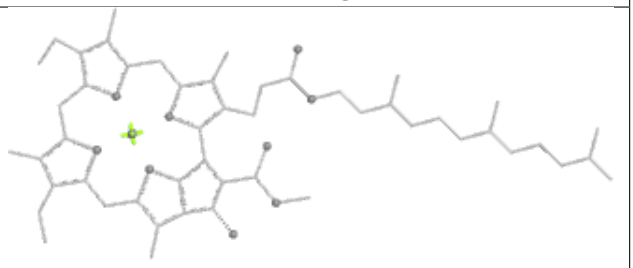
Bond lengths



Bond angles

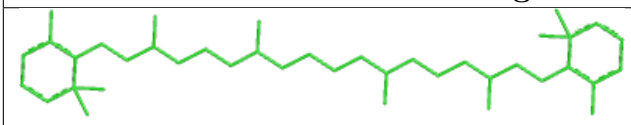


Torsions

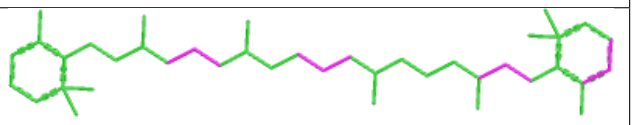


Rings

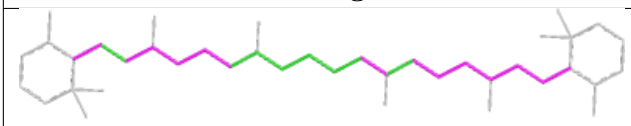
Ligand BCR A 4011



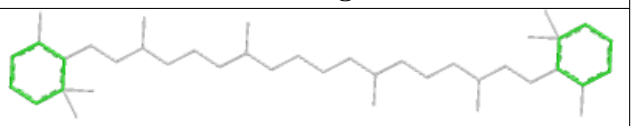
Bond lengths



Bond angles

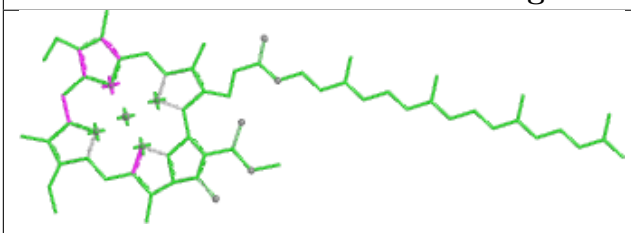


Torsions

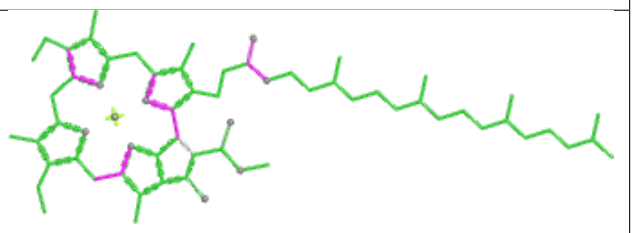


Rings

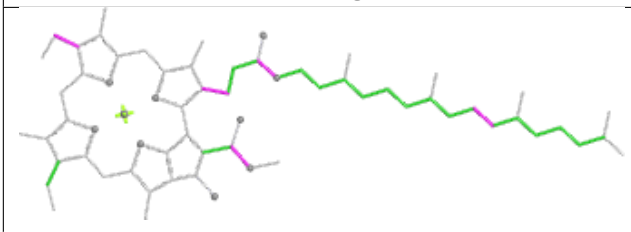
Ligand CLA n 511



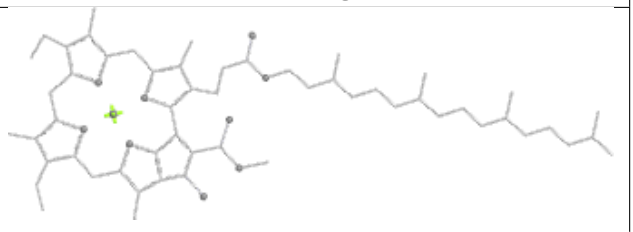
Bond lengths



Bond angles

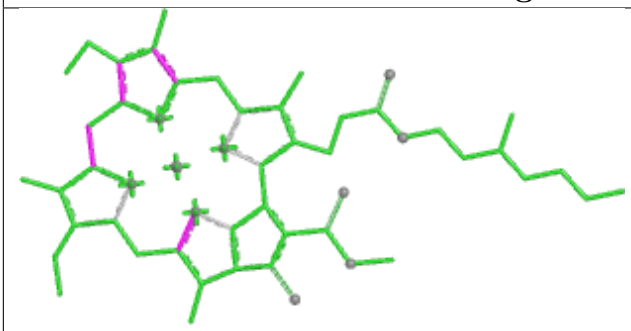


Torsions



Rings

Ligand CLA B 1220



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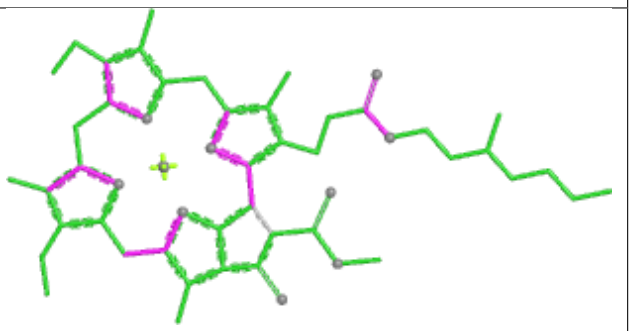
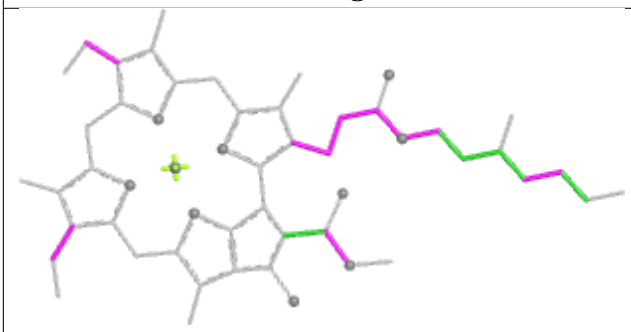
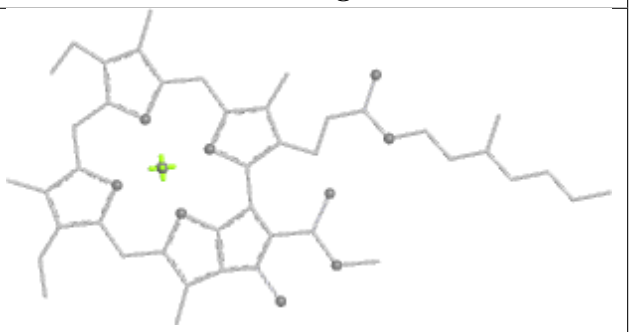


Bond angles

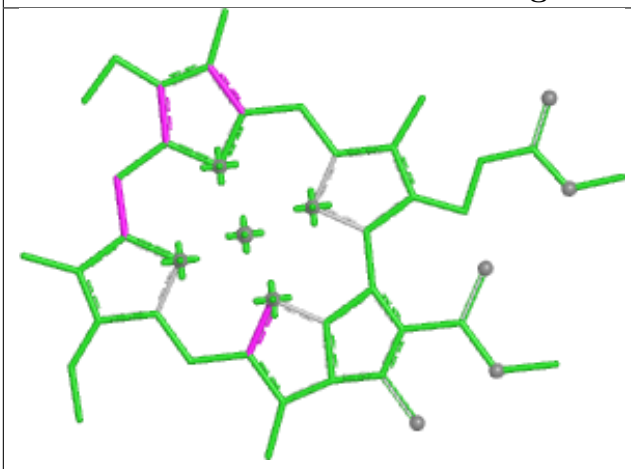


Torsions



Rings

Ligand CLA s 516



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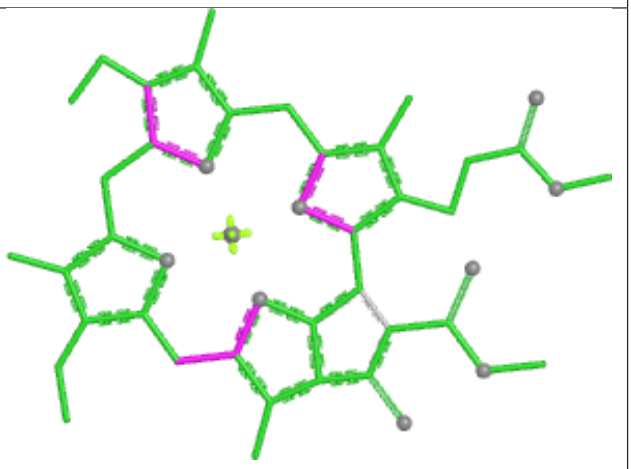
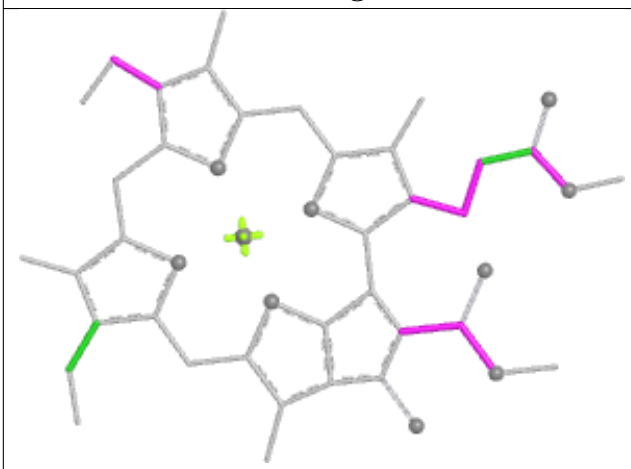
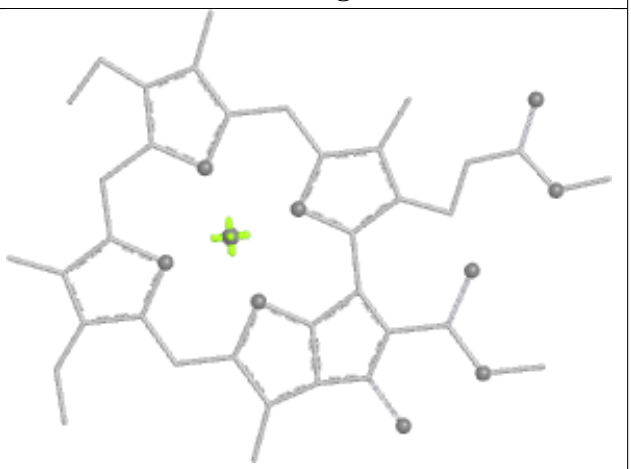


Bond angles

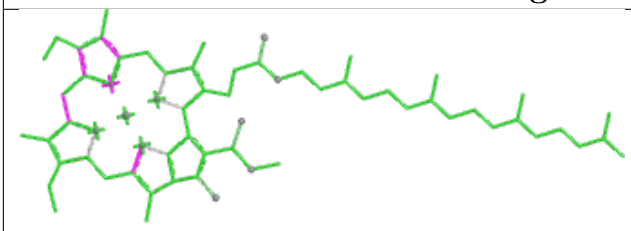


Torsions



Rings

Ligand CLA r 511



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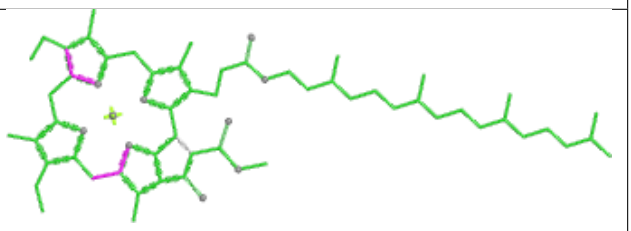
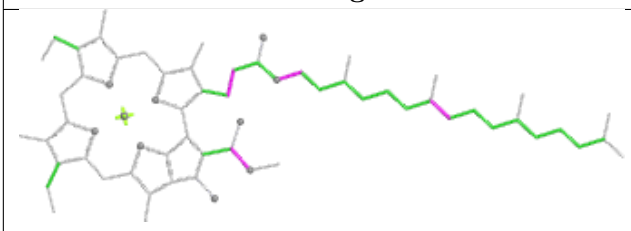


Bond angles



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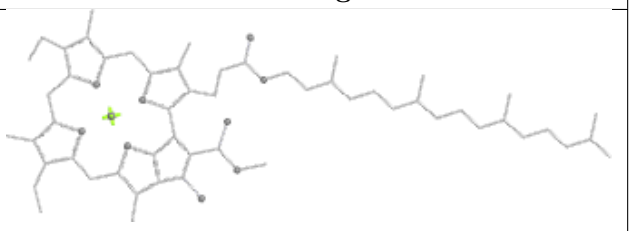
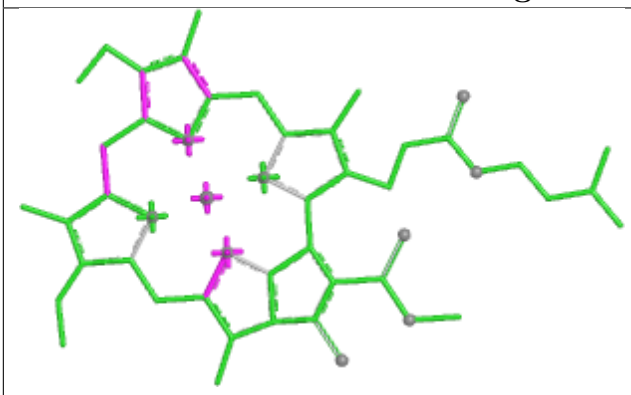
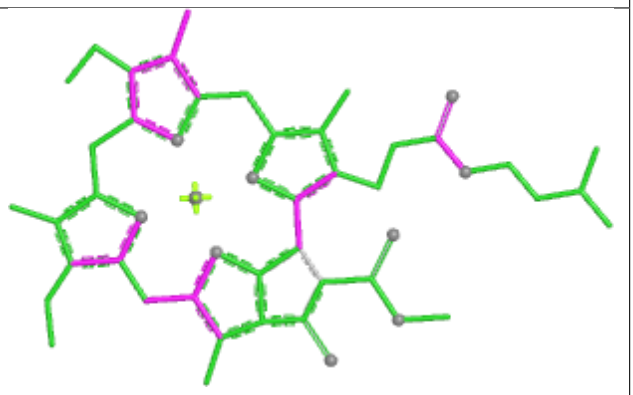


Rings

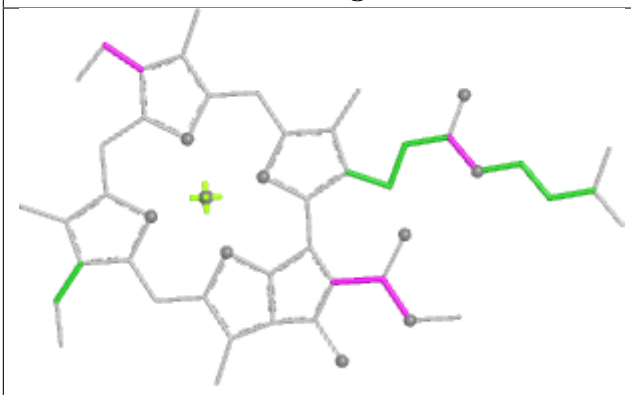
Ligand CLA G 1222



Bond lengths



Bond angles



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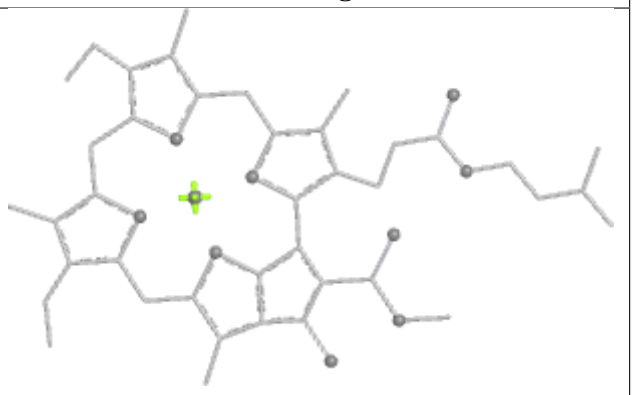
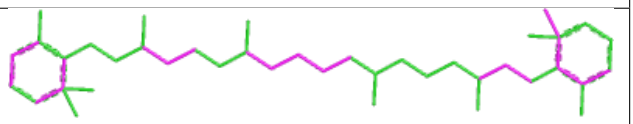


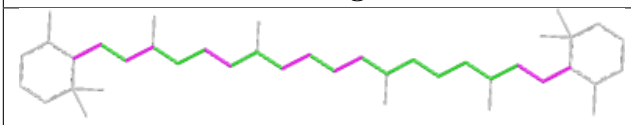
Rings

Ligand BCR W 604

Bond lengths



Bond angles



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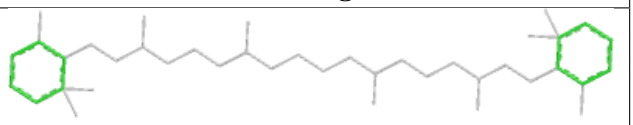
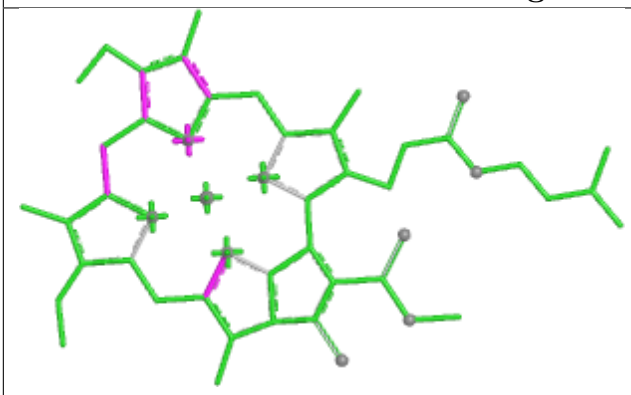


Rings

Ligand CLA h 502



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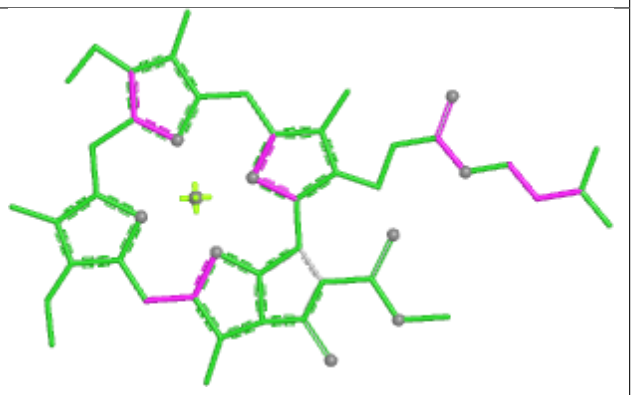
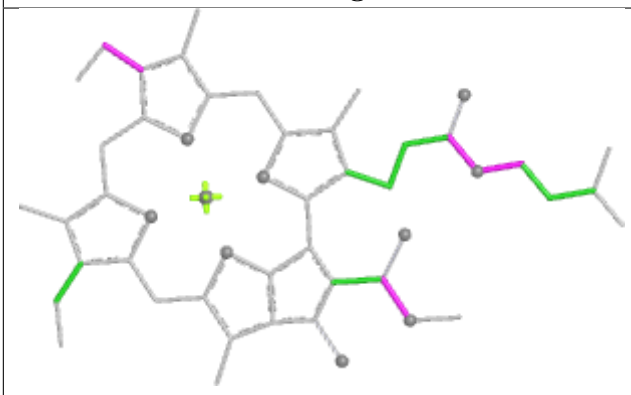


Bond angles



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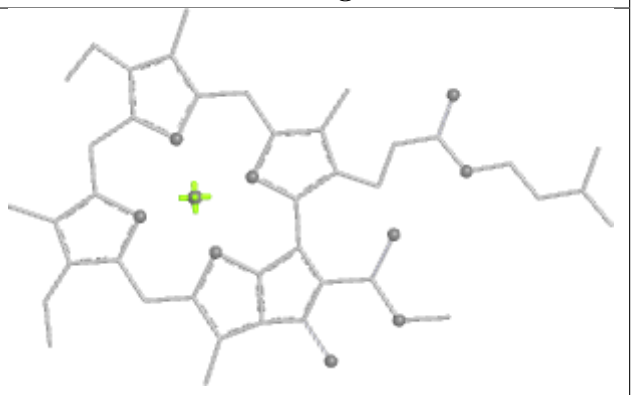
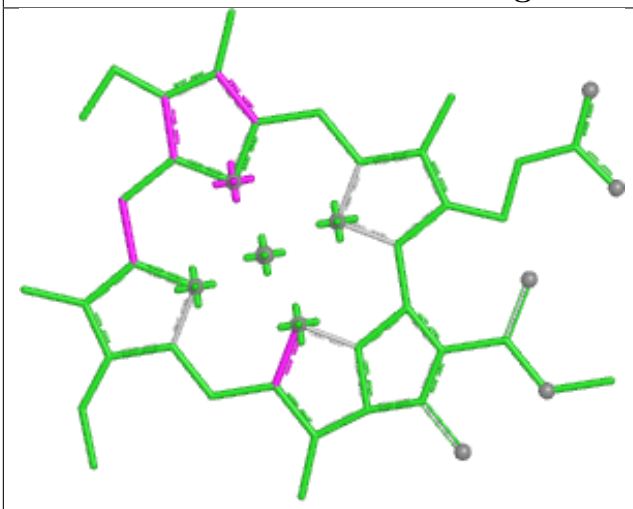


Rings

Ligand CLA G 1232



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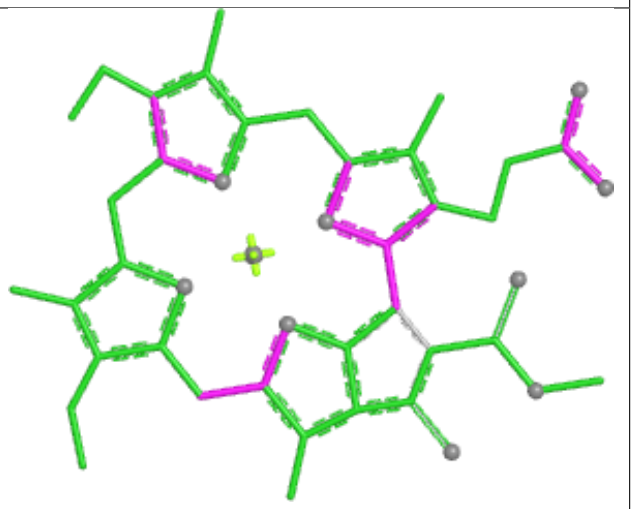
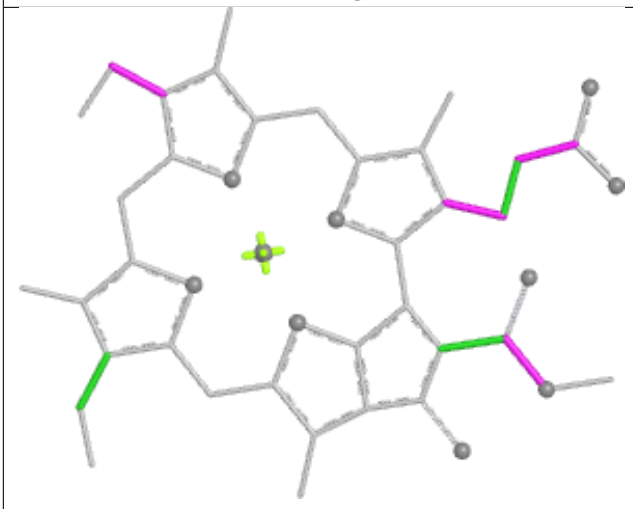


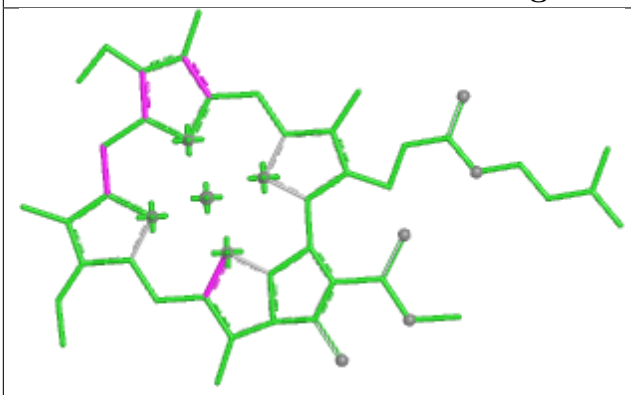
Bond angles



Torsions

Rings

Ligand CLA r 501



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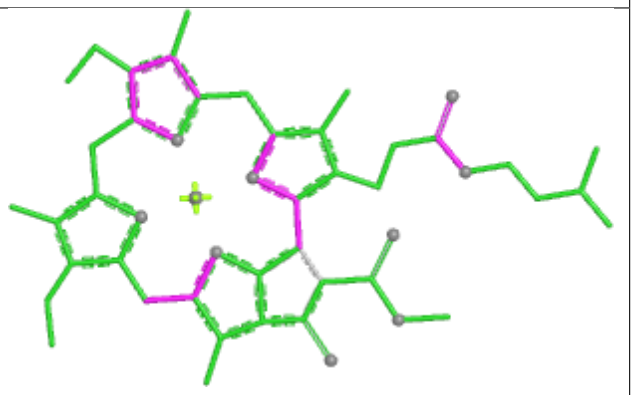
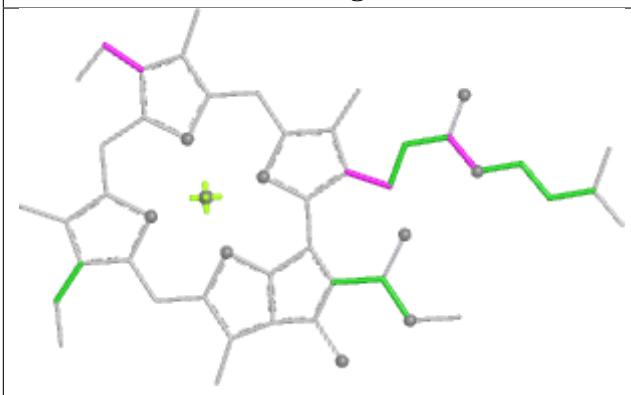
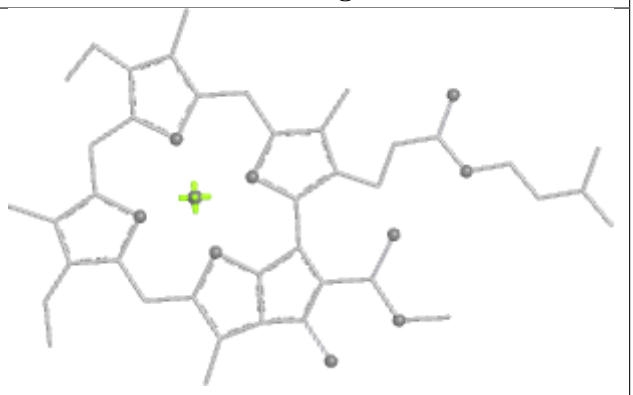


Bond angles

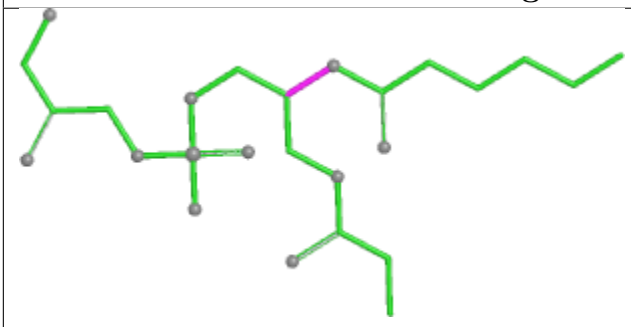


Torsions



Rings

Ligand LHG A 851



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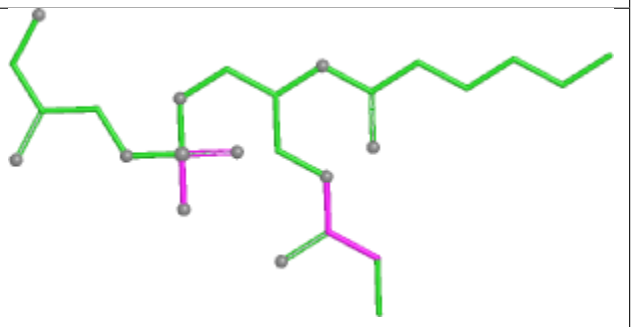
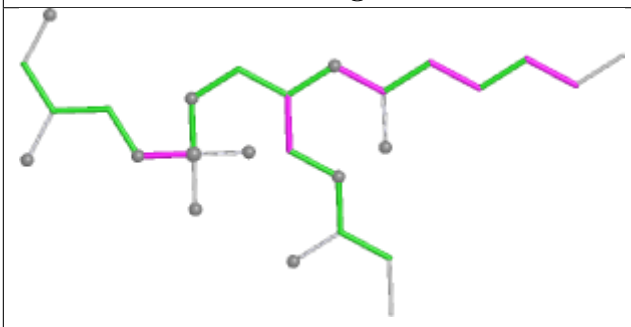


Bond angles



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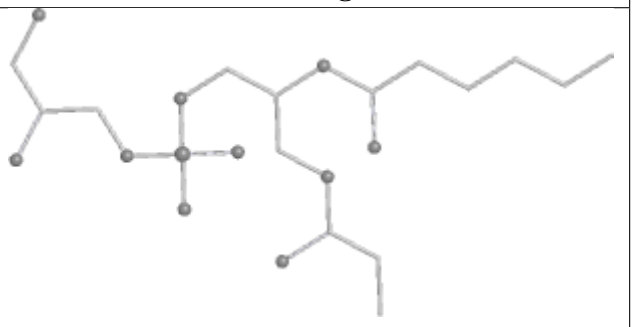
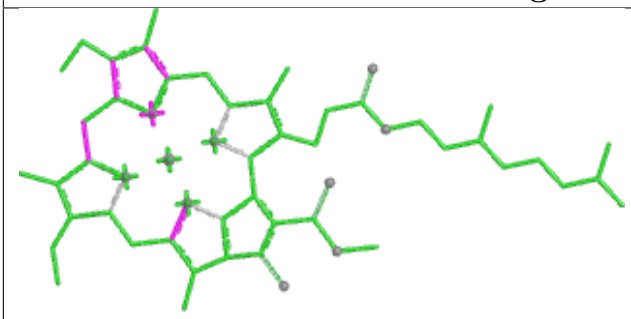


Rings

Ligand CLA s 517



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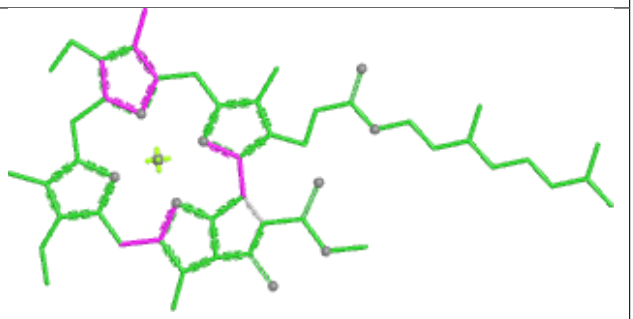
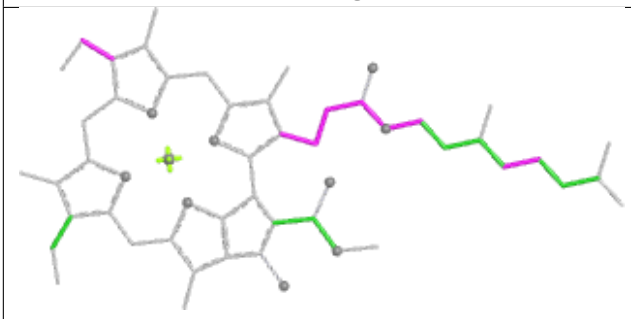
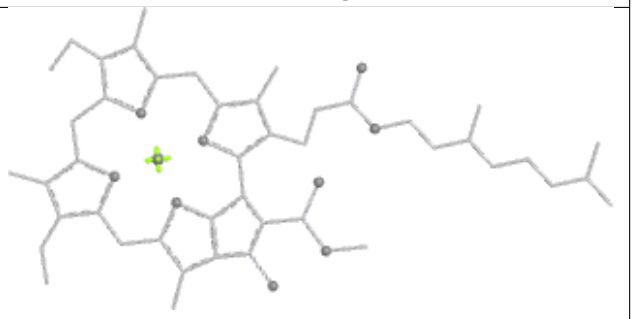


Bond angles

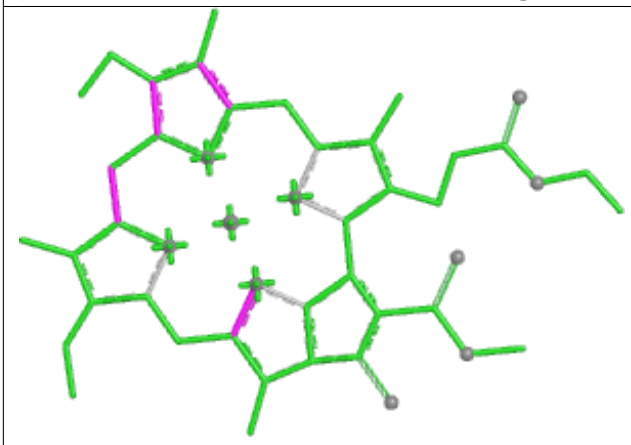


Torsions

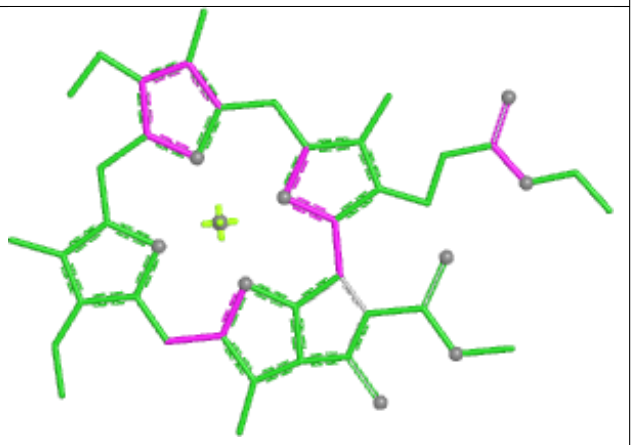


Rings

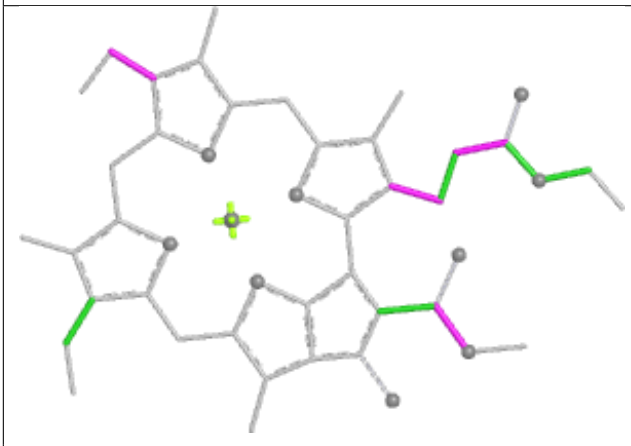
Ligand CLA A 1137



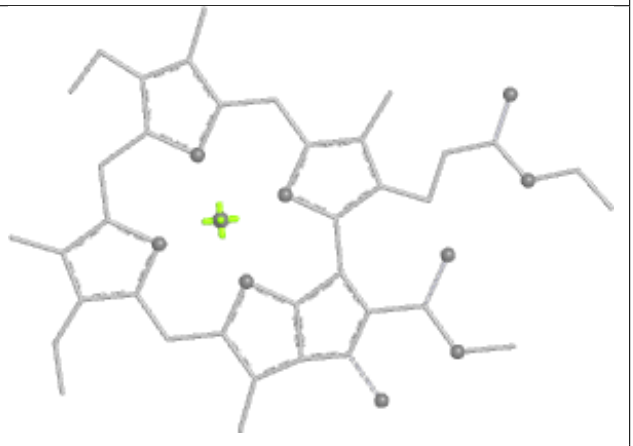
Bond lengths



Bond angles

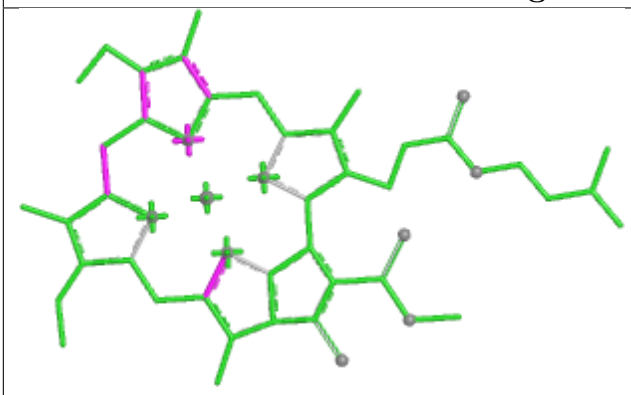


Torsions

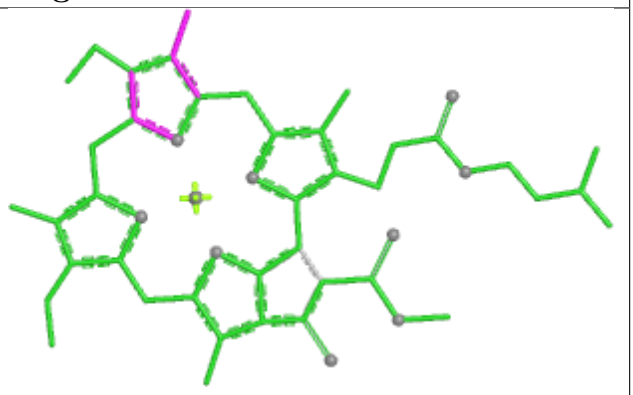


Rings

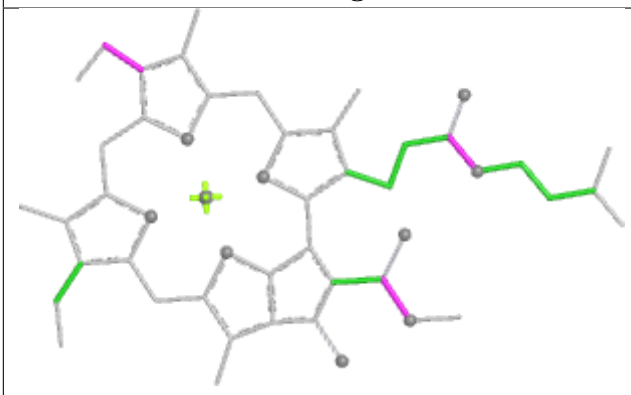
Ligand CLA g 502



Bond lengths



Bond angles



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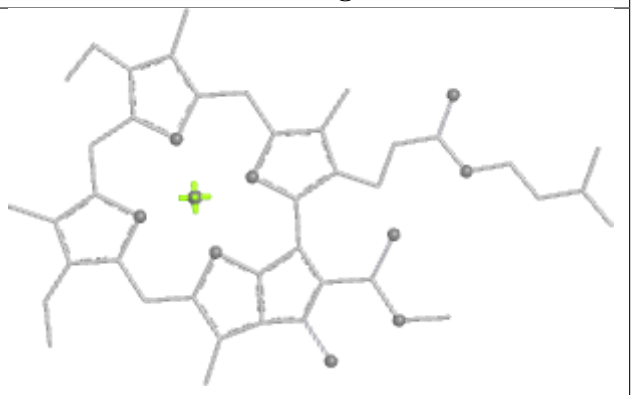
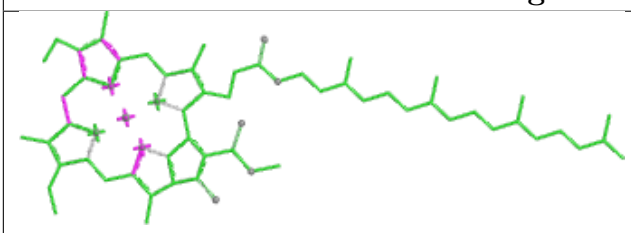
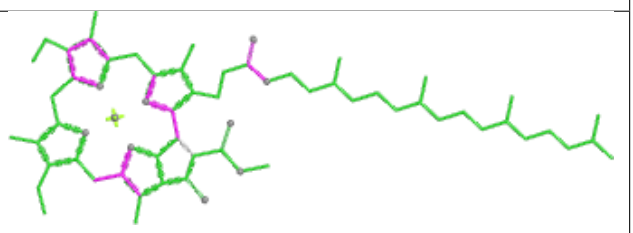


Rings

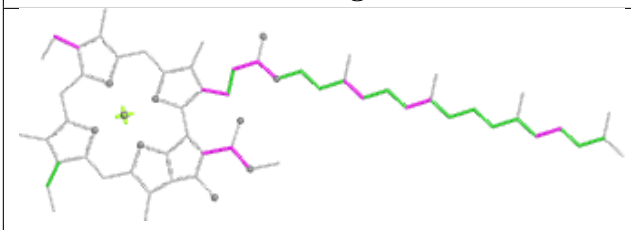
Ligand CLA v 509



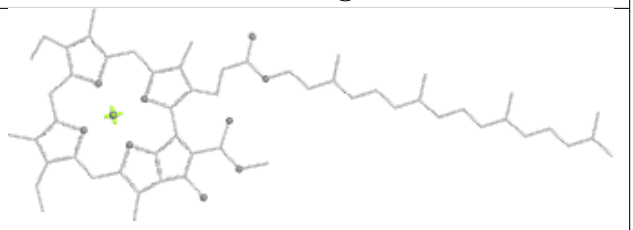
Bond lengths



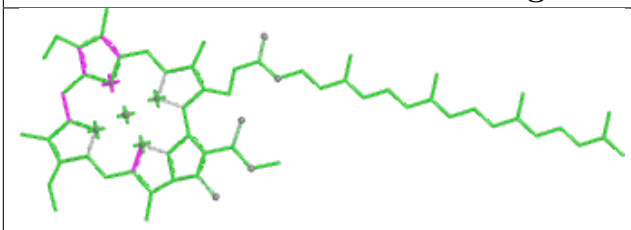
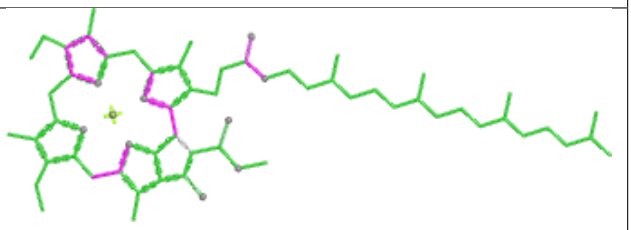
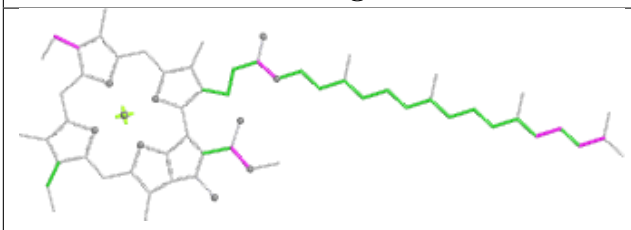
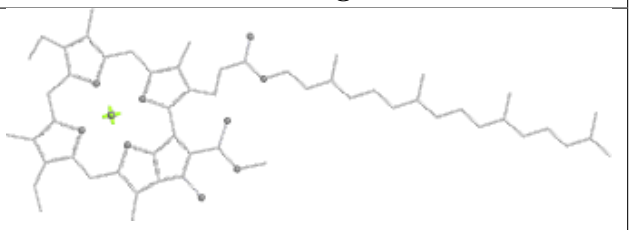
Bond angles

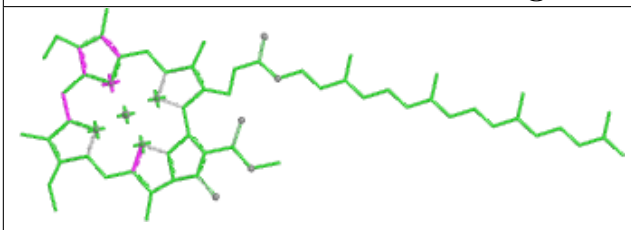
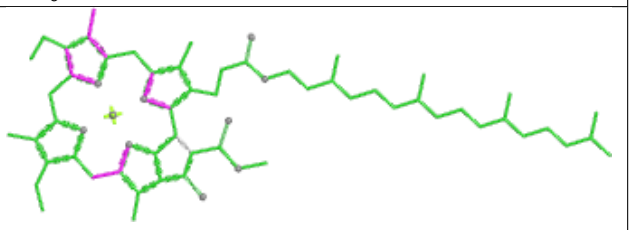
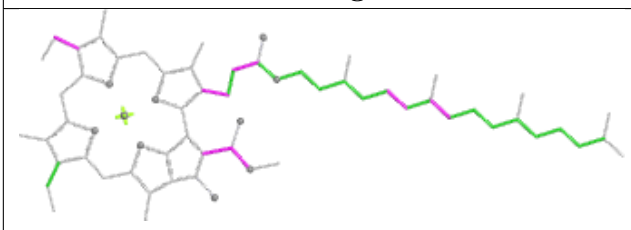
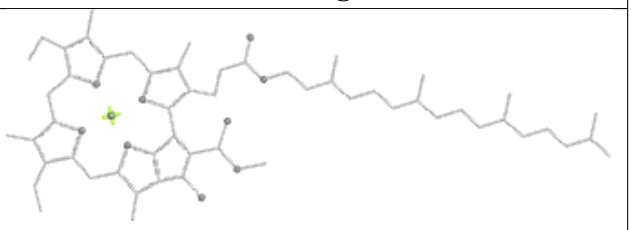


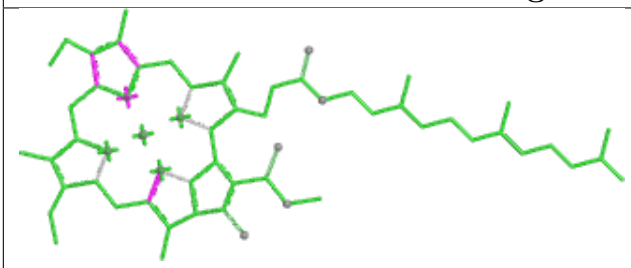
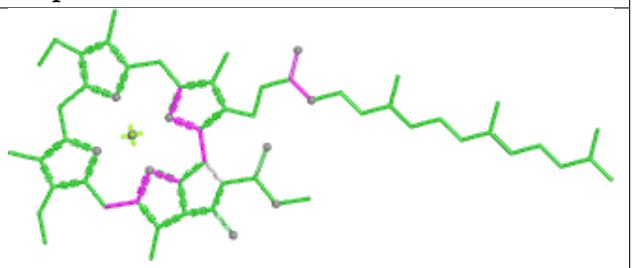
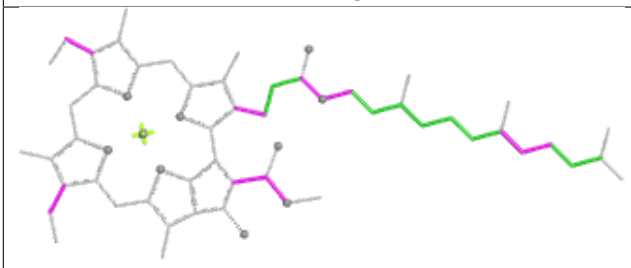
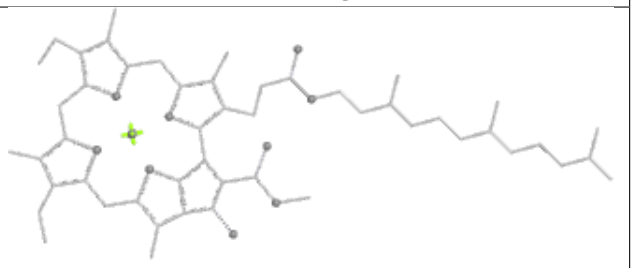
Torsions

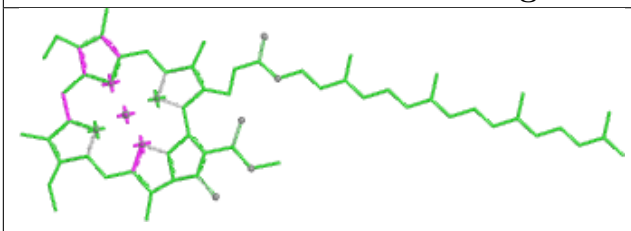
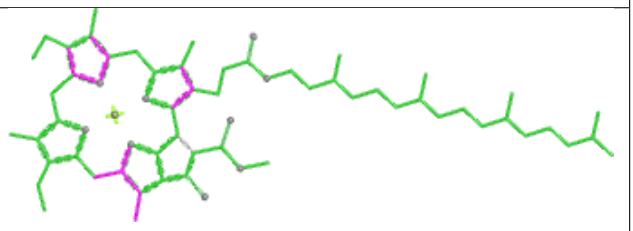
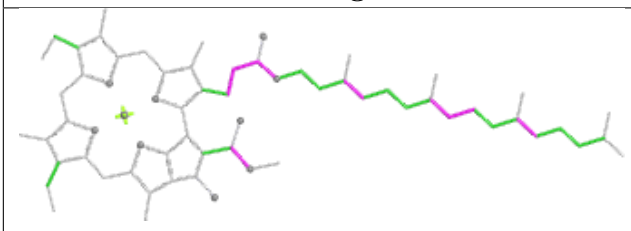
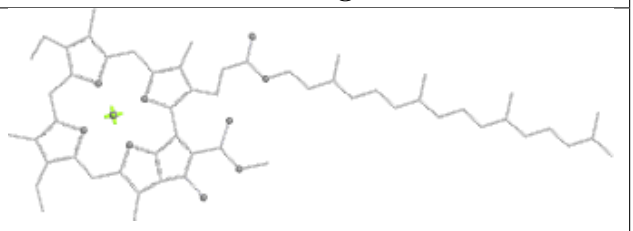


Rings

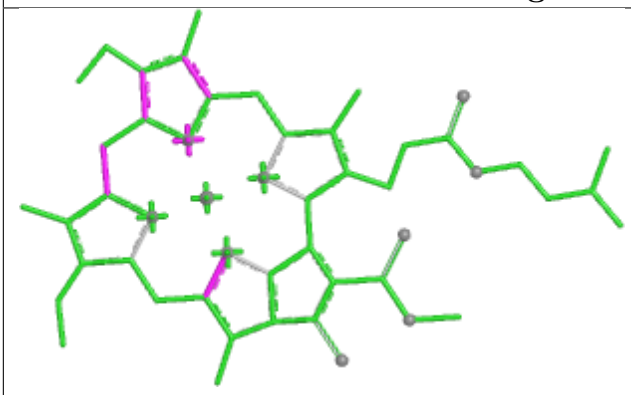
Ligand CLA h 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA y 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

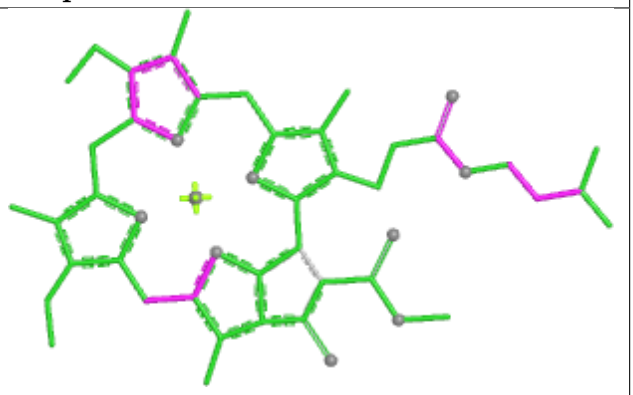
Ligand CLA p 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1013	
	
Bond lengths	Bond angles
	
Torsions	Rings

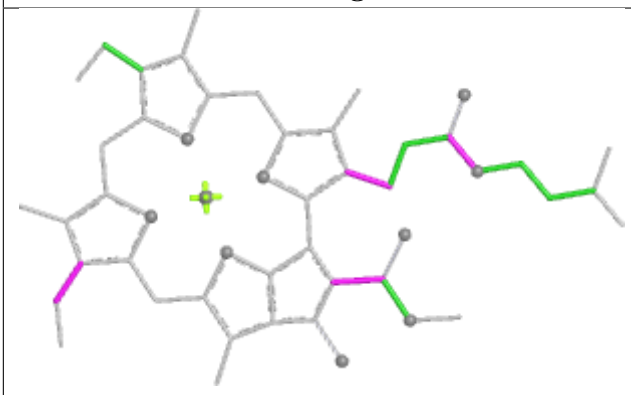
Ligand CLA q 501



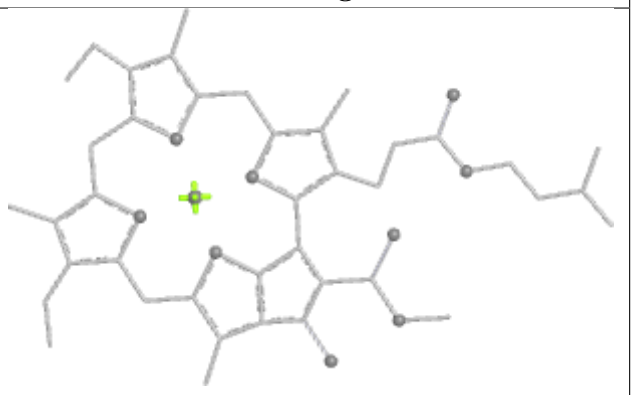
Bond lengths



Bond angles

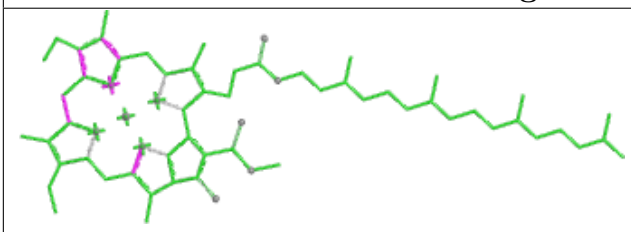


Torsions

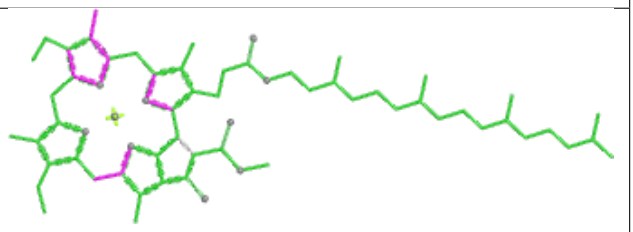


Rings

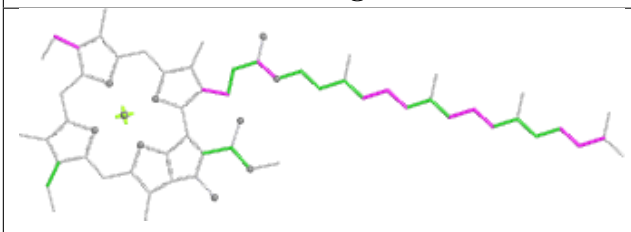
Ligand CLA a 1140



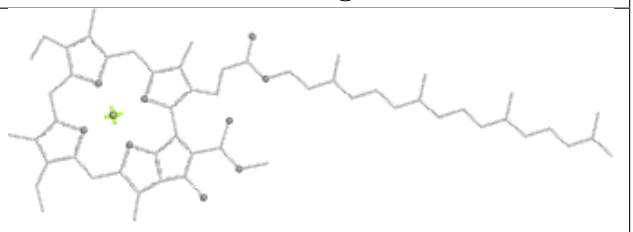
Bond lengths



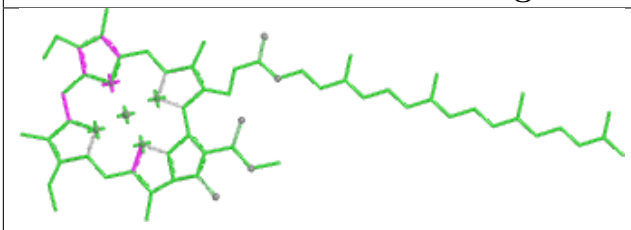
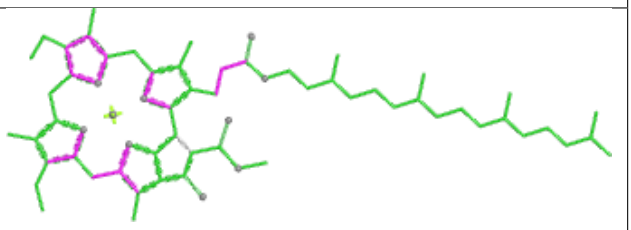
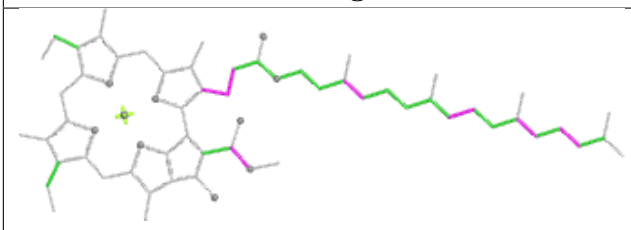
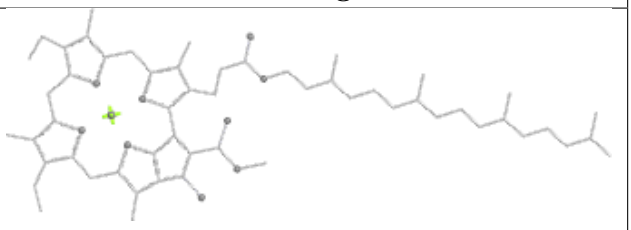
Bond angles

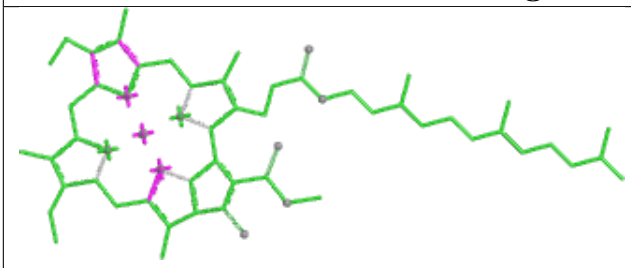
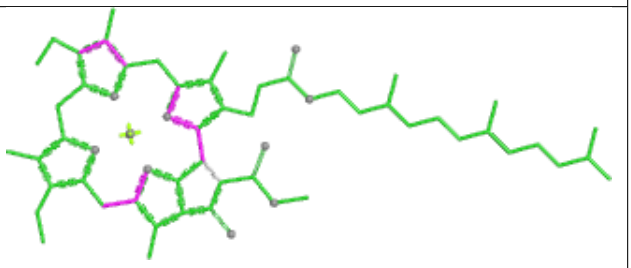
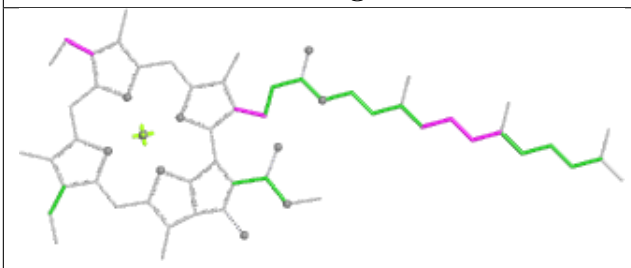
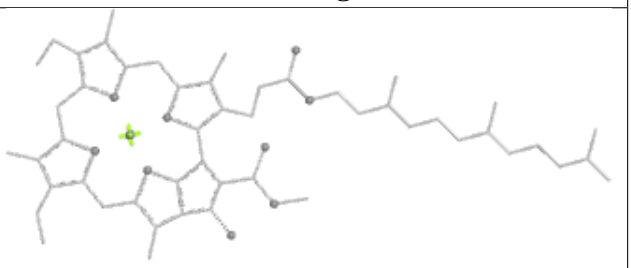


Torsions

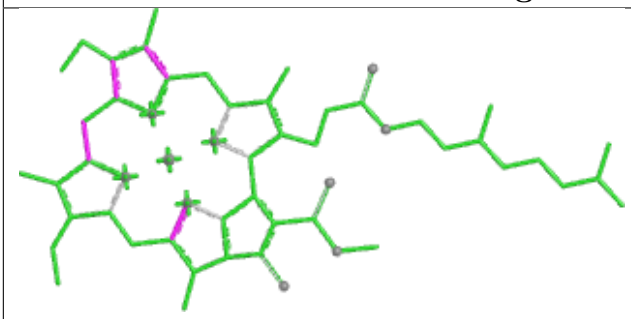


Rings

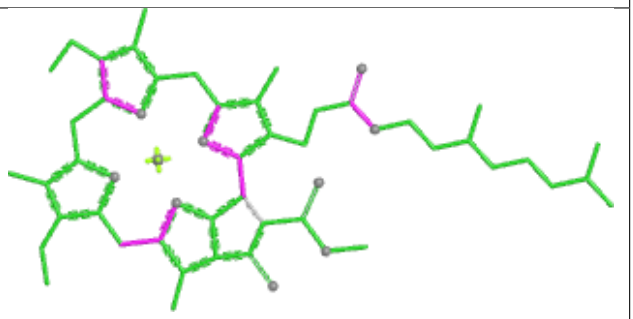
Ligand CLA H 1022	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA w 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

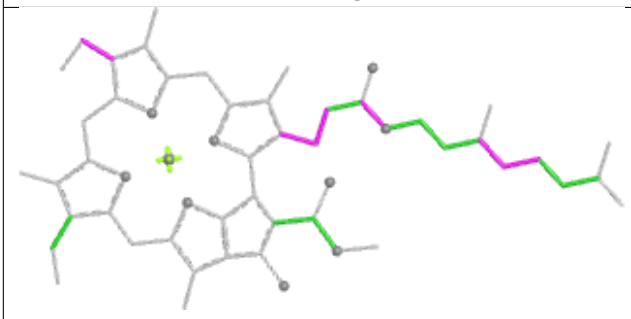
Ligand CLA B 1218



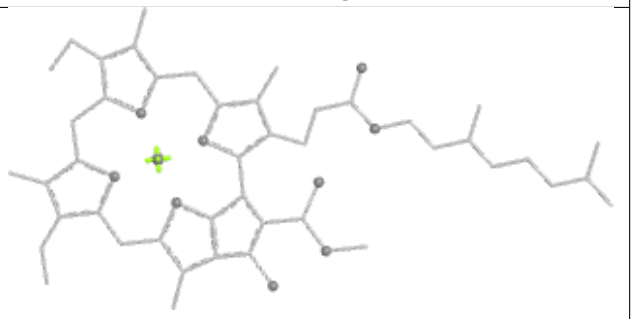
Bond lengths



Bond angles

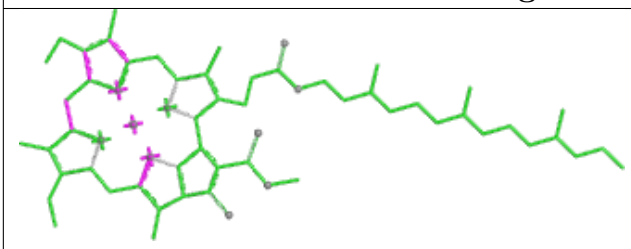


Torsions

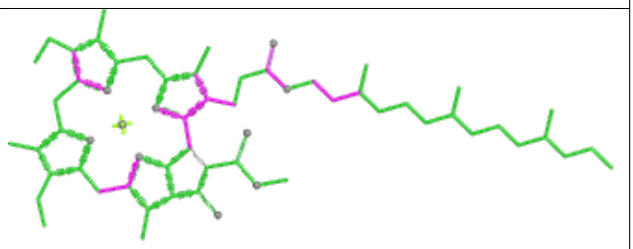


Rings

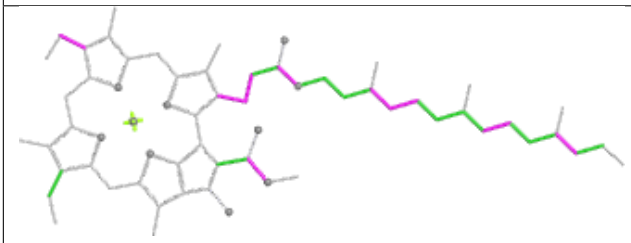
Ligand CLA b 1235



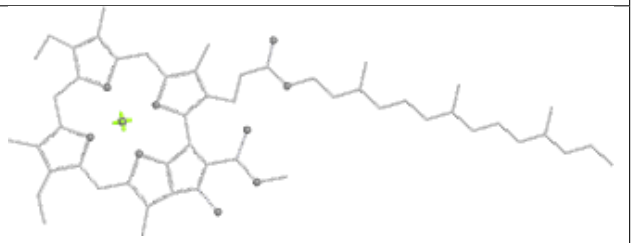
Bond lengths



Bond angles

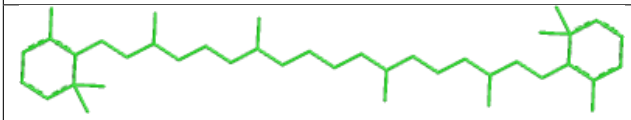


Torsions

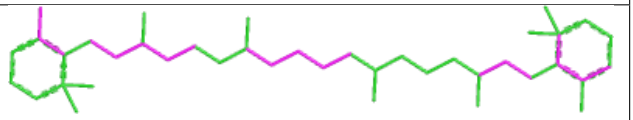


Rings

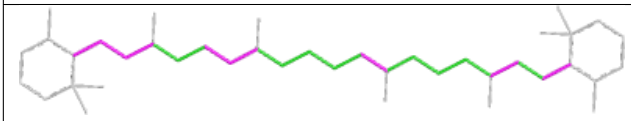
Ligand BCR J 4012



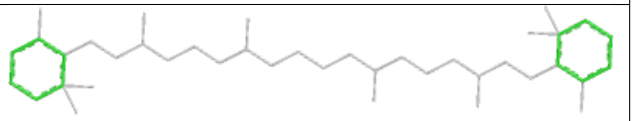
Bond lengths



Bond angles

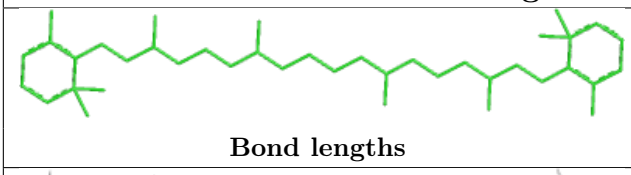


Torsions

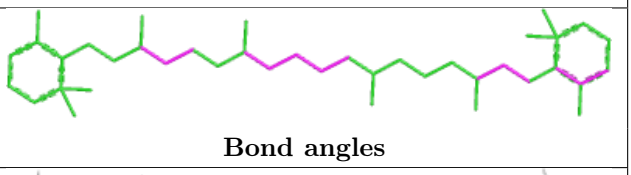


Rings

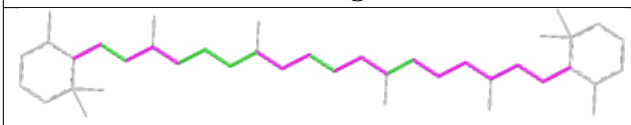
Ligand BCR X 604



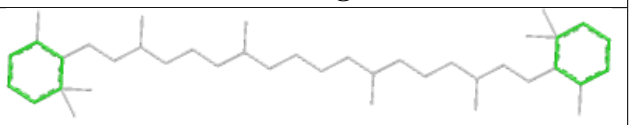
Bond lengths



Bond angles

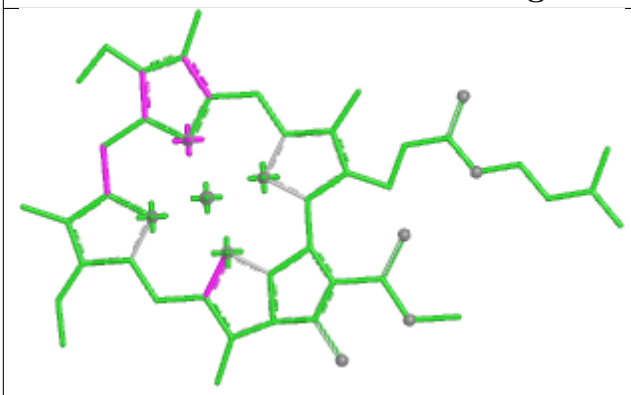


Torsions

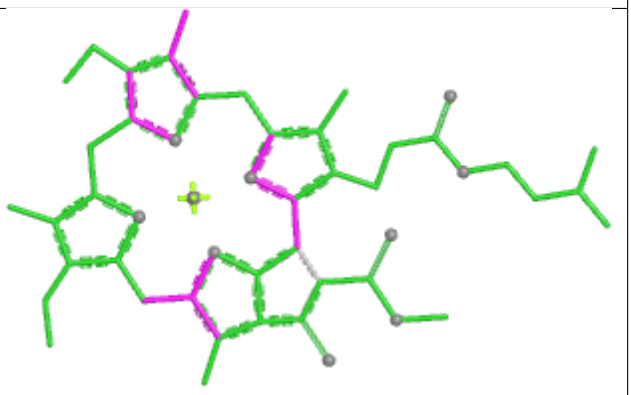


Rings

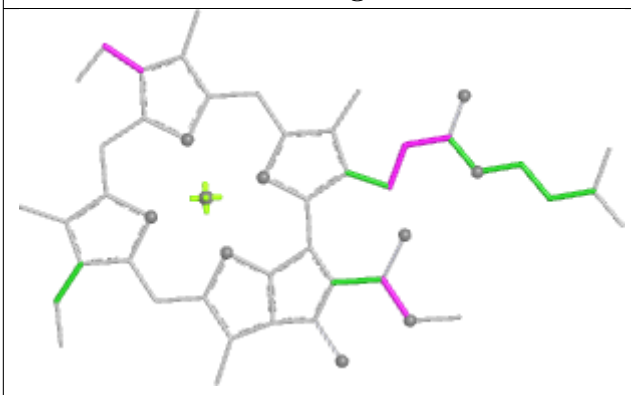
Ligand CLA u 514



Bond lengths



Bond angles



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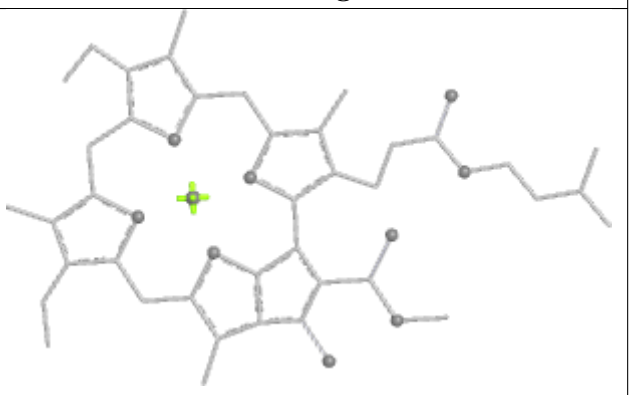
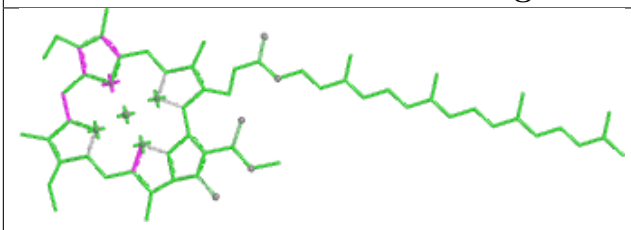
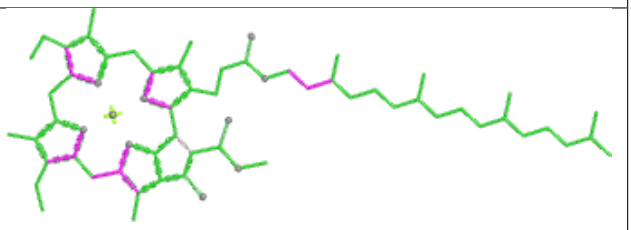


Rings

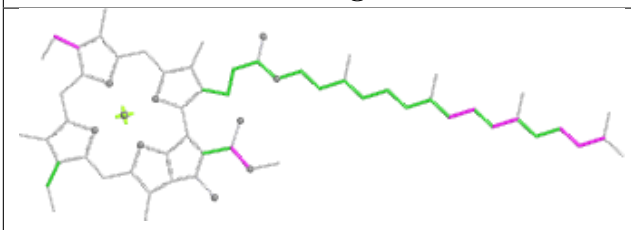
Ligand CLA H 1117



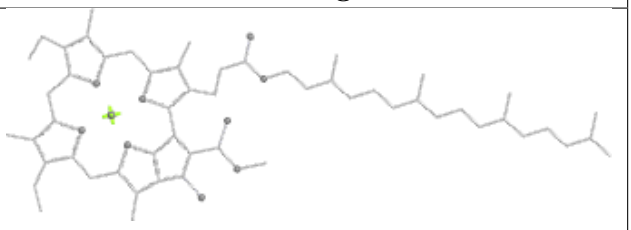
Bond lengths



Bond angles

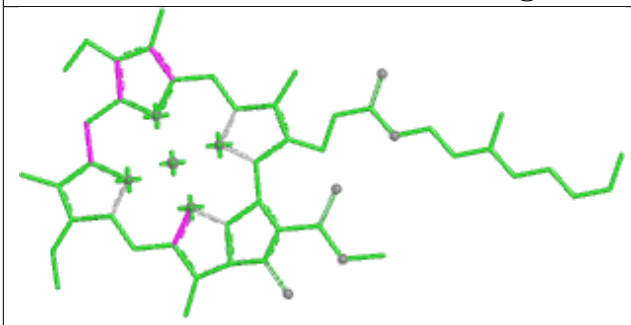


Torsions



Rings

Ligand CLA b 1201



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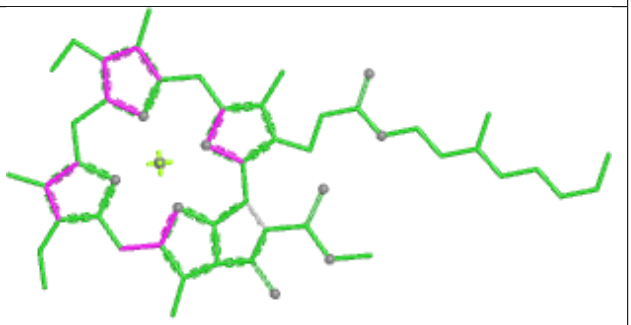
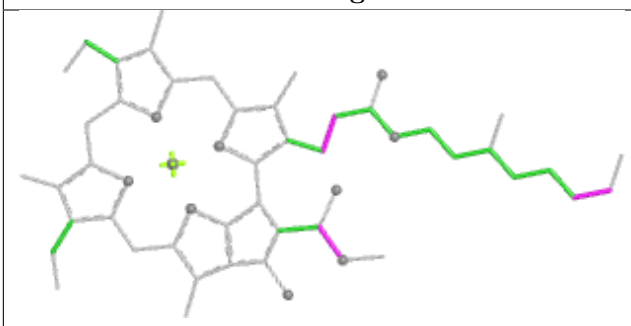


Bond angles



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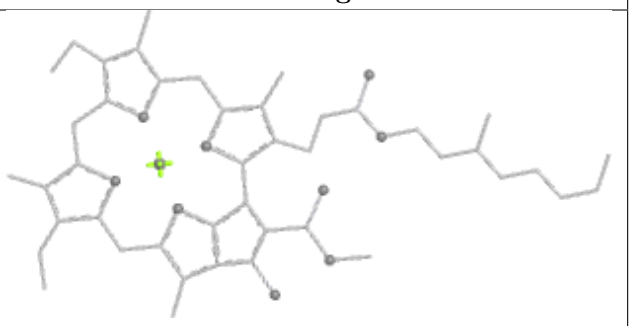
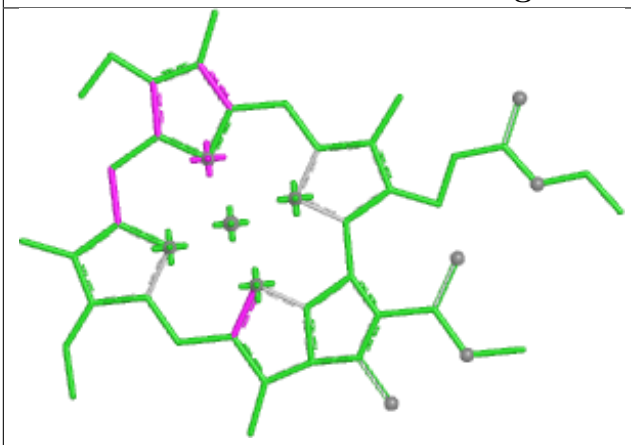


Rings

Ligand CLA H 1137



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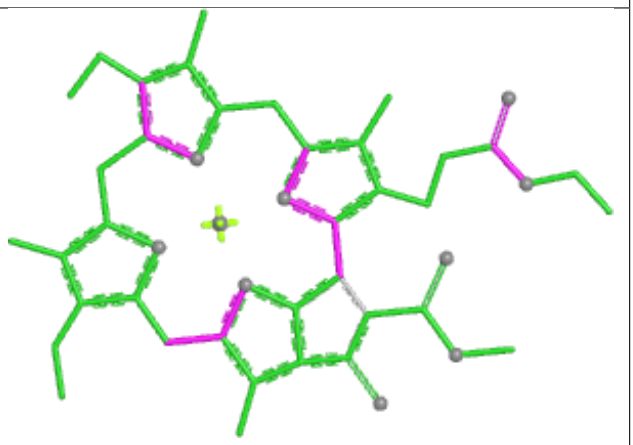
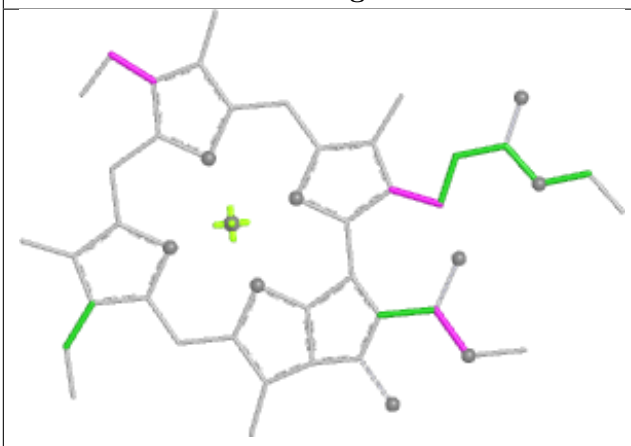
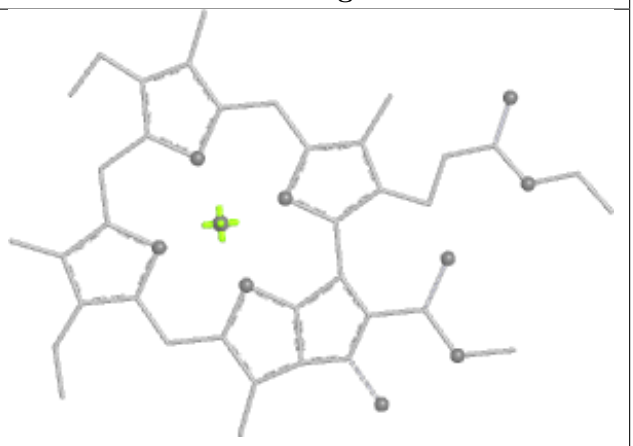


Bond angles

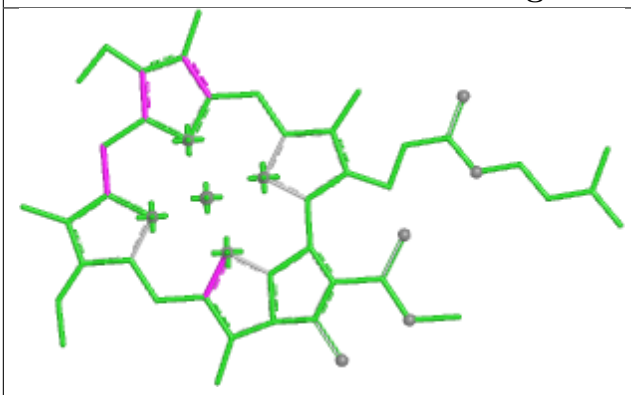


Torsions



Rings

Ligand CLA Z 514



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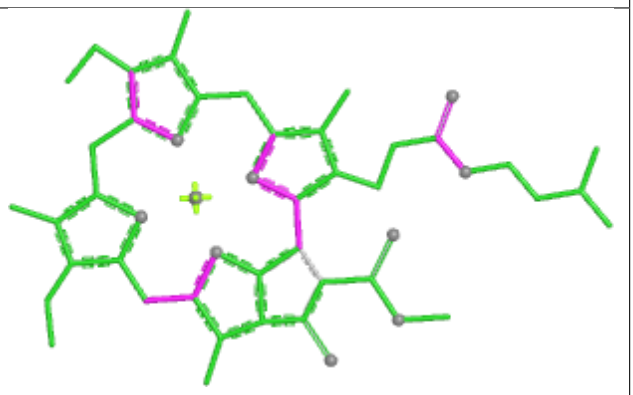
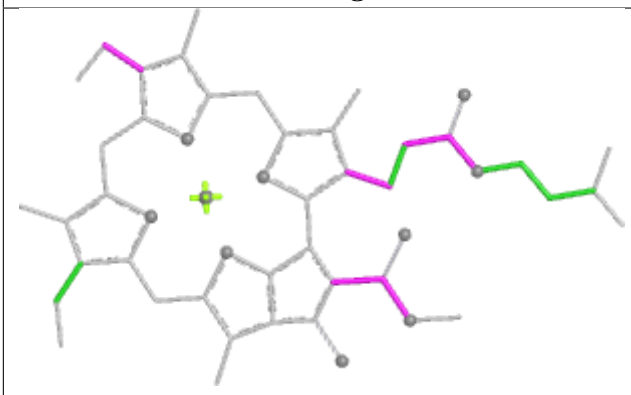
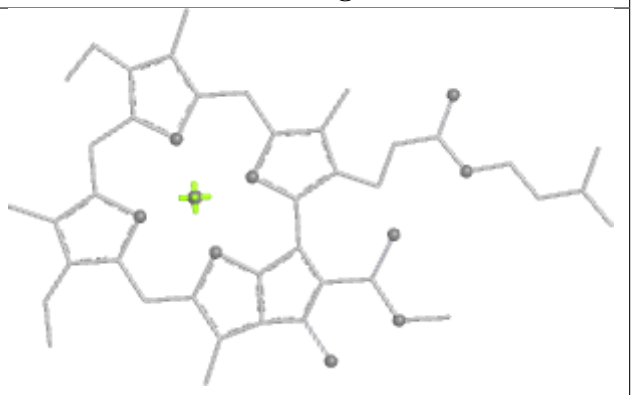


Bond angles

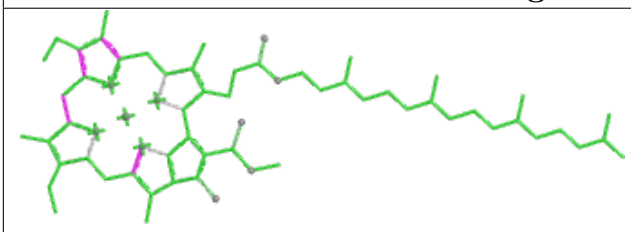


Torsions



Rings

Ligand CLA h 507



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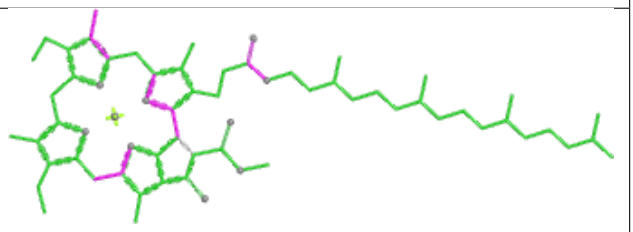
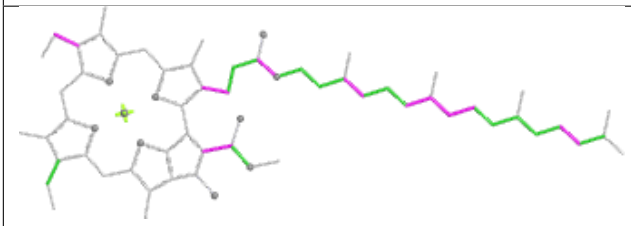


Bond angles



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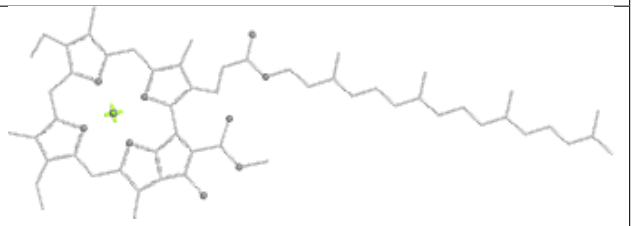
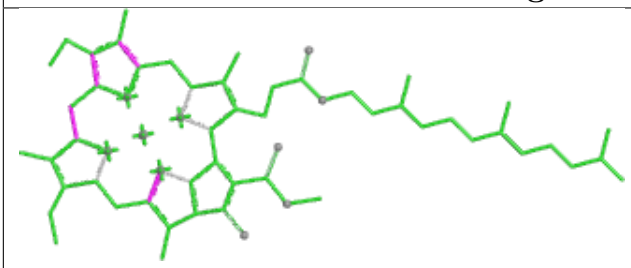


Rings

Ligand CLA n 504



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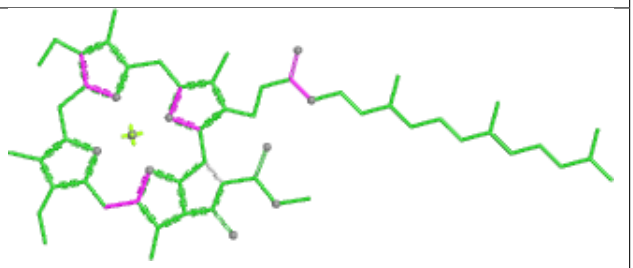
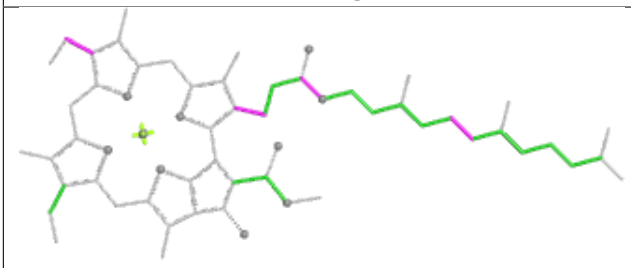


Bond angles



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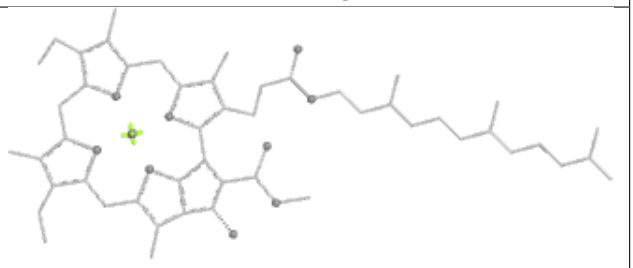
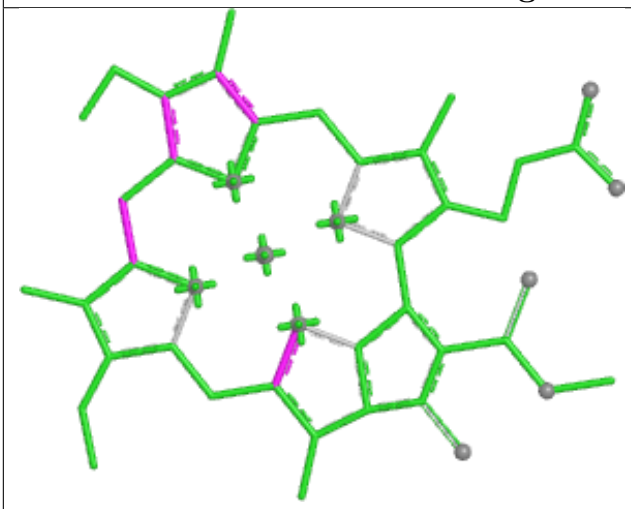


Rings

Ligand CLA b 1217



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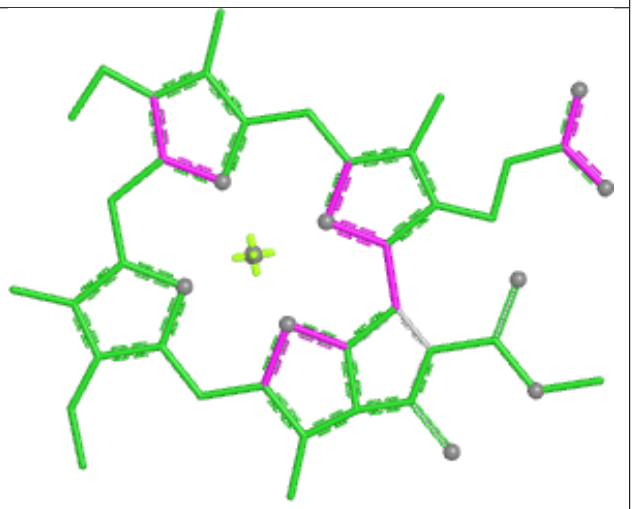
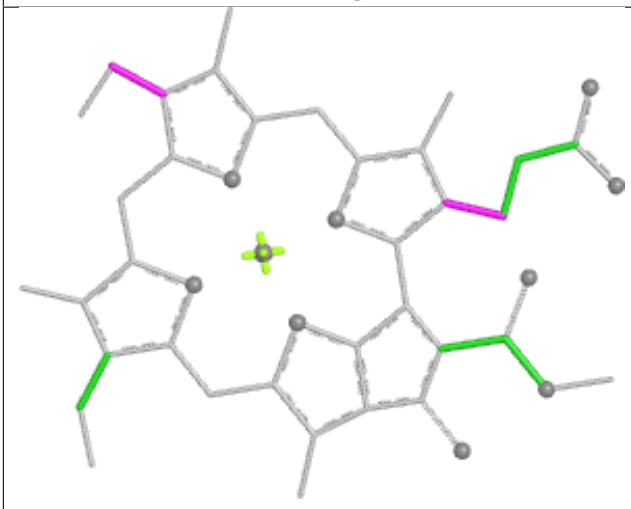


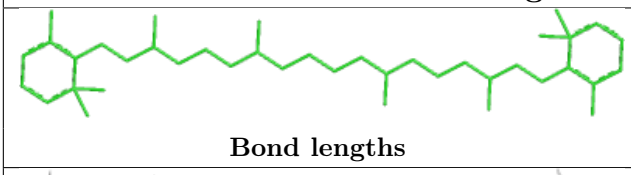
Bond angles



Torsions

Rings

Ligand BCR u 603



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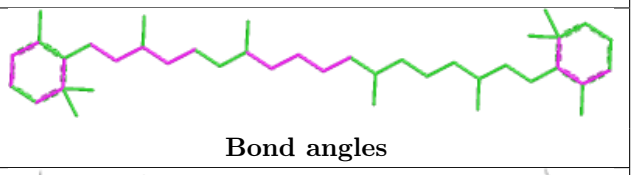

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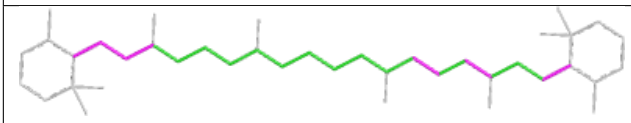

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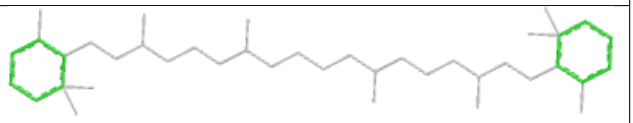
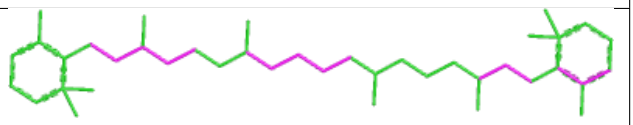


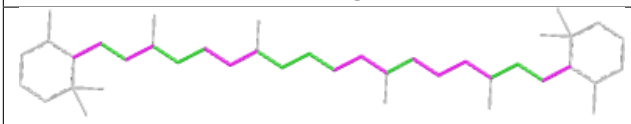
Rings

Ligand BCR t 601

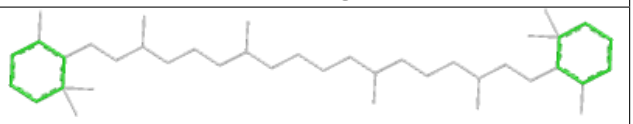
Bond lengths



Bond angles

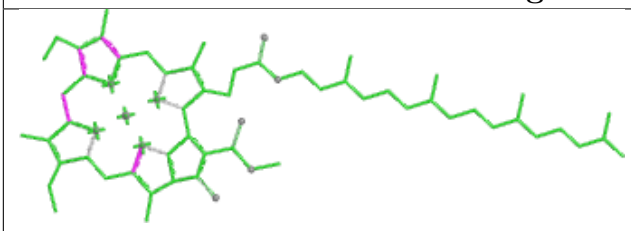


Torsions

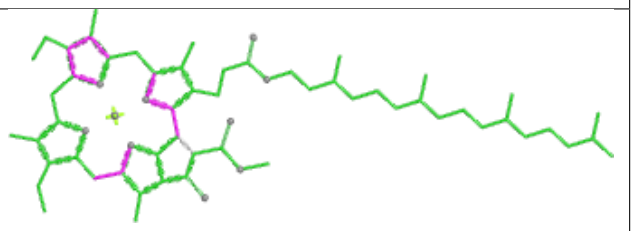


Rings

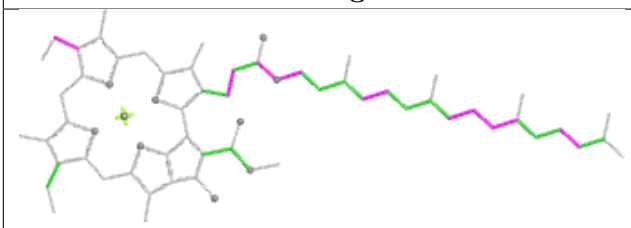
Ligand CLA Z 515



Bond lengths



Bond angles



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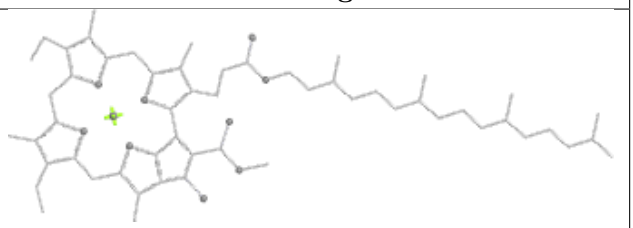
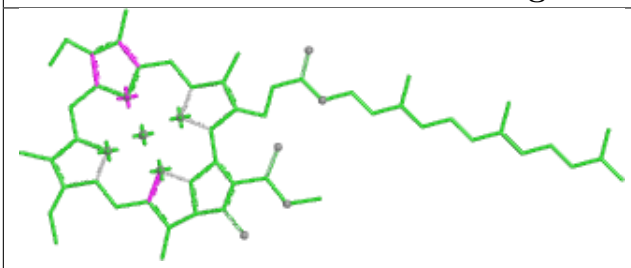
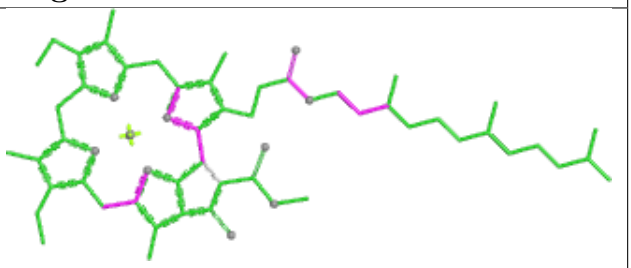
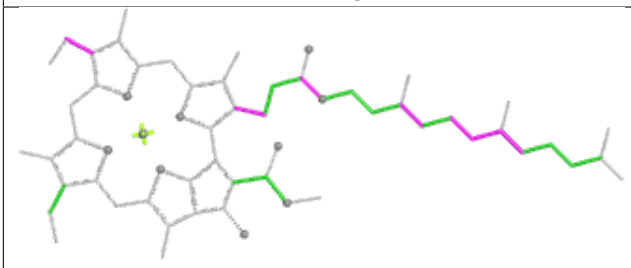
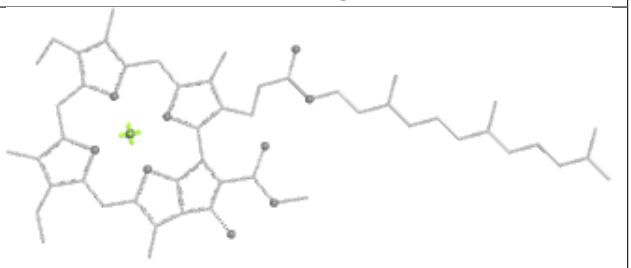
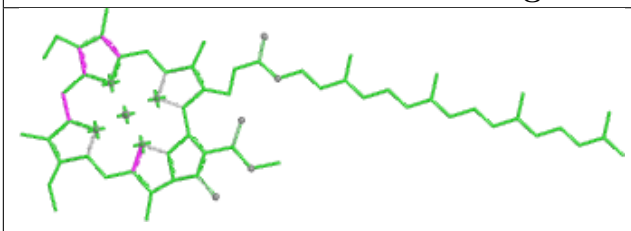
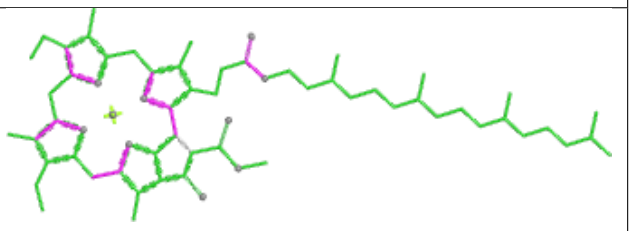
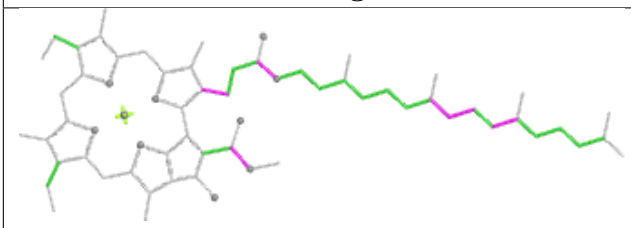
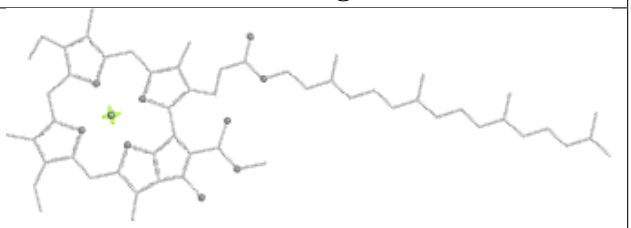
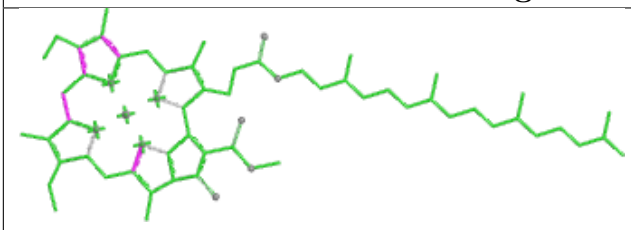


Rings

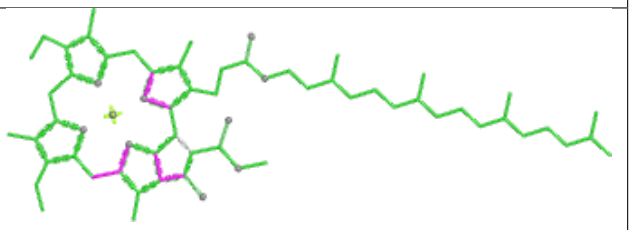
Ligand CLA g 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA X 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

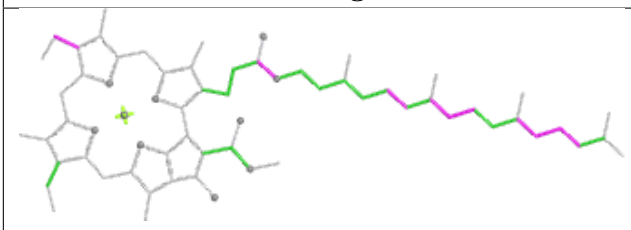
Ligand CLA A 1125



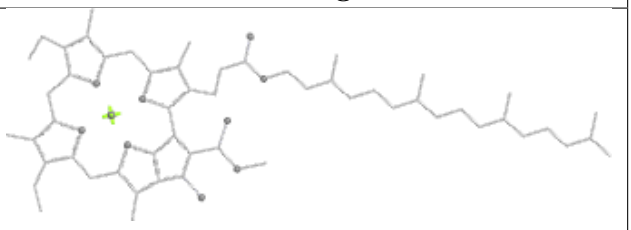
Bond lengths



Bond angles

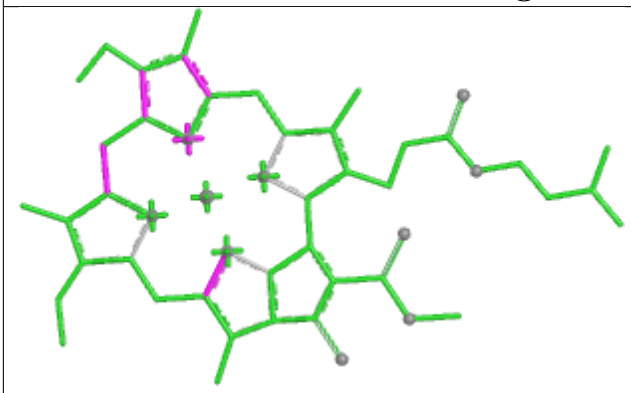


Torsions

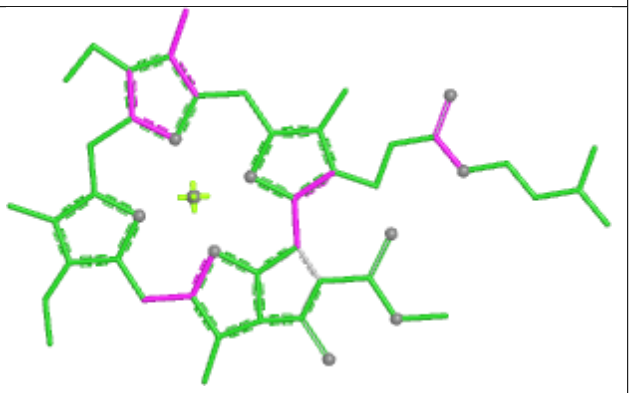


Rings

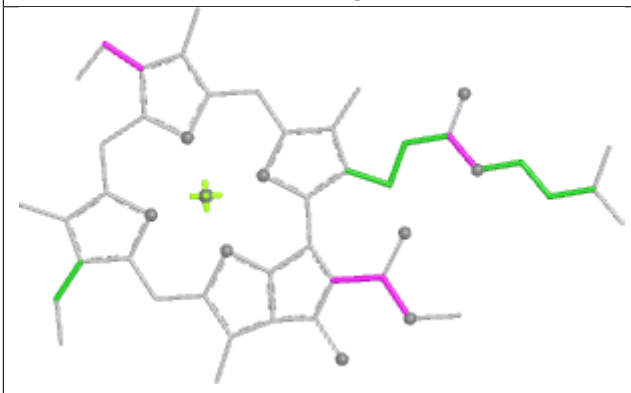
Ligand CLA B 1222



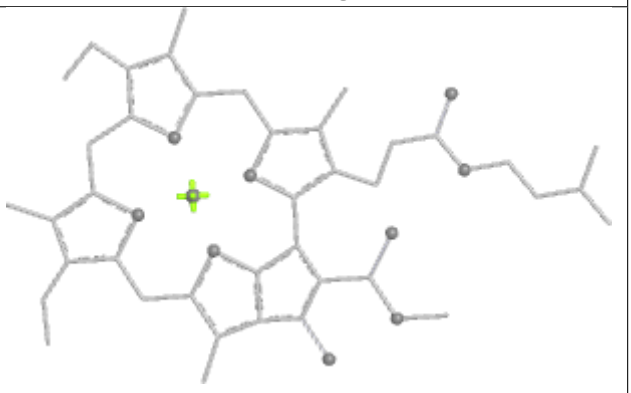
Bond lengths



Bond angles

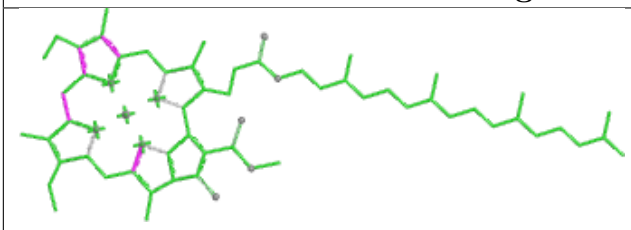


Torsions

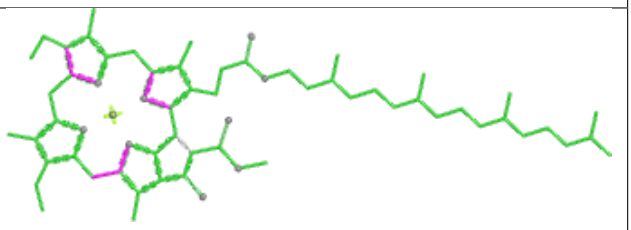


Rings

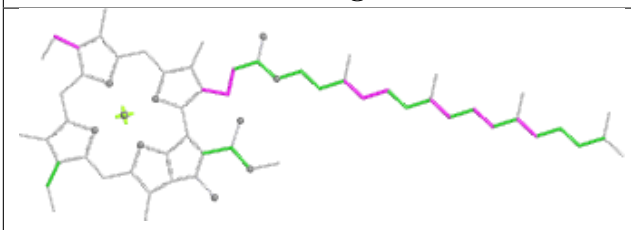
Ligand CLA B 1223



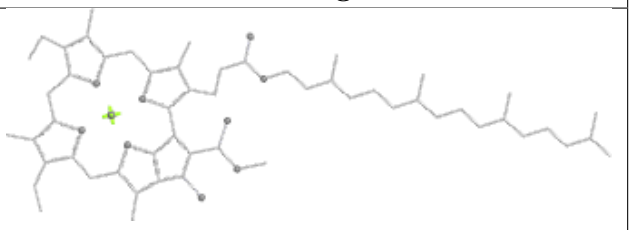
Bond lengths



Bond angles

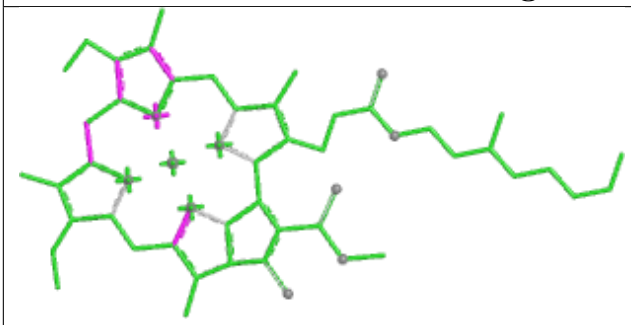


Torsions

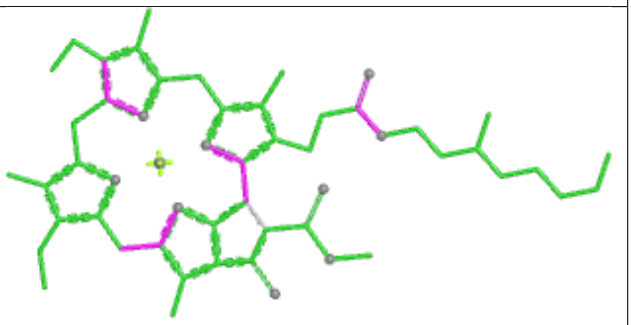


Rings

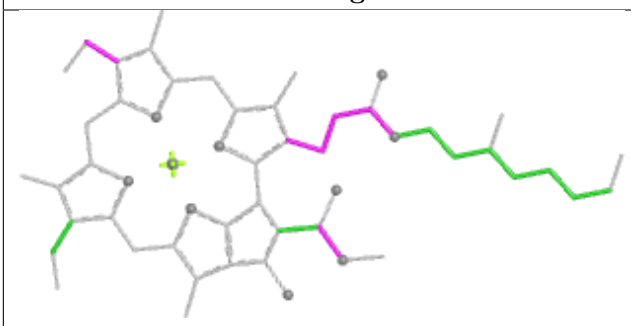
Ligand CLA a 1116



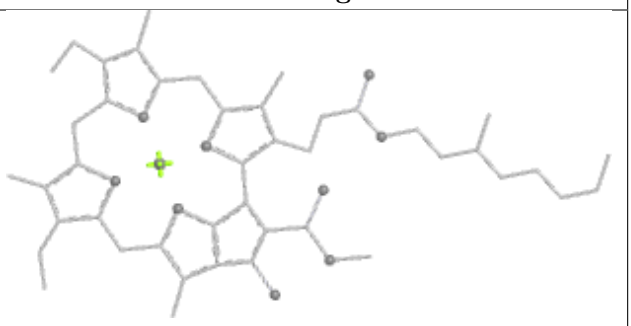
Bond lengths



Bond angles

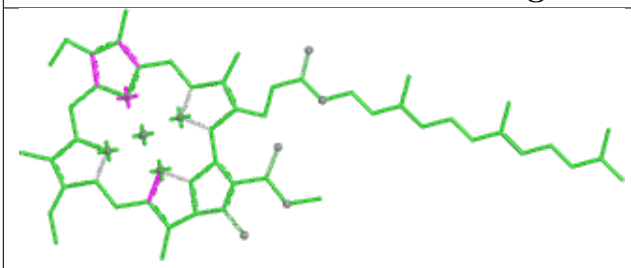


Torsions



Rings

Ligand CLA n 506



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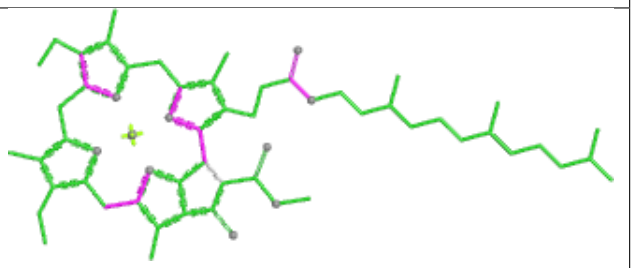
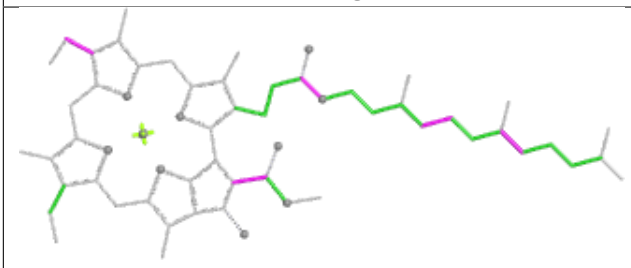
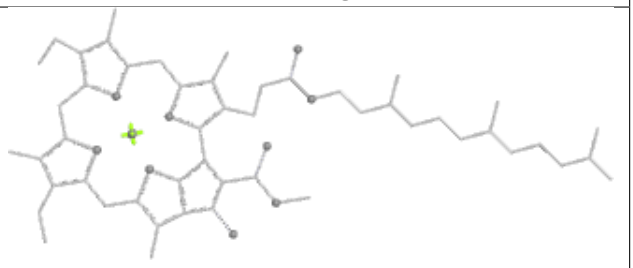


Bond angles

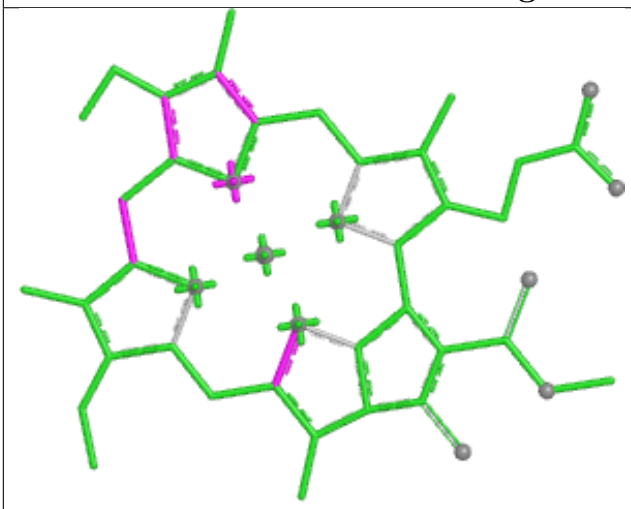


Torsions



Rings

Ligand CLA b 1232



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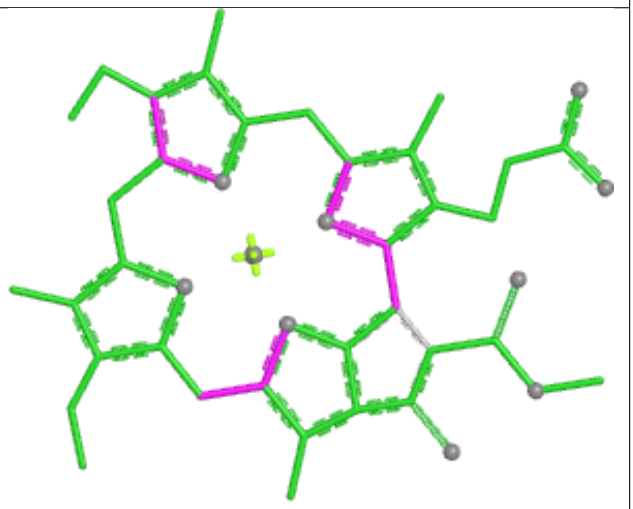
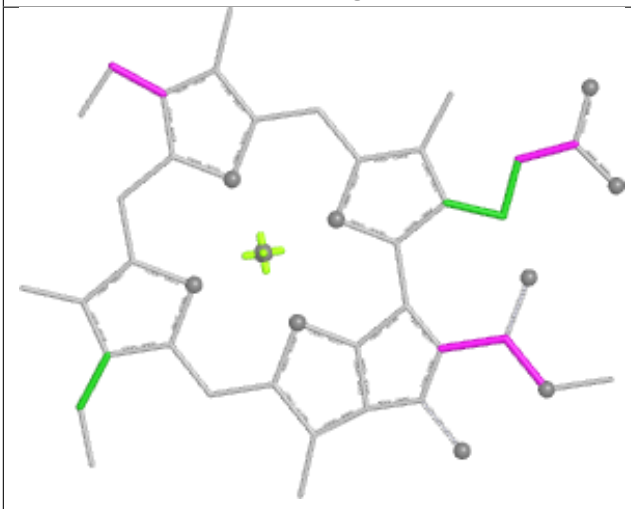


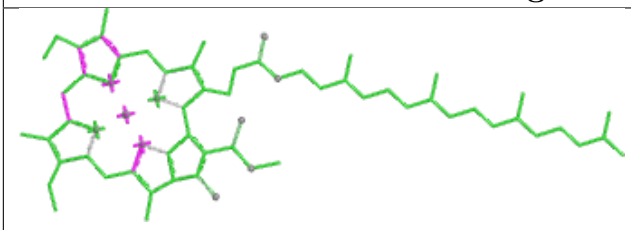
Bond angles



Torsions

Rings

Ligand CLA n 512



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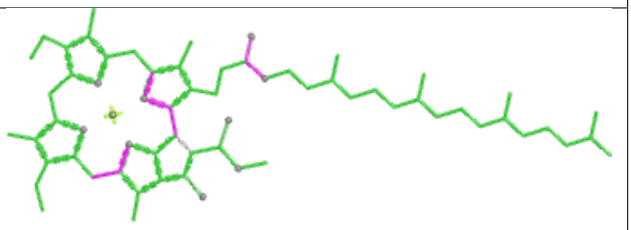
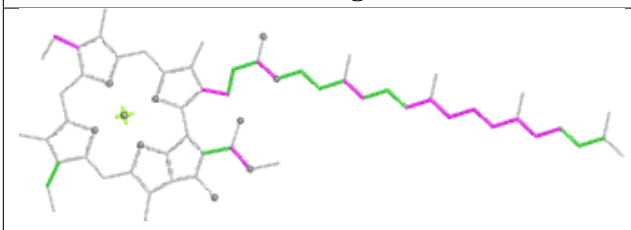
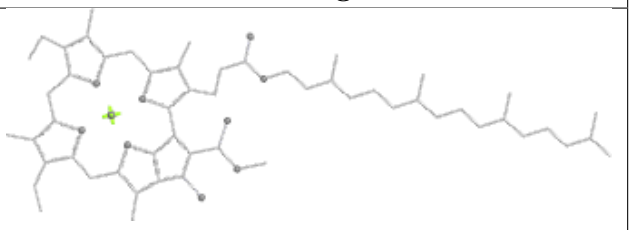


Bond angles

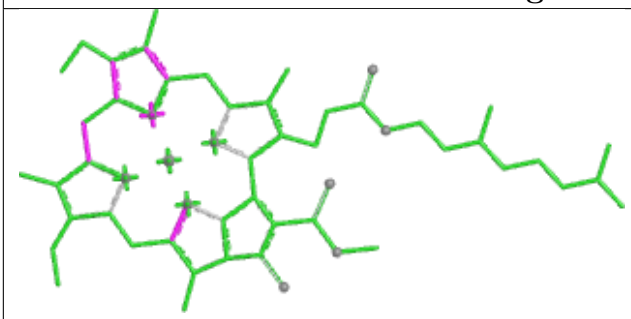


Torsions



Rings

Ligand CLA Z 517



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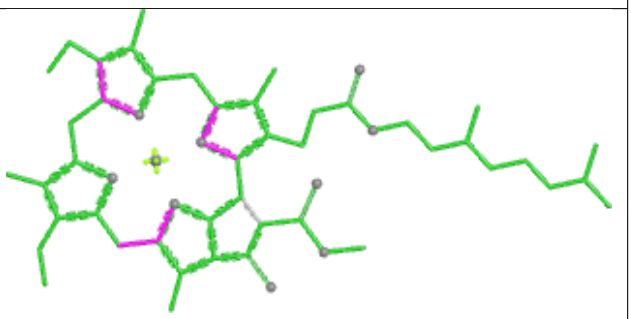
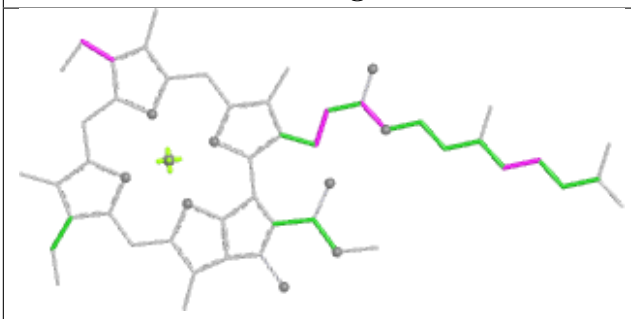
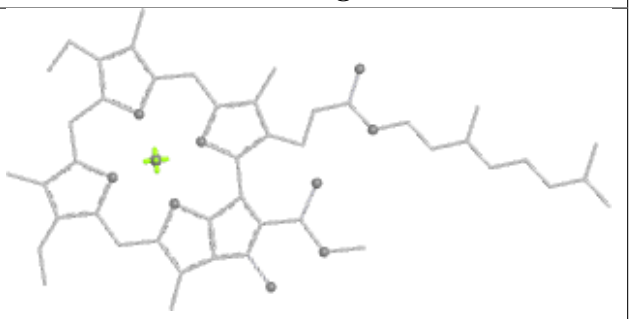


Bond angles

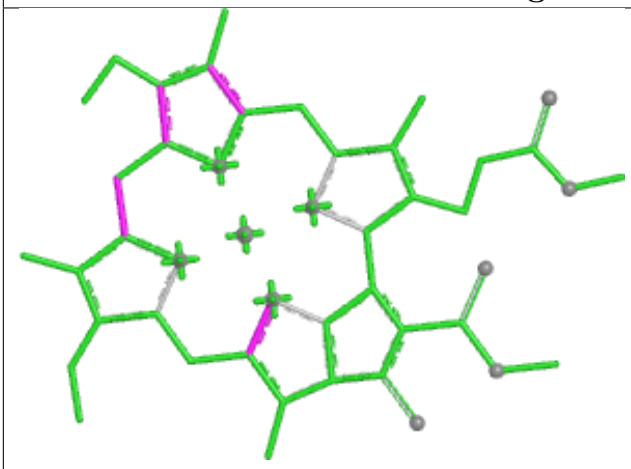


Torsions

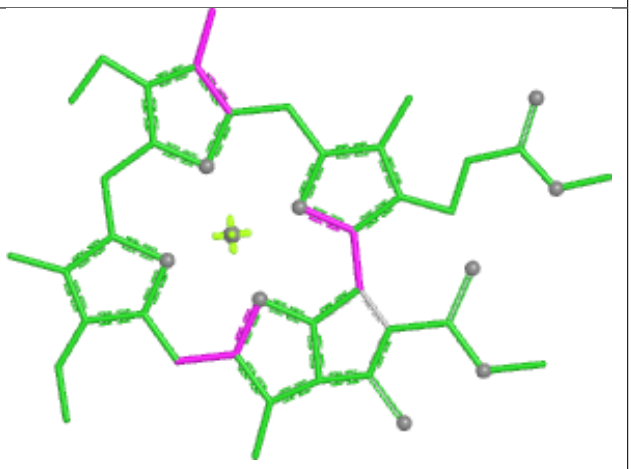


Rings

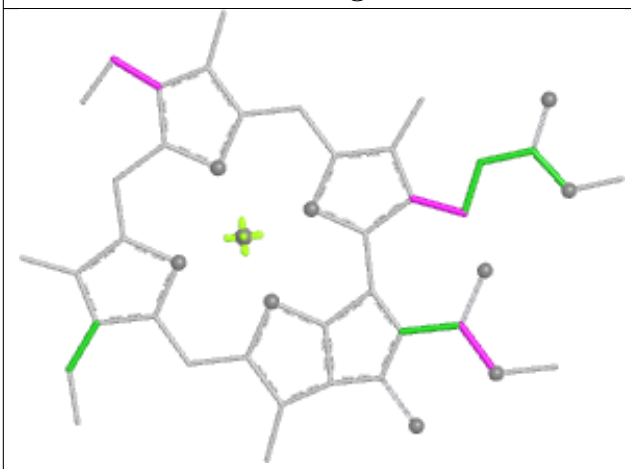
Ligand CLA v 516



Bond lengths



Bond angles



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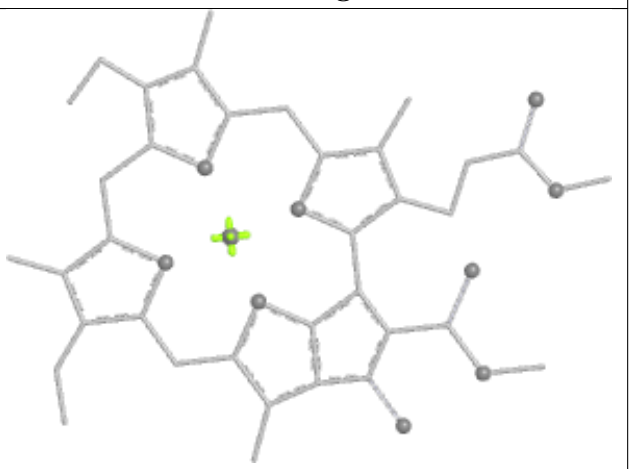
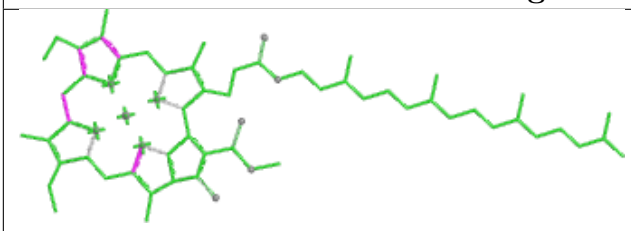


Rings

Ligand CLA y 509



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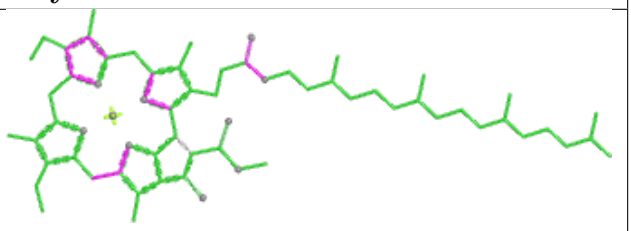

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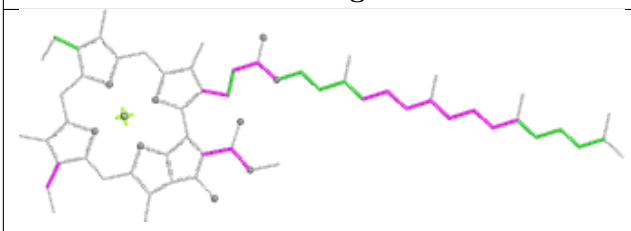

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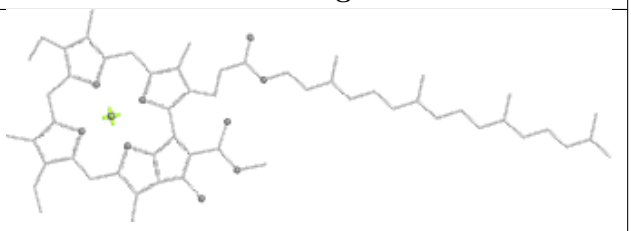
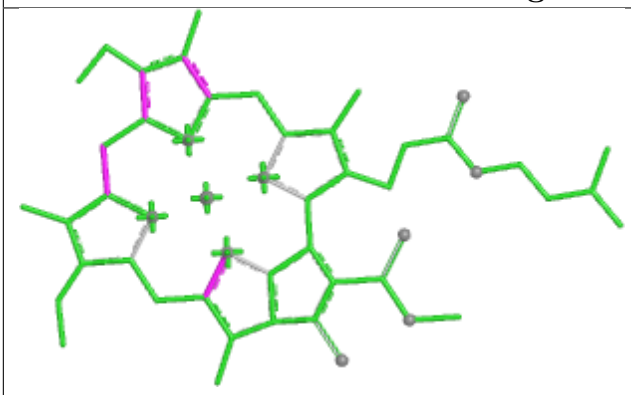


Rings

Ligand CLA n 501



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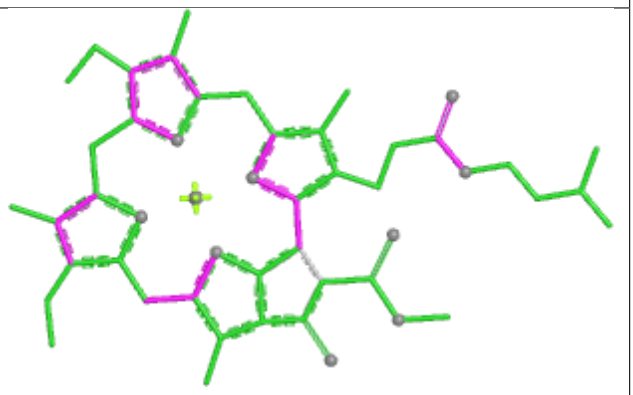
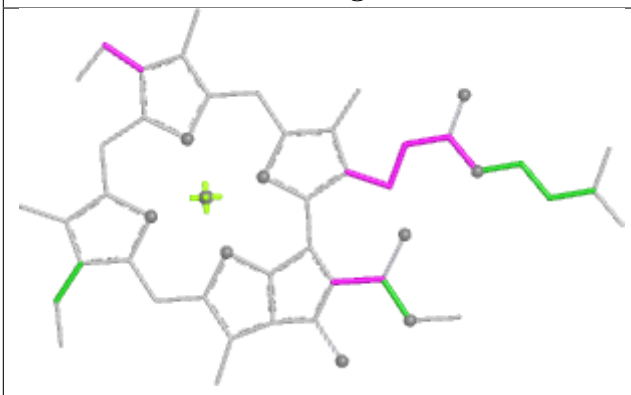


Bond angles



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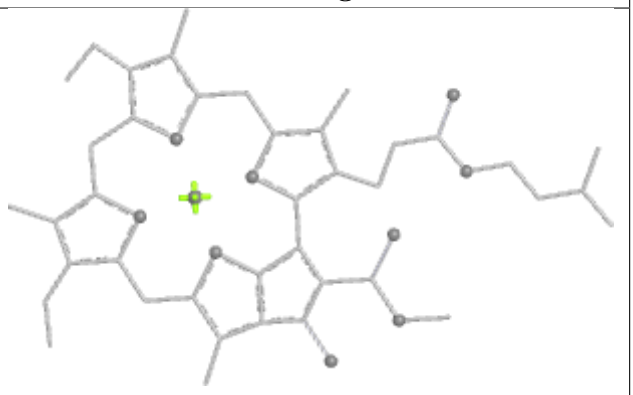
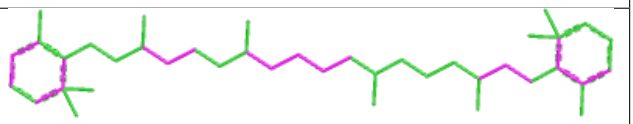


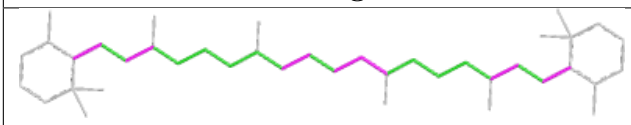
Rings

Ligand BCR s 602

Bond lengths



Bond angles



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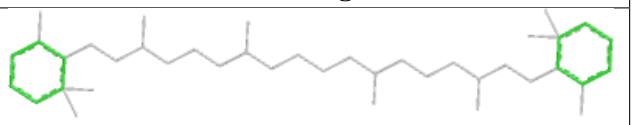
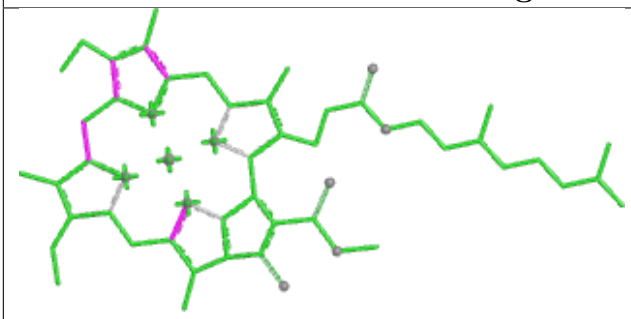
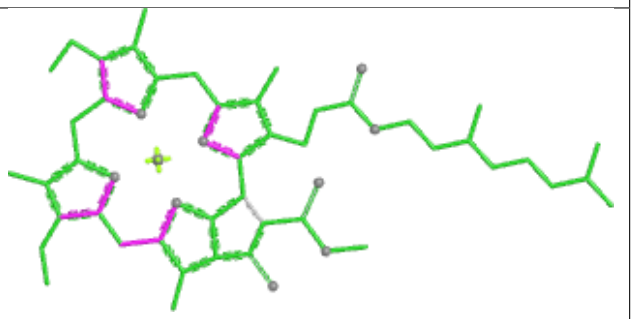


Rings

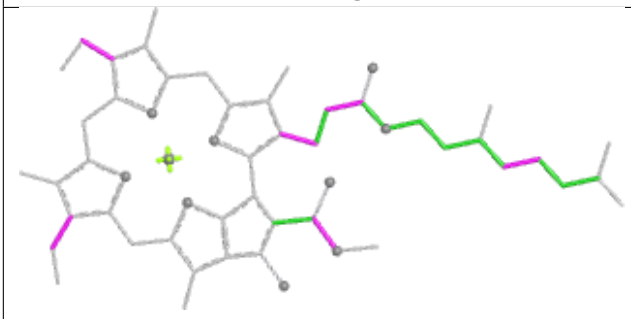
Ligand CLA B 1214



Bond lengths



Bond angles



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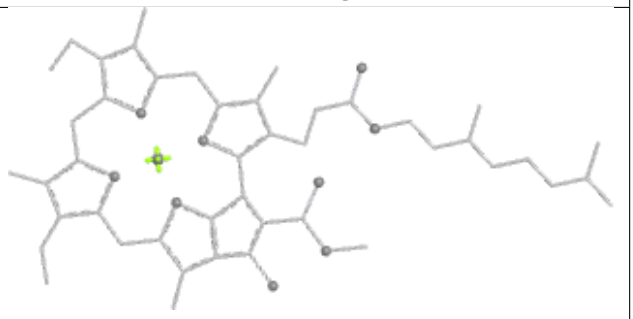
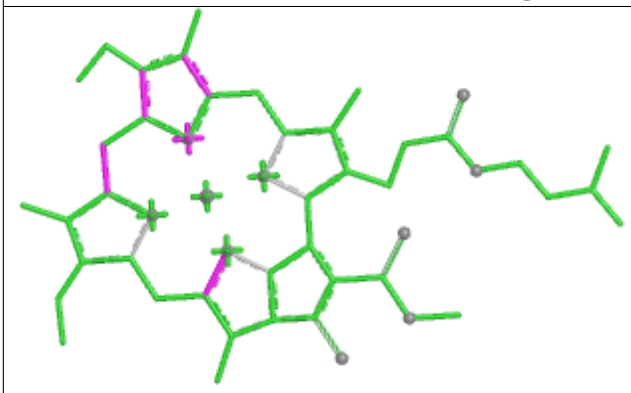


Rings

Ligand CLA b 1236



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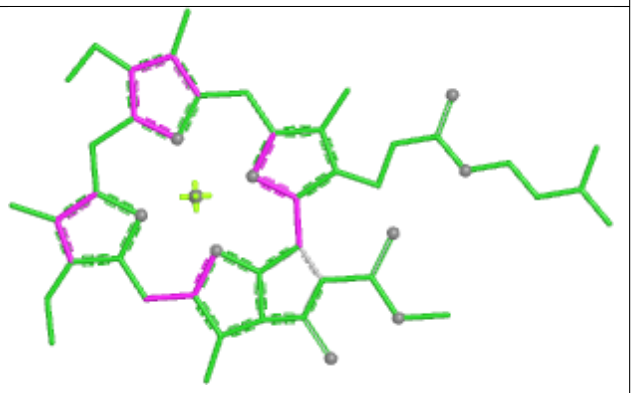
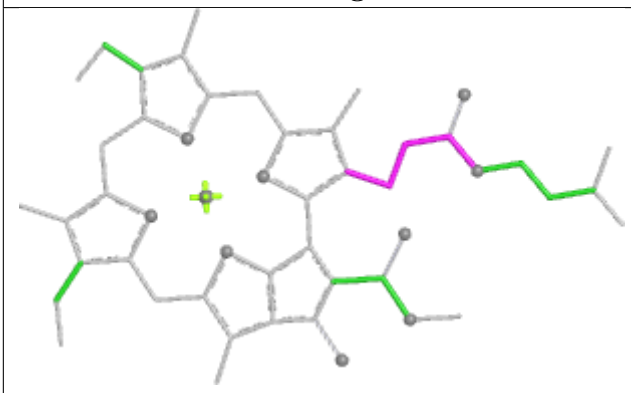
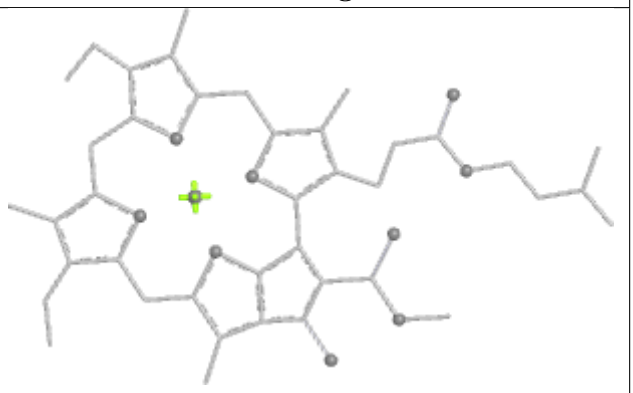


Bond angles

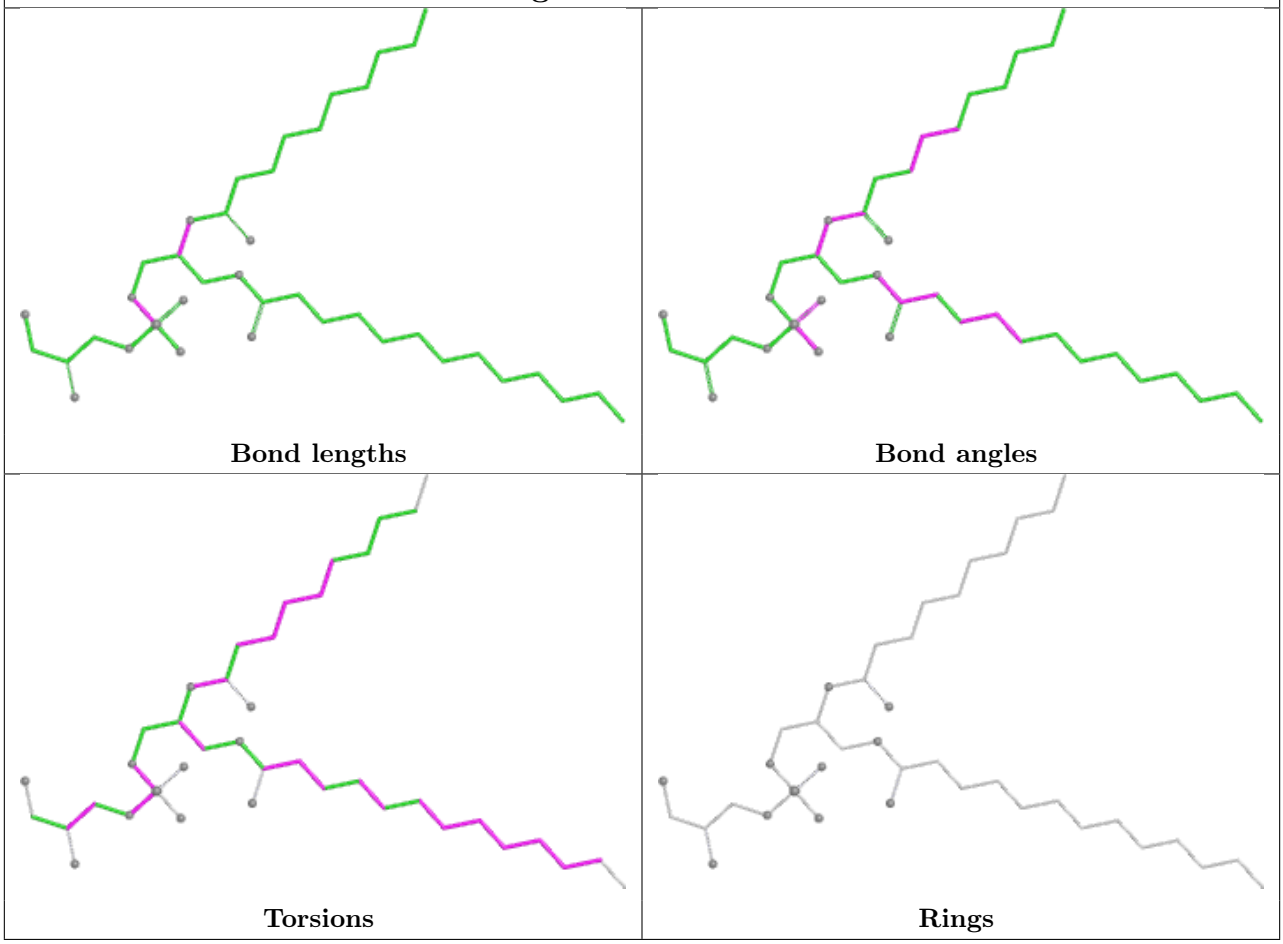


Torsions

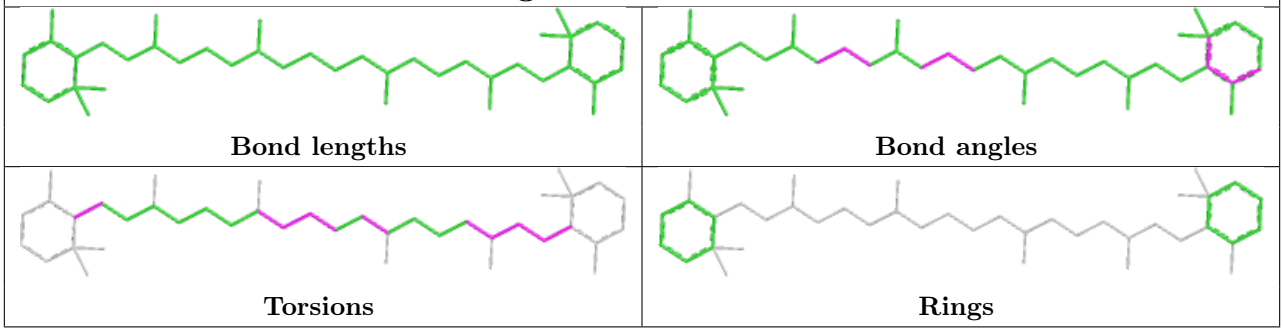


Rings

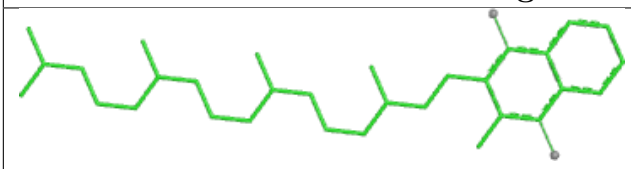
Ligand LHG i 103



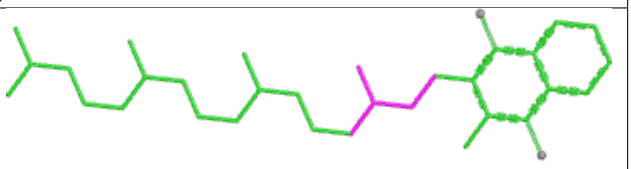
Ligand BCR b 4017



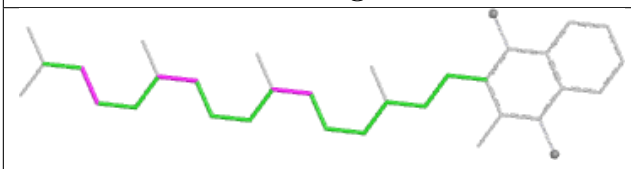
Ligand PQN a 2001



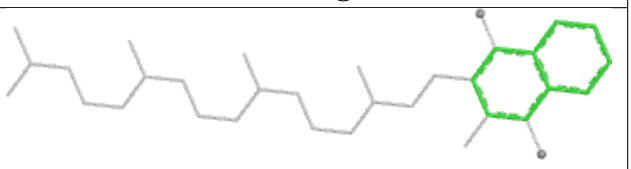
Bond lengths



Bond angles

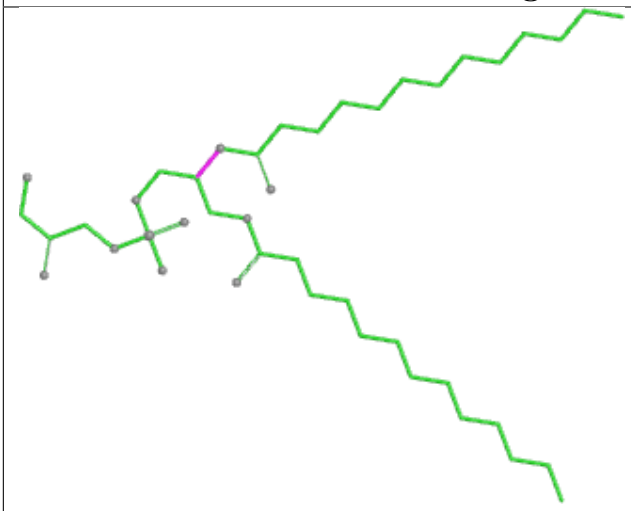


Torsions

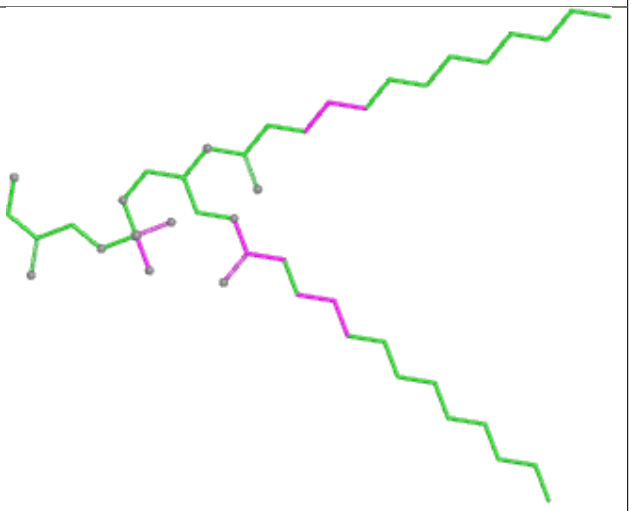


Rings

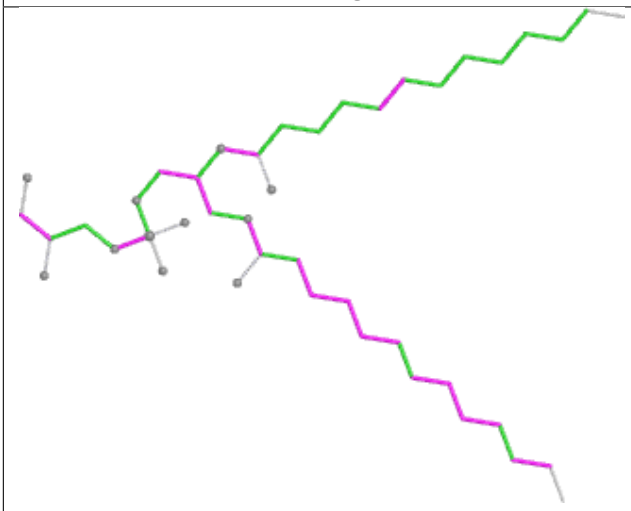
Ligand LHG A 849



Bond lengths



Bond angles



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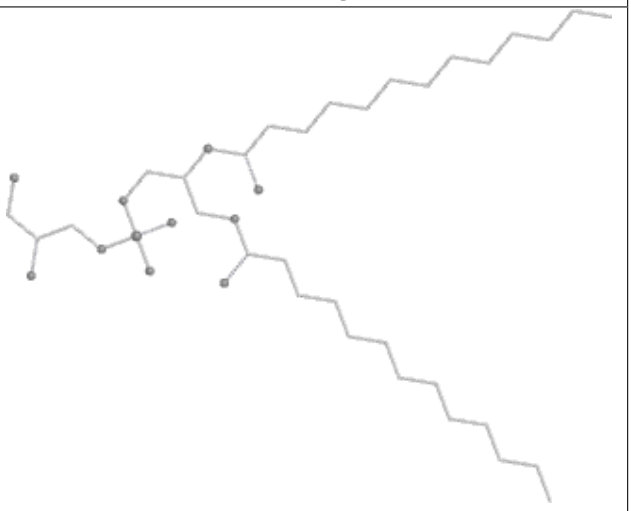
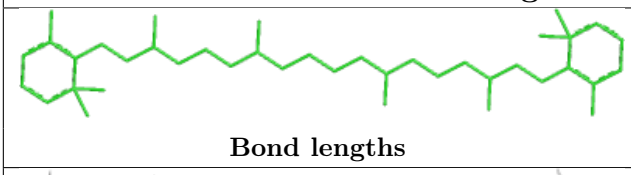
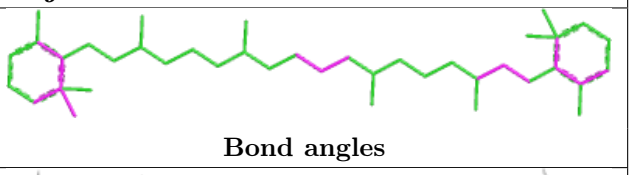


Rings

Ligand BCR j 4013



Bond lengths



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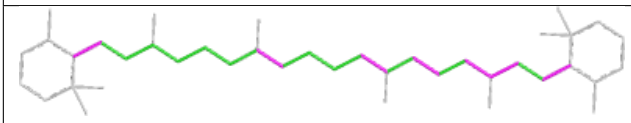
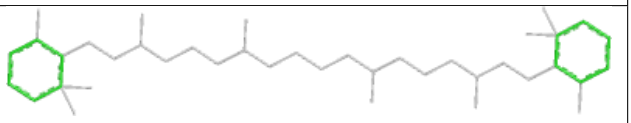
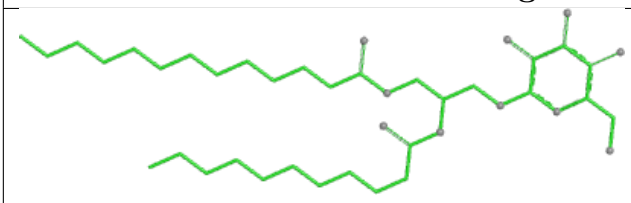


Torsions



Rings

Ligand LMG G 848



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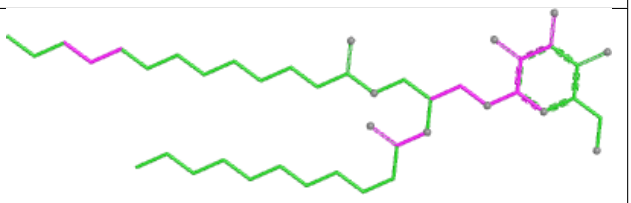

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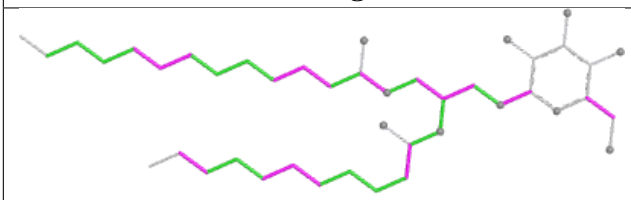

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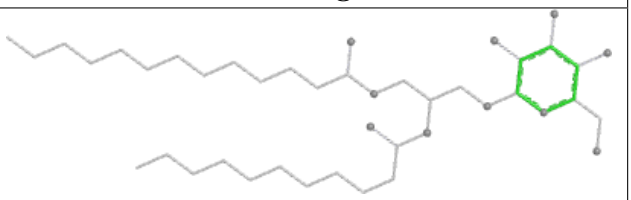
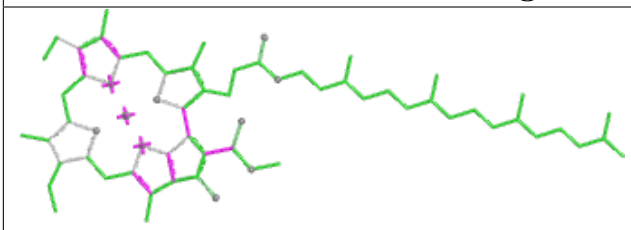


Rings

Ligand CL0 H 1011



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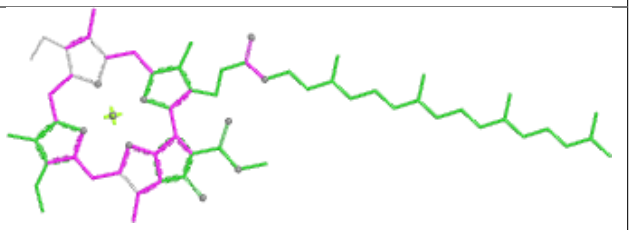

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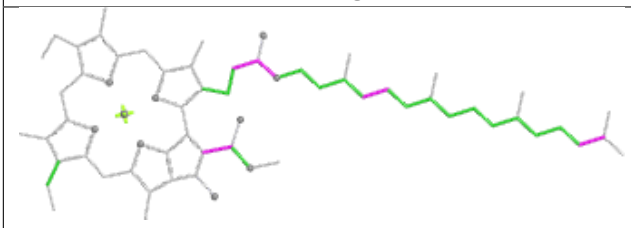

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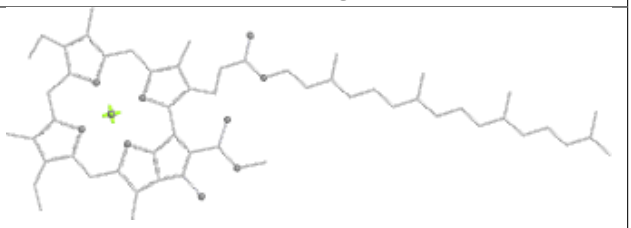
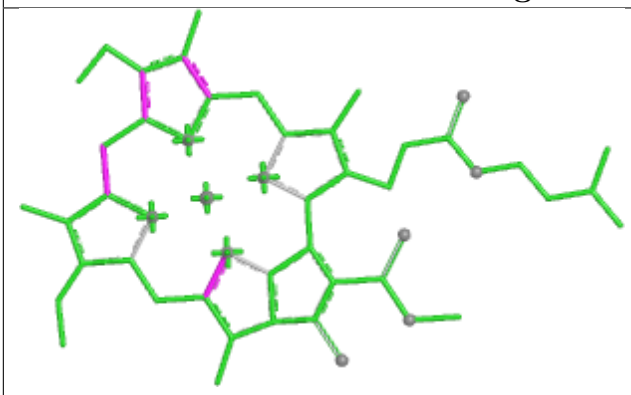


Rings

Ligand CLA G 1236



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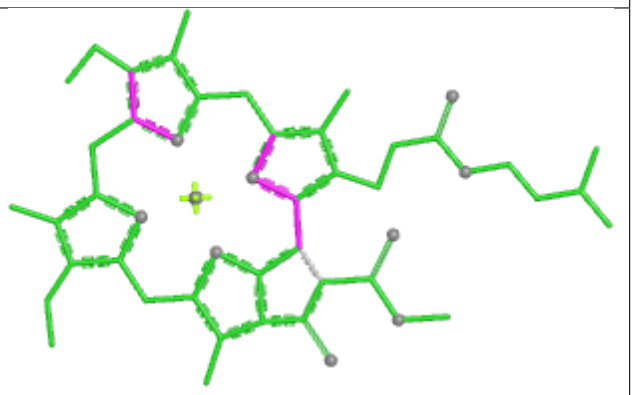

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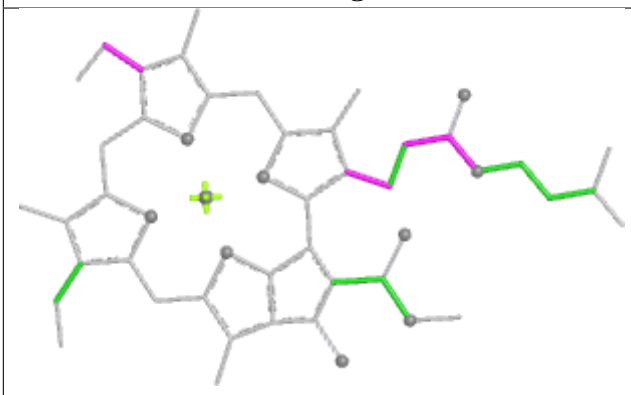

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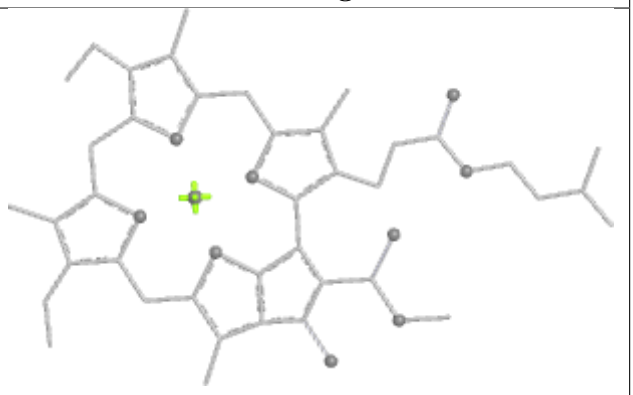
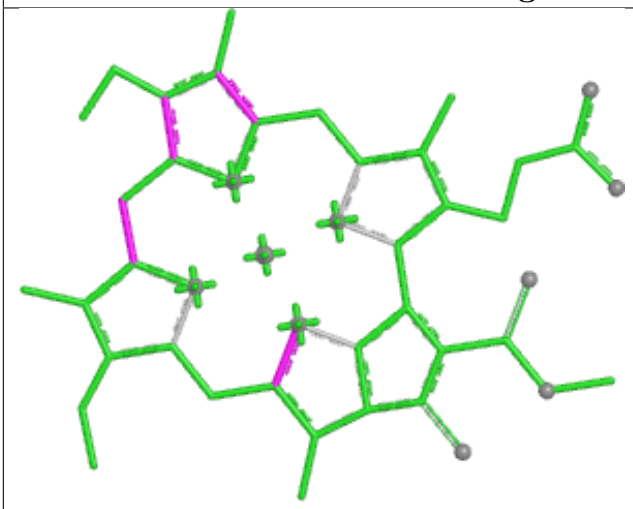


Rings

Ligand CLA b 1209



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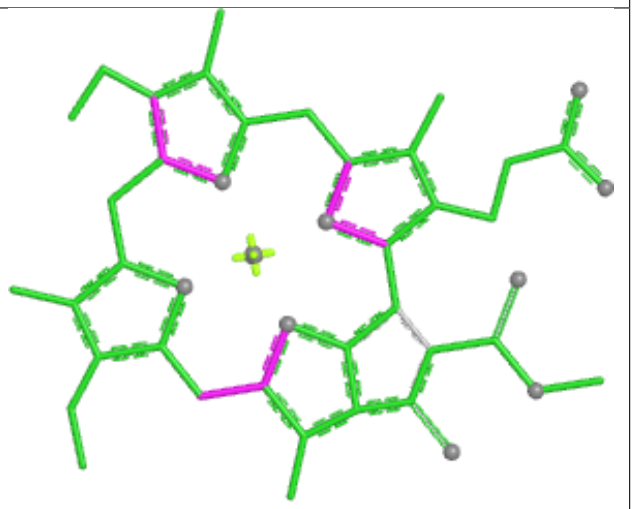

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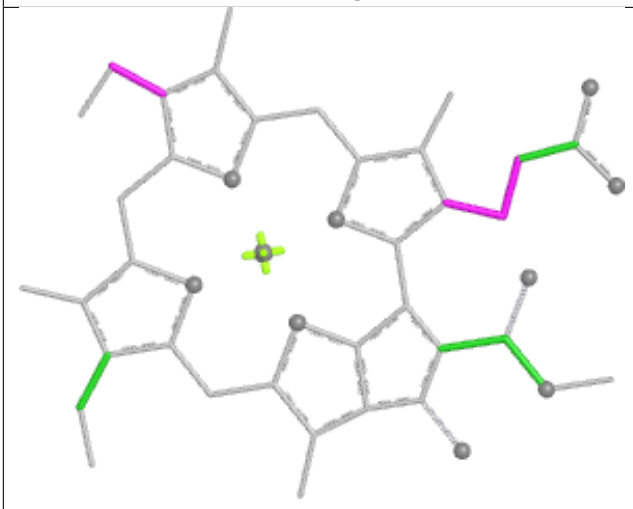
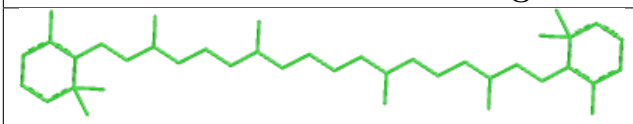


Torsions

Rings

Ligand BCR G 4017



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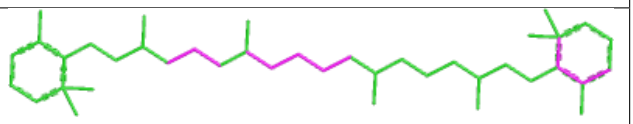

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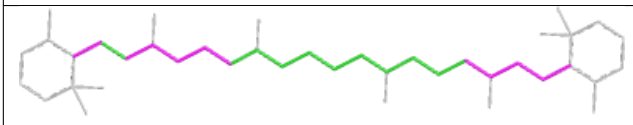

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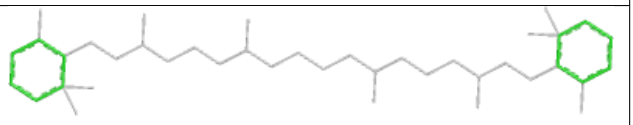
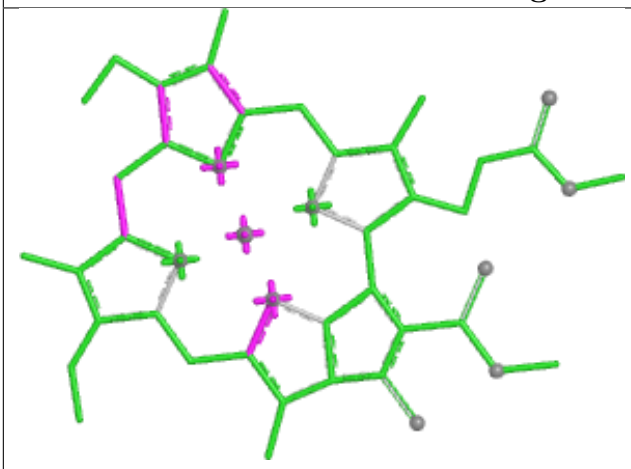


Rings

Ligand CLA s 503



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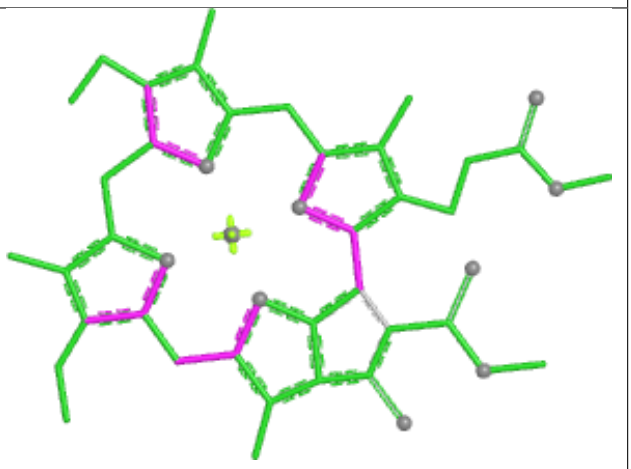

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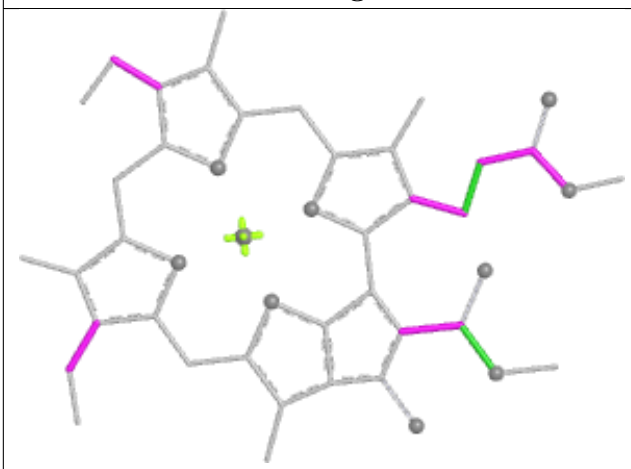

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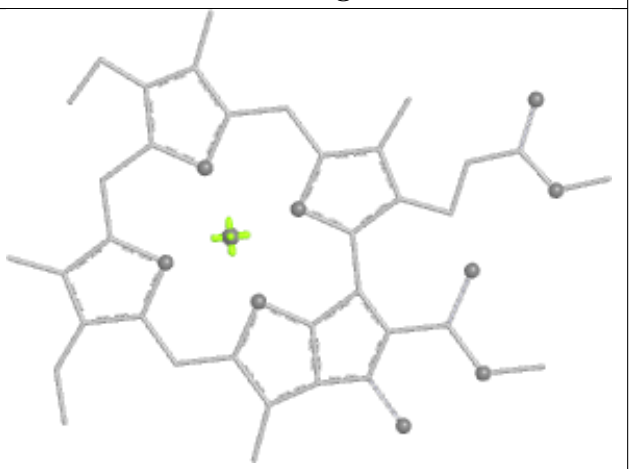
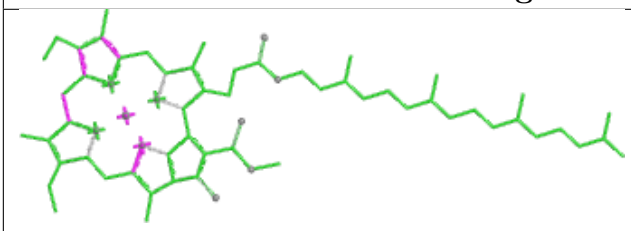


Rings

Ligand CLA B 1207



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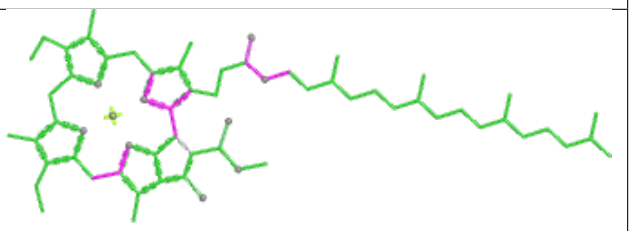

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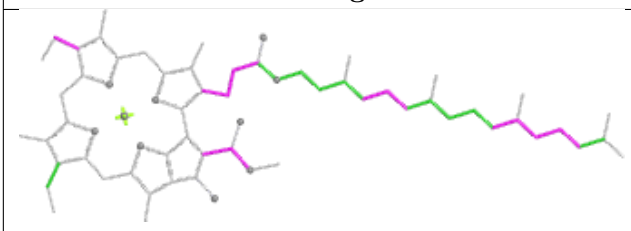

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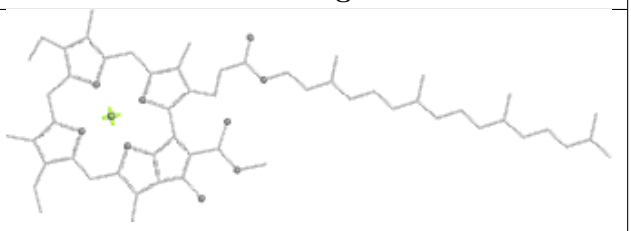
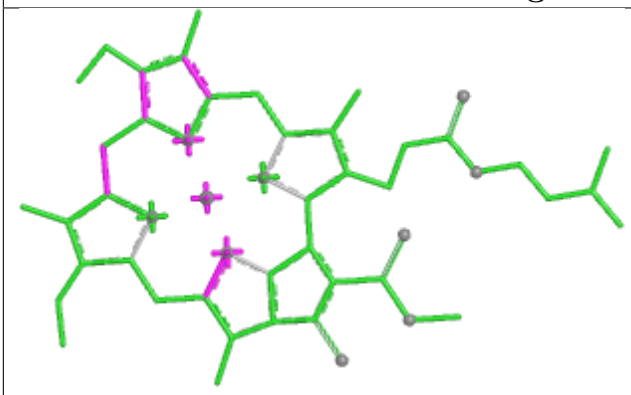


Rings

Ligand CLA n 502



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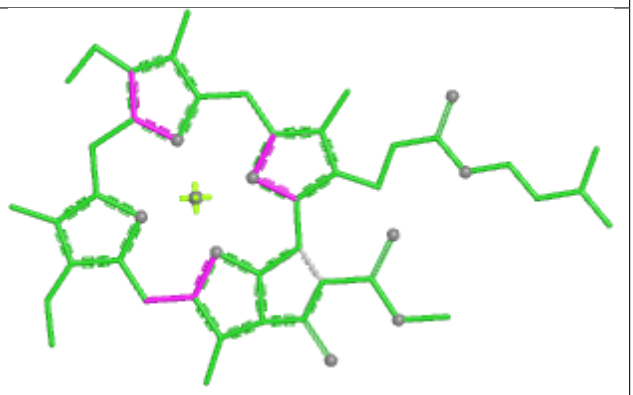
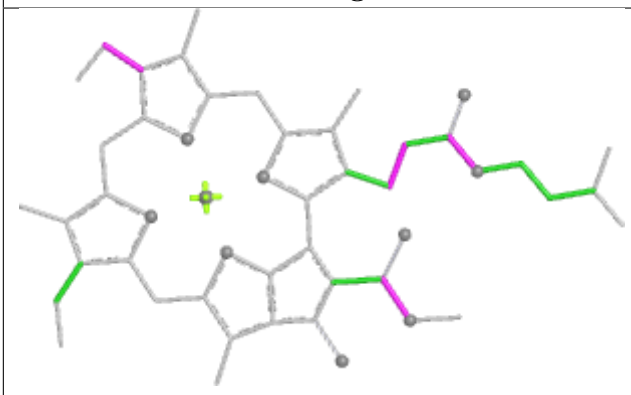


Bond angles



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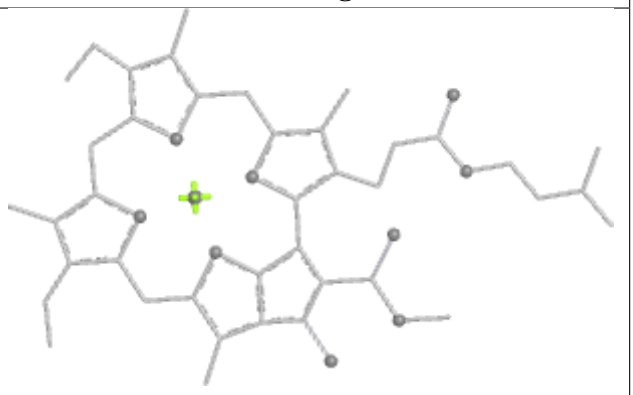
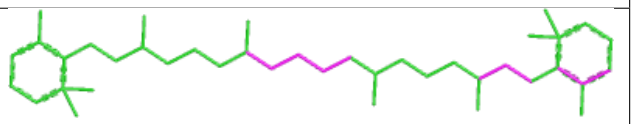


Rings

Ligand BCR r 602

Bond lengths



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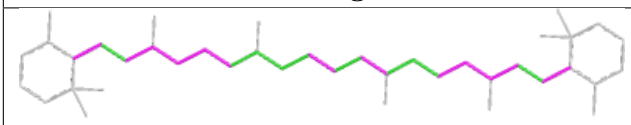

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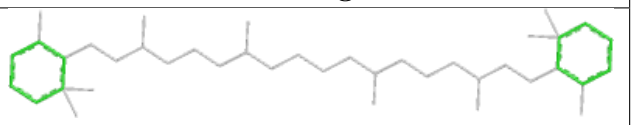
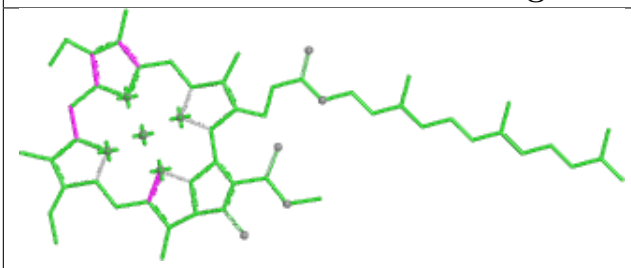


Rings

Ligand CLA u 510



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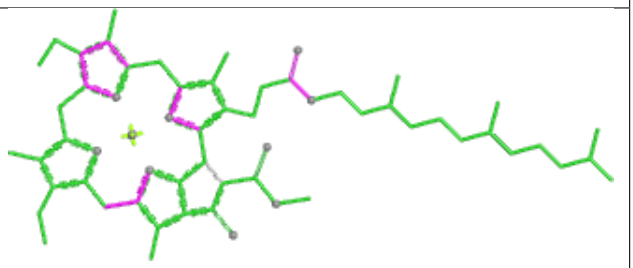
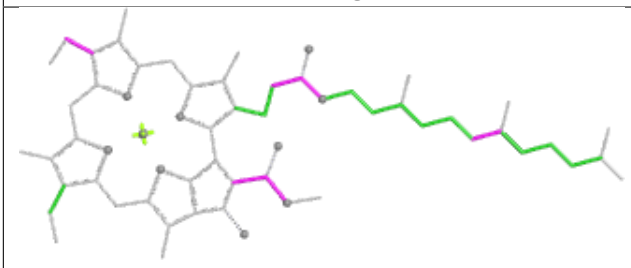


Bond angles



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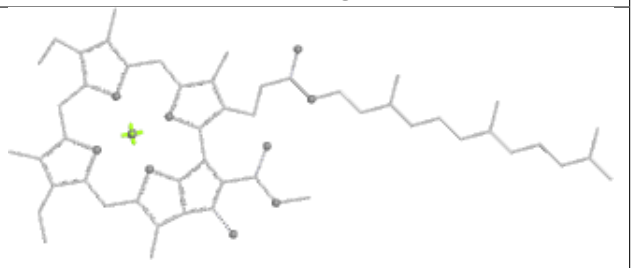
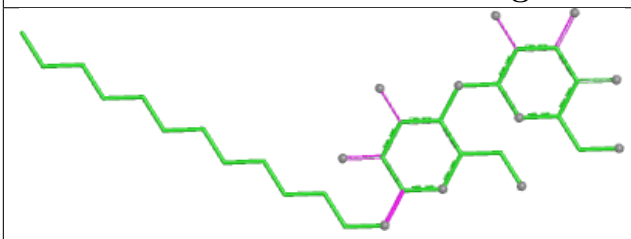


Rings

Ligand LMT A 4202



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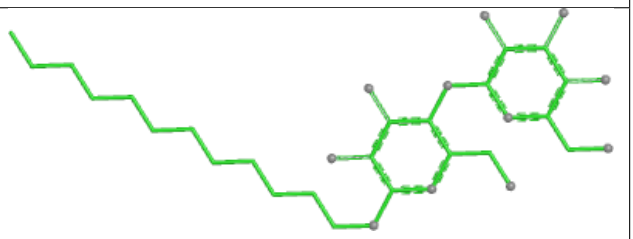
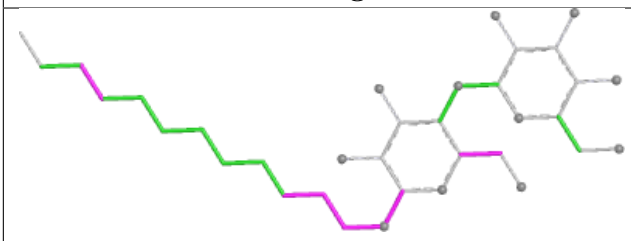


Bond angles



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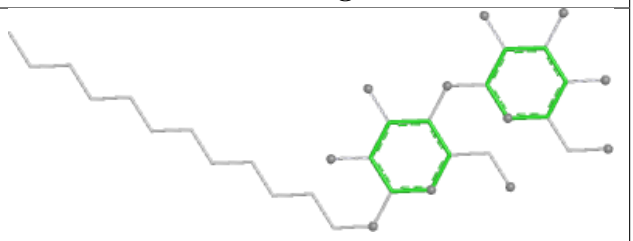
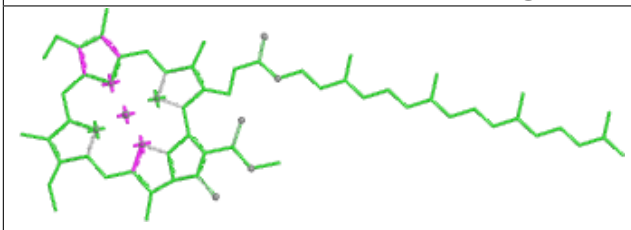
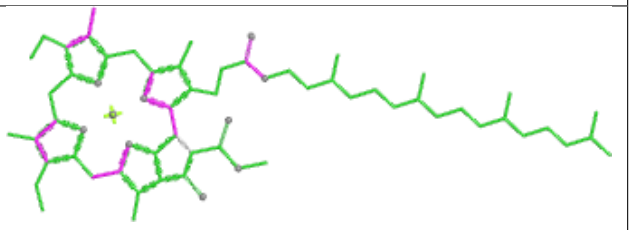
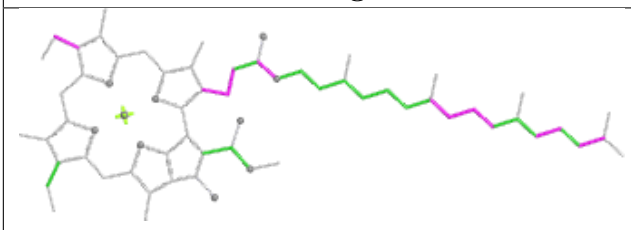
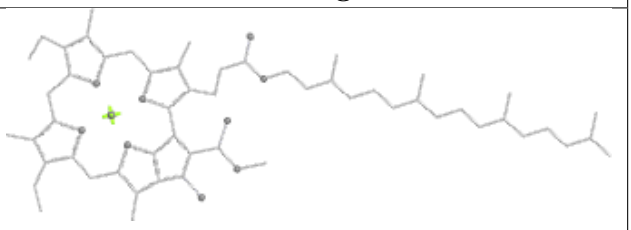
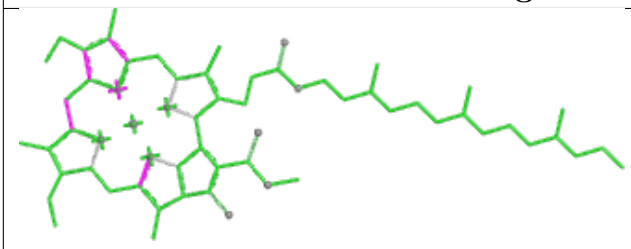
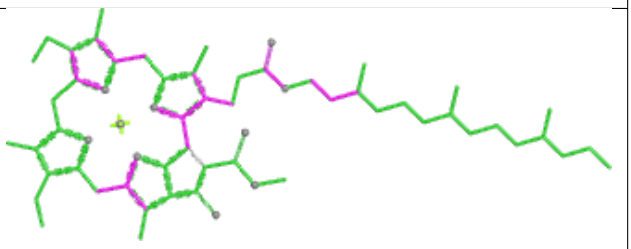
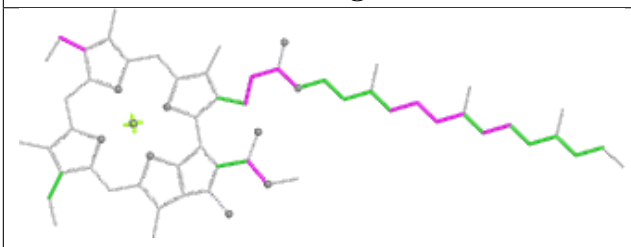
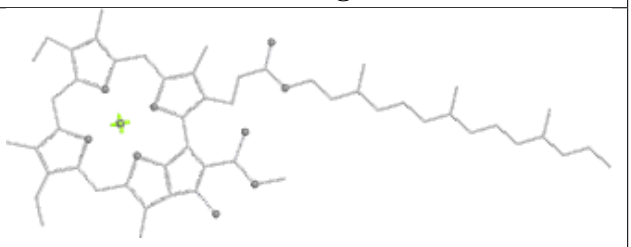
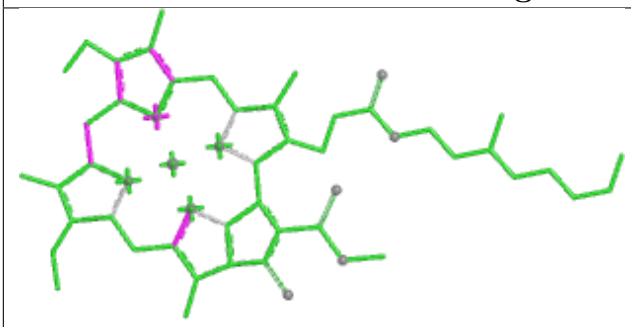


Rings

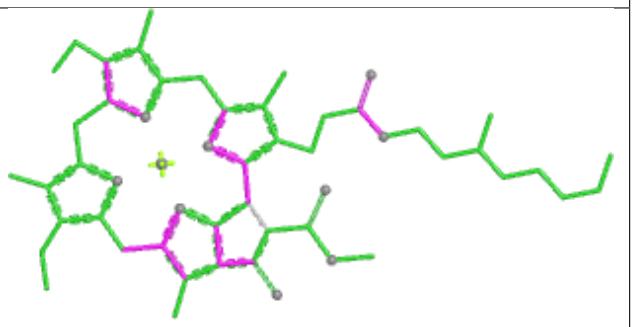
Ligand CLA a 1237	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1235	
 Bond lengths	 Bond angles
 Torsions	 Rings

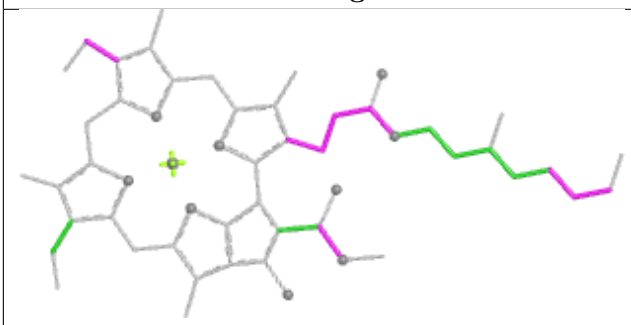
Ligand CLA A 1116



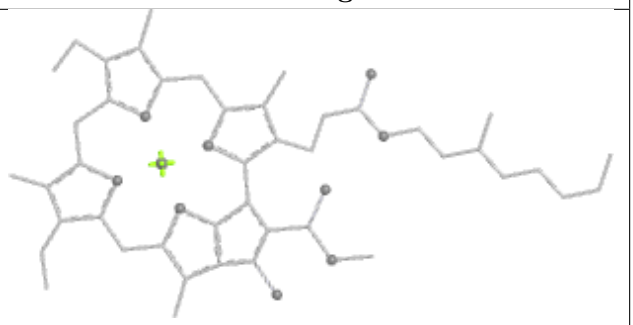
Bond lengths



Bond angles

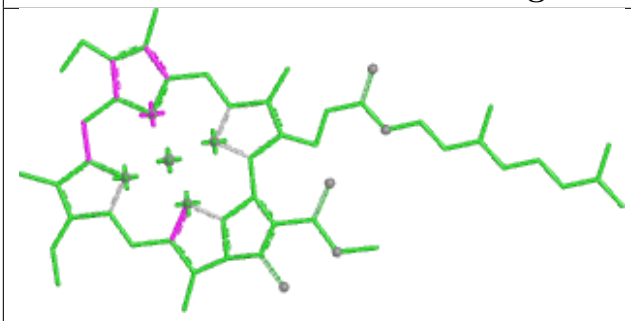


Torsions

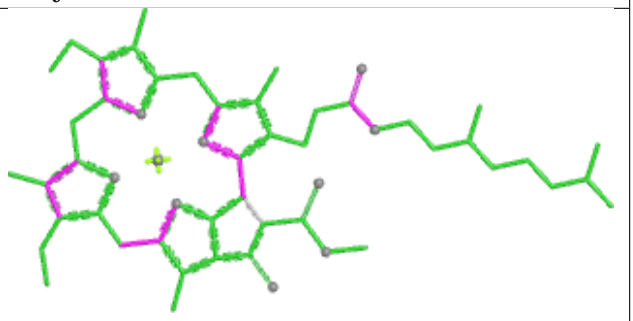


Rings

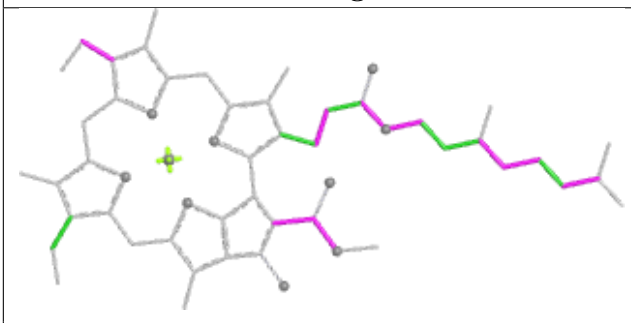
Ligand CLA y 517



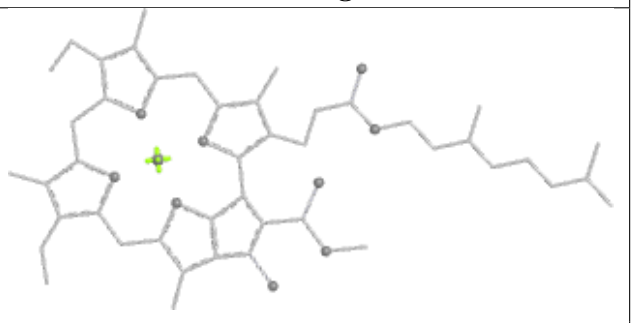
Bond lengths



Bond angles

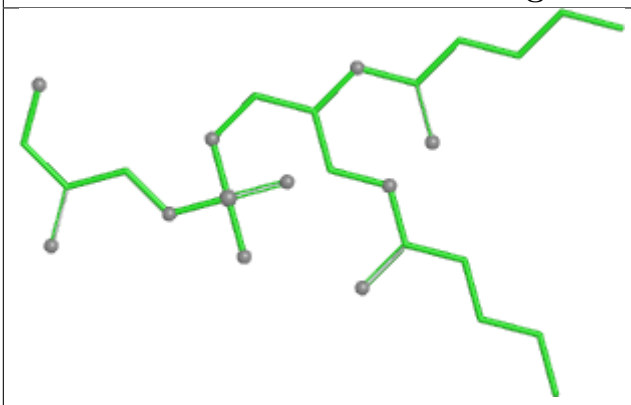


Torsions



Rings

Ligand LHG o 605



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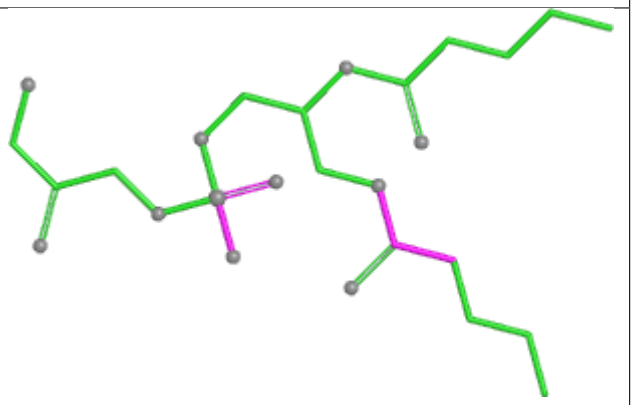
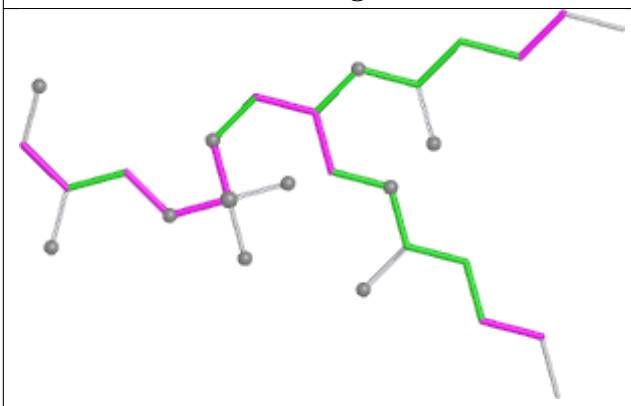
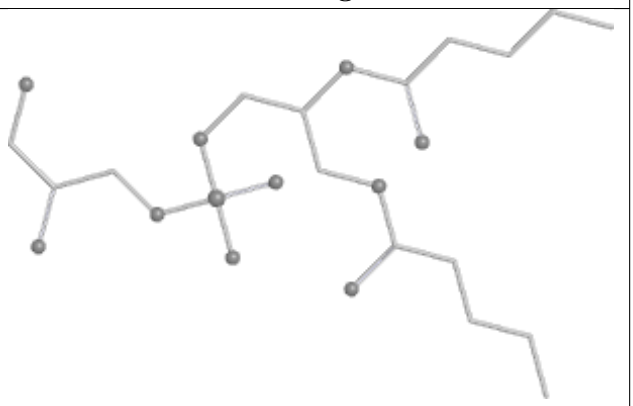


Bond angles

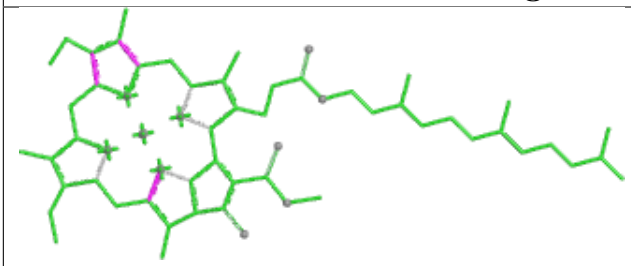


Torsions



Rings

Ligand CLA w 510



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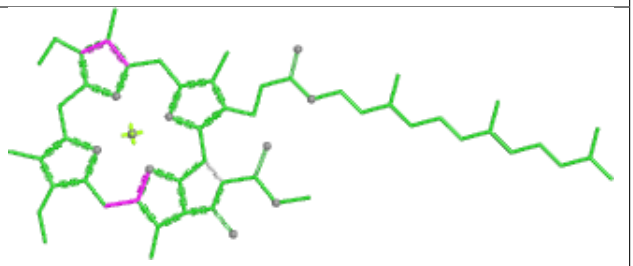
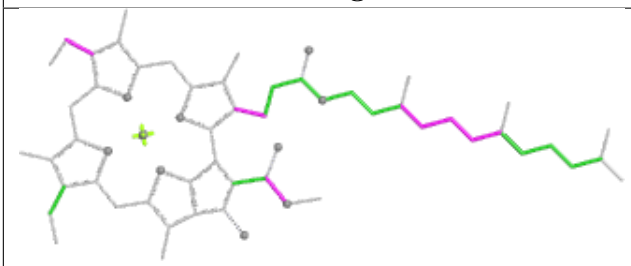


Bond angles



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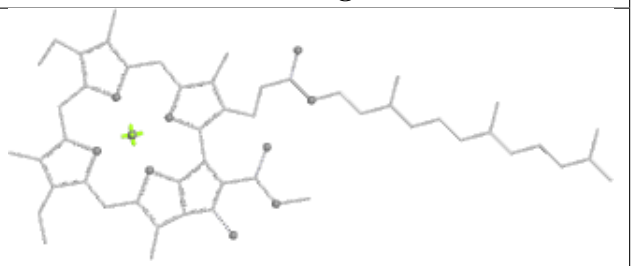
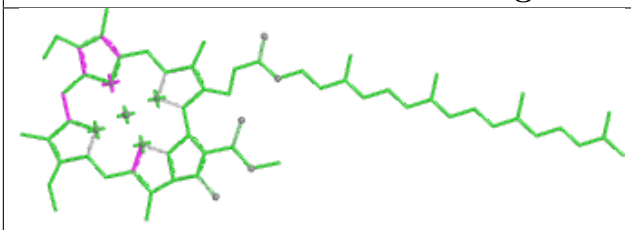
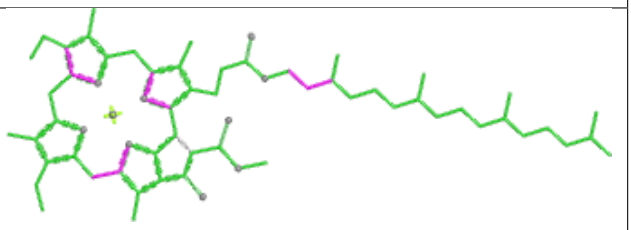


Rings

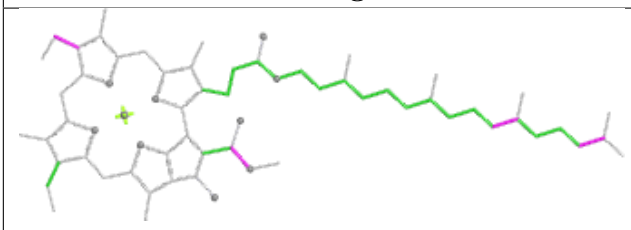
Ligand CLA A 1117



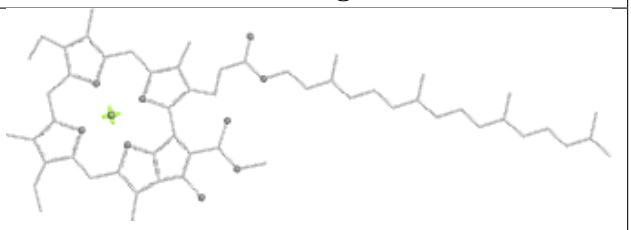
Bond lengths



Bond angles

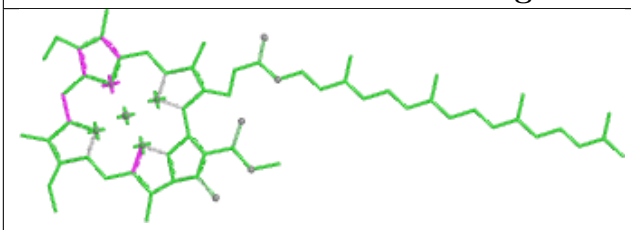


Torsions



Rings

Ligand CLA A 1104



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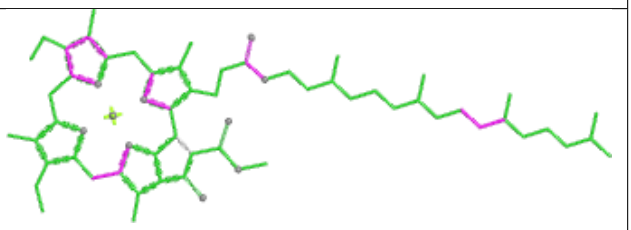
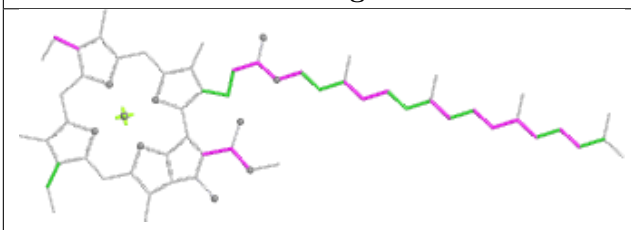


Bond angles



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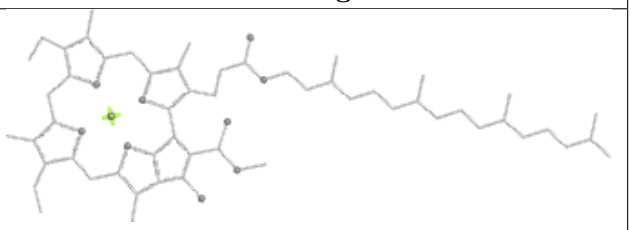
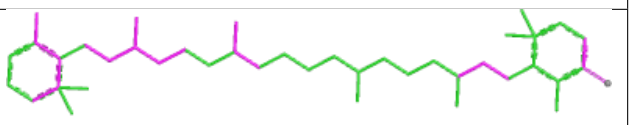


Rings

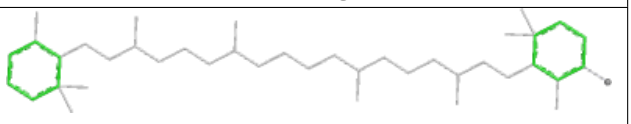
Ligand ECH i 4020

Bond lengths



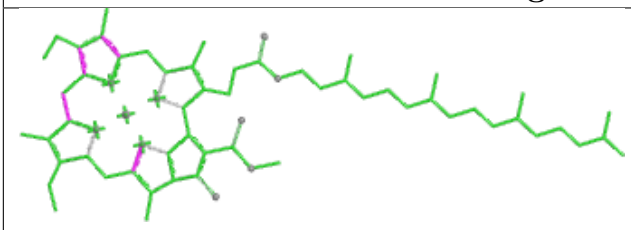
Bond angles

Torsions



Rings

Ligand CLA y 515



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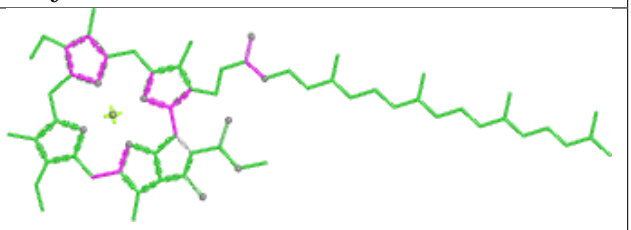
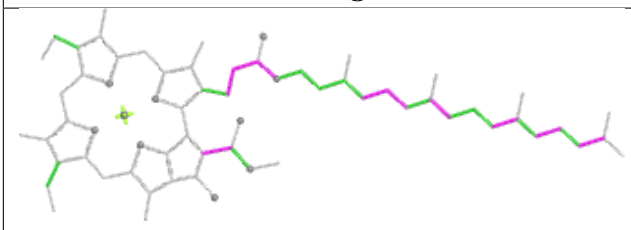


Bond angles



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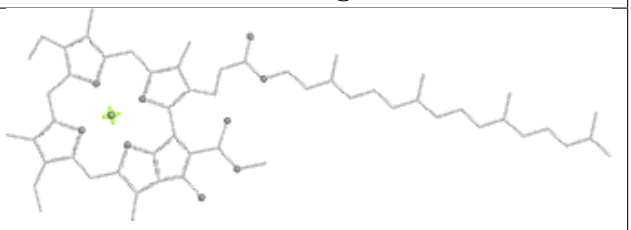
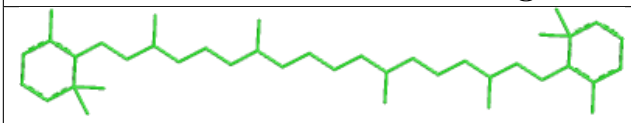


Rings

Ligand BCR J 4015



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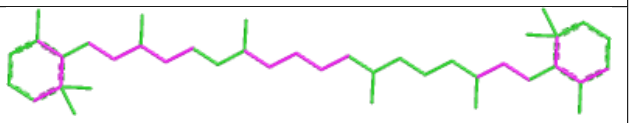
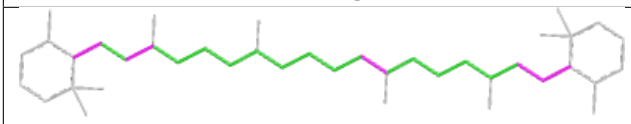


Bond angles



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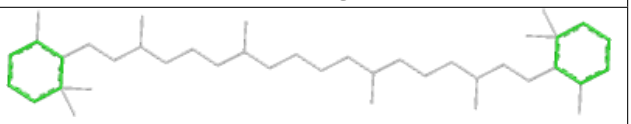
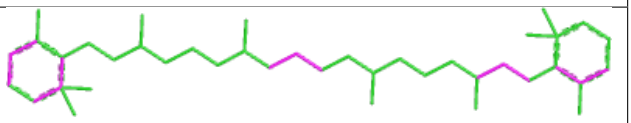


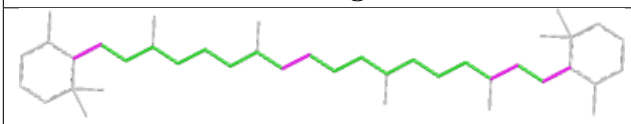
Rings

Ligand BCR k 4005

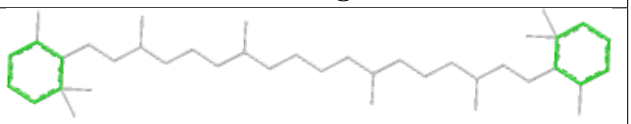
Bond lengths



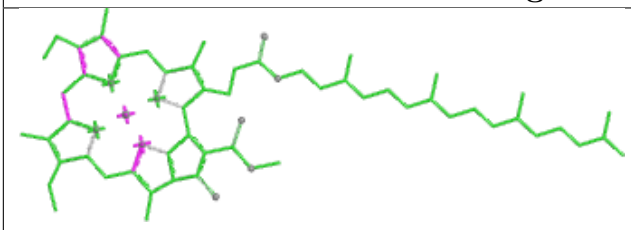
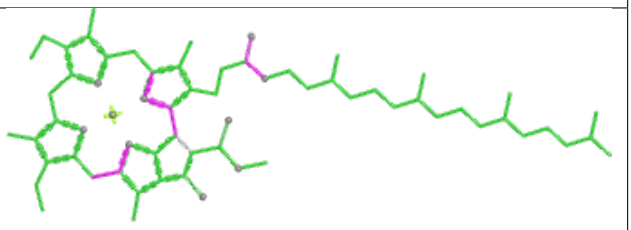
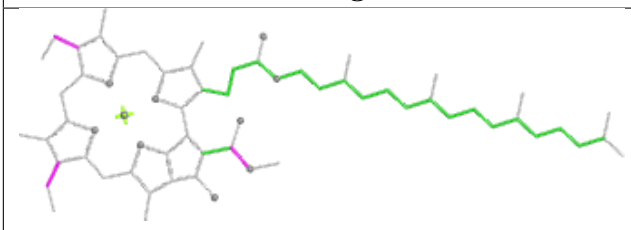
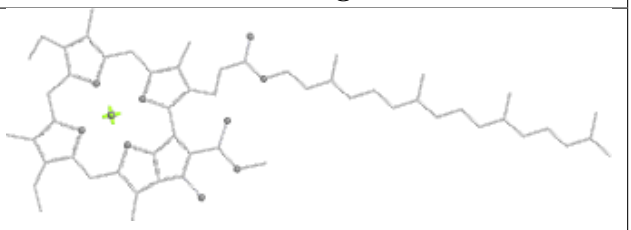
Bond angles

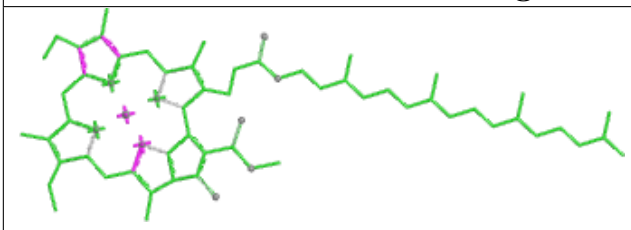
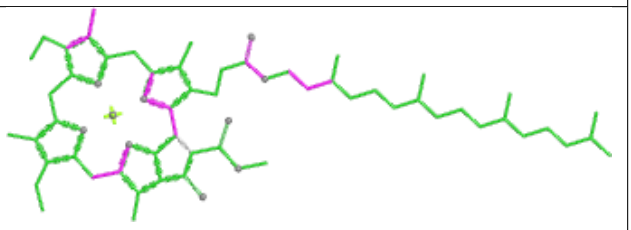
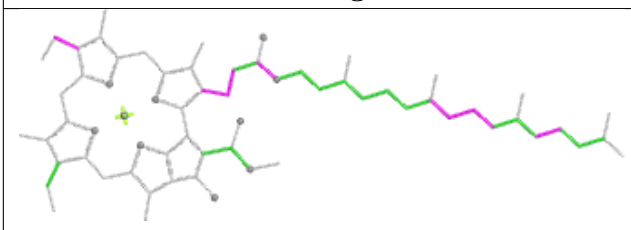
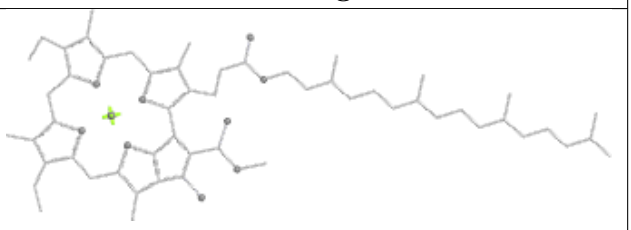


Torsions

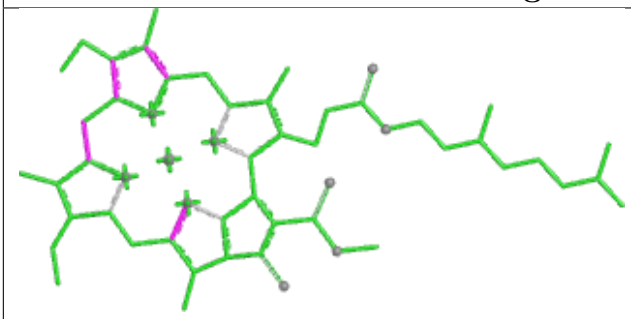


Rings

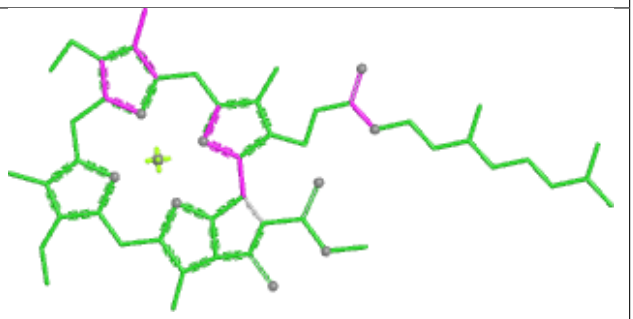
Ligand CLA Z 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1237	
	
Bond lengths	Bond angles
	
Torsions	Rings

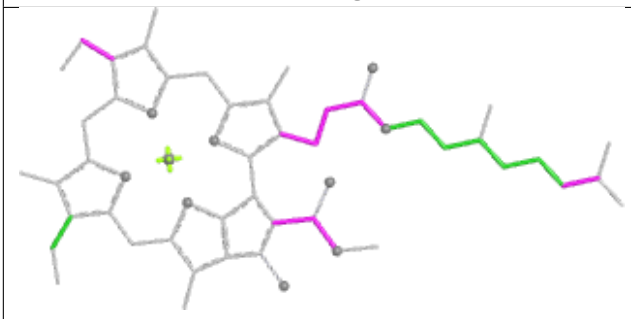
Ligand CLA Y 508



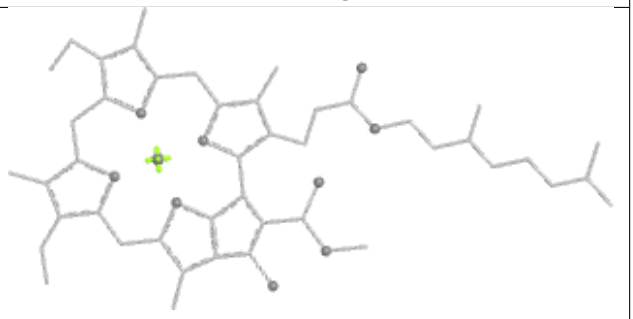
Bond lengths



Bond angles

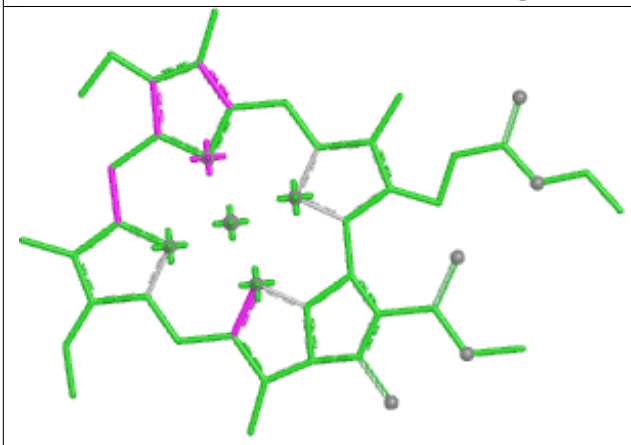


Torsions



Rings

Ligand CLA G 1216



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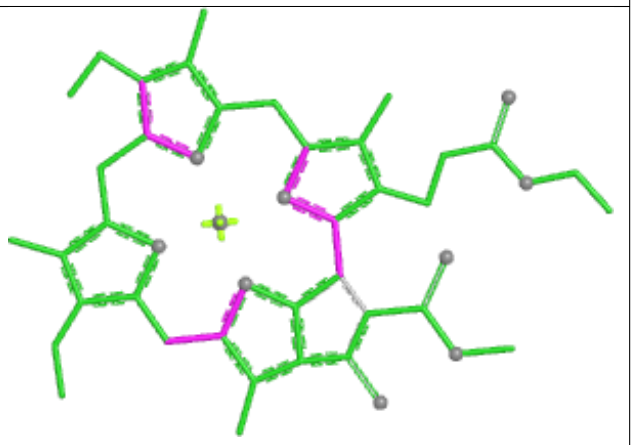
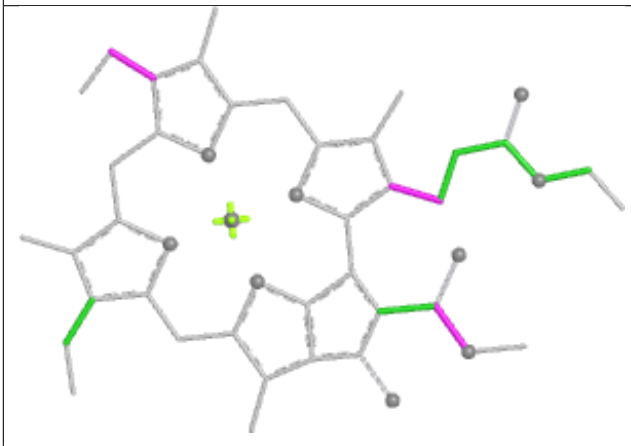


Bond angles



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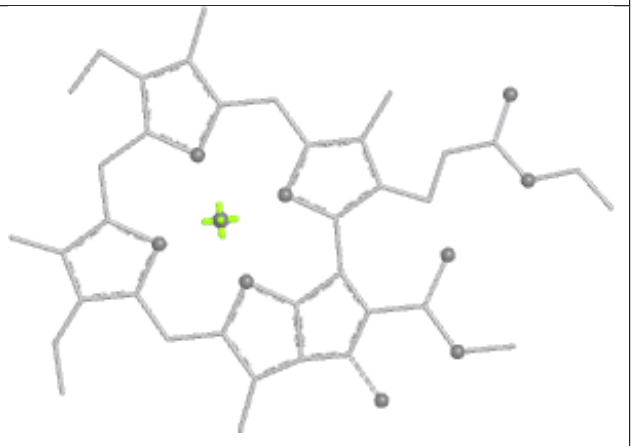
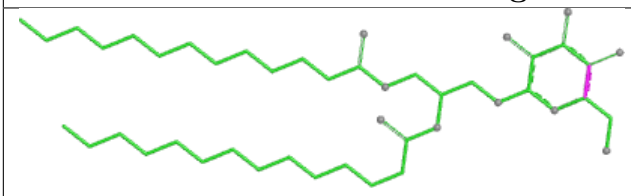
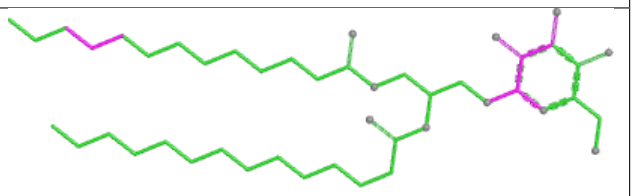


Rings

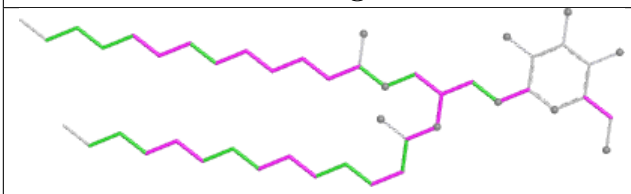
Ligand LMG H 4101



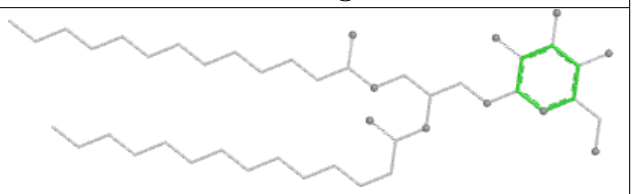
Bond lengths



Bond angles

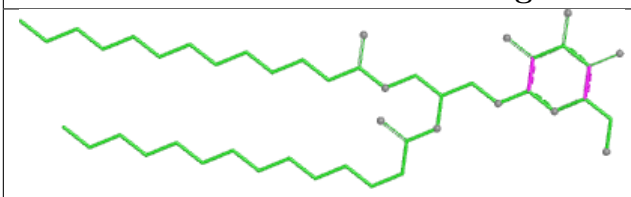


Torsions

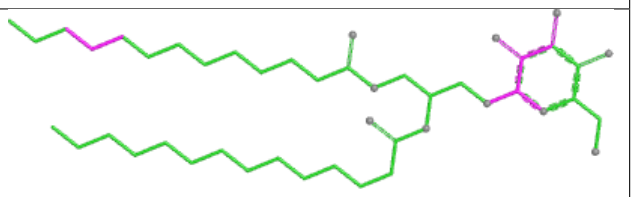


Rings

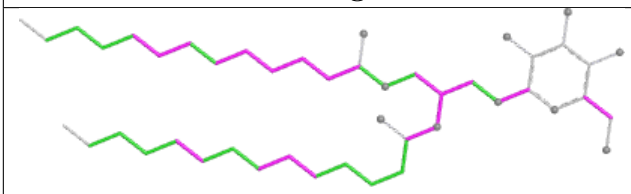
Ligand LMG a 4101



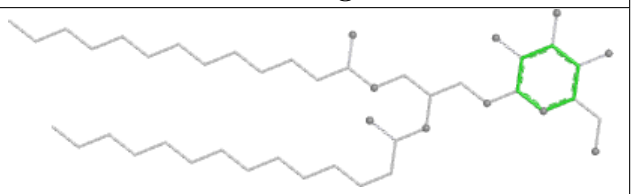
Bond lengths



Bond angles

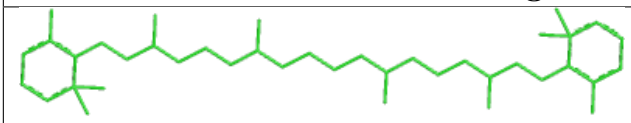


Torsions

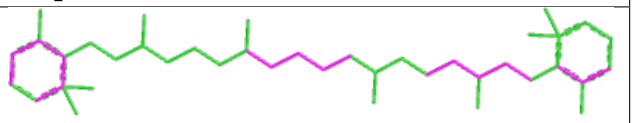


Rings

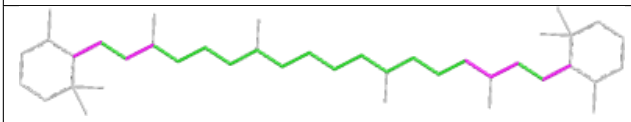
Ligand BCR p 601



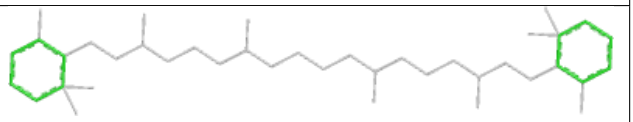
Bond lengths



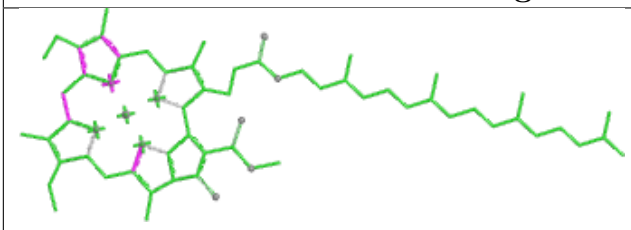
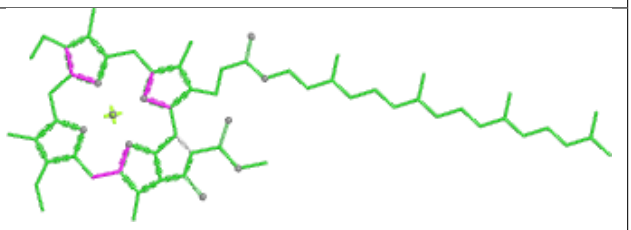
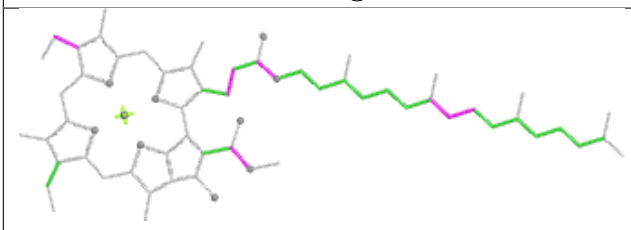
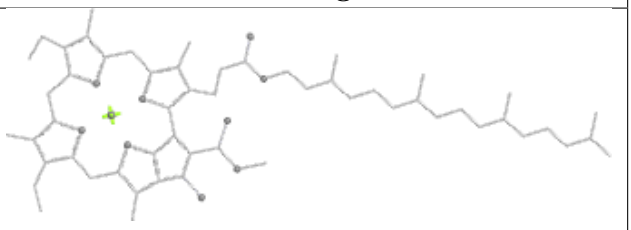
Bond angles

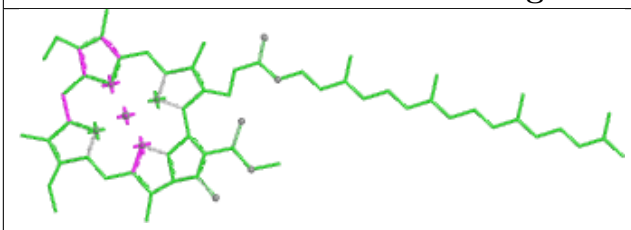
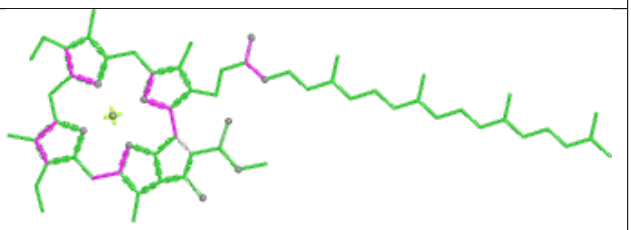
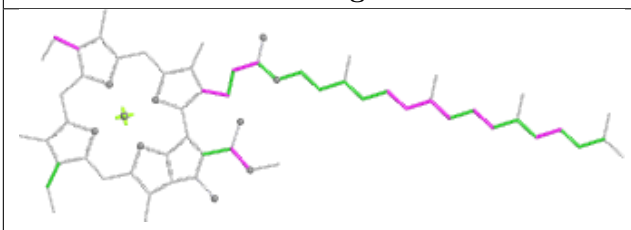
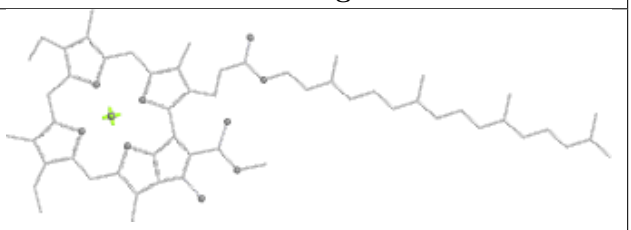


Torsions

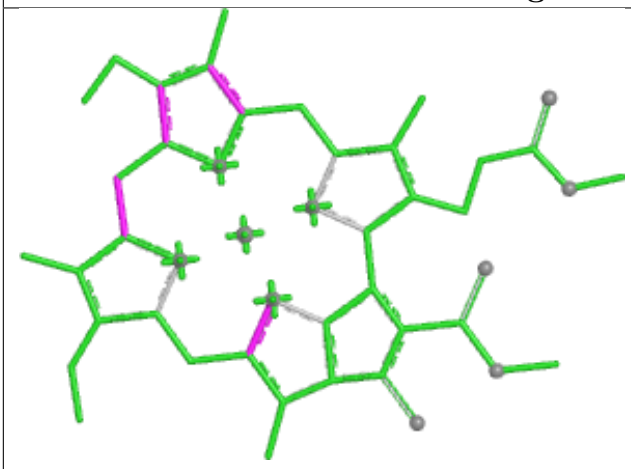


Rings

Ligand CLA H 1136	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Z 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 503



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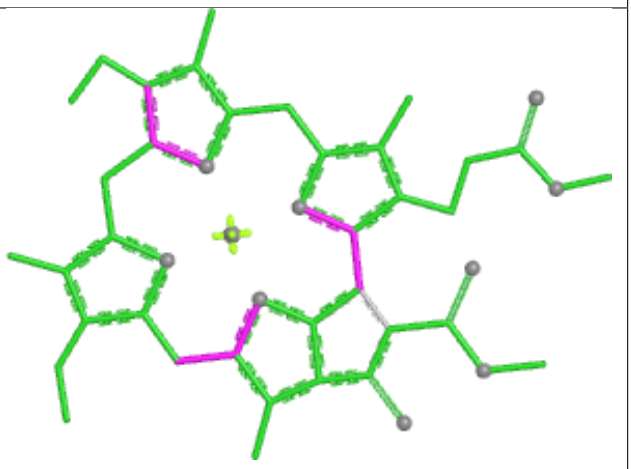
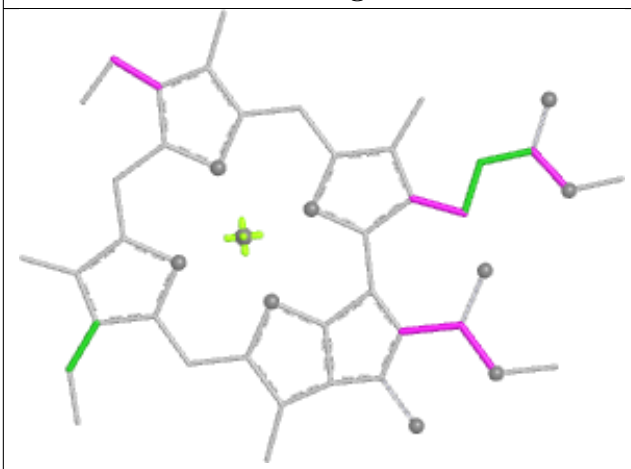
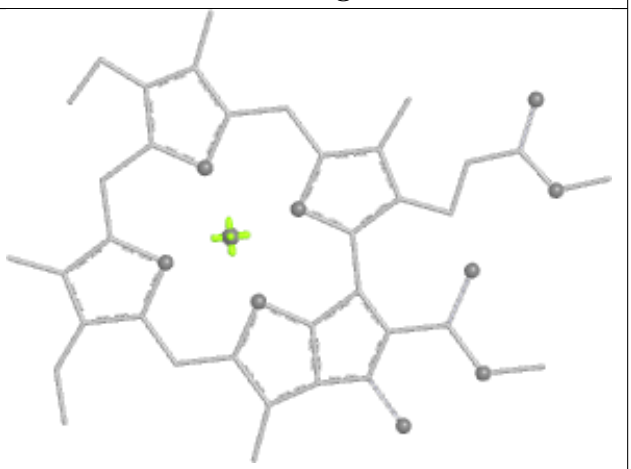


Bond angles

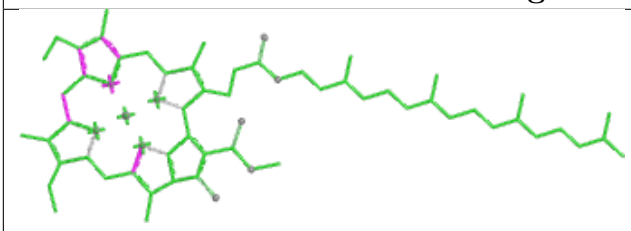


Torsions



Rings

Ligand CLA x 505



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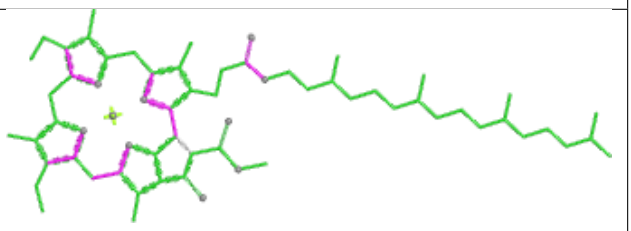

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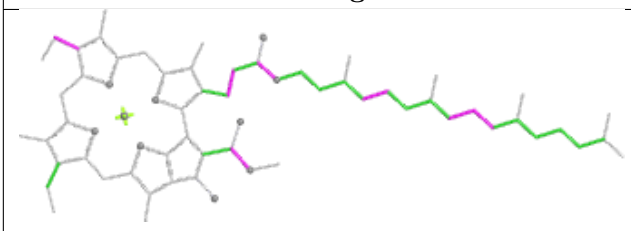

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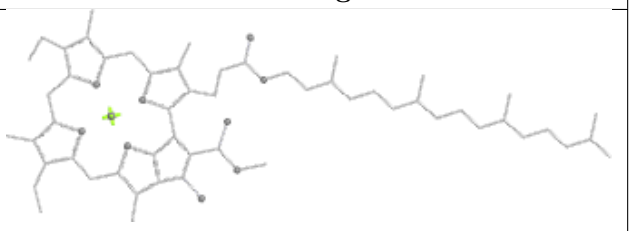
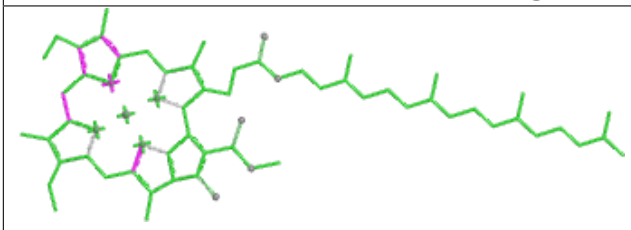


Rings

Ligand CLA v 507



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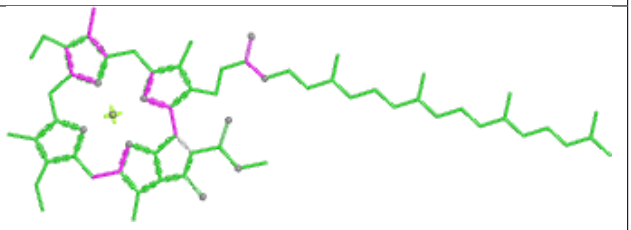
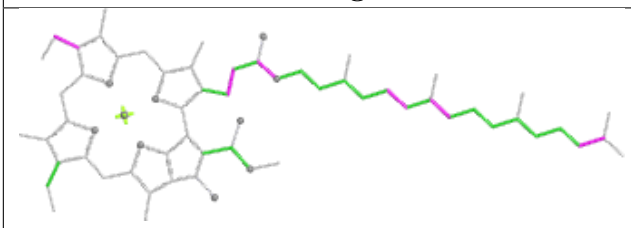


Bond angles



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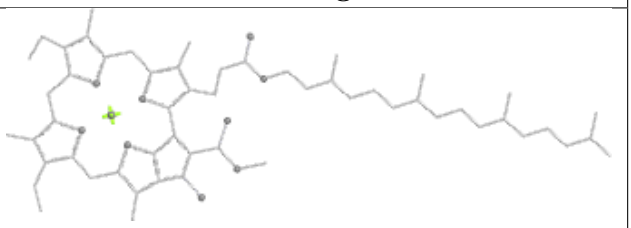
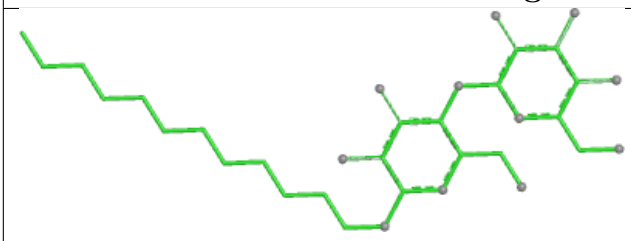


Rings

Ligand LMU g 606



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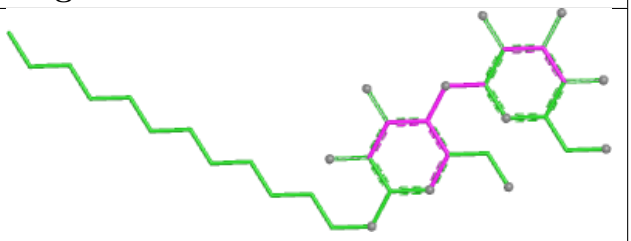
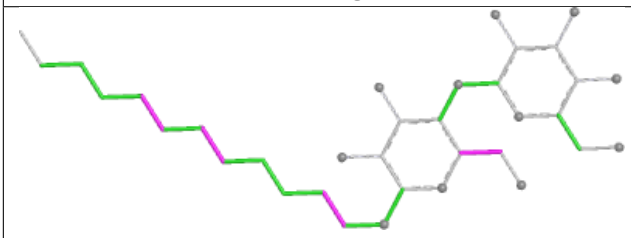
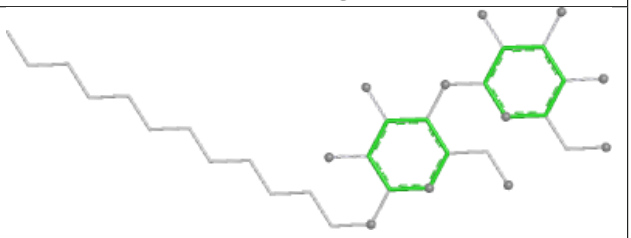


Bond angles

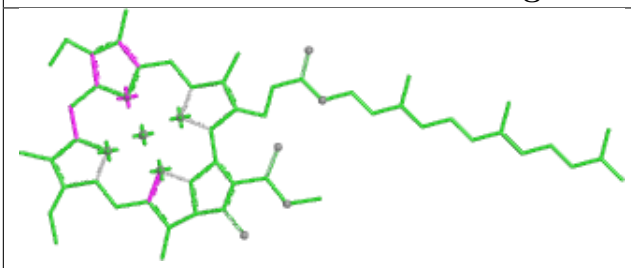


Torsions

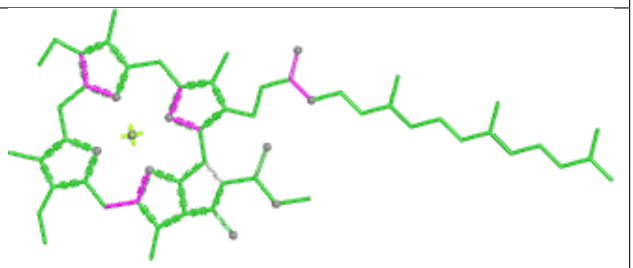


Rings

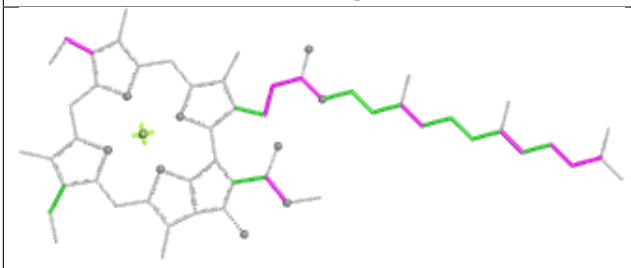
Ligand CLA l 1501



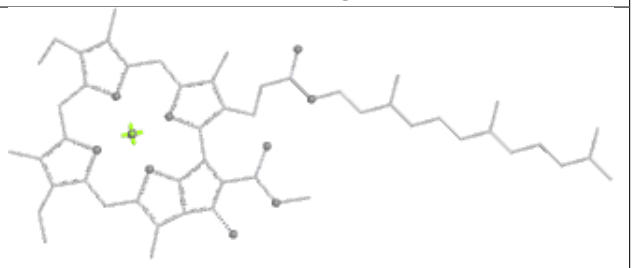
Bond lengths



Bond angles

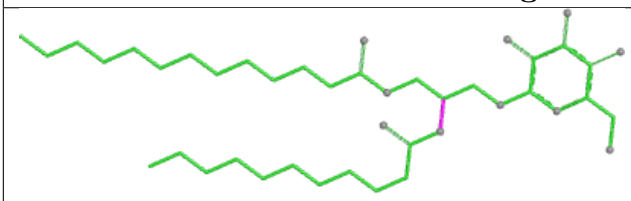


Torsions

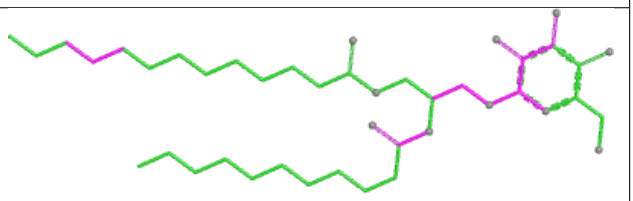


Rings

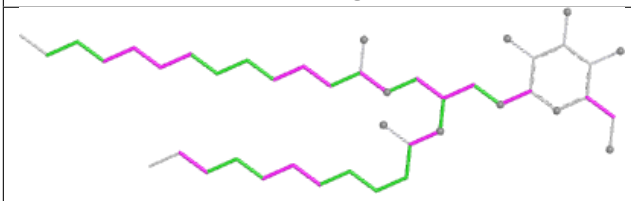
Ligand LMG B 848



Bond lengths



Bond angles



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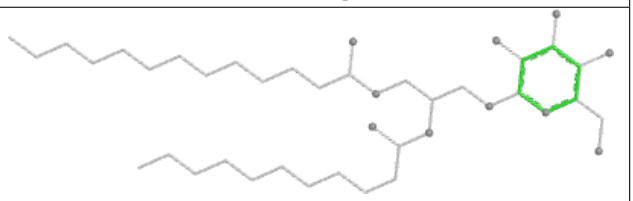
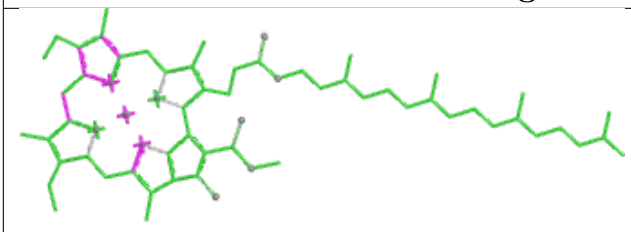
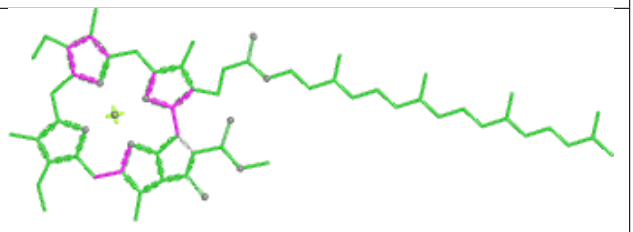


Rings

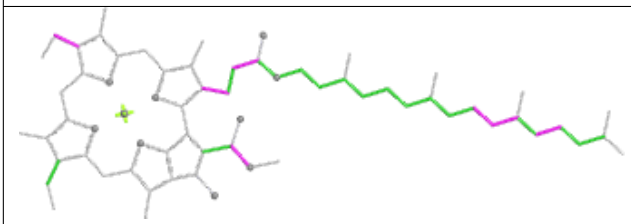
Ligand CLA b 1023



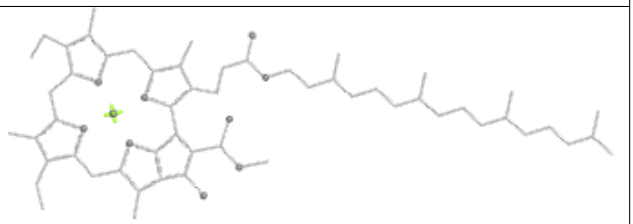
Bond lengths



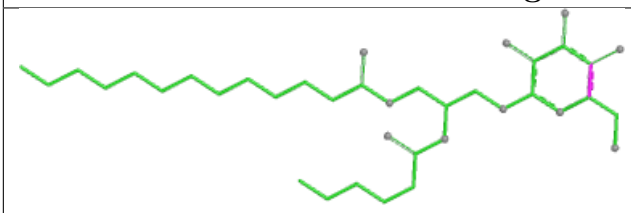
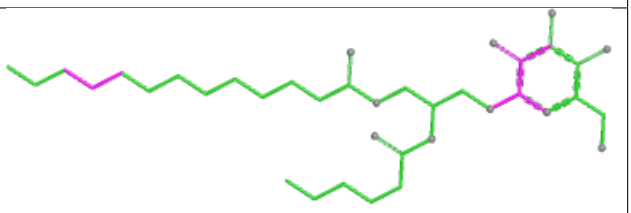
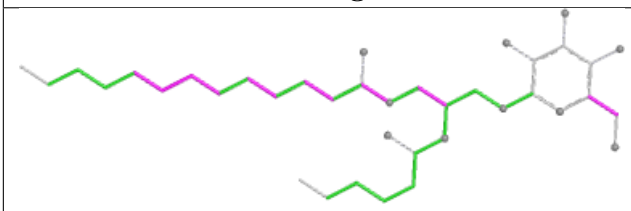
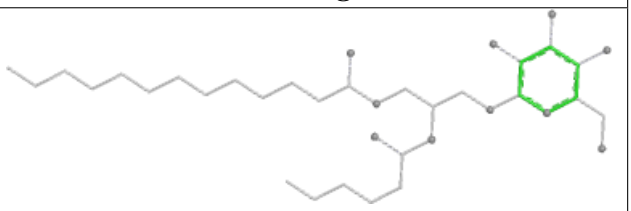
Bond angles

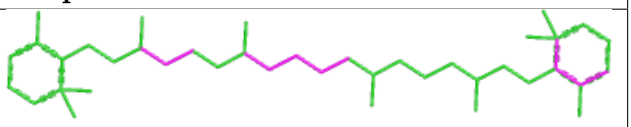
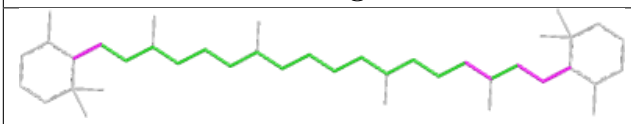
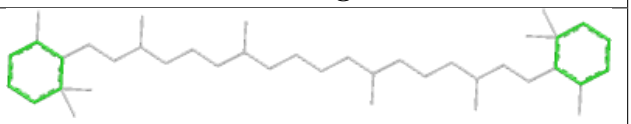


Torsions

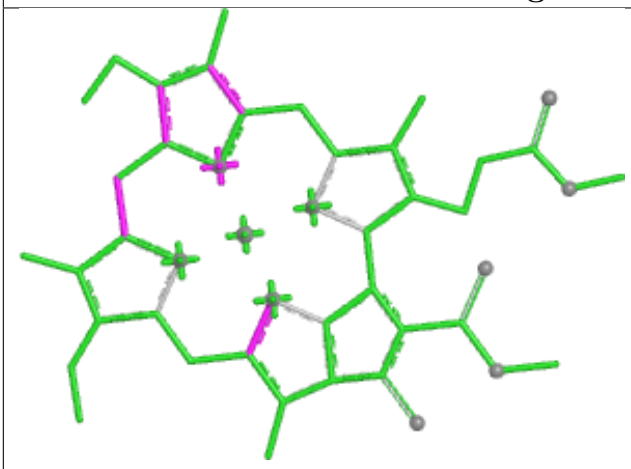


Rings

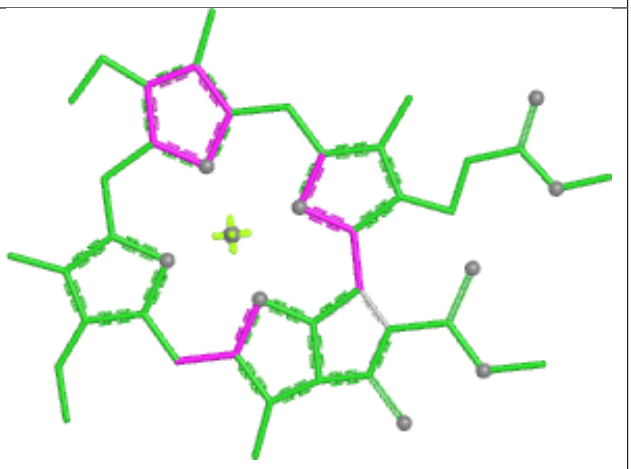
Ligand LMG a 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR q 603	
Bond lengths	 Bond angles
 Torsions	 Rings

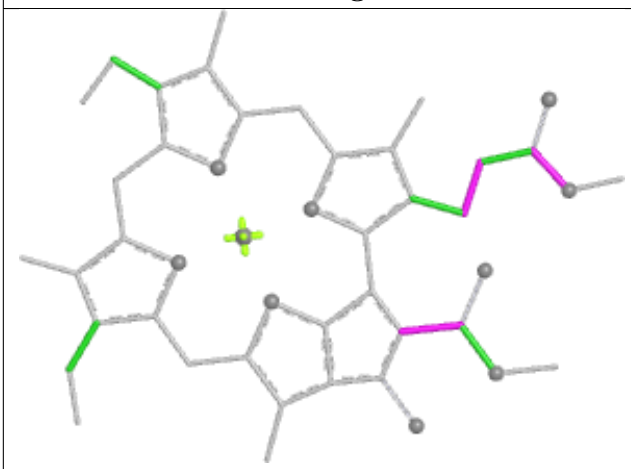
Ligand CLA h 503



Bond lengths



Bond angles



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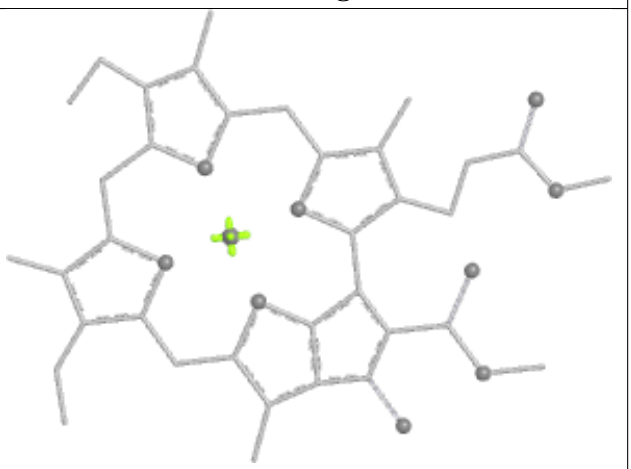
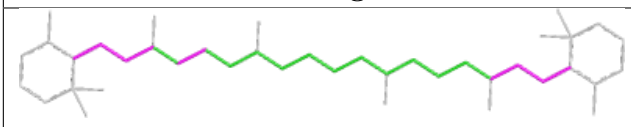


Rings

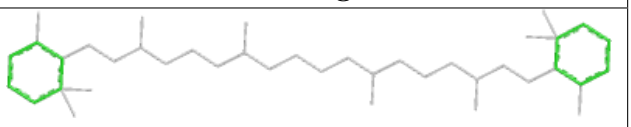
Ligand BCR h 603

Bond lengths

Bond angles

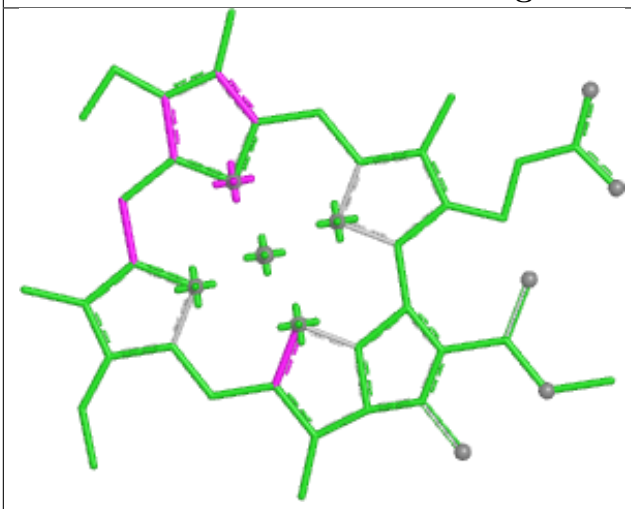


Torsions

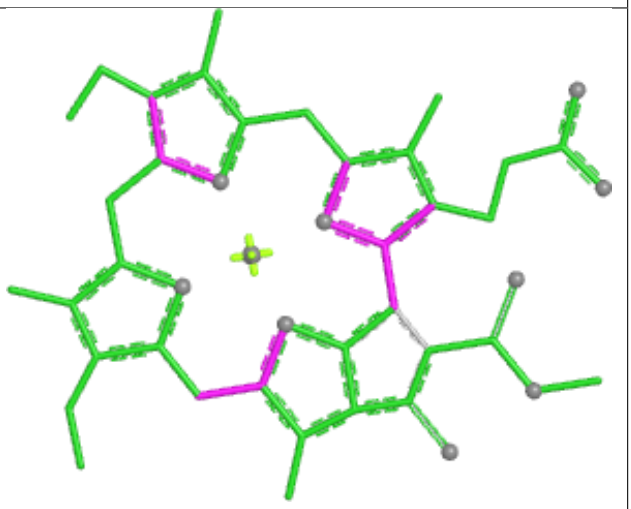


Rings

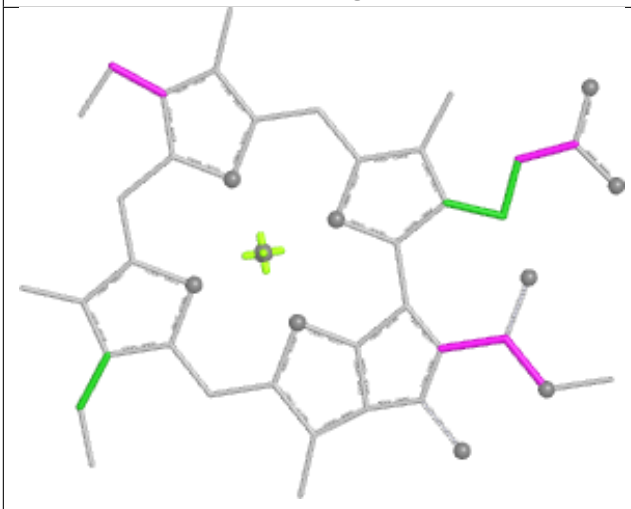
Ligand CLA B 1232



Bond lengths



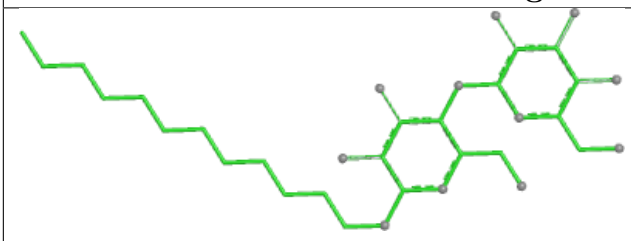
Bond angles



Torsions

Rings

Ligand LMU s 606



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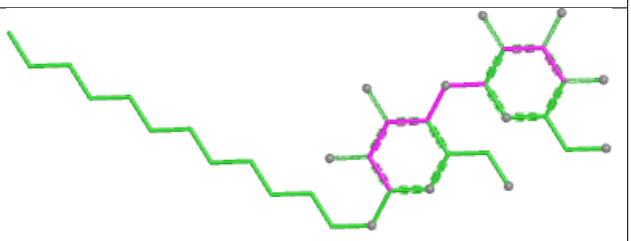
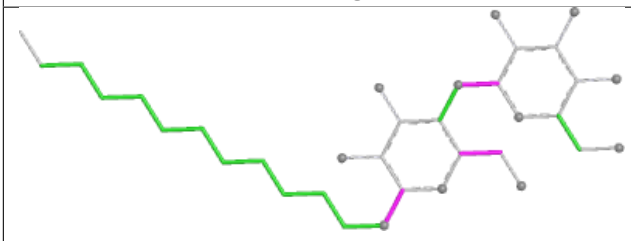
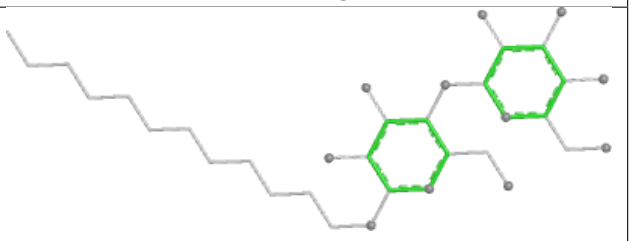


Bond angles

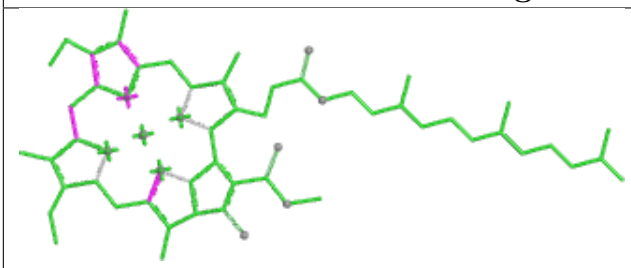


Torsions



Rings

Ligand CLA U 1501



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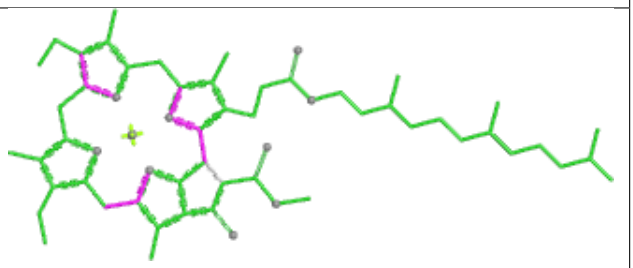
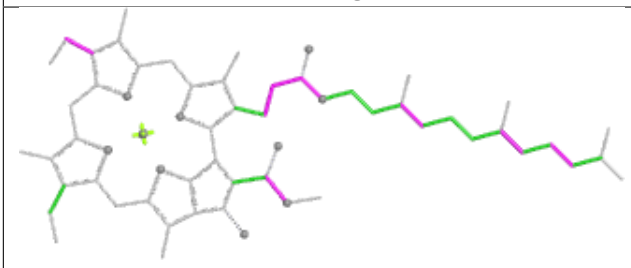
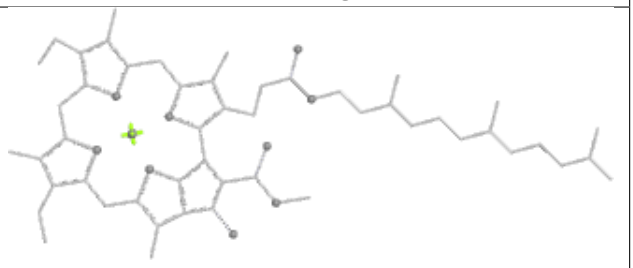


Bond angles

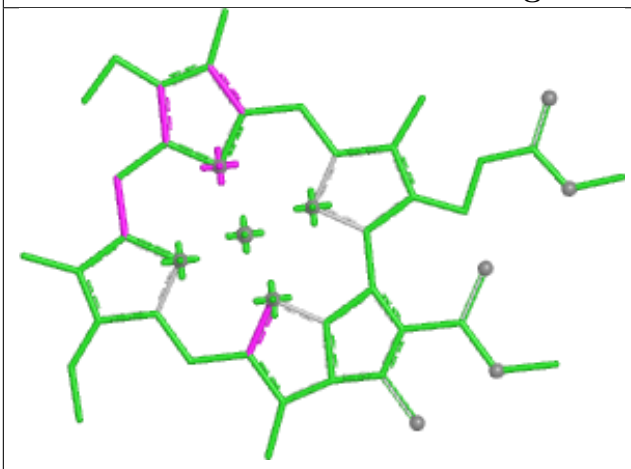


Torsions



Rings

Ligand CLA X 503



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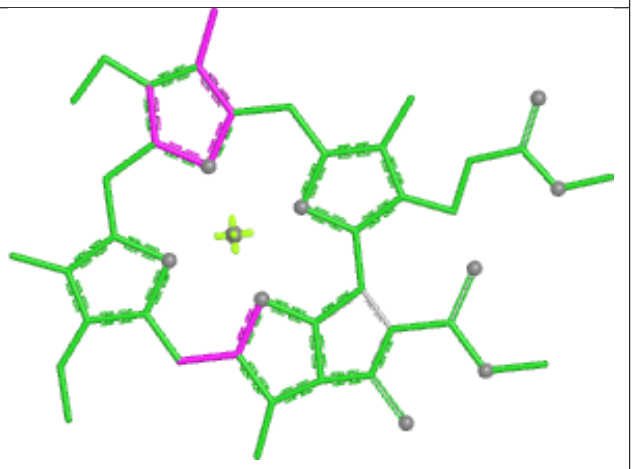
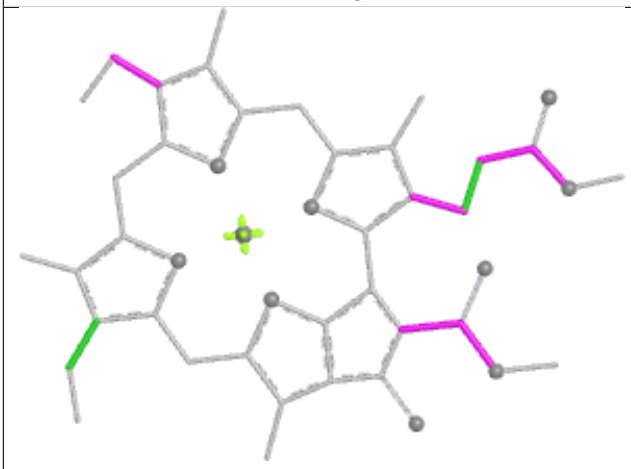
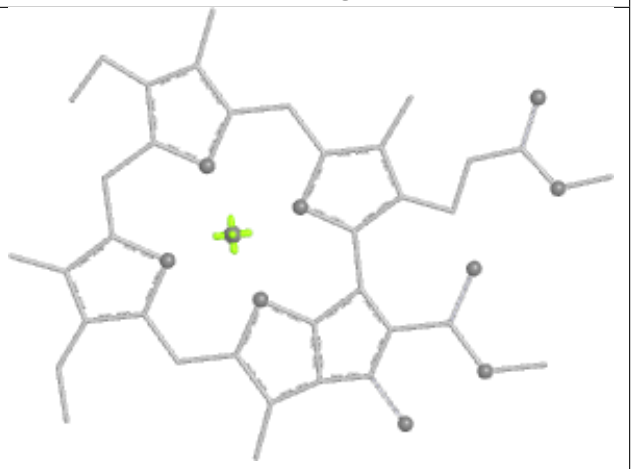


Bond angles

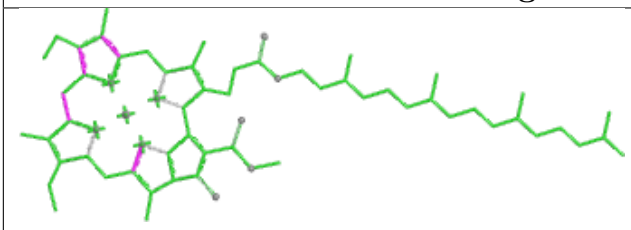


Torsions



Rings

Ligand CLA b 1204



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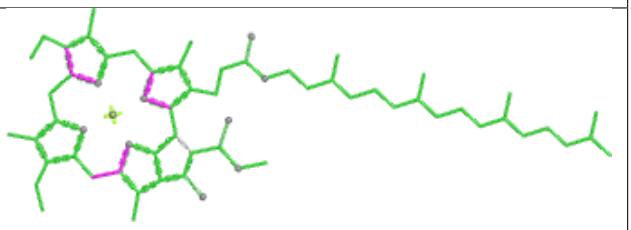
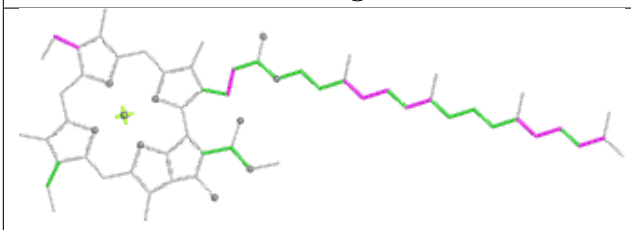
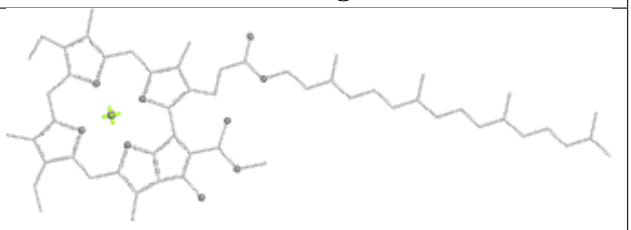


Bond angles

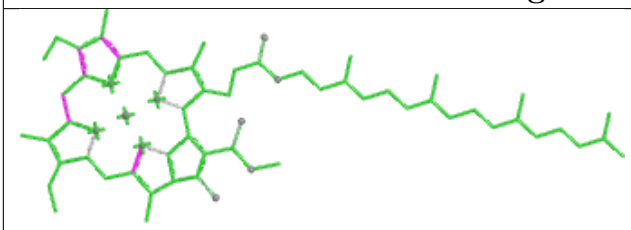


Torsions



Rings

Ligand CLA v 515



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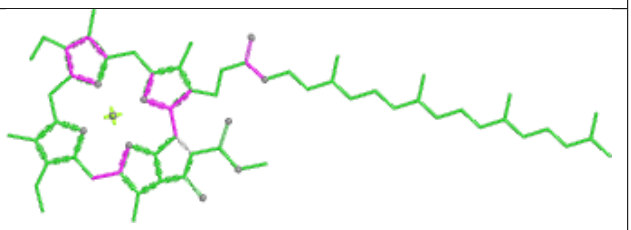
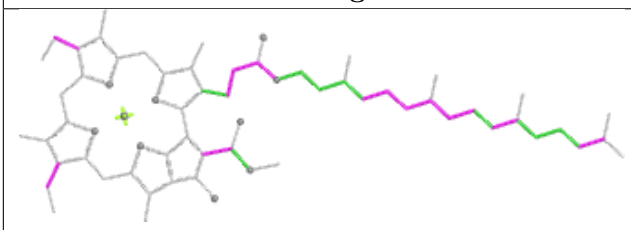
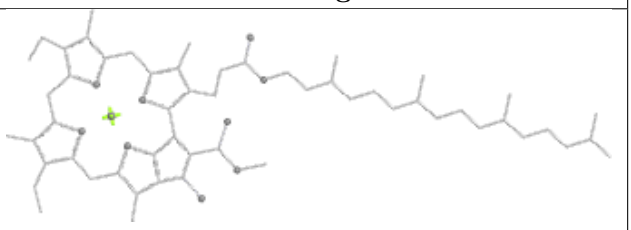


Bond angles

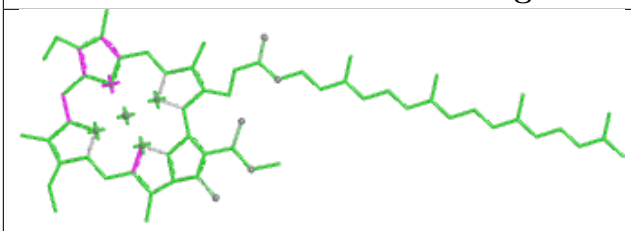


Torsions

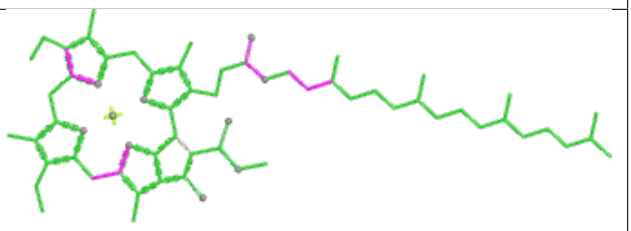


Rings

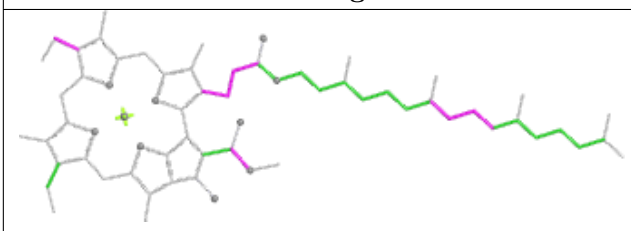
Ligand CLA H 1138



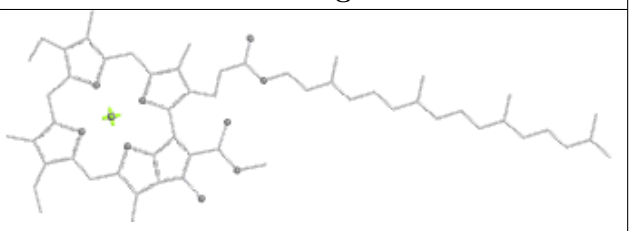
Bond lengths



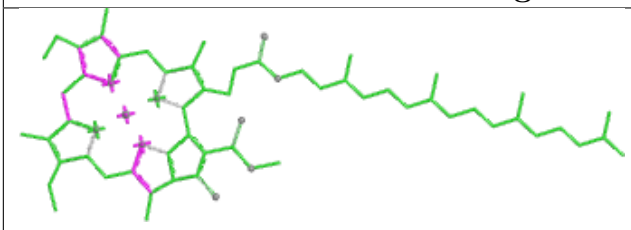
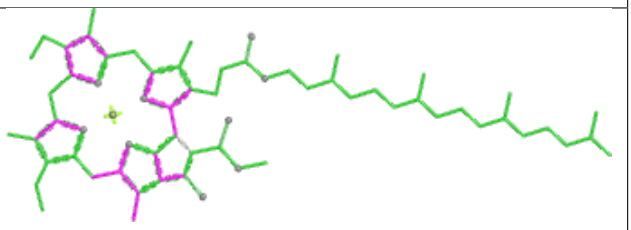
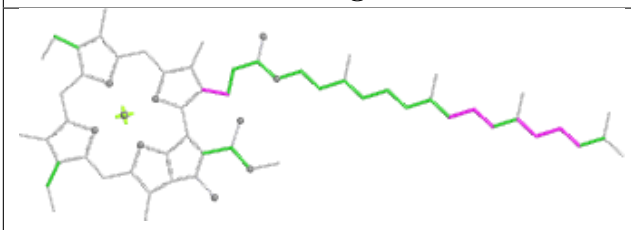
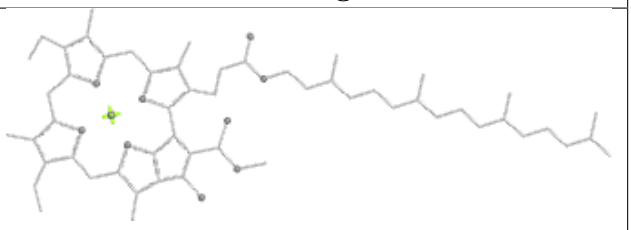
Bond angles

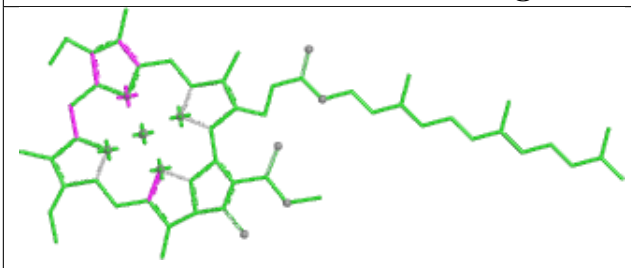
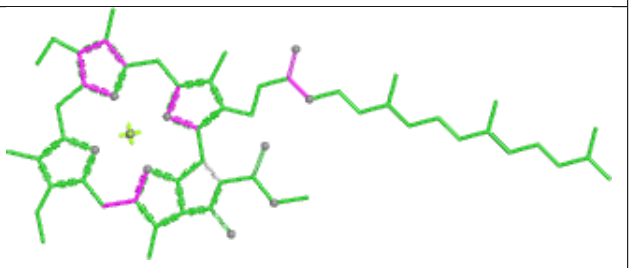
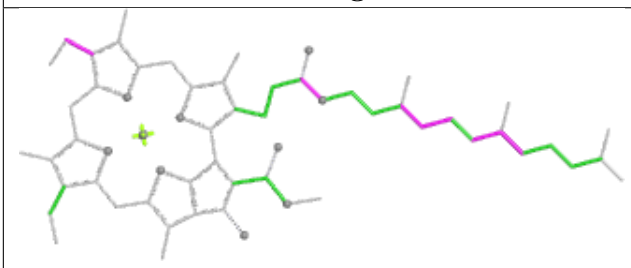
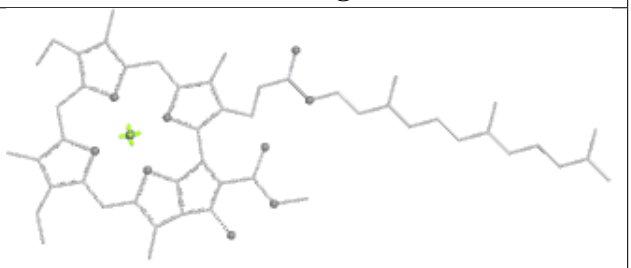


Torsions

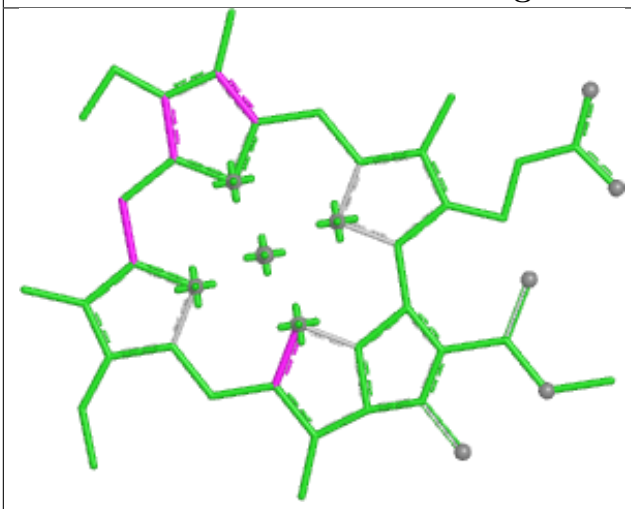


Rings

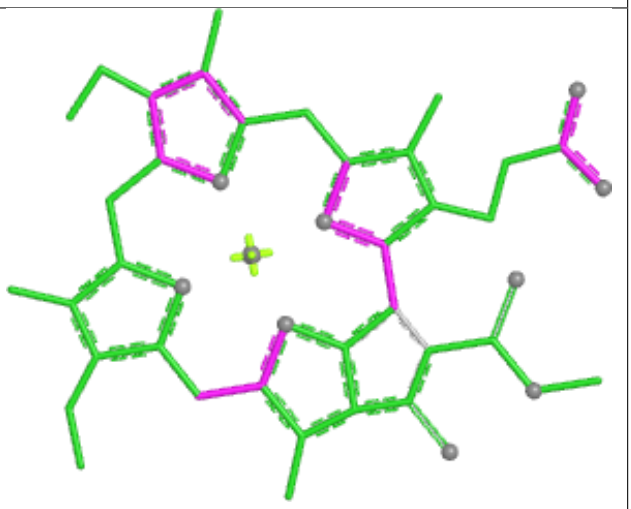
Ligand CLA G 1023	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA U 1502	
	
Bond lengths	Bond angles
	
Torsions	Rings

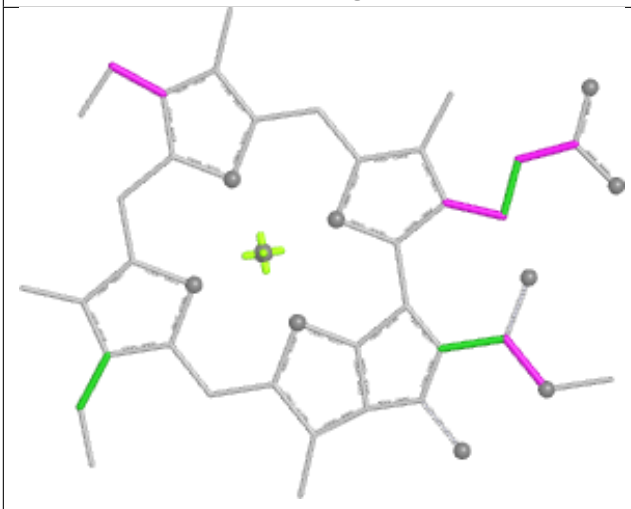
Ligand CLA G 1208



Bond lengths



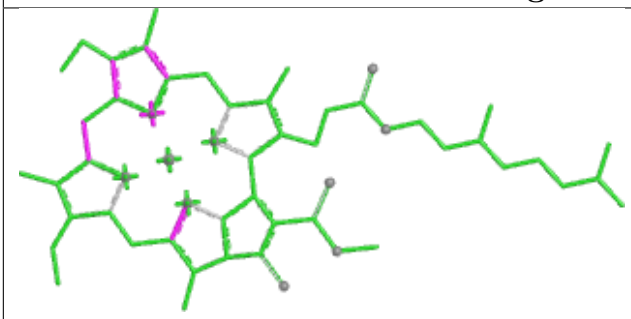
Bond angles



Torsions

Rings

Ligand CLA n 517



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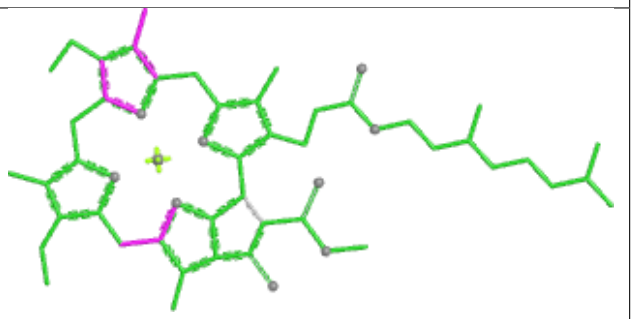
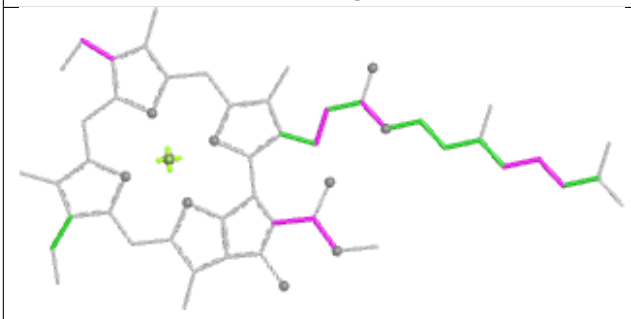
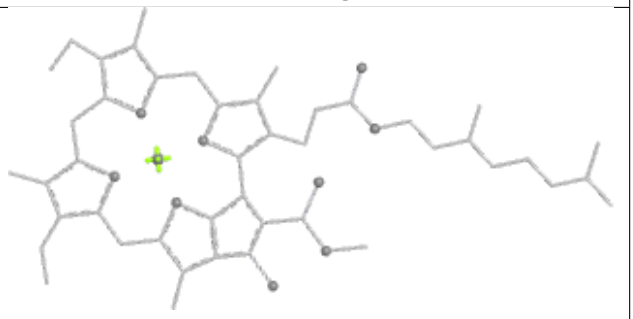


Bond angles

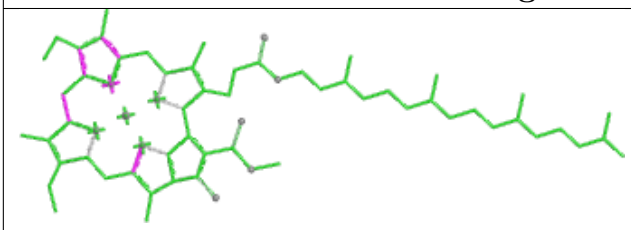


Torsions

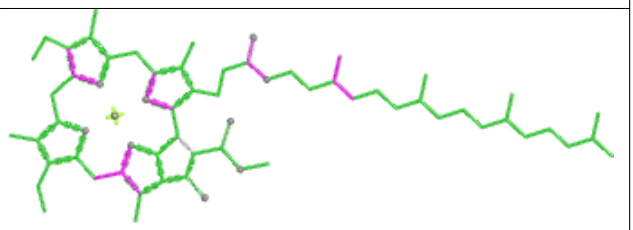


Rings

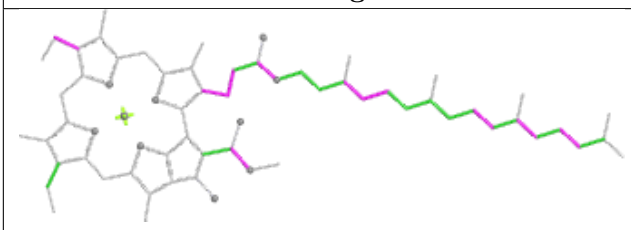
Ligand CLA b 1203



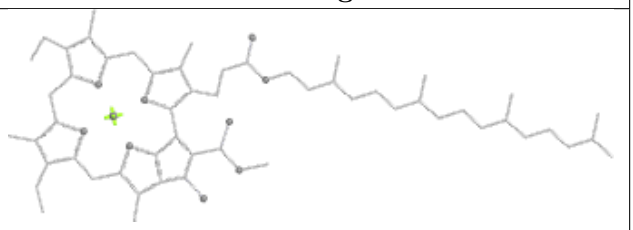
Bond lengths



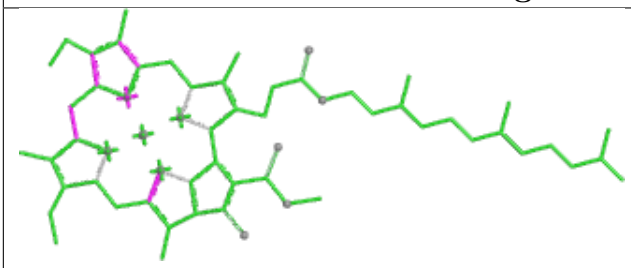
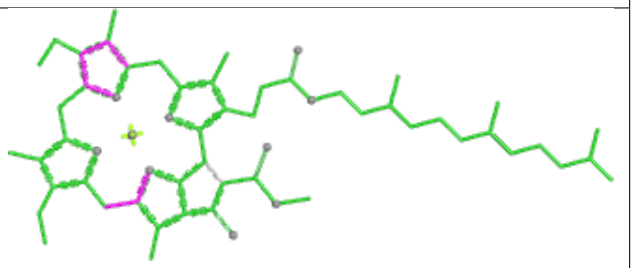
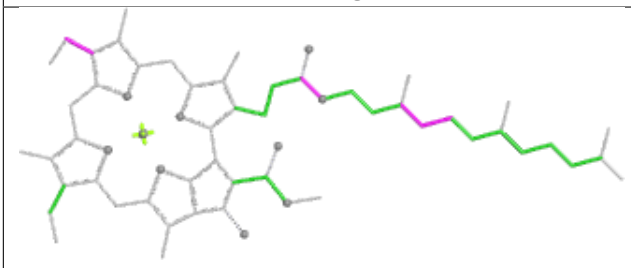
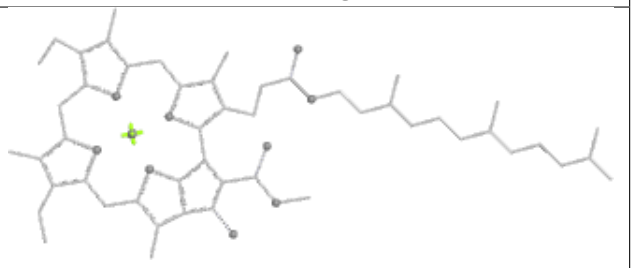
Bond angles

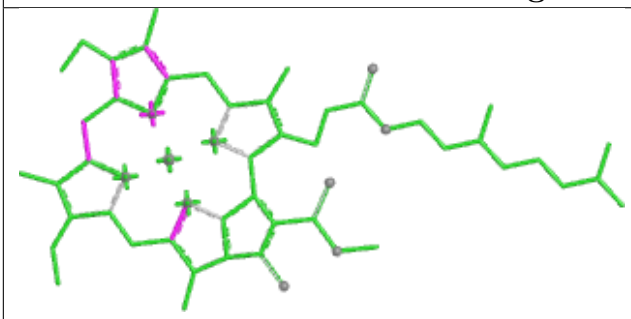
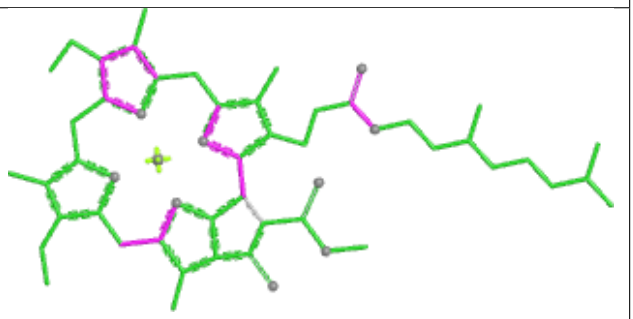
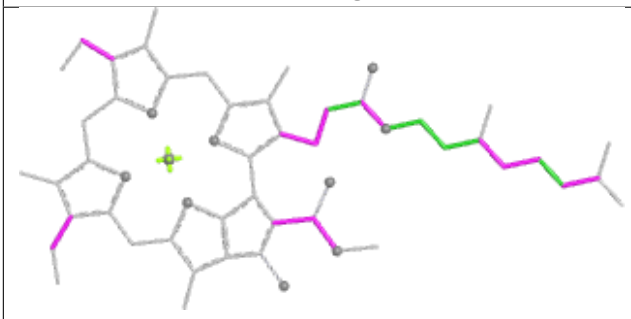
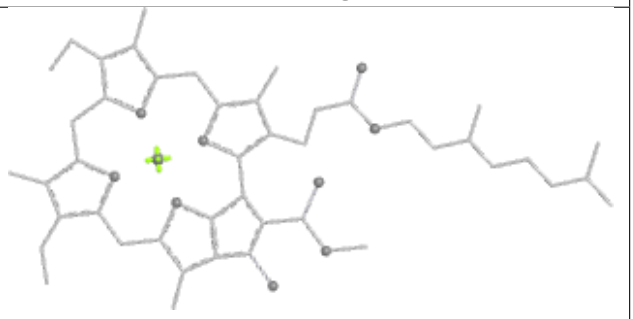


Torsions

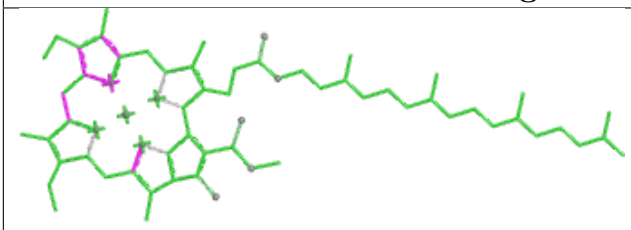


Rings

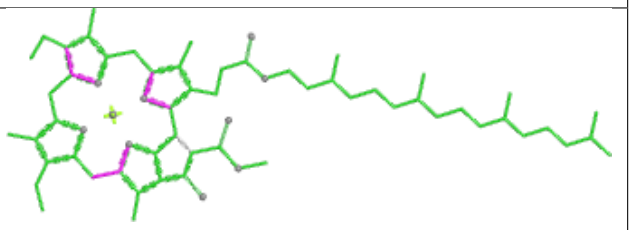
Ligand CLA H 1124	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA v 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

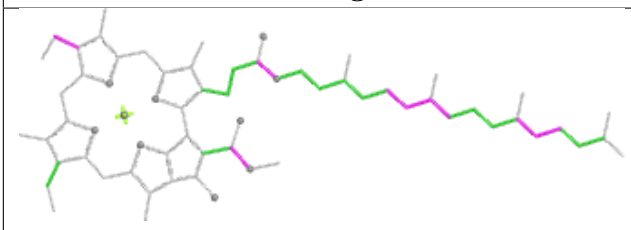
Ligand CLA a 1131



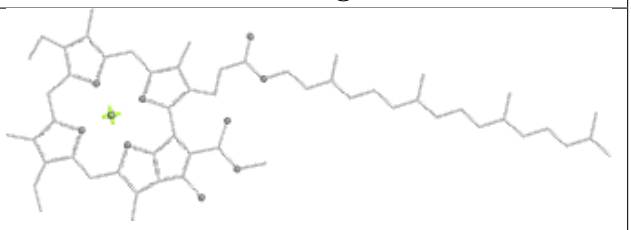
Bond lengths



Bond angles

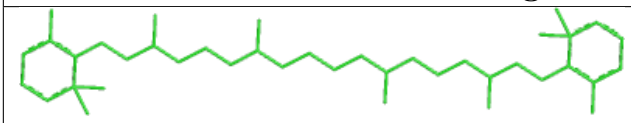


Torsions

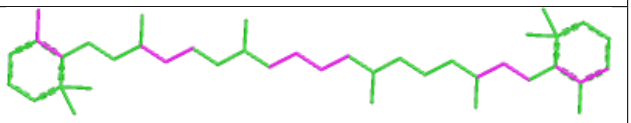


Rings

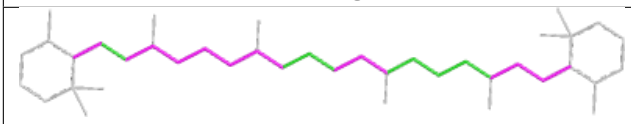
Ligand BCR w 604



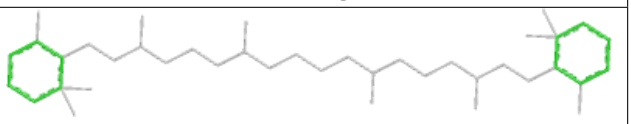
Bond lengths



Bond angles

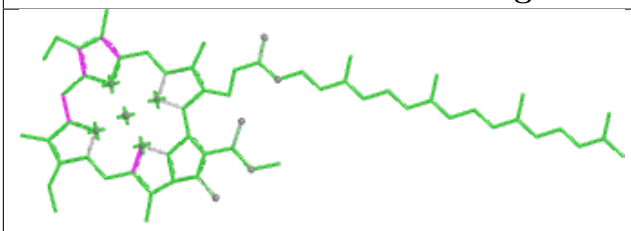


Torsions



Rings

Ligand CLA H 1125



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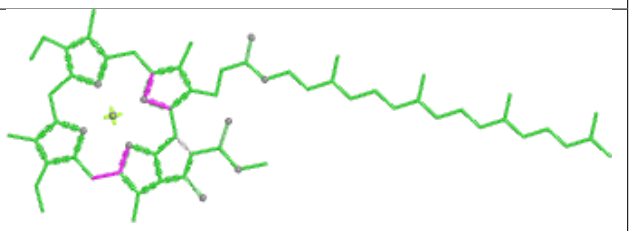
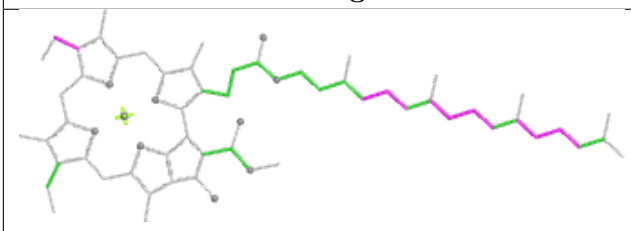
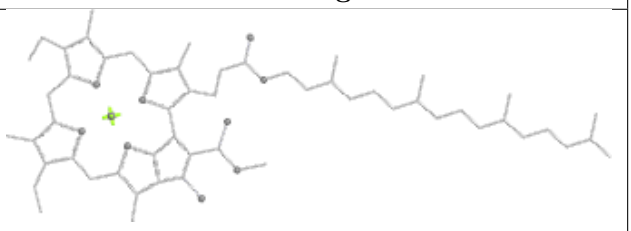


Bond angles

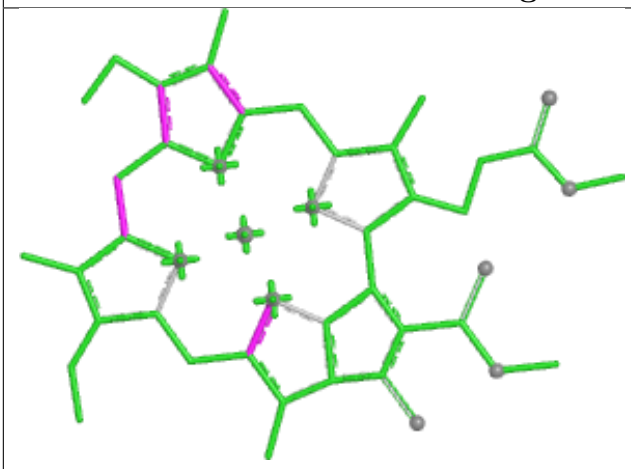


Torsions



Rings

Ligand CLA a 1801



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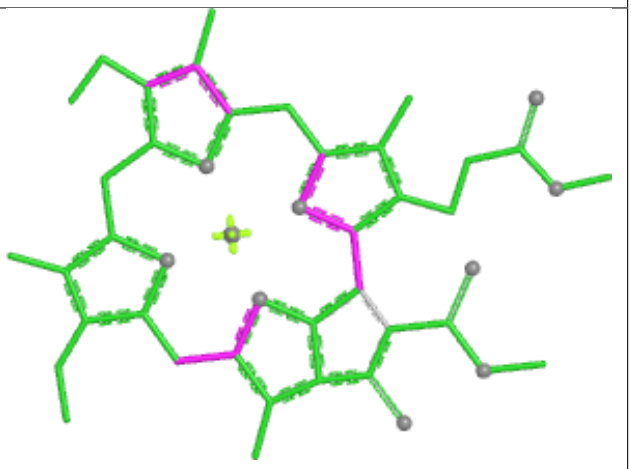
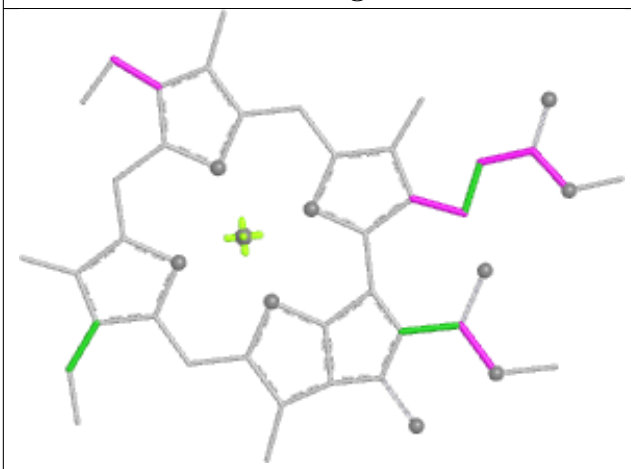
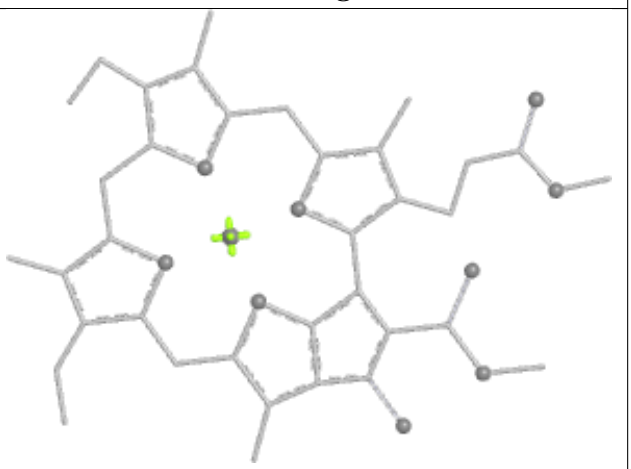


Bond angles

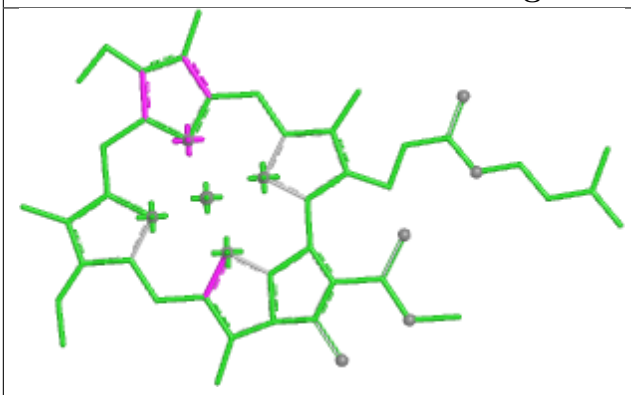


Torsions

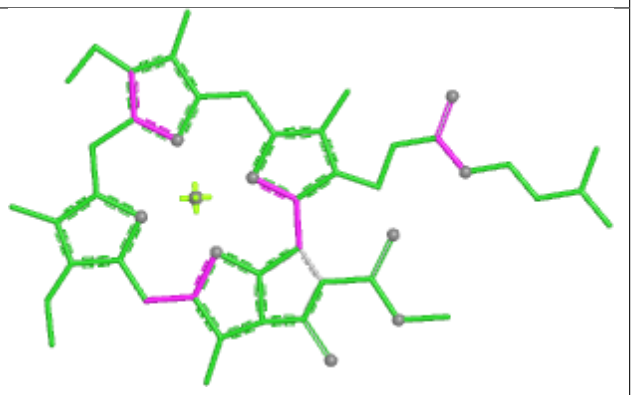


Rings

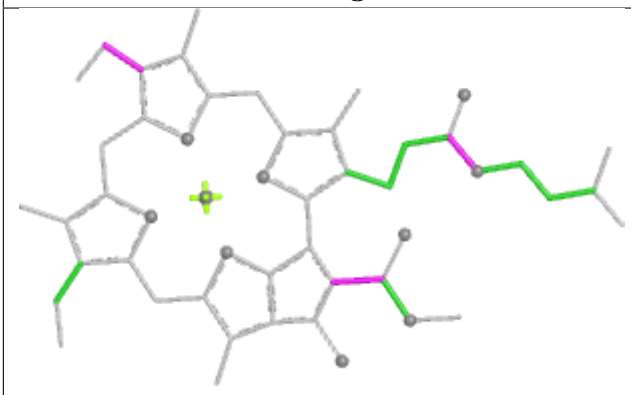
Ligand CLA Y 502



Bond lengths



Bond angles



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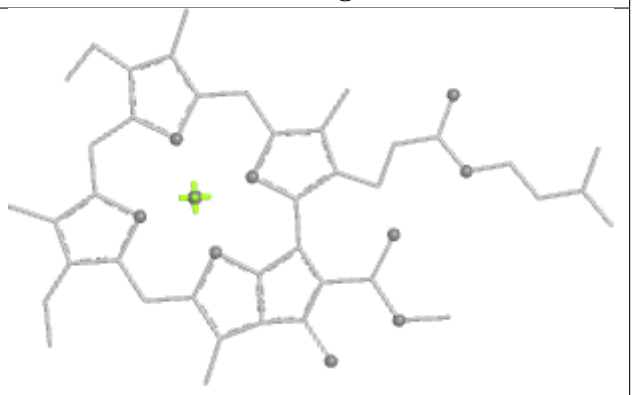
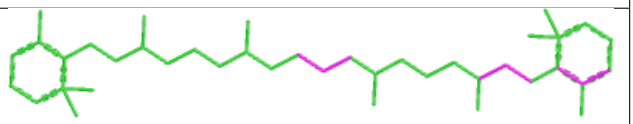


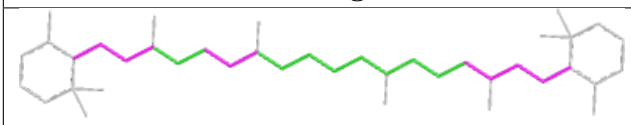
Rings

Ligand BCR A 4002

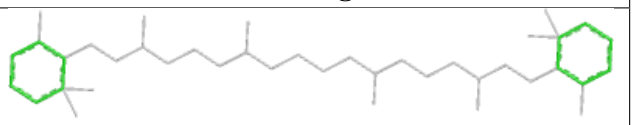
Bond lengths



Bond angles

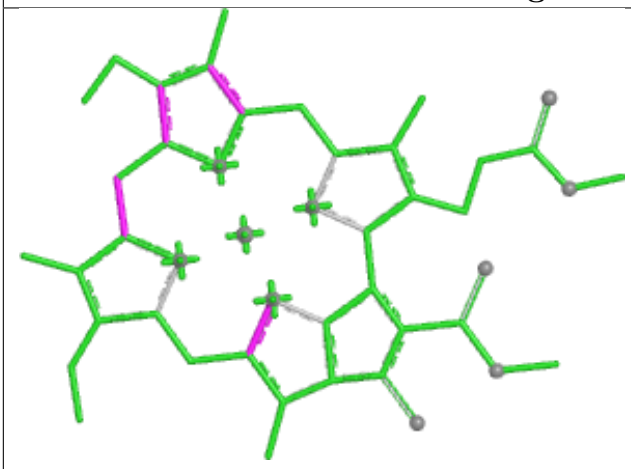


Torsions



Rings

Ligand CLA x 516



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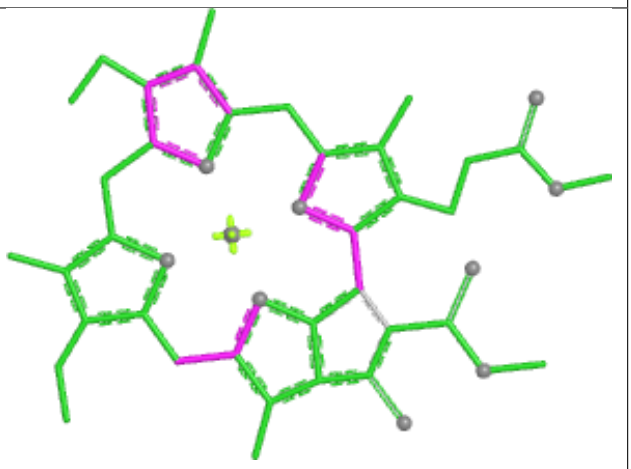
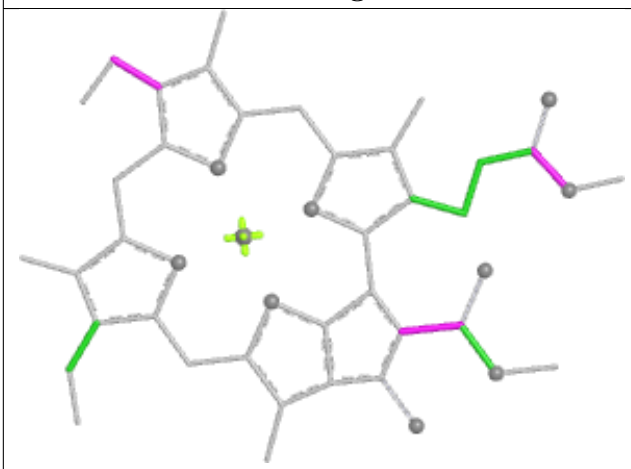


Bond angles



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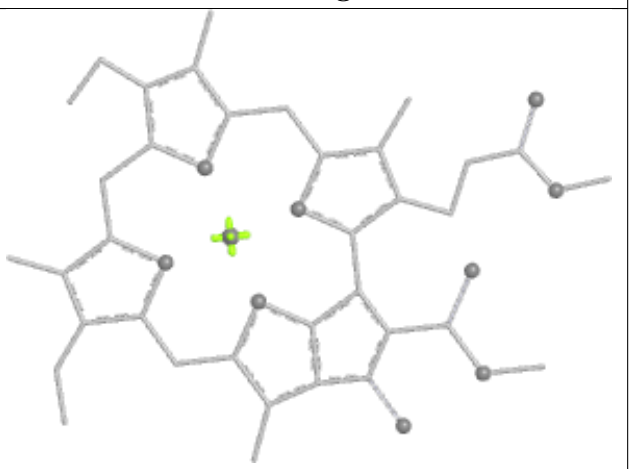
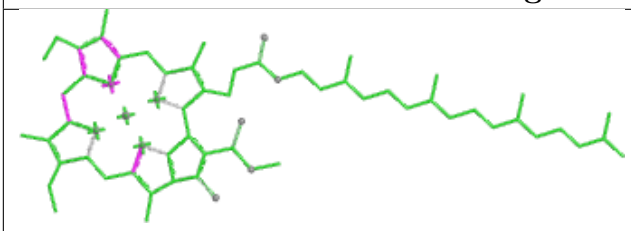
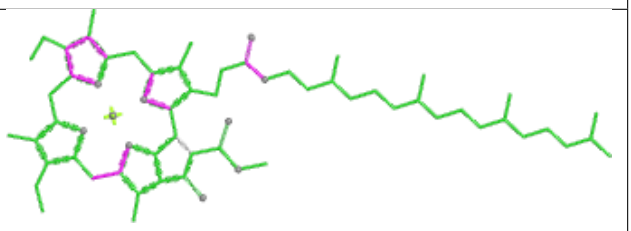


Rings

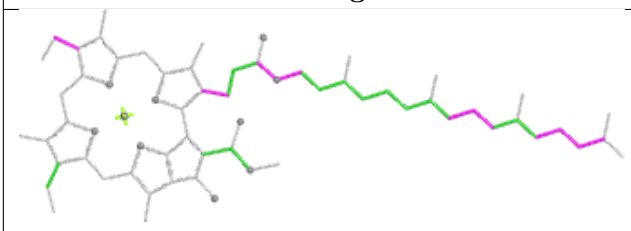
Ligand CLA w 509



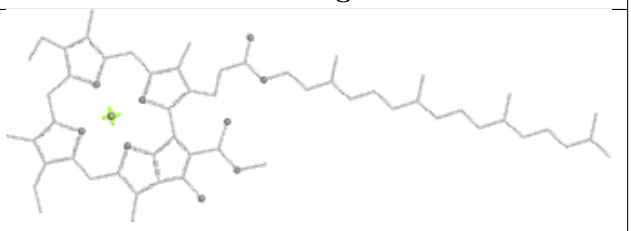
Bond lengths



Bond angles

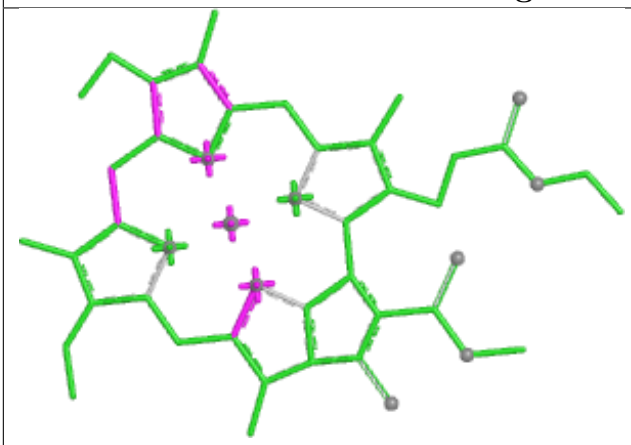


Torsions



Rings

Ligand CLA B 1216



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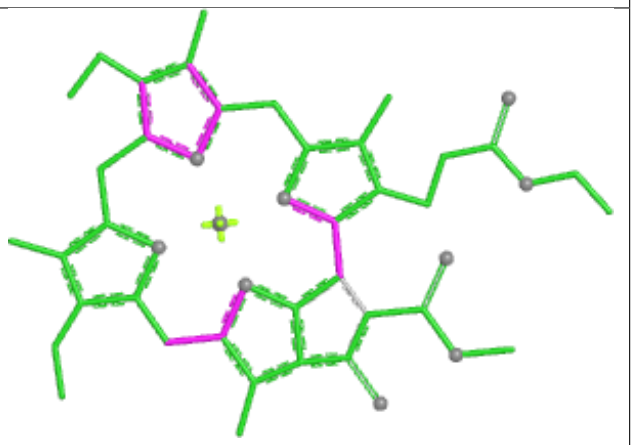
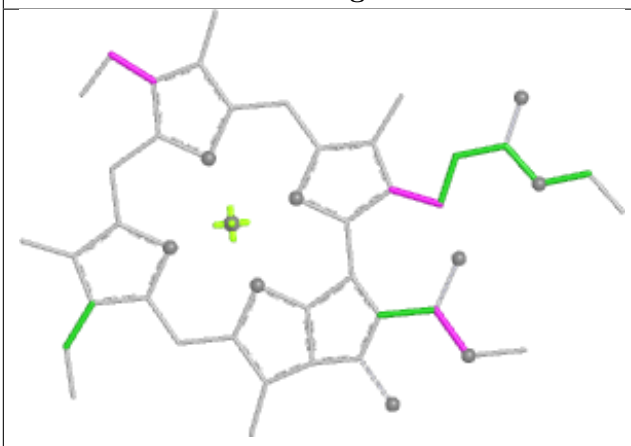
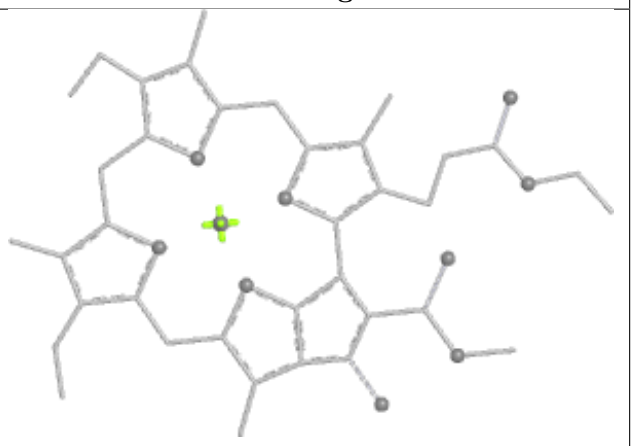


Bond angles



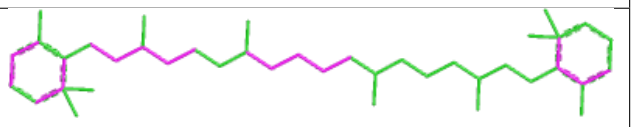
Torsions



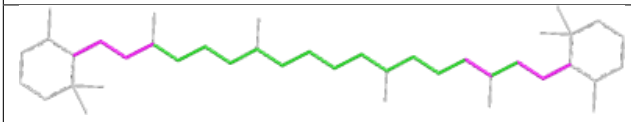
Rings

Ligand BCR o 603

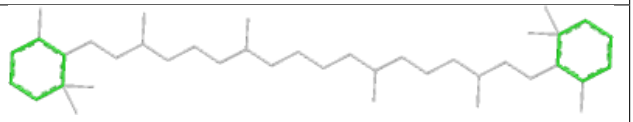
Bond lengths



Bond angles

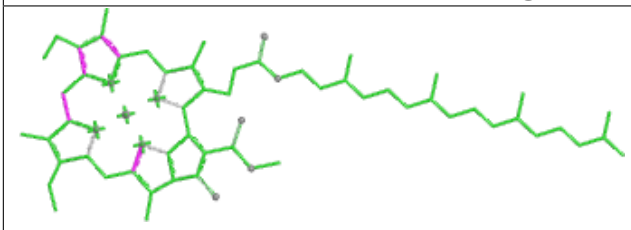


Torsions



Rings

Ligand CLA a 1109



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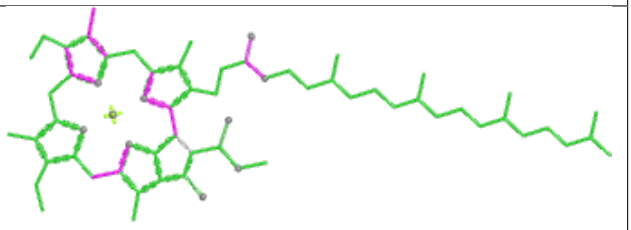
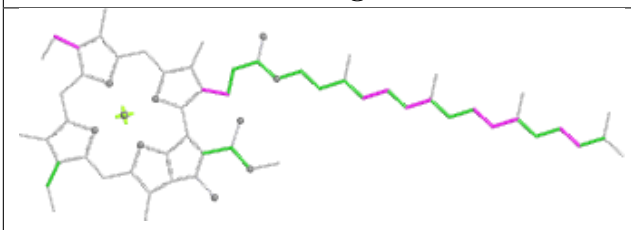


Bond angles



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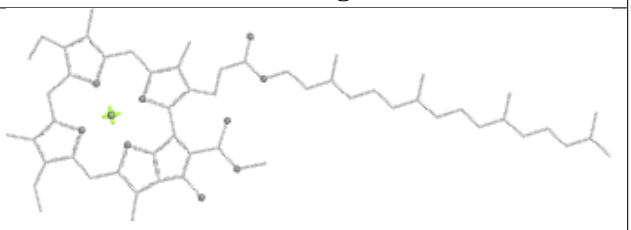
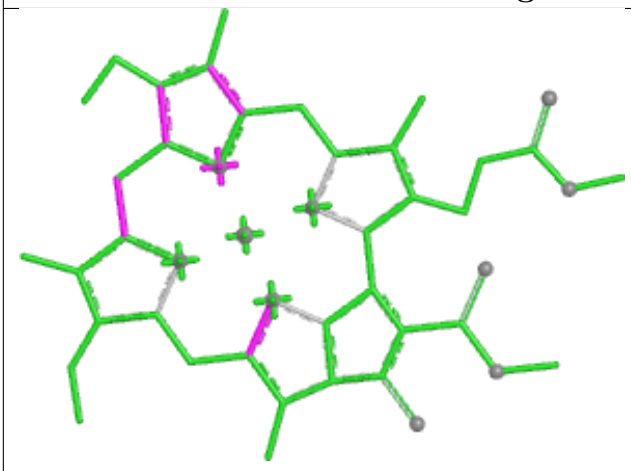
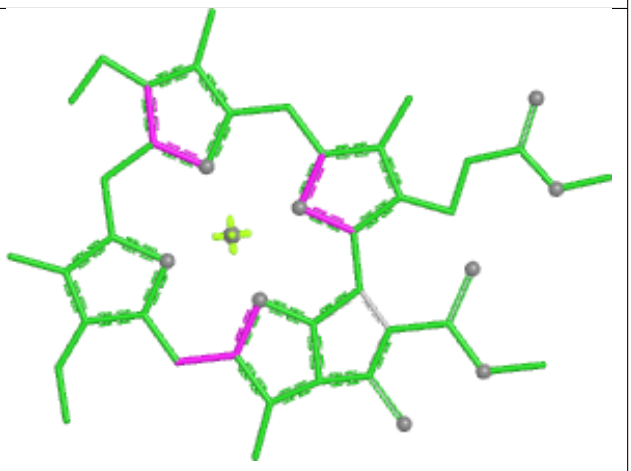


Rings

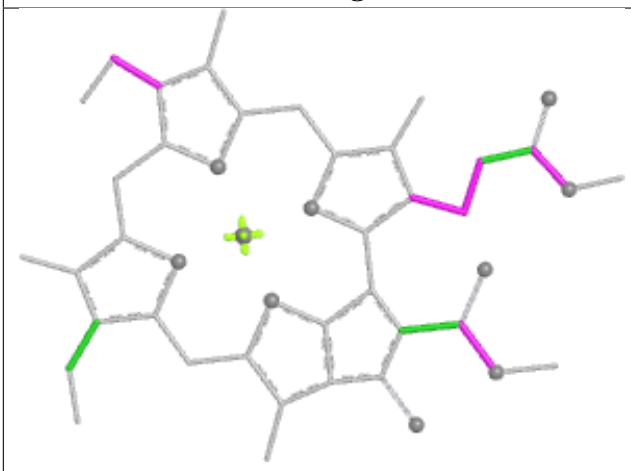
Ligand CLA F 1302



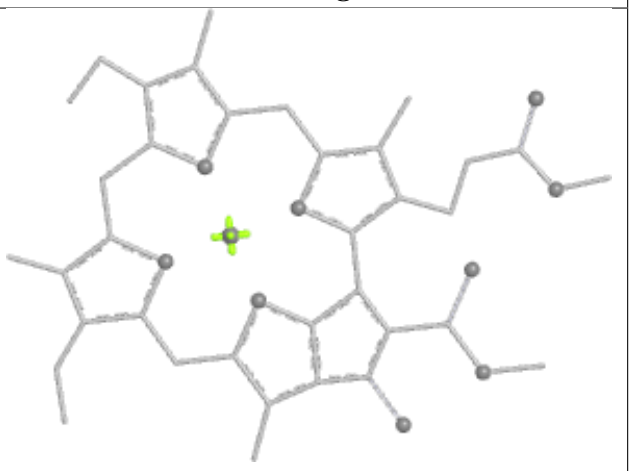
Bond lengths



Bond angles

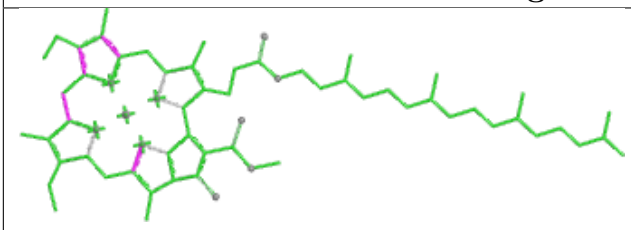


Torsions

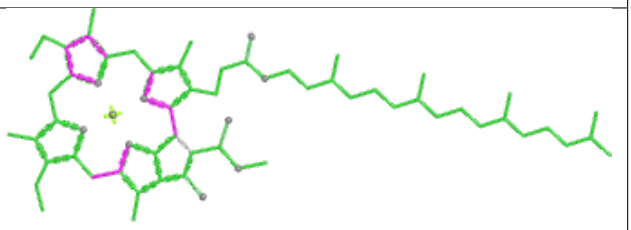


Rings

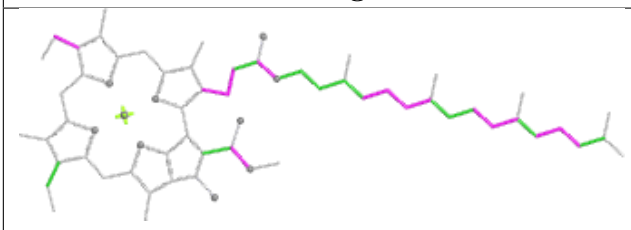
Ligand CLA n 515



Bond lengths



Bond angles



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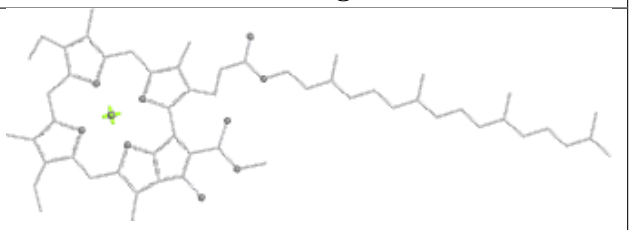
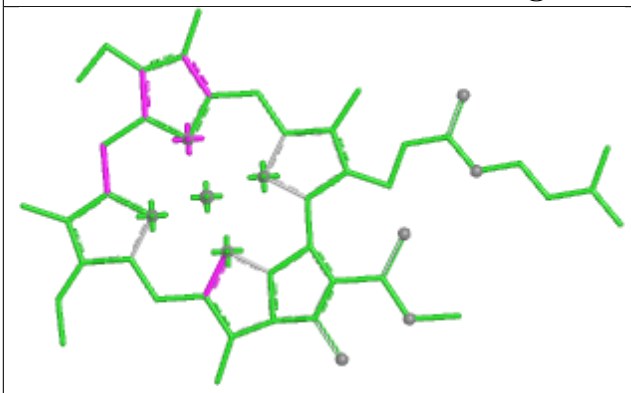
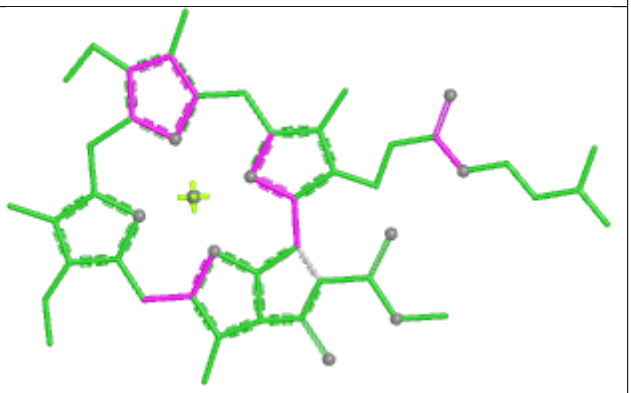


Rings

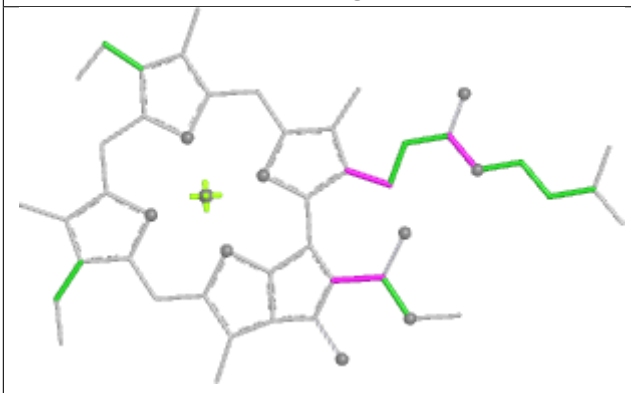
Ligand CLA x 501



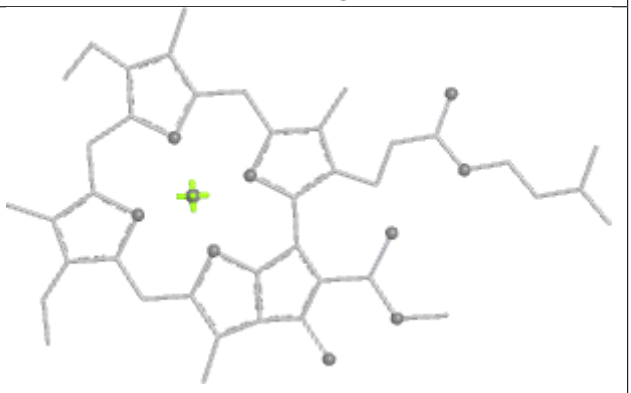
Bond lengths



Bond angles

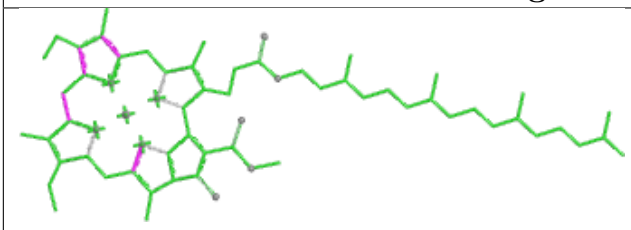


Torsions



Rings

Ligand CLA o 515



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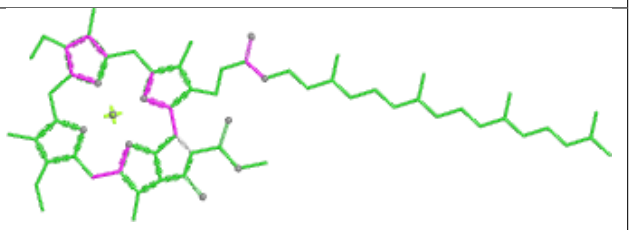
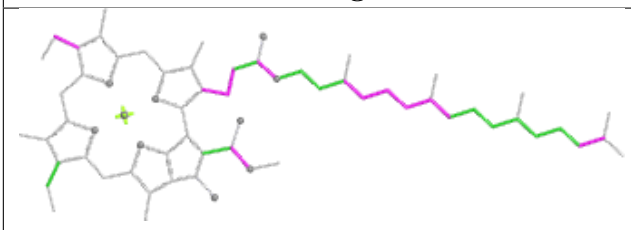
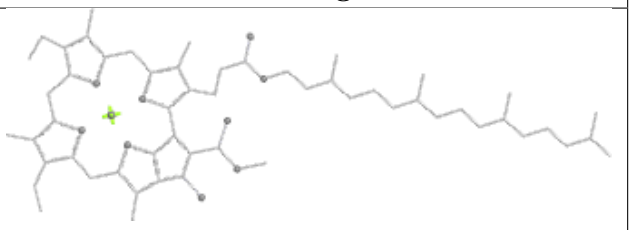


Bond angles

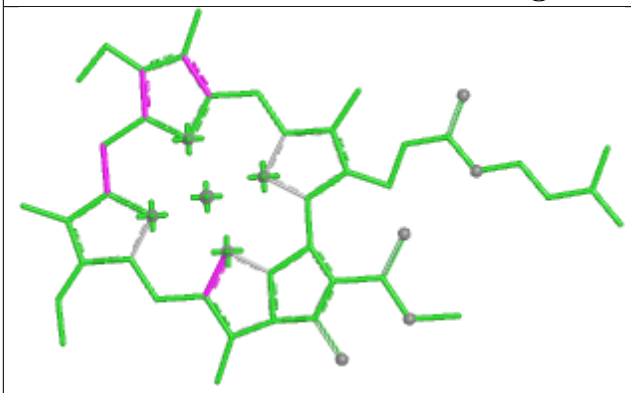


Torsions

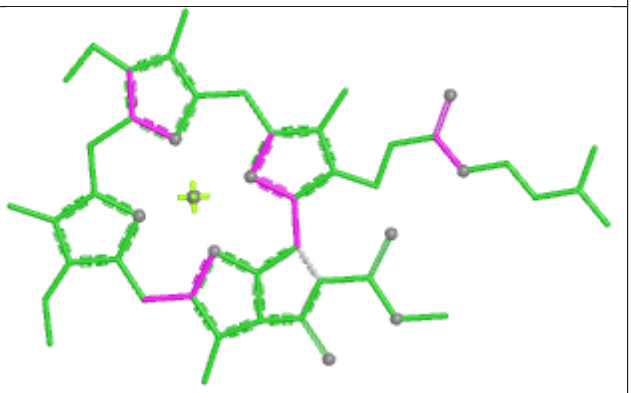


Rings

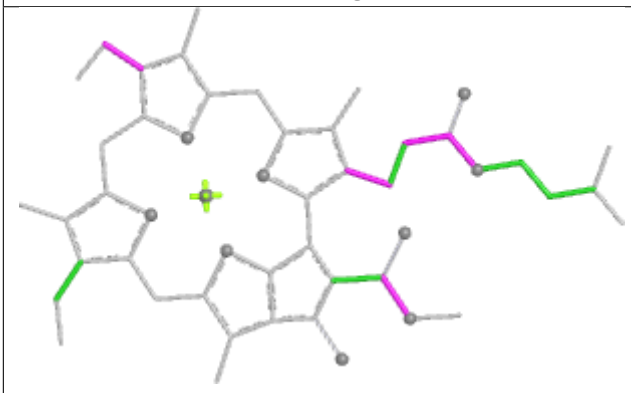
Ligand CLA t 514



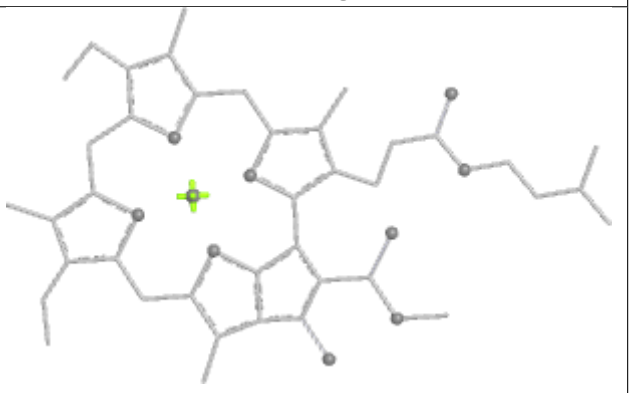
Bond lengths



Bond angles

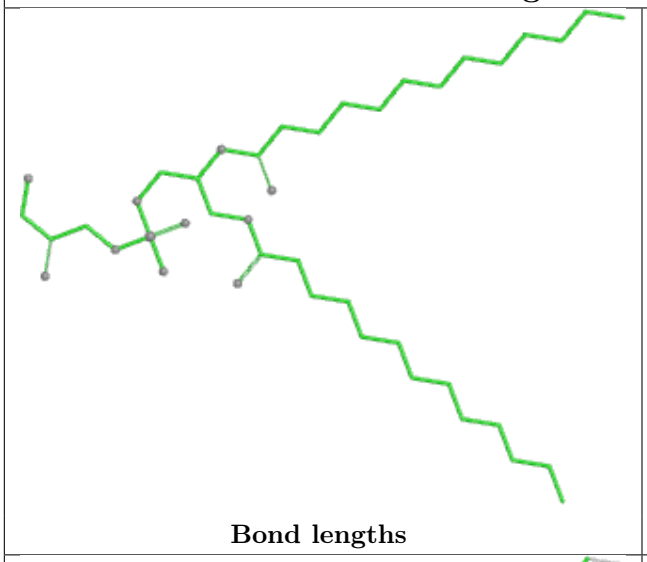


Torsions



Rings

Ligand LHG H 849



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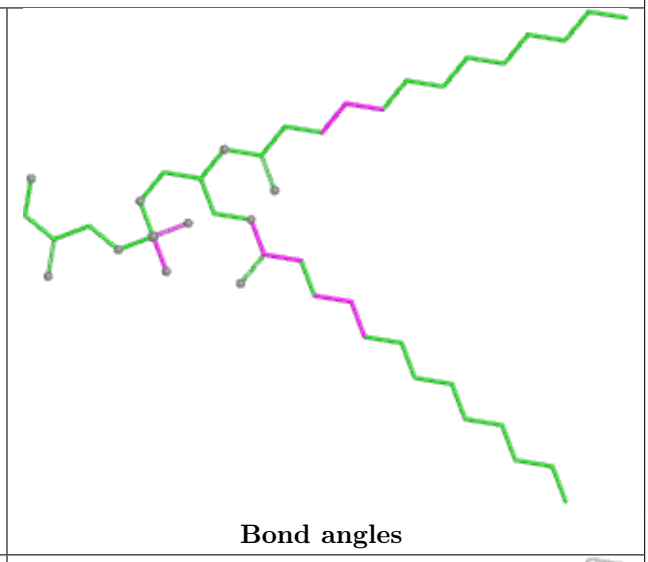
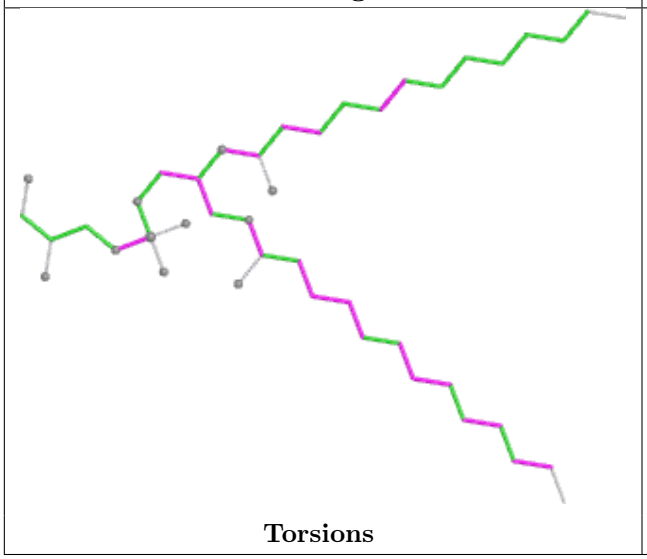


Bond angles



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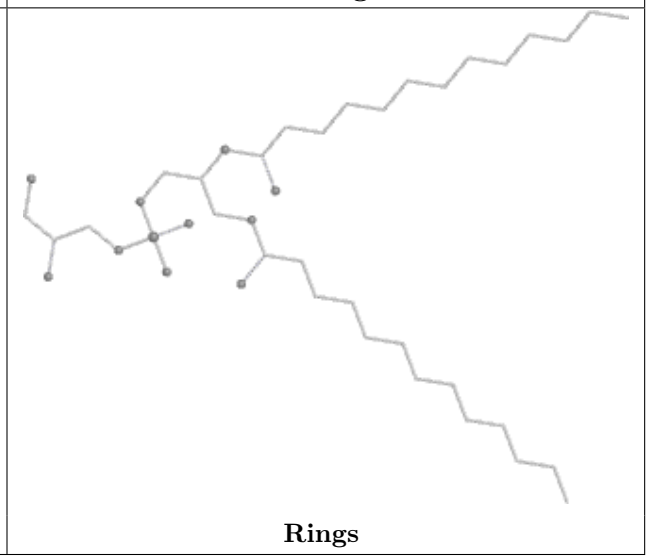
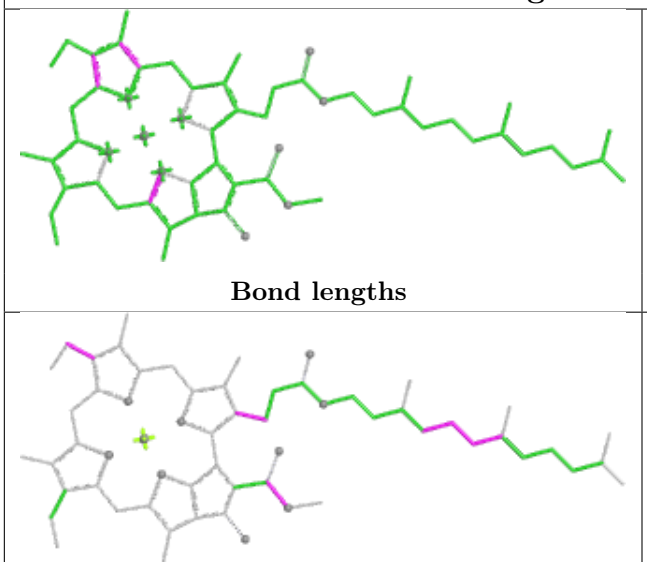


Rings

Ligand CLA Z 506



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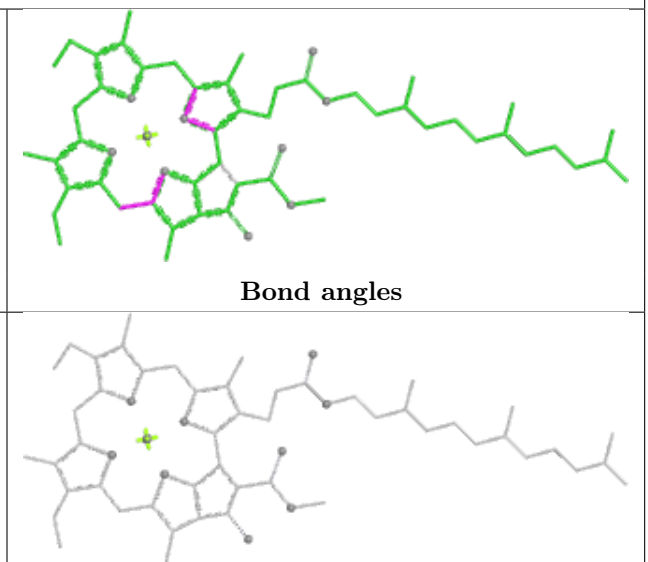
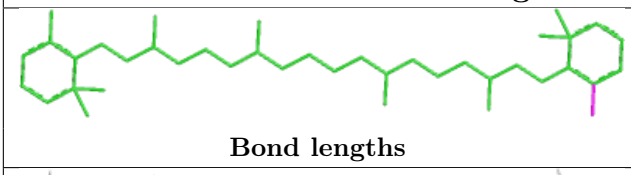


Bond angles

Torsions

Rings

Ligand BCR G 4014



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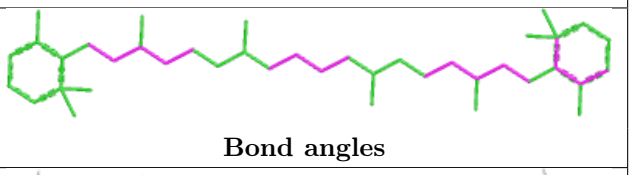
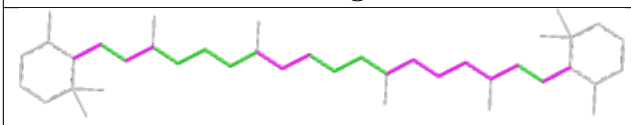


Bond angles



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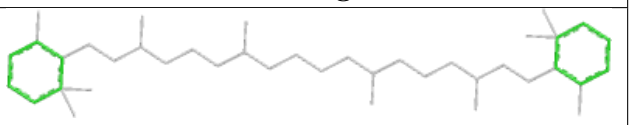
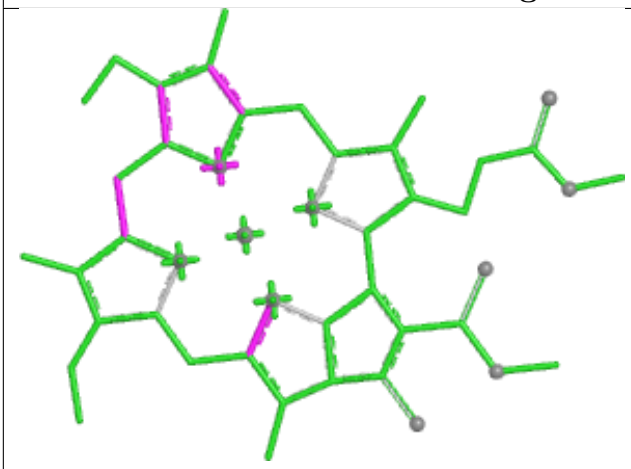


Rings

Ligand CLA a 1129



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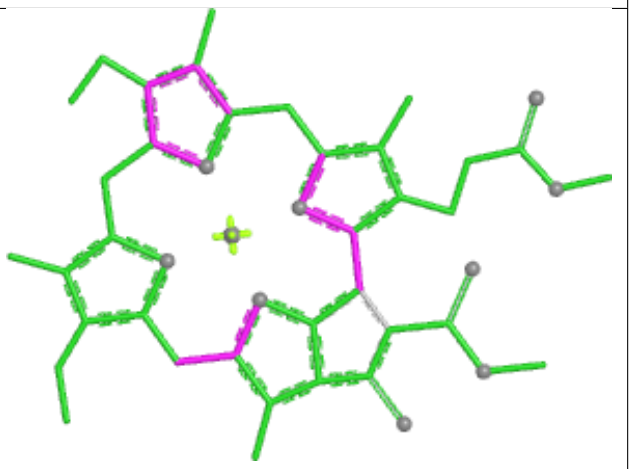
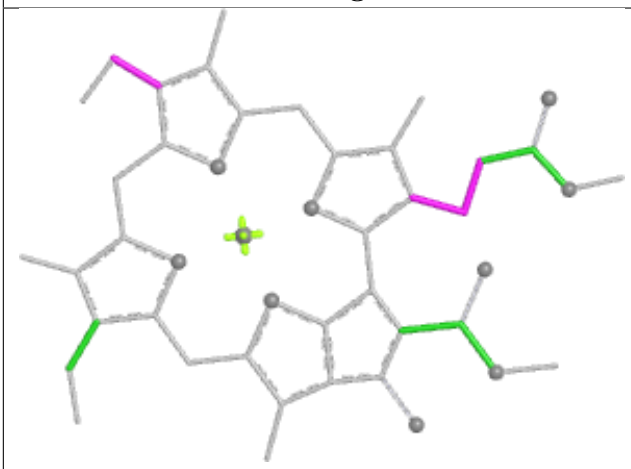


Bond angles



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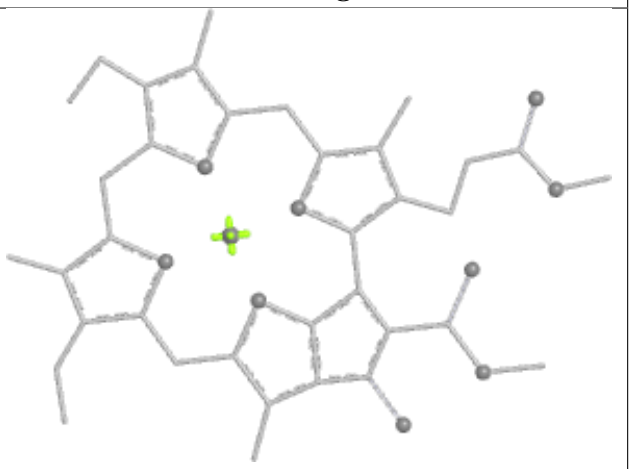
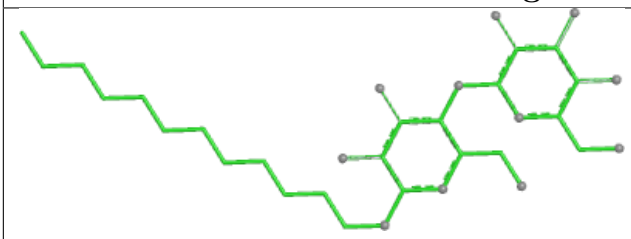


Rings

Ligand LMU p 606



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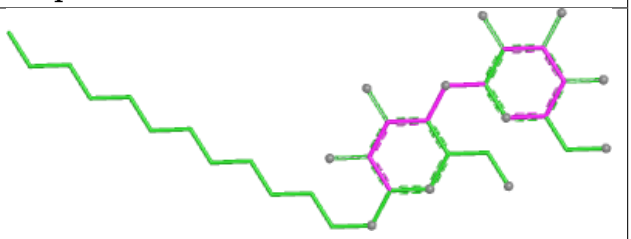
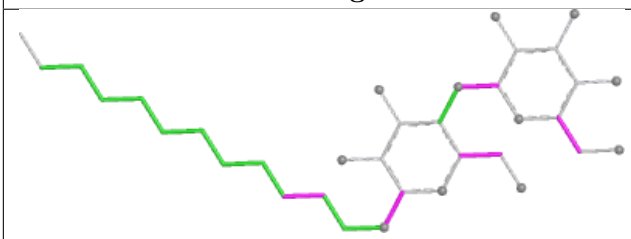


Bond angles



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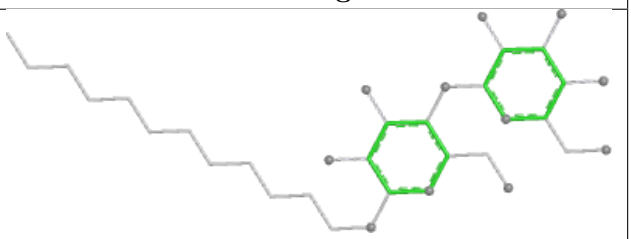
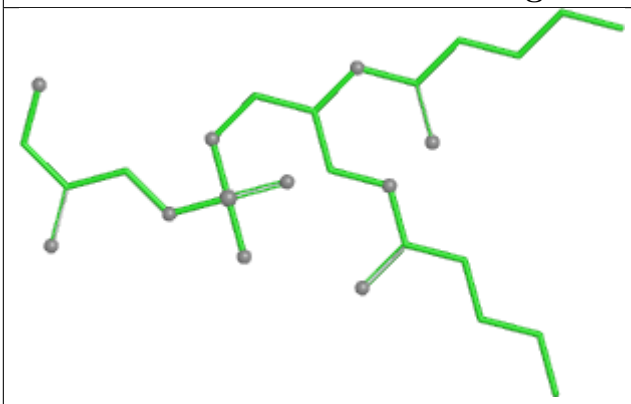


Rings

Ligand LHG u 605



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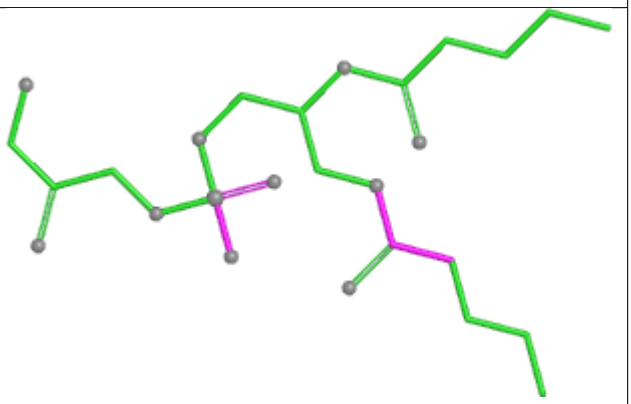
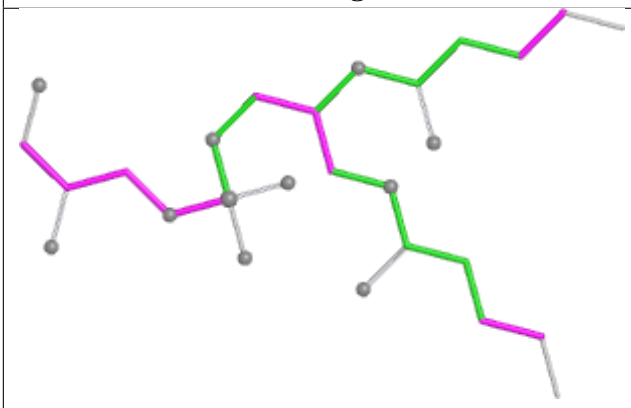


Bond angles



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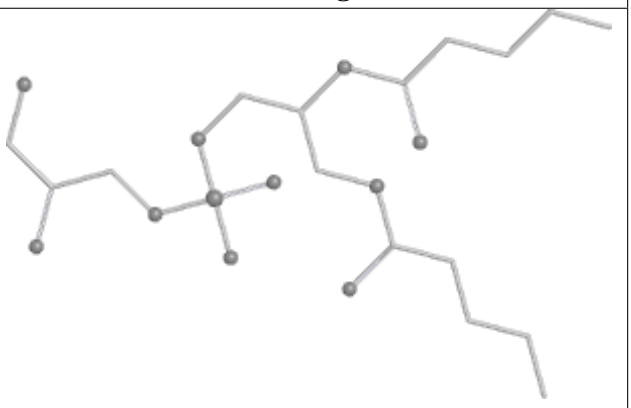
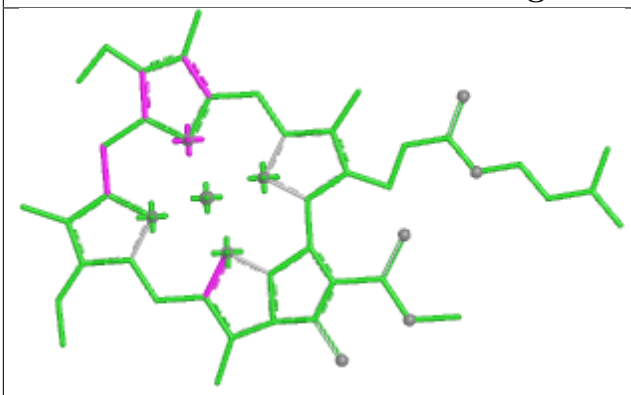


Rings

Ligand CLA p 514



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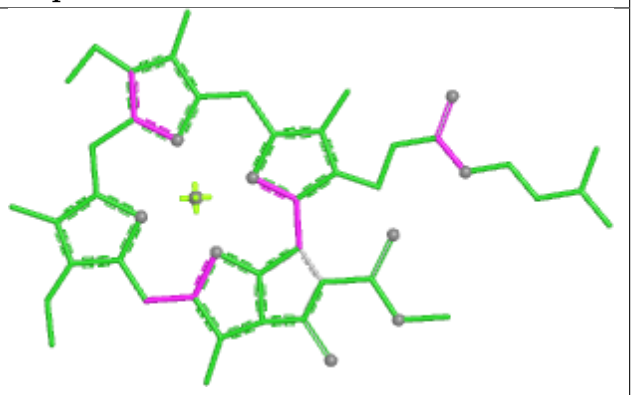
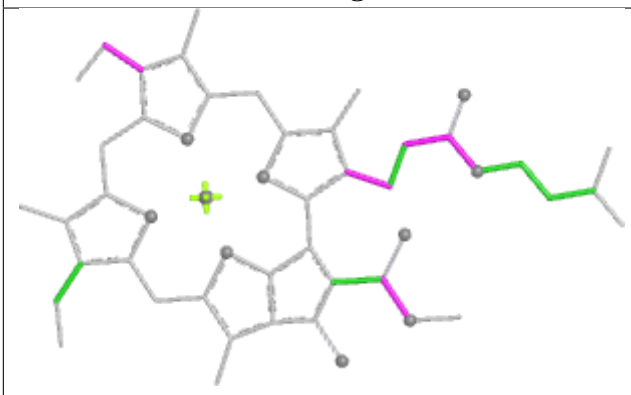


Bond angles



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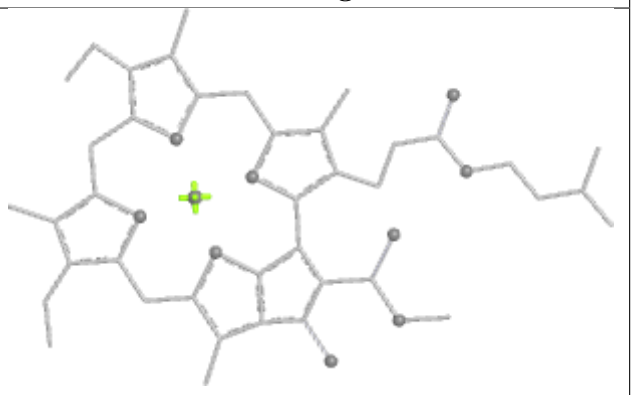
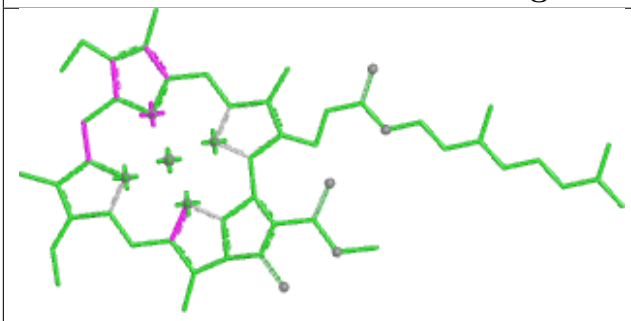
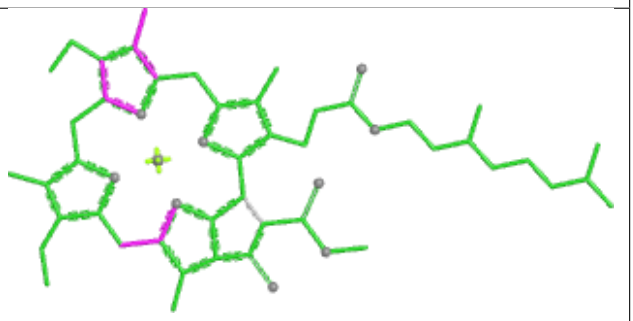


Rings

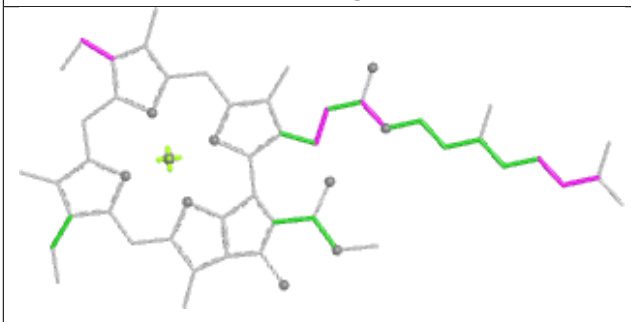
Ligand CLA t 517



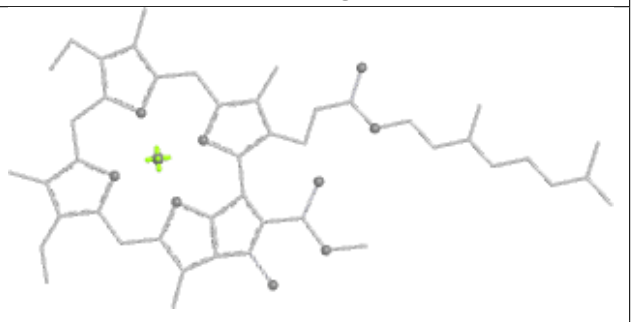
Bond lengths



Bond angles

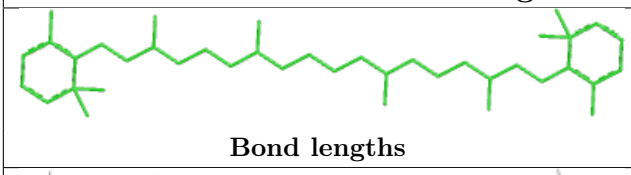


Torsions



Rings

Ligand BCR b 4005



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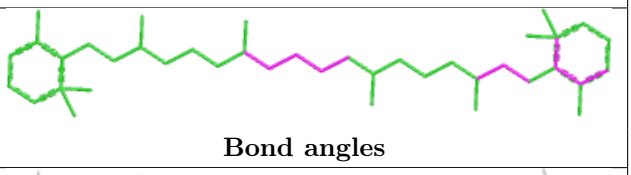
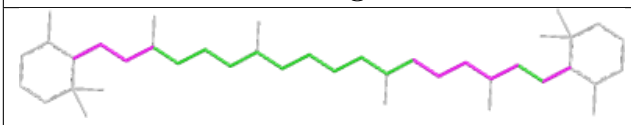


Bond angles



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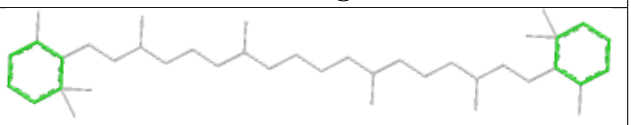
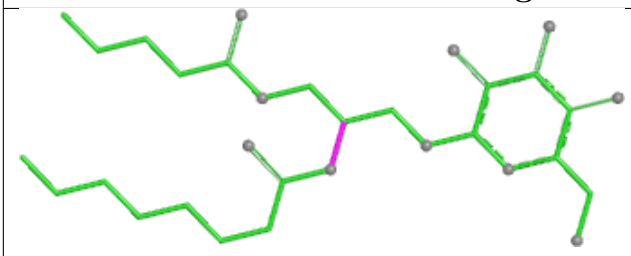


Rings

Ligand LMG a 4201



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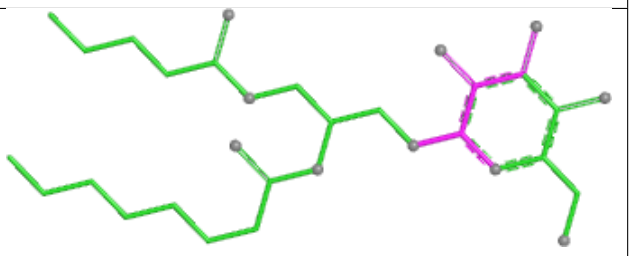
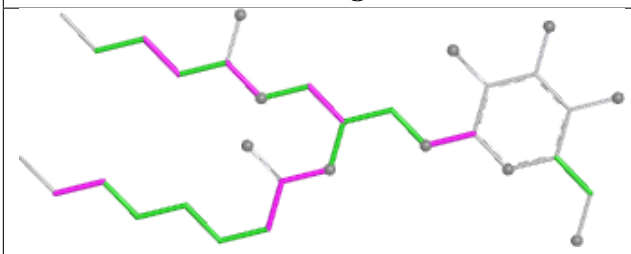


Bond angles



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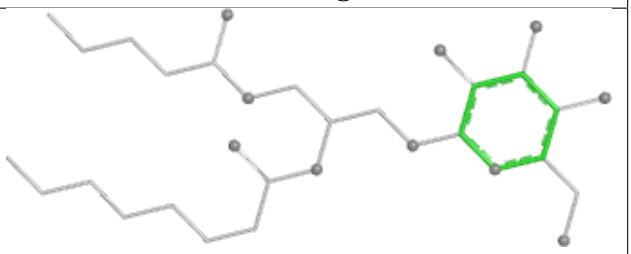
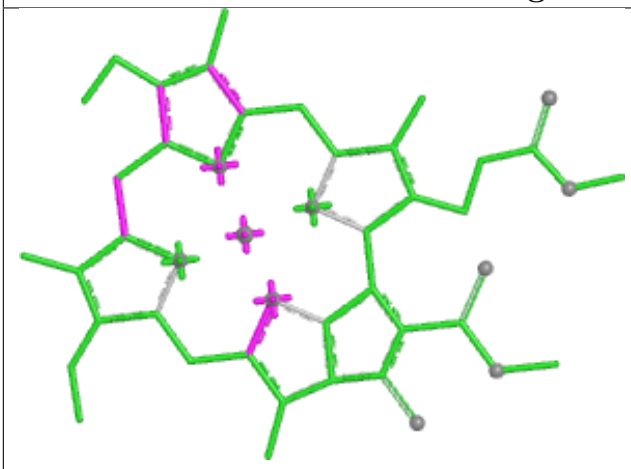


Rings

Ligand CLA y 503



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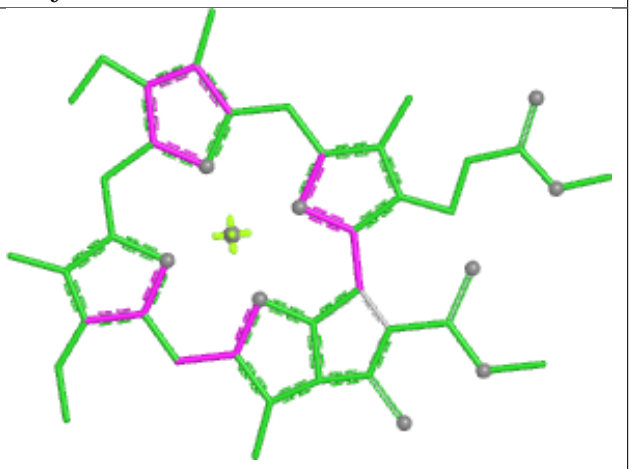
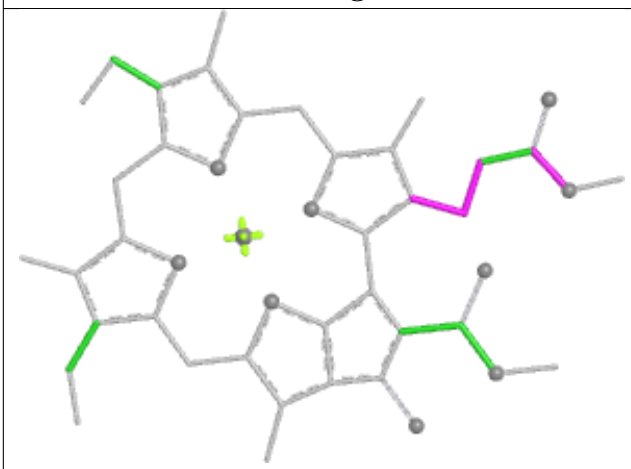
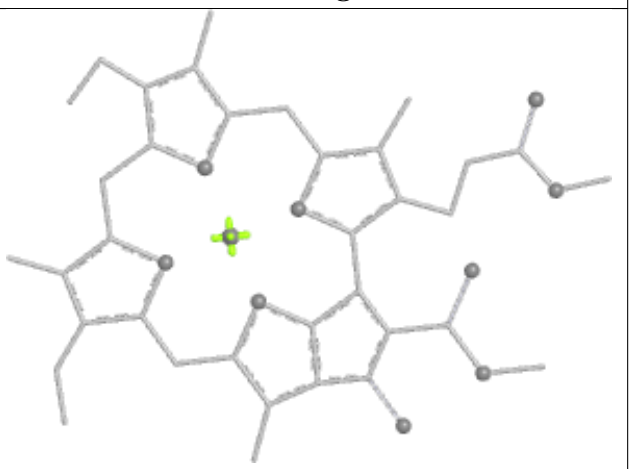


Bond angles

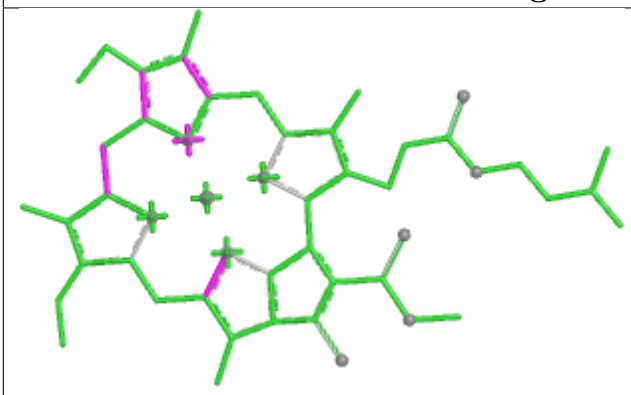


Torsions



Rings

Ligand CLA s 501



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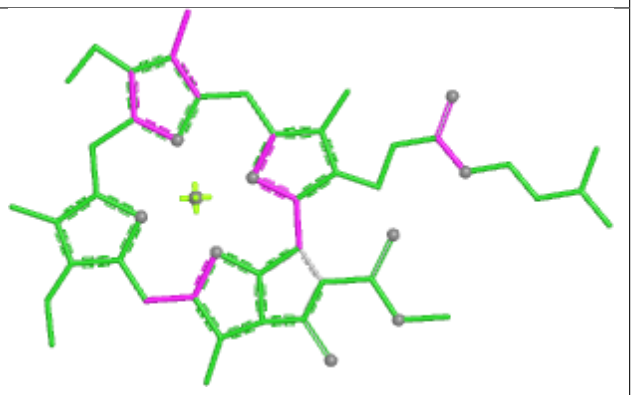
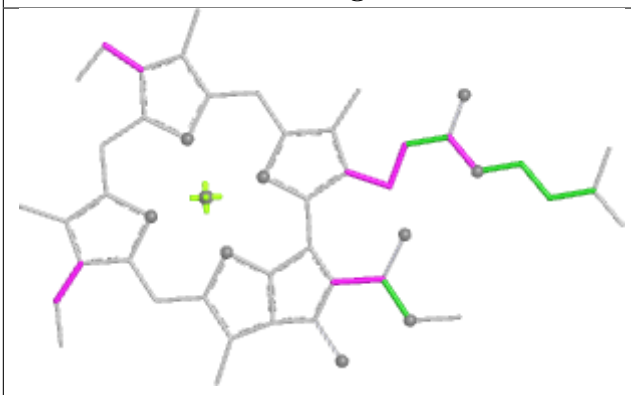
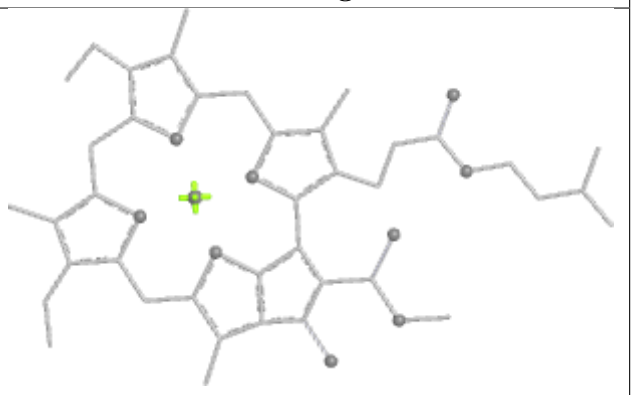


Bond angles

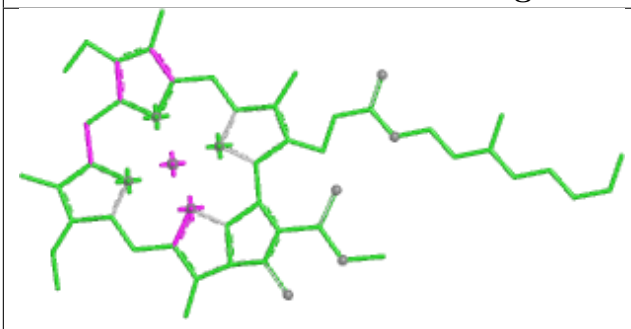


Torsions

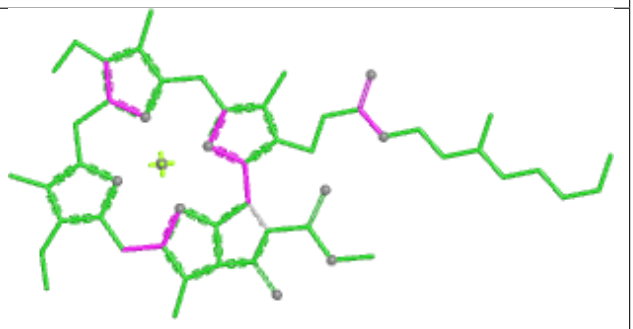


Rings

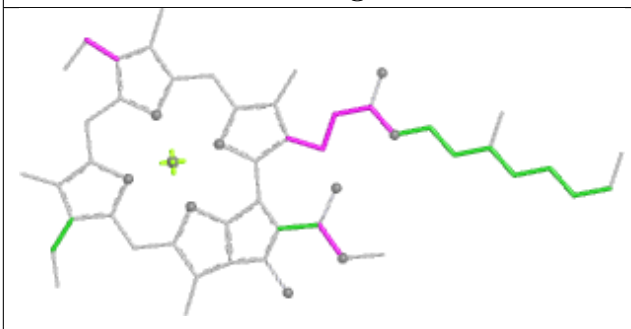
Ligand CLA H 1116



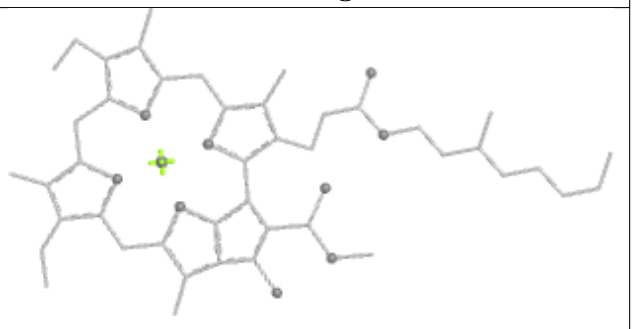
Bond lengths



Bond angles

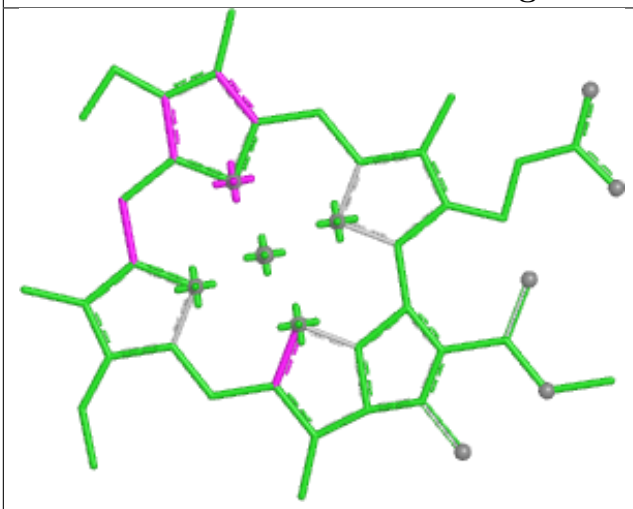


Torsions

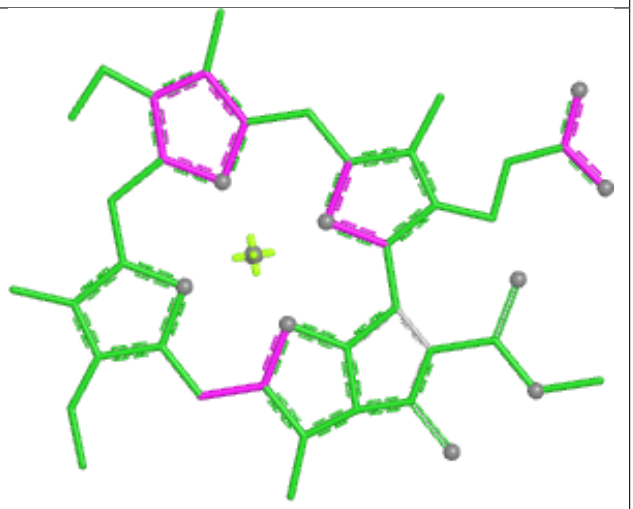


Rings

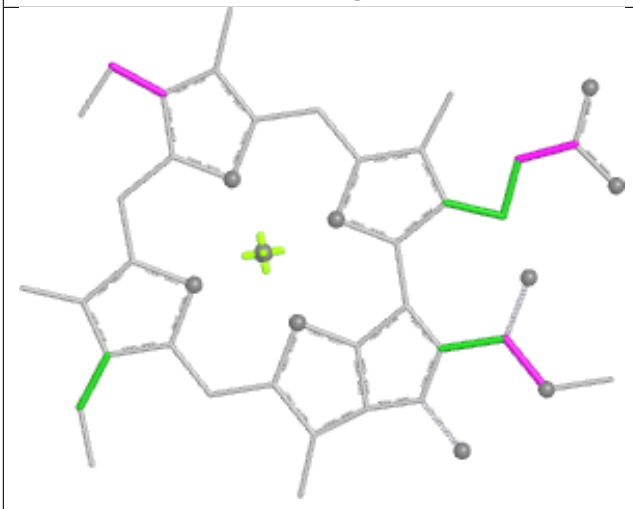
Ligand CLA J 1302



Bond lengths



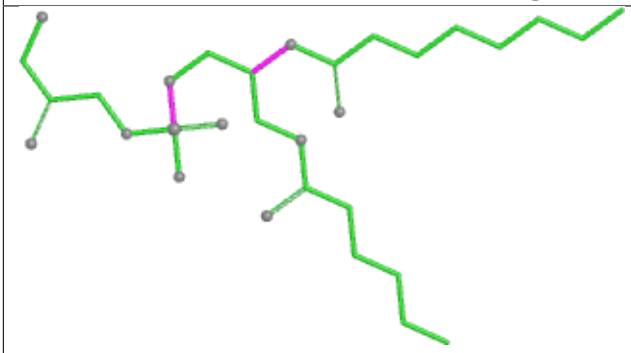
Bond angles



Torsions

Rings

Ligand LHG g 605



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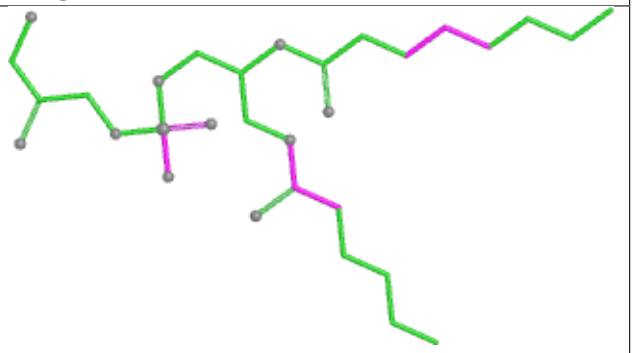
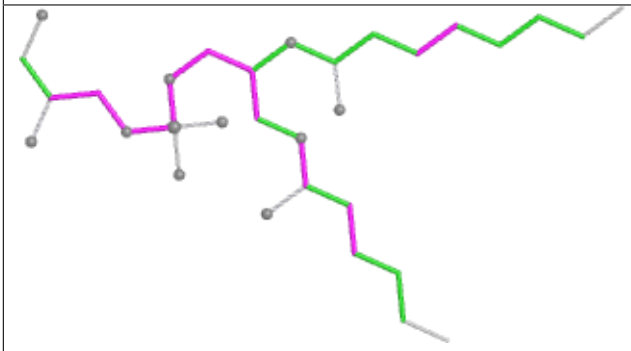
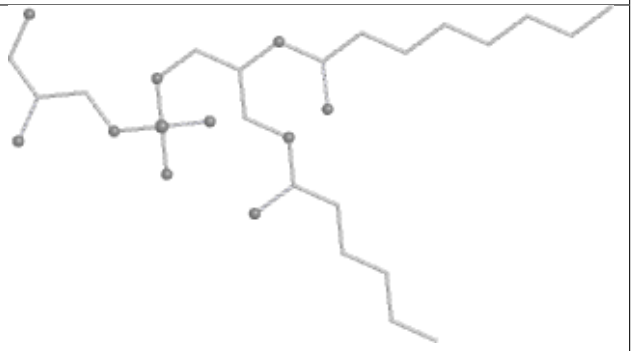


Bond angles

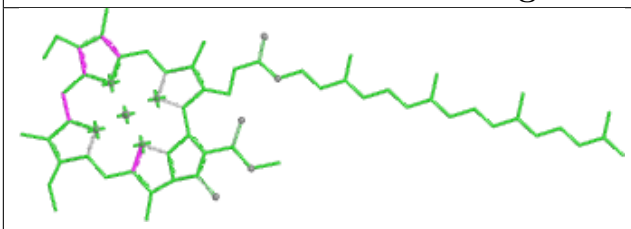


Torsions



Rings

Ligand CLA W 515



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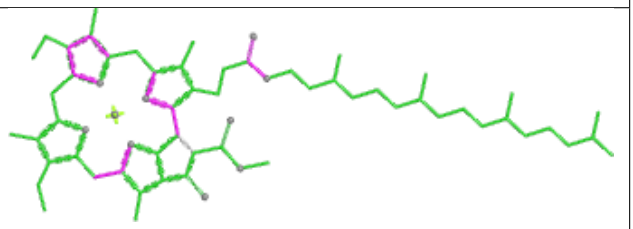
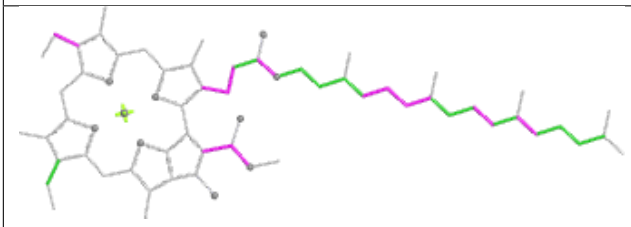
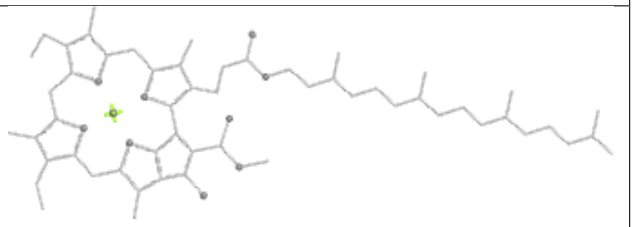


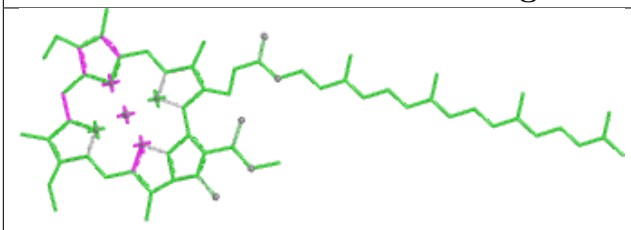
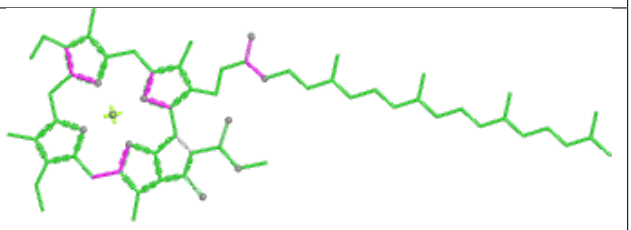
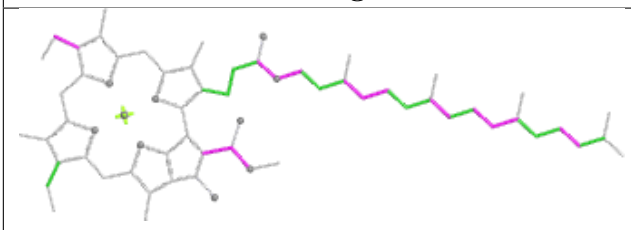
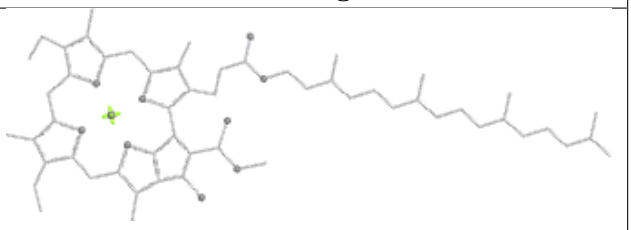
Bond angles

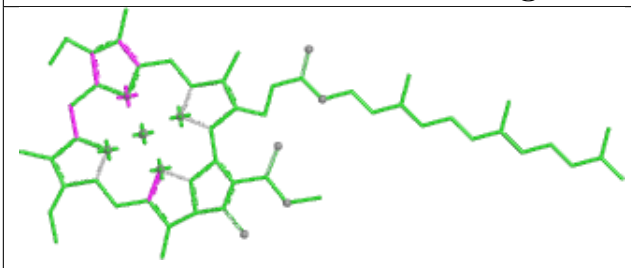
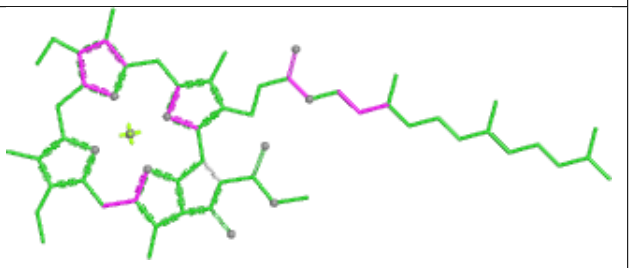
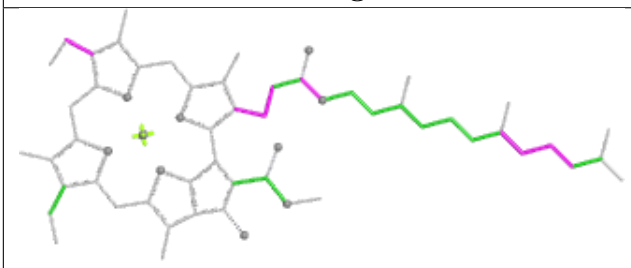
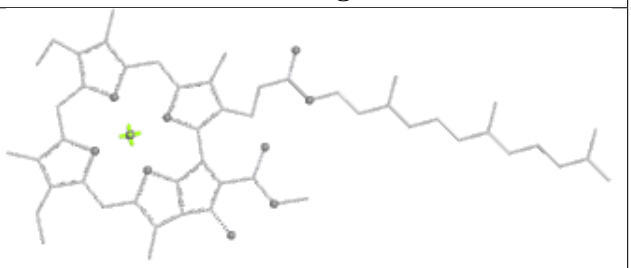


Torsions

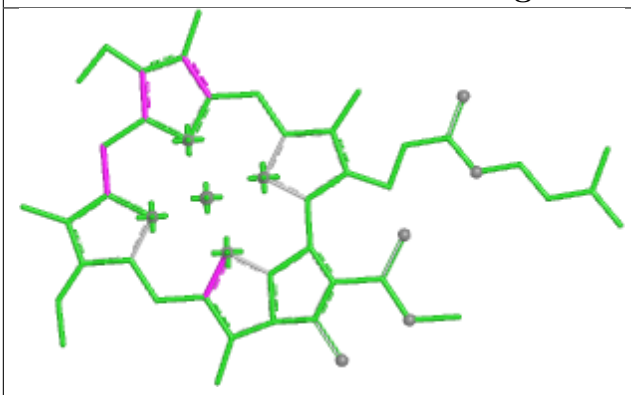


Rings

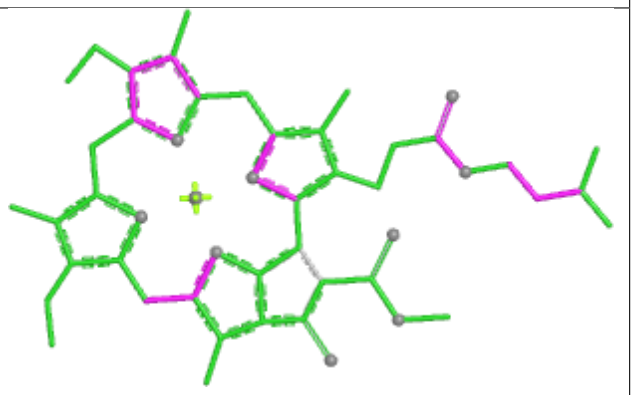
Ligand CLA a 1104	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1130	
	
Bond lengths	Bond angles
	
Torsions	Rings

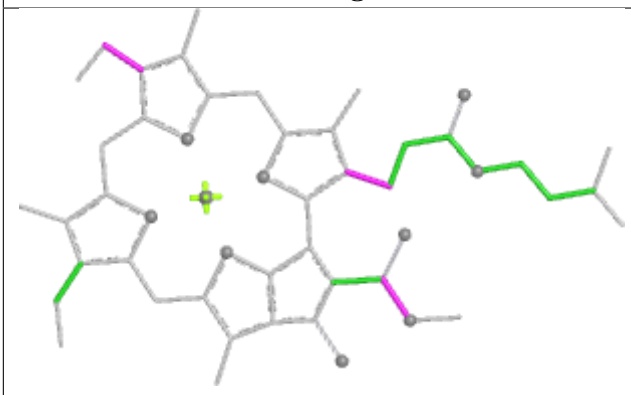
Ligand CLA H 1107



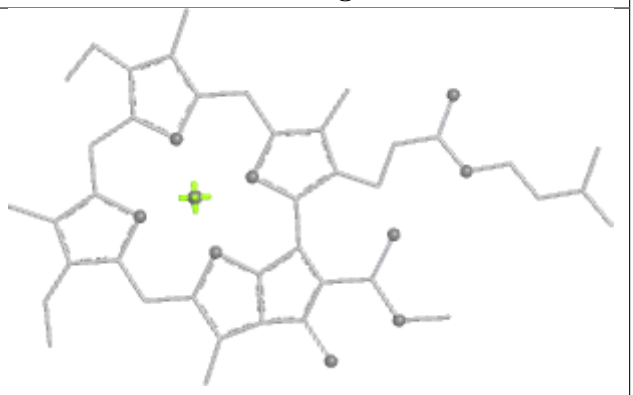
Bond lengths



Bond angles



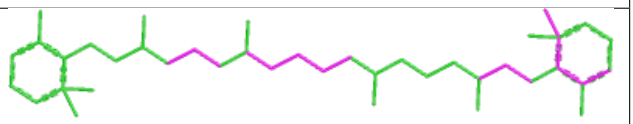
Torsions



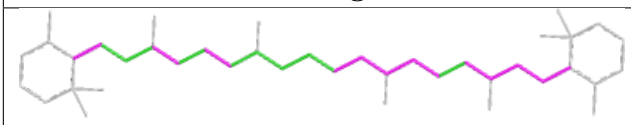
Rings

Ligand BCR b 4010

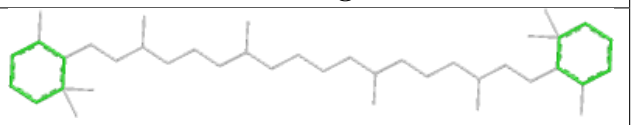
Bond lengths



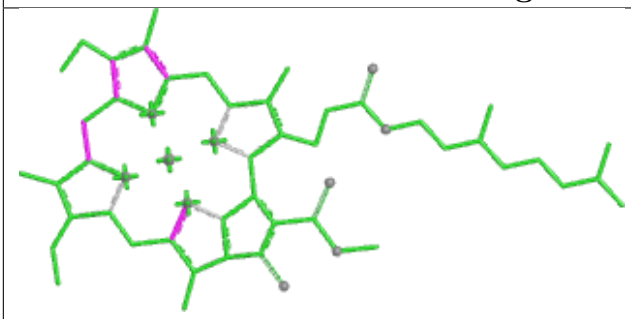
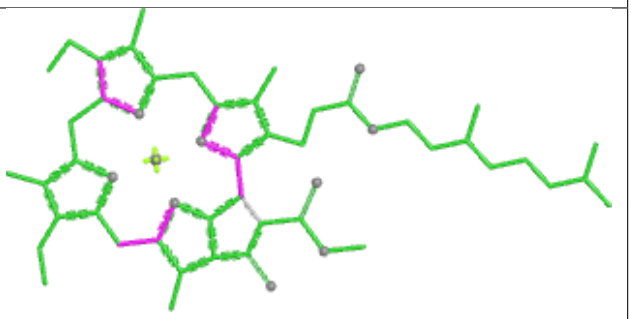
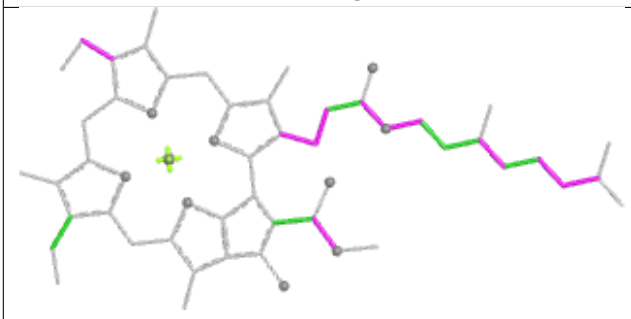
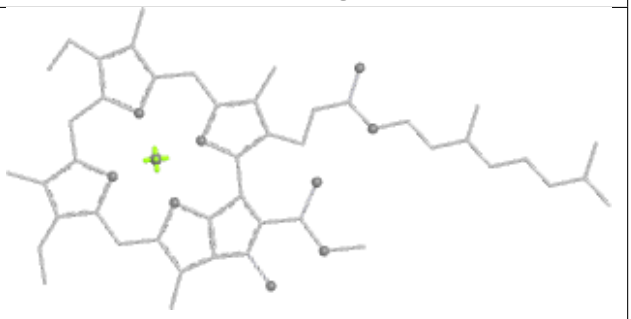
Bond angles

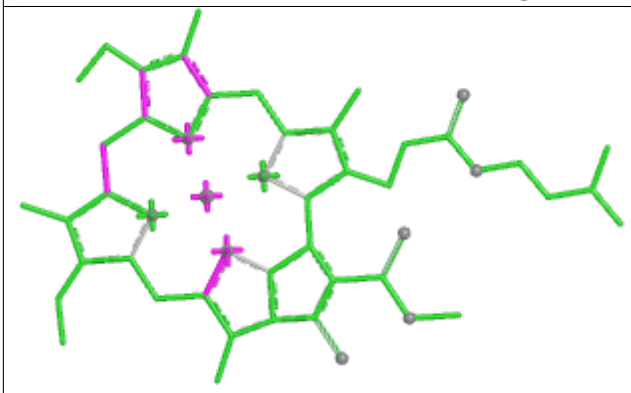
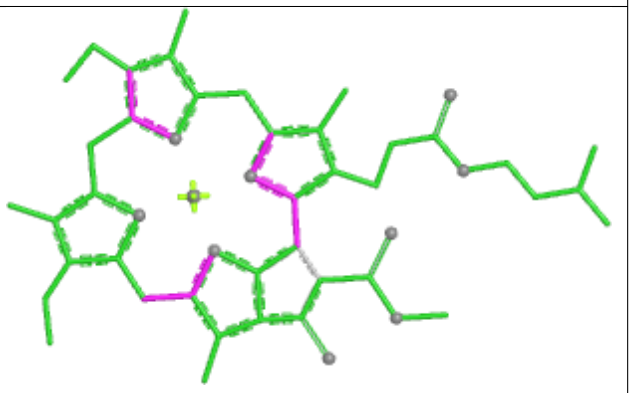
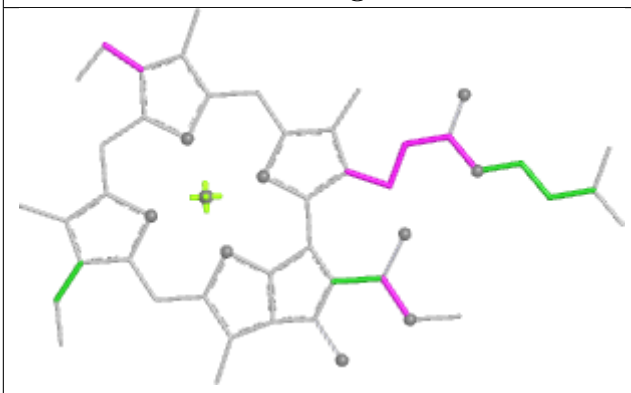
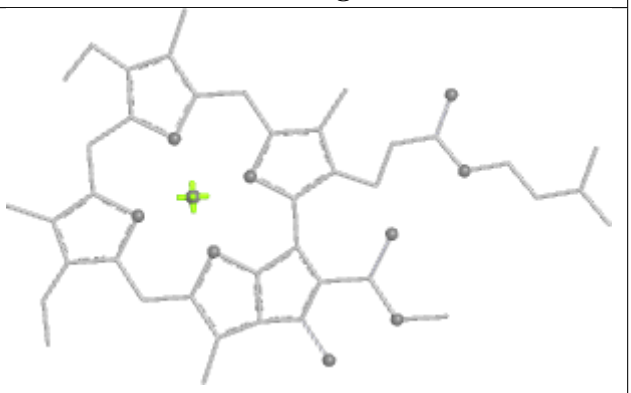


Torsions

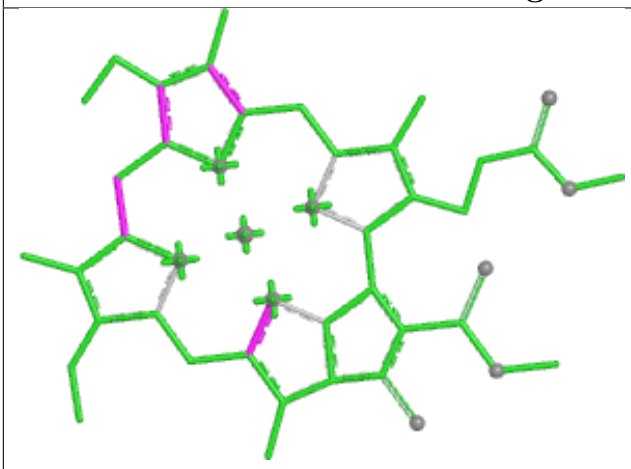


Rings

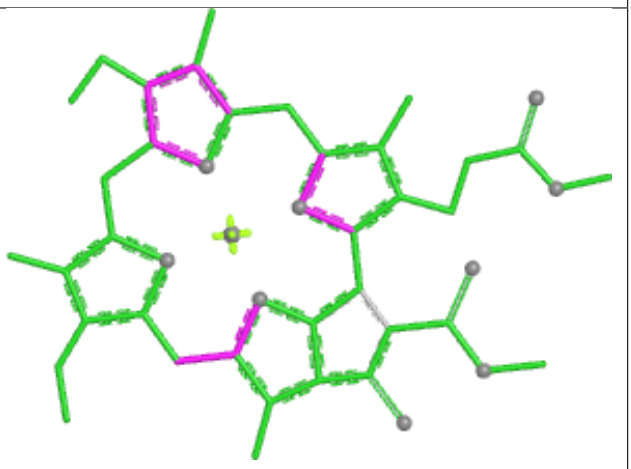
Ligand CLA B 1228	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1236	
	
Bond lengths	Bond angles
	
Torsions	Rings

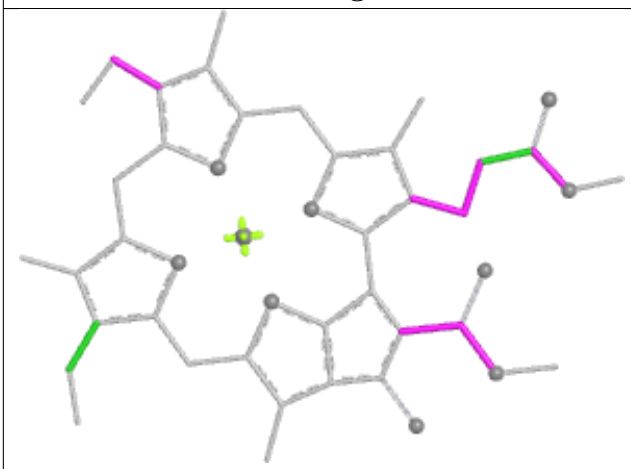
Ligand CLA Z 516



Bond lengths



Bond angles



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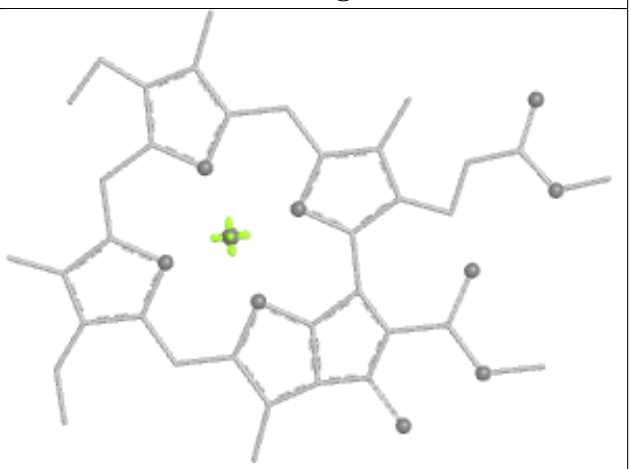
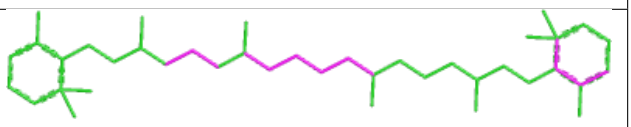


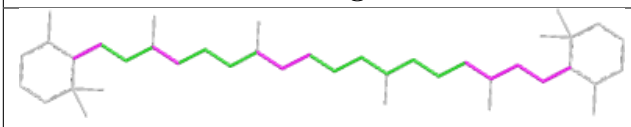
Rings

Ligand BCR B 4017

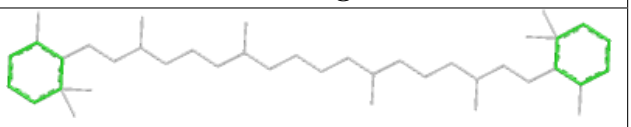
Bond lengths



Bond angles

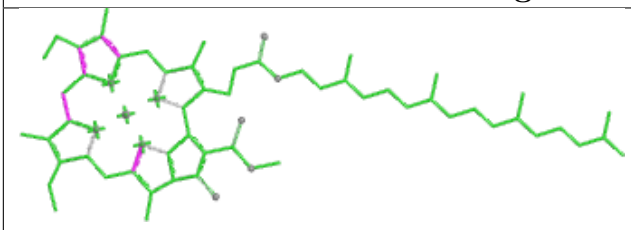


Torsions

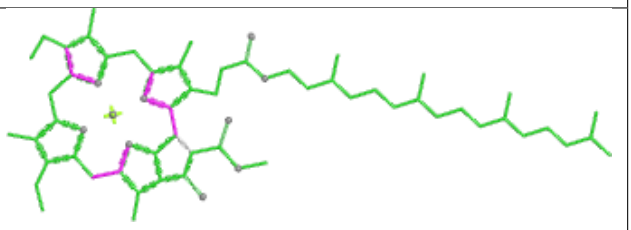


Rings

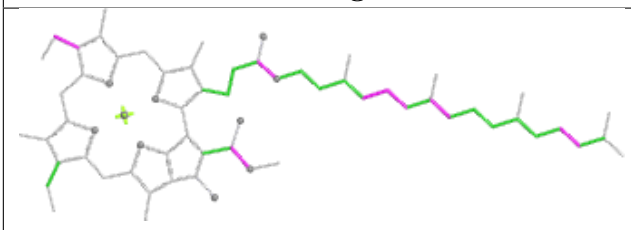
Ligand CLA H 1131



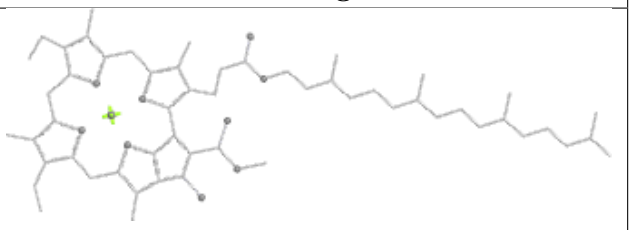
Bond lengths



Bond angles

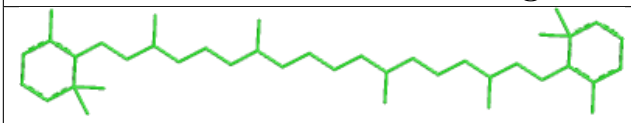


Torsions

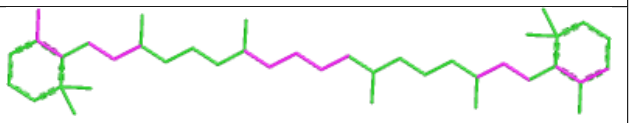


Rings

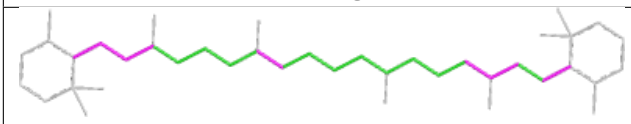
Ligand BCR Y 601



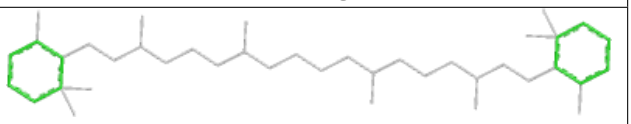
Bond lengths



Bond angles

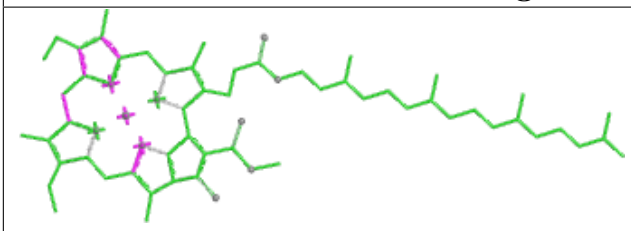


Torsions

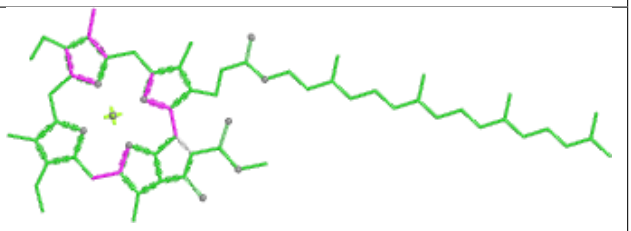


Rings

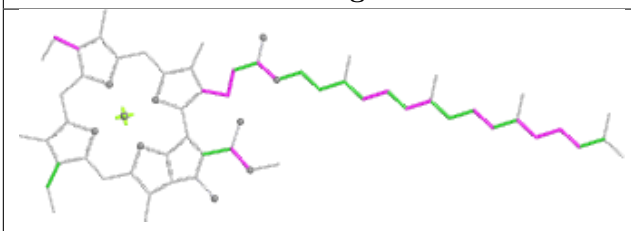
Ligand CLA B 1211



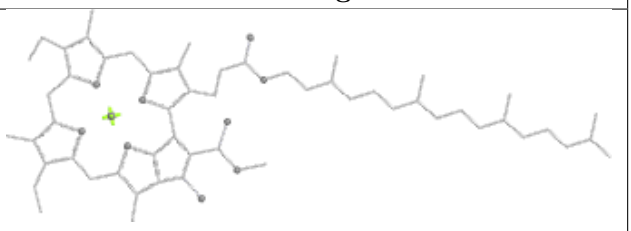
Bond lengths



Bond angles

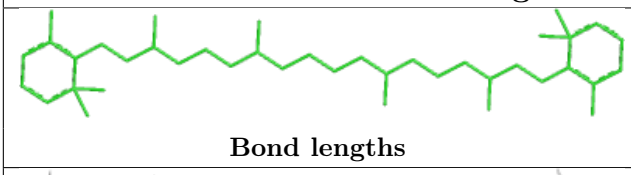


Torsions

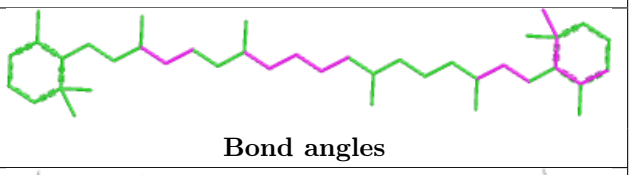


Rings

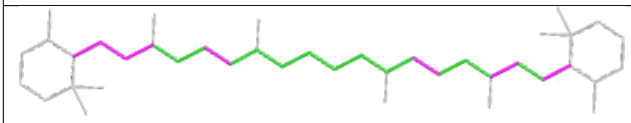
Ligand BCR K 4001



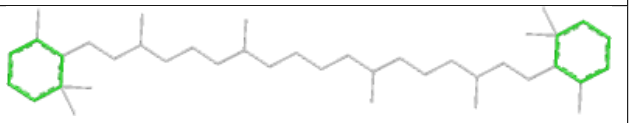
Bond lengths



Bond angles



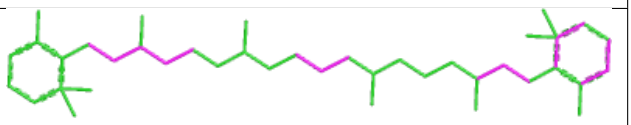
Torsions



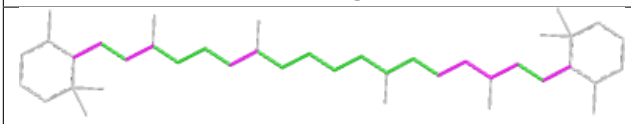
Rings

Ligand BCR n 601

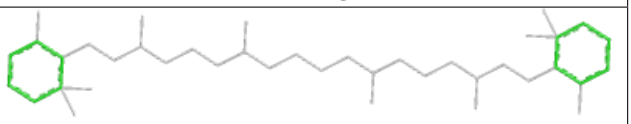
Bond lengths



Bond angles

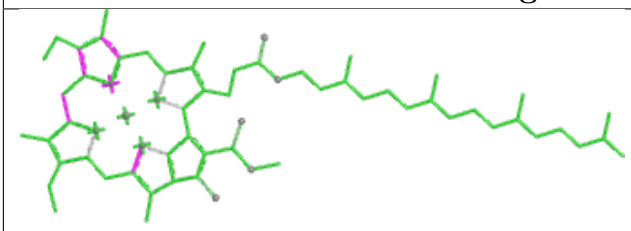


Torsions



Rings

Ligand CLA a 1117



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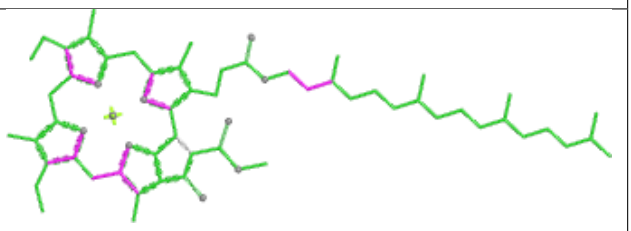
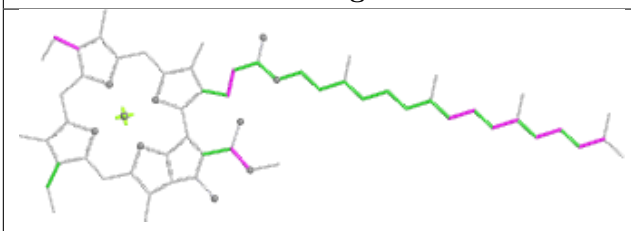
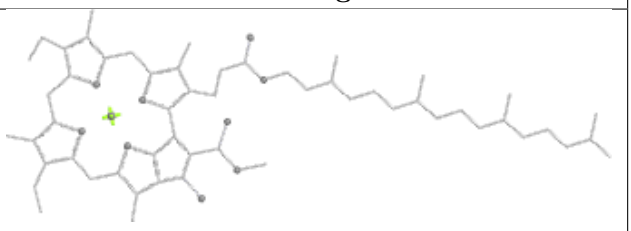


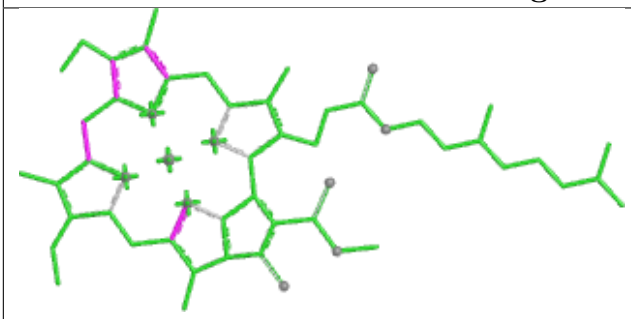
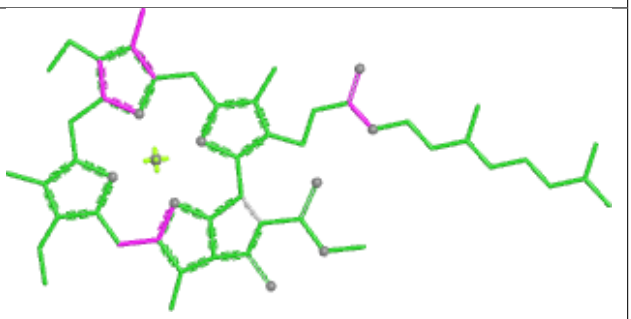
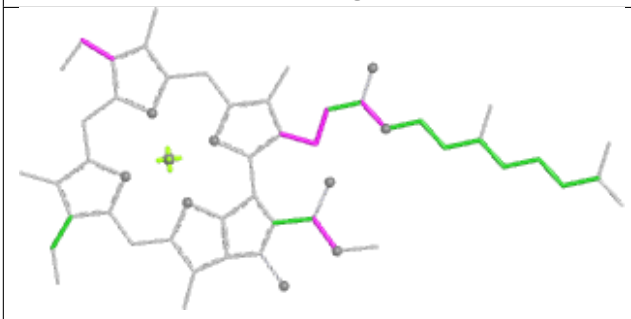
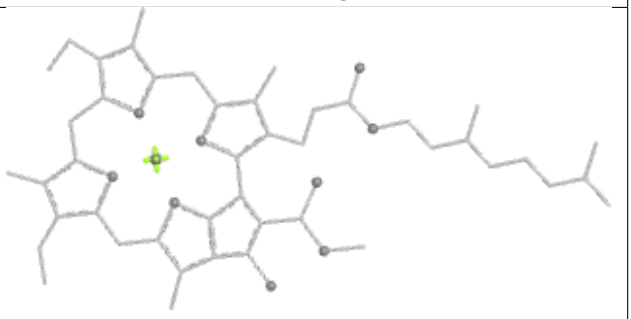
Bond angles

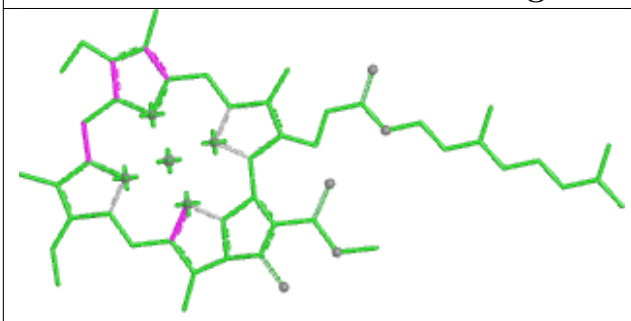
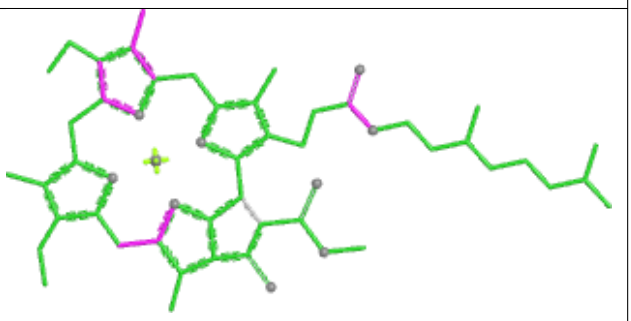
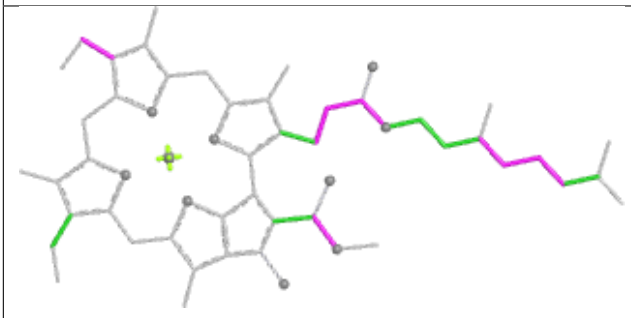
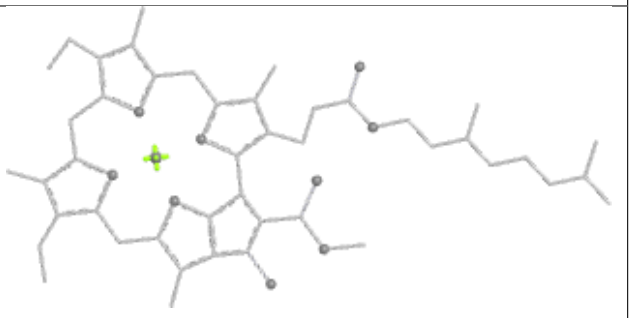


Torsions

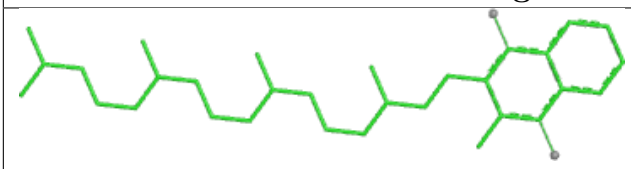


Rings

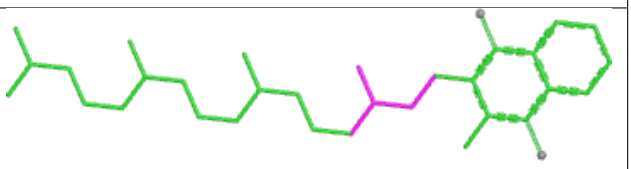
Ligand CLA t 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

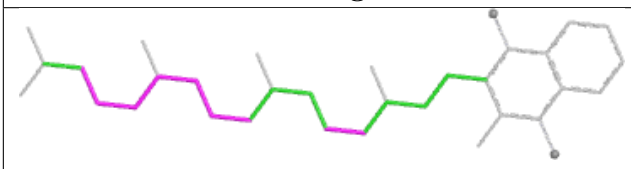
Ligand PQN B 2002



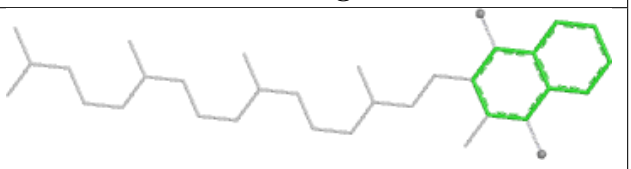
Bond lengths



Bond angles

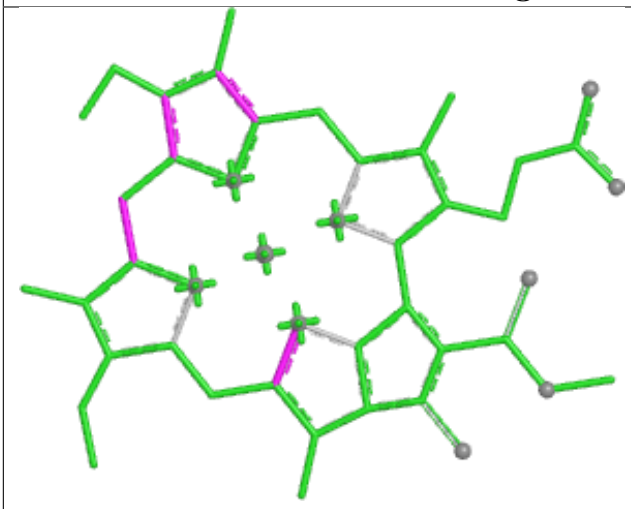


Torsions



Rings

Ligand CLA K 4003



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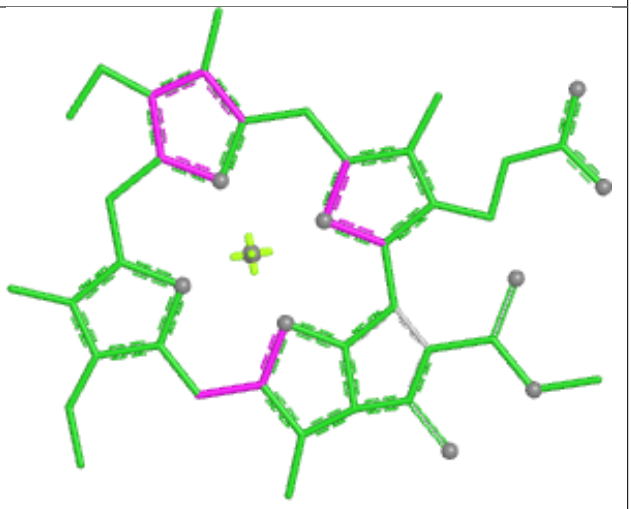
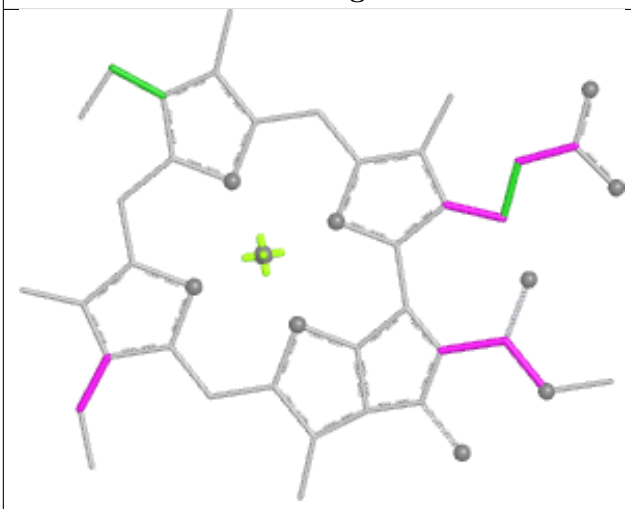
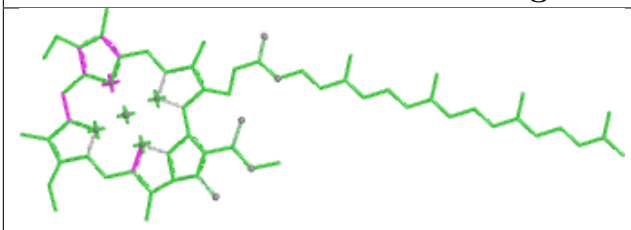
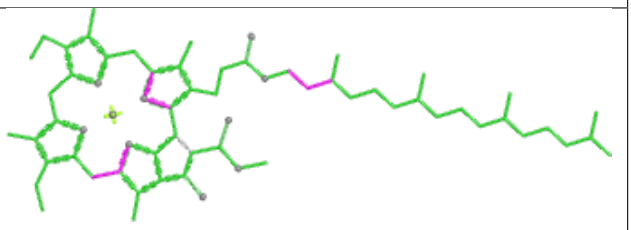
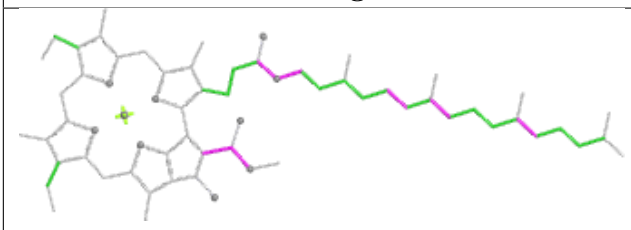
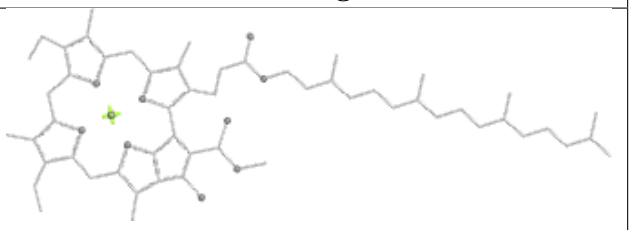


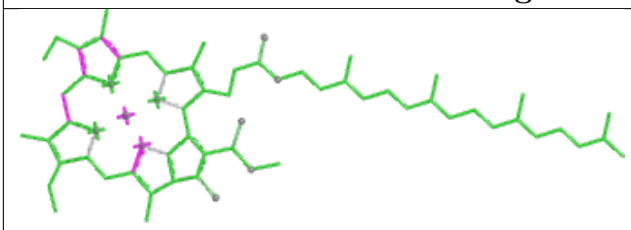
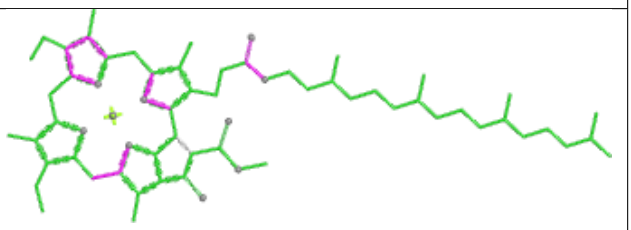
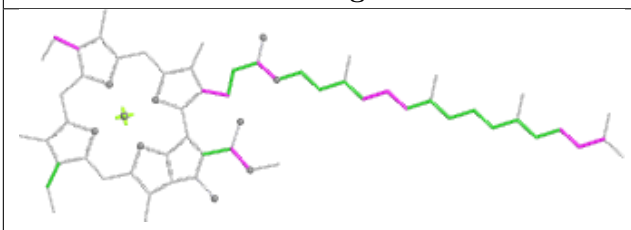
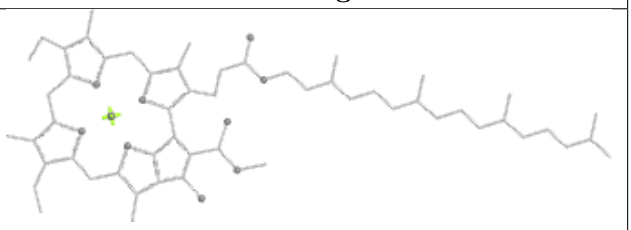
Bond angles



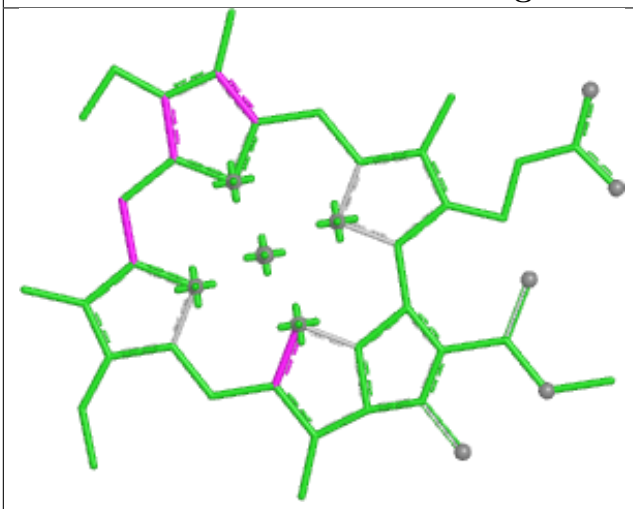
Torsions

Rings

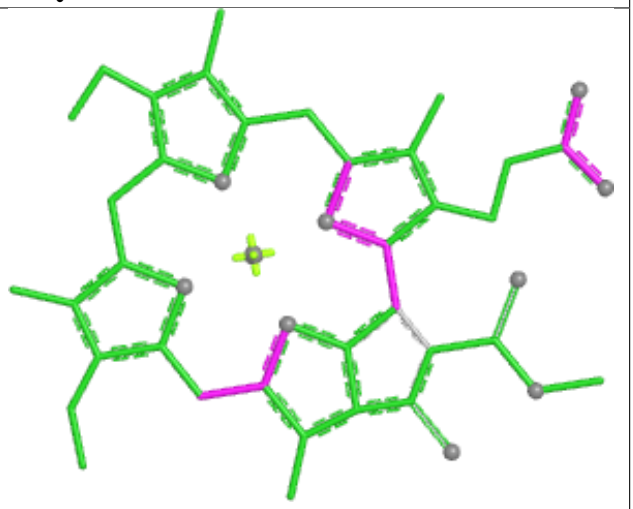
Ligand CLA r 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1140	
	
Bond lengths	Bond angles
	
Torsions	Rings

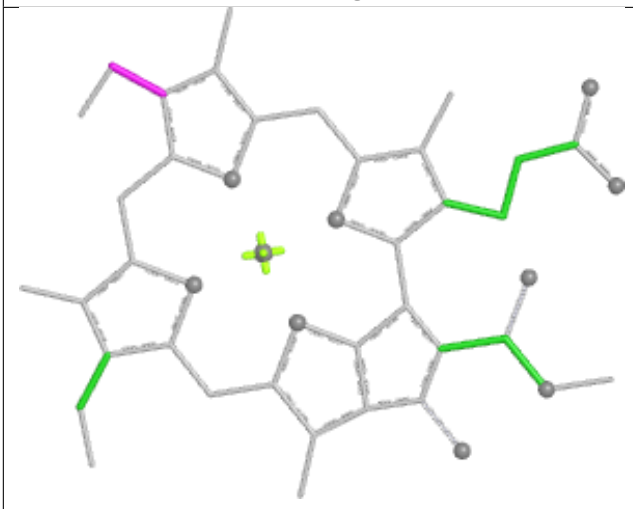
Ligand CLA Q 1301



Bond lengths



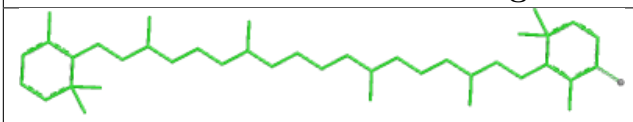
Bond angles



Torsions

Rings

Ligand ECH M 4021



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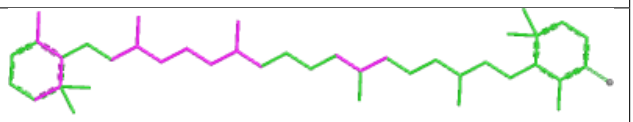

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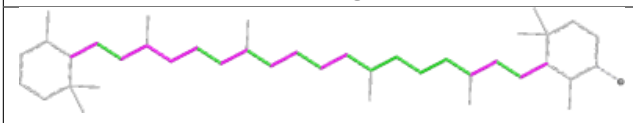
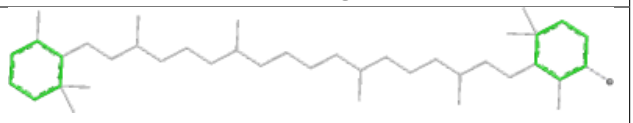
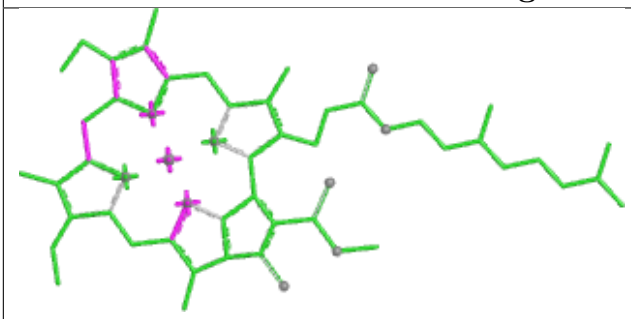


Torsions



Rings

Ligand CLA b 1213



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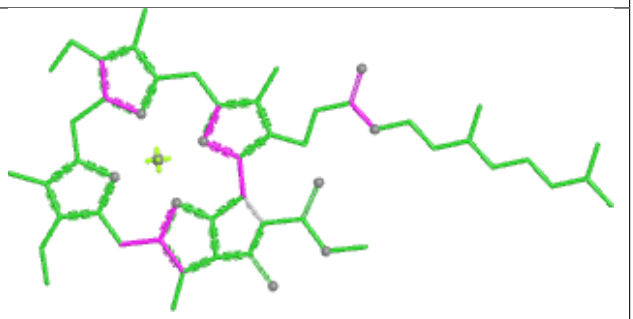
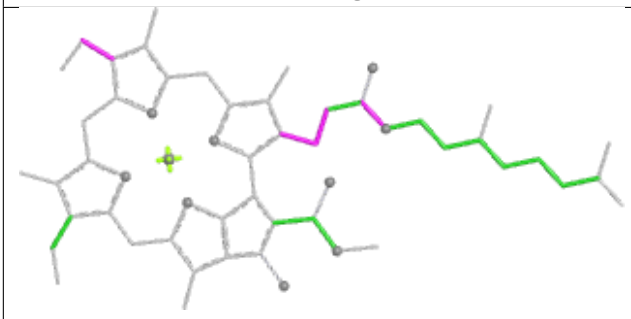


Bond angles



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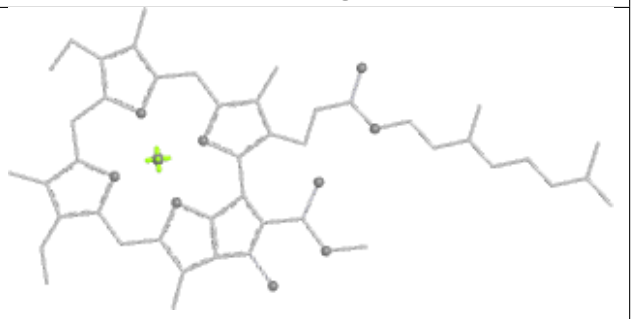
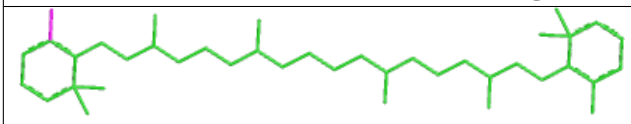


Rings

Ligand BCR r 601



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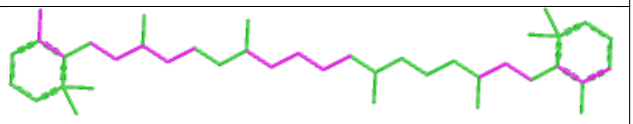
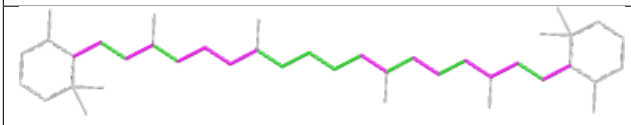


Bond angles



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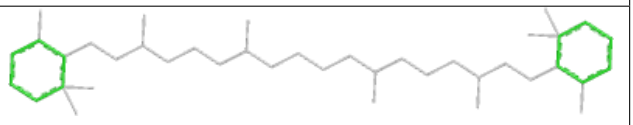
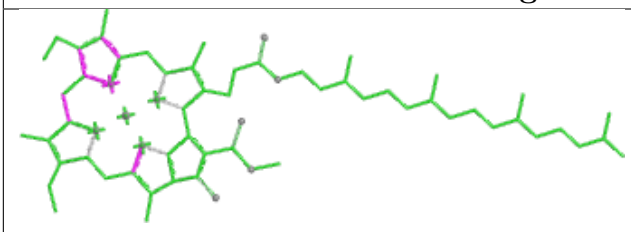


Rings

Ligand CLA a 1132



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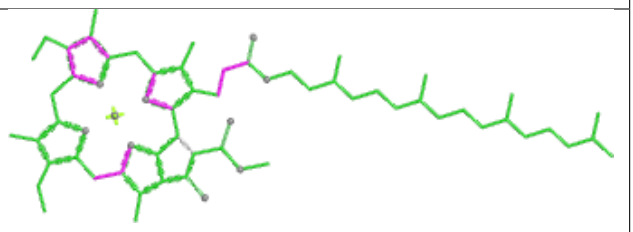
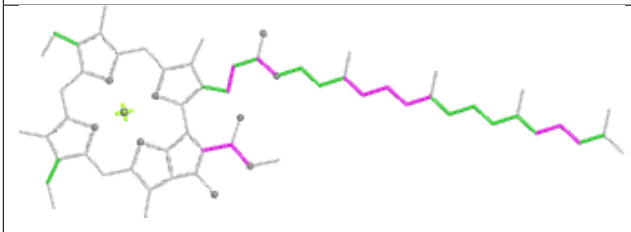
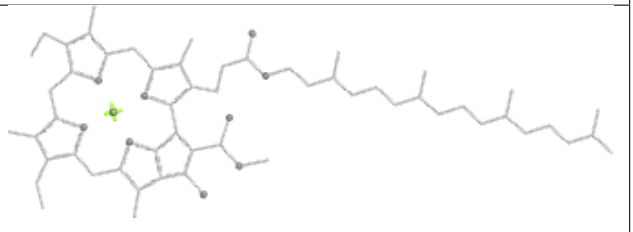


Bond angles

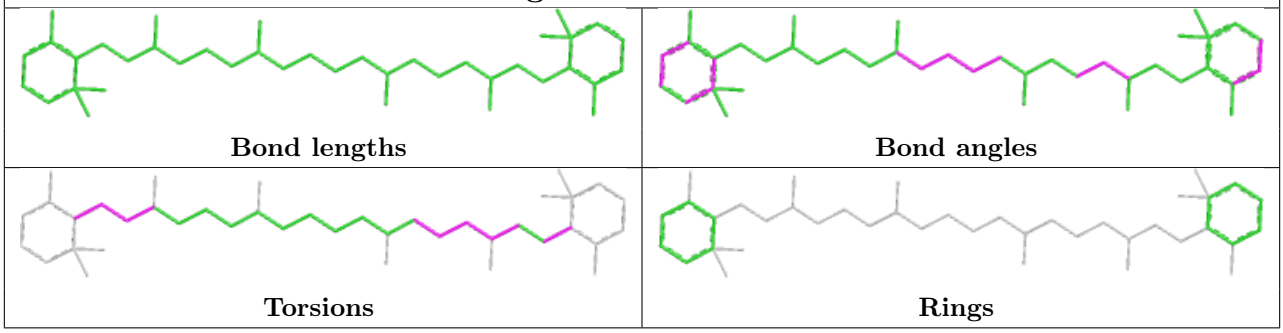


Torsions



Rings

Ligand BCR u 602



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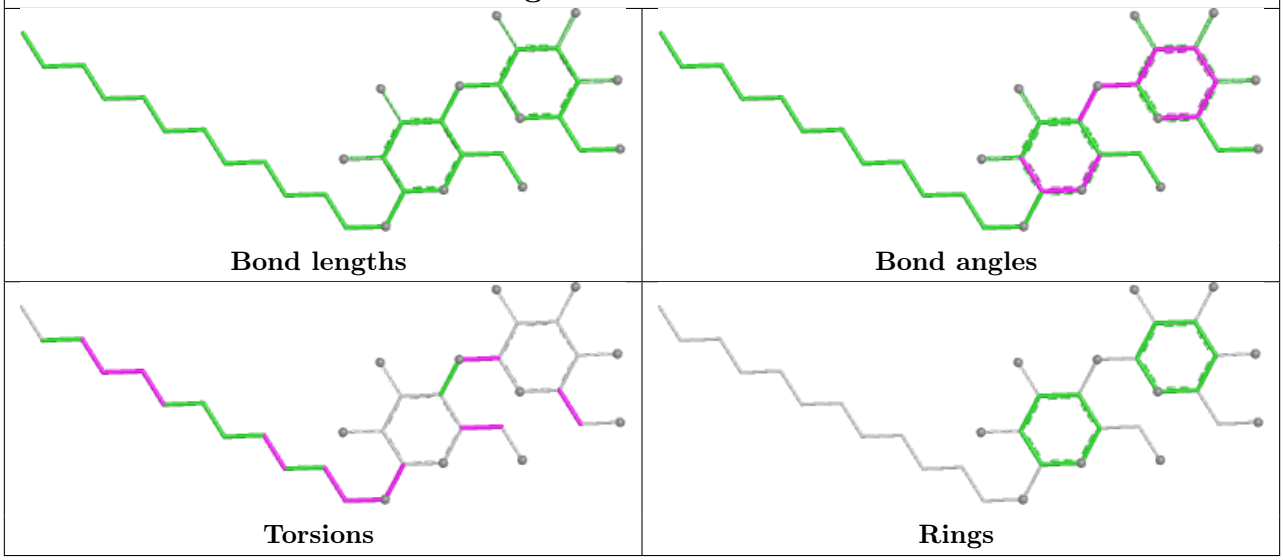
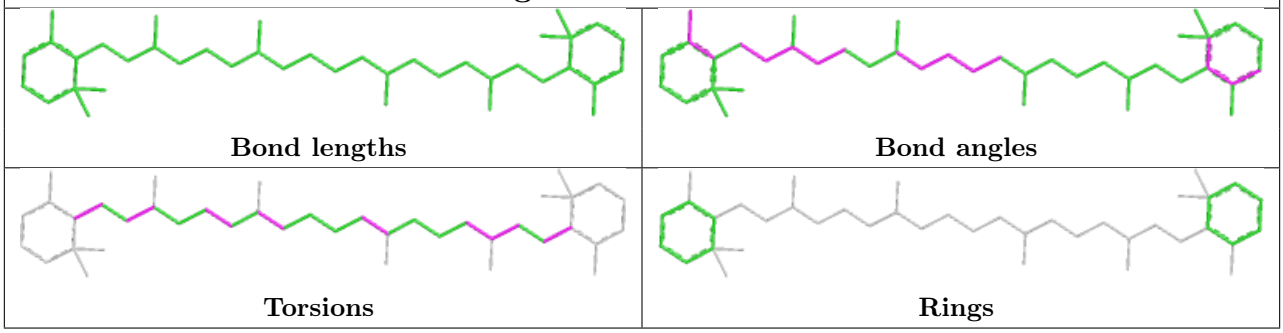


Ligand BCR R 4018



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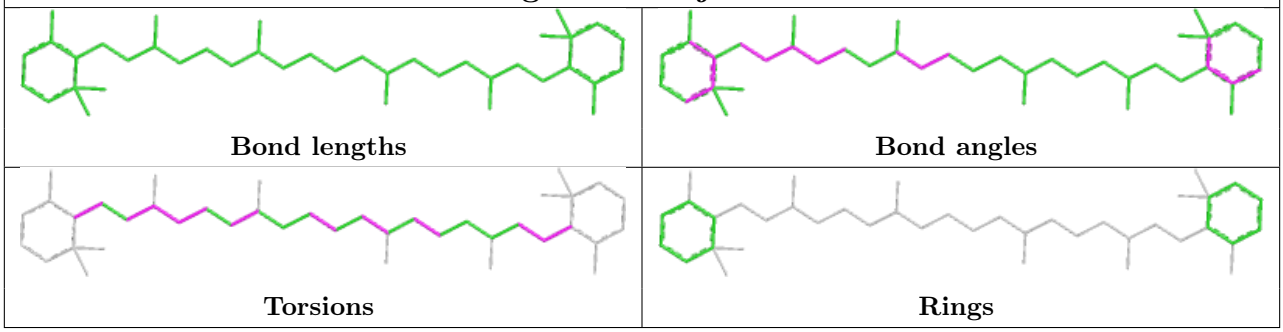

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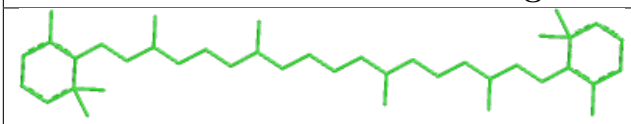
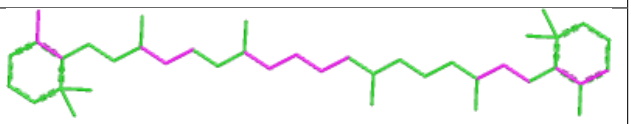
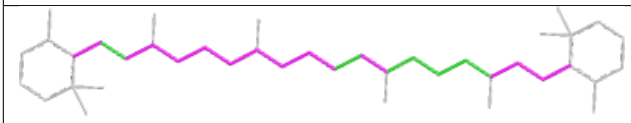


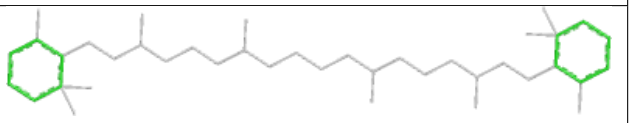
Bond lengths



Bond angles

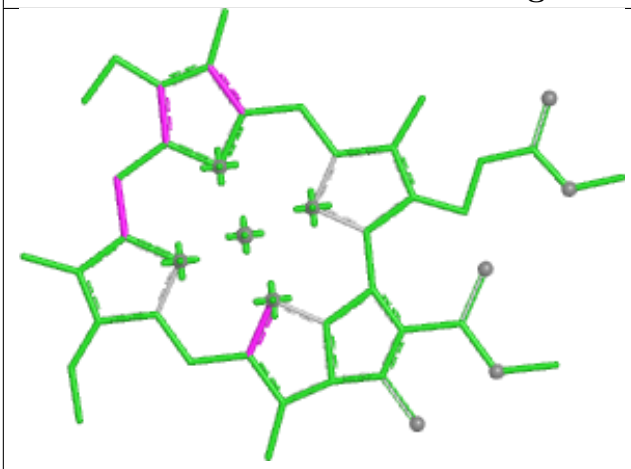


Torsions



Rings

Ligand CLA y 513



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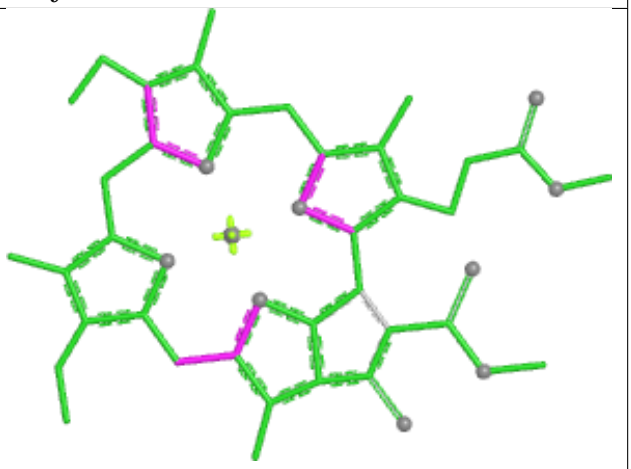
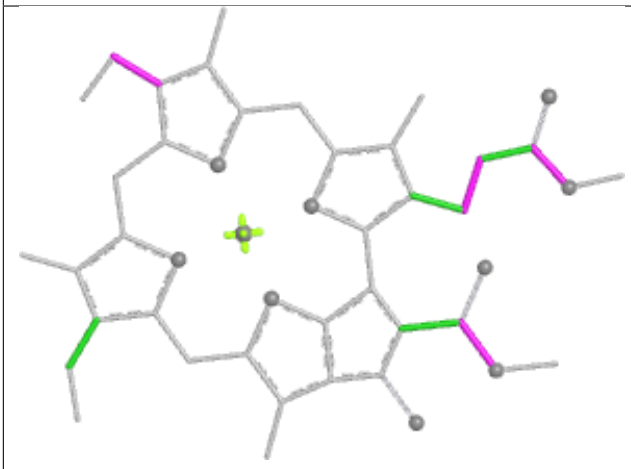


Bond angles



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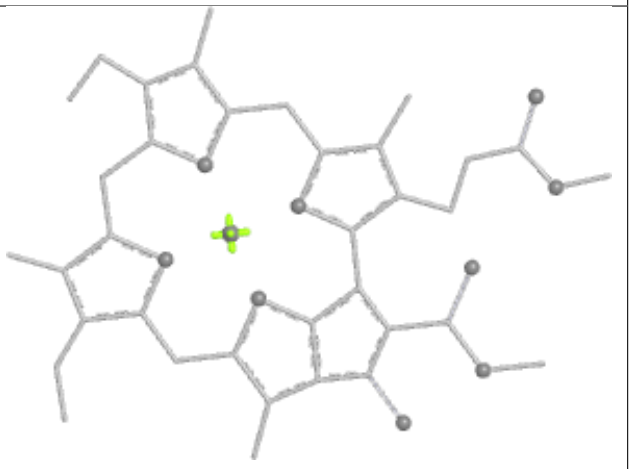
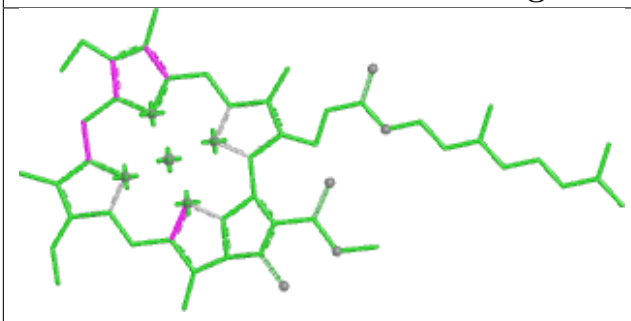


Rings

Ligand CLA q 508



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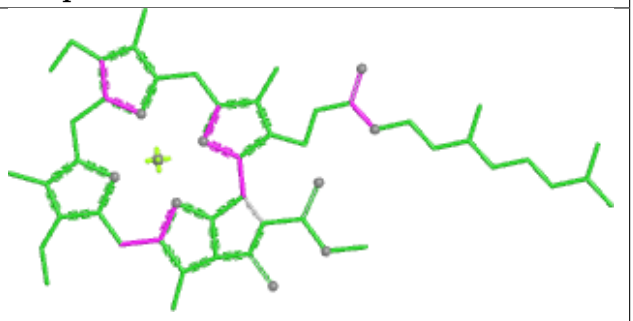

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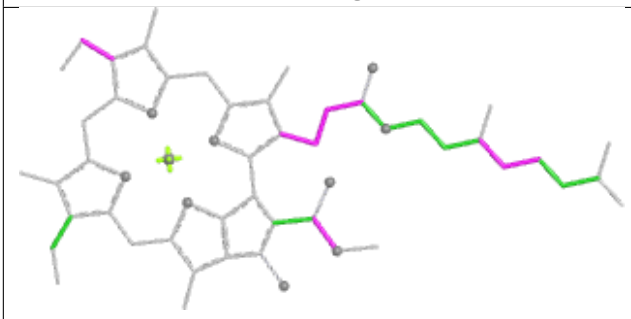

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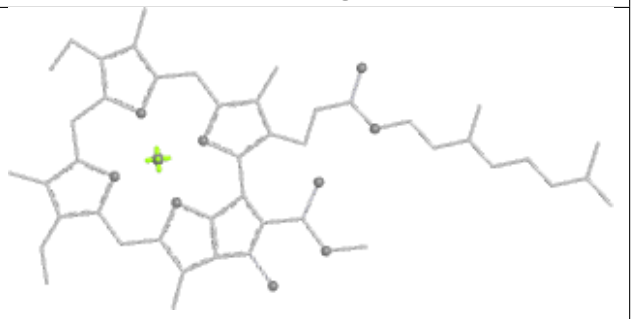
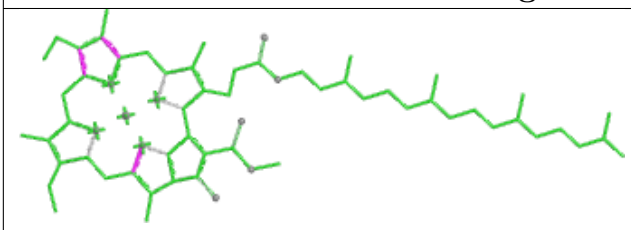


Rings

Ligand CLA W 510



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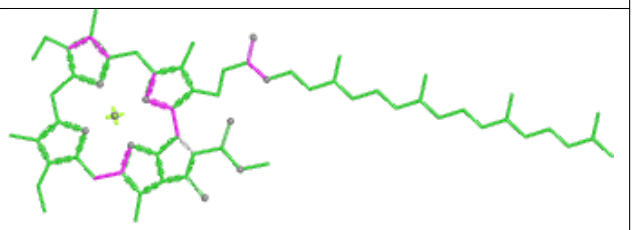

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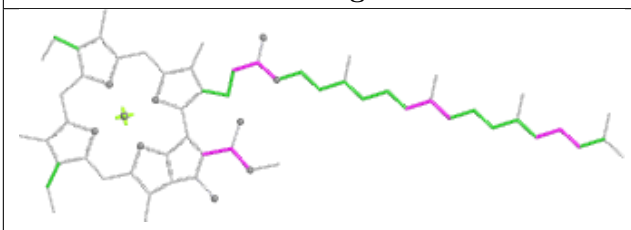

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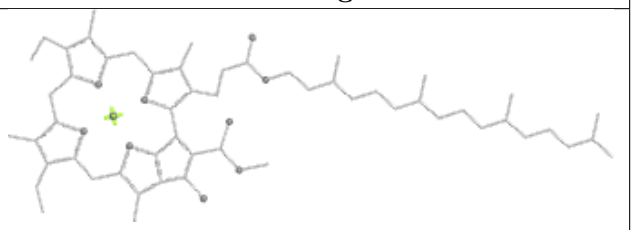
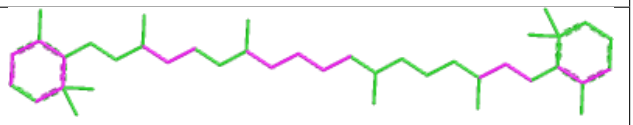


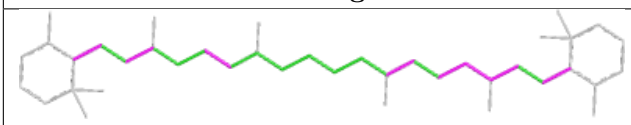
Rings

Ligand BCR Z 602

Bond lengths



Bond angles



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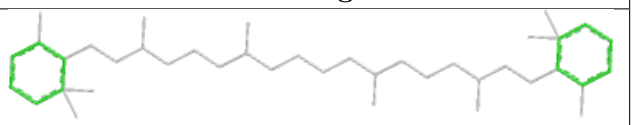
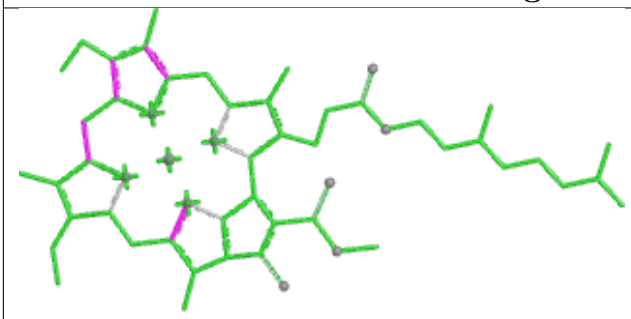


Rings

Ligand CLA X 508



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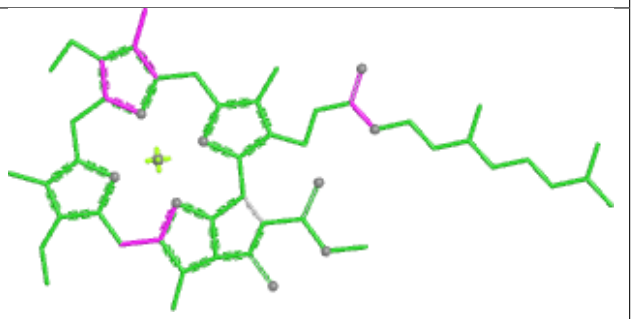

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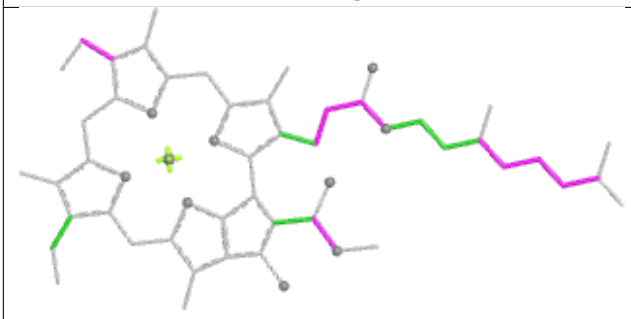

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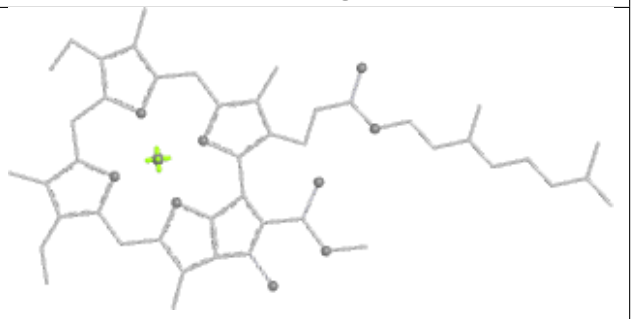
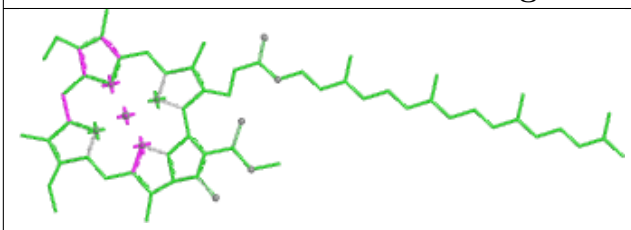


Rings

Ligand CLA a 1128



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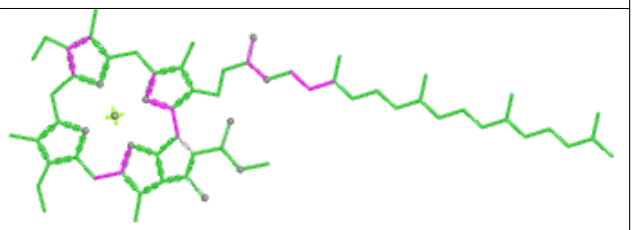
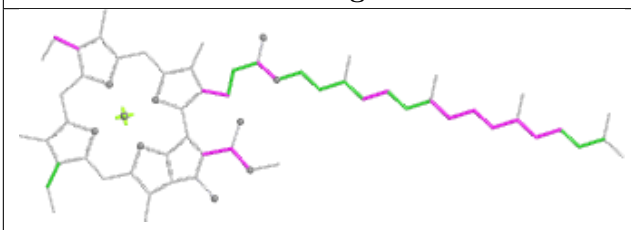


Bond angles



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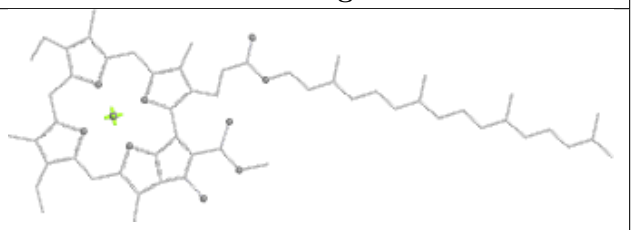
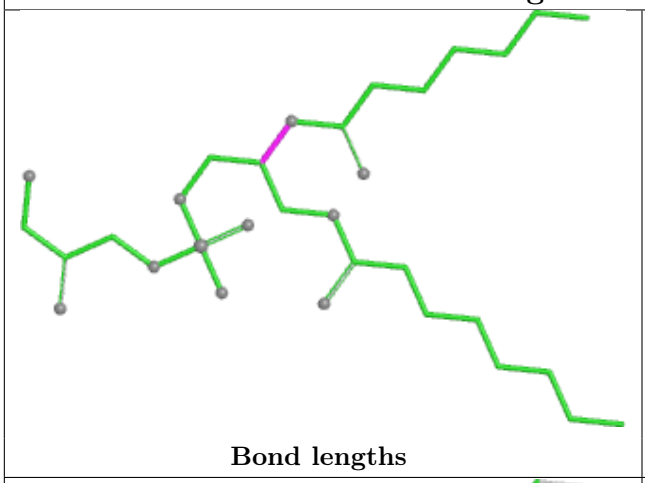


Rings

Ligand LHG p 605



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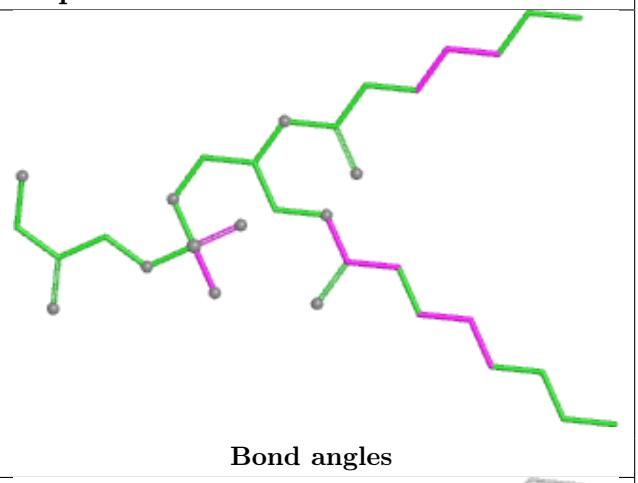
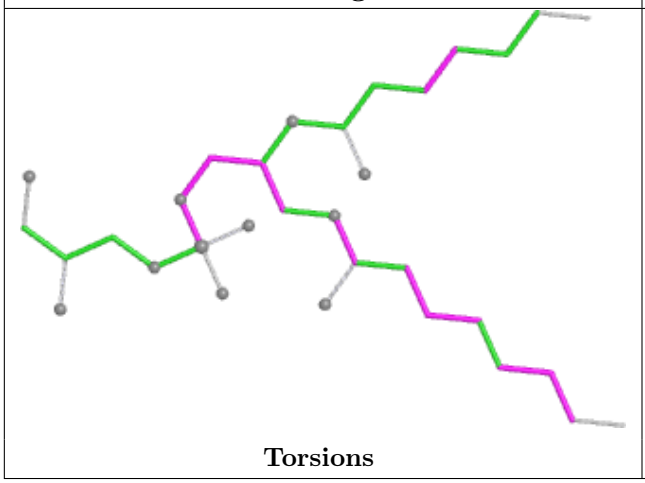


Bond angles



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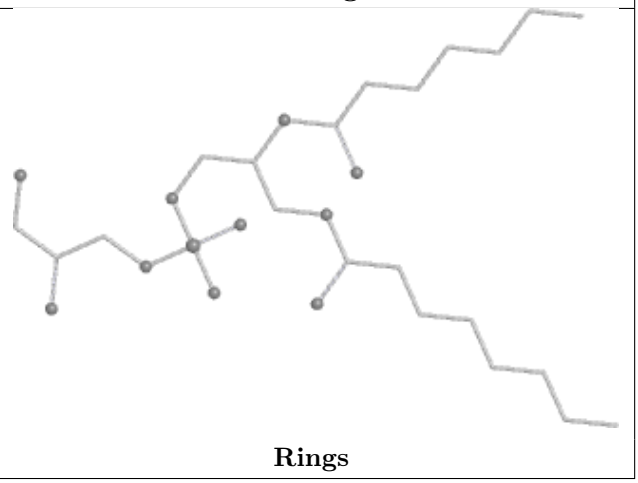
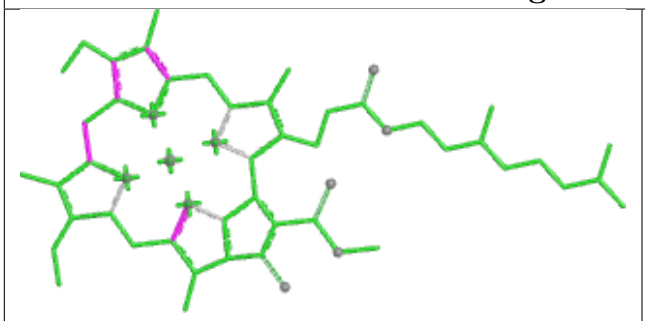


Rings

Ligand CLA x 517



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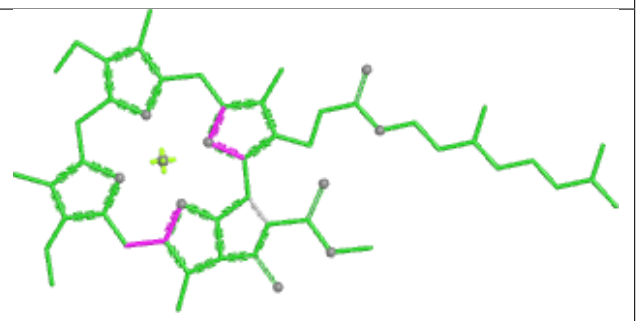
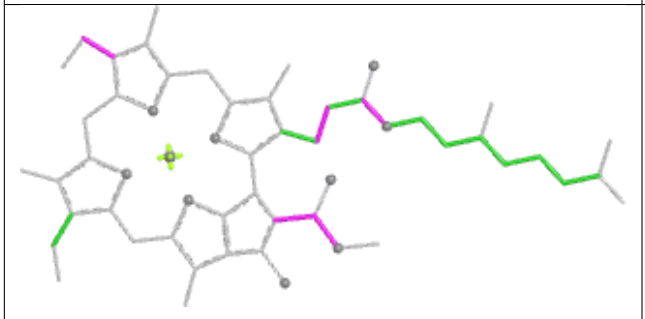


Bond angles



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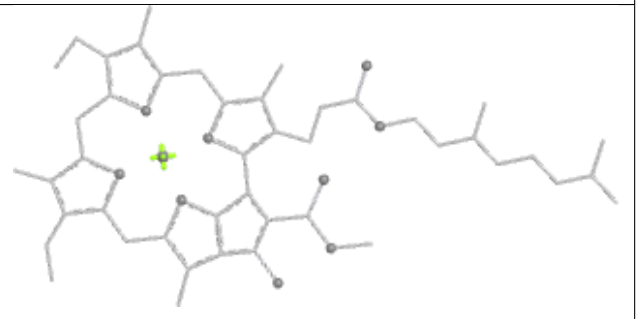
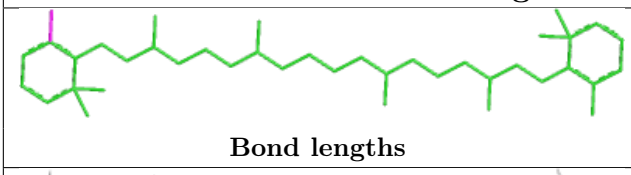


Rings

Ligand BCR H 4008



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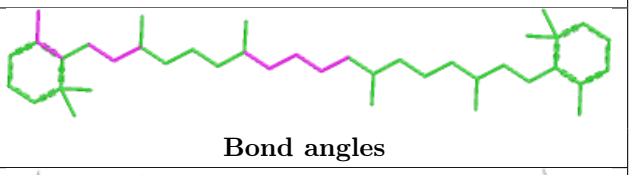
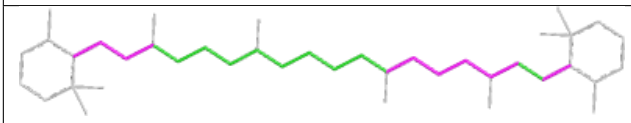


Bond angles



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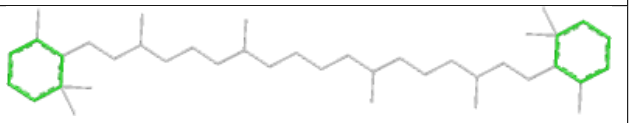
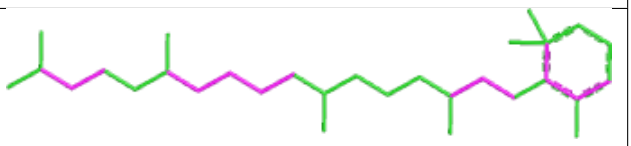


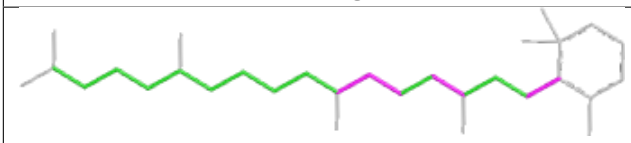
Rings

Ligand BCR b 4009

Bond lengths



Bond angles



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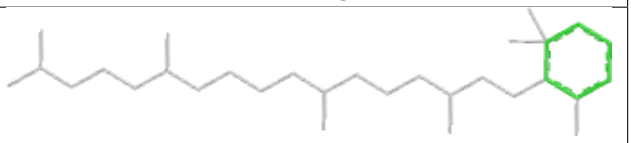
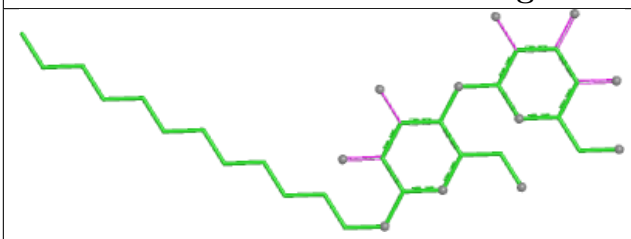


Rings

Ligand LMT a 4202



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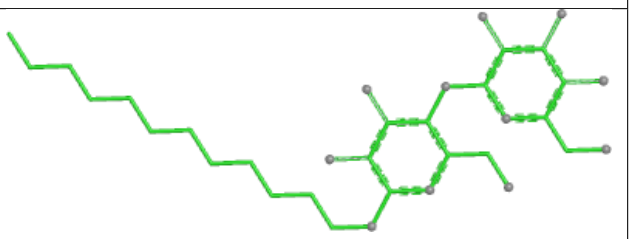
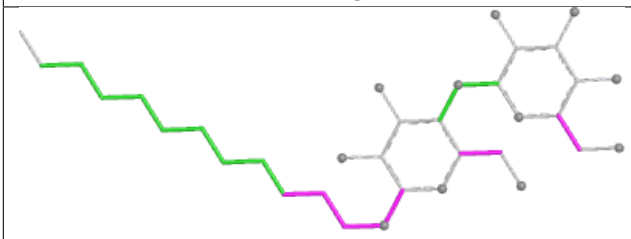


Bond angles



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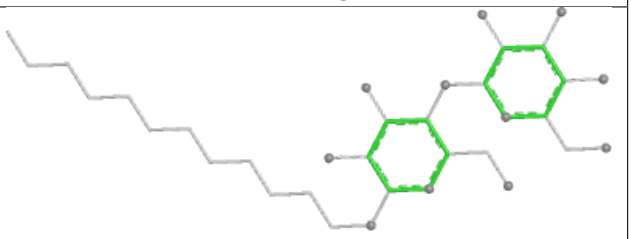
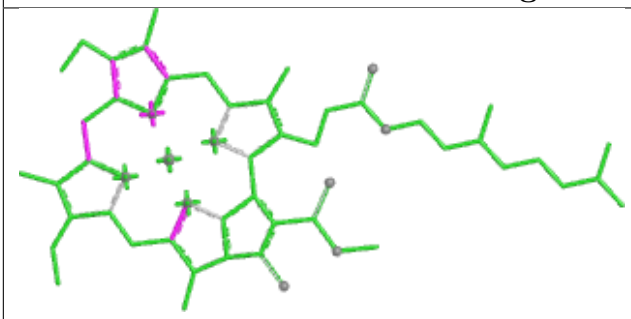
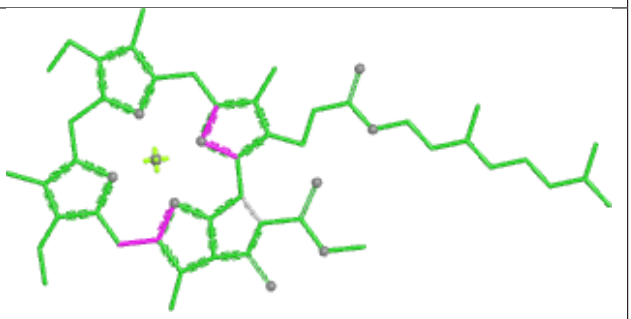
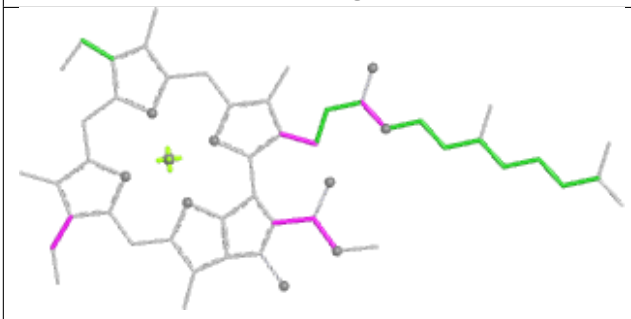
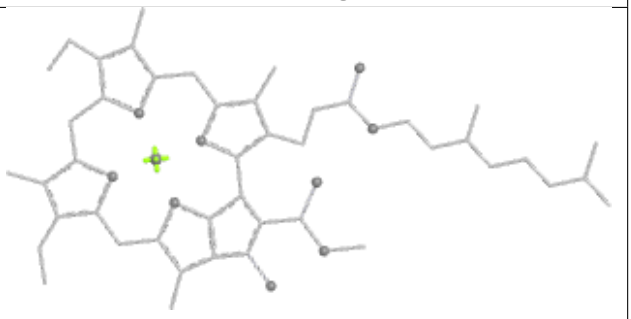
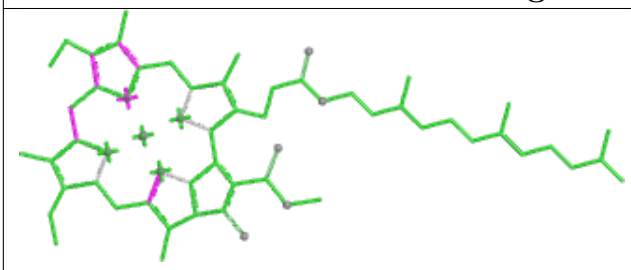
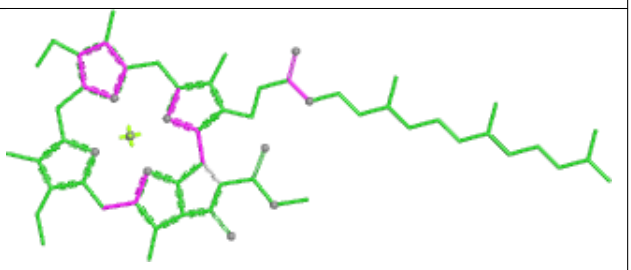
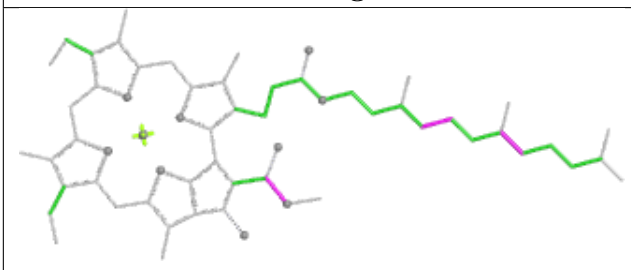
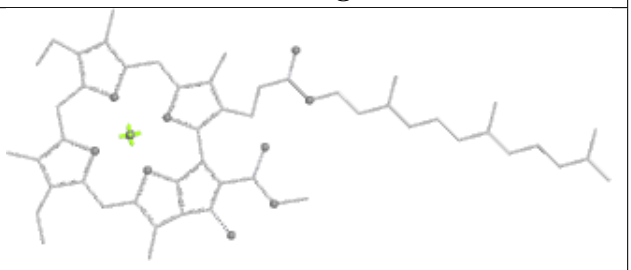
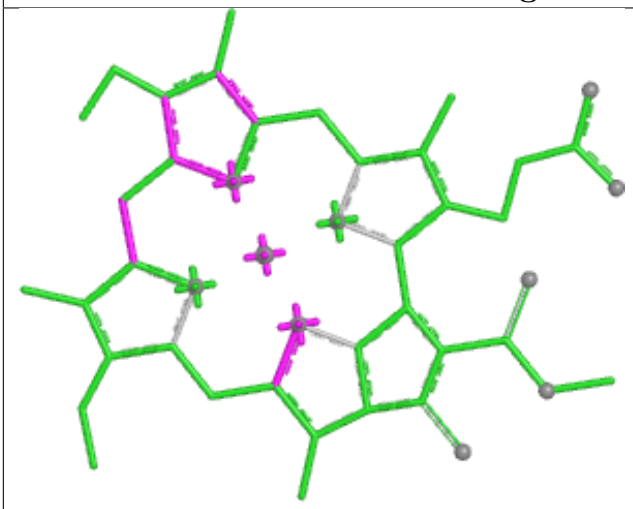


Rings

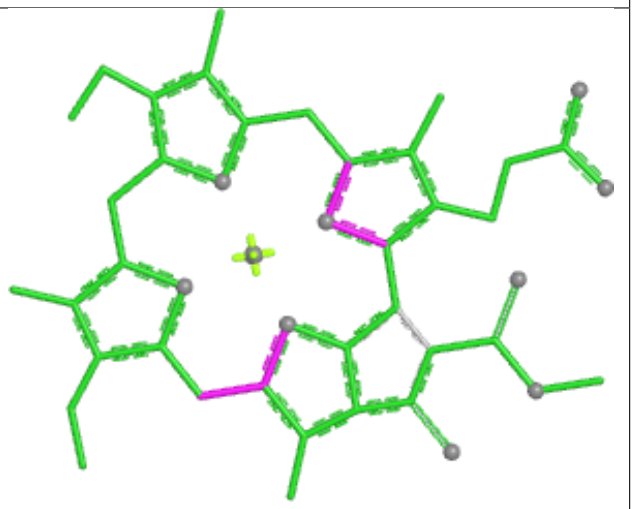
Ligand CLA a 1111	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA v 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

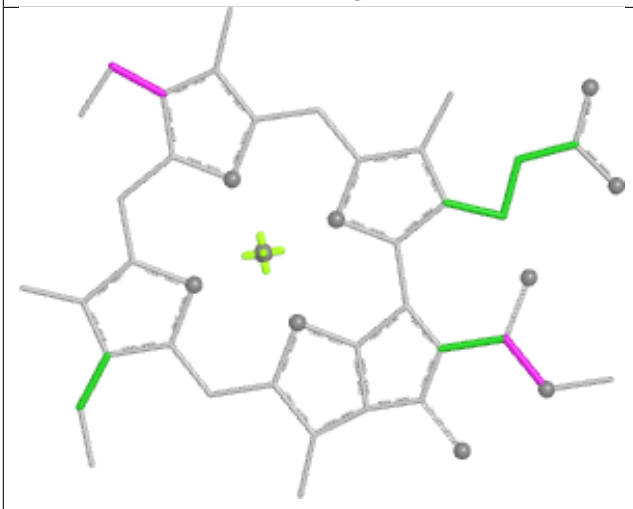
Ligand CLA a 1113



Bond lengths



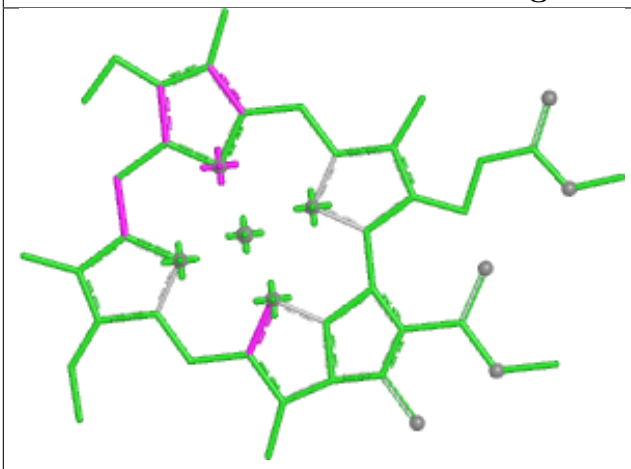
Bond angles



Torsions

Rings

Ligand CLA r 503



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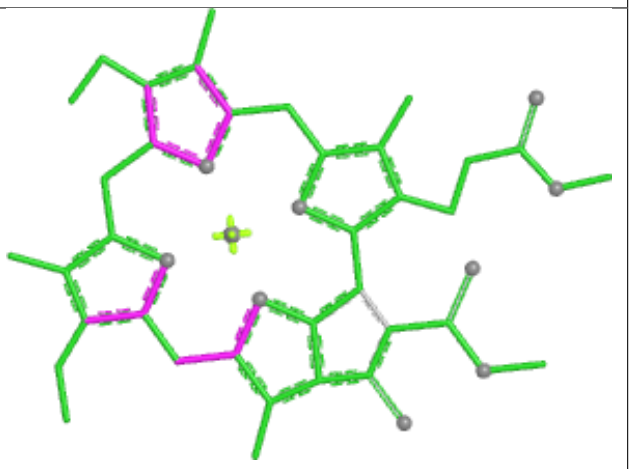

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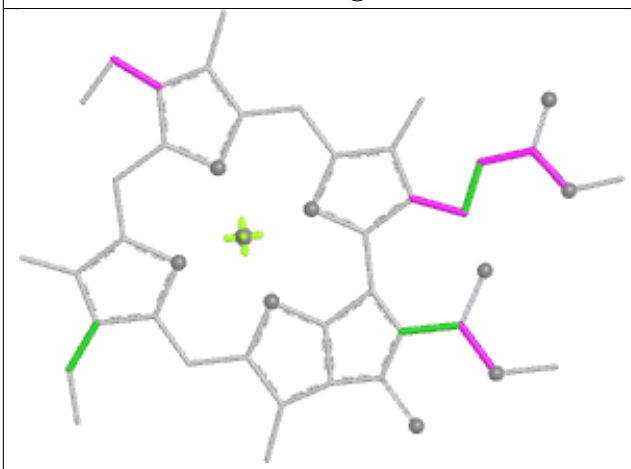

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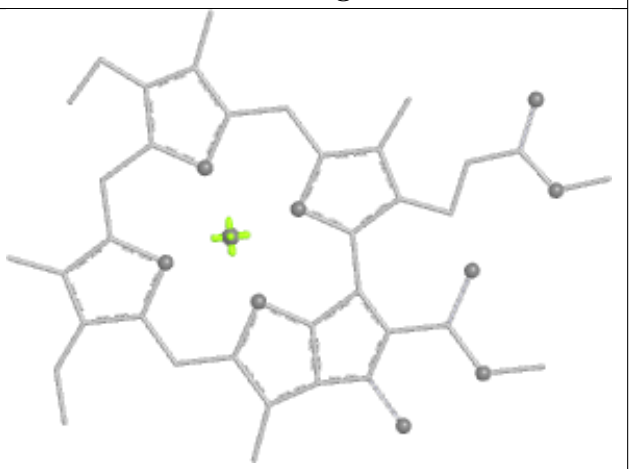
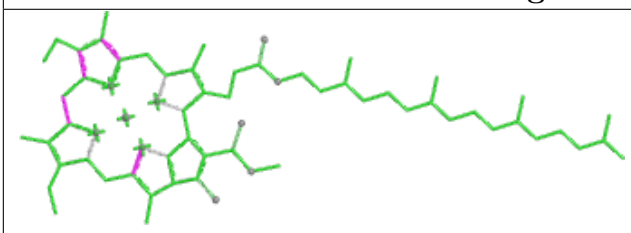


Rings

Ligand CLA u 507



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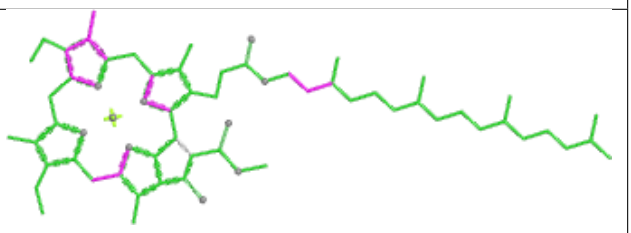
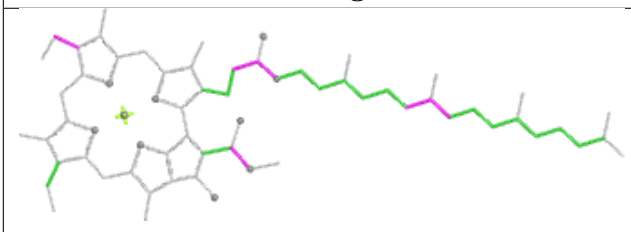
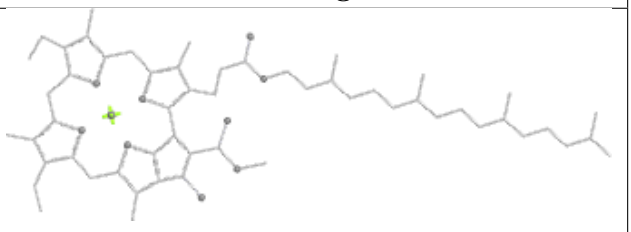


Bond angles

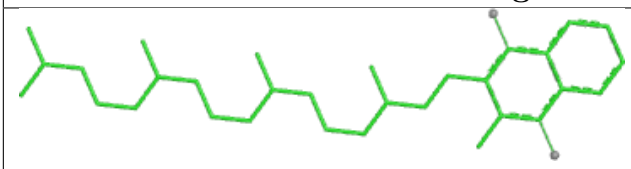


Torsions



Rings

Ligand PQN A 2001



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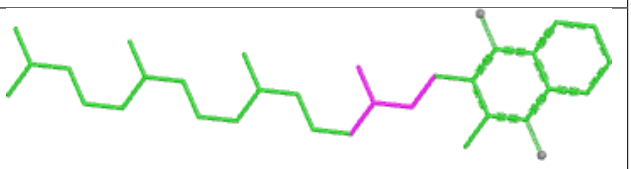

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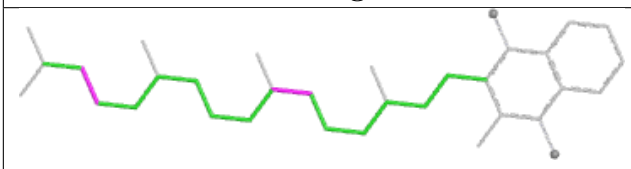
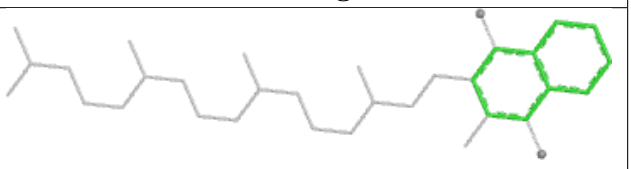
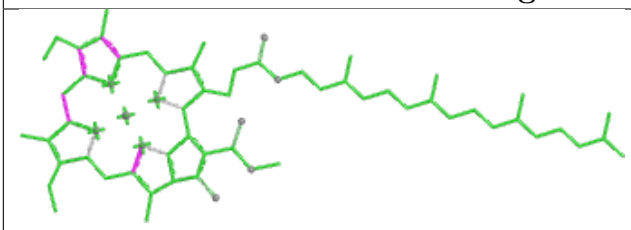


Torsions



Rings

Ligand CLA b 1223



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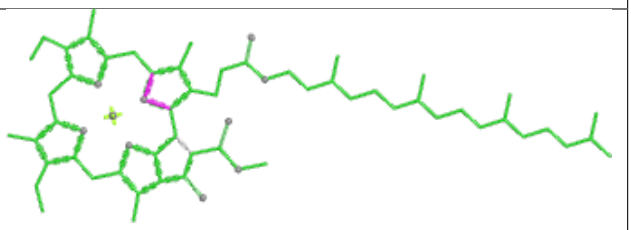
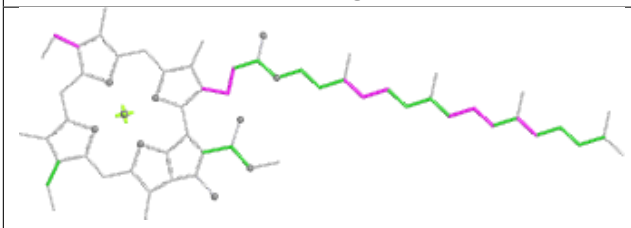


Bond angles



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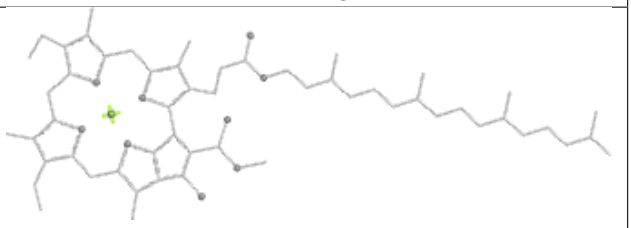
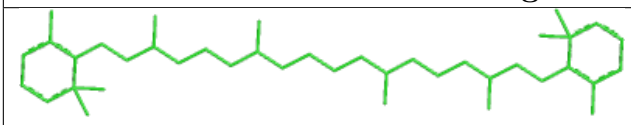


Rings

Ligand BCR l 4019



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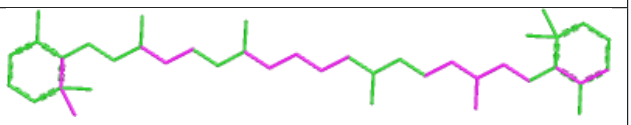
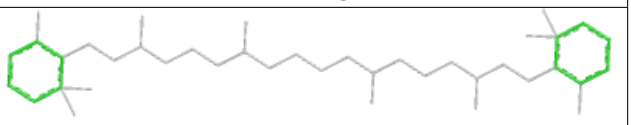


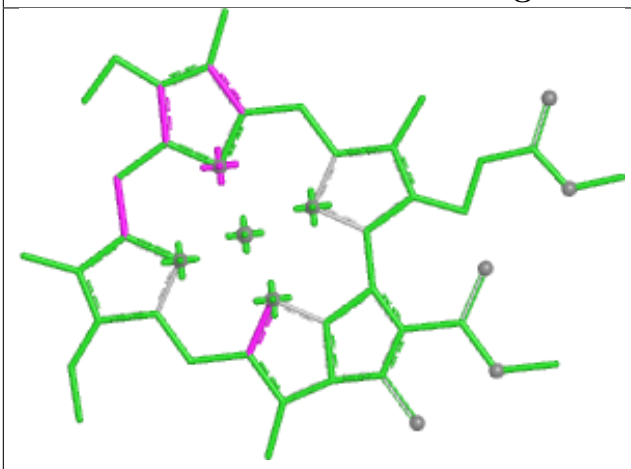
Bond angles

Torsions



Rings

Ligand CLA G 1240



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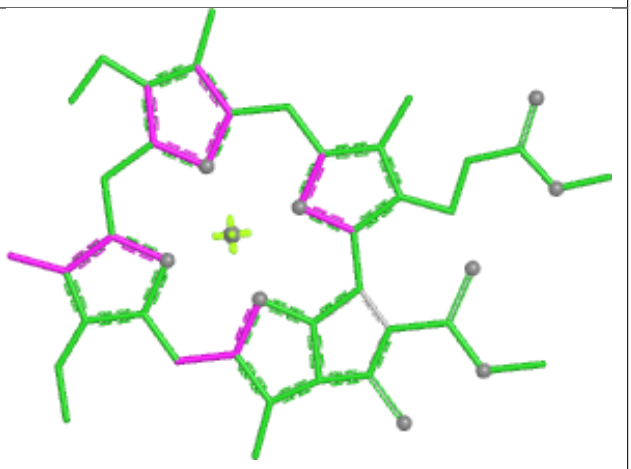
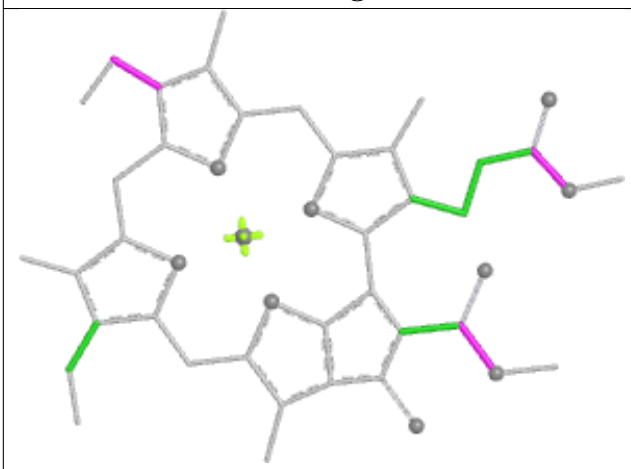


Bond angles



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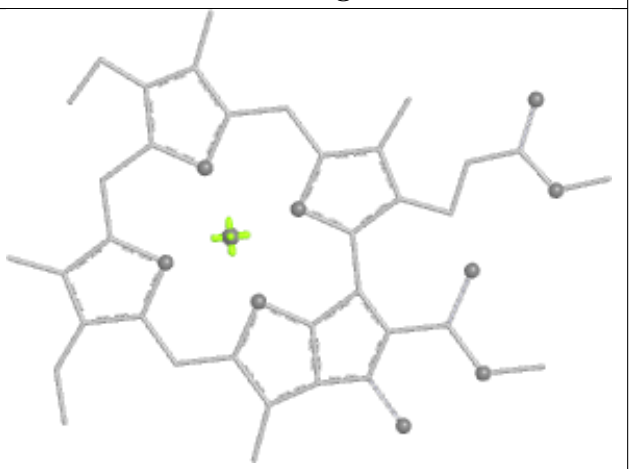
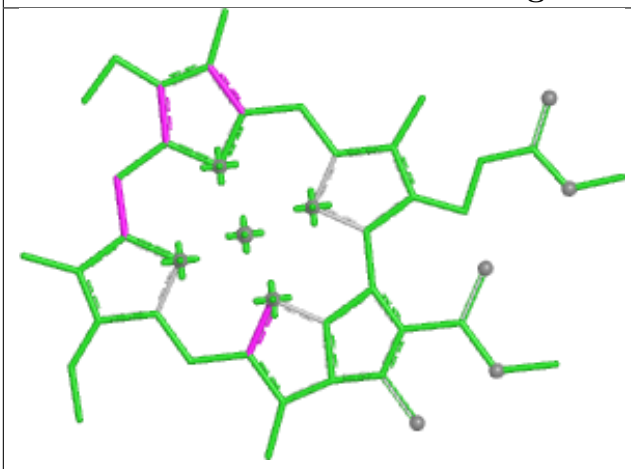


Rings

Ligand CLA h 513



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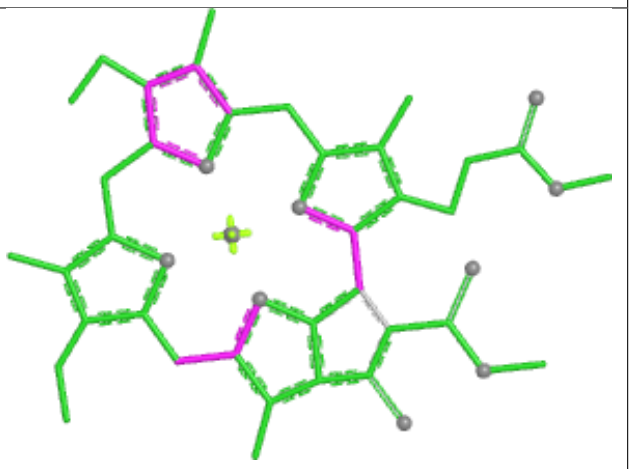

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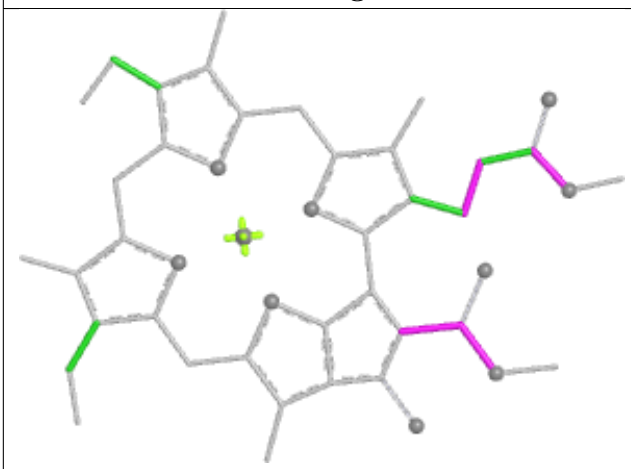

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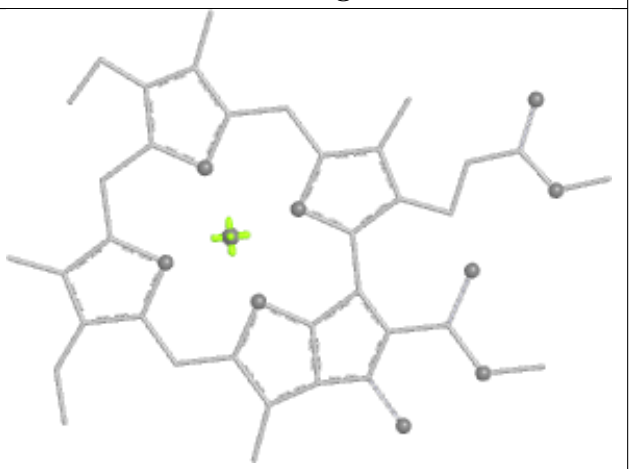
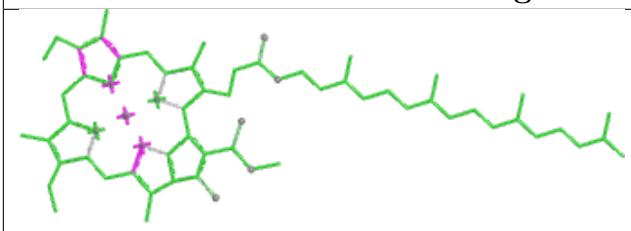


Rings

Ligand CLA G 1205



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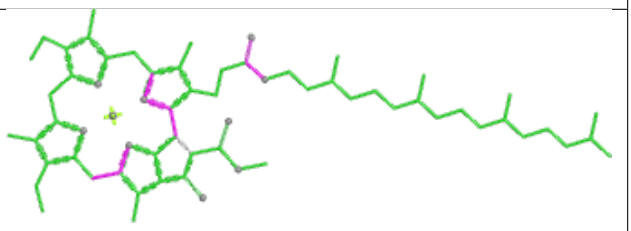
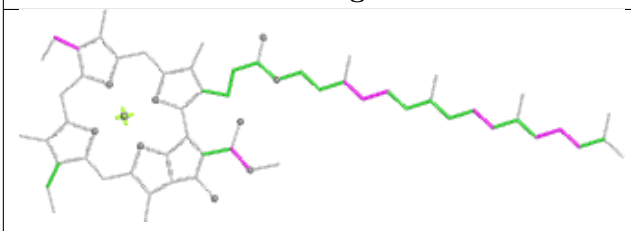


Bond angles



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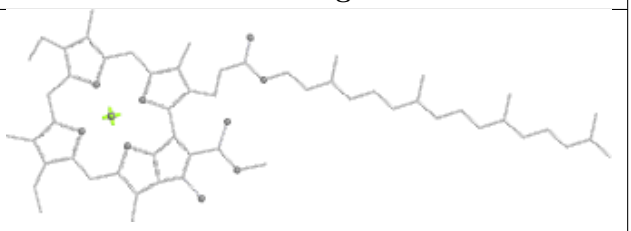
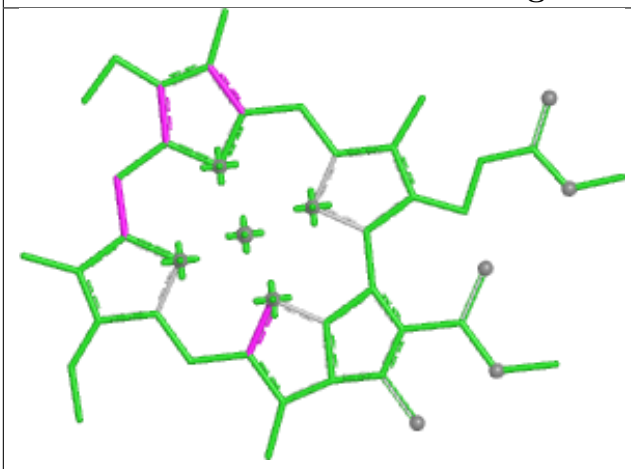


Rings

Ligand CLA v 513



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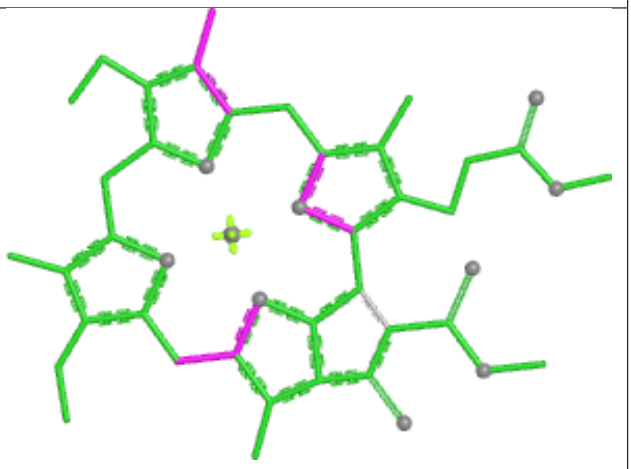

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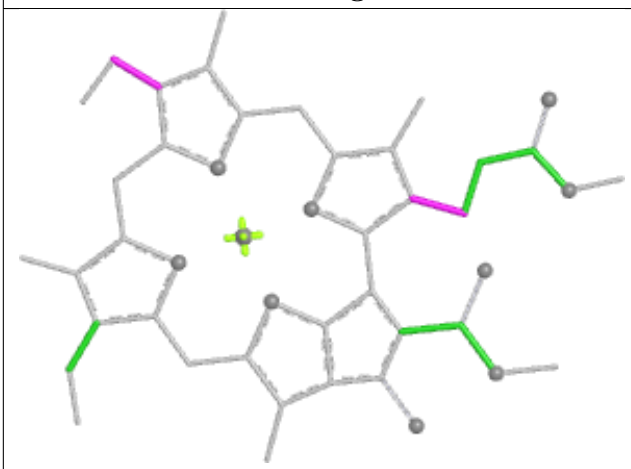

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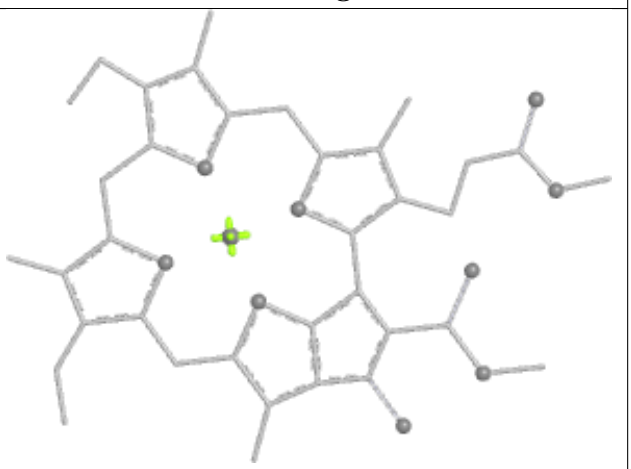
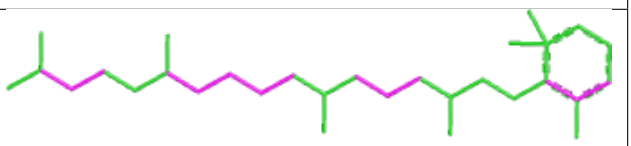


Rings

Ligand BCR G 4009

Bond lengths



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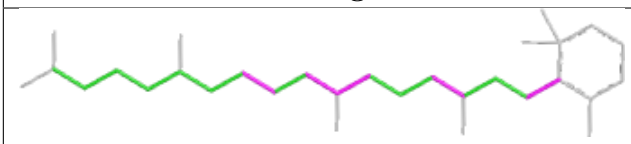

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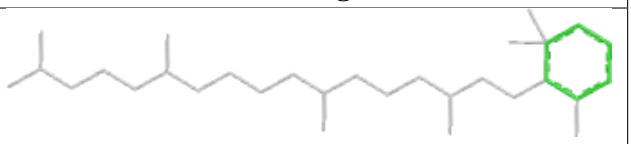
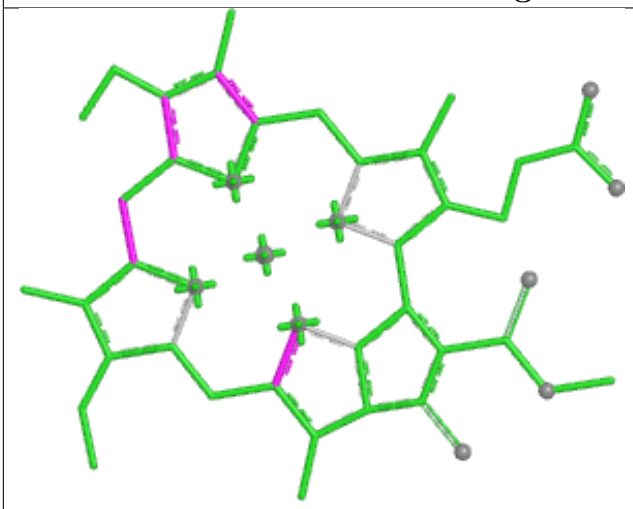


Rings

Ligand CLA H 1112



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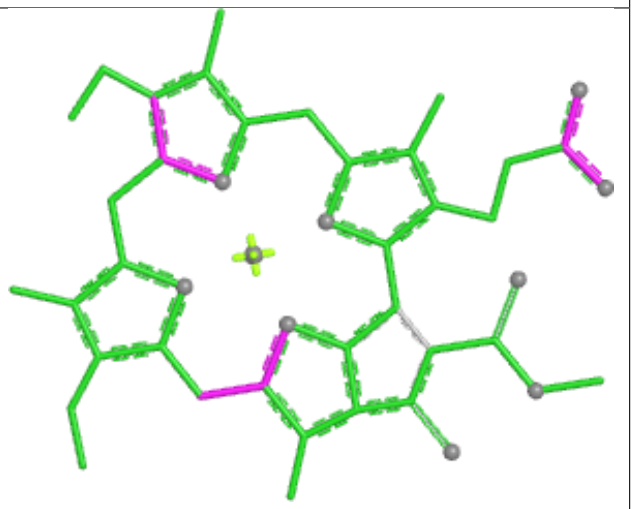
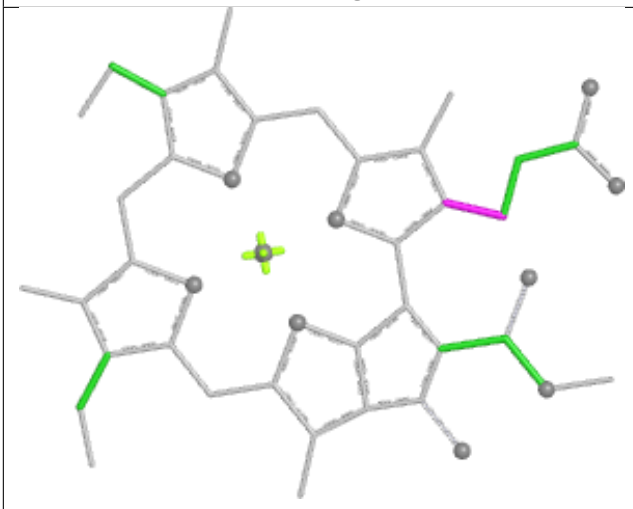


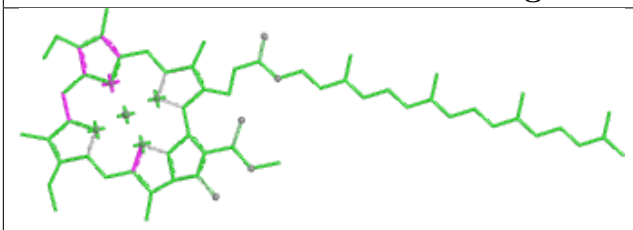
Bond angles



Torsions

Rings

Ligand CLA w 515



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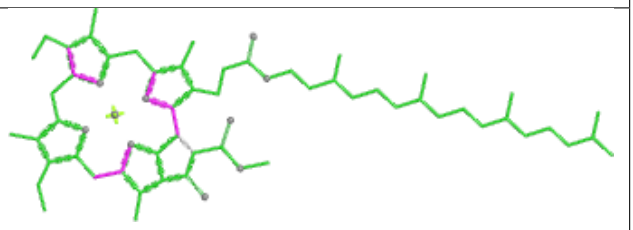

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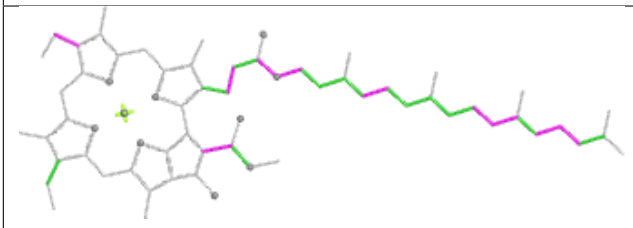

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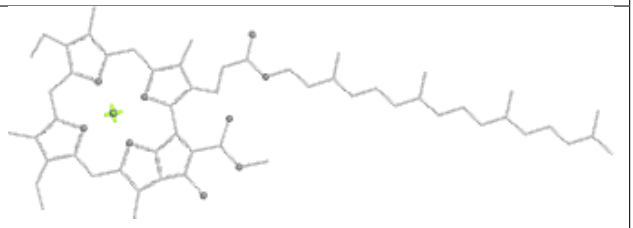
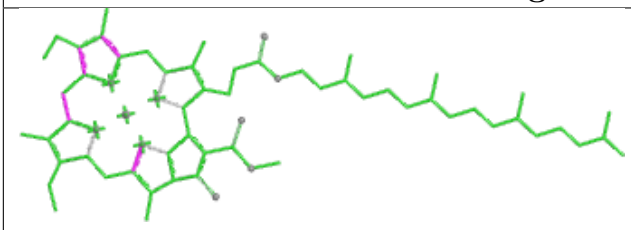
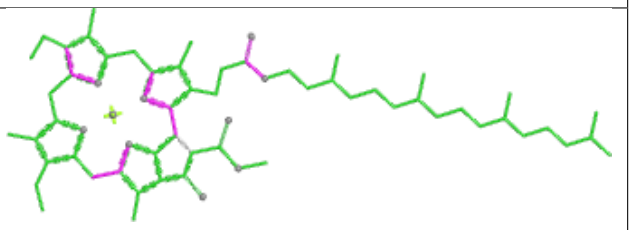
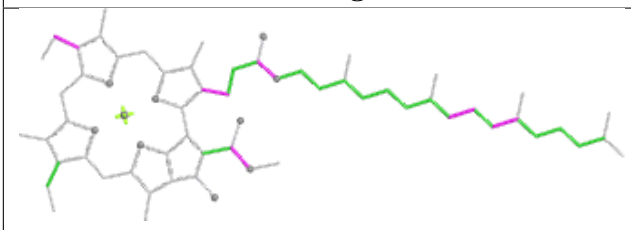
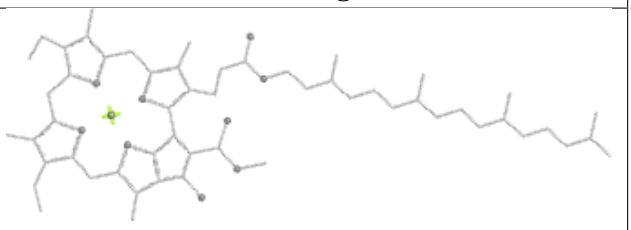
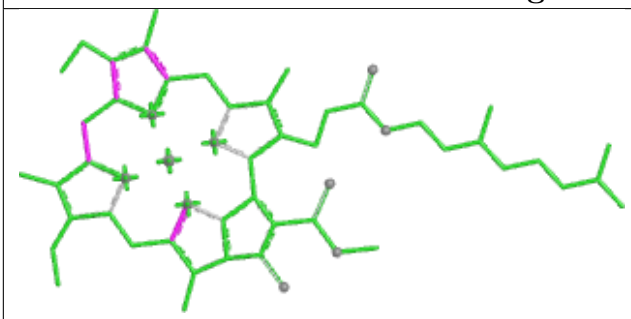
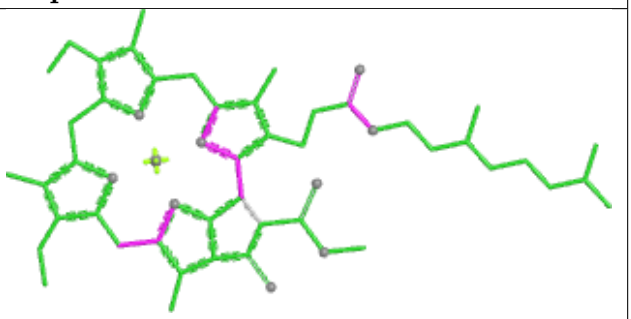
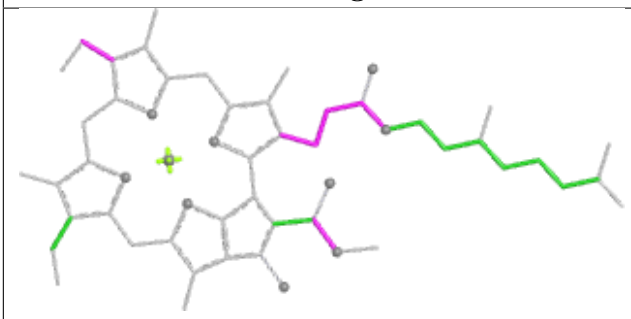
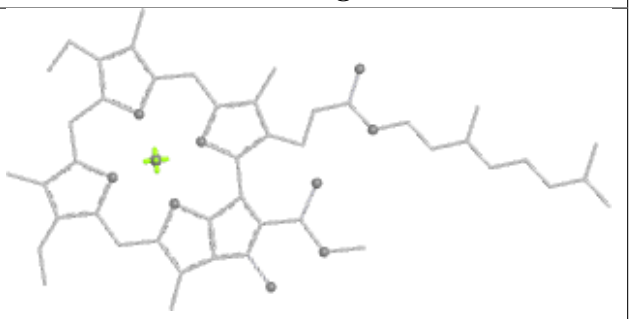
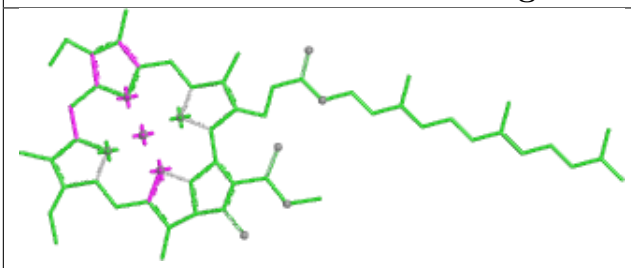
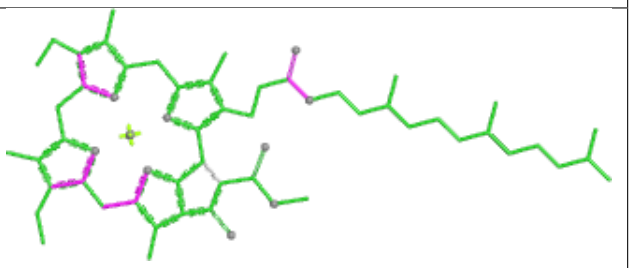
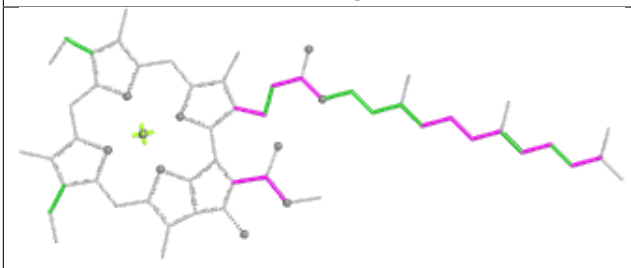
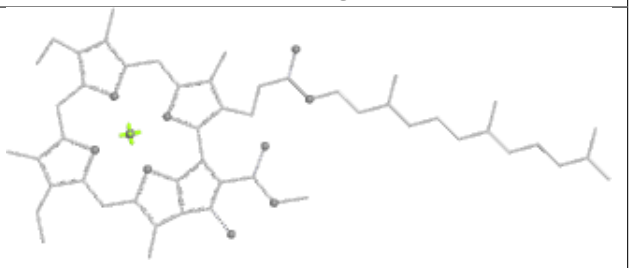


Rings

Ligand CLA o 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1226	
	
Bond lengths	Bond angles
	
Torsions	Rings

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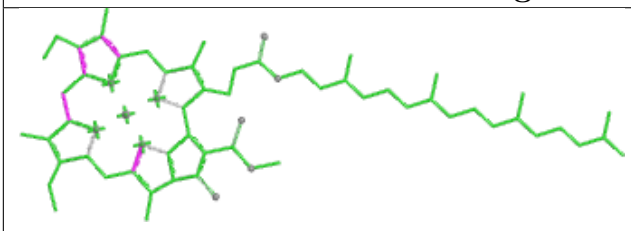
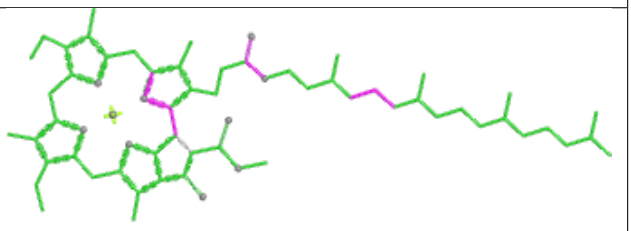
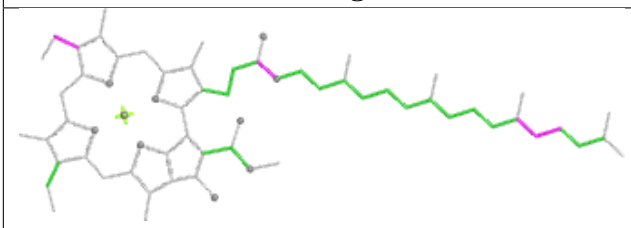
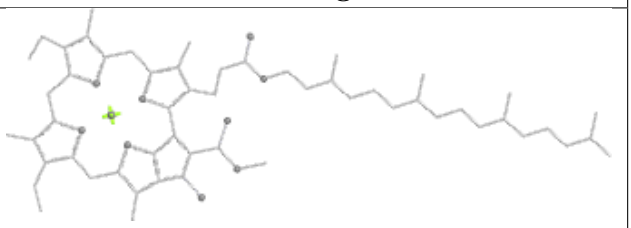
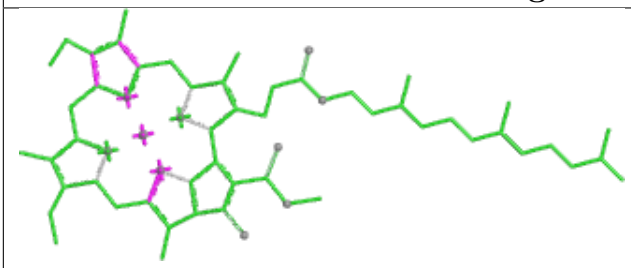
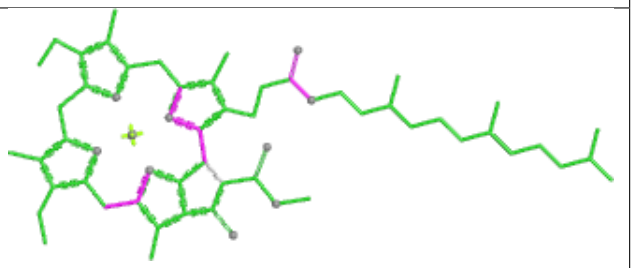
	
Bond lengths	Bond angles
	
Torsions	Rings

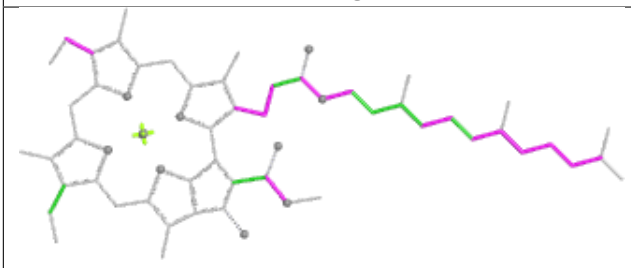
Ligand CLA o 506



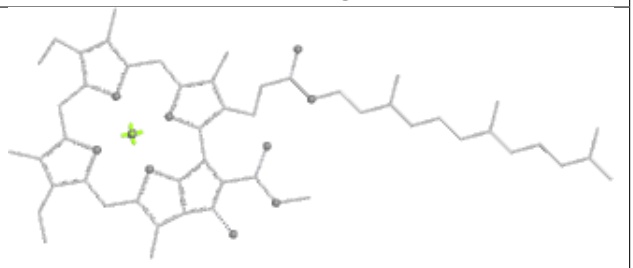
Bond lengths



Bond angles

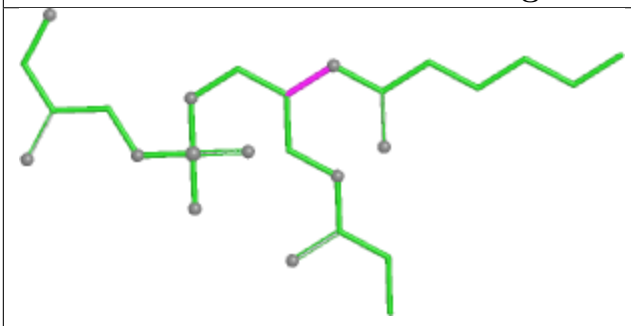


Torsions

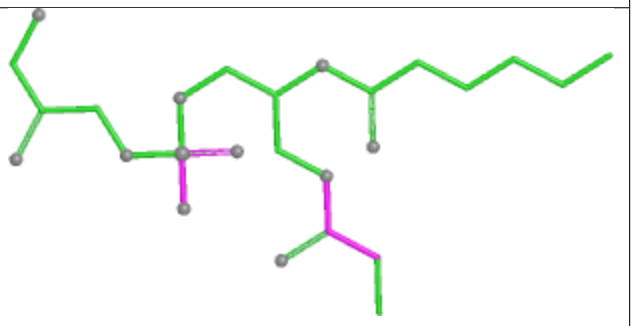


Rings

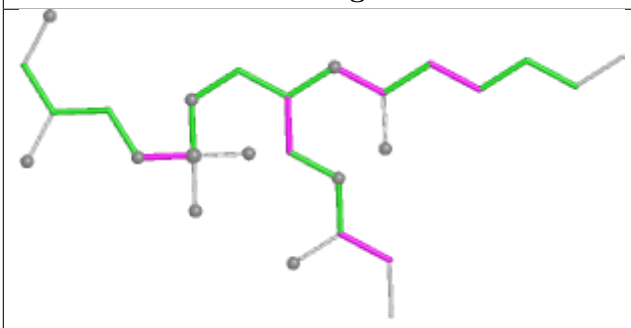
Ligand LHG H 851



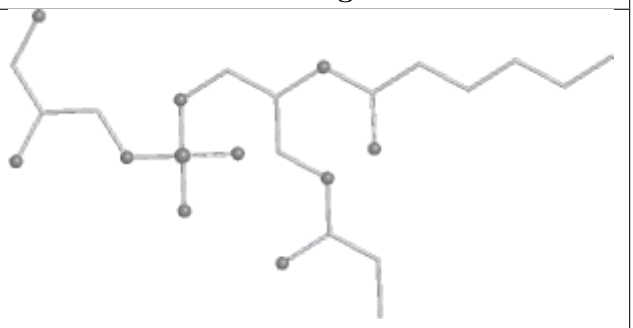
Bond lengths



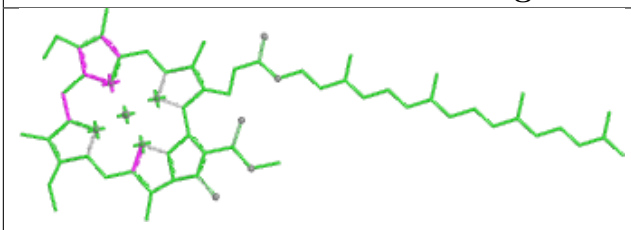
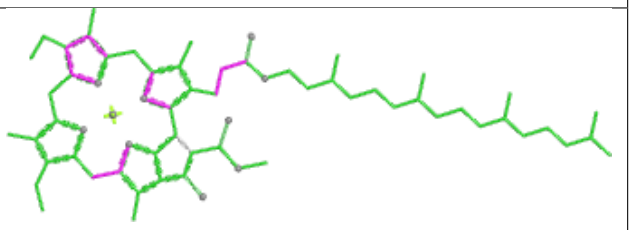
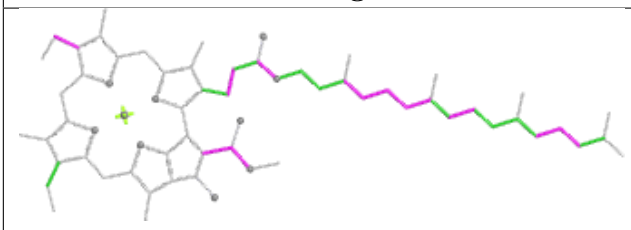
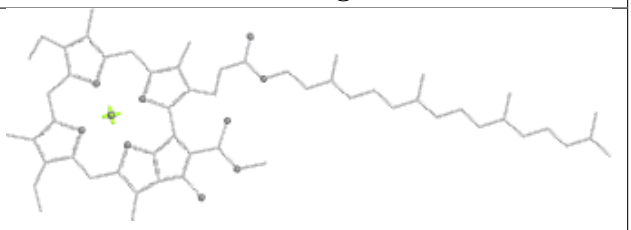
Bond angles

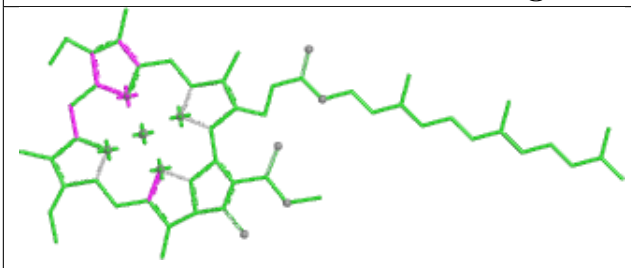
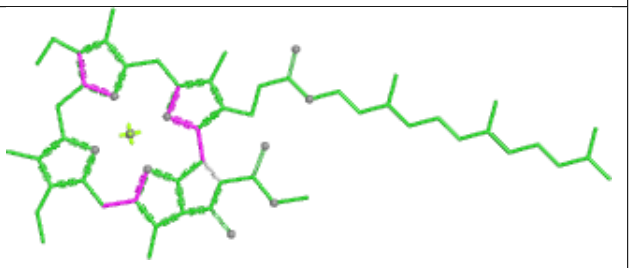
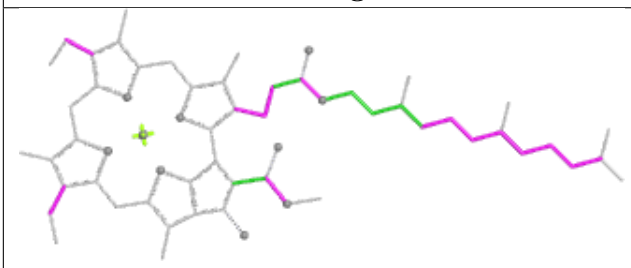
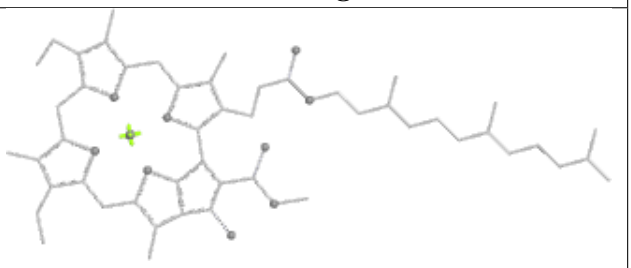


Torsions



Rings

Ligand CLA H 1132	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

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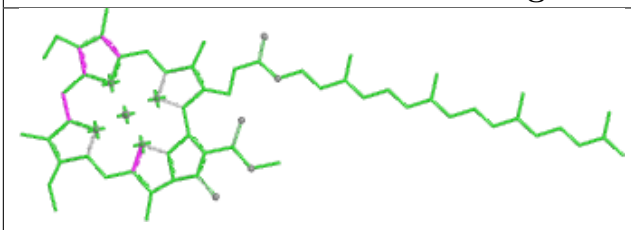	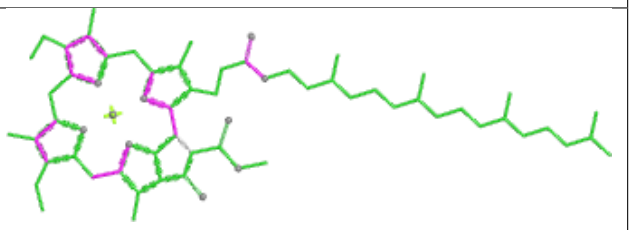
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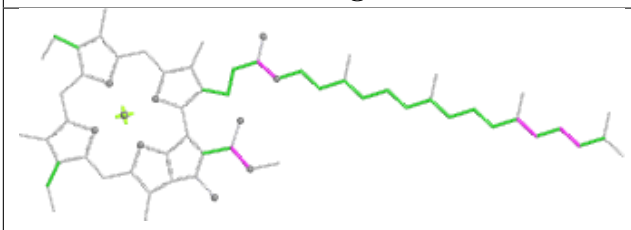	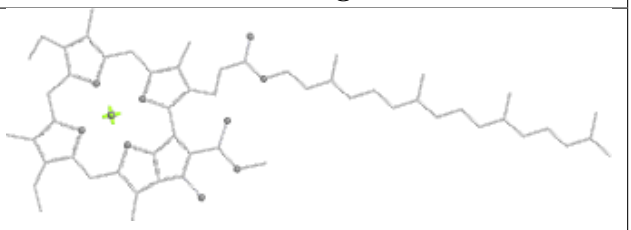
Torsions	Rings

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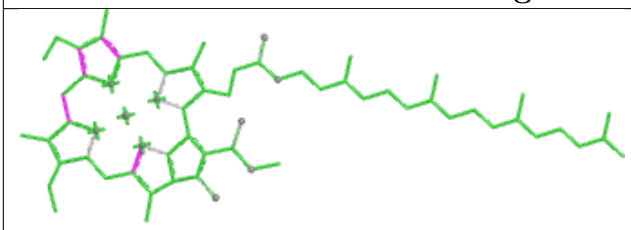
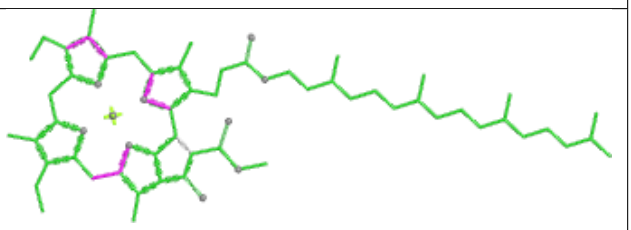
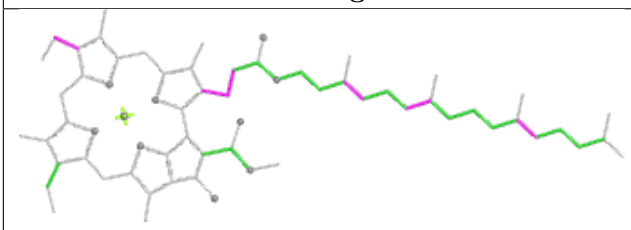
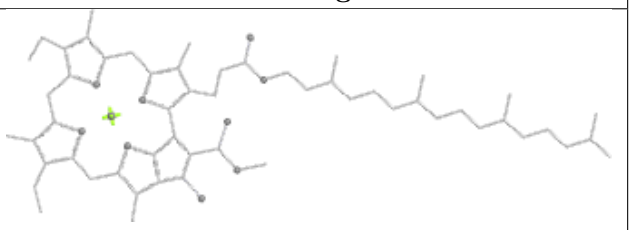
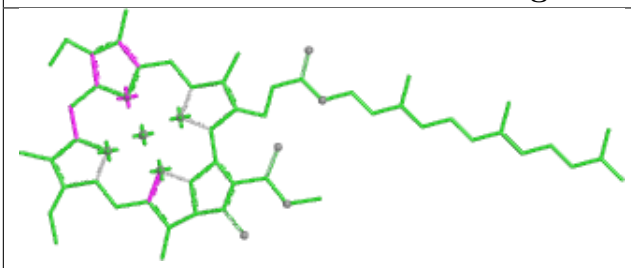
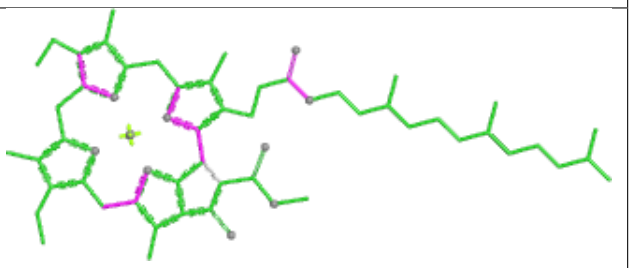
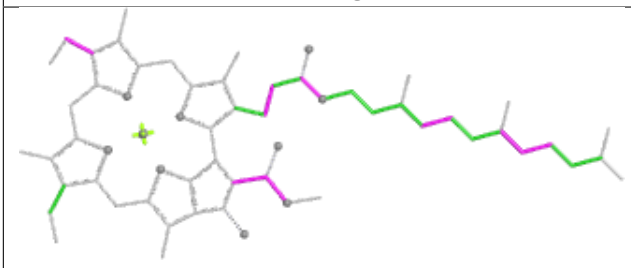
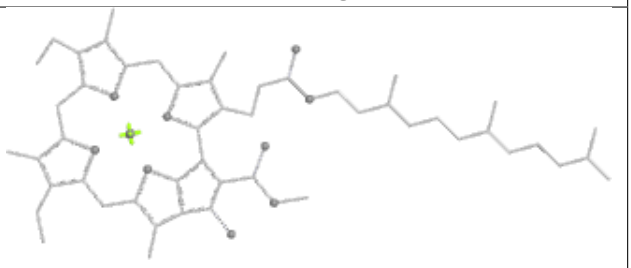
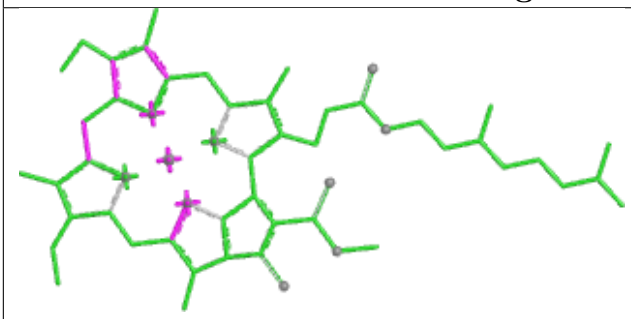
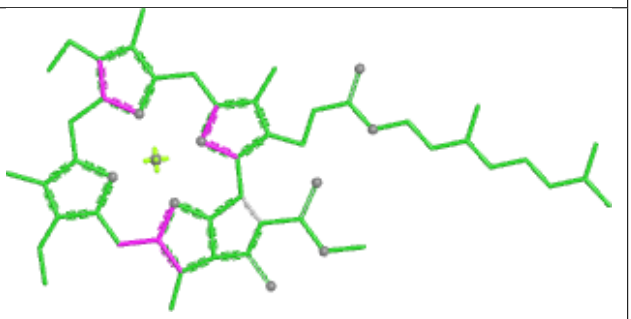
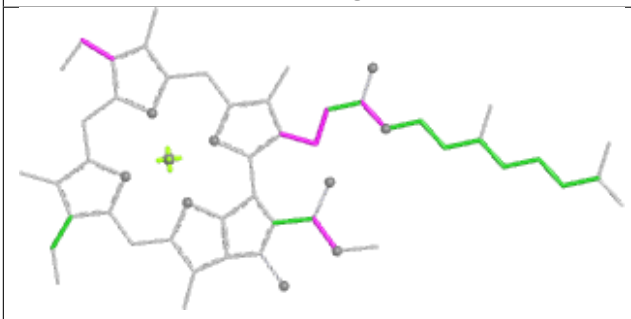
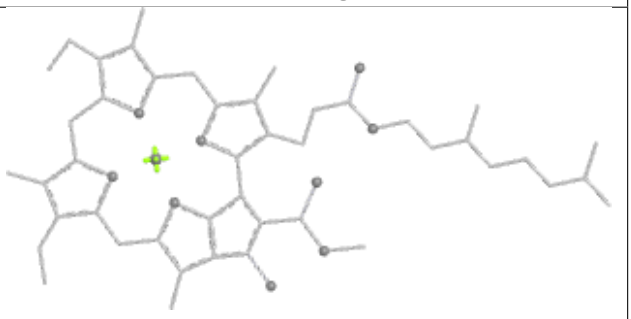
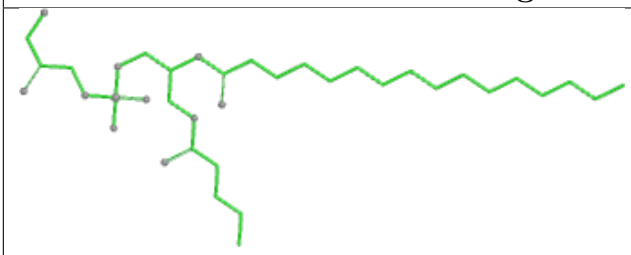
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA t 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1213	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG b 4018



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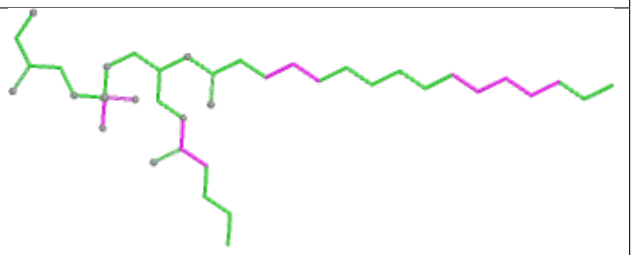
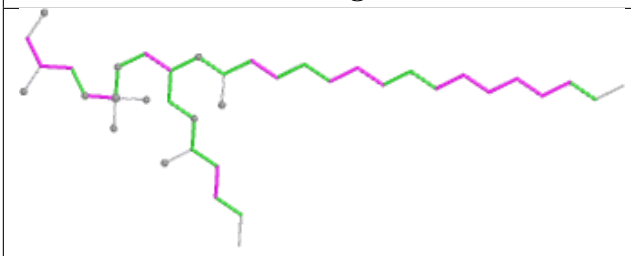
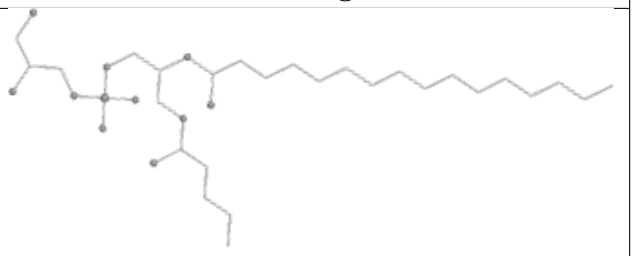


Bond angles

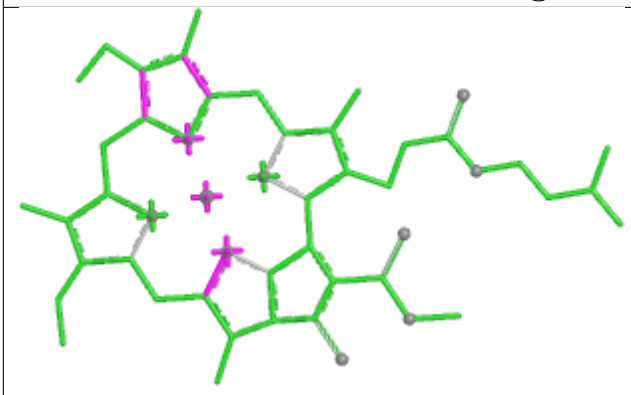


Torsions



Rings

Ligand CLA s 502



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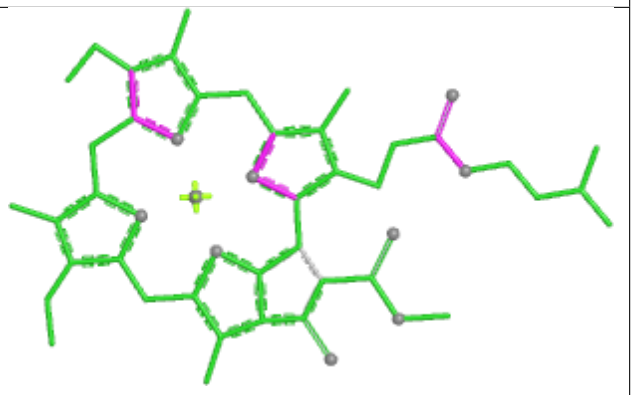
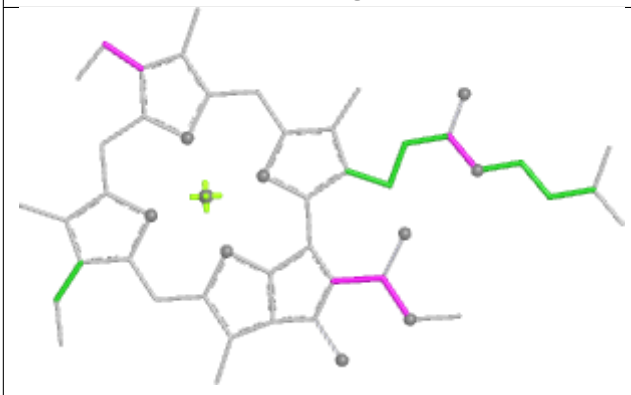
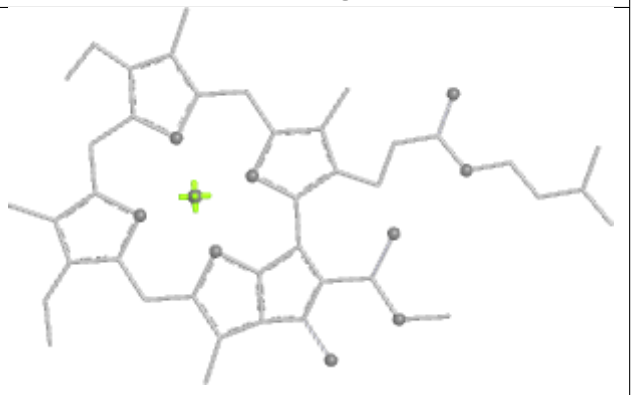


Bond angles

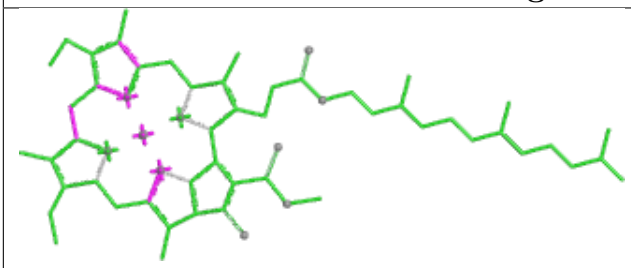


Torsions



Rings

Ligand CLA u 506



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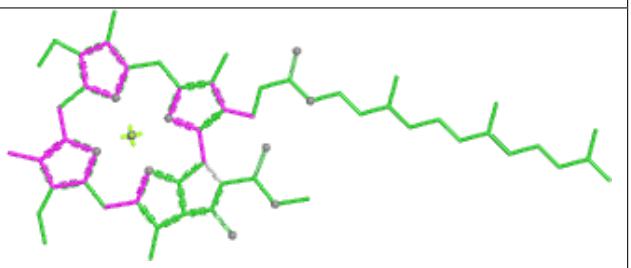
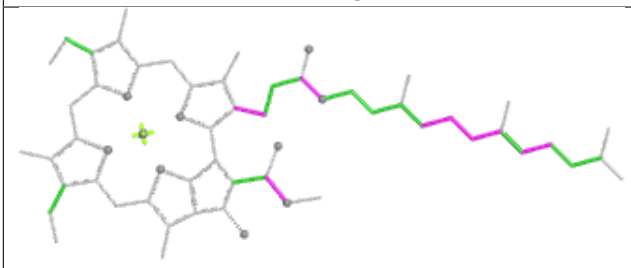
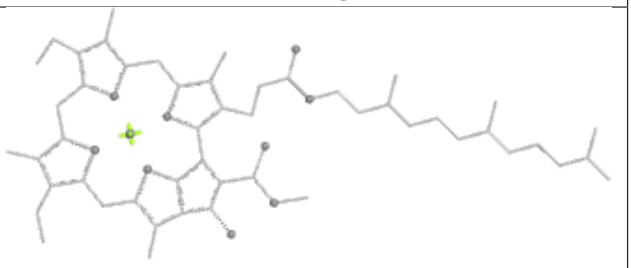


Bond angles

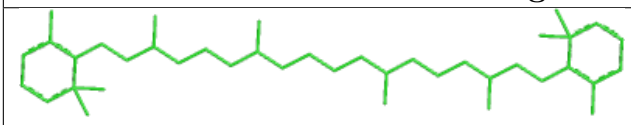


Torsions

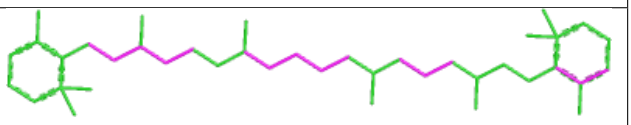


Rings

Ligand BCR s 603

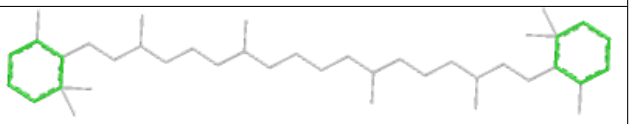


Bond lengths



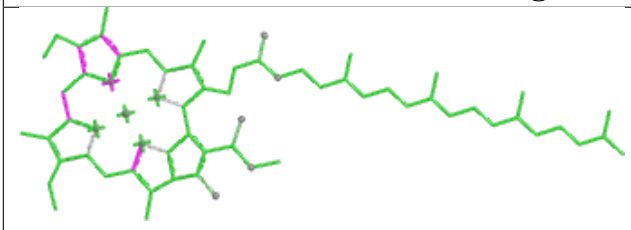
Bond angles

Torsions

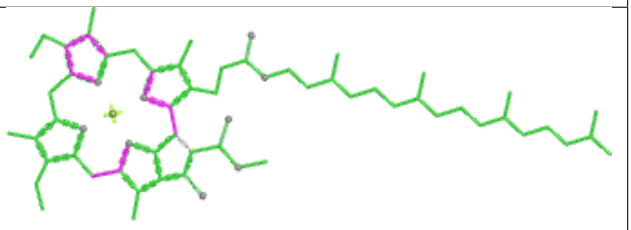


Rings

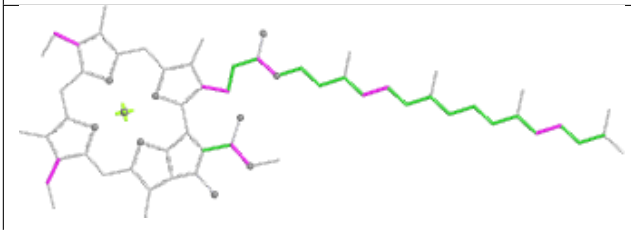
Ligand CLA r 509



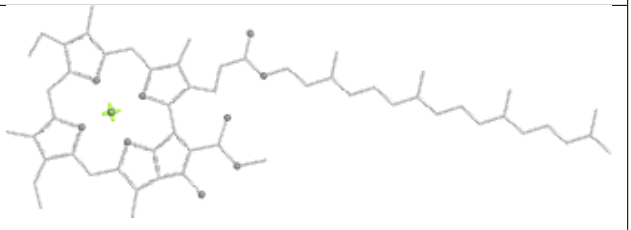
Bond lengths



Bond angles

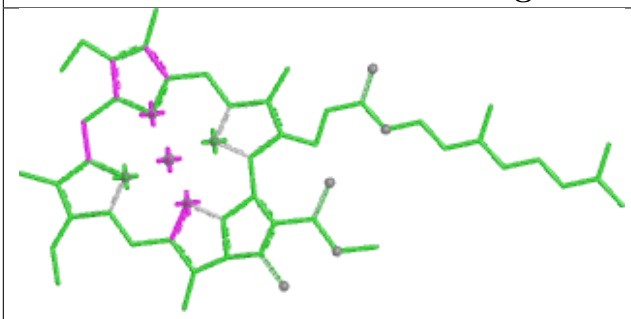


Torsions

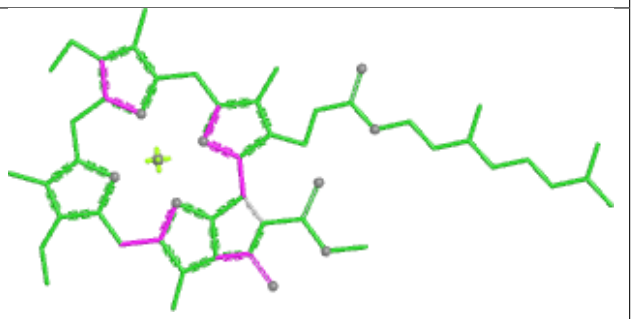


Rings

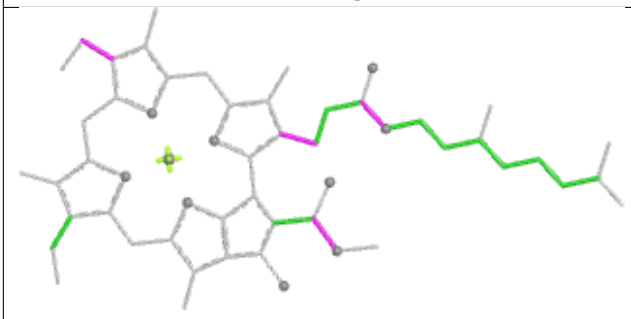
Ligand CLA A 1111



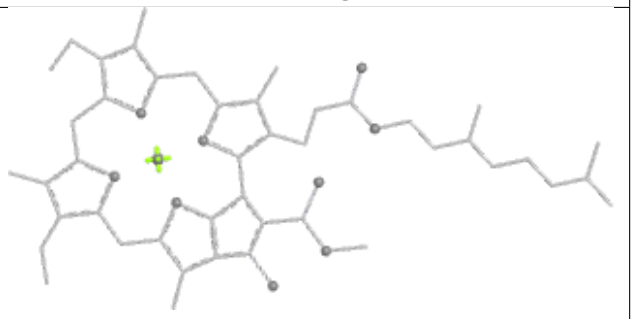
Bond lengths



Bond angles

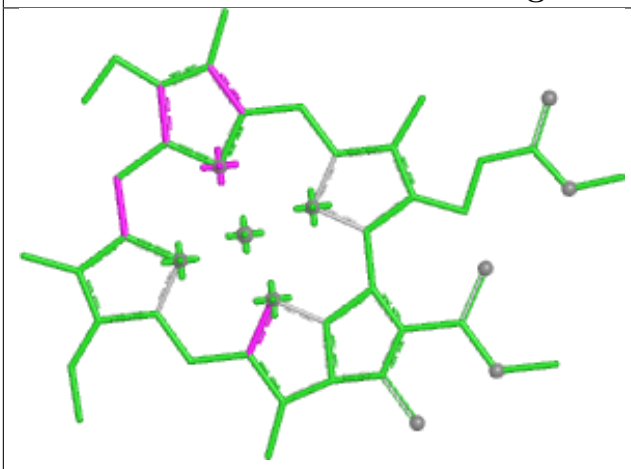


Torsions

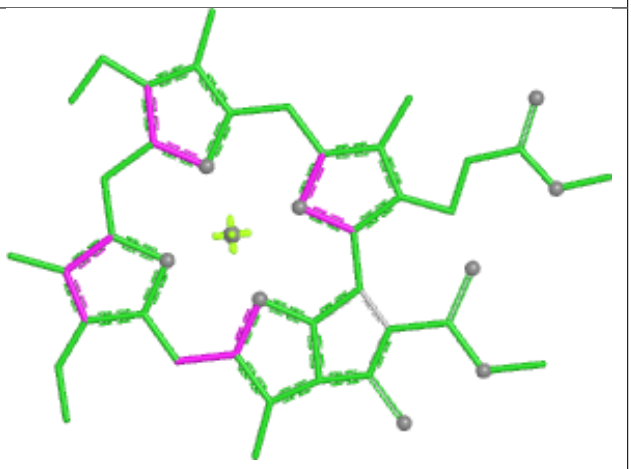


Rings

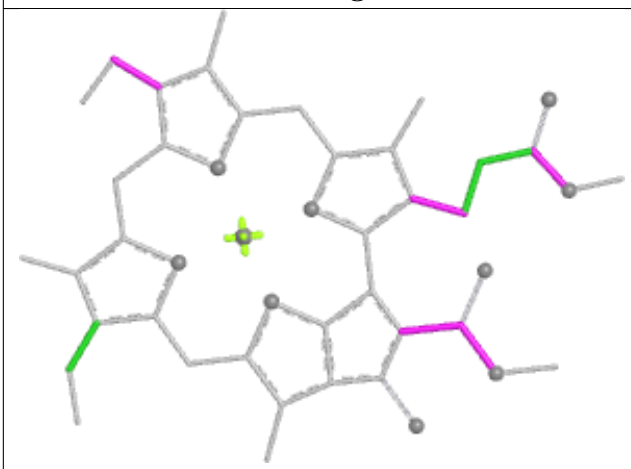
Ligand CLA n 513



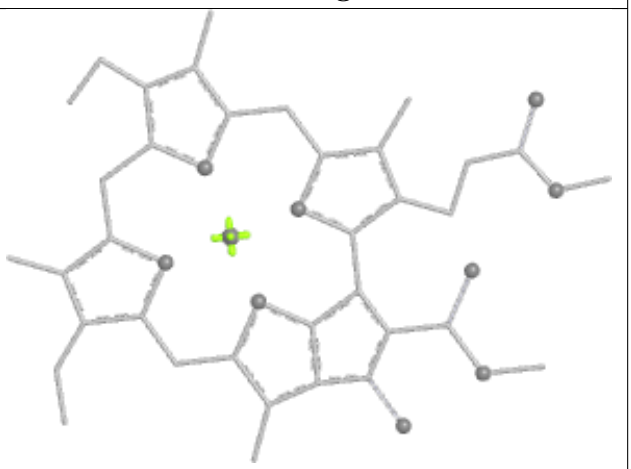
Bond lengths



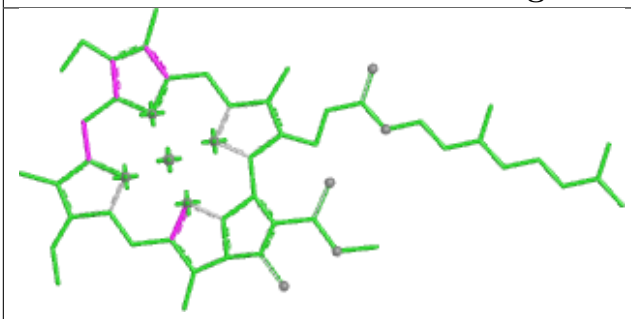
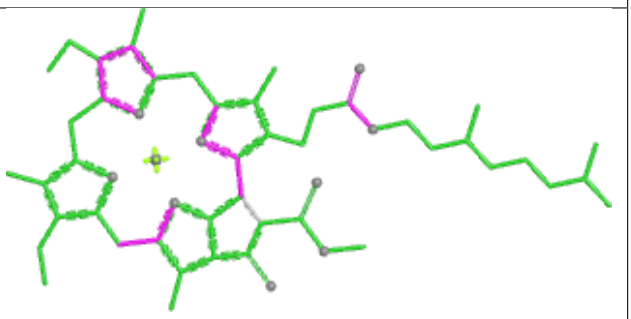
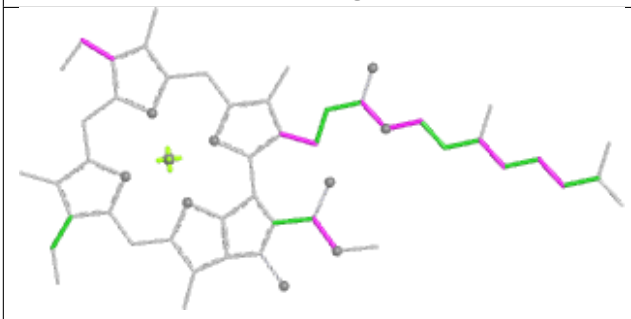
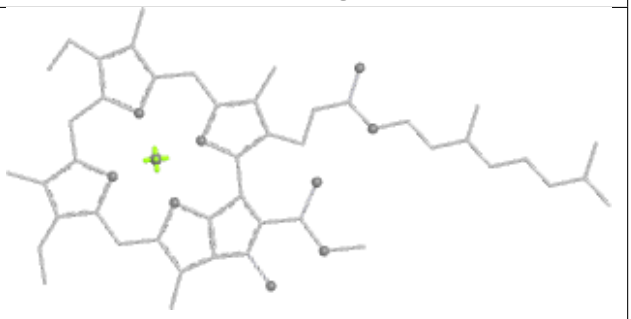
Bond angles



Torsions



Rings

Ligand CLA h 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

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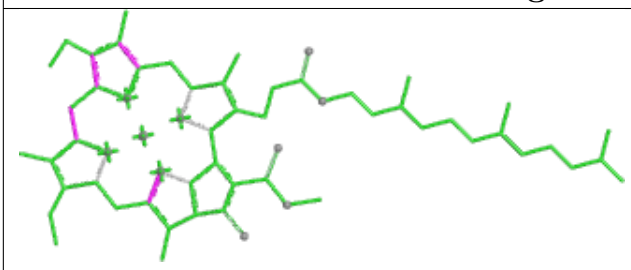
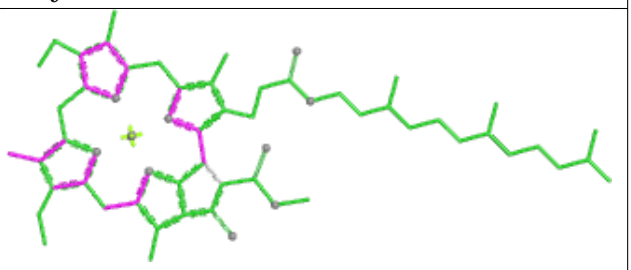
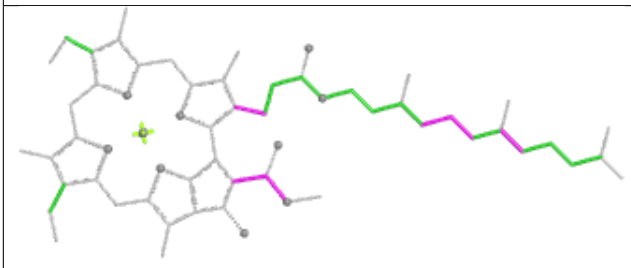
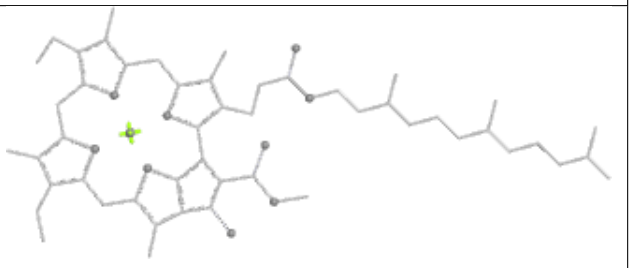
	
Bond lengths	Bond angles
	
Torsions	Rings

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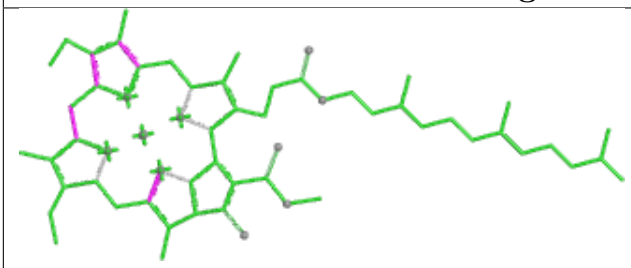
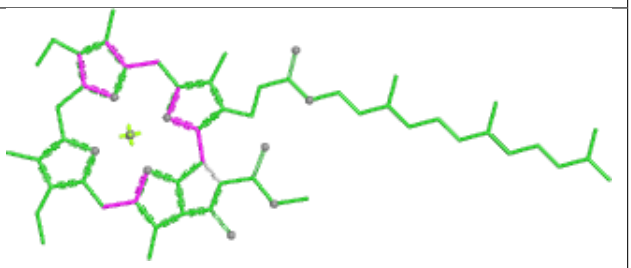
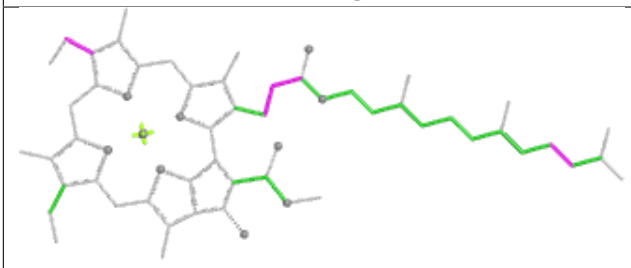
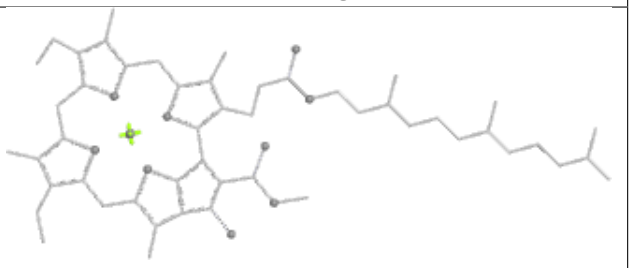
	
Bond lengths	Bond angles
	
Torsions	Rings

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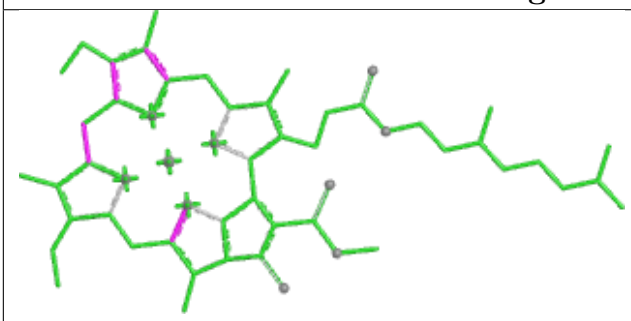
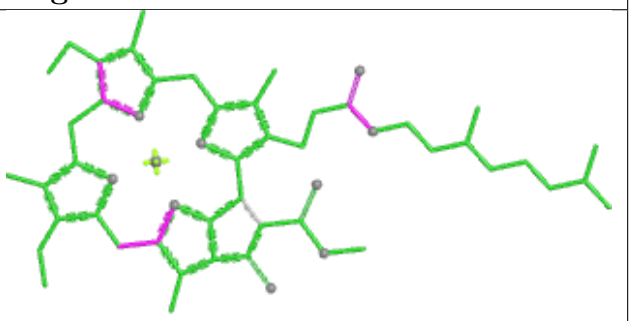
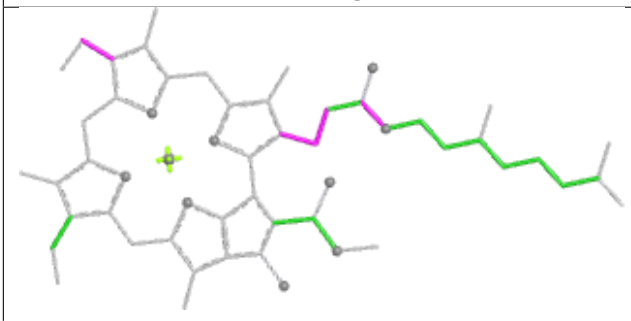
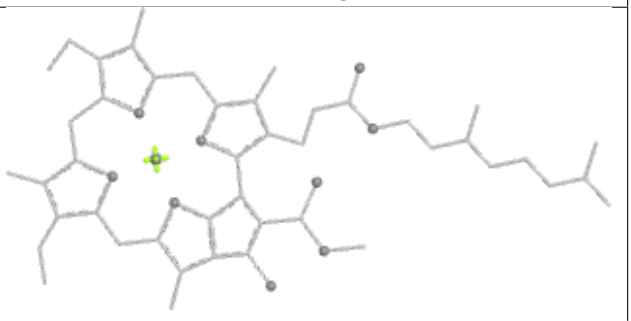
	
Bond lengths	Bond angles
	
Torsions	Rings

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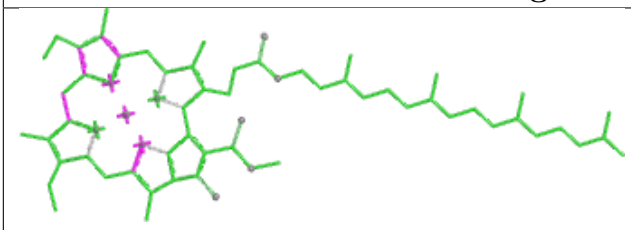
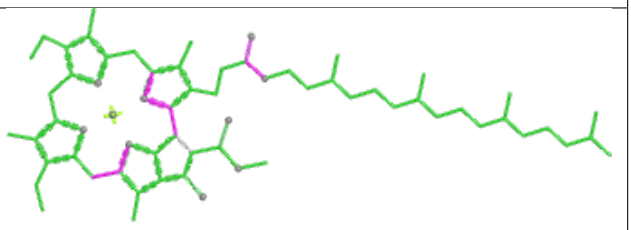
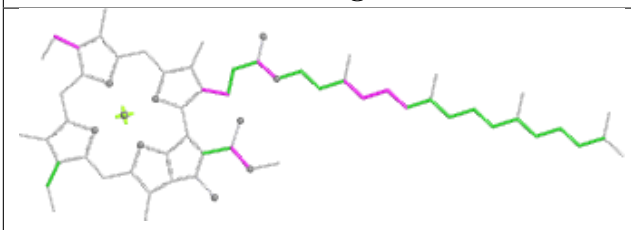
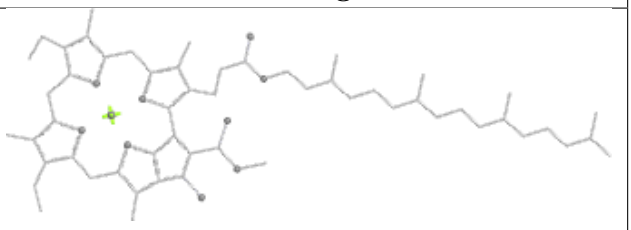
	
Bond lengths	Bond angles
	
Torsions	Rings

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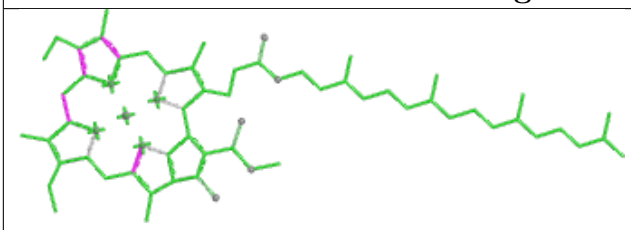
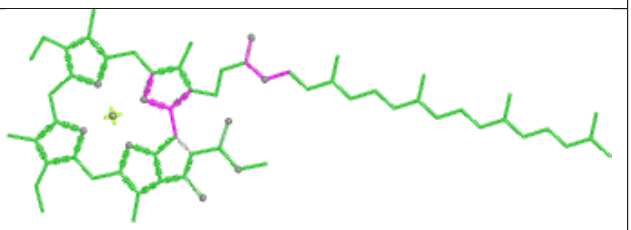
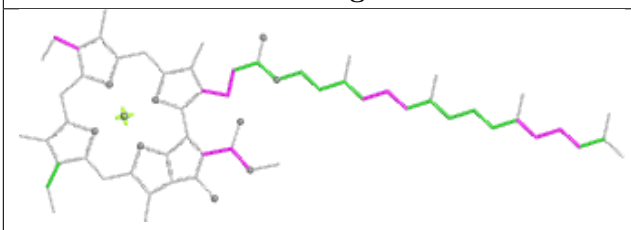
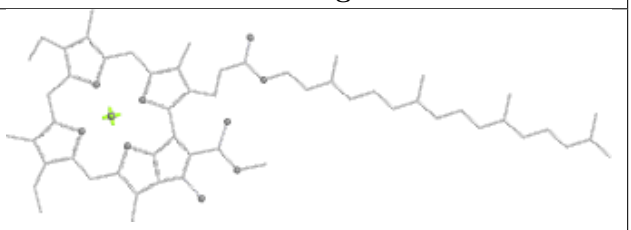
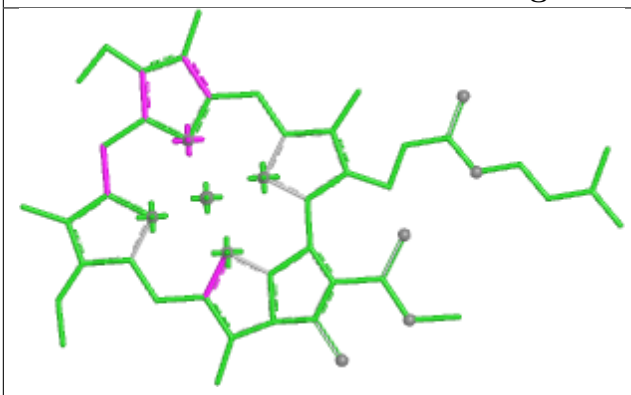
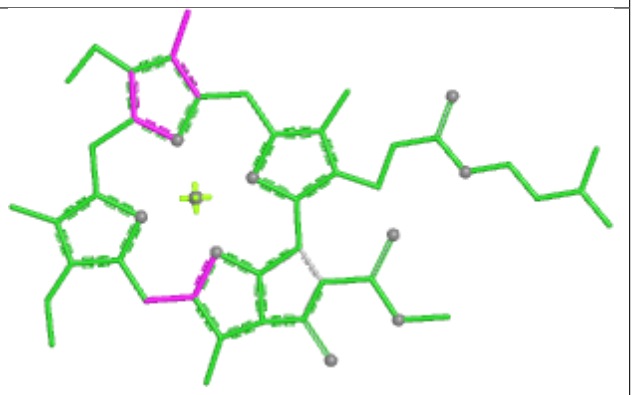
	
Bond lengths	Bond angles
	
Torsions	Rings

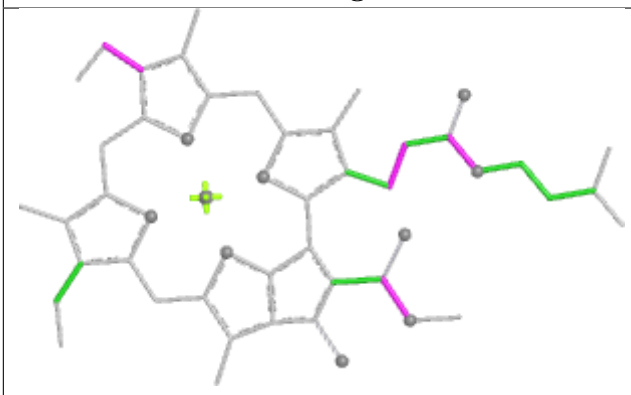
Ligand CLA r 502



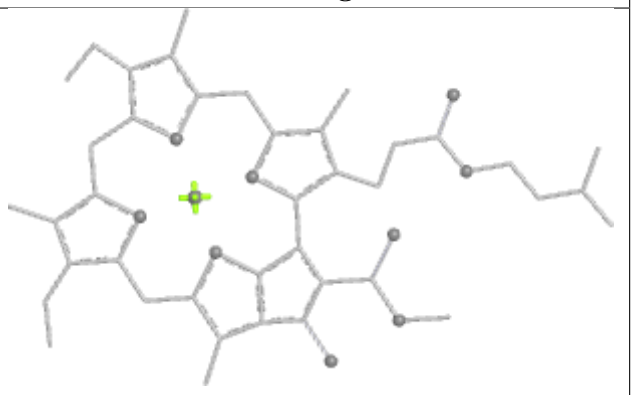
Bond lengths



Bond angles

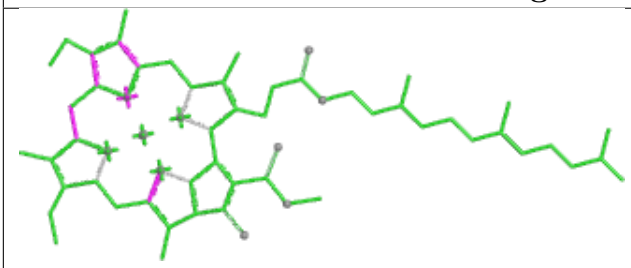


Torsions



Rings

Ligand CLA t 509



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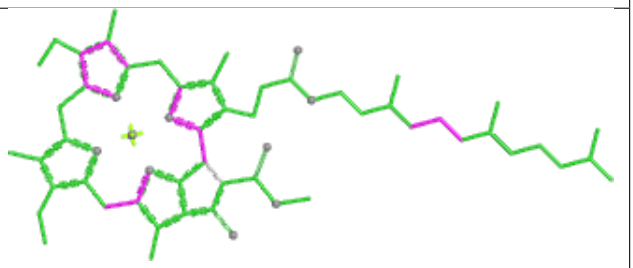
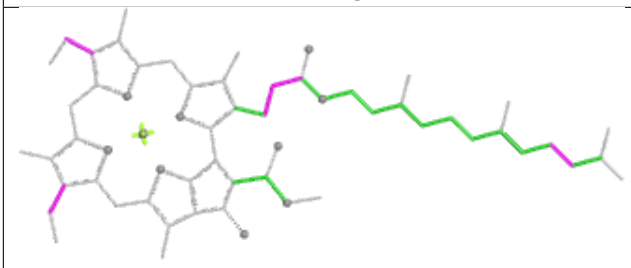


Bond angles



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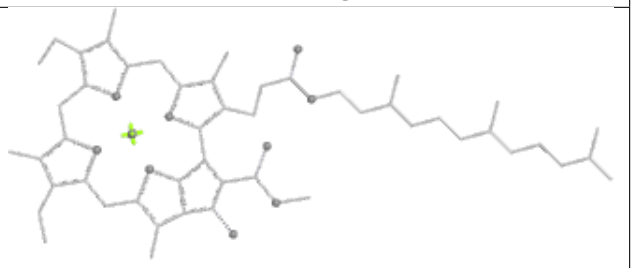
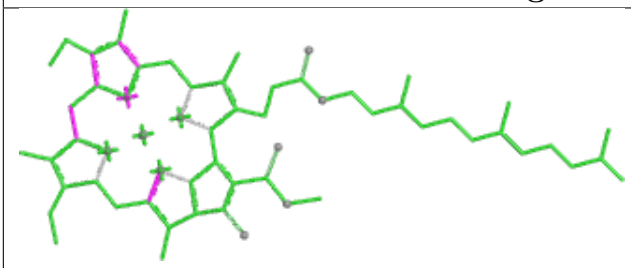
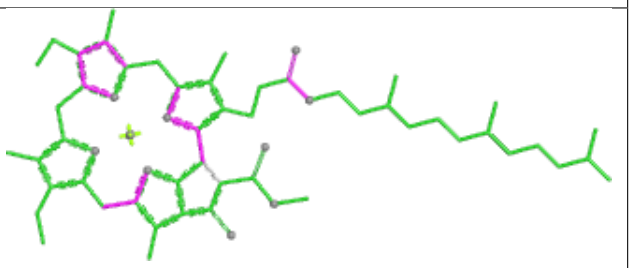
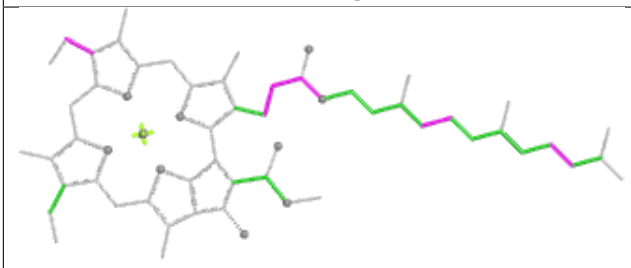
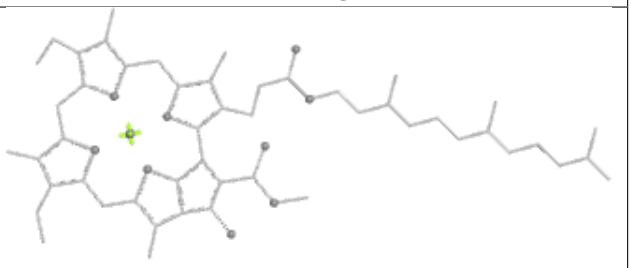
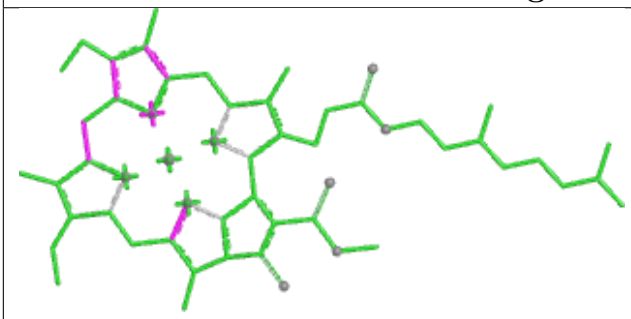
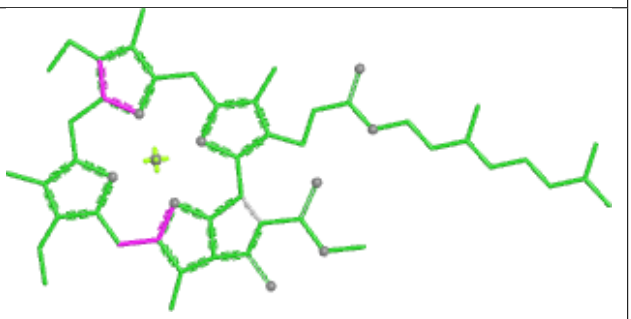
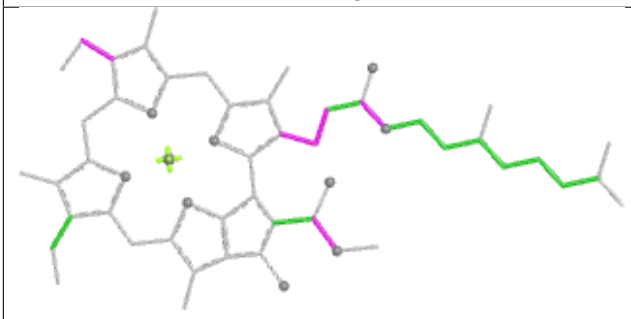
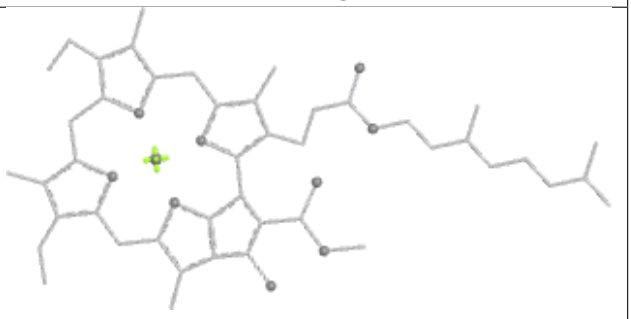
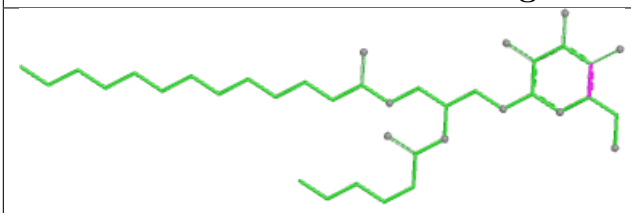


Rings

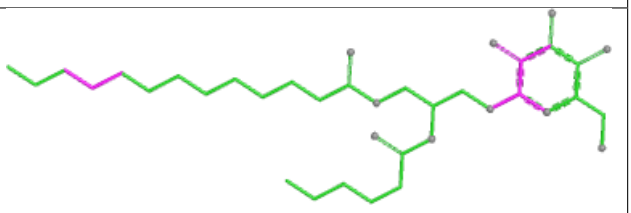
Ligand CLA u 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

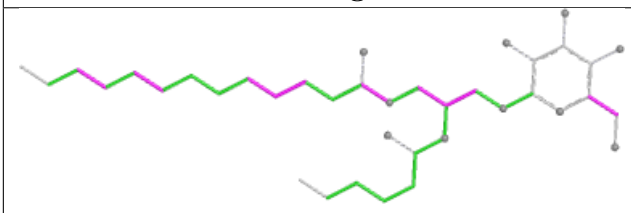
Ligand LMG A 852



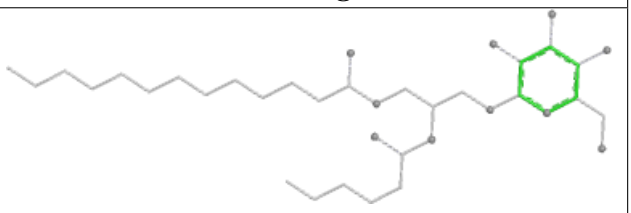
Bond lengths



Bond angles

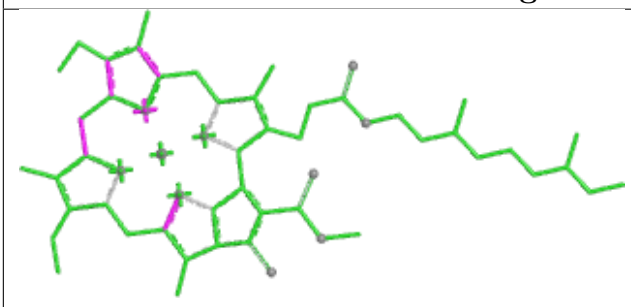


Torsions

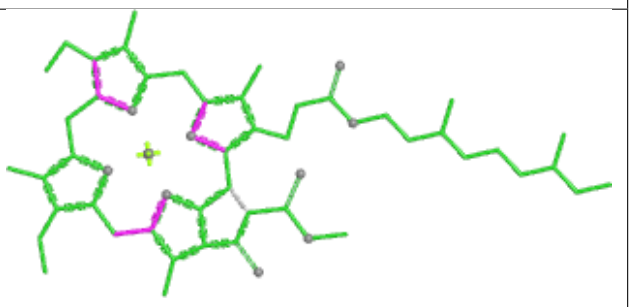


Rings

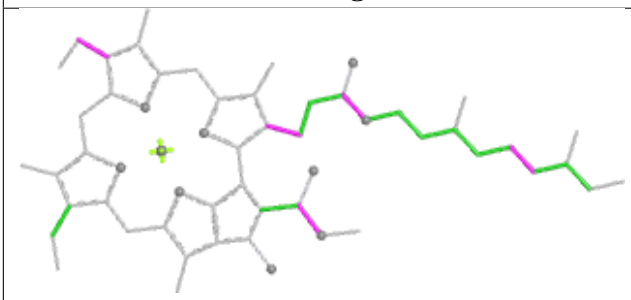
Ligand CLA a 1102



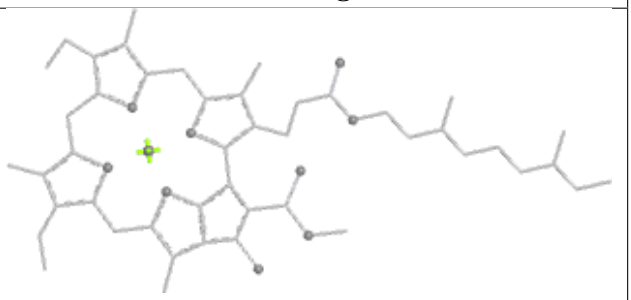
Bond lengths



Bond angles

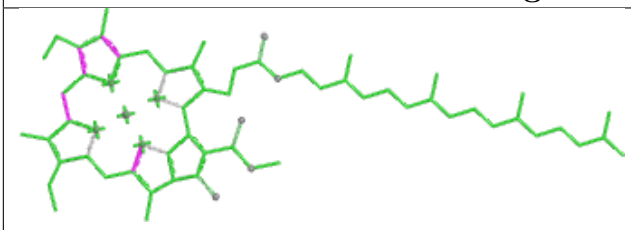


Torsions



Rings

Ligand CLA Y 510



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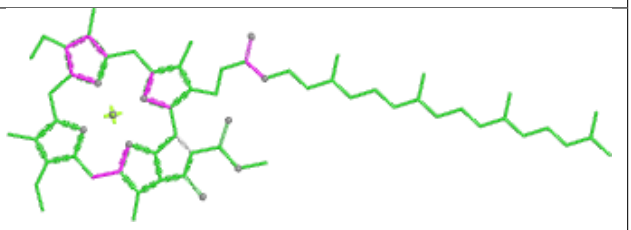

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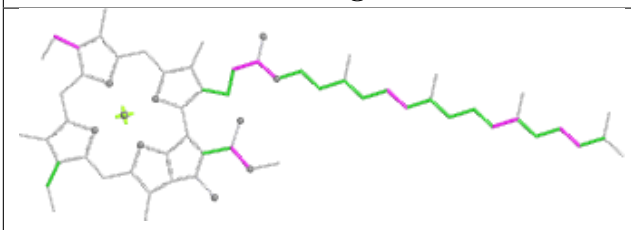

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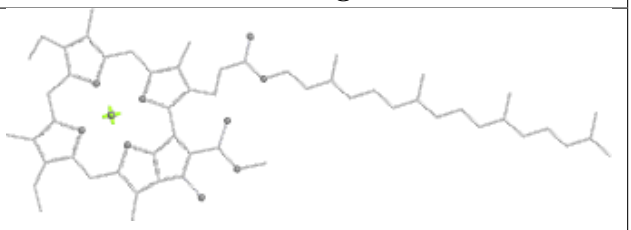
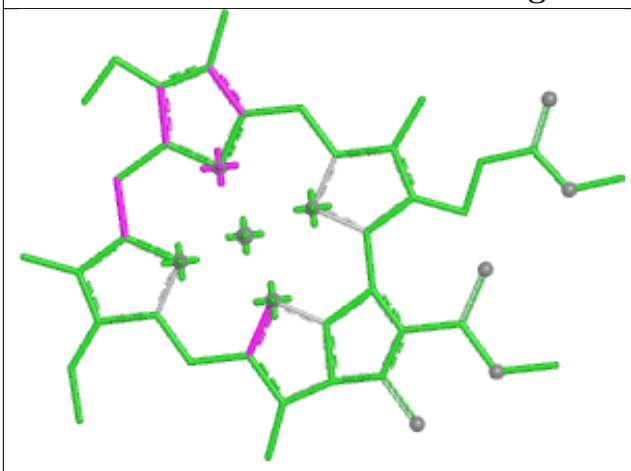


Rings

Ligand CLA o 516



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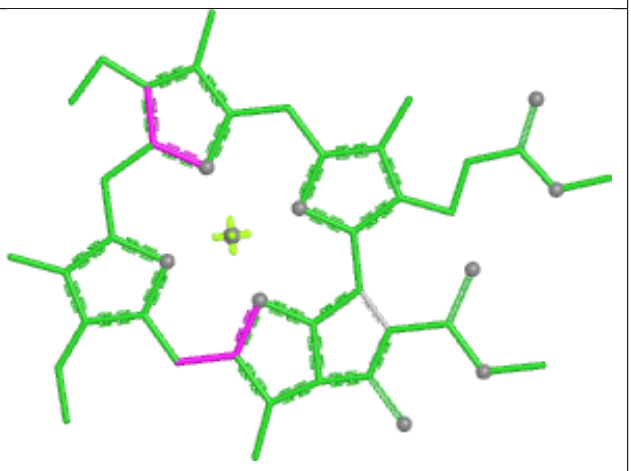
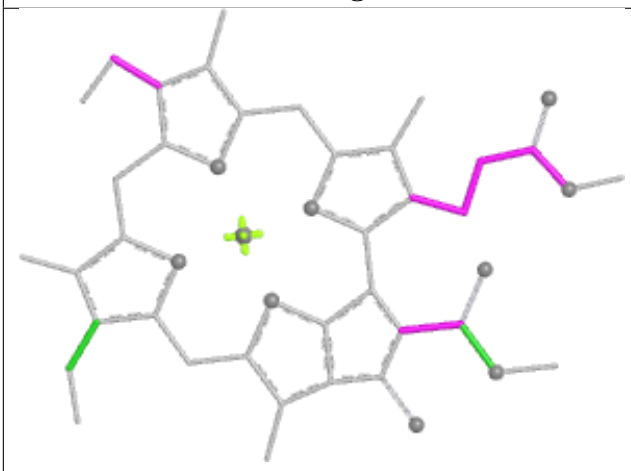


Bond angles



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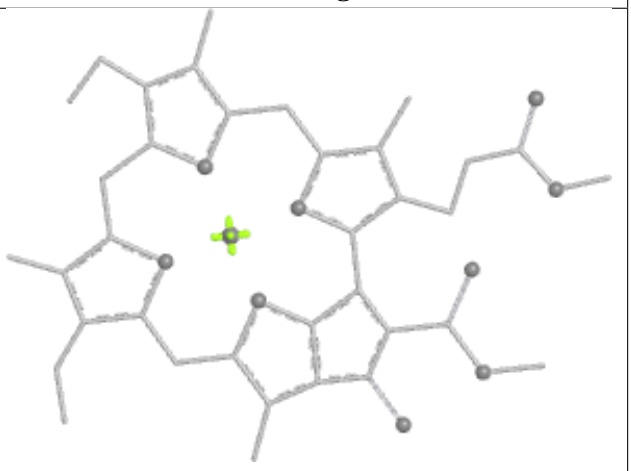
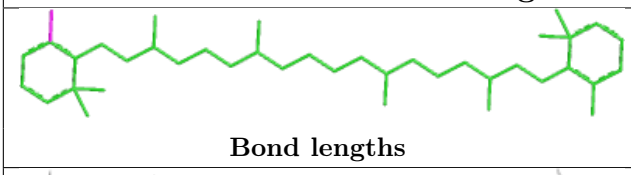


Rings

Ligand BCR a 4008



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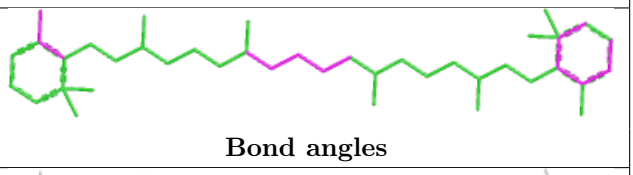

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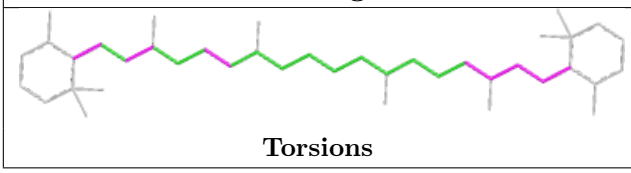
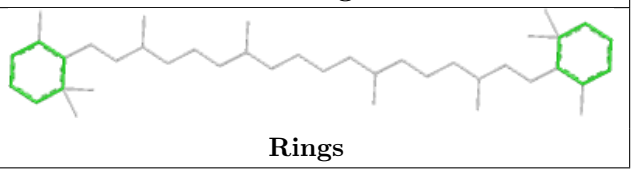
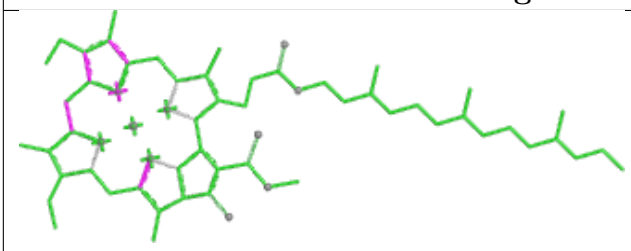


Torsions



Rings

Ligand CLA G 1235



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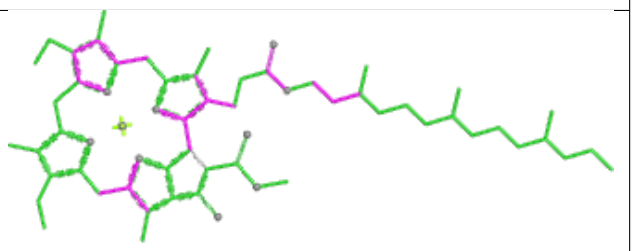
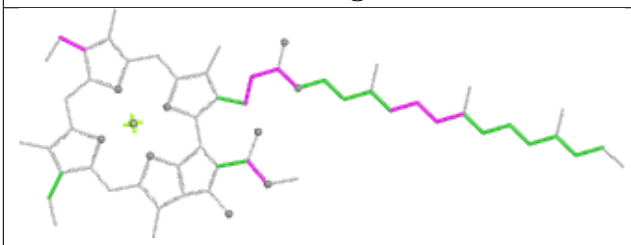


Bond angles



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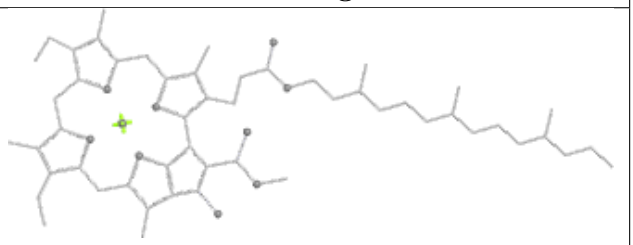
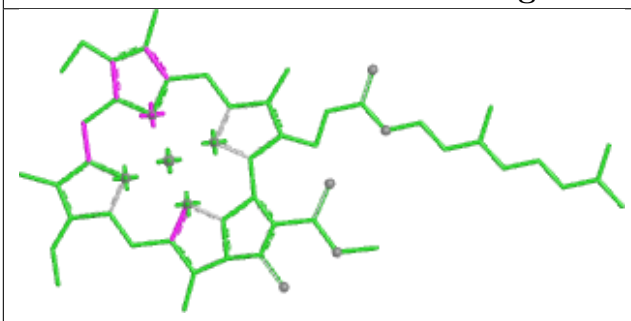


Rings

Ligand CLA b 1214



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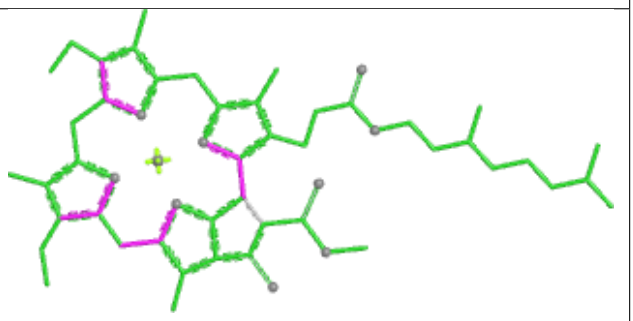

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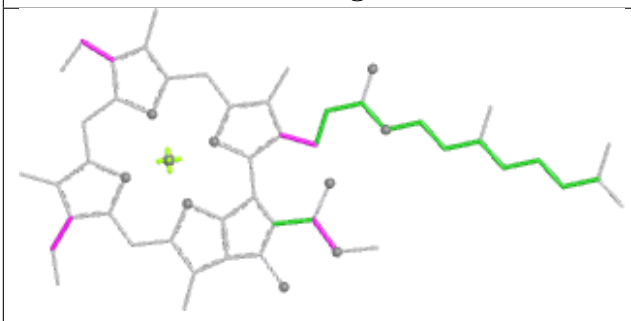

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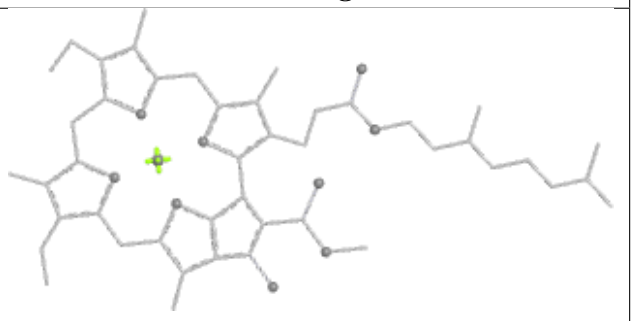
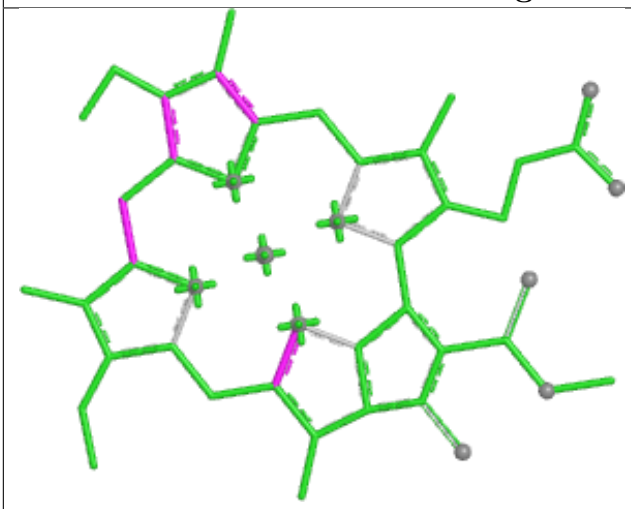


Rings

Ligand CLA B 1208



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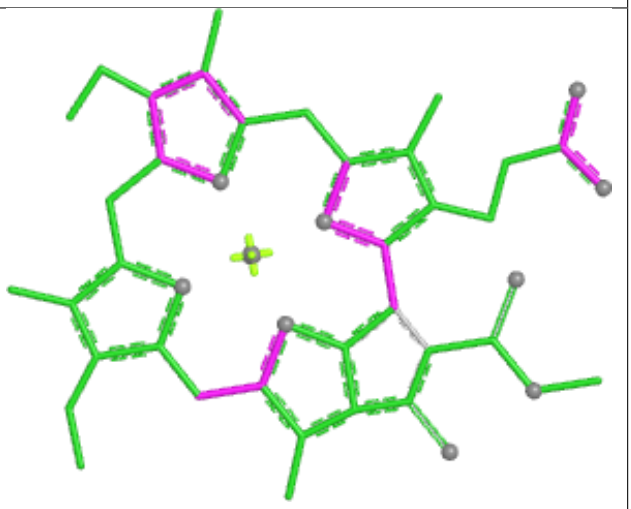

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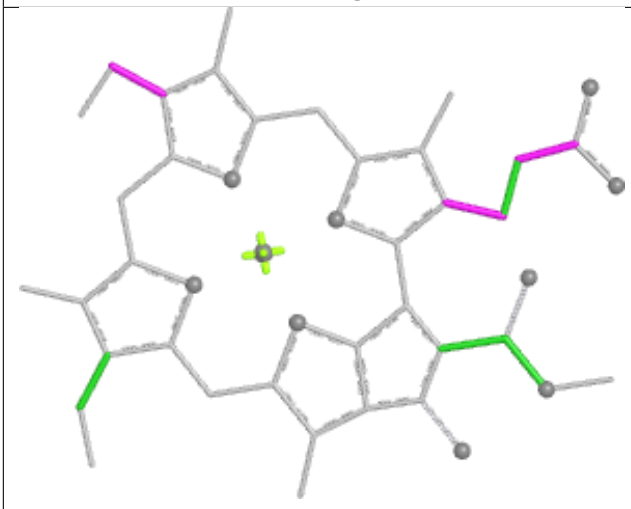
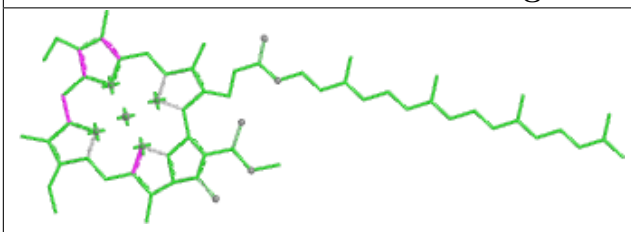


Torsions

Rings

Ligand CLA X 507



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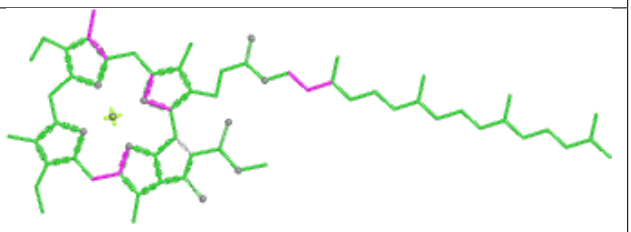

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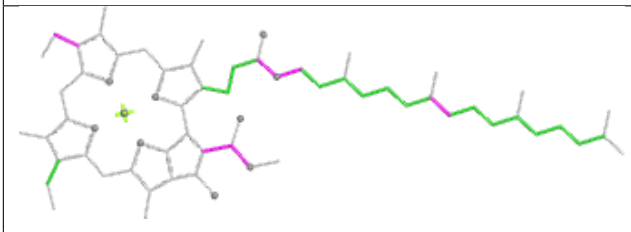

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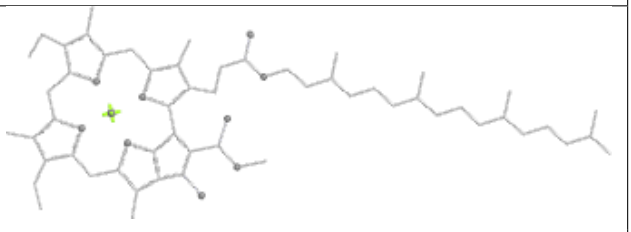
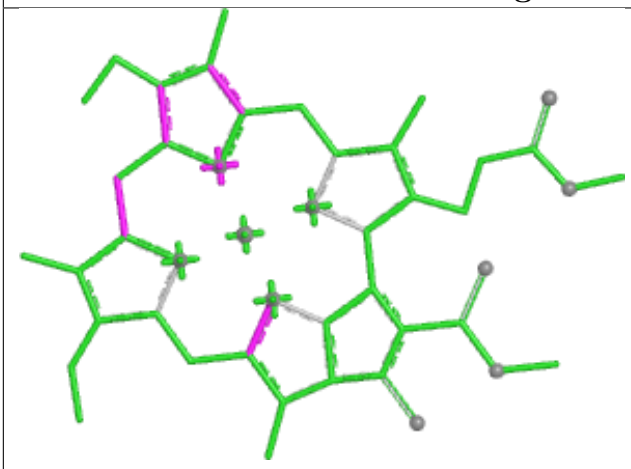


Rings

Ligand CLA H 1114



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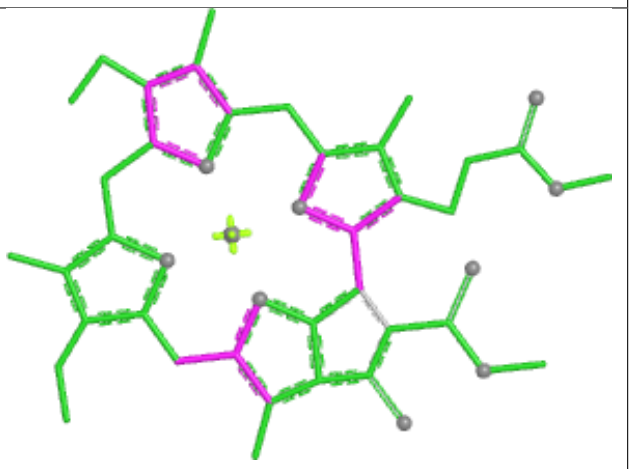

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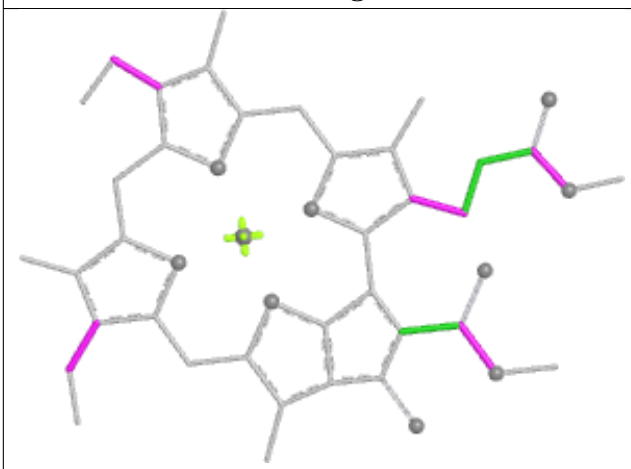

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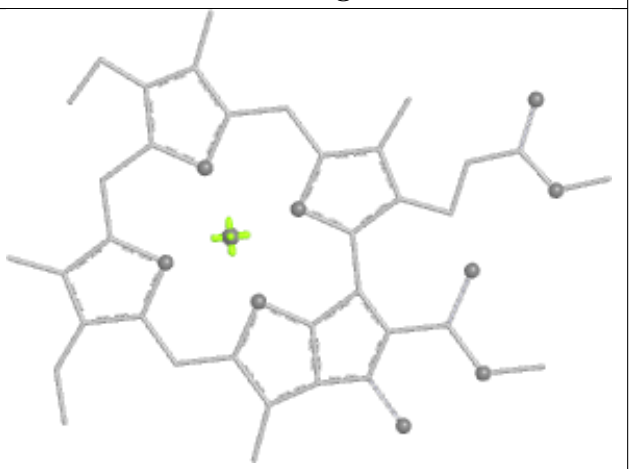
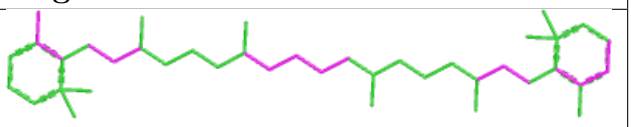


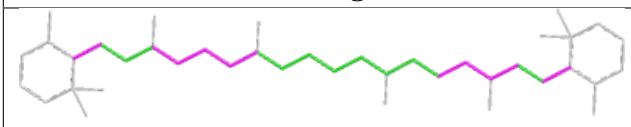
Rings

Ligand BCR g 602

Bond lengths



Bond angles



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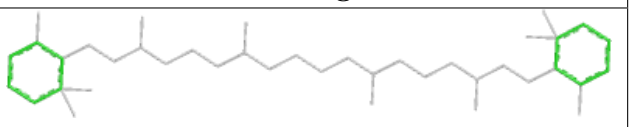
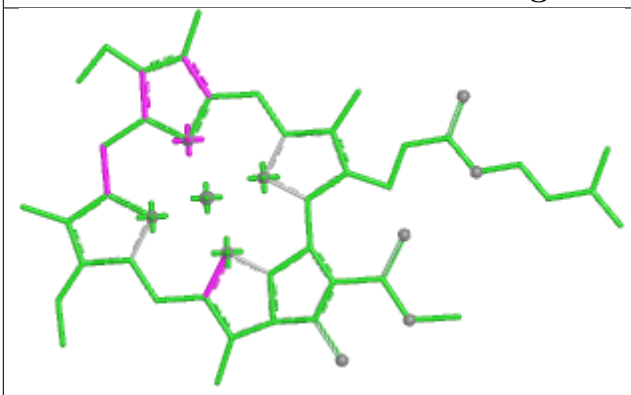


Rings

Ligand CLA s 514



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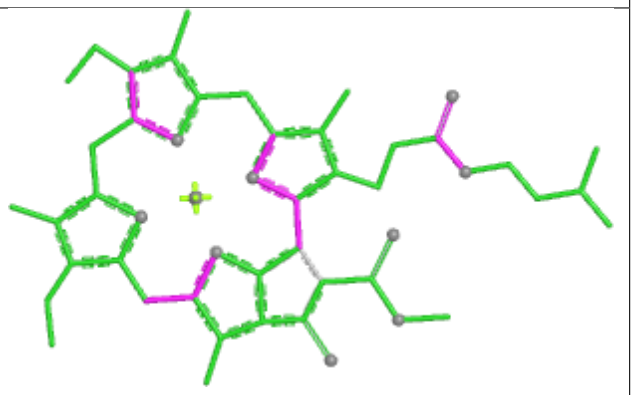

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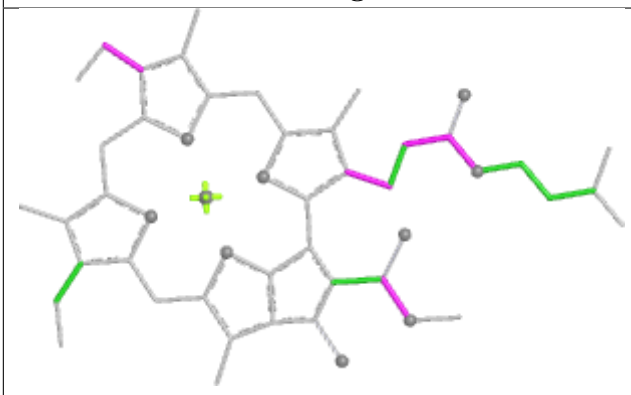

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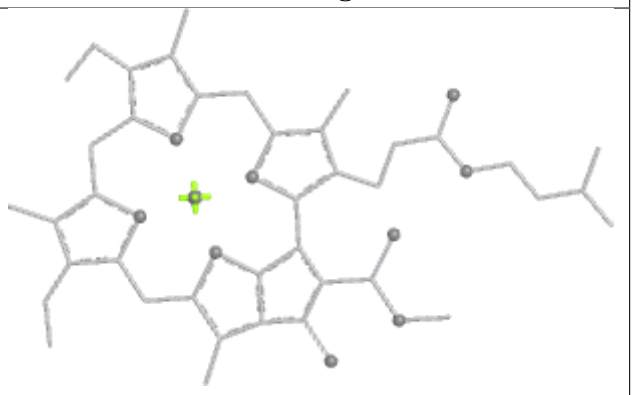
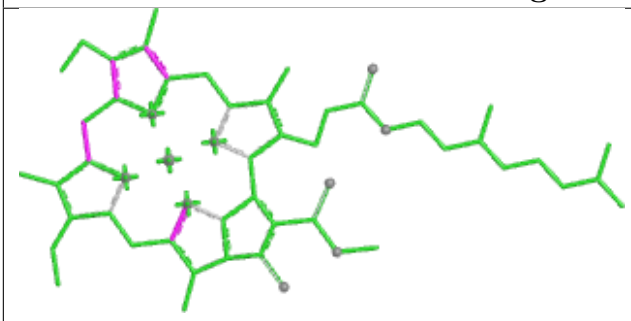


Rings

Ligand CLA r 517



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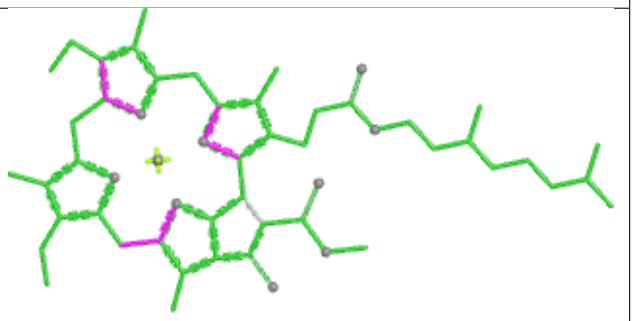
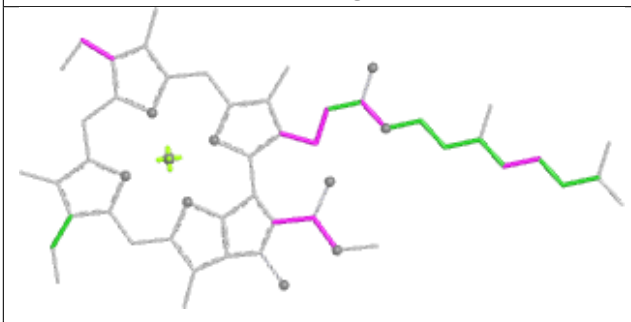


Bond angles



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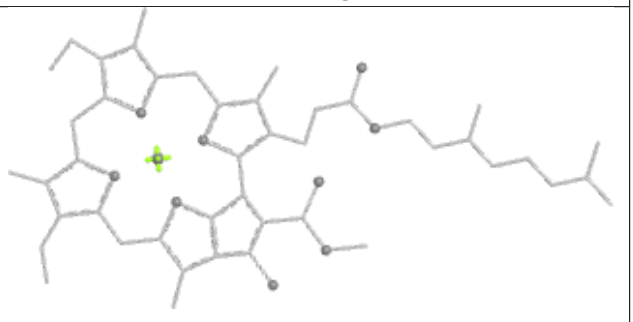
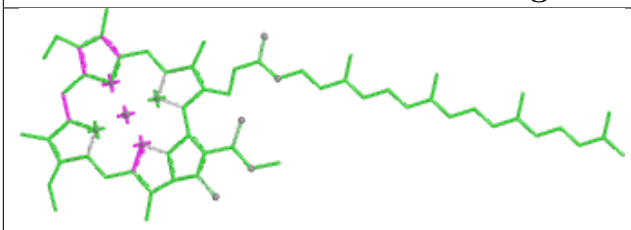
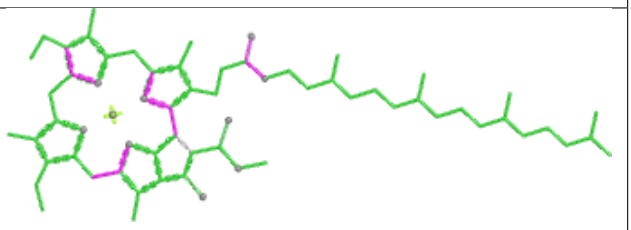
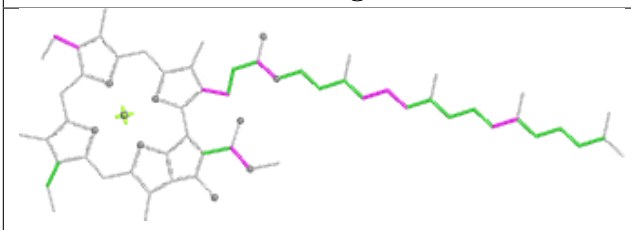
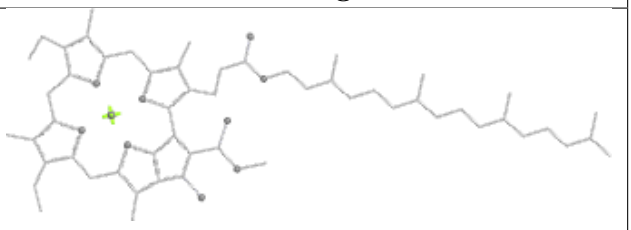
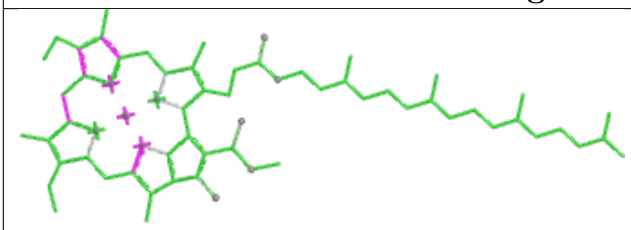
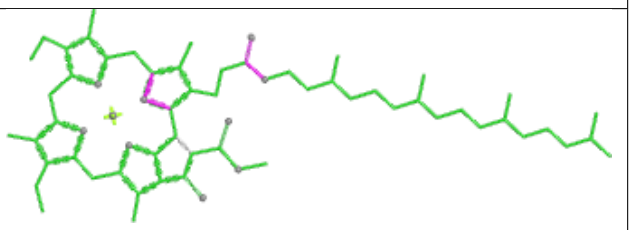
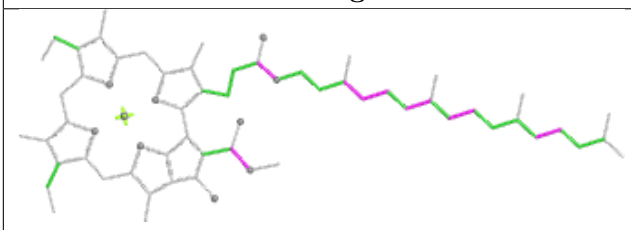
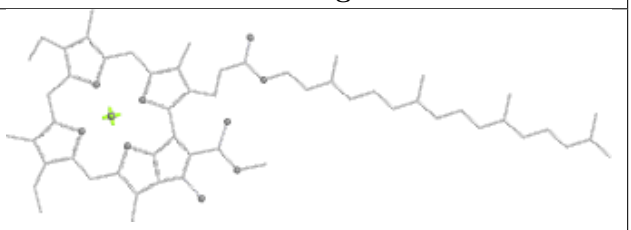
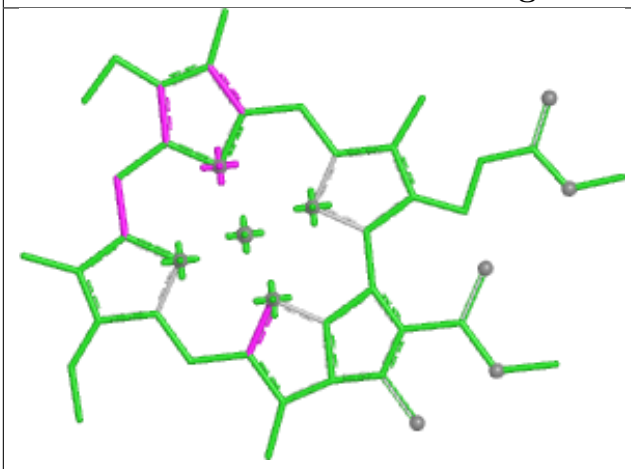


Rings

Ligand CLA t 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA u 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 513



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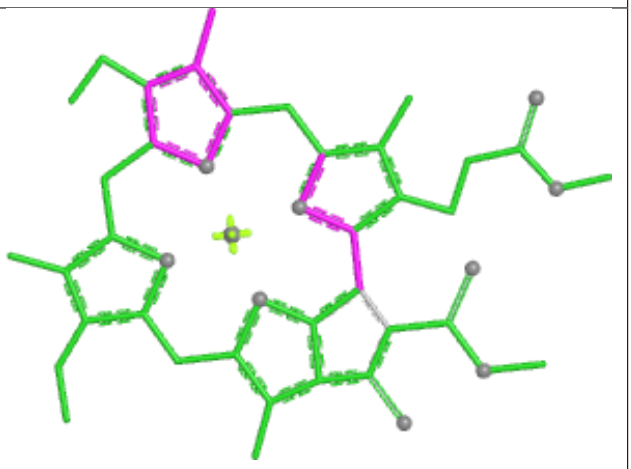
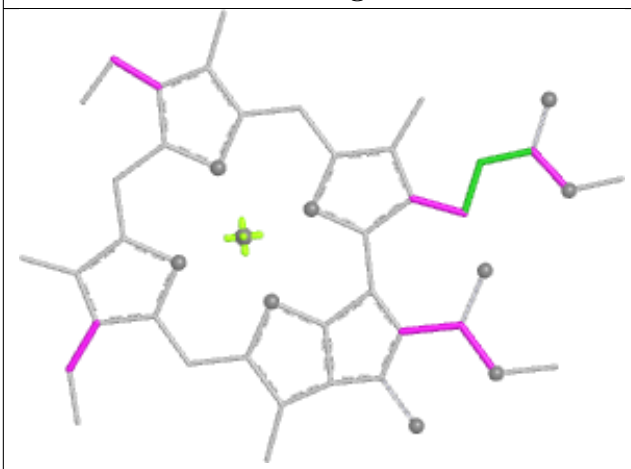
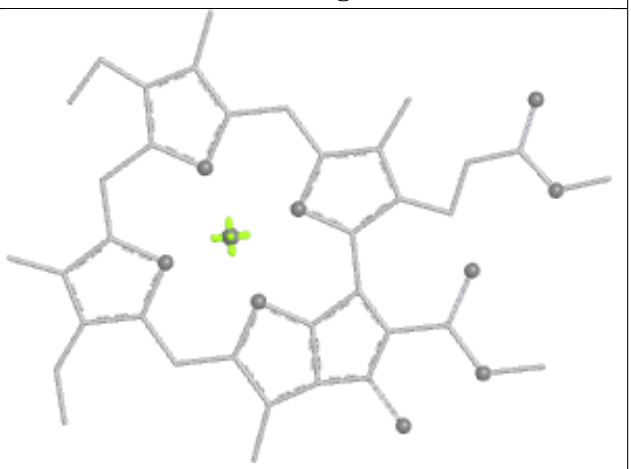


Bond angles



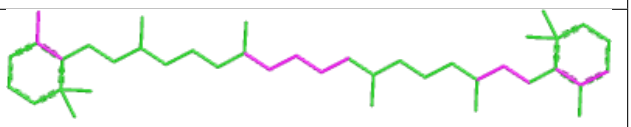
Torsions



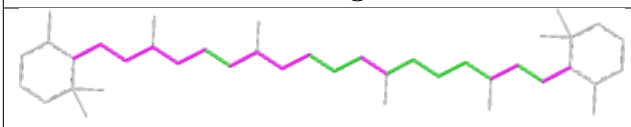
Rings

Ligand BCR s 604

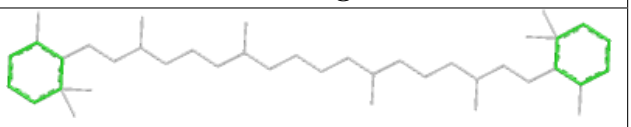
Bond lengths



Bond angles

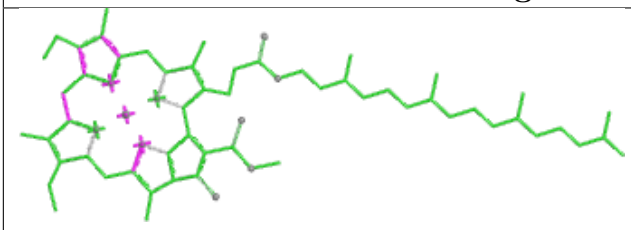


Torsions



Rings

Ligand CLA H 1127



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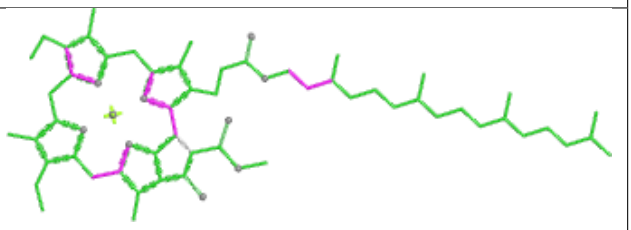

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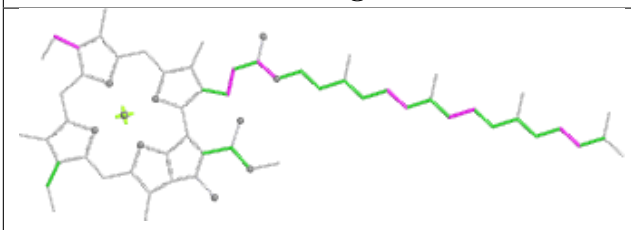

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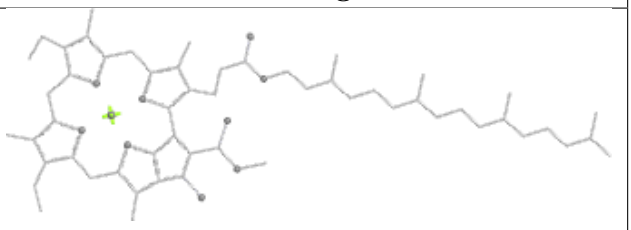
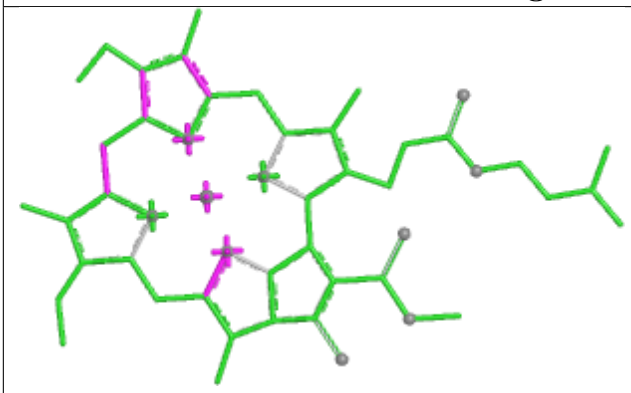


Rings

Ligand CLA u 502



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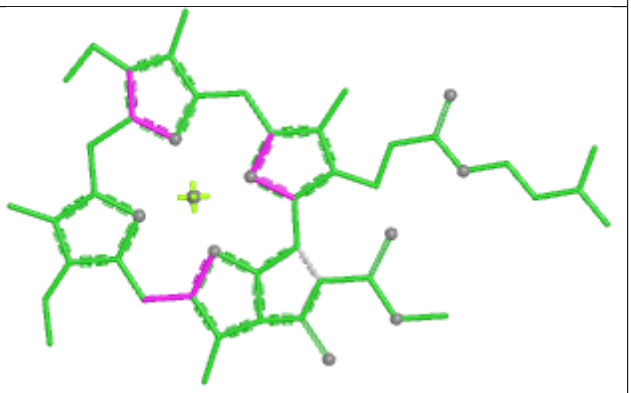
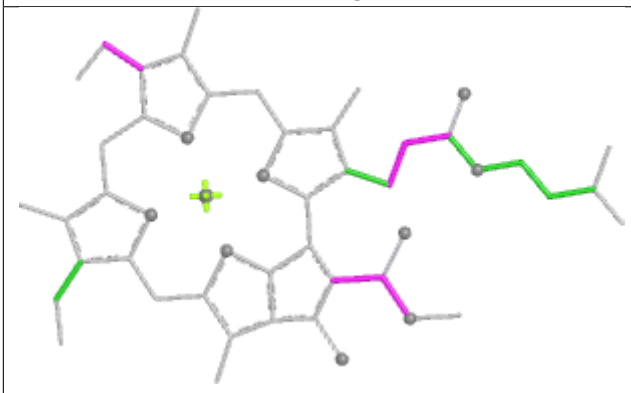


Bond angles



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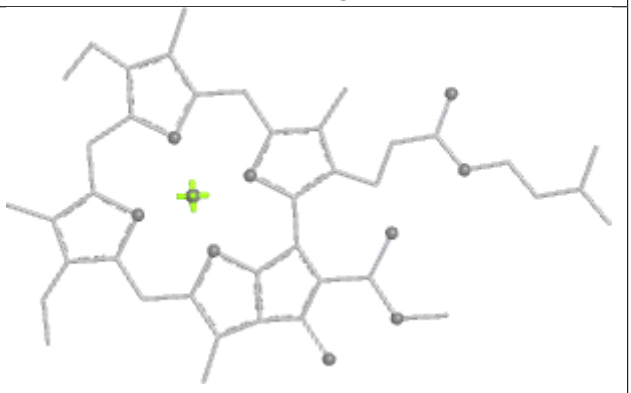
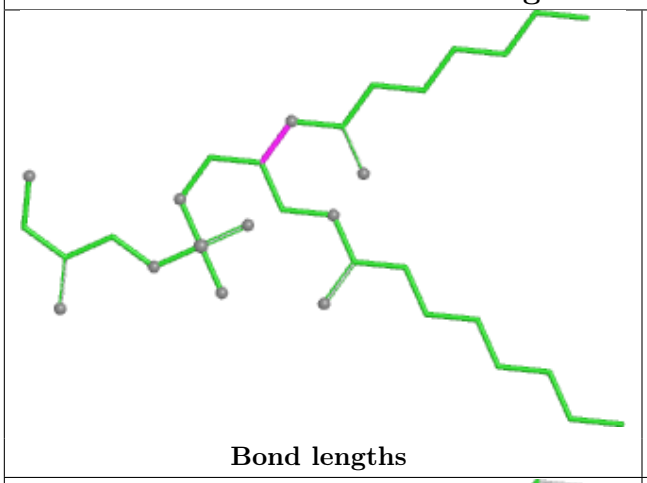


Rings

Ligand LHG Y 605



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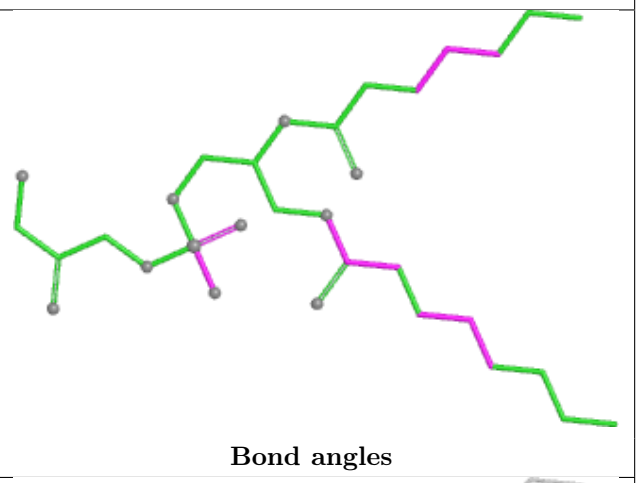
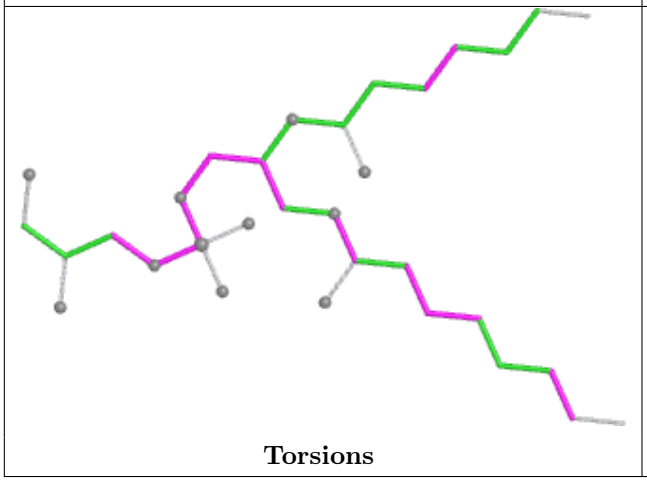


Bond angles



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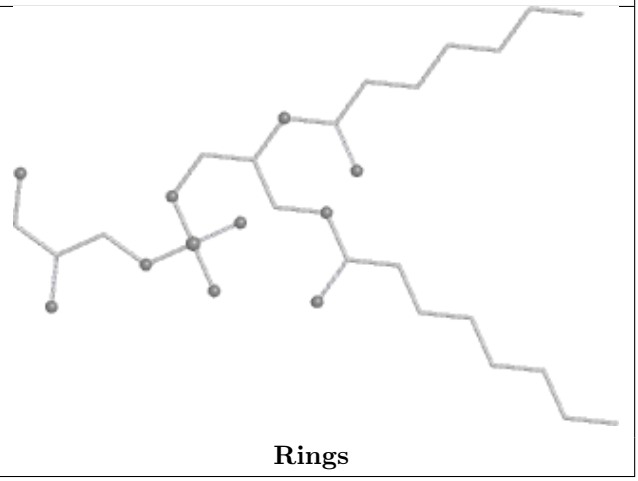
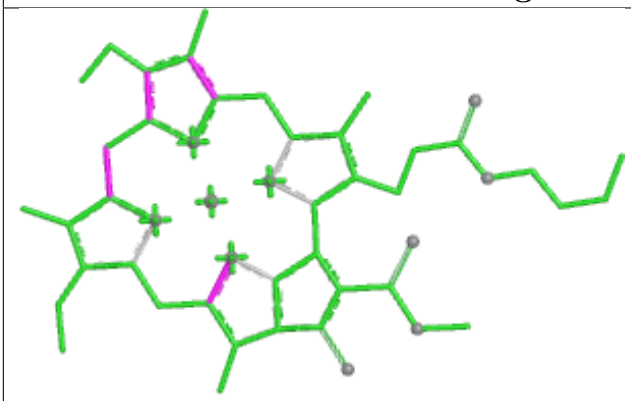


Rings

Ligand CLA A 1120



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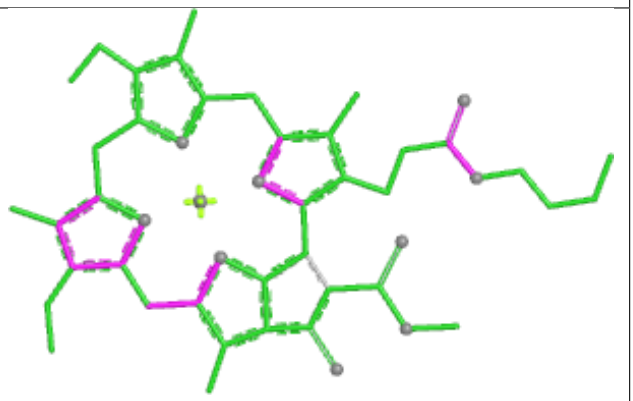
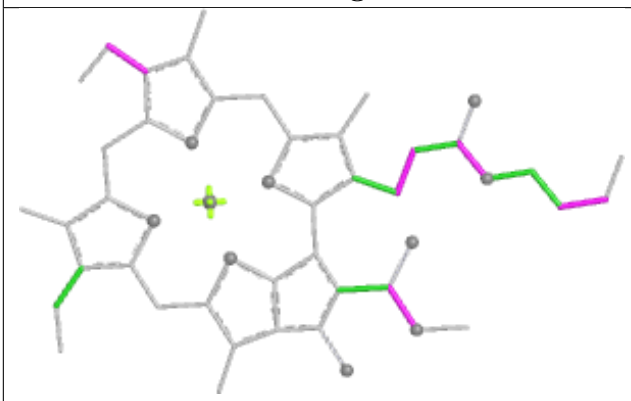


Bond angles



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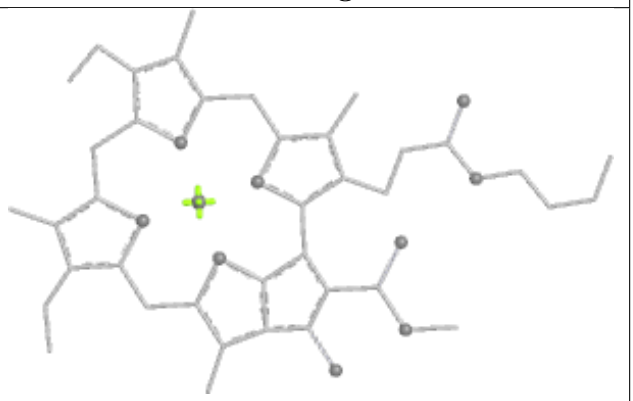
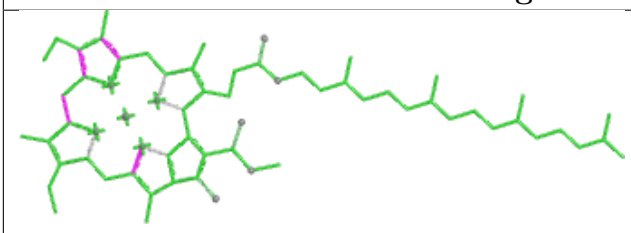


Rings

Ligand CLA B 1204



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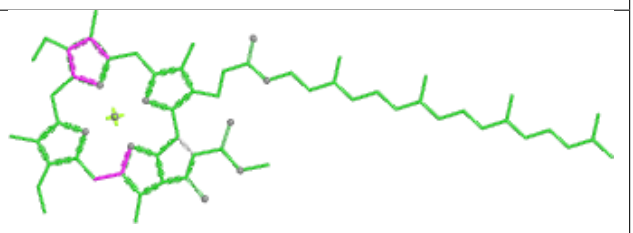
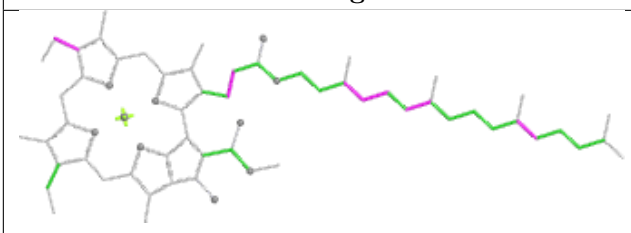


Bond angles



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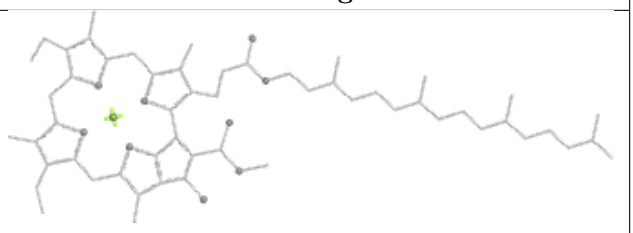
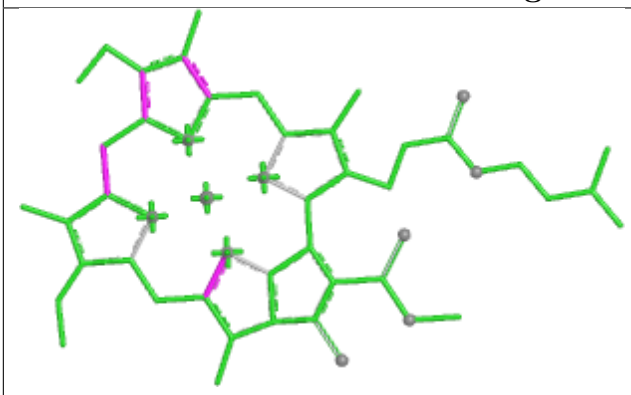


Rings

Ligand CLA w 513



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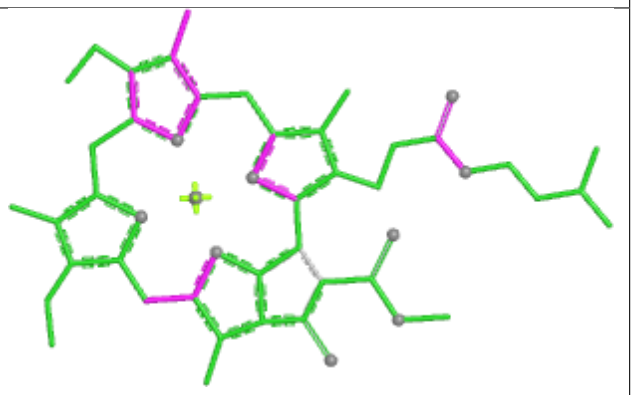

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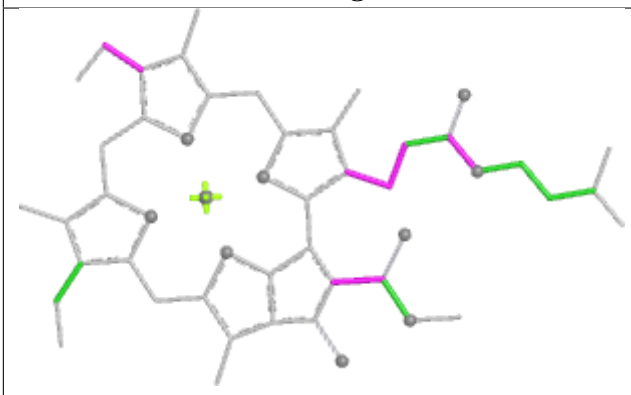

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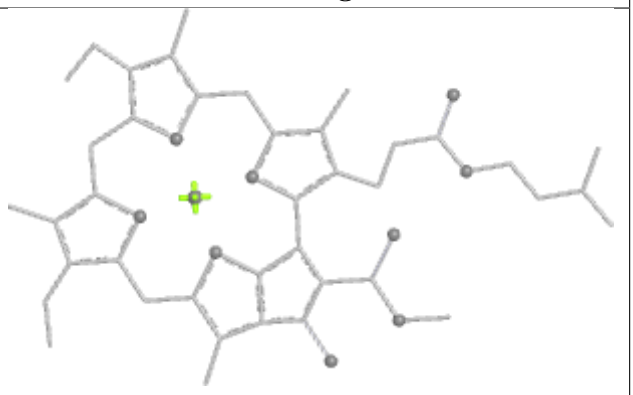

Rings

Ligand BCR X 601

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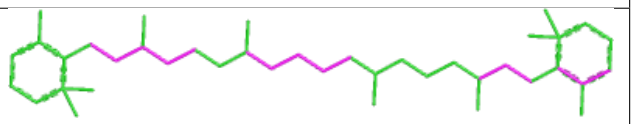

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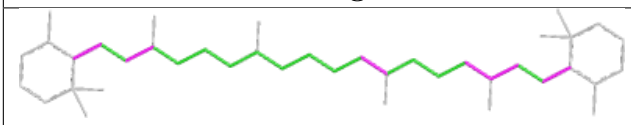

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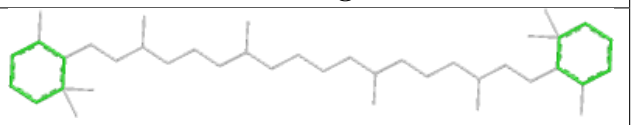
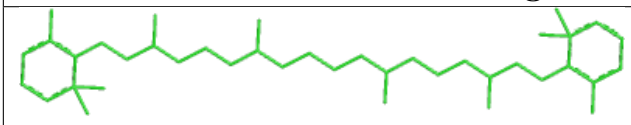


Rings

Ligand BCR Z 603



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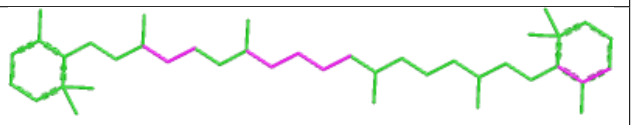
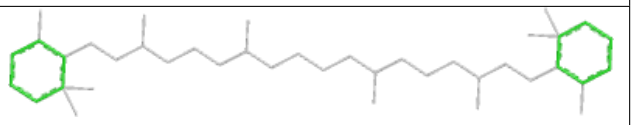


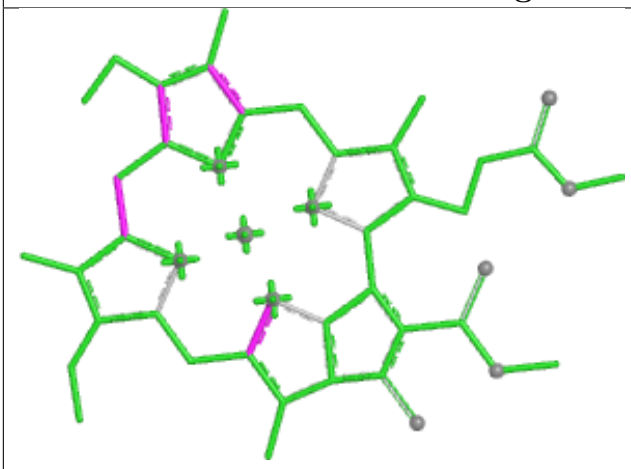
Bond angles

Torsions



Rings

Ligand CLA A 1801



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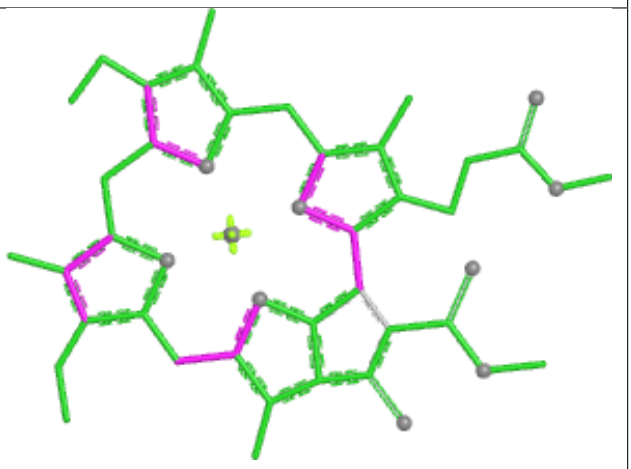

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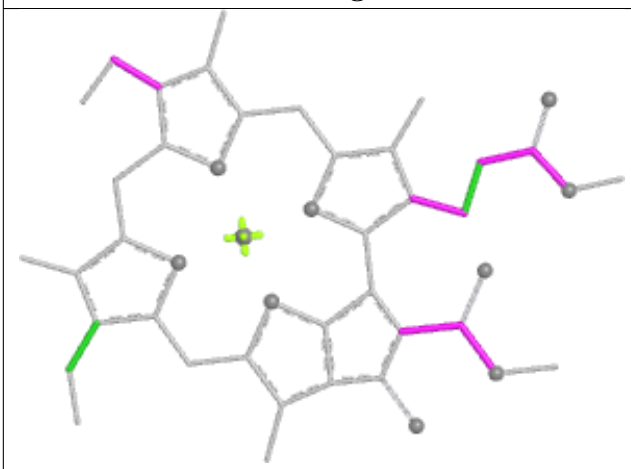

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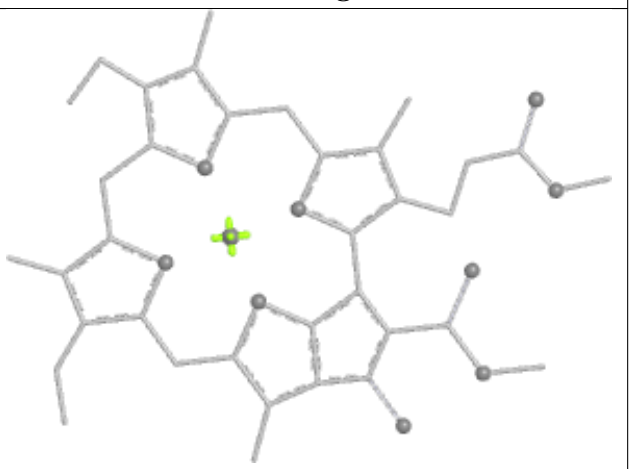
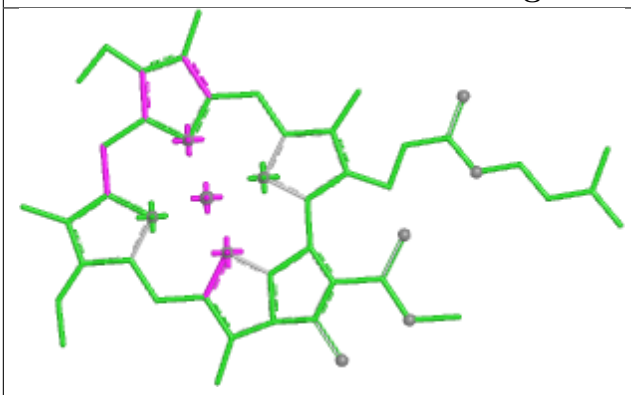


Rings

Ligand CLA X 502



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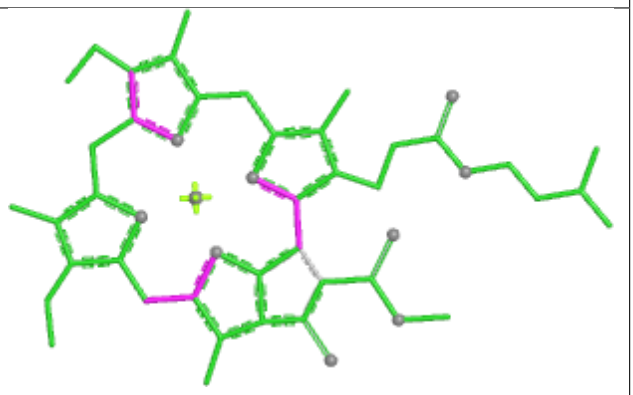

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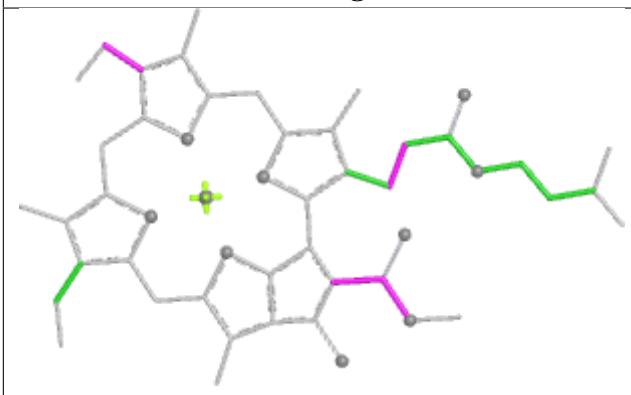

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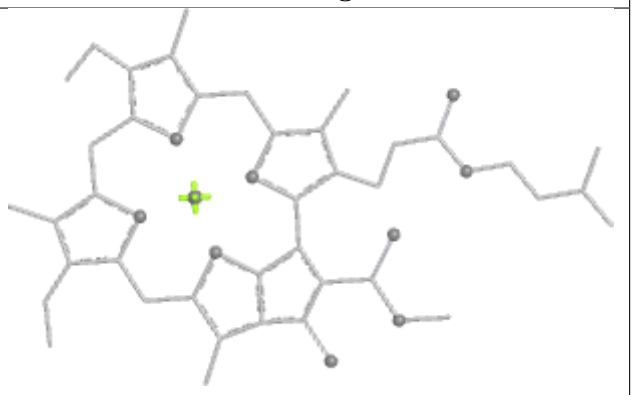
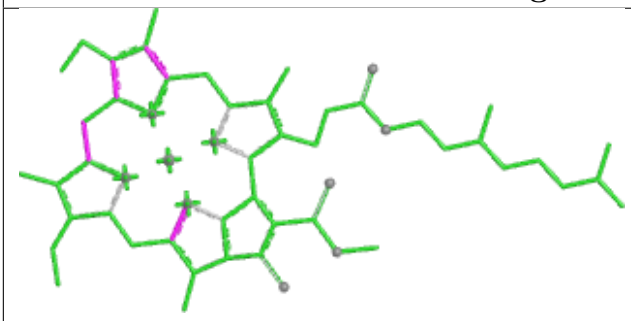


Rings

Ligand CLA r 508



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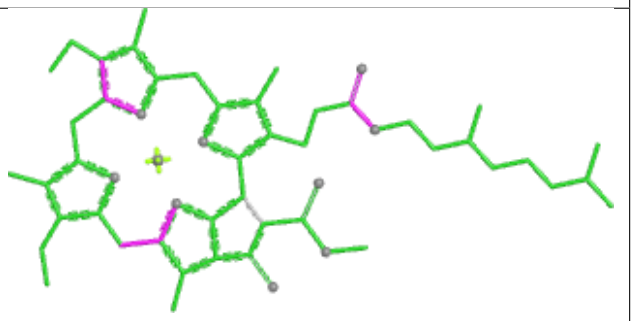
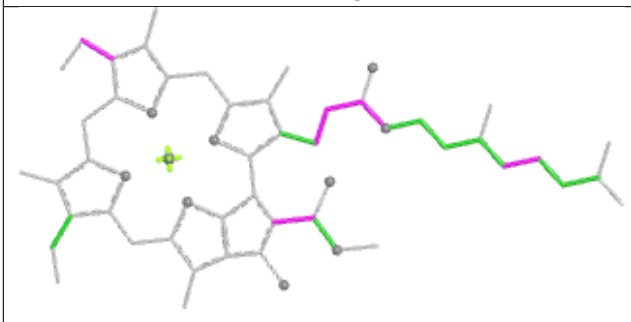


Bond angles



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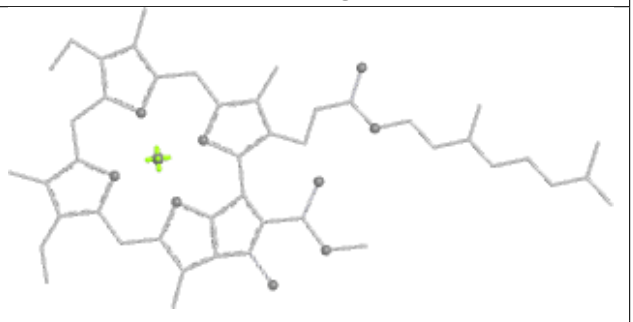
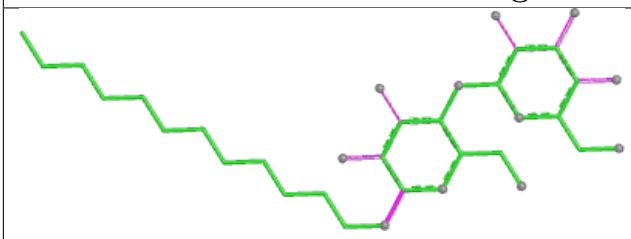


Rings

Ligand LMT U 4101



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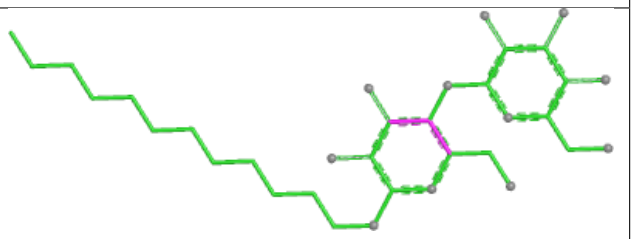
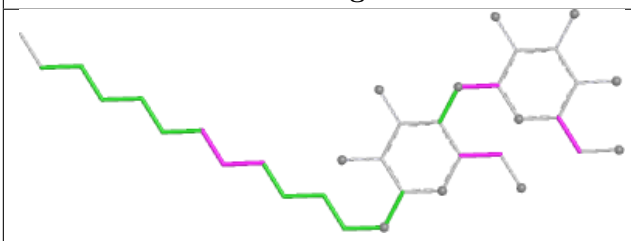


Bond angles



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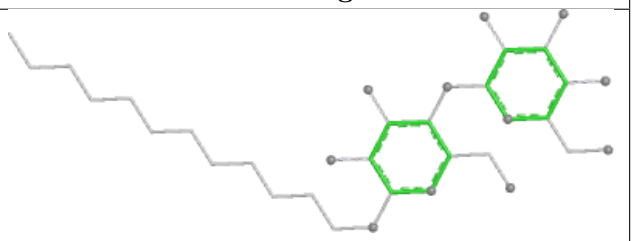
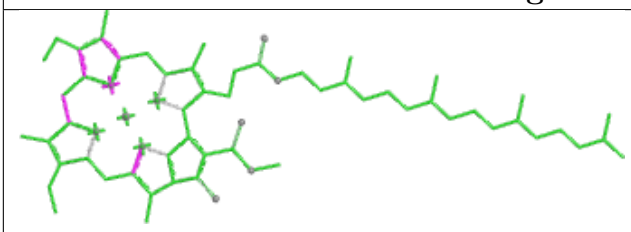


Rings

Ligand CLA Z 505



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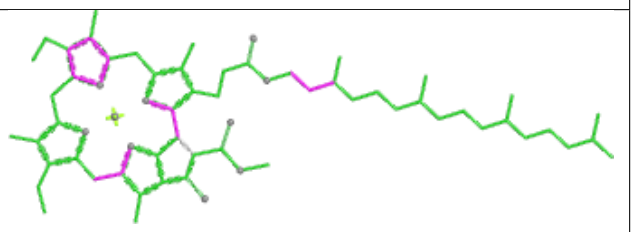
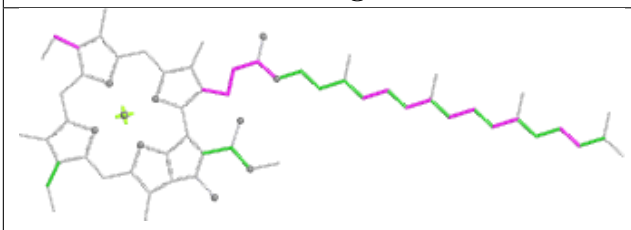


Bond angles



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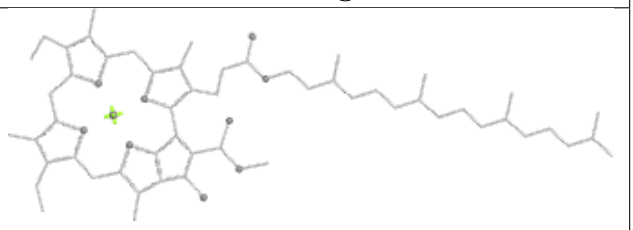
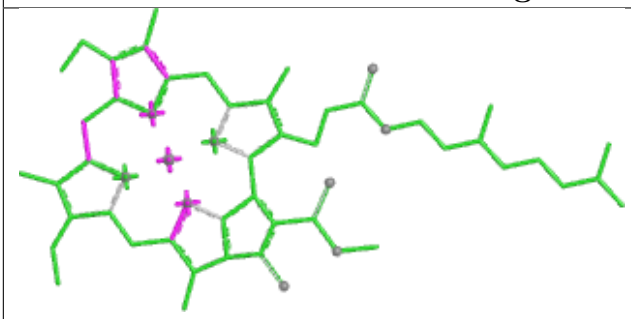
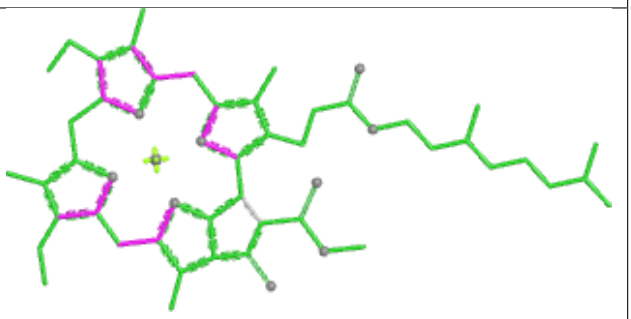
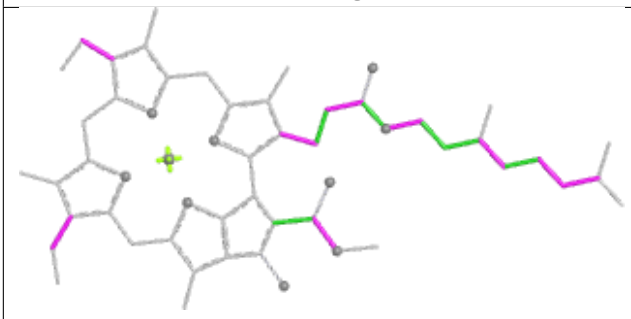
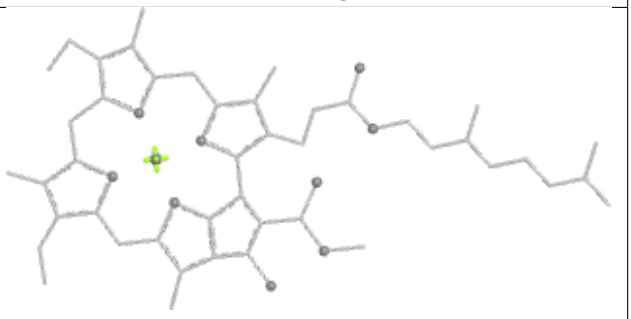
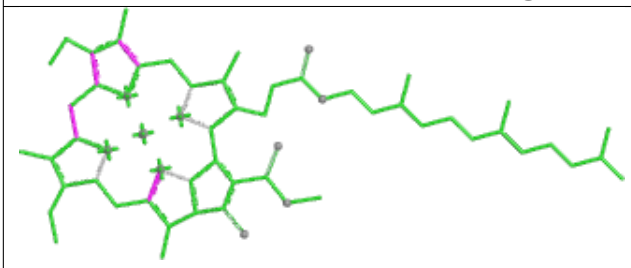
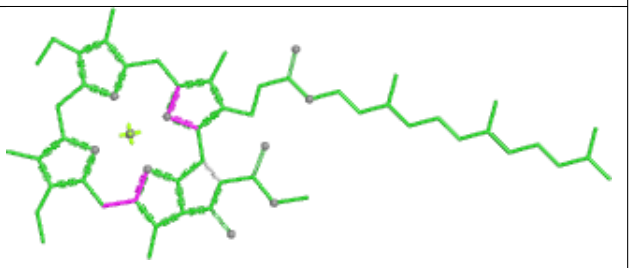
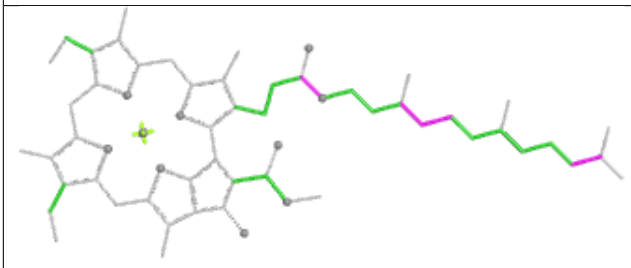
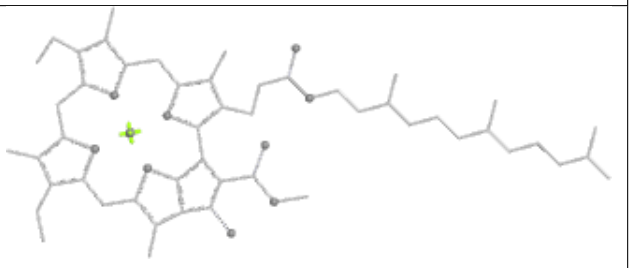
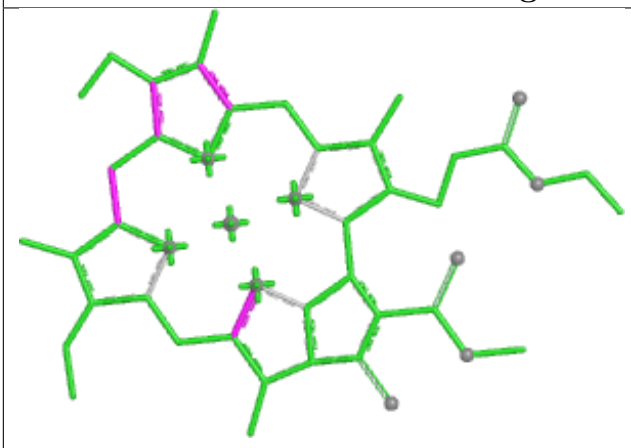


Rings

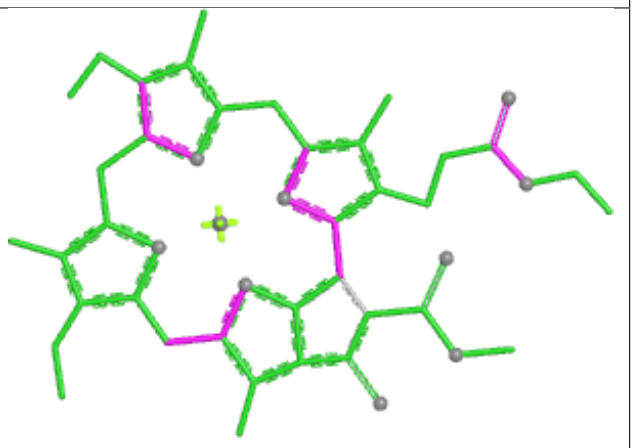
Ligand CLA G 1214	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1124	
	
Bond lengths	Bond angles
	
Torsions	Rings

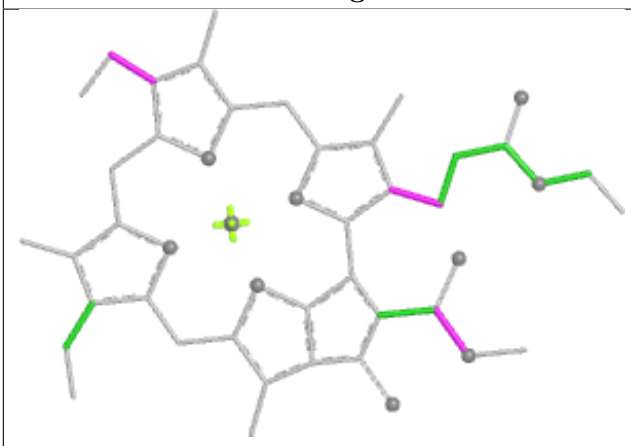
Ligand CLA a 1137



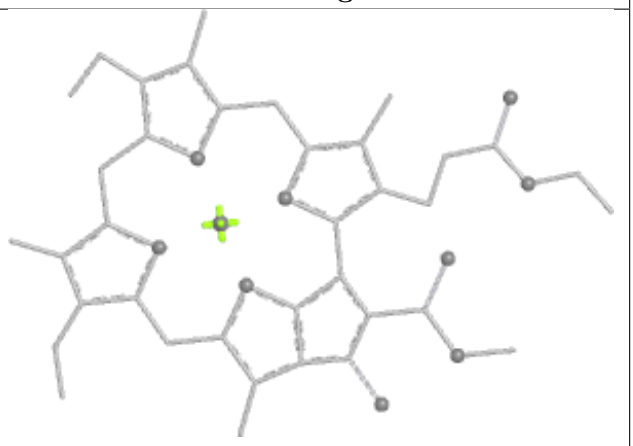
Bond lengths



Bond angles

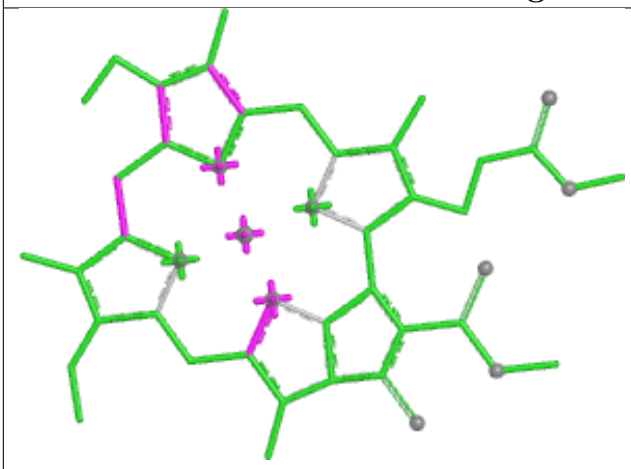


Torsions

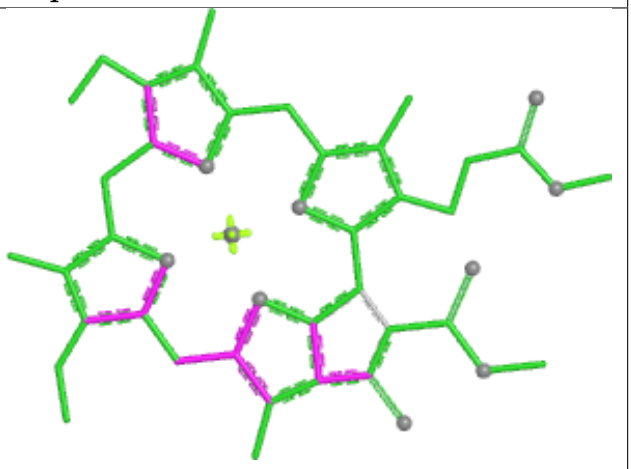


Rings

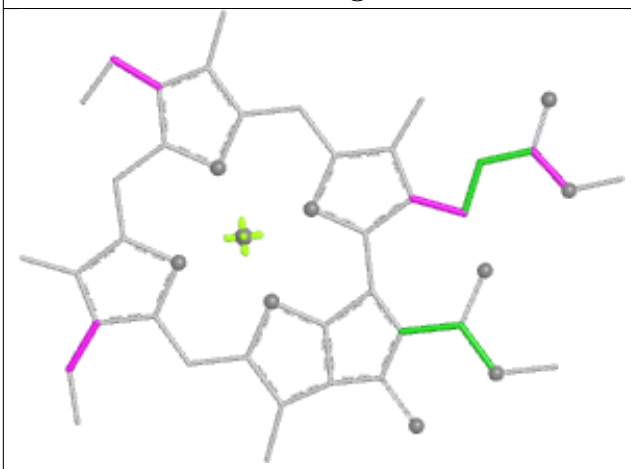
Ligand CLA p 503



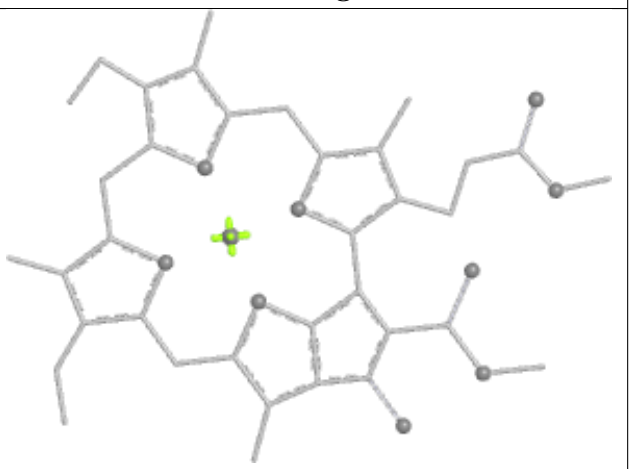
Bond lengths



Bond angles

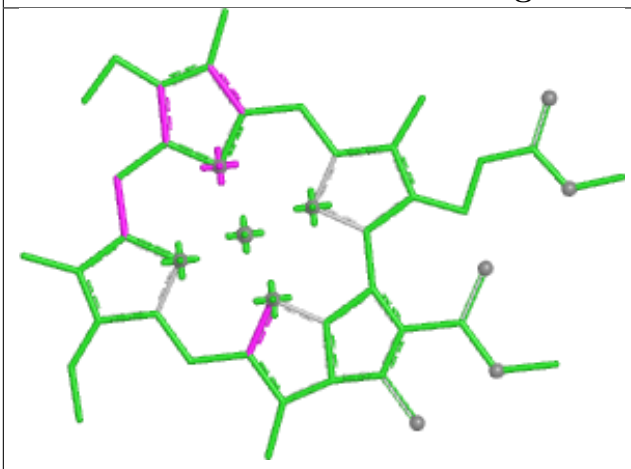


Torsions

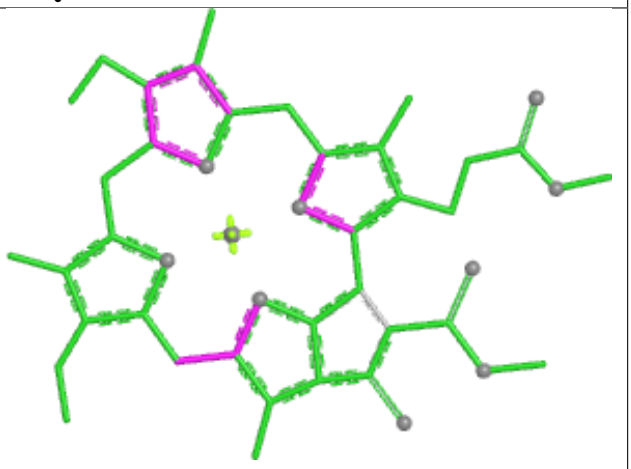


Rings

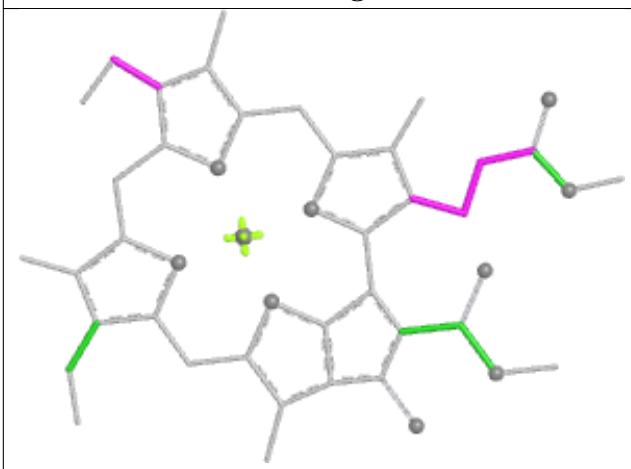
Ligand CLA Q 1302



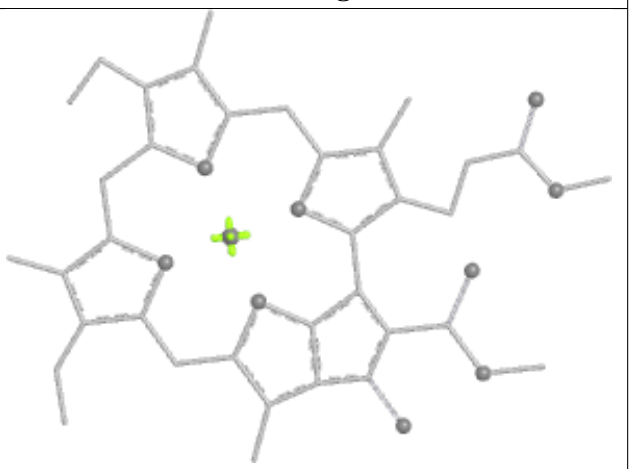
Bond lengths



Bond angles

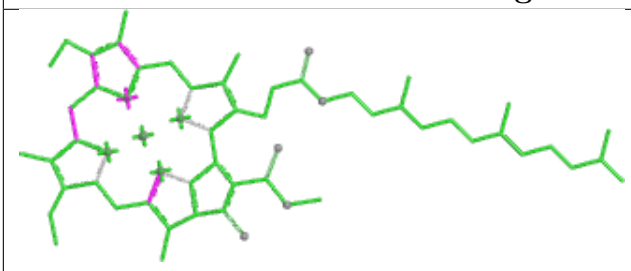


Torsions

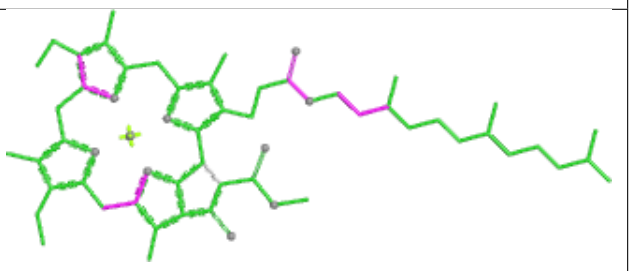


Rings

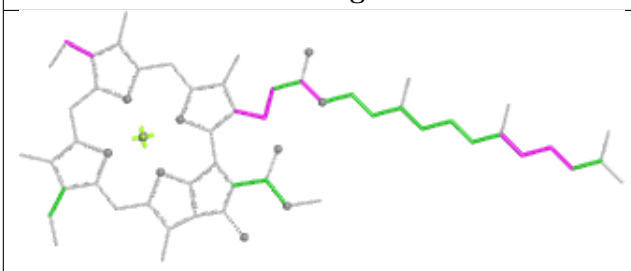
Ligand CLA A 1130



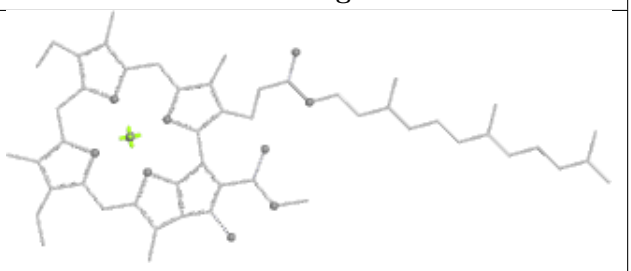
Bond lengths



Bond angles

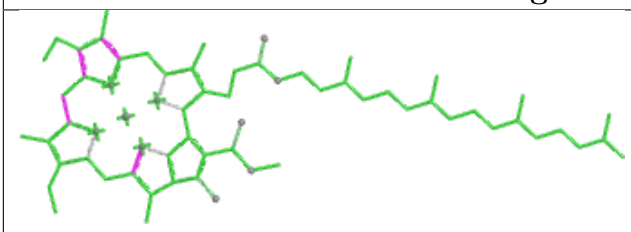


Torsions

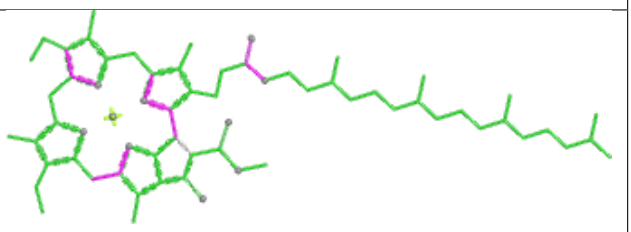


Rings

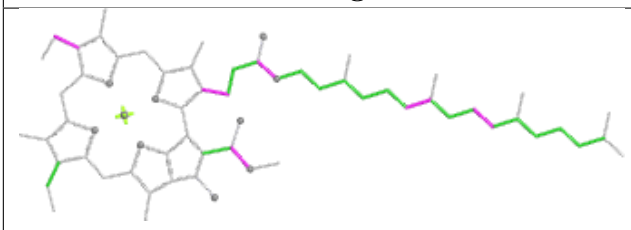
Ligand CLA t 511



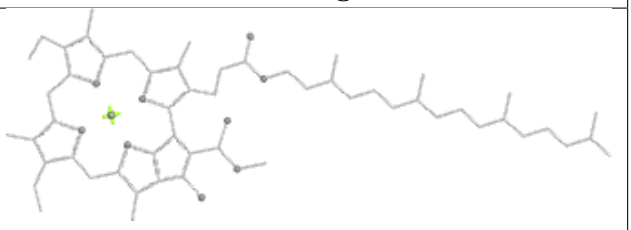
Bond lengths



Bond angles

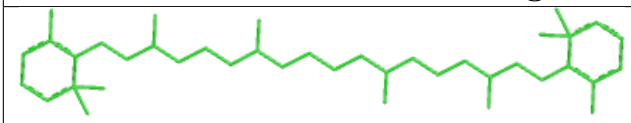


Torsions

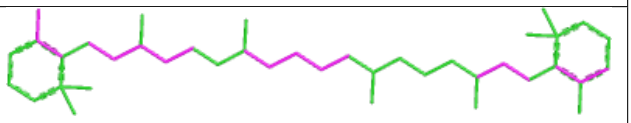


Rings

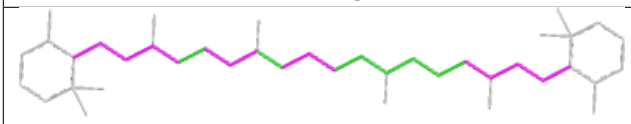
Ligand BCR x 602



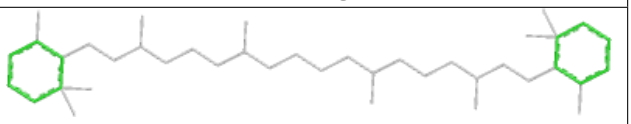
Bond lengths



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.

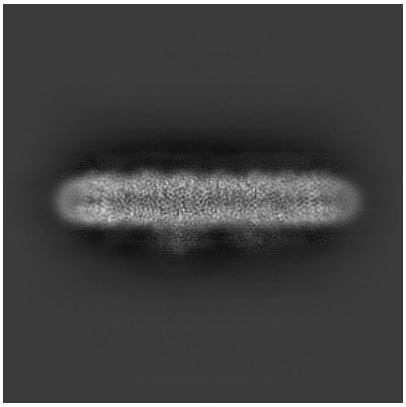
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26601. These allow visual inspection of the internal detail of the map and identification of artifacts.

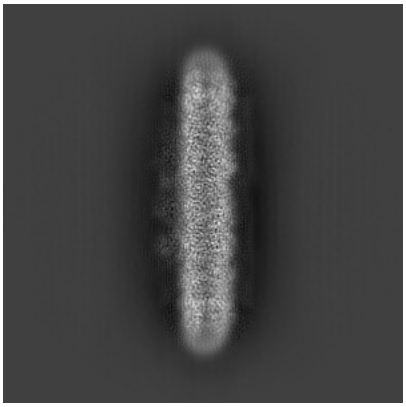
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

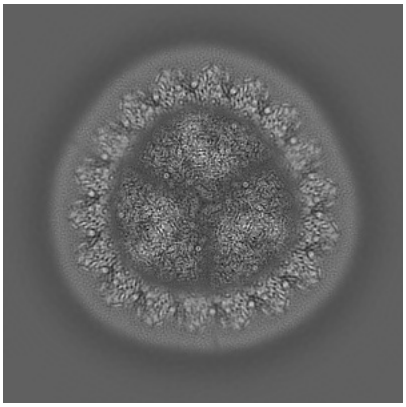
6.1.1 Primary map



X



Y

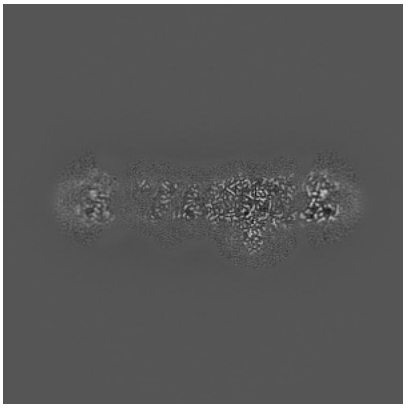


Z

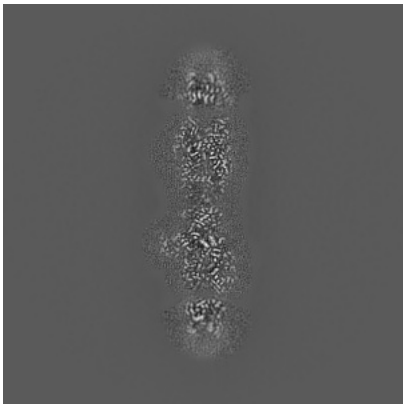
The images above show the map projected in three orthogonal directions.

6.2 Central slices

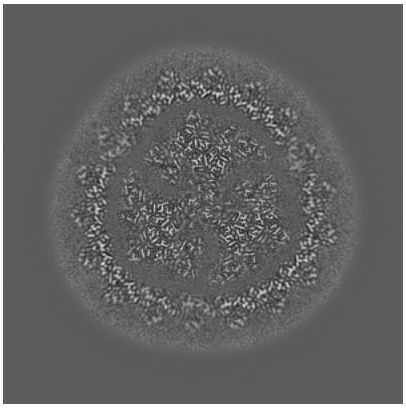
6.2.1 Primary map



X Index: 200



Y Index: 200

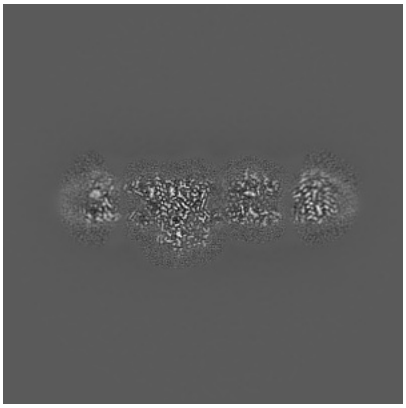


Z Index: 200

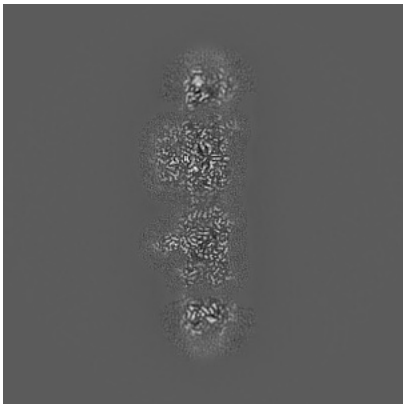
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

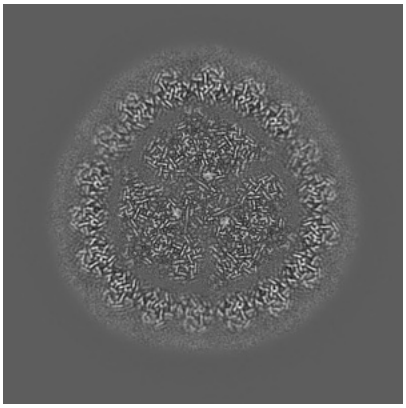
6.3.1 Primary map



X Index: 160



Y Index: 177

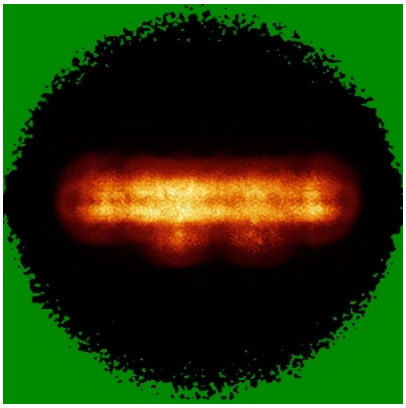


Z Index: 193

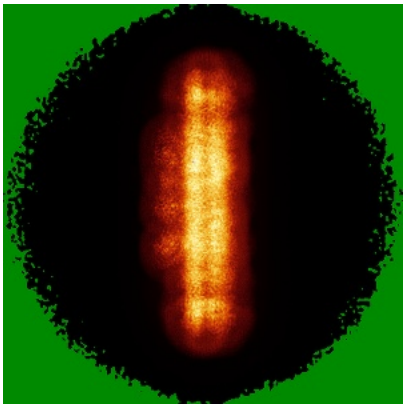
The images above show the largest variance slices of the map in three orthogonal directions.

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

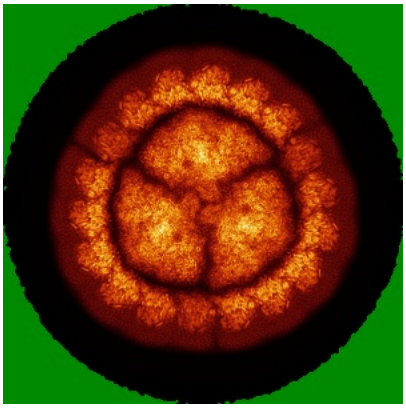
6.4.1 Primary map



X



Y

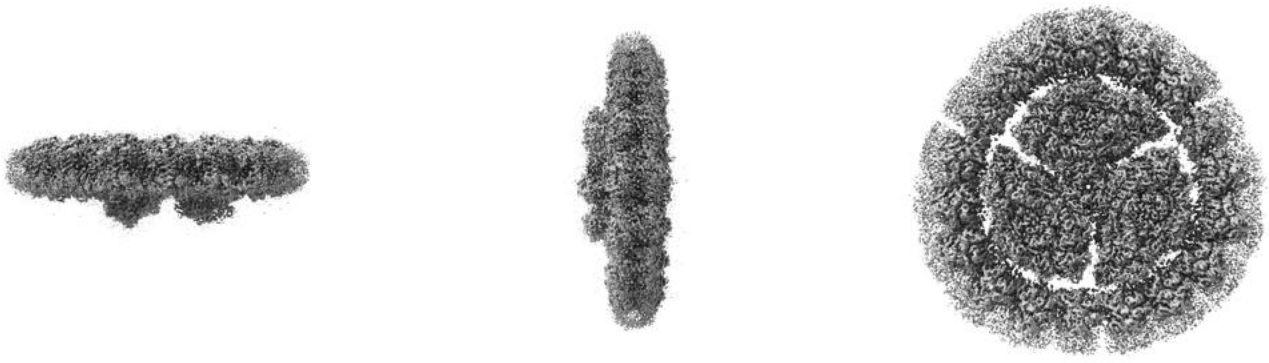


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 9.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

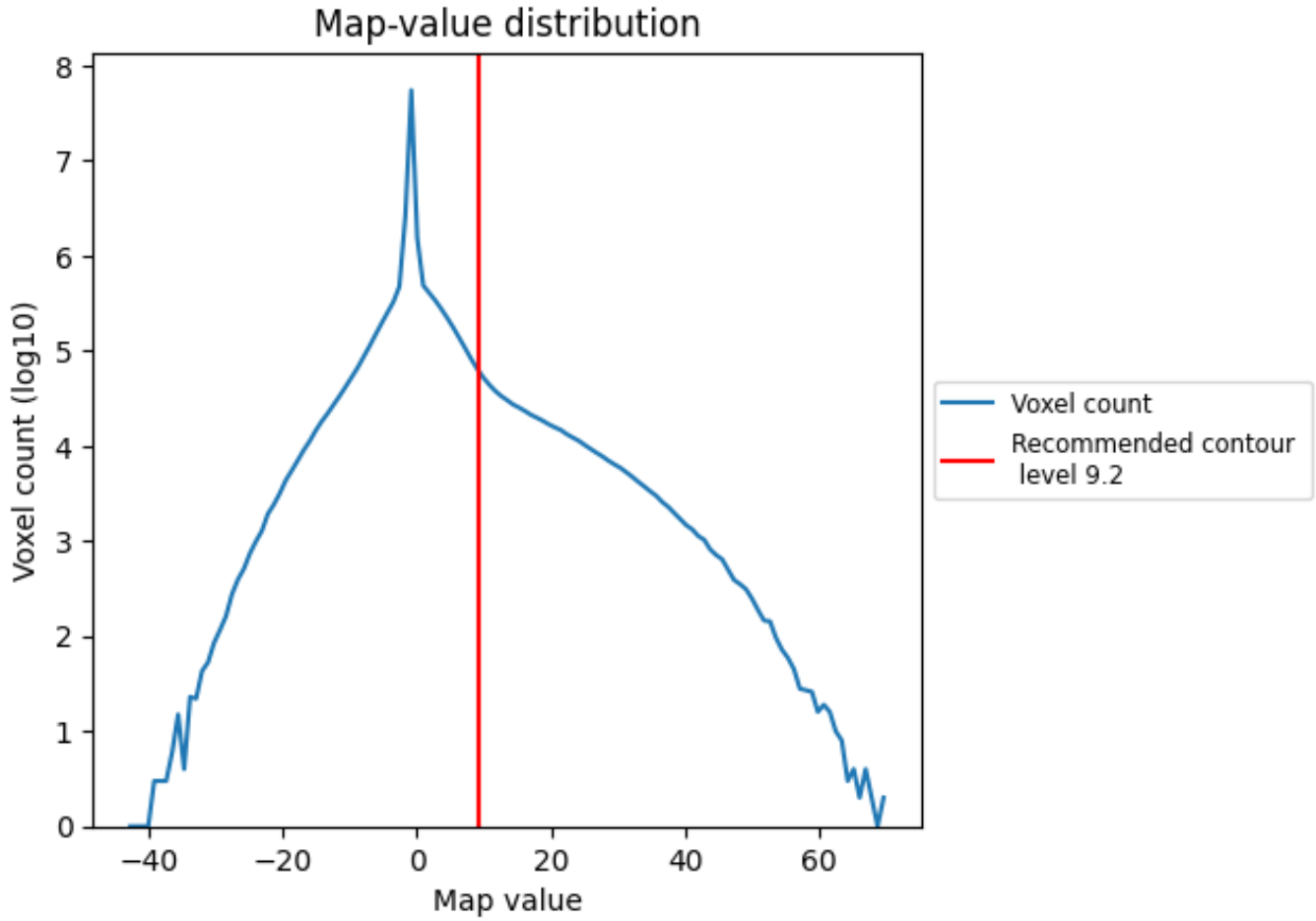
6.6 Mask visualisation (i)

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

7 Map analysis

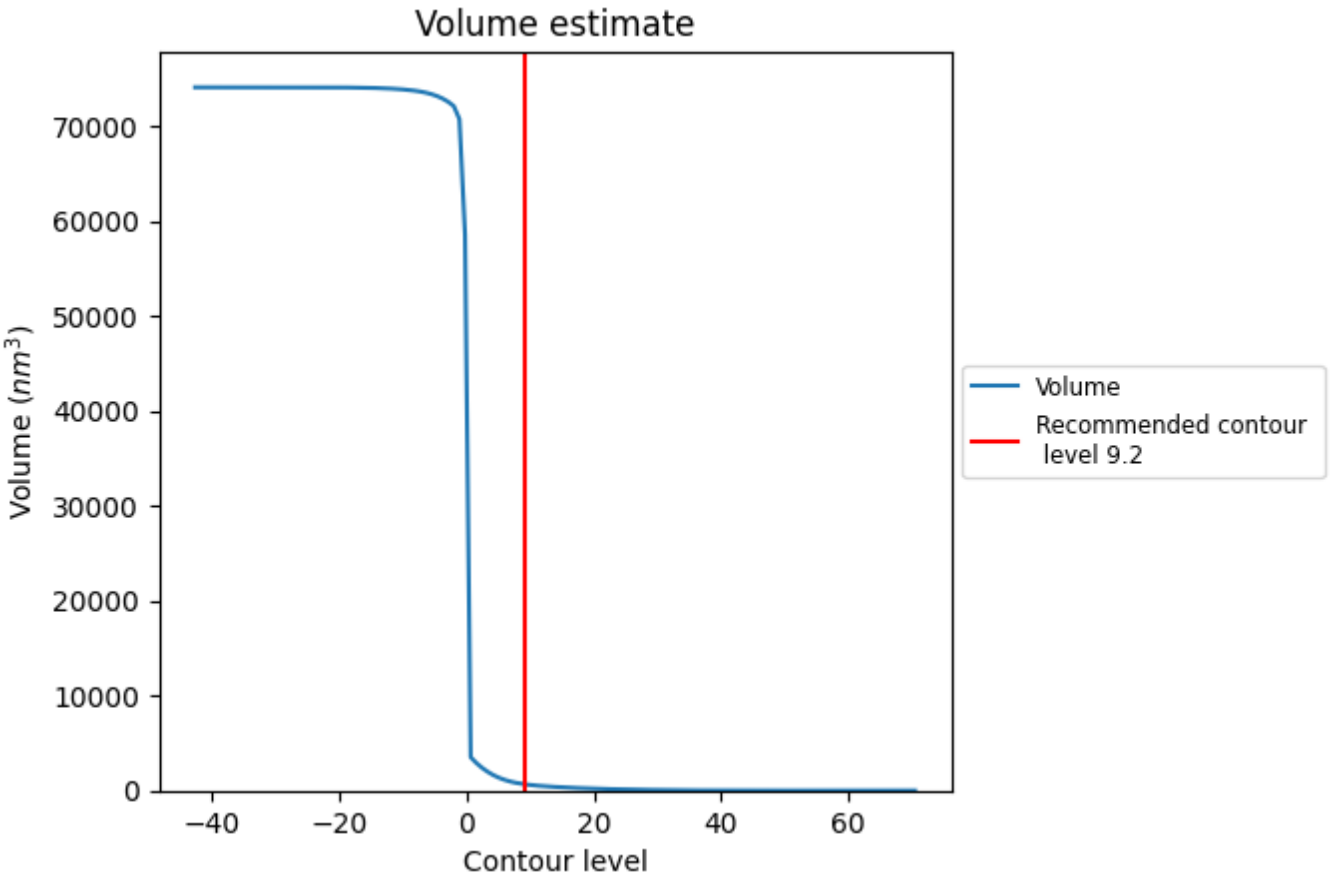
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

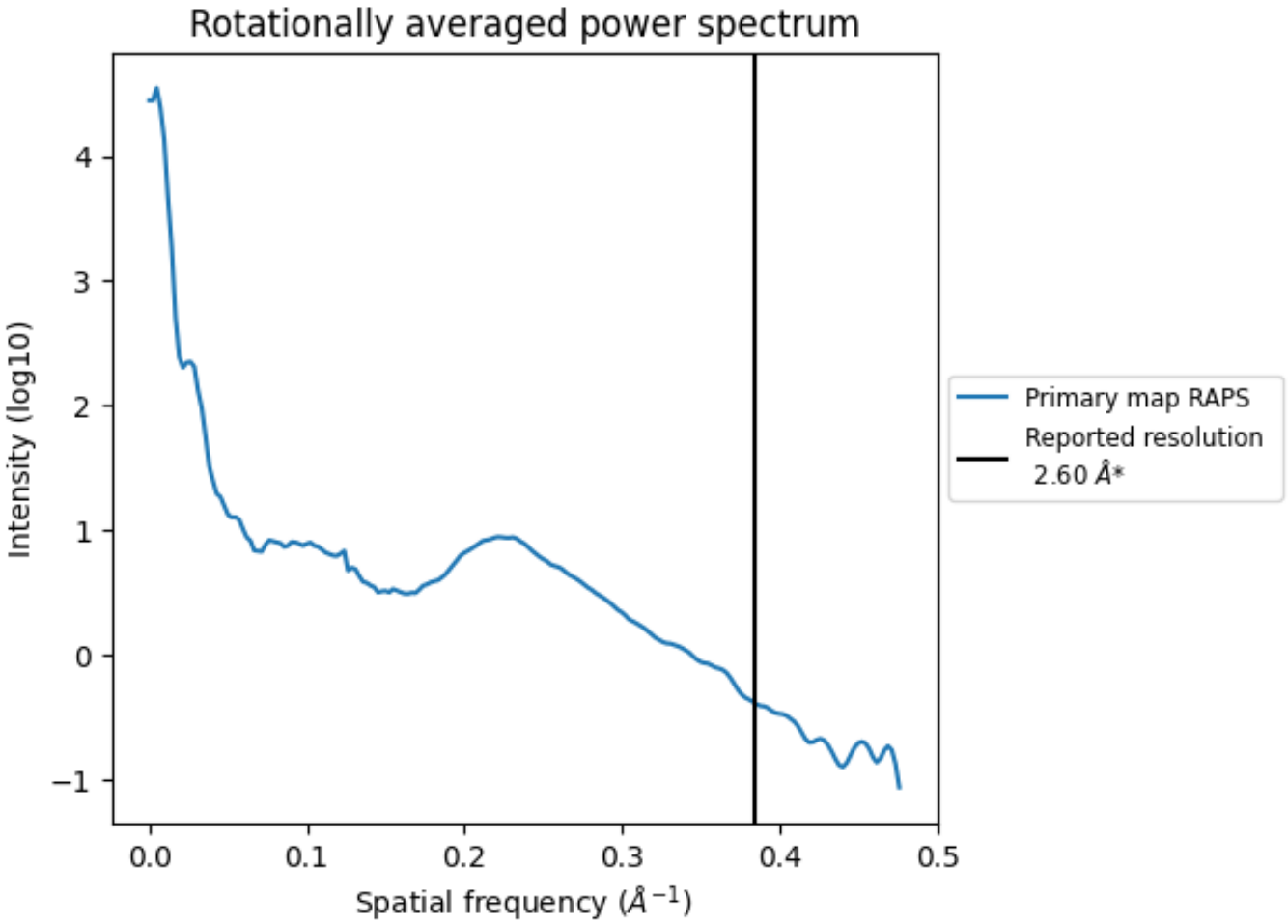
7.2 Volume estimate



The volume at the recommended contour level is 657 nm^3; this corresponds to an approximate mass of 594 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 0.385 $Å^{-1}$

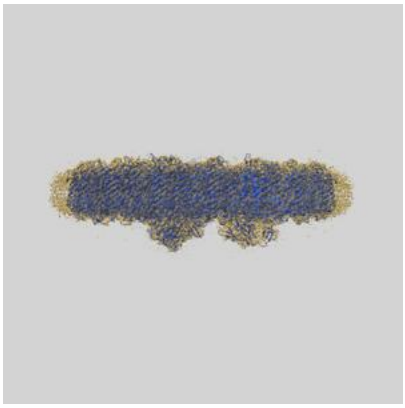
8 Fourier-Shell correlation

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

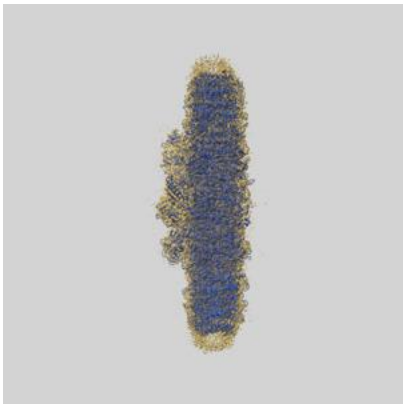
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26601 and PDB model 7UMH. Per-residue inclusion information can be found in section 3 on page 64.

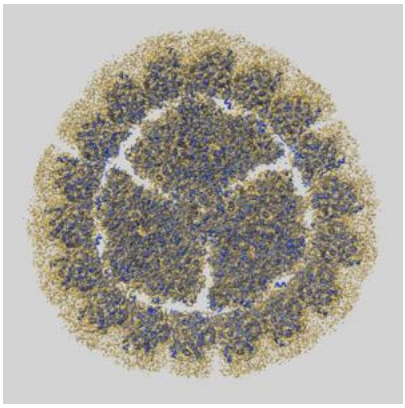
9.1 Map-model overlay



X



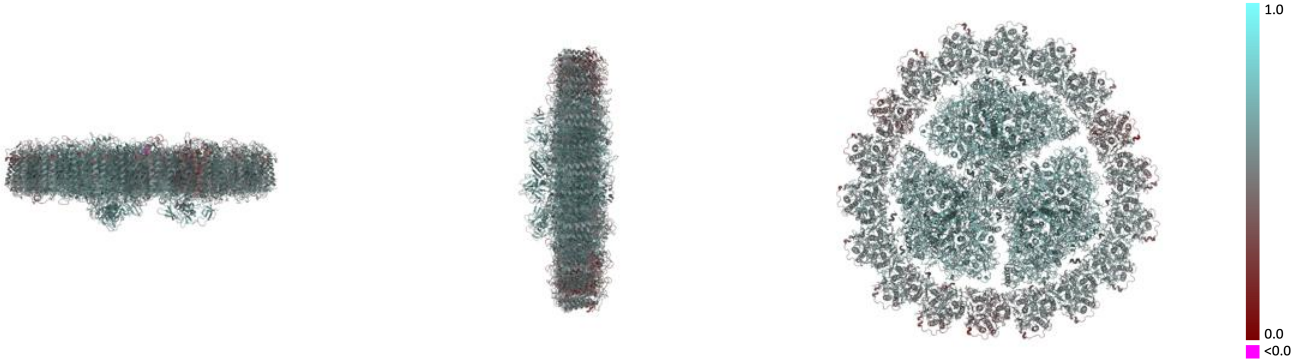
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

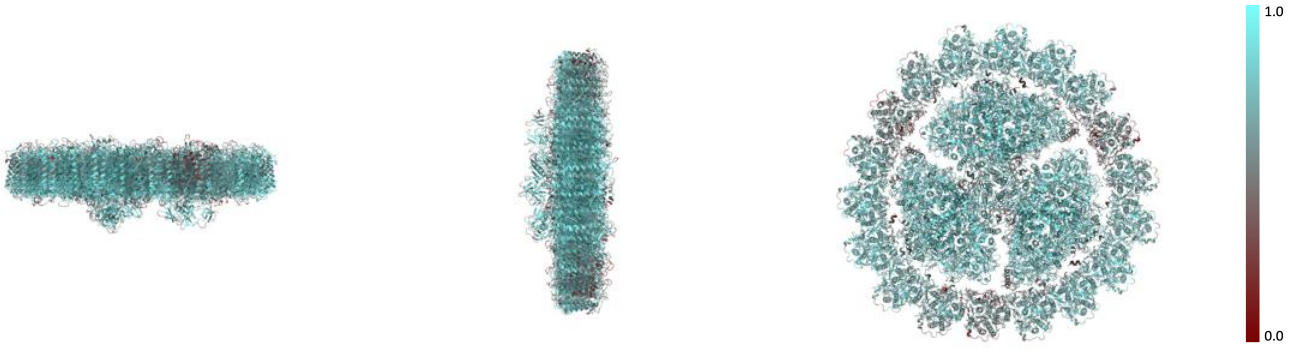
9.2 Q-score mapped to coordinate model (i)



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.

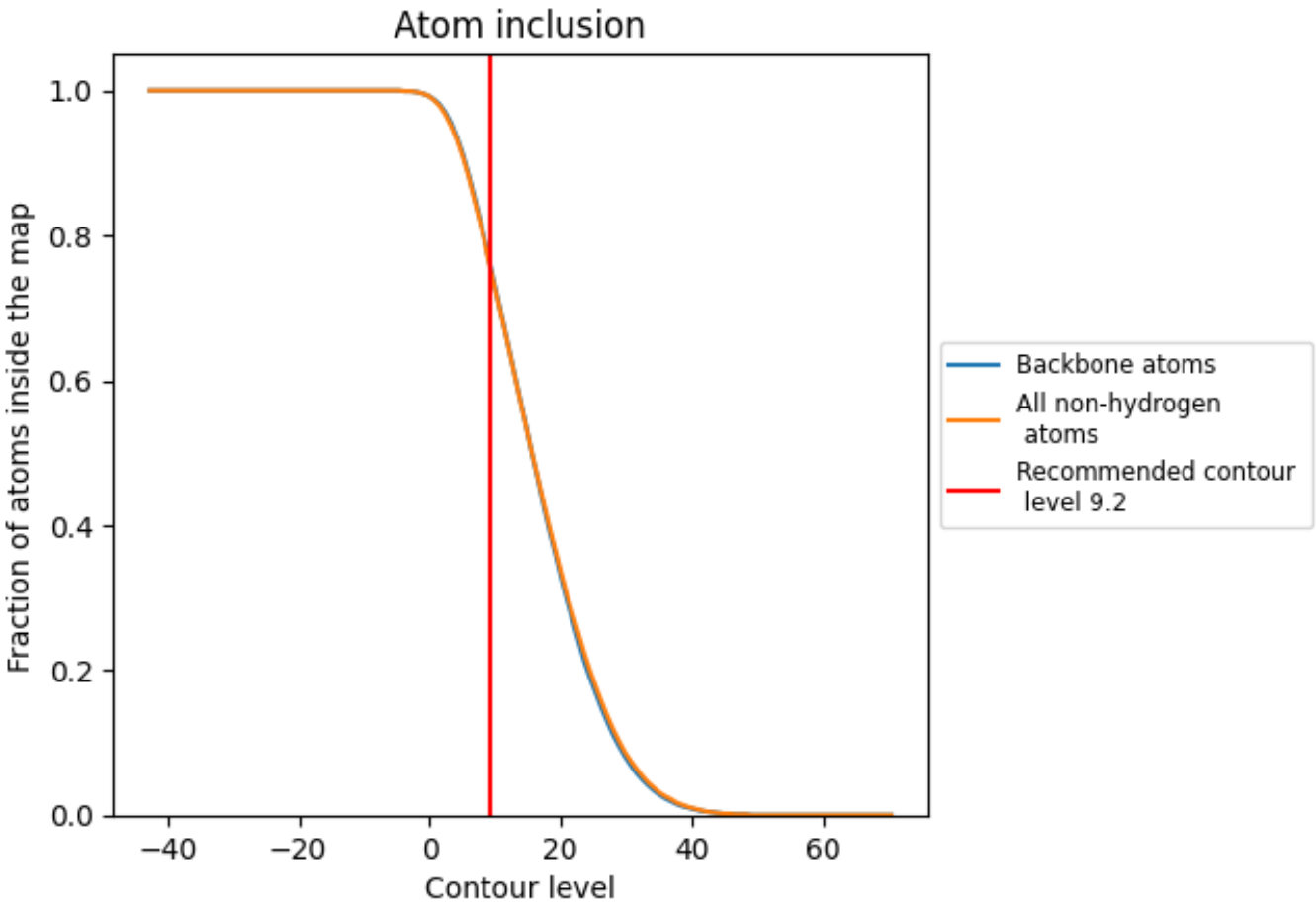
9.3 Atom inclusion mapped to coordinate model (i)



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 (9.2).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (9.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.5830
A	0.8500	0.6590
B	0.8530	0.6580
C	0.8720	0.6440
D	0.7320	0.6010
E	0.7110	0.5910
F	0.6610	0.6030
G	0.8570	0.6580
H	0.8550	0.6590
I	0.7320	0.6300
J	0.7310	0.6300
K	0.5930	0.5910
L	0.7710	0.6360
M	0.7140	0.6350
N	0.8740	0.6450
O	0.6800	0.5860
P	0.7240	0.6040
Q	0.6700	0.6070
R	0.7320	0.6350
S	0.7270	0.6340
T	0.6090	0.5850
U	0.7720	0.6400
V	0.6770	0.6170
W	0.6650	0.5000
X	0.7490	0.5360
Y	0.7840	0.5560
Z	0.7720	0.5460
a	0.8490	0.6620
b	0.8570	0.6610
c	0.8700	0.6500
d	0.7210	0.6020
e	0.6720	0.5800
f	0.6720	0.6070
g	0.7050	0.5260
h	0.5270	0.4200

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Chain	Atom inclusion	Q-score
i	0.7370	0.6290
j	0.7590	0.6360
k	0.6030	0.5890
l	0.7650	0.6350
m	0.7140	0.6350
n	0.6720	0.5010
o	0.7400	0.5370
p	0.7770	0.5570
q	0.7590	0.5430
r	0.6990	0.5170
s	0.7750	0.5550
t	0.6620	0.4980
u	0.7400	0.5300
v	0.5460	0.4350
w	0.7620	0.5450
x	0.6830	0.5150
y	0.5320	0.4260